Supporting Information

Palladium-catalyzed aerobic oxyarylthiolation of alkynone *O*-methyloximes

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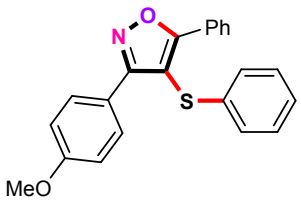
General methods

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 (GF_{254}). Unless otherwise noted, purchased chemicals were used without further purification.

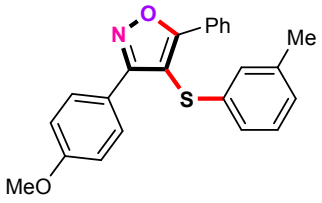
Typical procedure for the preparation of 4-sulfenylisoxazoles

O-Methyl oximes (0.20 mmol), arylhydrazine hydrochloride (0.32 mmol, 1.6 equiv.), elemental sulfur (S_8, 1.25 equiv.), IPr-Pd-Allyl-Cl (0.1 mol%), $[C_2OHmim]Cl$ (0.4 mmol), Cs_2CO_3 (0.4 mmol), and DMF (2 mL) were combined in an oven-dried Schlenk tube equipped with a stir bar. After the addition of all of the solid reagent, the balloon filled with O_2 was connected to the Schlenk tube via a syringe. The Schlenk tube was heated at 100 °C for 8 h. After the reaction was completed (monitored by TLC), the contents were cooled to room temperature, and then the balloon gas was released. After that, the reaction was quenched by water and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate) to afford the desired products.

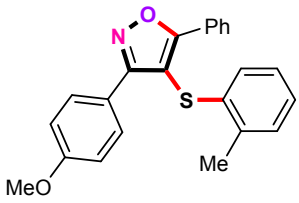
Characterization data for all products



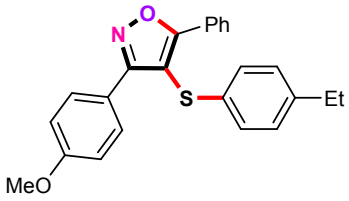
3-(4-Methoxyphenyl)-5-phenyl-4-(phenylthio)isoxazole (**3a**): Yield: 82% as a white solid; mp = 122 - 123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 - 8.13 (m, 2H), 7.88 - 7.77 (m, 2H), 7.51 - 7.47 (m, 3H), 7.44 - 7.36 (m, 3H), 7.02 (d, J = 8.8 Hz, 2H), 6.74 (d, J = 8.8 Hz, 2H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 165.1, 158.6, 130.9, 130.1, 128.9, 128.8, 128.7, 128.6, 128.4, 127.5, 127.2, 126.5, 115.0, 103.7, 55.4 ppm; ν_{max}(KBr)/cm^{-1} 3058, 2932, 1586, 1484, 1416, 1252, 820, 701; HRMS-ESI (m/z): calcd for $C_{22}H_{17}NNaO_2S$, $[M+Na]^+$: 382.0872, found 382.0871.



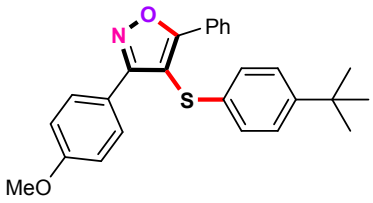
3-(4-Methoxyphenyl)-5-phenyl-4-(m-tolylthio)isoxazole (**3b**): Yield: 86% as a yellow solid; mp = 136 - 138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 - 7.95 (m, 2H), 7.83 (d, J = 7.2 Hz, 2H), 7.42 (q, J = 6.0 Hz, 3H), 7.36 (t, J = 7.6 Hz, 1H), 7.30 (d, J = 7.6 Hz, 1H), 7.03 (d, J = 8.4 Hz, 2H), 6.73 (d, J = 8.4 Hz, 2H), 3.72 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 165.0, 158.6, 138.6, 131.6, 129.9, 128.8, 128.8, 128.7, 128.5, 128.4, 128.1, 127.0, 126.6, 124.7, 115.0, 103.5, 55.2, 21.5 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1568, 1520, 1488, 1416, 1255, 752; HRMS-ESI (m/z): calcd for $C_{23}H_{19}NNaO_2S$, $[M+Na]^+$: 396.1029, found 396.1035.



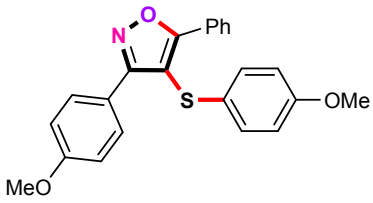
3-(4-Methoxyphenyl)-5-phenyl-4-(o-tolylthio)isoxazole (**3c**): Yield: 81% as a yellow solid; mp = 121 - 123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 - 8.26 (m, 2H), 7.62 - 7.48 (m, 3H), 7.36 (td, J = 8.0, 4.0 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 7.21 (d, J = 4.4 Hz, 2H), 6.96 (d, J = 8.6 Hz, 2H), 6.68 (d, J = 8.6 Hz, 2H), 3.75 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 166.7, 158.8, 137.6, 130.9, 130.8, 130.3, 130.2, 129.6, 128.9, 127.8, 127.3, 125.6, 125.4, 114.6, 106.6, 55.3, 19.9 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2936, 1582, 1516, 1470, 1412, 1256, 754; HRMS-ESI (m/z): calcd for $C_{23}H_{19}NNaO_2S$, $[M+Na]^+$: 396.1029, found 396.1033.



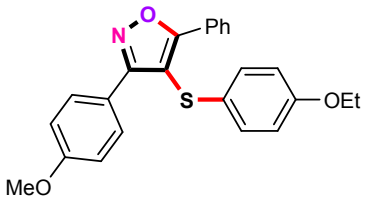
4-((4-Ethylphenyl)thio)-3-(4-methoxyphenyl)-5-phenylisoxazole (**3d**): Yield: 85% as a white solid; mp = 142 - 143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 7.2 Hz, 2H), 7.49 - 7.37 (m, 3H), 7.32 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 8.4 Hz, 2H), 6.75 (d, J = 8.4 Hz, 2H), 3.72 (s, 3H), 2.70 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 165.0, 158.3, 147.4, 129.9, 128.7, 128.6, 128.4, 128.3, 127.5, 126.8, 124.6, 115.0, 102.8, 55.3, 28.8, 15.3 ppm; ν_{max}(KBr)/cm^{-1} 3055, 2946, 1586, 1486, 1412, 1245, 765; HRMS-ESI (m/z): calcd for $C_{24}H_{21}NNaO_2S$, $[M+Na]^+$: 410.1185, found 410.1192.



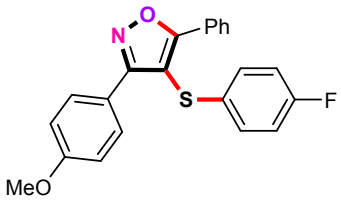
4-((4-(*tert*-Butyl)phenyl)thio)-3-(4-methoxyphenyl)-5-phenylisoxazole (**3e**): Yield: 86% as a white solid; mp = 148 - 149 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 7.0 Hz, 2H), 7.49 - 7.38 (m, 3H), 7.29 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 8.4 Hz, 2H), 6.75 (d, J = 8.4 Hz, 2H), 3.72 (s, 3H), 2.67 (t, J = 7.6 Hz, 2H), 1.65 (dd, J = 15.2, 7.8 Hz, 2H), 1.38 (dq, J = 14.4, 7.2 Hz, 2H), 0.94 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 165.1, 158.5, 146.3, 129.8, 128.8, 128.7, 128.5, 128.5, 127.4, 126.7, 124.6, 115.0, 102.9, 55.4, 35.8, 33.3, 22.4, 13.9 ppm; ν_{max}(KBr)/cm^{-1} 3052, 2938, 1605, 1556, 1476, 1426, 1248, 759; HRMS-ESI (m/z): calcd for $C_{26}H_{25}NNaO_2S$, $[M+Na]^+$: 438.1498, found 438.1504.



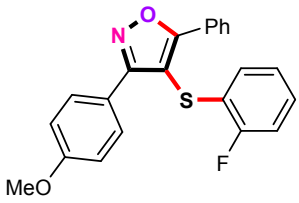
3-(4-Methoxyphenyl)-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**3f**): Yield: 75% as a white solid; mp = 137 - 138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 - 7.70 (m, 2H), 7.62 (d, J = 8.2 Hz, 2H), 7.50 - 7.43 (m, 4H), 7.05 (s, 1H), 6.96 (d, J = 8.2 Hz, 2H), 6.89 (d, J = 8.2 Hz, 1H), 4.02 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 159.7, 152.6, 138.2, 137.2, 134.4, 129.7, 128.5, 128.4, 126.8, 126.7, 125.3, 118.2, 114.7, 113.8, 62.6, 55.3 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2948, 1588, 1526, 1495, 1436, 1235, 758; HRMS-ESI (m/z): calcd for $C_{23}H_{19}NNaO_3S$, $[M+Na]^+$: 412.0978, found 412.0975.



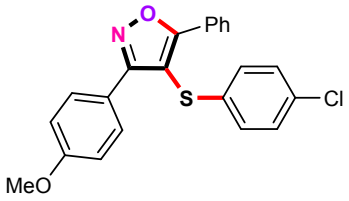
4-((4-Ethoxyphenyl)thio)-3-(4-methoxyphenyl)-5-phenylisoxazole (**3g**): Yield: 72% as a yellow solid; mp = 115 - 117 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.8 Hz, 2H), 7.90 - 7.77 (m, 2H), 7.51 - 7.37 (m, 3H), 7.04 (d, J = 8.8 Hz, 2H), 6.98 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 4.10 (q, J = 7.0 Hz, 2H), 3.75 (s, 3H), 1.45 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 165.0, 161.2, 158.4, 129.9, 129.1, 128.8, 128.5, 128.4, 126.8, 119.8, 115.0, 114.8, 101.7, 63.6, 55.2, 14.7 ppm; ν_{max}(KBr)/cm^{-1} 3048, 2932, 1603, 1516, 1496, 1251, 756; HRMS-ESI (m/z): calcd for $C_{24}H_{21}NNaO_3S$, $[M+Na]^+$: 426.1134, found 426.1137.



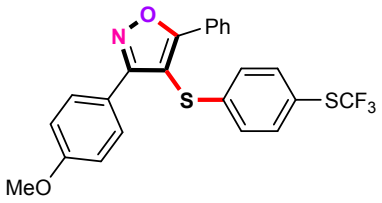
4-((4-Fluorophenyl)thio)-3-(4-methoxyphenyl)-5-phenylisoxazole (**3h**): Yield: 73% as a yellow solid; mp = 133 - 134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 - 8.09 (m, 2H), 7.76 (d, J = 7.2 Hz, 2H), 7. 45 - 7.36 (m, 3H), 7.16 (t, J = 8.4 Hz, 2H), 7.00 (d, J = 8.4 Hz, 2H), 6.72 (d, J = 8.4 Hz, 2H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 165.2, 164.4 (d, J = 252.7 Hz), 158.7, 130.0, 129.8 (d, J = 8.6 Hz), 128.8, 128.7, 128.6, 128.2, 126.2, 123.7 (d, J = 3.4 Hz), 116.4 (d, J = 21.9 Hz), 115.1, 103.2, 55.3 ppm; ν_{max}(KBr)/cm^{-1} 3042, 2929, 1640, 1488, 1424, 1269, 756; HRMS-ESI (m/z): calcd for $C_{22}H_{16}FNNaO_2S$, $[M+Na]^+$: 400.0778, found 400.0781.



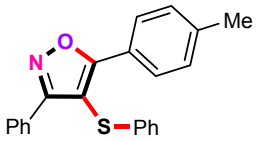
4-((2-Fluorophenyl)thio)-3-(4-methoxyphenyl)-5-phenylisoxazole (**3i**): Yield: 66% as a yellow solid; mp = 128 - 129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 7.2 Hz, 2H), 7.72 (t, J = 7.2 Hz, 1H), 7.53 (dd, J = 13.6, 7.2 Hz, 1H), 7.48 - 7.36 (m, 3H), 7.22 (d, J = 5.2 Hz, 1H), 7.20 (d, J = 9.4 Hz, 1H), 6.98 (d, J = 8.4 Hz, 2H), 6.68 (d, J = 8.4 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 163.8, 160.2 (d, J = 254.6 Hz), 158.8, 132.8 (d, J = 8.6 Hz), 131.0, 129.8, 129.7, 128.6, 128.5, 126.1, 124.4 (d, J = 3.8 Hz), 116.5 (d, J = 21.4 Hz), 115.8 (d, J = 13.6 Hz), 114.8, 107.7, 55.3 ppm; ν_{max}(KBr)/cm^{-1} 3058, 2926, 1646, 1556, 1474, 1416, 1287, 758; HRMS-ESI (m/z): calcd for $C_{22}H_{16}FNNaO_2S$, $[M+Na]^+$: 400.0778, found 400.0783.



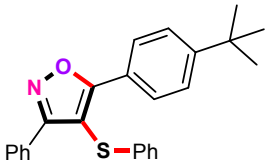
4-((4-Chlorophenyl)thio)-3-(4-methoxyphenyl)-5-phenylisoxazole (**3j**): Yield: 72% as a white solid; mp = 126 - 128 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 6.4 Hz, 2H), 7.58 - 7.39 (m, 5H), 6.99 (d, J = 8.4 Hz, 2H), 6.75 (d, J = 8.4 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 165.2, 158.7, 137.2, 130.2, 129.4, 128.9, 128.7, 128.6, 128.6, 128.2, 126.3, 125.7, 115.1, 104.3, 55.3 ppm; ν_{max}(KBr)/cm^{-1} 3060, 2928, 1589, 1556, 1482, 1434, 1246, 746; HRMS-ESI (m/z): calcd for $C_{22}H_{16}ClNNaO_2S$, $[M+Na]^+$: 416.0482, found 416.0485.



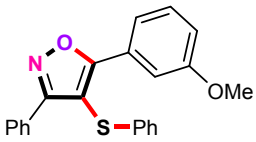
3-(4-Methoxyphenyl)-5-phenyl-4-((4-((trifluoromethyl)thio)phenyl)thio)isoxazole (**3k**): Yield: 61% as a white solid; mp = 147 - 148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 - 8.09 (m, 2H), 7.89 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H), 7.58 - 7.44 (m, 3H), 7.06 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 163.9, 158.6, 136.1, 132.6, 131.1, 130.8, 129.7, 129.0, 128.9, 127.5, 127.8 (q, J = 257.8 Hz), 115.2, 104.0, 55.4 ppm; ν_{max}(KBr)/cm^{-1} 3050, 2934, 1592, 1536, 1491, 1256, 757; HRMS-ESI (m/z): calcd for $C_{23}H_{16}F_3NNaO_2S_2$, $[M+Na]^+$: 482.0467, found 482.0466.



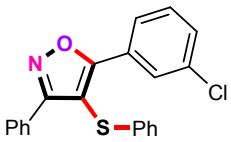
3-Phenyl-4-(phenylthio)-5-(p-tolyl)isoxazole (**4a**): Yield: 87% as a yellow solid; mp = 112 - 113 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 - 8.11 (m, 2H), 7.88 - 7.80 (m, 3H), 7.51 - 7.43 (m, 4H), 7.44 - 7.35 (m, 2H), 7.03 - 6.99 (m, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 165.2, 135.8, 132.7, 130.8, 130.2, 130.0, 128.9, 128.6, 128.5, 127.6, 126.8, 126.3, 125.8, 102.4, 20.9 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2928, 1586, 1470, 1410, 758; HRMS-ESI (m/z): calcd for $C_{22}H_{17}NNaOs$, $[M+Na]^+$: 366.0923, found 366.0928.



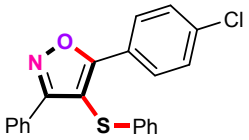
5-(4-(*tert*-Butyl)phenyl)-3-phenyl-4-(phenylthio)isoxazole (**4b**): Yield: 90% as a yellow solid; mp = 134 - 135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 - 8.09 (m, 2H), 7.88 - 7.83 (m, 2H), 7.54 - 7.48 (m, 3H), 7.44 - 7.38 (m, 3H), 7.22 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.0 Hz, 2H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 165.0, 149.1, 130.8, 129.8, 129.0, 128.7, 128.7, 128.5, 127.5, 126.8, 126.4, 126.2, 125.8, 102.5, 34.4, 31.2 ppm; ν_{max}(KBr)/cm^{-1} 3052, 2956, 1652, 1561, 1471, 1412, 1260, 764; HRMS-ESI (m/z): calcd for $C_{25}H_{24}NOS$, $[M+H]^+$: 386.1573, found 386.1575.



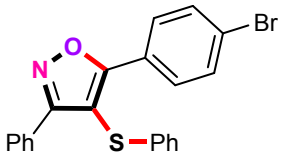
5-(3-Methoxyphenyl)-3-phenyl-4-(phenylthio)isoxazole (**4c**): Yield: 78% as a yellow yellow solid; mp = 106 - 108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 - 8.08 (m, 2H), 7.86 (d, J = 7.2 Hz, 2H), 7.52 - 7.46 (m, 3H), 7.42 (q, J = 6.8 Hz, 3H), 7.14 (q, J = 8.2 Hz, 1H), 6.72 (d, J = 8.2 Hz, 1H), 6.66 (d, J = 6.8 Hz, 2H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 165.1, 160.2, 137.5, 131.0, 130.1, 130.0, 128.7, 128.5, 128.6, 128.2, 127.6, 127.0, 118.2, 111.8, 111.7, 101.7, 55.2 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2938, 1678, 1582, 1526, 1468, 1413, 1245, 764; HRMS-ESI (m/z): calcd for $C_{22}H_{18}NO_2S$, $[M+H]^+$: 360.1053, found 360.1056.



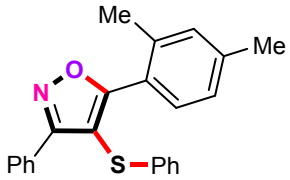
5-(3-Chlorophenyl)-3-phenyl-4-(phenylthio)isoxazole (**4d**): Yield: 76% as a yellow solid; mp = 131 - 132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (dd, J = 7.6, 2.8 Hz, 2H), 7.80 (dd, J = 7.6, 2.4 Hz, 2H), 7.53 - 7.46 (m, 3H), 7.45 - 7.38 (m, 3H), 7.17 - 7.06 (m, 3H), 6.95 (dt, J = 7.6, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 165.0, 138.2, 135.3, 131.2, 130.5, 130.2, 128.8, 128.5, 128.4, 128.0, 127.5, 126.9, 126.2, 125.8, 124.0, 101.0 ppm; ν_{max}(KBr)/cm^{-1} 3060, 2928, 1684, 1567, 1516, 1455, 1410, 1259, 863; HRMS-ESI (m/z): calcd for $C_{21}H_{14}ClNNaOS$, $[M+Na]^+$: 386.0377, found 386.0381.



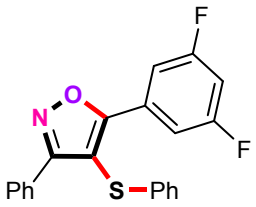
5-(4-Chlorophenyl)-3-phenyl-4-(phenylthio)isoxazole (**4e**): Yield: 80% as a yellow solid; mp = 138 - 139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 - 8.11 (m, 2H), 7.82 (d, J = 7.6 Hz, 2H), 7.55 - 7.48 (m, 3H), 7.47 - 7.38 (m, 3H), 7.19 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 165.0, 134.6, 131.8, 131.2, 130.2, 129.6, 128.8, 128.5, 128.4, 128.0, 127.5, 127.4, 126.8, 101.6 ppm; ν_{max}(KBr)/cm^{-1} 3052, 2928, 1636, 1551, 1470, 1412, 1267, 811, 758; HRMS-ESI (m/z): calcd for $C_{21}H_{15}ClNOS$, $[M+H]^+$: 364.0557, found 364.0562.



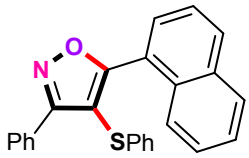
5-(4-Bromophenyl)-3-phenyl-4-(phenylthio)isoxazole (**4f**): Yield: 72% as a yellow solid; mp = 152 - 154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 - 8.05 (m, 2H), 7.94 - 7.80 (m, 2H), 7.56 - 7.48 (m, 3H), 7.45 - 7.36 (m, 3H), 7.33 (d, J = 8.4 Hz, 2H), 6.98 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 165.0, 135.4, 132.3, 131.1, 130.2, 128.8, 128.7, 128.6, 128.0, 127.7, 127.4, 126.9, 119.8, 101.3 ppm; ν_{max}(KBr)/cm^{-1} 3046, 2929, 1556, 1510, 1462, 1413, 1256, 768; HRMS-ESI (m/z): calcd for $C_{21}H_{15}BrNOS$, $[M+H]^+$: 408.0052, found 408.0055.



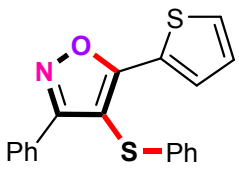
5-(2,4-Dimethylphenyl)-3-phenyl-4-(phenylthio)isoxazole (**4g**): Yield: 84% as a yellow solid; mp = 101 - 102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, J = 7.2, 3.6 Hz, 2H), 7.89 - 7.79 (m, 3H), 7.56 - 7.45 (m, 5H), 7.42 (dt, J = 8.8, 4.2 Hz, 3H), 2.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 165.3, 139.0, 135.9, 130.8, 130.0, 129.2, 128.9, 128.7, 128.6, 127.5, 126.8, 125.8, 123.6, 97.6, 21.3 ppm; ν_{max}(KBr)/cm^{-1} 3052, 2928, 1680, 1575, 1508, 1455, 1266, 865; HRMS-ESI (m/z): calcd for $C_{23}H_{19}NNaOS$, $[M+Na]^+$: 380.1080, found 380.1086.



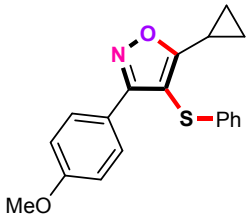
5-(3,5-Difluorophenyl)-3-phenyl-4-(phenylthio)isoxazole (**4h**): Yield: 69% as a yellow solid; mp = 143 - 144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, J = 7.2, 2.6 Hz, 2H), 7.82 (dd, J = 7.6, 2.0 Hz, 2H), 7.54 - 7.49 (m, 3H), 7.46 - 7.38 (m, 3H), 6.99 (dd, J = 18.0, 8.4 Hz, 1H), 6.94 - 6.87 (m, 1H), 6.84 - 6.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 164.9, 151.3 (dd, J = 176.7, 12.3 Hz), 148.8 (dd, J = 175.4, 13.5 Hz), 132.2 (dd, J = 5.8, 3.6 Hz), 131.3, 130.2, 128.8, 128.7, 128.5, 127.8, 127.5, 126.9, 122.5 (dd, J = 6.8, 3.2 Hz), 118.2 (d, J = 18.4 Hz), 115.8 (d, J = 19.9 Hz), 101.7 ppm; ν_{max}(KBr)/cm^{-1} 3050, 2928, 1654, 1593, 1498, 1426, 1270, 795; HRMS-ESI (m/z): calcd for $C_{21}H_{13}F_2NNaOS$, $[M+Na]^+$: 388.0578, found 388.0582.



