

Supporting Information

Palladium-catalyzed three-component cascade *S*-transfer reaction in ionic

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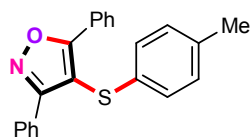
General methods

Melting points were measured using a melting point instrument and are uncorrected. ^1H 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.

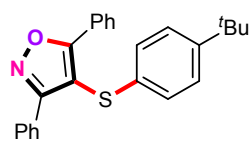
Typical procedure for the preparation of 4-sulfenylisoxazoles

A 15 mL vial was charged with *O*-methyl oxime **1** (0.20 mmol), **2** (0.40 mmol), **3** (0.30 mmol), NHC-Pd(II) (0.25 mol %), and [Bmim]Cl (2 mL). After being heated at 80 °C under air for 12 h, the reaction was quenched by water and extracted with CH₂Cl₂ three times. The combined organic layers were dried over anhydrous Na₂SO₄ and evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate) to afford the desired products.

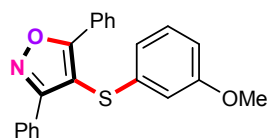
Characterization data for all products



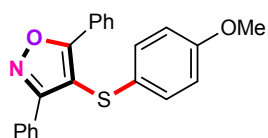
3,5-Diphenyl-4-(*p*-tolylthio)isoxazole (**4a**): Yield: 81% (55.6 mg) as a yellow solid; mp = 89.4 - 90.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.18 - 8.08 (m, 2H), 7.86 - 7.79 (m, 3H), 7.50 - 7.42 (m, 4H), 7.42 - 7.33 (m, 2H), 7.01 - 6.98 (m, 3H), 2.24 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 172.3, 165.2, 135.9, 132.6, 130.9, 130.1, 130.0, 128.8, 128.6, 128.5, 127.5, 126.9, 126.3, 125.9, 102.4, 20.9 ppm; ν_{max}(KBr)/cm⁻¹ 3051, 2926, 1567, 1470, 755, 702; MS (EI) m/z 77, 105, 238, 314, 343; HRMS-ESI (m/z): calcd for C₂₂H₁₇NNaOs, [M+Na]⁺: 366.0923, found 366.0927.



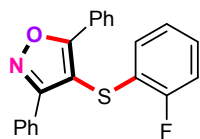
4-((4-*tert*-Butyl)phenylthio)-3,5-diphenylisoxazole (**4b**): Yield: 87% (67.0 mg) as a yellow solid; mp = 105.8 - 107.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.22 - 8.07 (m, 2H), 7.85 - 7.81 (m, 2H), 7.50 - 7.43 (m, 3H), 7.42 - 7.36 (m, 3H), 7.21 (d, *J* = 8.2 Hz, 2H), 7.02 (d, *J* = 8.2 Hz, 2H), 1.24 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 172.2, 165.1, 149.2, 130.9, 129.9, 129.0, 128.8, 128.6, 128.5, 127.5, 126.9, 126.4, 126.2, 125.9, 102.6, 34.4, 31.2 ppm; ν_{max}(KBr)/cm⁻¹ 3060, 2955, 1639, 1561, 1471, 1267, 760, 694; MS (EI) m/z 77, 105, 280, 328, 370, 385; HRMS-ESI (m/z): calcd for C₂₅H₂₃NNaOs, [M+Na]⁺: 408.1393, found 408.1394.