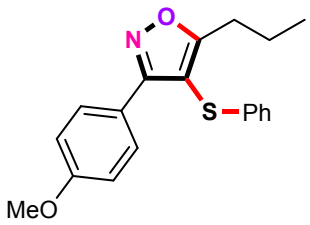
5-(Naphthalen-1-yl)-3-phenyl-4-(phenylthio)isoxazole (**4i**): Yield: 78% as a yellow solid; mp = 123 - 125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 - 8.10 (m, 2H), 7.84 (d, J = 7.6 Hz, 2H), 7.73 (dd, J = 12.8, 8.8 Hz, 2H), 7.65 (d, J = 7.6 Hz, 1H), 7.54 - 7.36 (m, 9H), 7.22 (d, J = 9.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 165.3, 133.8, 133.7, 131.6, 131.1, 130.1, 129.1, 128.8, 128.6, 128.5, 128.1, 127.9, 127.6, 127.1, 127.0, 126.9, 125.8, 124.2, 123.7, 101.6 ppm; ν_{max}(KBr)/cm^{-1} 3036, 2928, 1635, 1552, 1453, 1412, 1266, 746; HRMS-ESI (m/z): calcd for $C_{25}H_{17}NNaOS$, $[M+Na]^+$: 402.0923, found 402.0927.



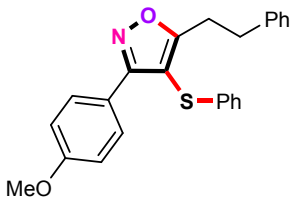
3-Phenyl-4-(phenylthio)-5-(thiophen-2-yl)isoxazole (**4j**): Yield: 66% as a yellow solid; mp = 97 - 98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 - 8.13 (m, 2H), 7.95 - 7.80 (m, 2H), 7.60 - 7.45 (m, 3H), 7.44 - 7.35 (m, 3H), 7.12 (d, J = 5.2 Hz, 1H), 6.82 - 6.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 164.5, 133.8, 131.0, 130.7, 130.0, 129.2, 129.0, 128.8, 128.6, 127.8, 127.3, 126.8, 125.8, 105.6 ppm; ν_{max}(KBr)/cm^{-1} 3046, 2928, 1656, 1552, 1450, 1410, 767; HRMS-ESI (m/z): calcd for $C_{19}H_{13}NNaOS_2$, $[M+Na]^+$: 358.0331, found 358.0334.



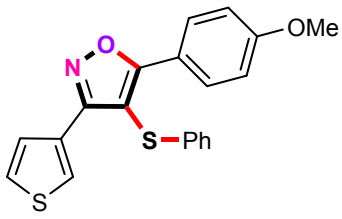
5-Cyclopropyl-3-(4-methoxyphenyl)-4-(phenylthio)isoxazole (**4l**): Yield: 80% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.2 Hz, 2H), 7.49 - 7.36 (m, 3H), 7.06 (d, J = 8.2 Hz, 2H), 6.78 (d, J = 8.2 Hz, 2H), 3.72 (s, 3H), 2.48 - 2.20 (m, 1H), 1.31 - 1.26 (m, 2H), 1.18 - 1.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.4, 163.6, 158.4, 129.8, 128.7, 128.5, 128.4, 128.3, 127.3, 114.9, 103.3, 55.5, 8.8, 8.2 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2936, 1576, 1480, 1410, 1250, 754; HRMS-ESI (m/z): calcd for $C_{19}H_{17}NNaO_2S$, $[M+Na]^+$: 346.0872, found 346.0875.



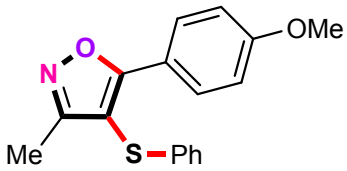
3-(4-Methoxyphenyl)-4-(phenylthio)-5-propylisoxazole (**4m**): Yield: 80% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, J = 7.6, 2.0 Hz, 2H), 7.45 - 7.40 (m, 3H), 7.06 (d, J = 8.8 Hz, 2H), 6.79 (d, J = 8.8 Hz, 2H), 3.75 (s, 3H), 2.89 (t, J = 7.6 Hz, 2H), 2.13 - 1.65 (m, 2H), 0.98 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 163.1, 158.3, 134.4, 129.7, 128.7, 128.5, 128.3, 127.0, 114.8, 104.2, 55.3, 28.0, 20.9, 13.8 ppm; ν_{max}(KBr)/cm^{-1} 3046, 2936, 1572, 1486, 1413, 1244, 756; HRMS-ESI (m/z): calcd for $C_{19}H_{19}NNaO_2S$, $[M+Na]^+$: 348.1029, found 348.1032.



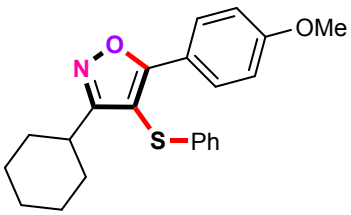
3-(4-Methoxyphenyl)-5-phenethyl-4-(phenylthio)isoxazole (**4n**): Yield: 73% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.2 Hz, 2H), 7.49 - 7.38 (m, 3H), 7.28 (dd, J = 16.8, 9.2 Hz, 3H), 7.20 (d, J = 7.2 Hz, 2H), 6.89 (d, J = 8.2 Hz, 2H), 6.72 (d, J = 8.0 Hz, 2H), 3.72 (s, 3H), 3.24 (t, J = 7.8 Hz, 2H), 3.06 (t, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 163.1, 158.3, 140.0, 129.8, 129.0, 128.8, 128.6, 128.4, 128.3, 126.6, 126.5, 114.8, 104.9, 55.2, 33.2, 28.1 ppm; ν_{max}(KBr)/cm^{-1} 3044, 2938, 1588, 1516, 1472, 1258, 756; HRMS-ESI (m/z): calcd for $C_{24}H_{21}NNaO_2S$, $[M+Na]^+$: 410.1185, found 410.1189.



5-(4-Methoxyphenyl)-4-(phenylthio)-3-(thiophen-3-yl)isoxazole (**4o**): Yield: 71% as a white solid; mp = 106 - 107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 4.2 Hz, 1H), 7.88 (d, J = 7.2 Hz, 2H), 7.54 (d, J = 5.2 Hz, 1H), 7.50 - 7.41 (m, 3H), 7.17 (t, J = 4.8 Hz, 1H), 7.08 (d, J = 8.8 Hz, 2H), 6.75 (d, J = 8.8 Hz, 2H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 164.4, 158.4, 130.2, 130.1, 129.1, 128.8, 128.6, 128.4, 128.1, 127.8, 127.7, 126.2, 115.0, 102.4, 55.4 ppm; ν_{max}(KBr)/cm^{-1} 3038, 2927, 1576, 1488, 1414, 1246, 758; HRMS-ESI (m/z): calcd for $C_{20}H_{15}NNaO_2S_2$, $[M+Na]^+$: 388.0436, found 388.0440.

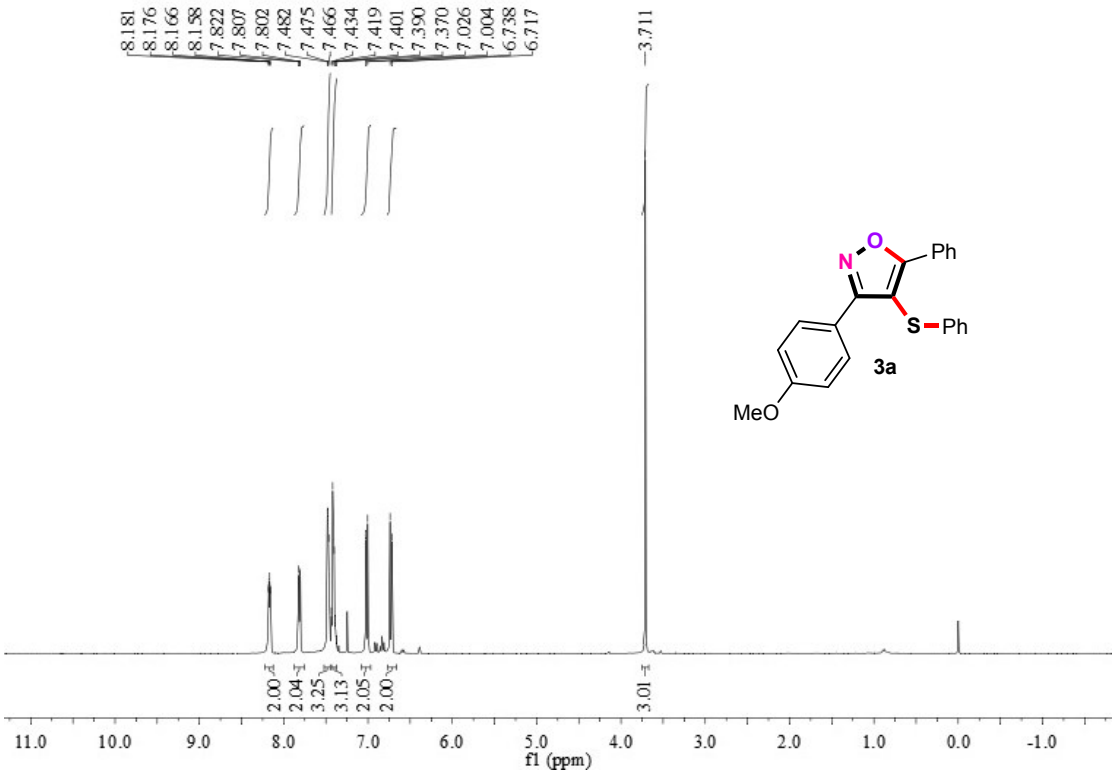


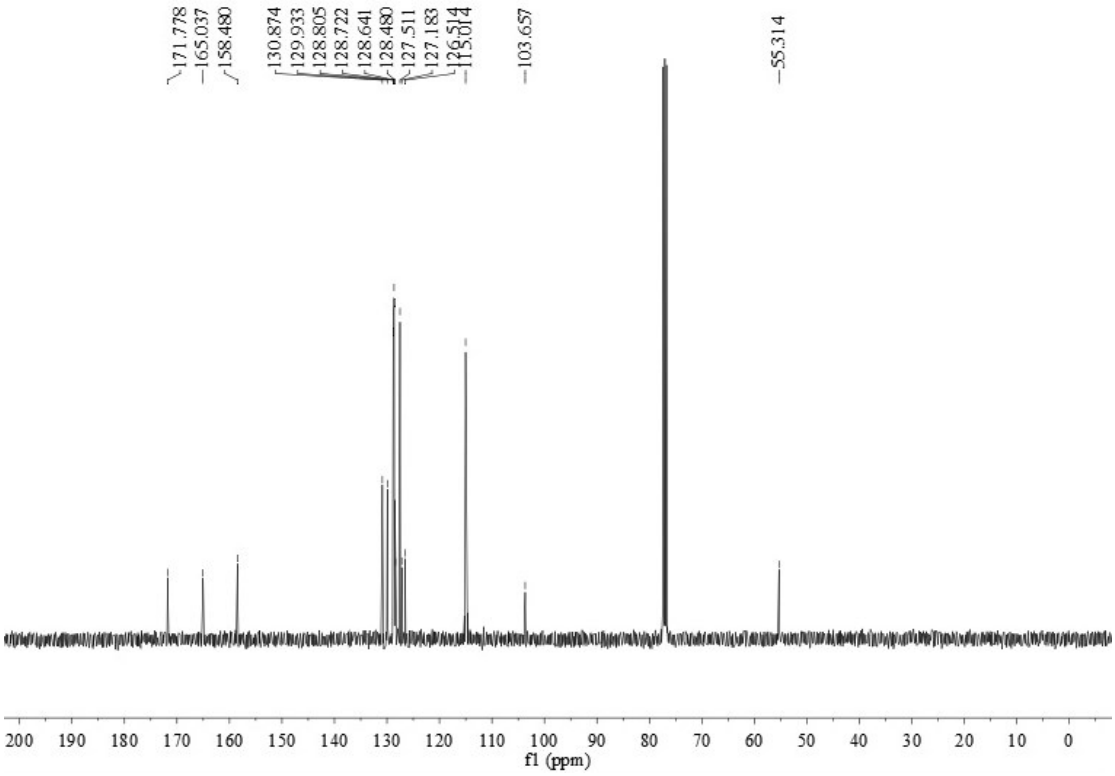
5-(4-Methoxyphenyl)-3-methyl-4-(phenylthio)isoxazole (**4q**): Yield: 81% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 - 8.04 (m, 2H), 7.57 - 7.42 (m, 3H), 7.11 (d, J = 8.8 Hz, 2H), 6.80 (d, J = 8.8 Hz, 2H), 3.75 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 163.7, 158.5, 130.6, 129.0, 128.7, 127.5, 127.2, 125.8, 115.0, 104.7, 55.5, 10.2 ppm; ν_{max}(KBr)/cm^{-1} 3048, 2932, 1558, 1482, 1416, 1250, 753; HRMS-ESI (m/z): calcd for $C_{17}H_{15}NNaO_2S$, $[M+Na]^+$: 320.0716, found 320.0718.

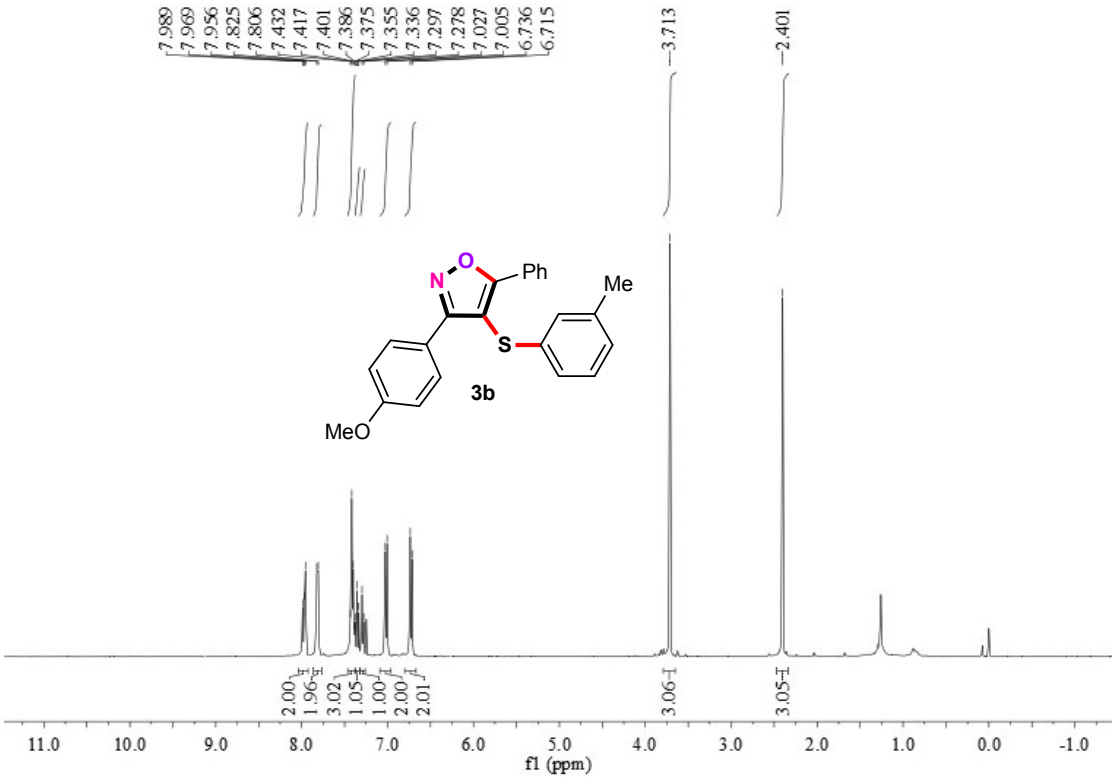


3-Cyclohexyl-5-(4-methoxyphenyl)-4-(phenylthio)isoxazole (**4r**): Yield: 64% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 - 8.08 (m, 2H), 7.53 - 7.36 (m, 3H), 7.08 (d, J = 8.8 Hz, 2H), 6.79 (d, J = 8.8 Hz, 2H), 3.72 (s, 3H), 2.88 - 2.72 (m, 1H), 1.95 - 1.86 (m, 2H), 1.84 - 1.76 (m, 2H), 1.73 - 1.67 (m, 1H), 1.60 (dd, J = 11.6, 7.2 Hz, 2H), 1.35 - 1.25 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 170.3, 158.6, 130.5, 128.8, 128.6, 127.4, 127.2, 126.8, 115.0, 103.4, 55.5, 35.7, 31.4, 26.2, 25.8 ppm; ν_{max}(KBr)/cm^{-1} 3038, 2946, 1580, 1488, 1414, 1258, 758; HRMS-ESI (m/z): calcd for $C_{22}H_{23}NNaO_2S$, $[M+Na]^+$: 388.1342, found 388.1346.

^{1}H and ^{13}C NMR spectra of compounds 3



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7.278
7.027
7.005
6.736
6.715
3.713
2.401
N
O
Ph
Me
S
MeO
3b
2.00
1.96
3.02
1.05
1.00
2.00
2.01
3.06
3.05
11.0
10.0
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6.0
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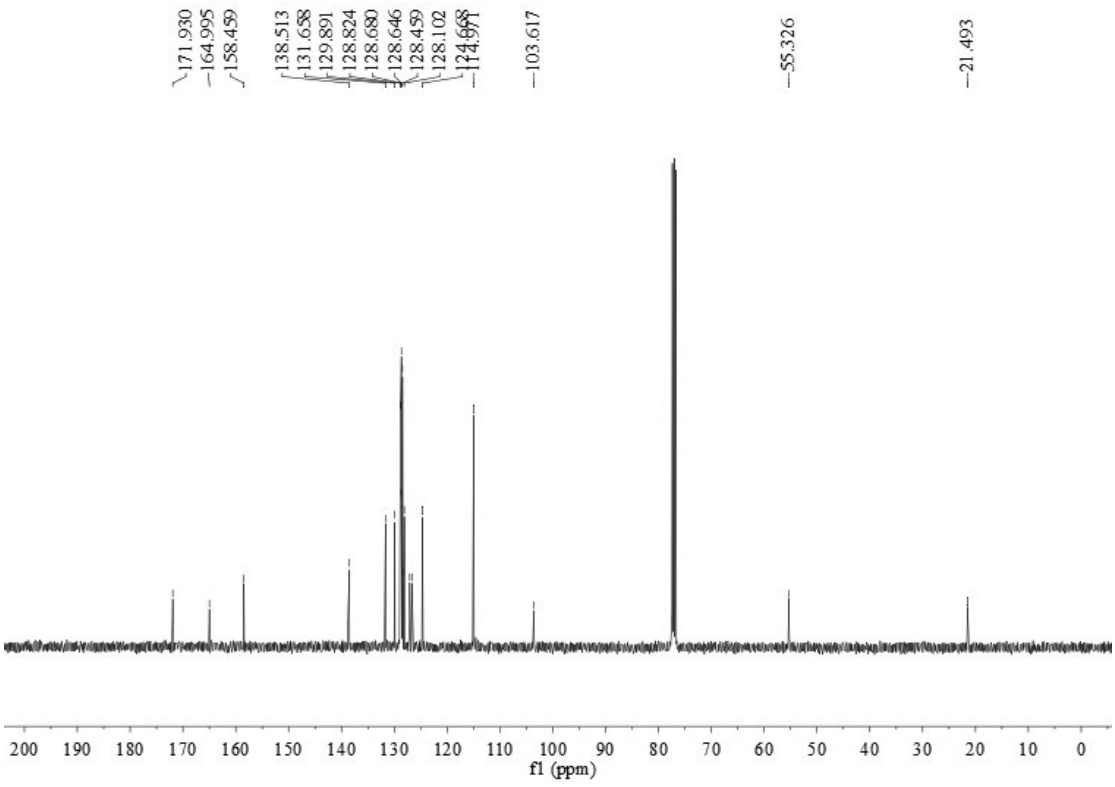
f1 (ppm)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55.326
21.493
200
190
180
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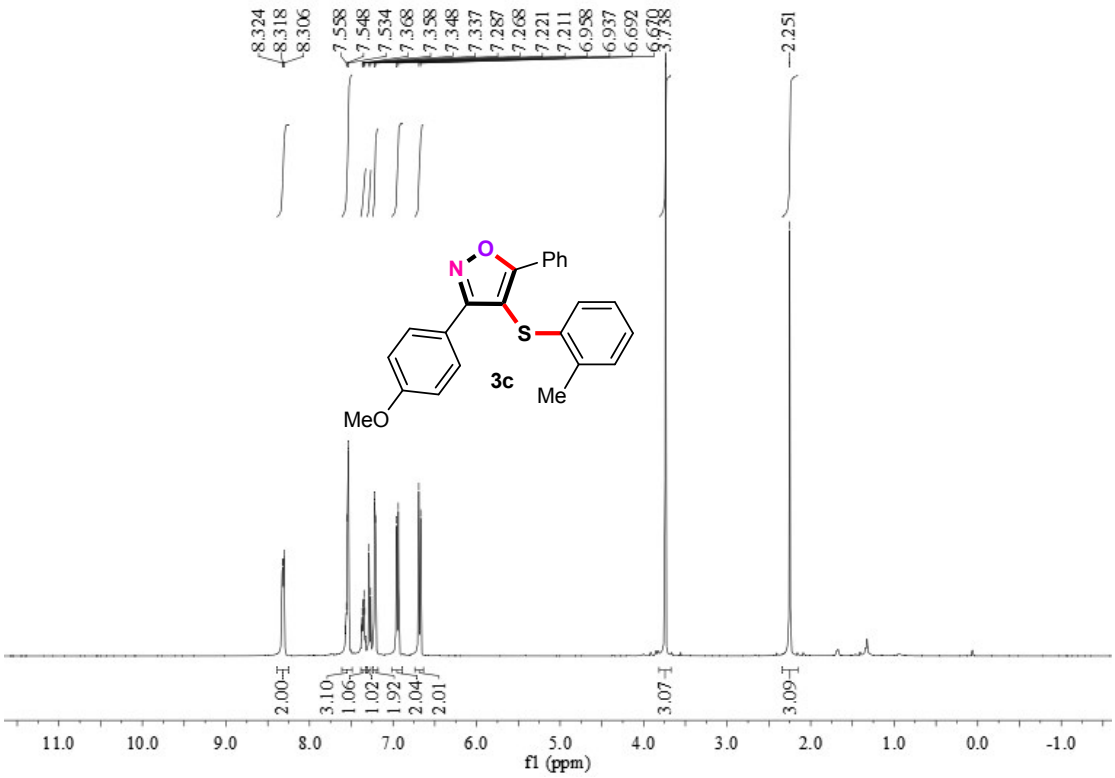
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.211
6.958
6.937
6.692
6.670
3.738
2.251
O
N
Ph
S
3c
Me
MeO
2.00
3.10
1.06
1.02
1.92
2.04
2.01
3.07
3.09
11.0
10.0
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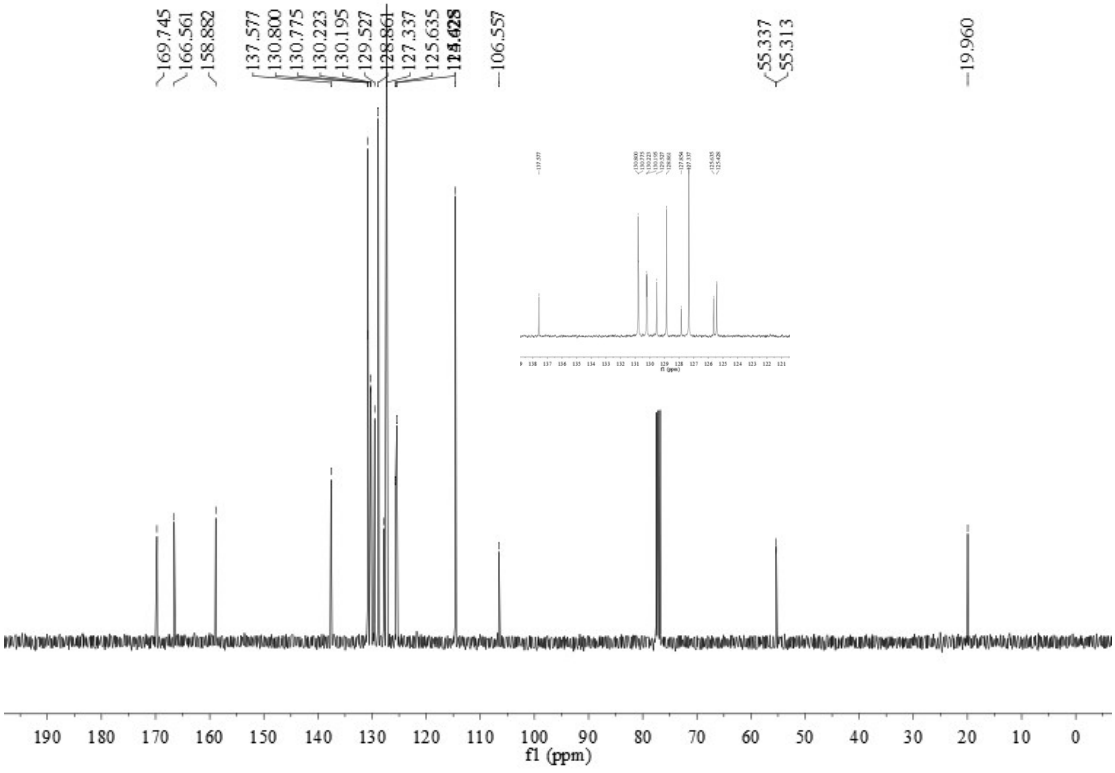
f1 (ppm)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55.337
55.313
19.960
190
180
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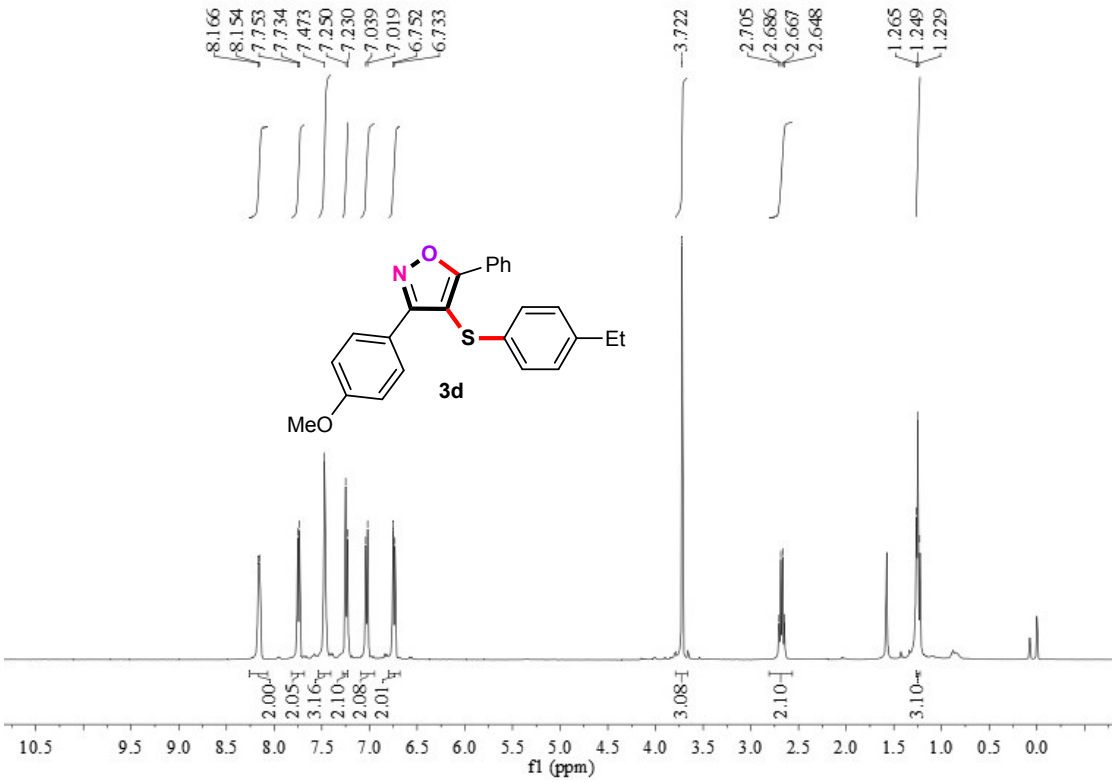
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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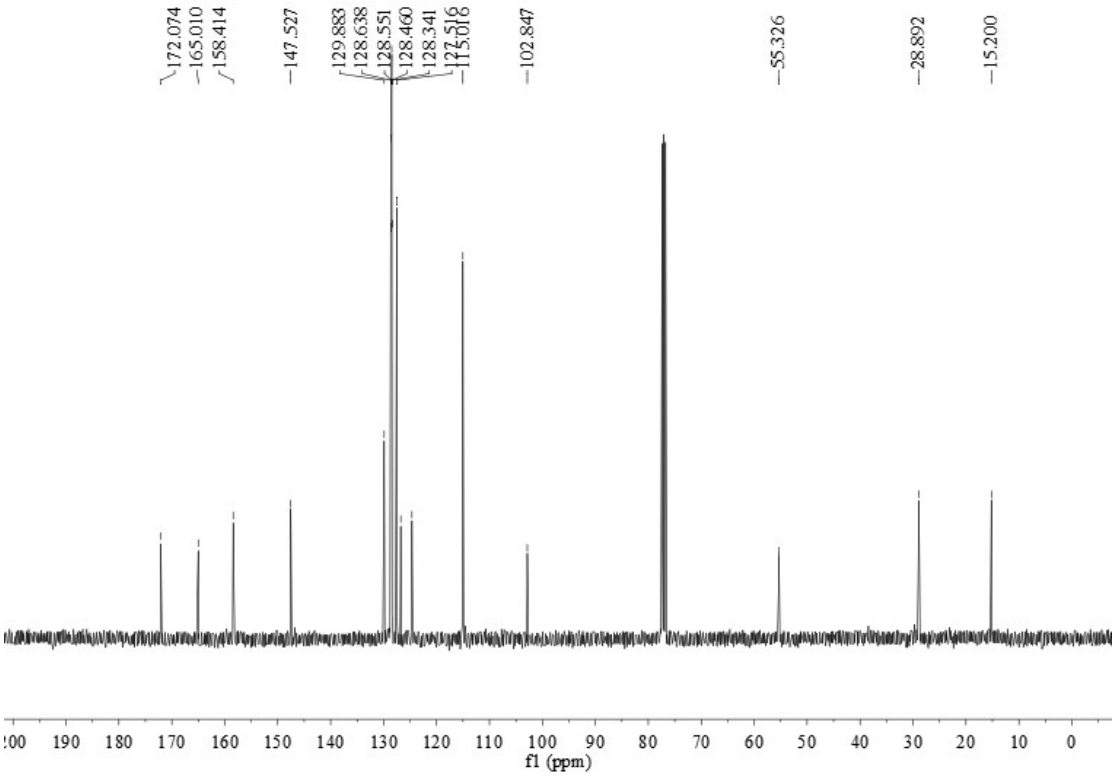
2.686
2.667
2.648
1.265
1.249
1.229
Ph
O
N
S
Et
MeO
3d
2.00
2.05
3.16
2.10
2.08
2.01
3.08
2.10
3.10
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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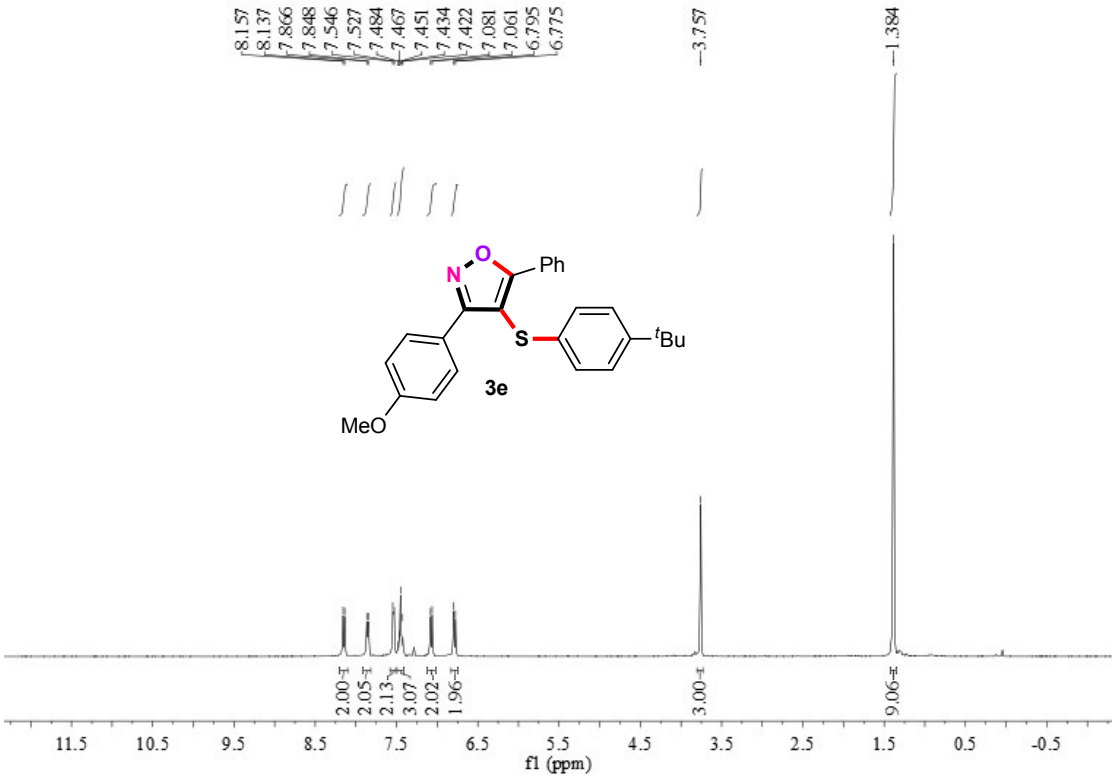
28.892
15.200
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.137
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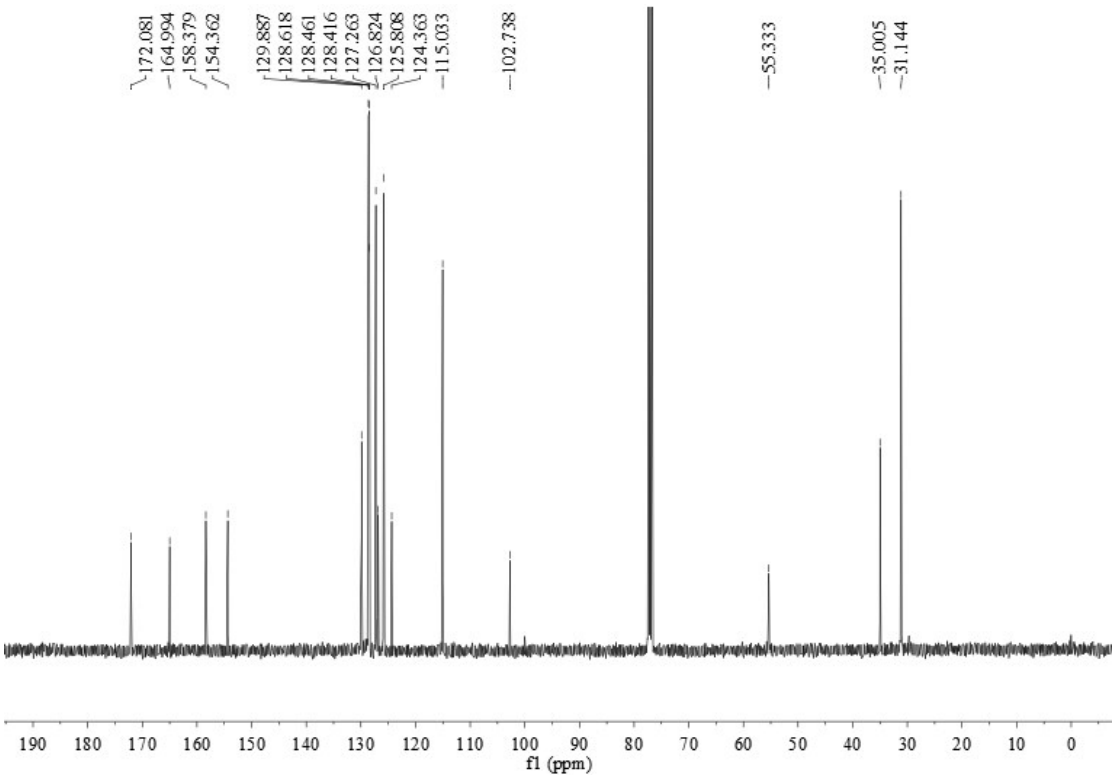
7.848
7.546
7.527
7.484
7.467
7.451
7.434
7.422
7.081
7.061
6.795
6.775
3.757
1.384
N
O
Ph
S
tBu
MeO
3e
2.00
2.05
2.13
3.07
2.02
1.96
3.00
9.06
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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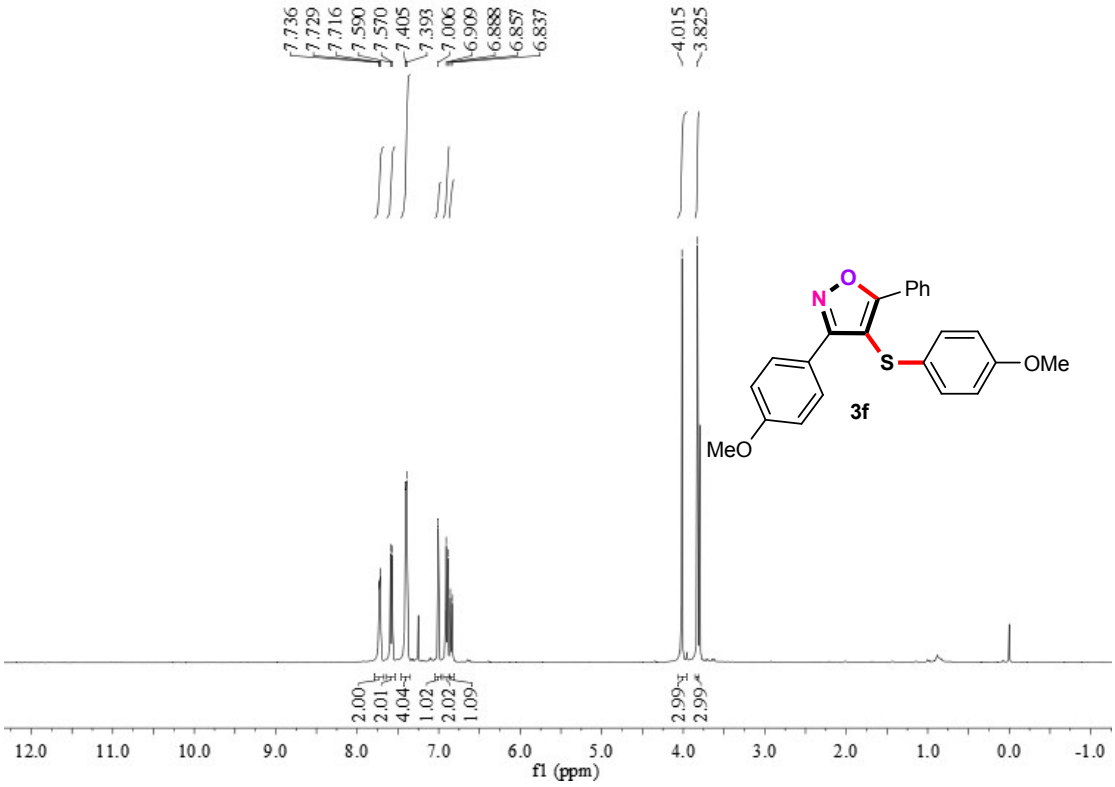
164.994
158.379
154.362
129.887
128.618
128.461
128.416
127.263
126.824
125.808
124.363
115.033
102.738
55.333
35.005
31.144
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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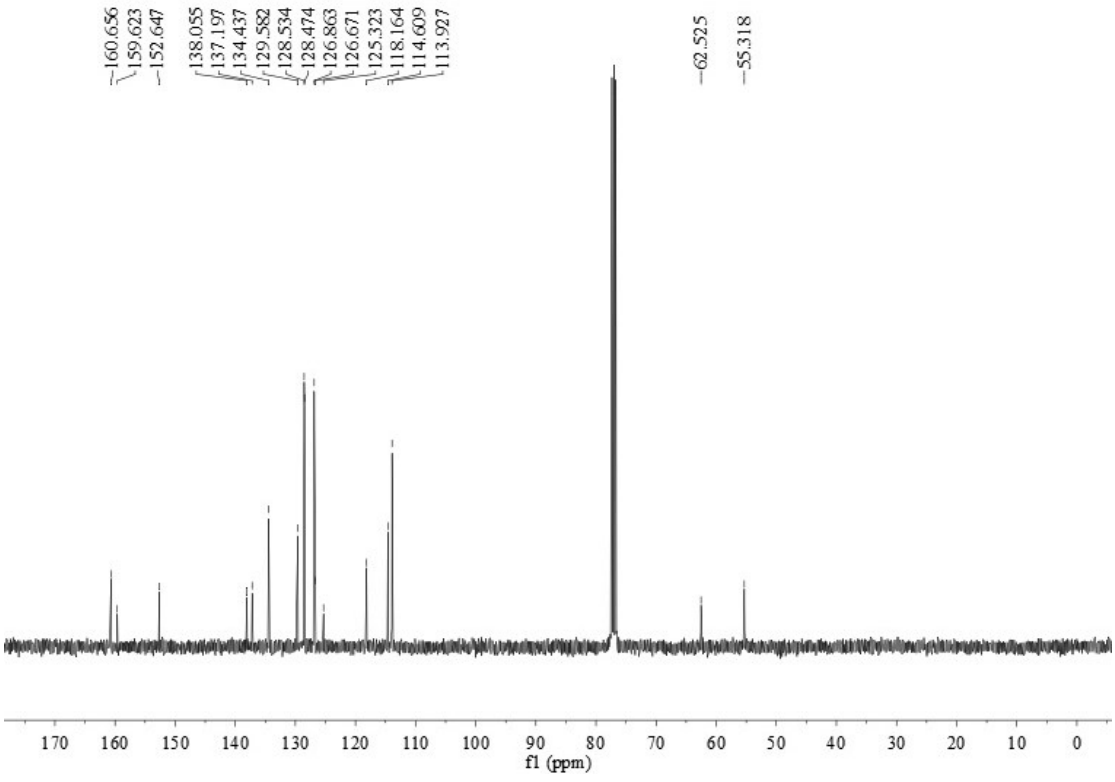
7.716
7.590
7.570
7.405
7.393
7.006
6.909
6.888
6.857
6.837
4.015
3.825
2.00
2.01
4.04
1.02
2.02
1.09
2.99
2.99
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)
N
O
Ph
S
OMe
MeO
3f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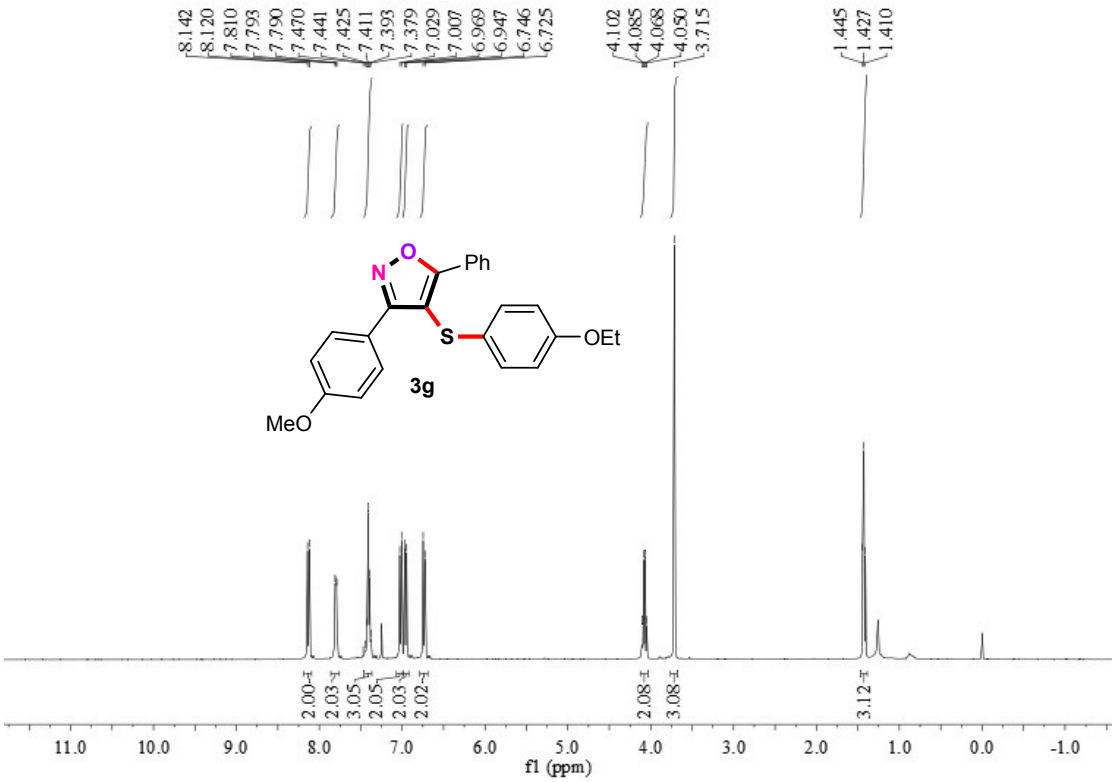
159.623
152.647
138.055
137.197
134.437
129.582
128.534
128.474
126.863
126.671
125.323
118.164
114.609
113.927
62.525
55.318
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.120
7.810
7.793
7.790
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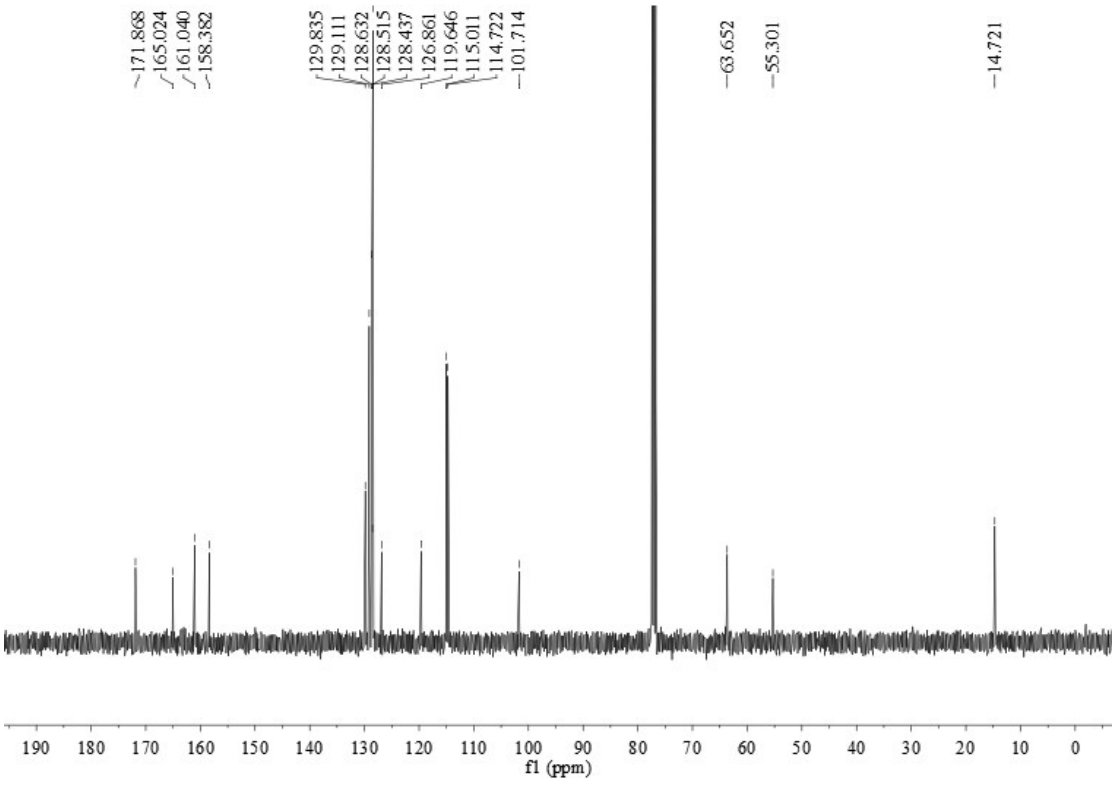
7.441
7.425
7.411
7.393
7.379
7.029
7.007
6.969
6.947
6.746
6.725
4.102
4.085
4.068
4.050
3.715
1.445
1.427
1.410
N
O
Ph
S
OEt
MeO
3g
2.00
2.03
3.05
2.05
2.03
2.02
2.08
3.08
3.12
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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161.040
158.382
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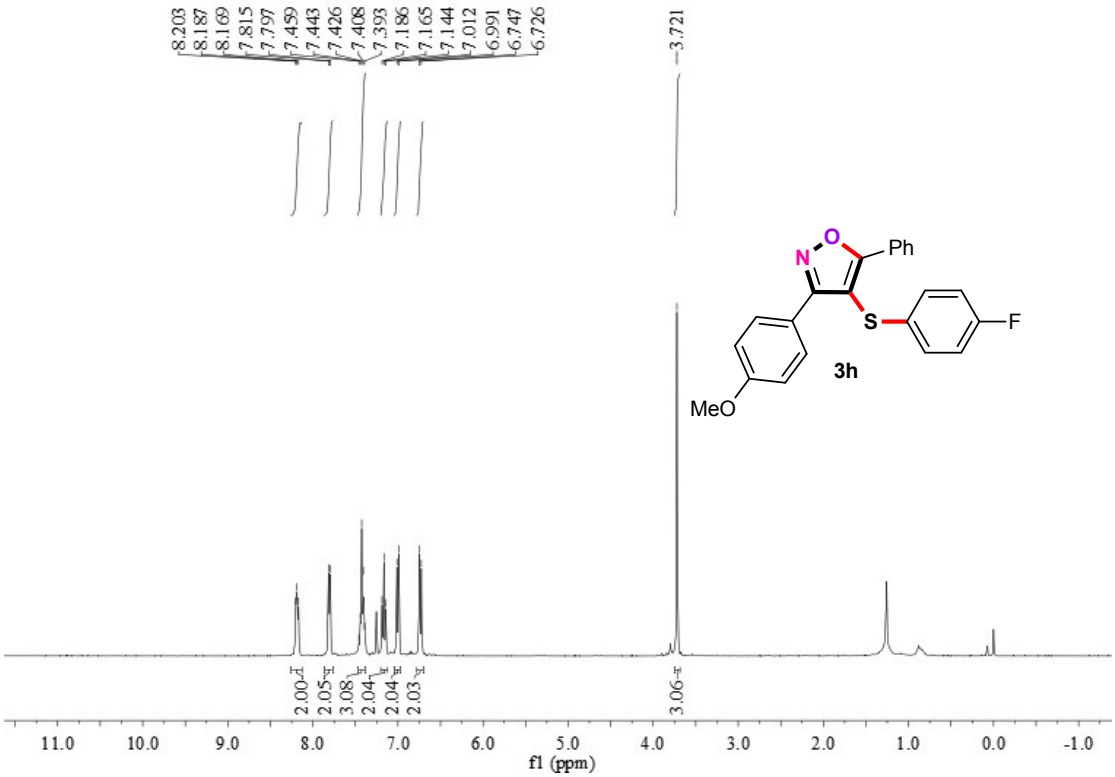
129.111
128.632
128.515
128.437
126.861
119.646
115.011
114.722
101.714
63.652
55.301
14.721
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.169
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7.797
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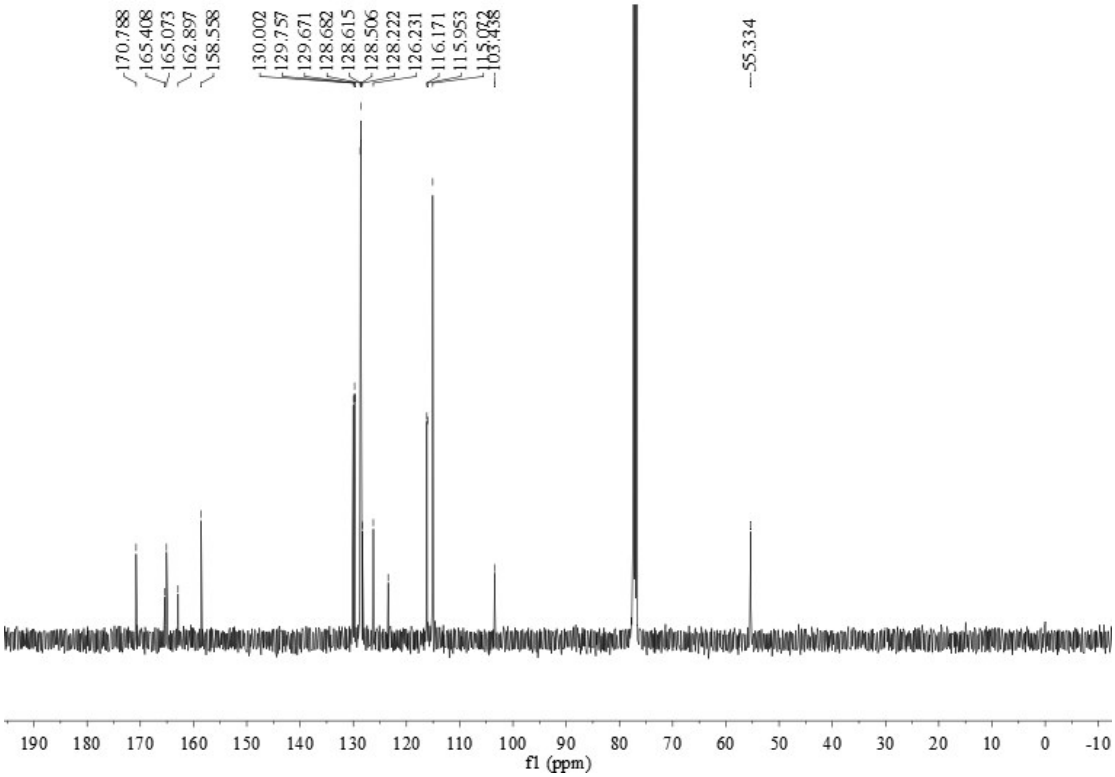
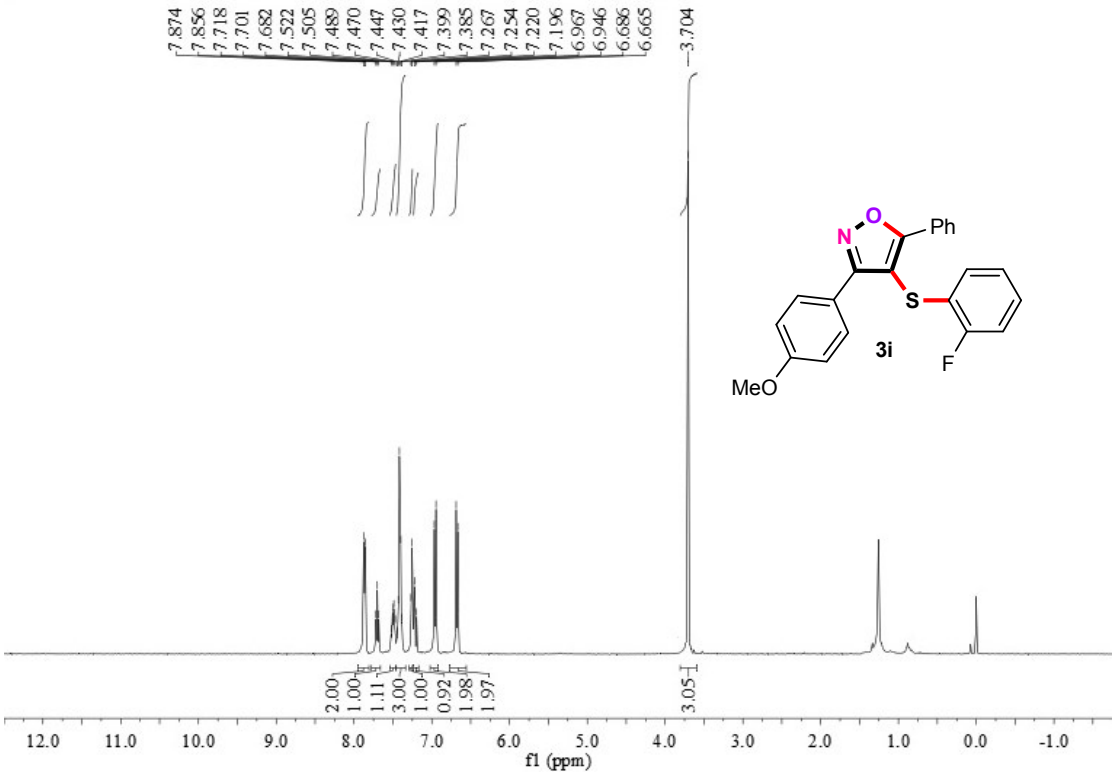
7.443
7.426
7.408
7.393
7.186
7.165
7.144
7.012
6.991
6.747
6.726
3.721
Ph
N
O
S
F
MeO
3h
2.00
2.05
3.08
2.04
2.04
2.03
3.06
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