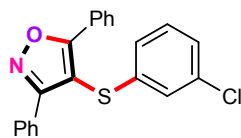
4-((3-Methoxyphenyl)thio)-3,5-diphenylisoxazole (**4c**): Yield: 76% (54.6 mg) as a yellow solid; mp = 89.6 - 90.1 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.18 - 8.06 (m, 2H), 7.82 (d, $J = 7.2$ Hz, 2H), 7.49 - 7.43 (m, 3H), 7.40 (q, $J = 6.4$ Hz, 3H), 7.11 (q, $J = 8.0$ Hz, 1H), 6.70 (d, $J = 8.0$ Hz, 1H), 6.65 (d, $J = 6.8$ Hz, 2H), 3.67 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.5, 165.1, 160.3, 137.6, 131.0, 130.2, 130.0, 128.8, 128.6, 128.5, 128.2, 127.5, 127.0, 118.3, 111.7, 111.6, 101.8, 55.2 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3062, 2931, 1677, 1580, 1469, 1243, 767, 694; MS (EI) m/z 77, 105, 151, 254, 359; HRMS-ESI (m/z): calcd for $\text{C}_{22}\text{H}_{17}\text{NNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 382.0872, found 382.0877.



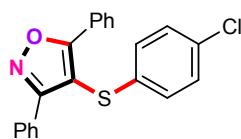
4-((4-Methoxyphenyl)thio)-3,5-diphenylisoxazole (**4d**): Yield: 78% (56.0 mg) as a yellow solid; mp = 110.3 - 111.5 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.23 - 8.12 (m, 2H), 7.87 - 7.77 (m, 2H), 7.52 - 7.46 (m, 3H), 7.44 - 7.36 (m, 3H), 7.01 (d, $J = 8.8$ Hz, 2H), 6.73 (d, $J = 8.8$ Hz, 2H), 3.71 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 171.8, 165.0, 158.5, 130.9, 129.9, 128.8, 128.7, 128.6, 128.5, 128.4, 127.5, 127.2, 126.5, 115.0, 103.7, 55.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3062, 2933, 1583, 1480, 1250, 819, 701; MS (EI) m/z 77, 105, 151, 254, 316, 359; HRMS-ESI (m/z): calcd for $\text{C}_{22}\text{H}_{17}\text{NNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 382.0872, found 382.0874.



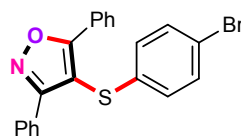
4-((2-Fluorophenyl)thio)-3,5-diphenylisoxazole (**4e**): Yield: 70% (48.6 mg) as a yellow solid; mp = 102.5 - 104.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.10 - 7.99 (m, 2H), 7.79 - 7.67 (m, 2H), 7.44 - 7.35 (m, 4H), 7.31 (q, *J* = 6.0 Hz, 2H), 6.99 (dd, *J* = 13.4, 6.4 Hz, 1H), 6.91 (t, *J* = 9.0 Hz, 1H), 6.85 - 6.71 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 172.6, 165.1, 159.5 (d, *J* = 245.5 Hz), 131.1, 130.1, 128.9, 128.6, 128.4, 128.1, 127.9, 127.5, 126.9, 125.9, 124.9 (d, *J* = 3.5 Hz), 123.3 (d, *J* = 16.7 Hz), 115.7 (d, *J* = 20.8 Hz), 100.4 ppm; ν_{max}(KBr)/cm⁻¹ 3062, 2921, 1645, 1548, 1457, 1267, 824, 753; MS (EI) *m/z* 77, 105, 138, 242, 347; HRMS-ESI (*m/z*): calcd for C₂₁H₁₄FNNaOS, [M+Na]⁺: 370.0672, found 370.0676.



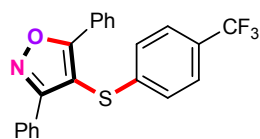
4-((3-Chlorophenyl)thio)-3,5-diphenylisoxazole (**4f**): Yield: 74% (53.7 mg) as a yellow solid; mp = 107.6 - 109.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.09 (dd, *J* = 7.6, 2.4 Hz, 2H), 7.79 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.51 - 7.44 (m, 3H), 7.43 - 7.36 (m, 3H), 7.16 - 7.04 (m, 3H), 6.94 (dt, *J* = 7.6, 1.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 172.6, 165.0, 138.3, 135.3, 131.2, 130.4, 130.2, 128.9, 128.6, 128.5, 128.0, 127.5, 126.8, 126.2, 125.7, 124.0, 101.0 ppm; ν_{max}(KBr)/cm⁻¹ 3061, 2923, 1684, 1567, 1455, 1259, 864, 773; MS (EI) *m/z* 77, 105, 155, 231, 334, 363; HRMS-ESI (*m/z*): calcd for C₂₁H₁₄ClNNaOS, [M+Na]⁺: 386.0377, found 386.0378.