170.788
165.408
165.073
162.897
158.558
130.002
129.757
129.671
128.682
128.615
128.506
128.222
126.231
116.171
115.953
115.072
163.438
55.334
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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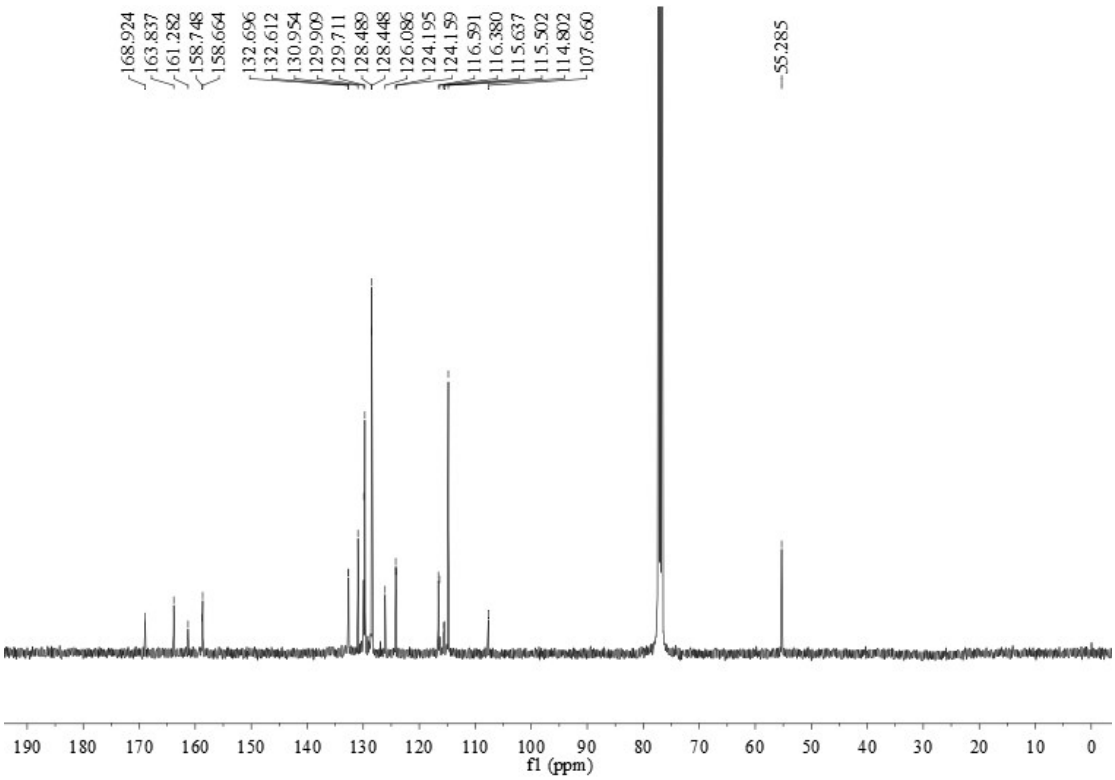
7.718
7.701
7.682
7.522
7.505
7.489
7.470
7.447
7.430
7.417
7.399
7.385
7.267
7.254
7.220
7.196
6.967
6.946
6.686
6.665
3.704
2.00
1.00
1.11
3.00
1.00
0.92
1.98
1.97
3.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)
O
N
Ph
S
F
MeO
3i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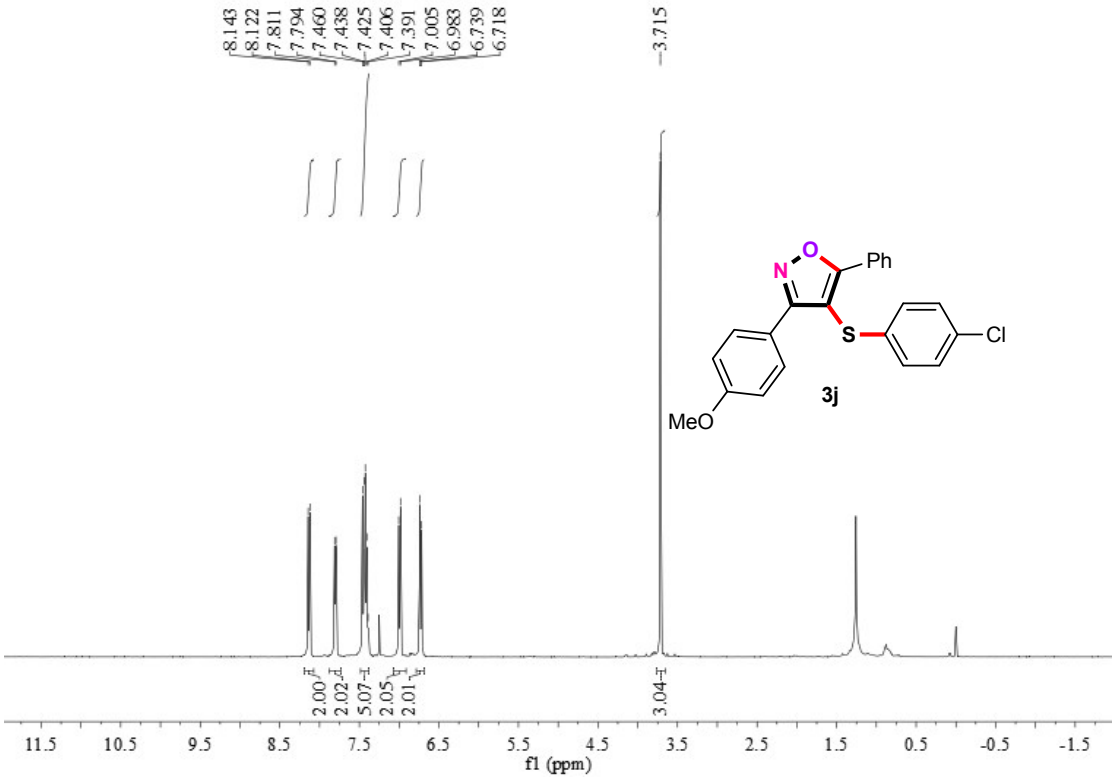
163.837
161.282
158.748
158.664
132.696
132.612
130.954
129.909
129.711
128.489
128.448
126.086
124.195
124.159
116.591
116.380
115.637
115.502
114.802
107.660
55.285
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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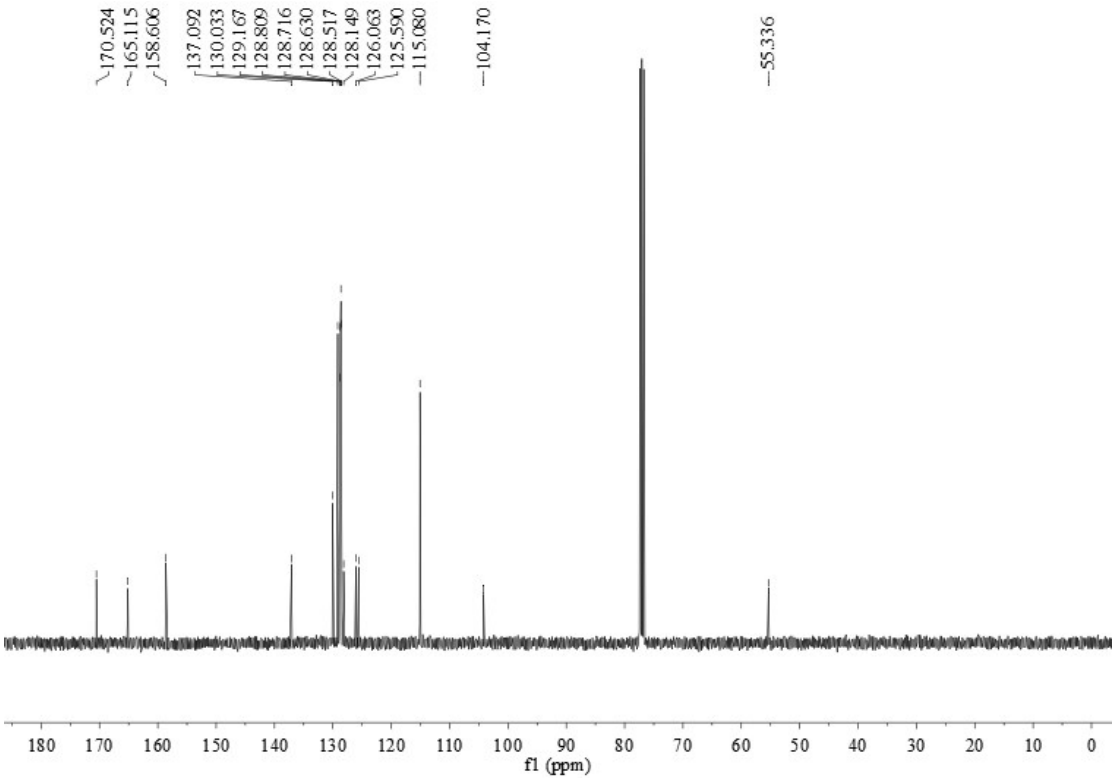
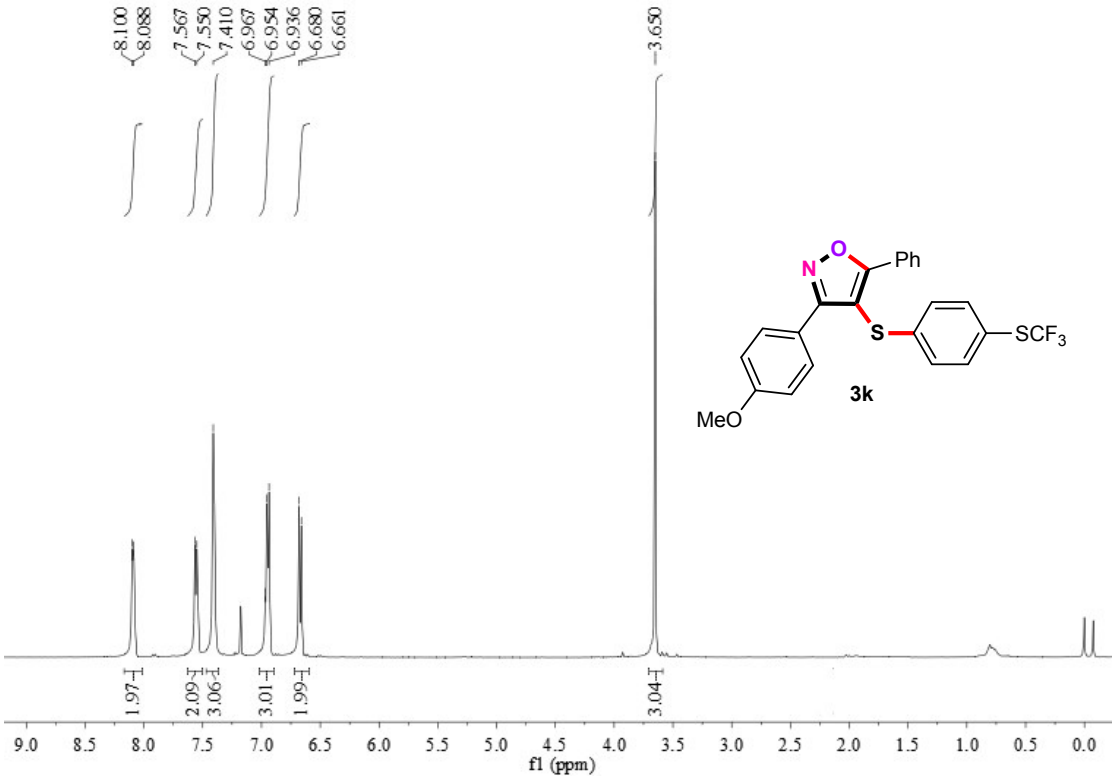
7.460
7.438
7.425
7.406
7.391
7.005
6.983
6.739
6.718
3.715
Ph
O
N
S
Cl
MeO
3j
2.00
2.02
5.07
2.05
2.01
3.04
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)


170.524
165.115
158.606
137.092
130.033
129.167
128.809
128.716
128.630
128.517
128.149
126.063
125.590
115.080
104.170
55.336
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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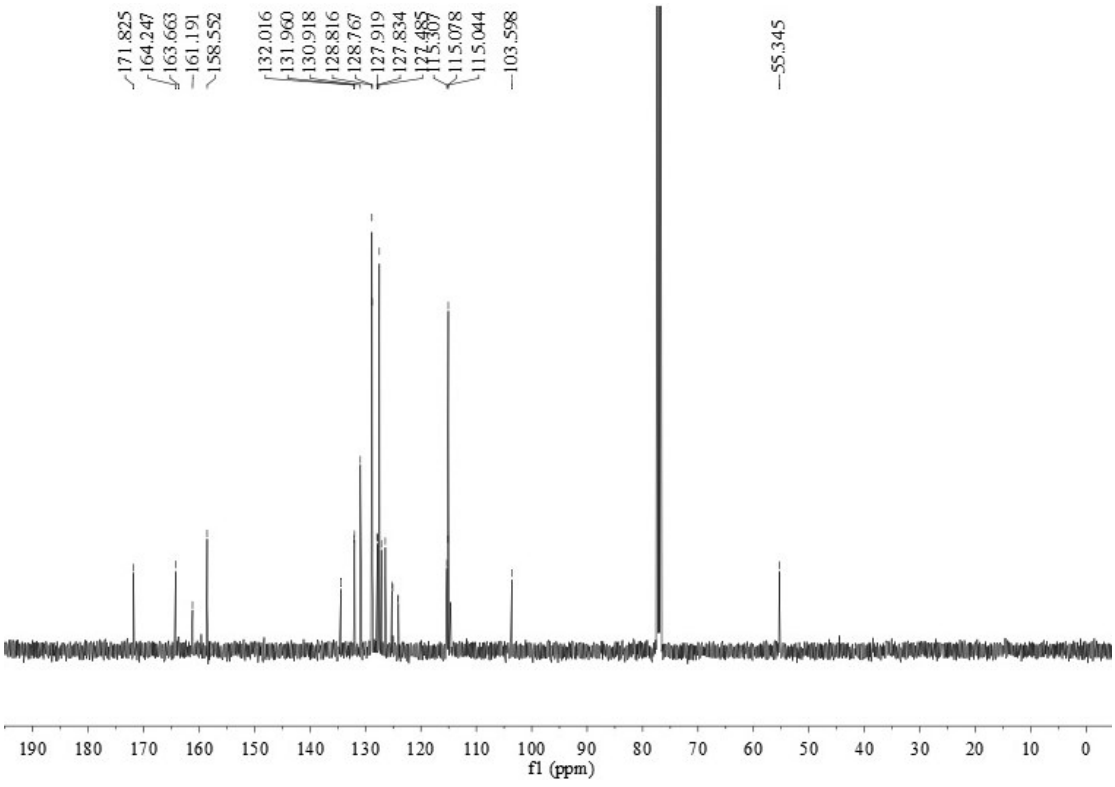
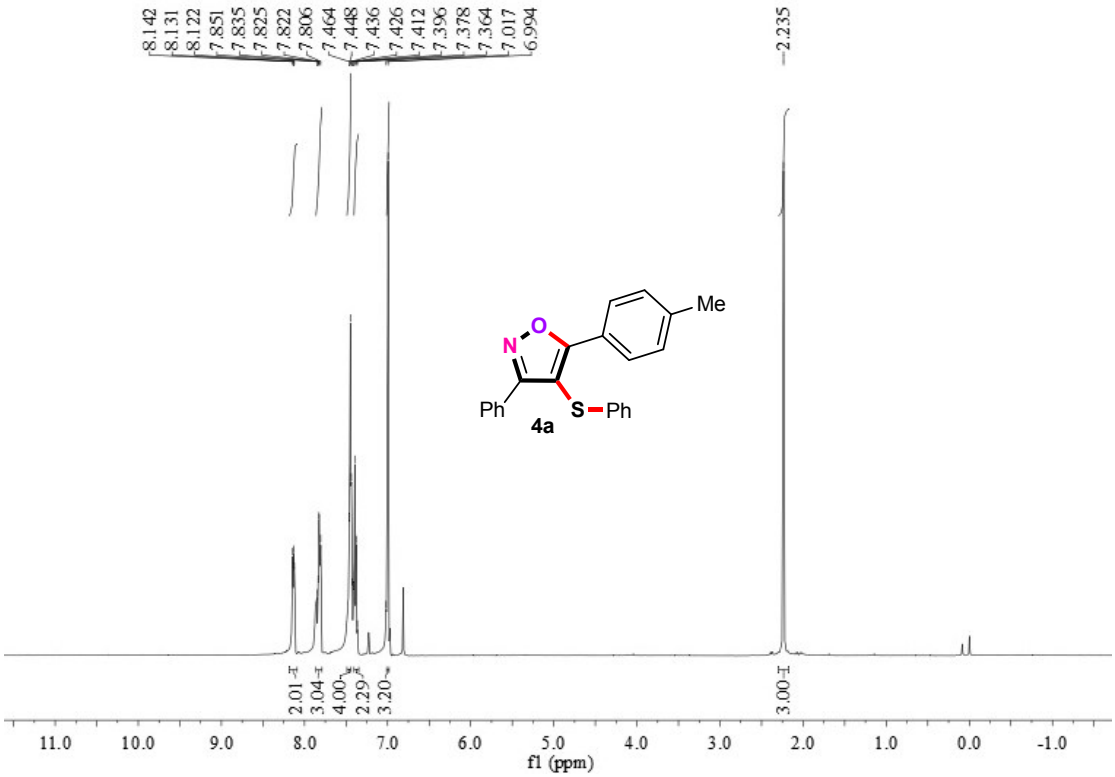
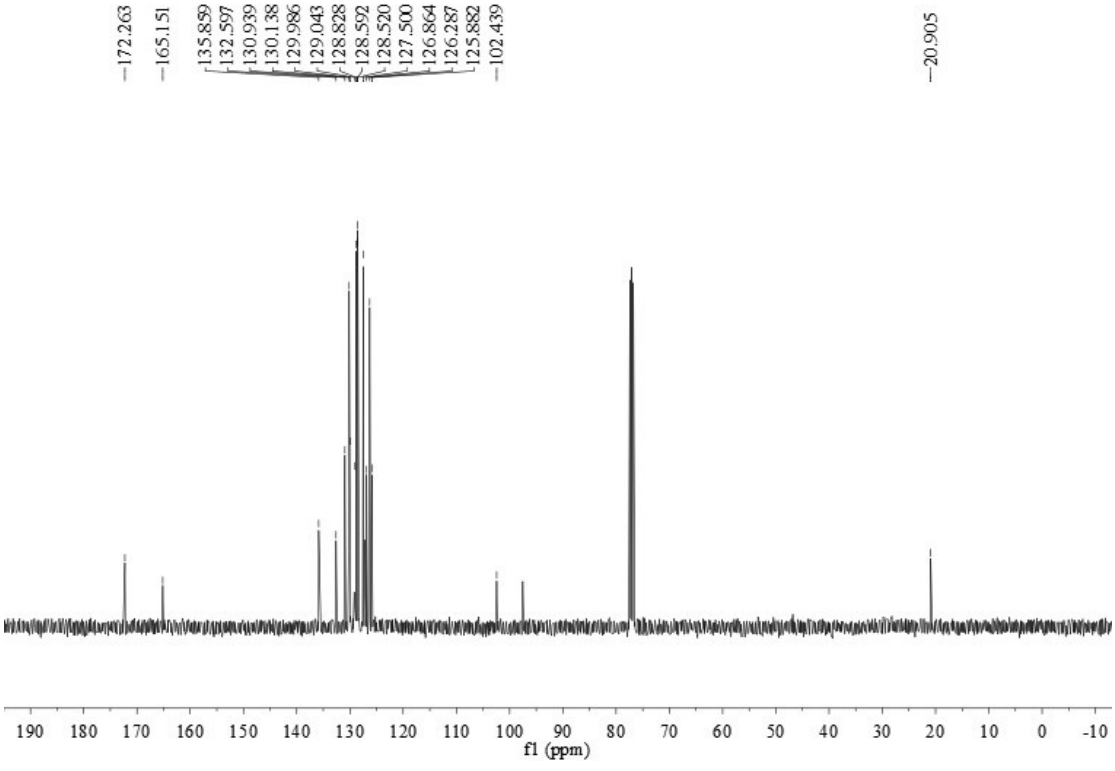
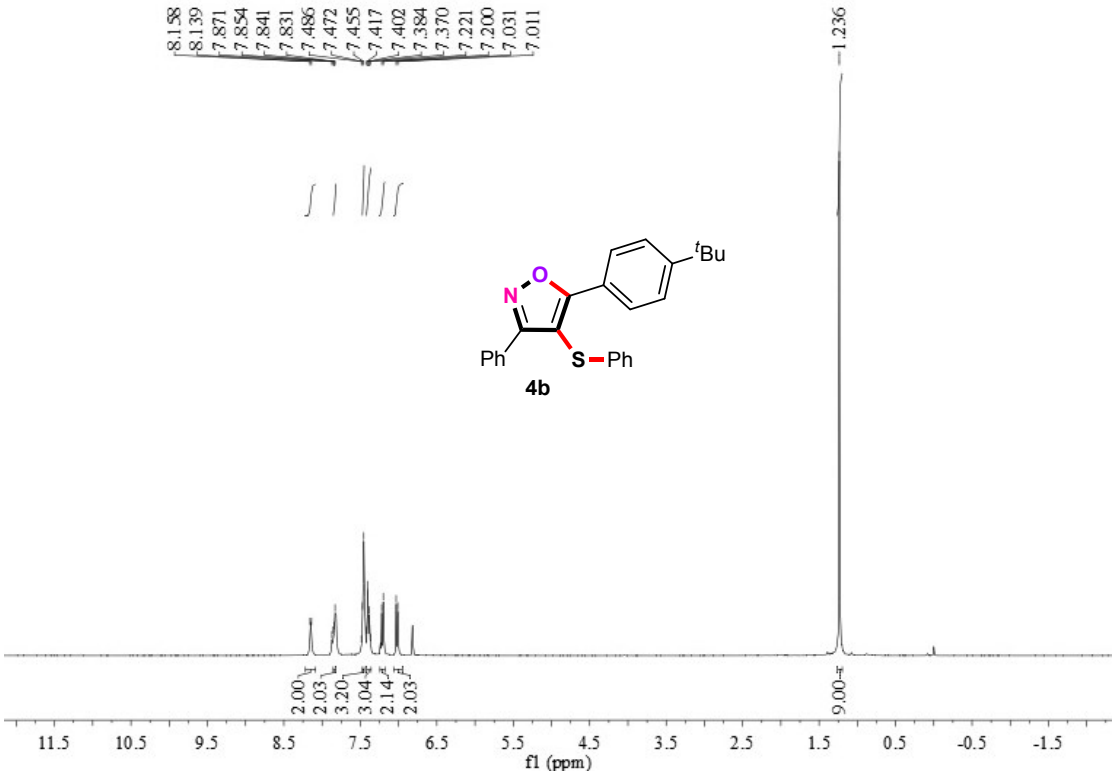
8.088
7.567
7.550
7.410
6.967
6.954
6.936
6.680
6.661
3.650
1.97
2.09
3.06
3.01
1.99
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
N
O
Ph
S
SCF3
MeO
3k


171.825
164.247
163.663
161.191
158.552
132.016
131.960
130.918
128.816
128.767
127.919
127.834
127.485
115.307
115.078
115.044
103.598
55.345
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compounds 4



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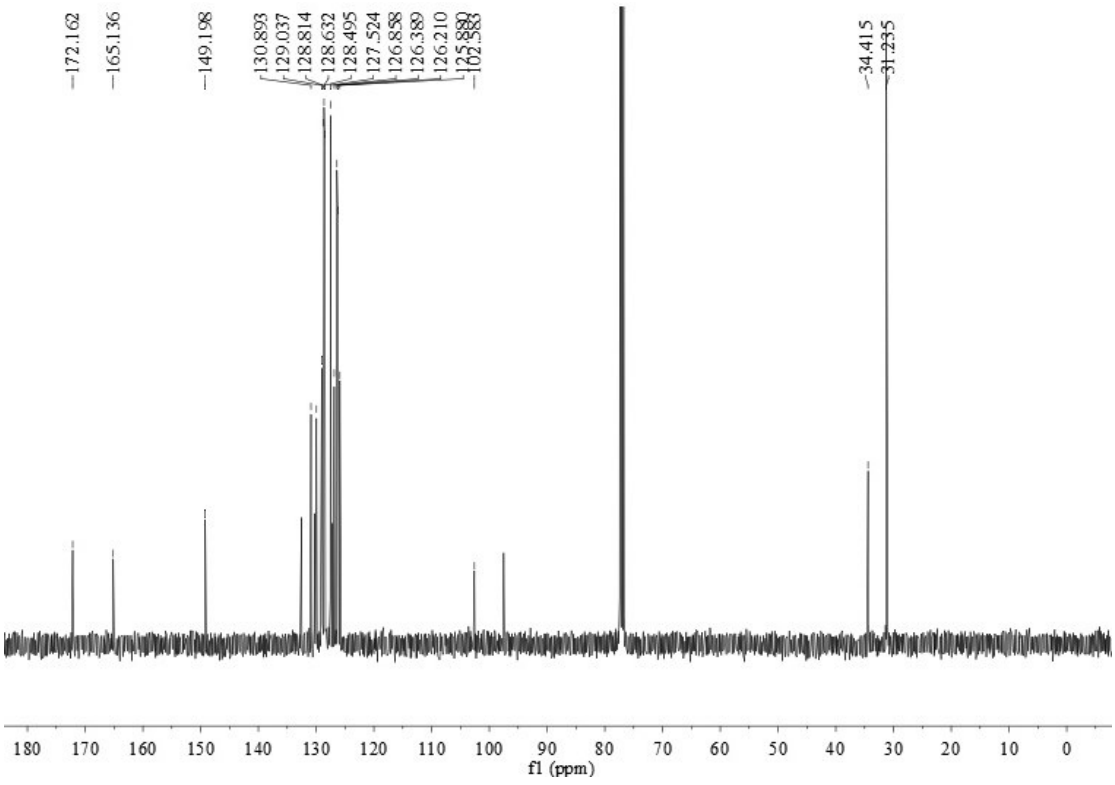
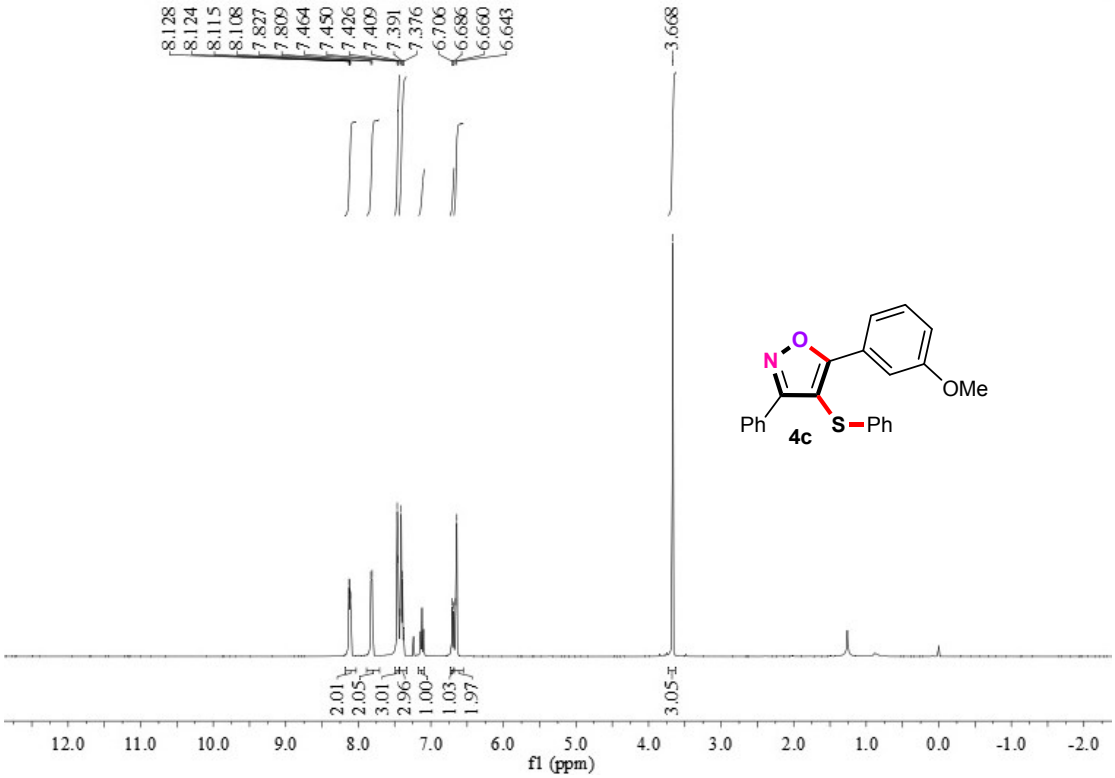
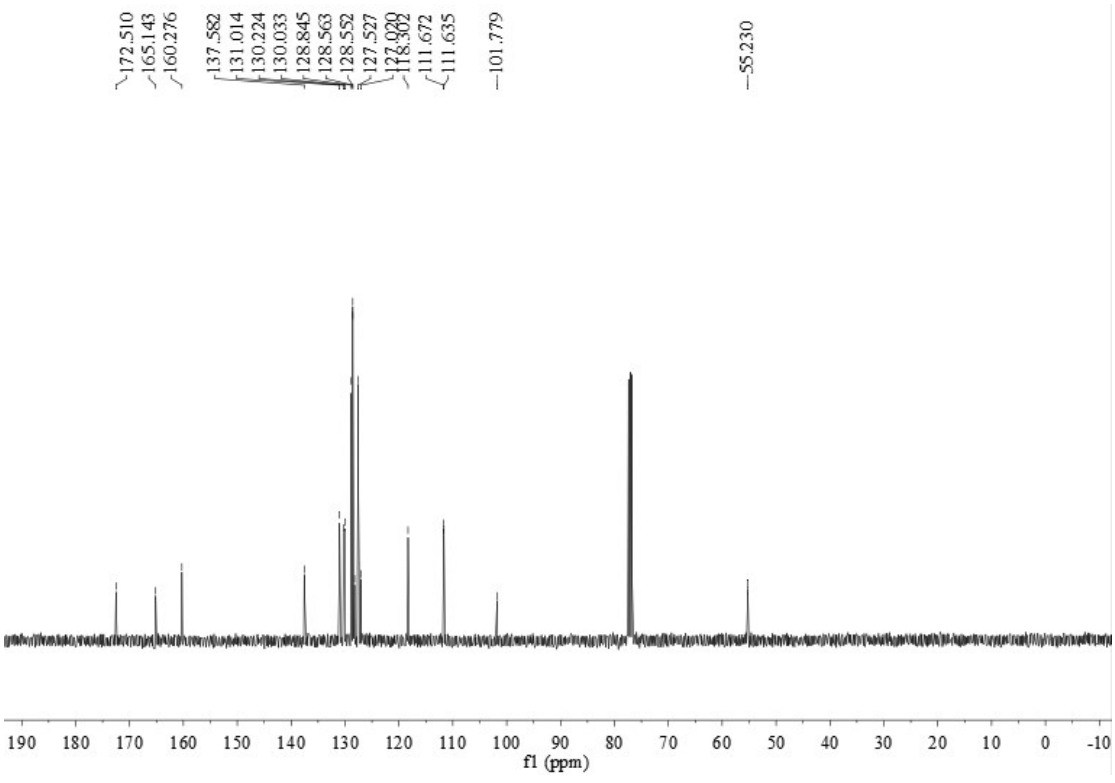
7.402
7.384
7.370
7.221
7.200
7.031
7.011
1.236
tBu
N
O
Ph
S
Ph
4b
2.00
2.03
3.20
3.04
2.14
2.03
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)


172.162
165.136
149.198
130.893
129.037
128.814
128.632
128.495
127.524
126.858
126.389
126.210
34.415
31.235
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.128
8.124
8.115
8.108
7.827
7.809
7.464
7.450
7.426
7.409
7.391
7.376
6.706
6.686
6.660
6.643
3.668
2.01
2.05
3.01
2.96
1.00
1.03
1.97
3.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)
N
O
OMe
Ph
S
Ph
4c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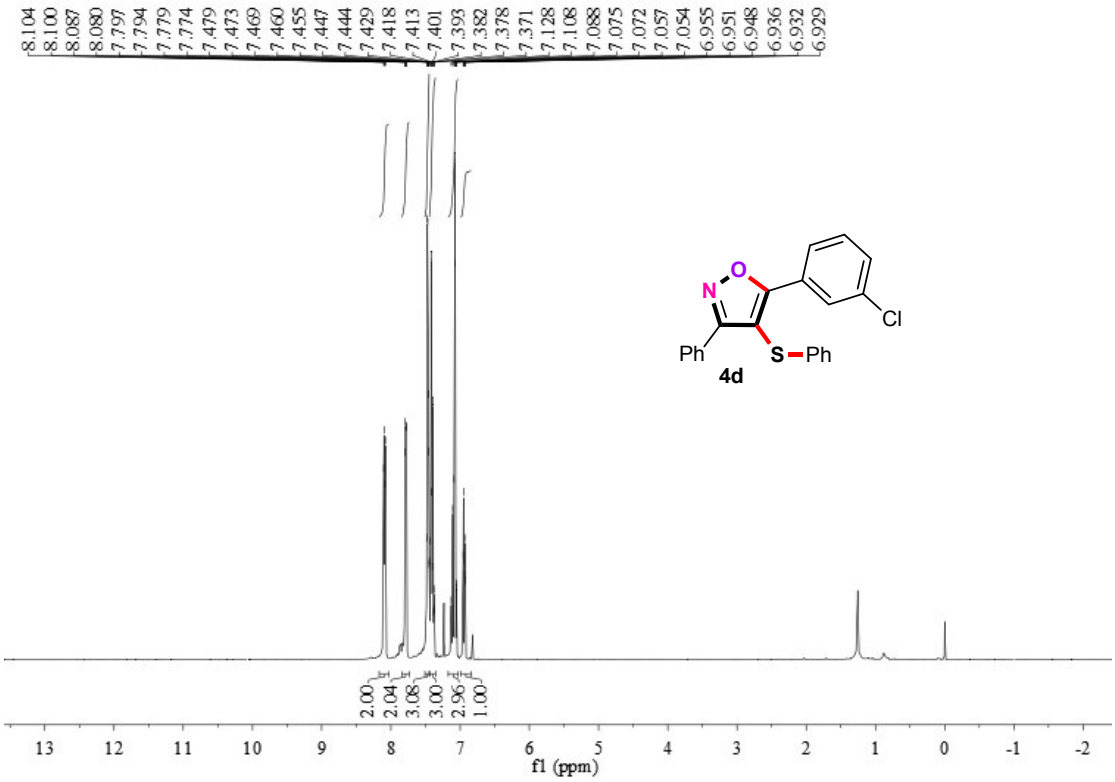
160.276
137.582
131.014
130.224
130.033
128.845
128.563
128.552
127.527
127.020
118.302
111.672
111.635
101.779
55.230
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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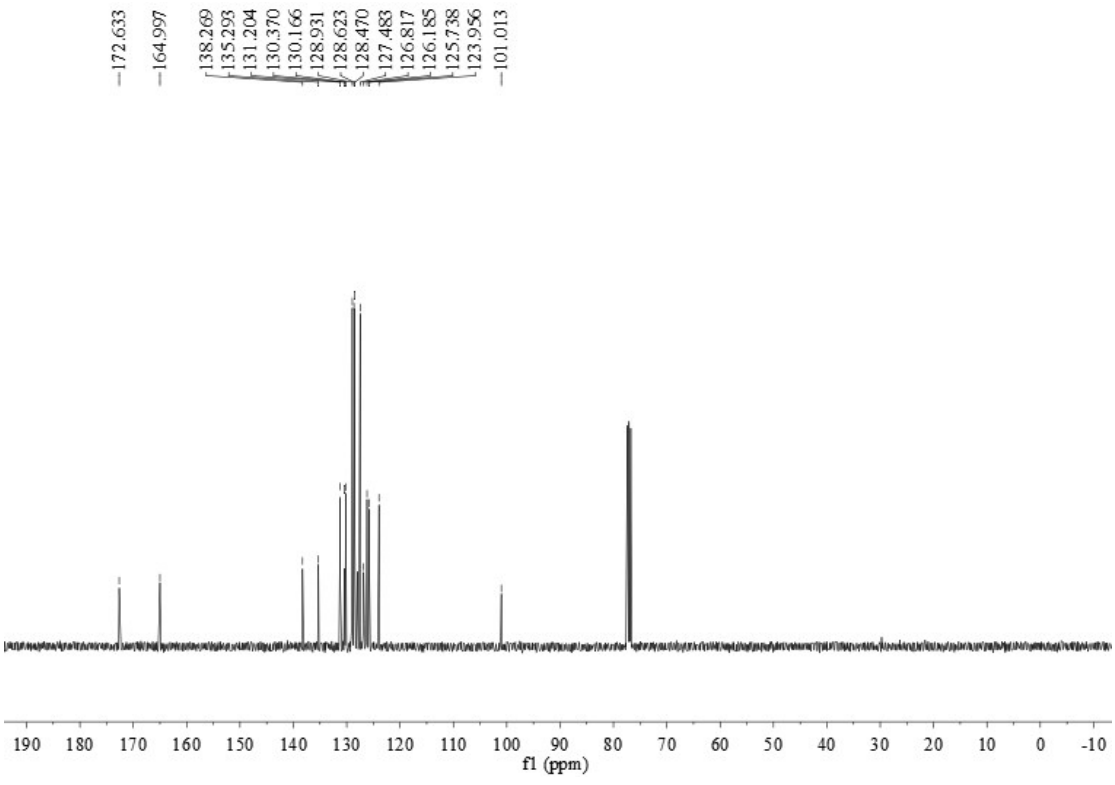
8.080
7.797
7.794
7.779
7.774
7.479
7.473
7.469
7.460
7.455
7.447
7.444
7.429
7.418
7.413
7.401
7.393
7.382
7.378
7.371
7.128
7.108
7.088
7.075
7.072
7.057
7.054
6.955
6.951
6.948
6.936
6.932
6.929
2.00
2.04
3.08
3.00
2.96
1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)
O
N
Cl
Ph
S
Ph
4d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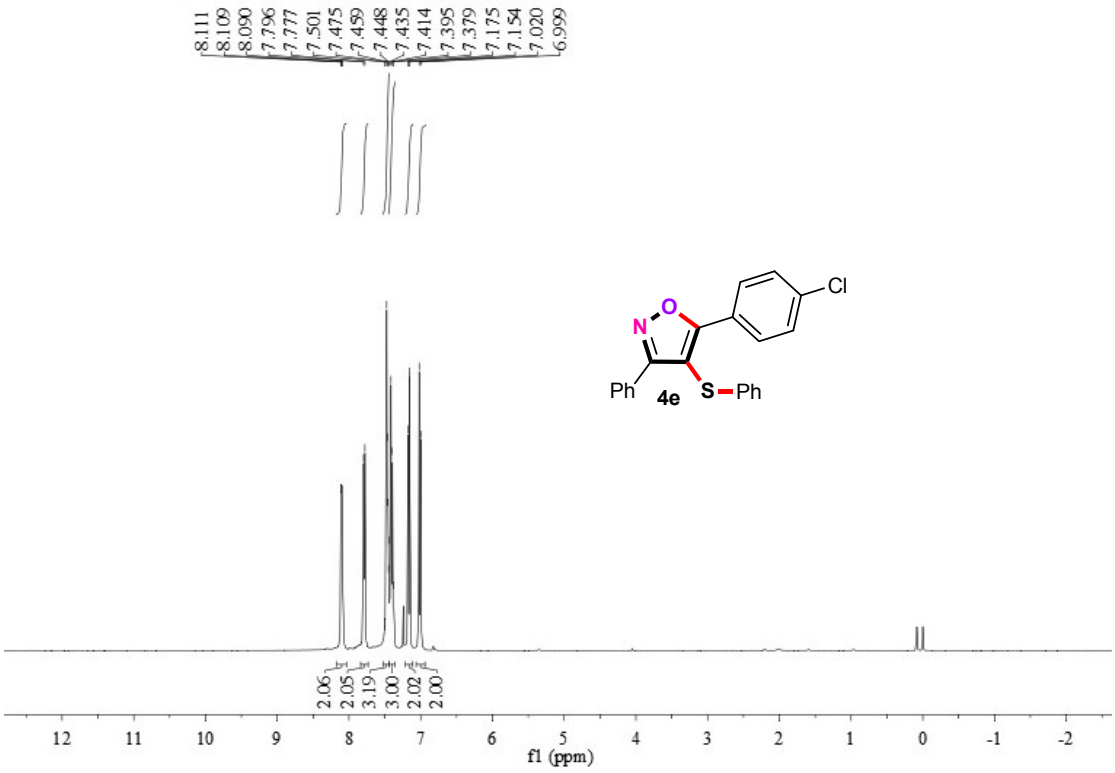
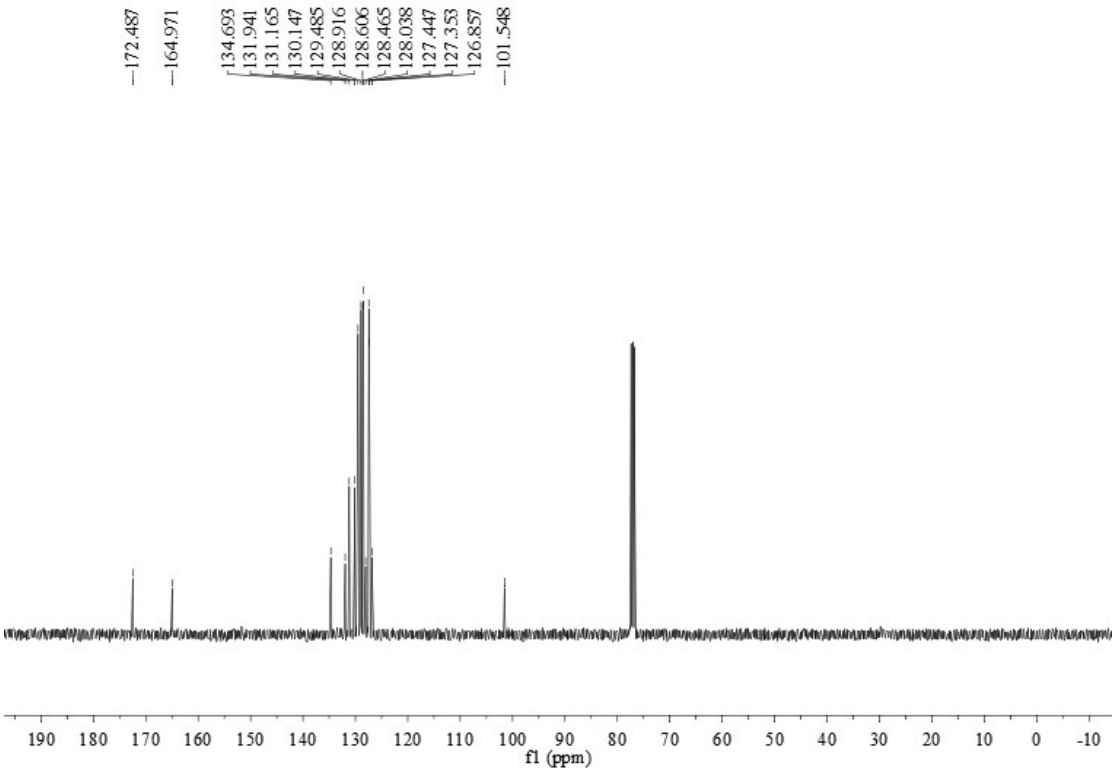
131.204
130.370
130.166
128.931
128.623
128.470
127.483
126.817
126.185
125.738
123.956
101.013
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.111
8.109
8.090
7.796
7.777
7.501
7.475
7.459
7.448
7.435
7.414
7.395
7.379
7.175
7.154
7.020
6.999
Cl
O
N
Ph
4e
S
Ph
2.06
2.05
3.19
3.00
2.02
2.00
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)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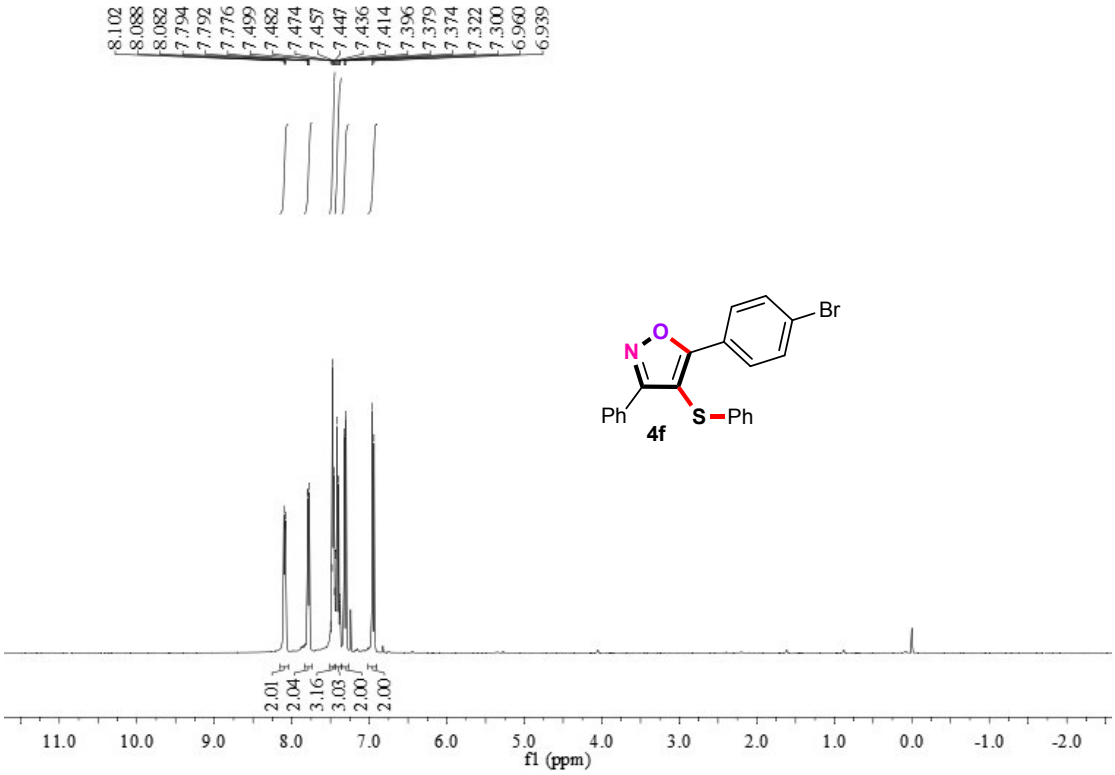
128.916
128.606
128.465
128.038
127.447
127.353
126.857
101.548
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.482
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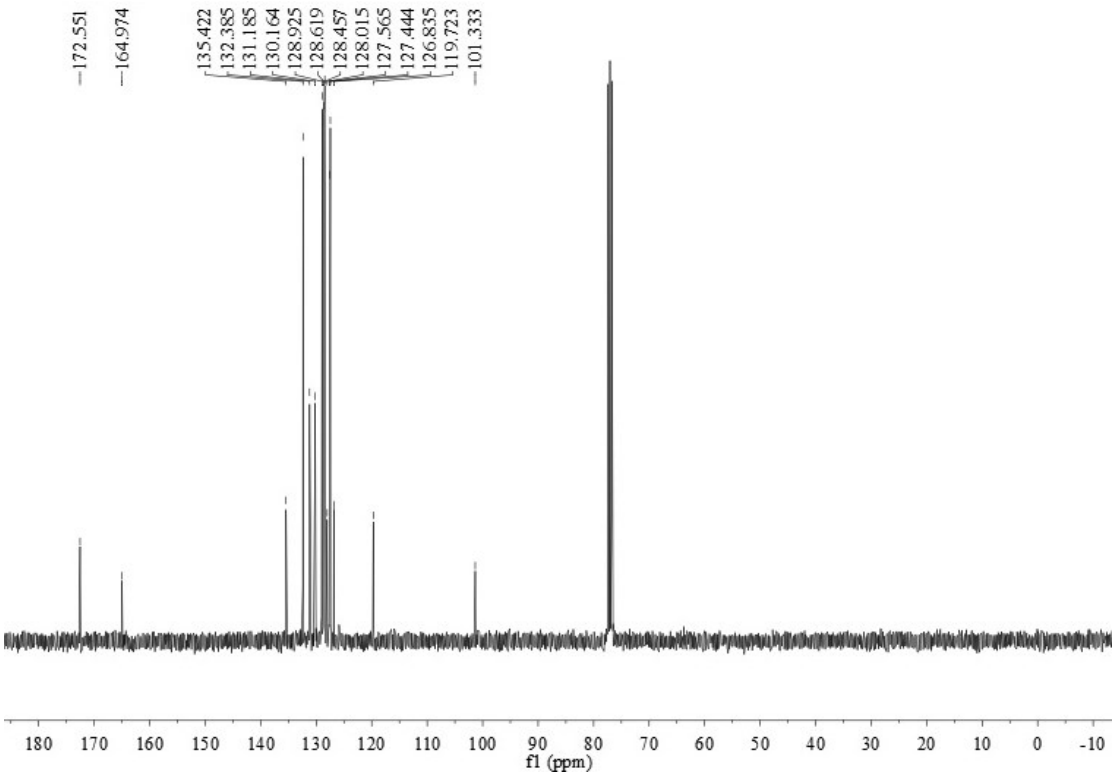
7.457
7.447
7.436
7.414
7.396
7.379
7.374
7.322
7.300
6.960
6.939
Br
N
O
Ph
S
Ph
4f
2.01
2.04
3.16
3.03
2.00
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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101.333
180
170
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100
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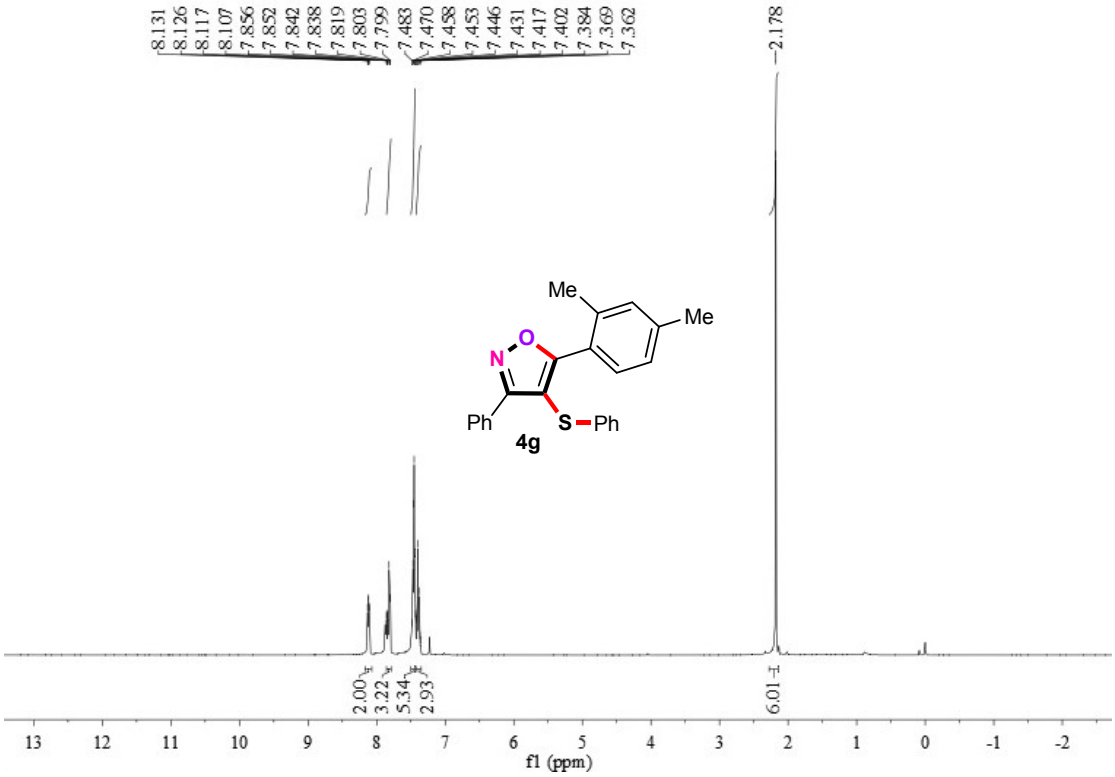
50
40
30
20
10
0
-10
f1 (ppm)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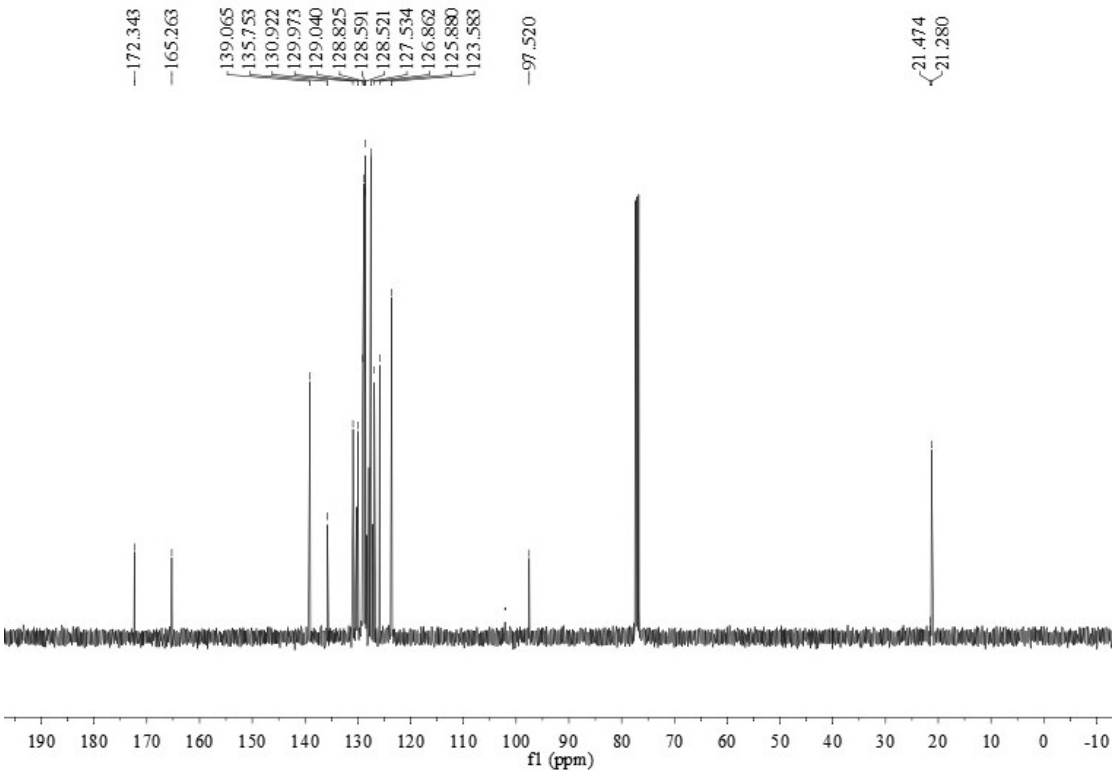
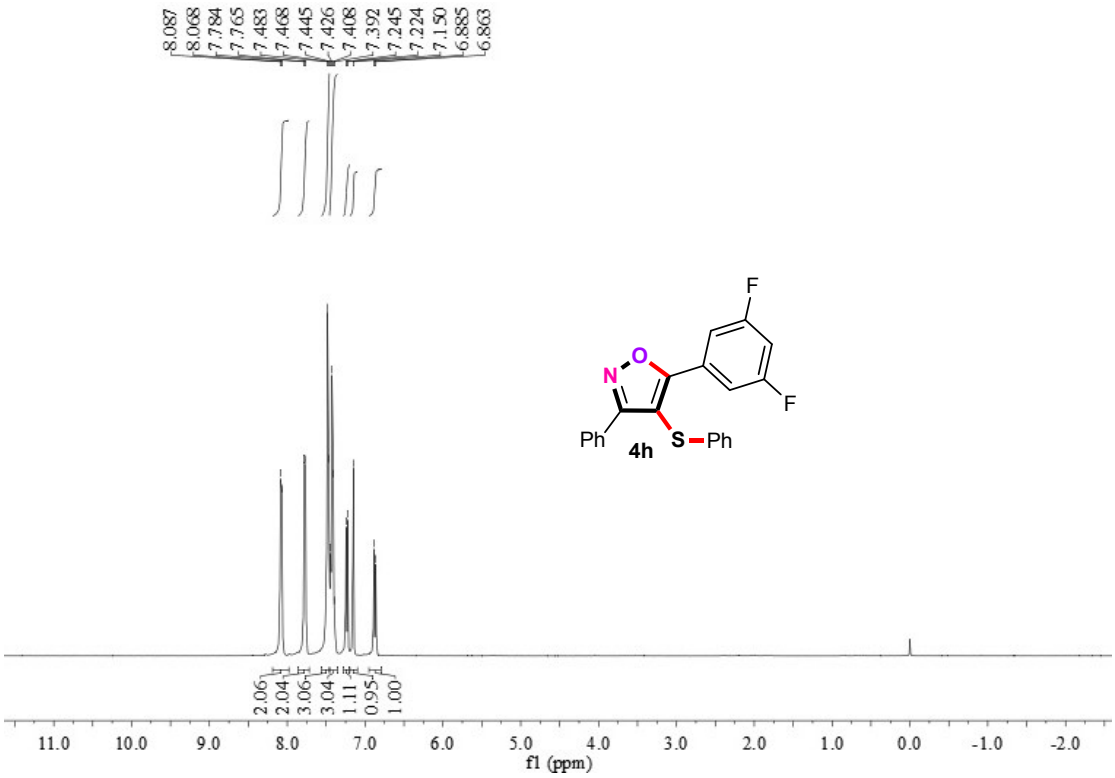
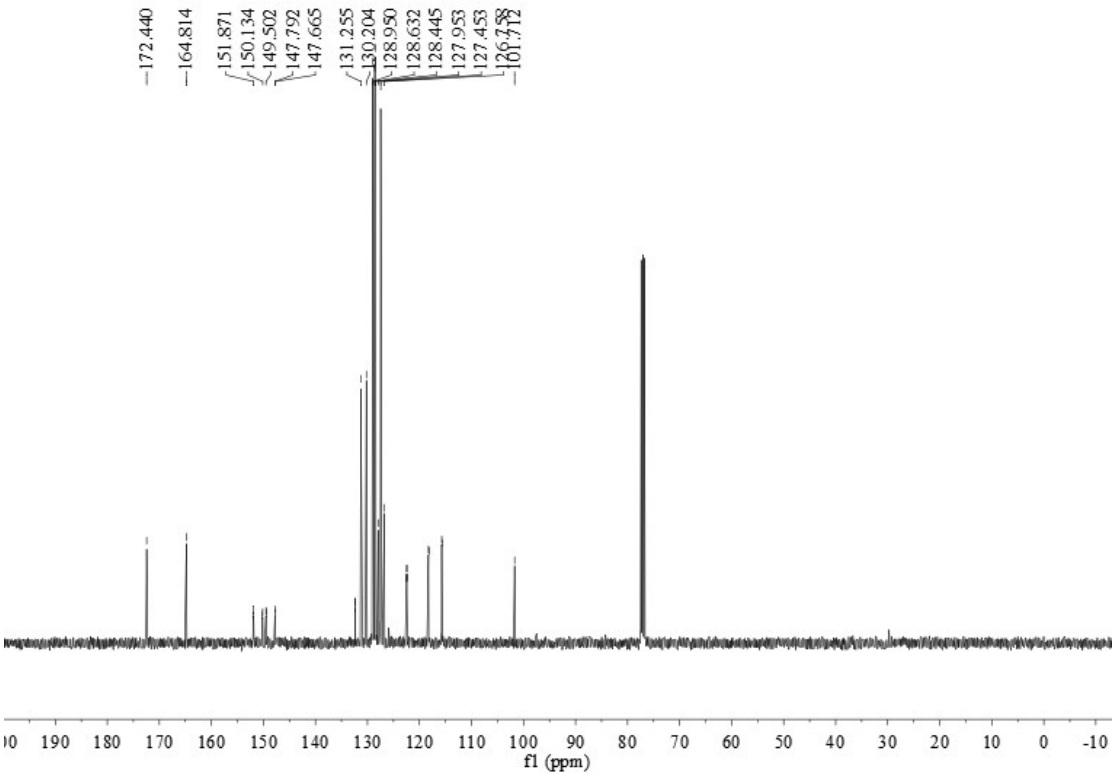
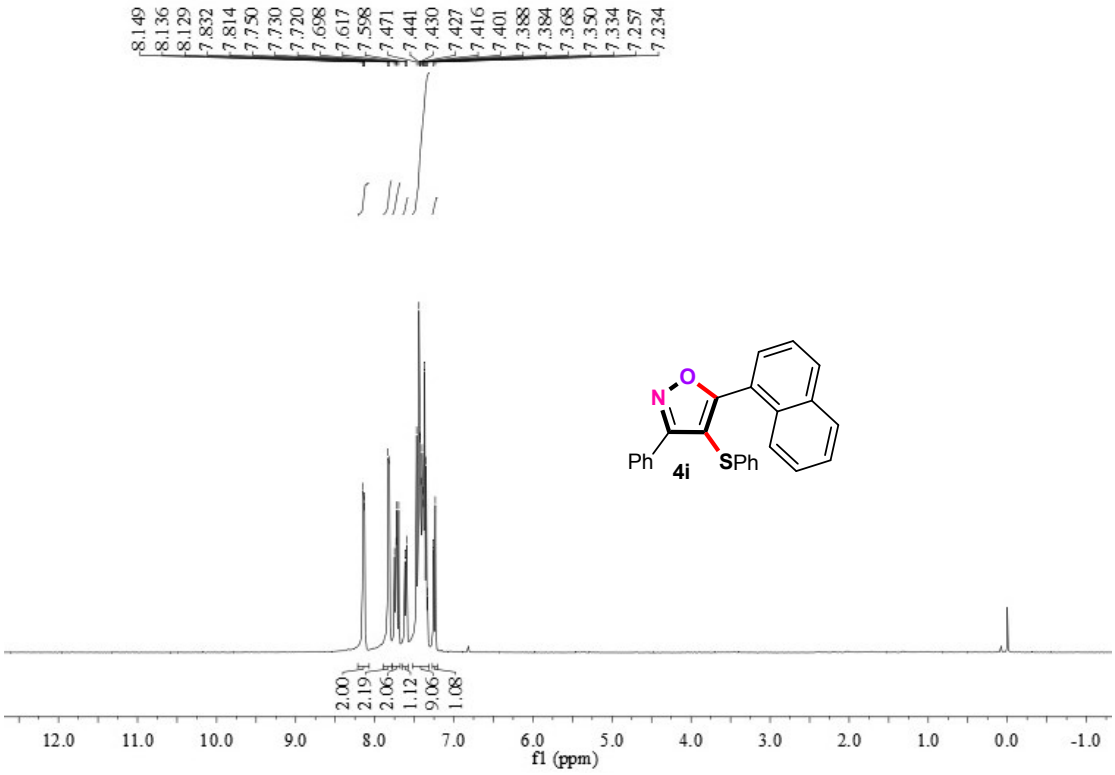
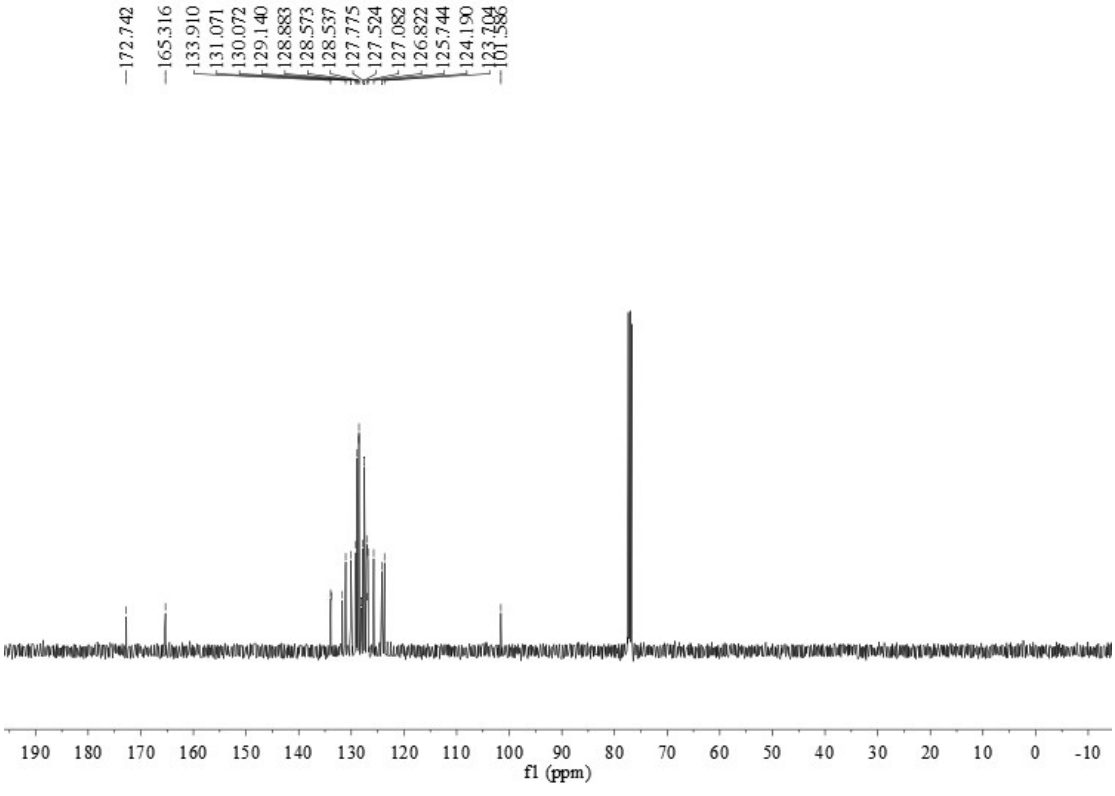
7.458
7.453
7.446
7.431
7.417
7.402
7.384
7.369
7.362
2.178
Me
Me
O
N
Ph
S
Ph
4g
2.00
3.22
5.34
2.93
6.01
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

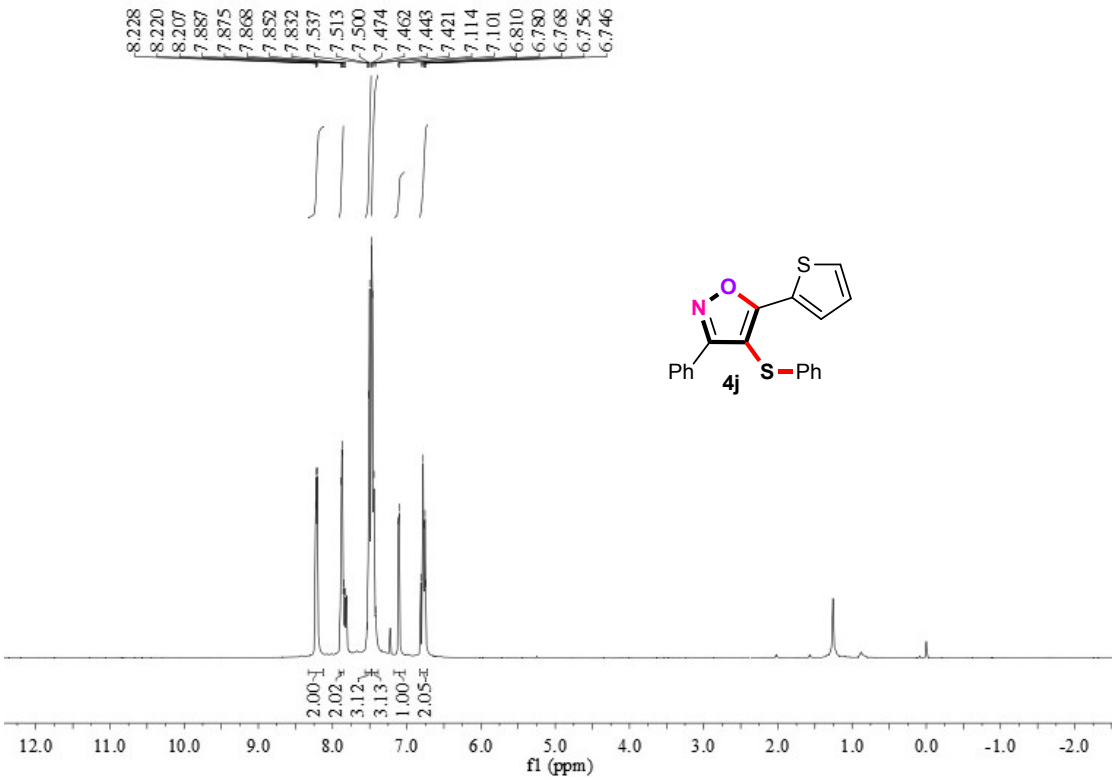

172.343
165.263
139.065
135.753
130.922
129.973
129.040
128.825
128.591
128.521
127.534
126.862
125.880
123.583
97.520
21.474
21.280
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

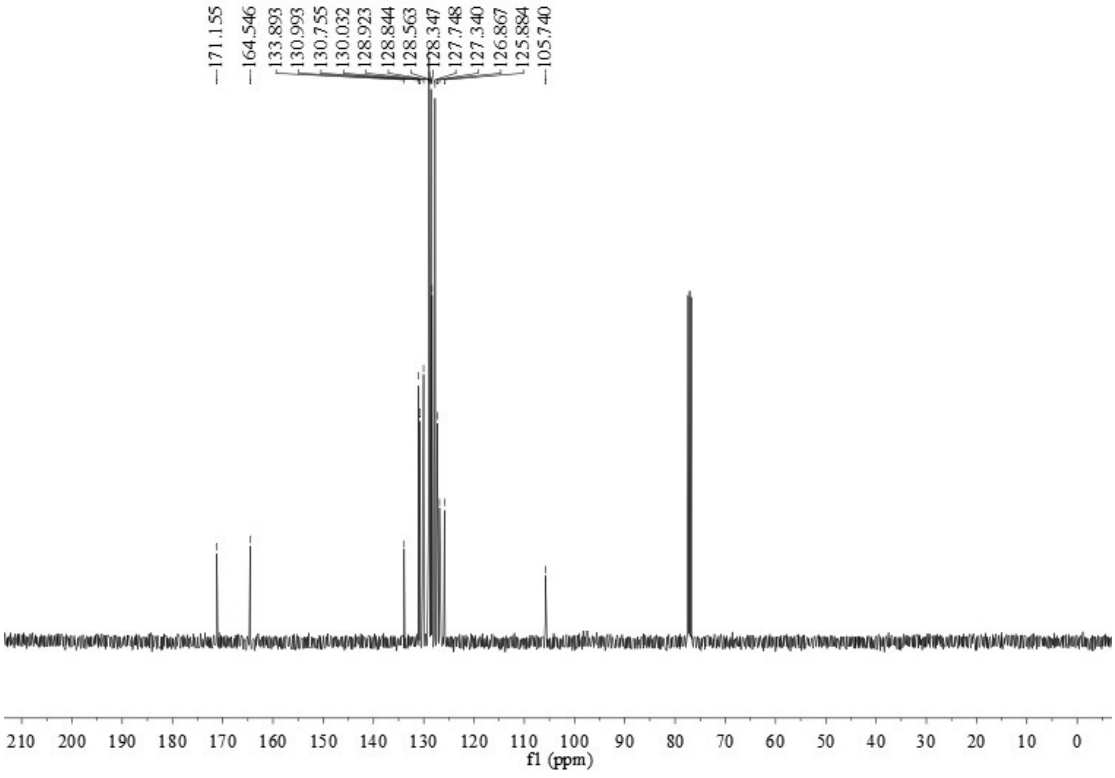

8.087
8.068
7.784
7.765
7.483
7.468
7.445
7.426
7.408
7.392
7.245
7.224
7.150
6.885
6.863
F
F
N
O
Ph
S
Ph
4h
2.06
2.04
3.06
3.04
1.11
0.95
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)

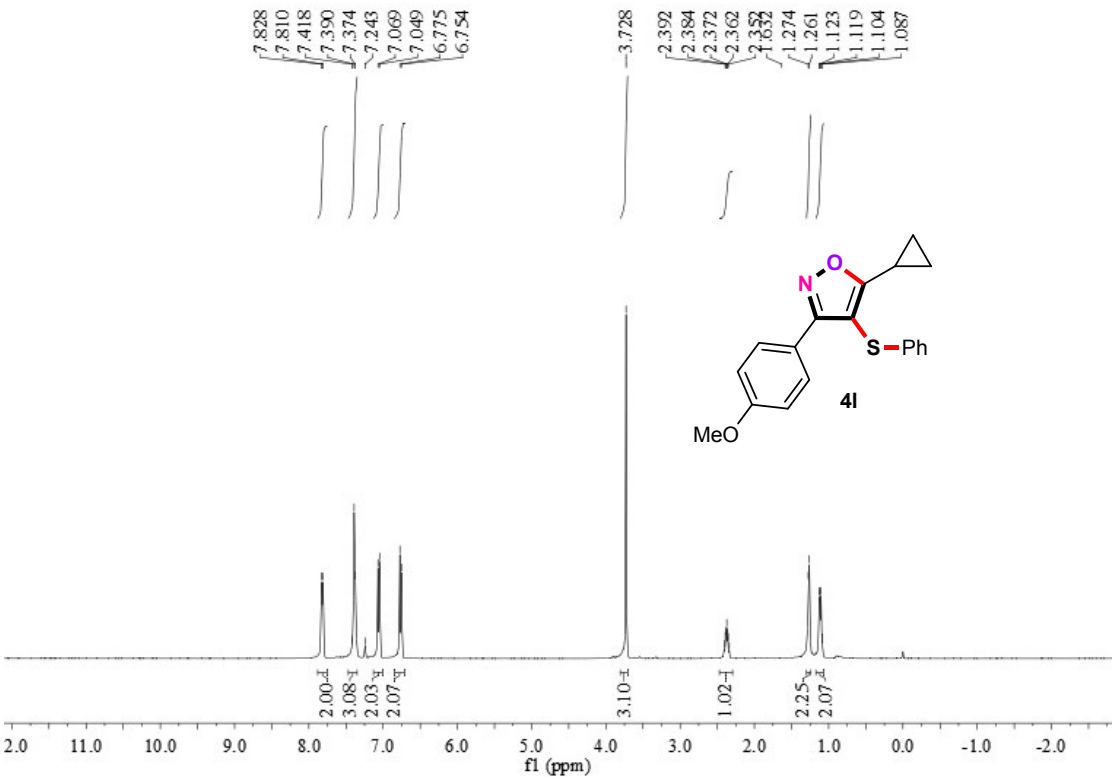

172.440
164.814
151.871
150.134
149.502
147.792
147.665
131.255
130.204
128.950
128.632
128.445
127.953
127.453
126.758
101.712
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

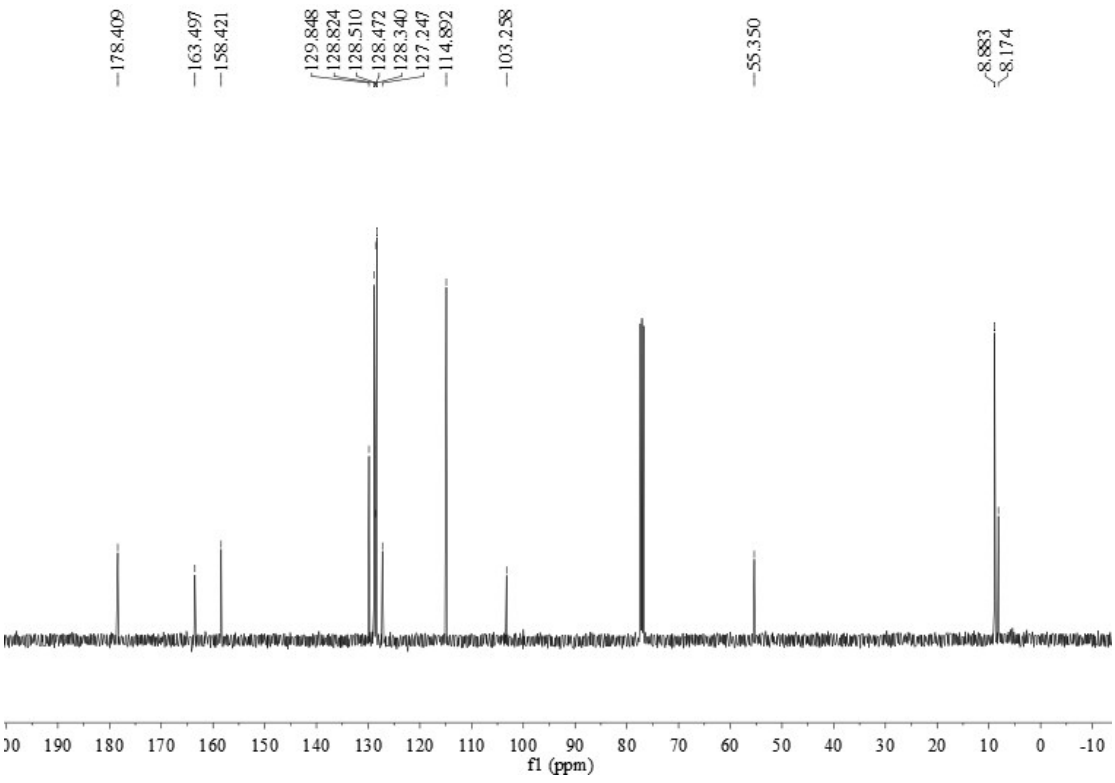

8.149
8.136
8.129
7.832
7.814
7.750
7.730
7.720
7.698
7.617
7.598
7.471
7.441
7.430
7.427
7.416
7.401
7.388
7.384
7.368
7.350
7.334
7.257
7.234
N
O
Ph
SPh
4i
2.00
2.19
2.06
1.12
9.06
1.08
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

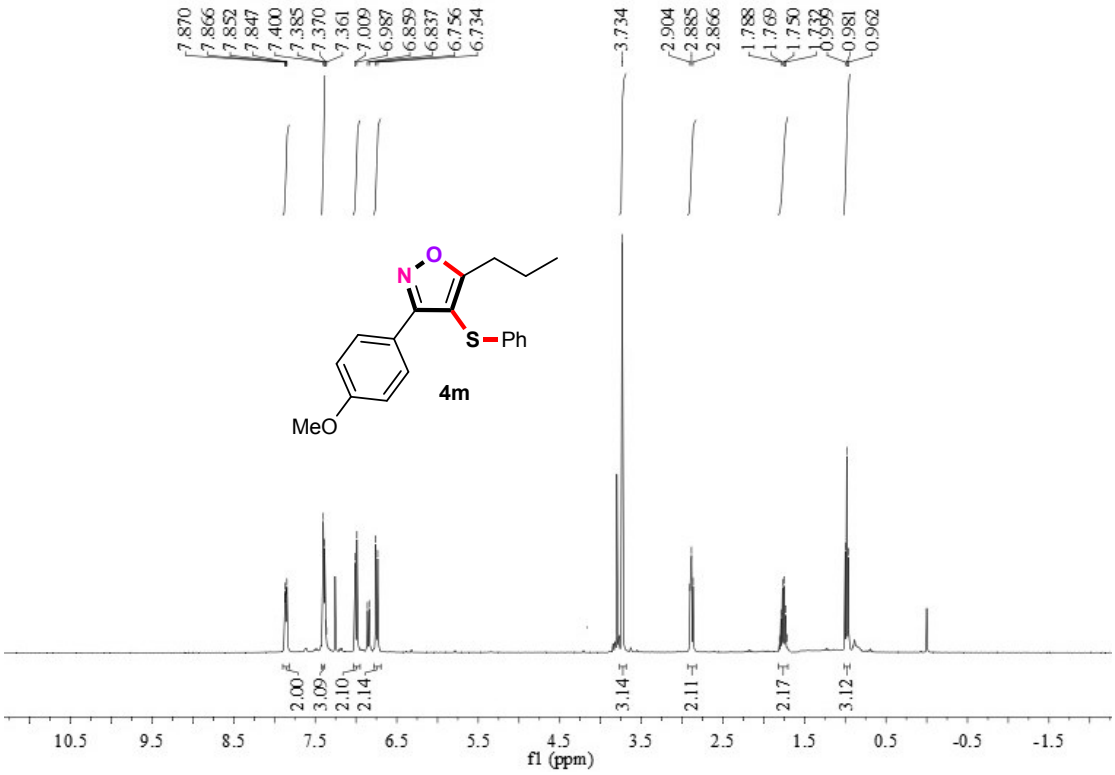

172.742
165.316
133.910
131.071
130.072
129.140
128.883
128.573
128.537
127.775
127.524
127.082
126.822
125.744
124.190
123.704
101.585
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

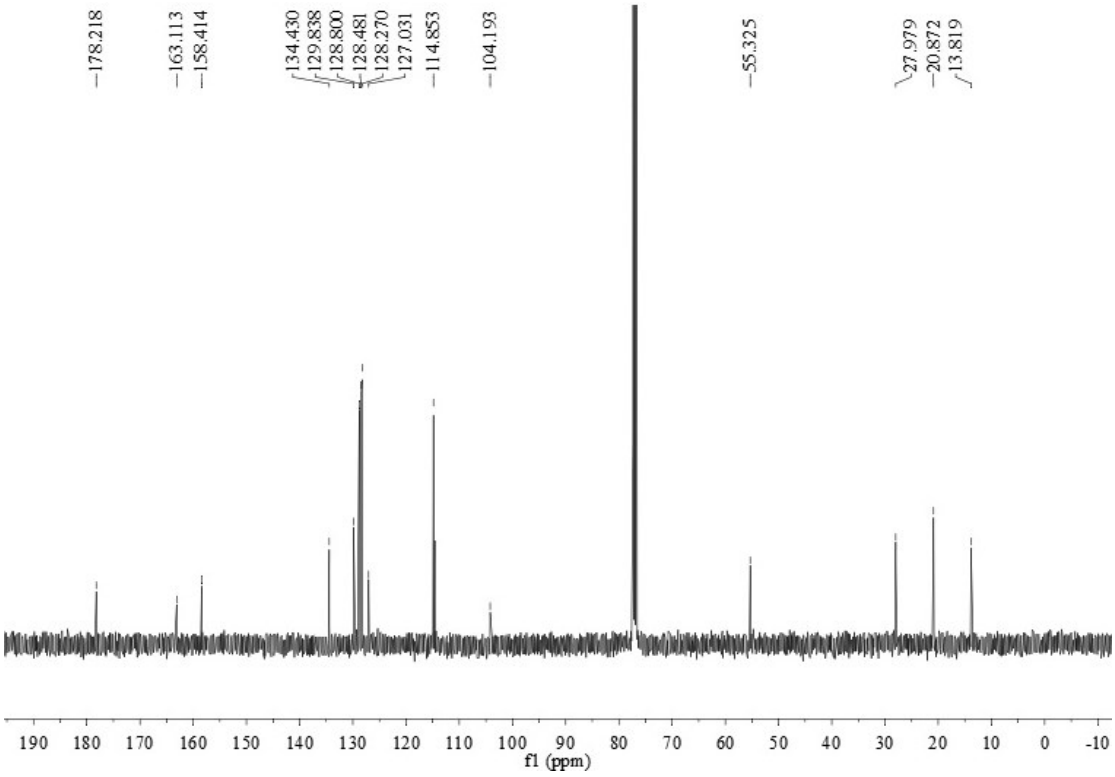

8.228
8.220
8.207
7.887
7.875
7.868
7.852
7.832
7.537
7.513
7.500
7.474
7.462
7.443
7.421
7.114
7.101
6.810
6.780
6.768
6.756
6.746
2.00
2.02
3.12
3.13
1.00
2.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)
S
O
N
Ph
S
Ph
4j

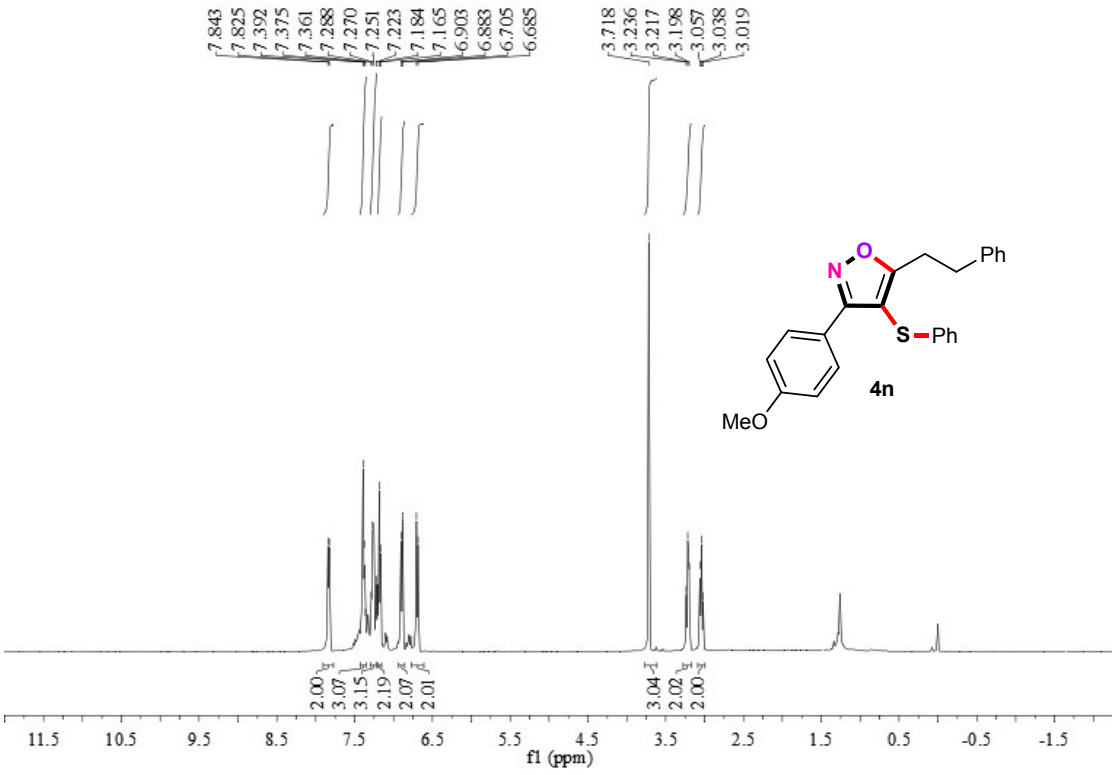

171.155
164.546
133.893
130.993
130.755
130.032
128.923
128.844
128.563
128.347
127.748
127.340
126.867
125.884
105.740
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

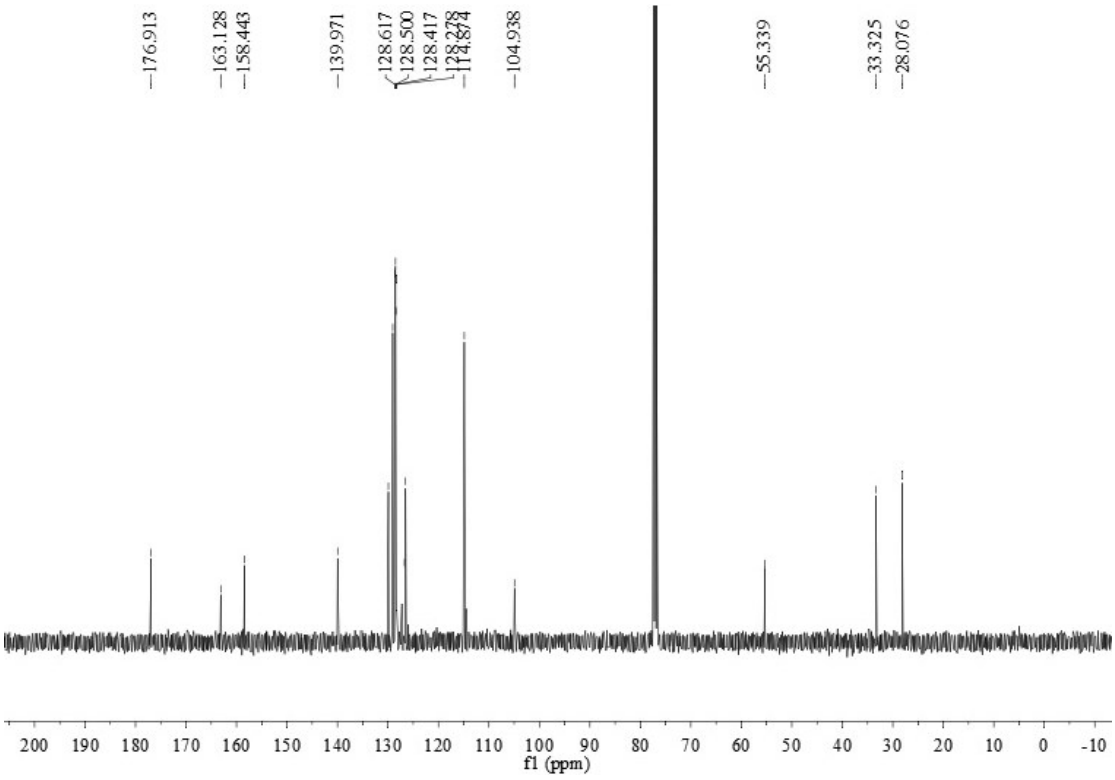

7.828
7.810
7.418
7.390
7.374
7.243
7.069
7.049
6.775
6.754
3.728
2.392
2.384
2.372
2.362
1.274
1.261
1.123
1.119
1.104
1.087
O
N
S
Ph
MeO
4l
2.00
3.08
2.03
2.07
3.10
1.02
2.25
2.07
2.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)

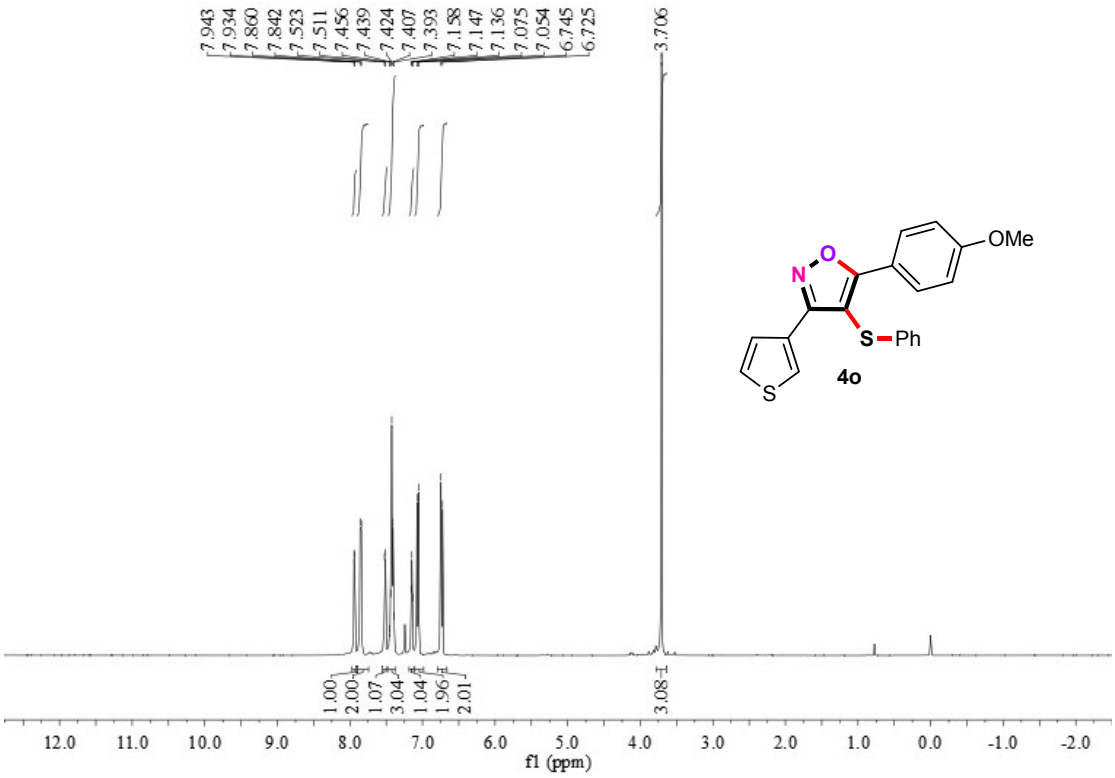

178.409
163.497
158.421
129.848
128.824
128.510
128.472
128.340
127.247
114.892
103.258
55.350
8.883
8.174
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

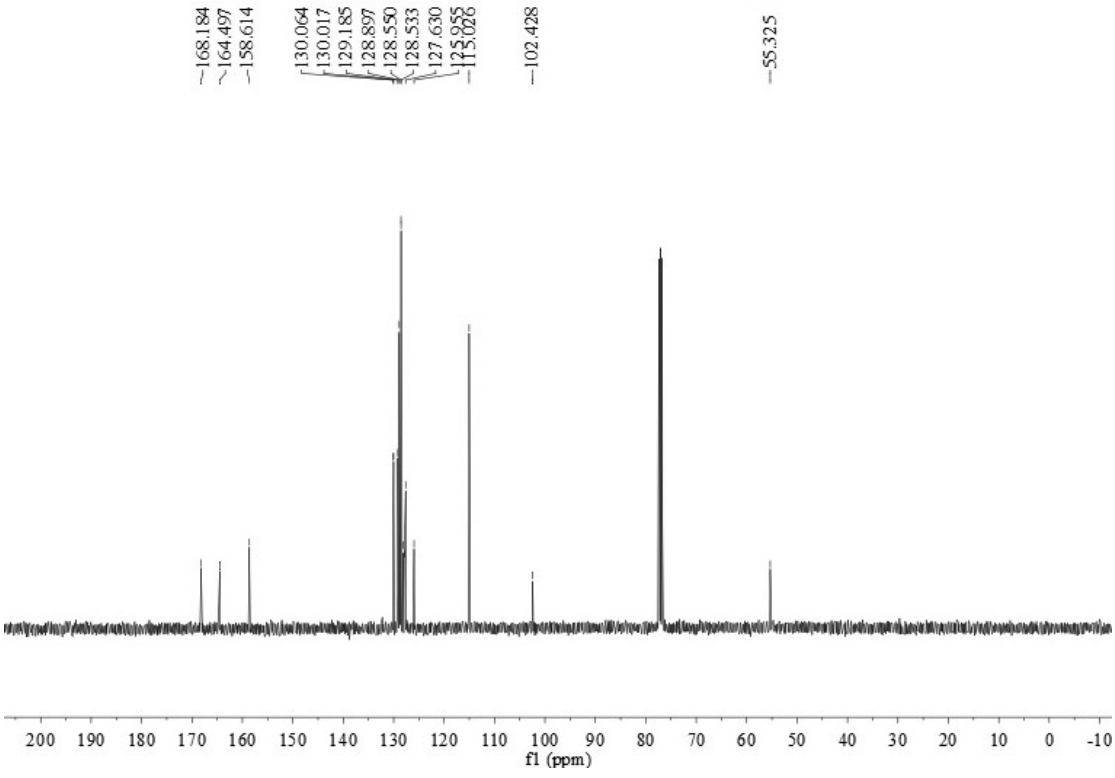

7.870
7.866
7.852
7.847
7.400
7.385
7.370
7.361
7.009
6.987
6.859
6.837
6.756
6.734
3.734
2.904
2.885
2.866
1.788
1.769
1.750
1.732
0.999
0.981
0.962
N
O
S
Ph
MeO
4m
2.00
3.09
2.10
2.14
3.14
2.11
2.17
3.12
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

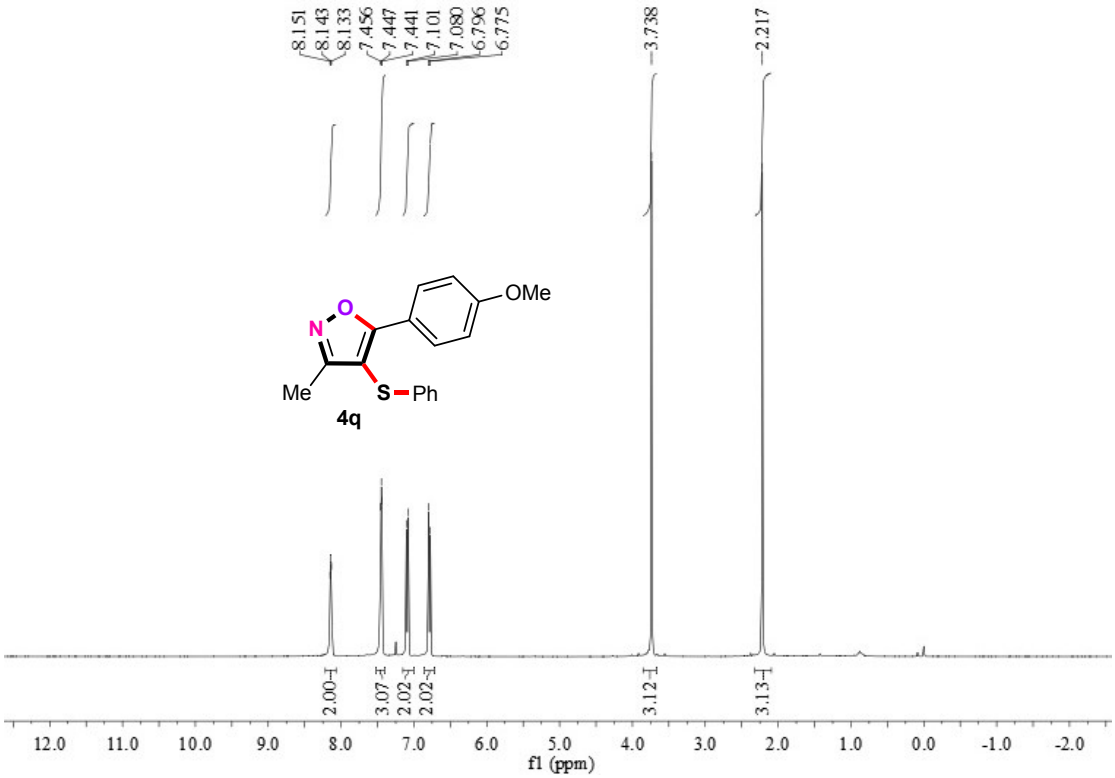

178.218
163.113
158.414
134.430
129.838
128.800
128.481
128.270
127.031
114.853
104.193
55.325
27.979
20.872
13.819
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

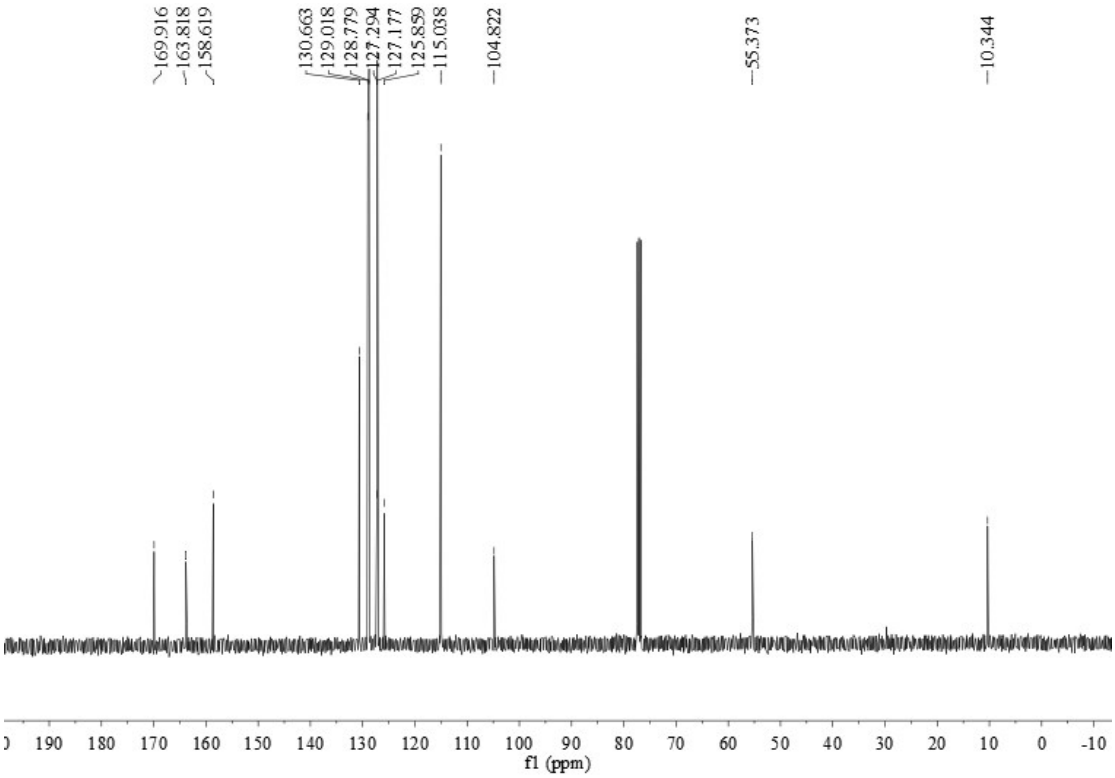

7.843
7.825
7.392
7.375
7.361
7.288
7.270
7.251
7.223
7.184
7.165
6.903
6.883
6.705
6.685
3.718
3.236
3.217
3.198
3.057
3.038
3.019
2.00
3.07
3.15
2.19
2.07
2.01
3.04
2.02
2.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)
O
N
Ph
S
Ph
MeO
4n


176.913
163.128
158.443
139.971
128.617
128.500
128.417
104.938
55.339
33.325
28.076
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.943
7.934
7.860
7.842
7.523
7.511
7.456
7.439
7.424
7.407
7.393
7.158
7.147
7.136
7.075
7.054
6.745
6.725
3.706
OMe
N
O
S
Ph
S
4o
1.00
2.00
1.07
3.04
1.04
1.96
2.01
3.08
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)


168.184
164.497
158.614
130.064
130.017
129.185
128.897
128.550
128.533
127.630
125.955
115.026
102.428
55.325
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.151
8.143
8.133
7.456
7.447
7.441
7.101
7.080
6.796
6.775
3.738
2.217
OMe
N
O
Me
S
Ph
4q
2.00
3.07
2.02
2.02
3.12
3.13
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


169.916
163.818
158.619
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128.779
127.294
127.177
125.859
115.038
104.822
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10.344
190
180
170
160
150
140
130
120
110
100
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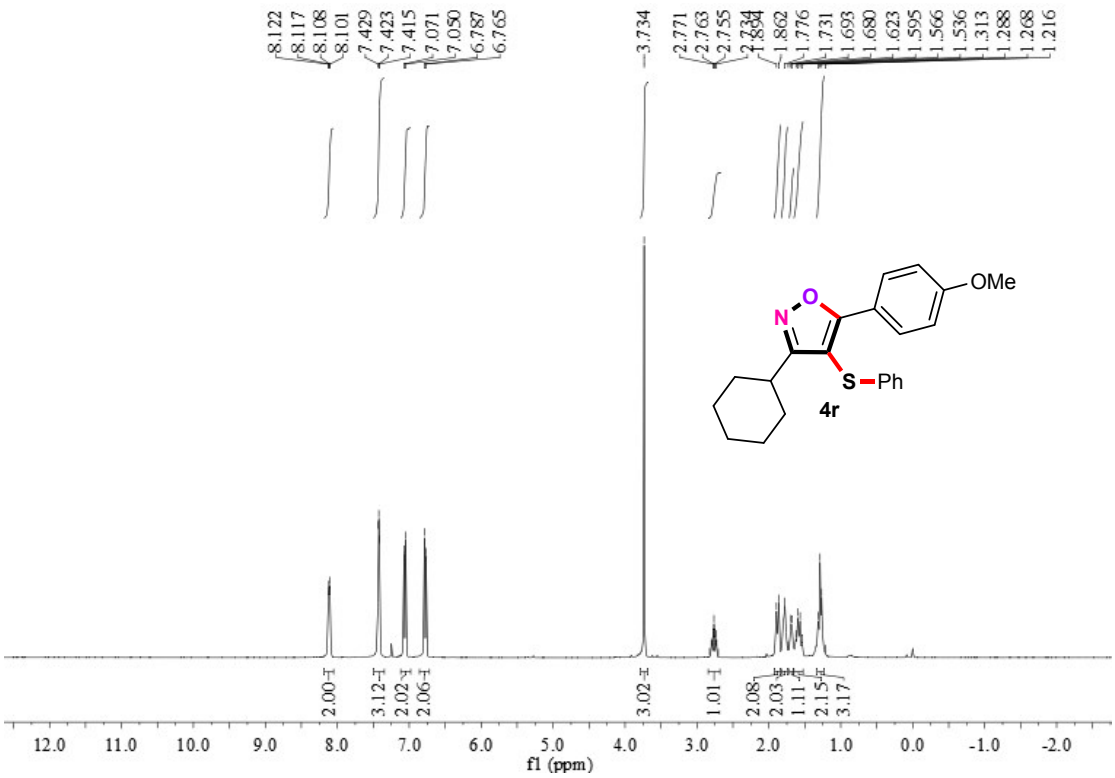
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.122
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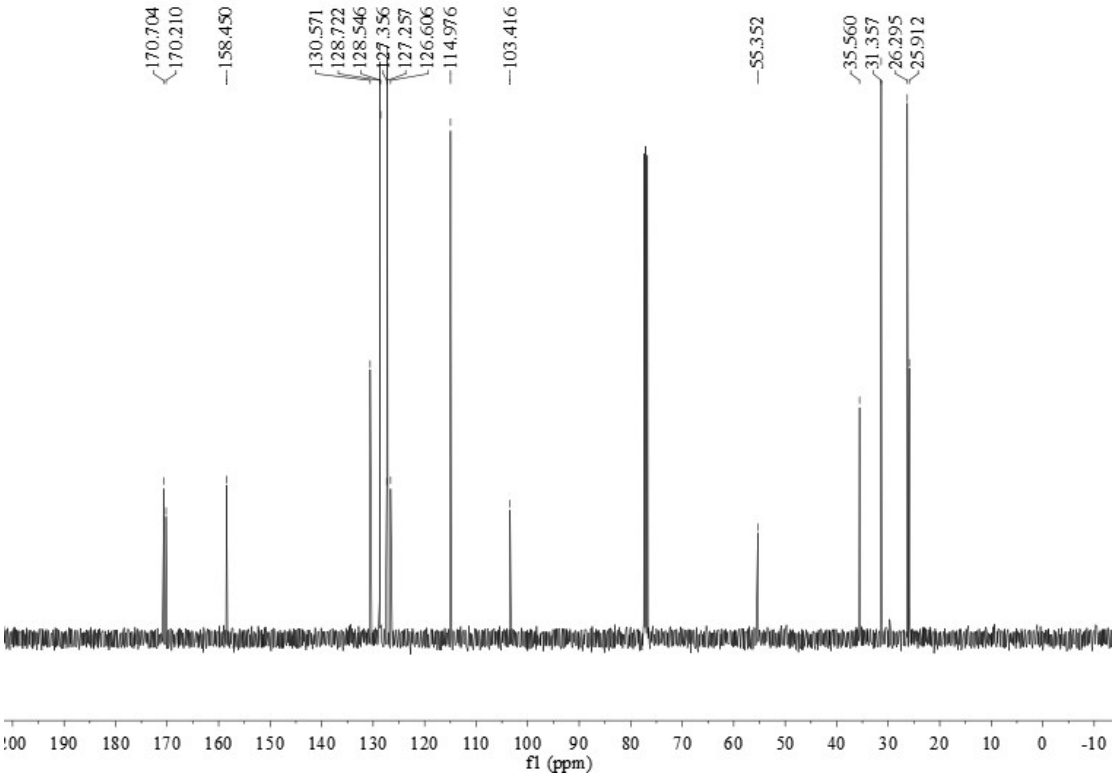
8.108
8.101
7.429
7.423
7.415
7.071
7.050
6.787
6.765
3.734
2.771
2.763
2.755
2.734
1.862
1.776
1.731
1.693
1.680
1.623
1.595
1.566
1.536
1.313
1.288
1.268
1.216
OMe
N
O
S
Ph
4r
2.00
3.12
2.02
2.06
3.02
1.01
2.08
2.03
1.11
2.15
3.17
f1 (ppm)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170.210
158.450
130.571
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128.546
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127.257
126.606
114.976
103.416
55.352
35.560
31.357
26.295
25.912
f1 (ppm)