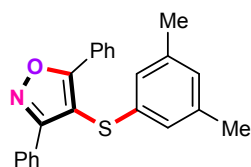
4-((4-Chlorophenyl)thio)-3,5-diphenylisoxazole (**4g**): Yield: 75% (54.5 mg) as a yellow solid; mp = 131.7 - 133.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.20 - 8.05 (m, 2H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.53 - 7.45 (m, 3H), 7.44 - 7.36 (m, 3H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 172.5, 165.0, 134.7, 131.9, 131.2, 130.2, 129.5, 128.9, 128.6, 128.5, 128.0, 127.5, 127.4, 126.9, 101.6 ppm; $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$ 3056, 2918, 1641, 1550, 1470, 1267, 811, 756; MS (EI) *m/z* 77, 155, 197, 258, 334, 363; HRMS-ESI (*m/z*): calcd for C₂₁H₁₄ClNNaOS, [M+Na]⁺: 386.0377, found 386.0381.



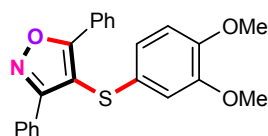
4-((4-Bromophenyl)thio)-3,5-diphenylisoxazole (**4h**): Yield: 63% (51.3 mg) as a yellow solid; mp = 135.8 - 137.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.17 - 8.02 (m, 2H), 7.90 - 7.71 (m, 2H), 7.51 - 7.45 (m, 3H), 7.44 - 7.37 (m, 3H), 7.31 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 172.6, 165.0, 135.4, 132.4, 131.2, 130.2, 128.9, 128.6, 128.5, 128.0, 127.6, 127.4, 126.8, 119.7, 101.3 ppm; $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$ 3065, 2922, 1557, 1462, 1256, 765, 688; MS (EI) *m/z* 77, 105, 199, 304, 380, 407; HRMS-ESI (*m/z*): calcd for C₂₁H₁₅BrNOS, [M+H]⁺: 408.0052, found 408.0048.



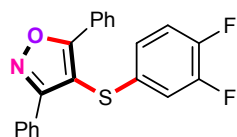
3,5-Diphenyl-4-((4-(trifluoromethyl)phenyl)thio)isoxazole (**4i**): Yield: 56% (44.5 mg) as a yellow solid; mp = 140.4 - 141.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.78 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.55 - 7.45 (m, 4H), 7.45 - 7.34 (m, 4H), 7.18 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 165.0, 141.4, 141.3, 131.3, 130.2, 129.0, 128.7, 128.4, 127.9, 127.4, 126.7, 126.2 (q, *J* = 3.8 Hz), 125.7, 125.6 (q, *J* = 256.5 Hz), 100.4 ppm; ν_{max}(KBr)/cm⁻¹ 3060, 2922, 1658, 1553, 1487, 1268, 824, 761; MS (EI) *m/z* 77, 1105, 189, 265, 292, 397; HRMS-ESI (*m/z*): calcd for C₂₂H₁₅F₃NOS, [M+H]⁺: 398.0821, Found 398.0817.



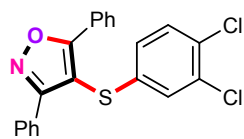
4-((3,5-Dimethylphenyl)thio)-3,5-diphenylisoxazole (**4k**): Yield: 82% (58.5 mg) as a yellow solid; mp = 90.4 - 91.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.12 (dd, *J* = 6.8, 3.2 Hz, 2H), 7.86 - 7.78 (m, 3H), 7.53 - 7.43 (m, 5H), 7.39 (dt, *J* = 8.8, 4.4 Hz, 3H), 2.18 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 172.3, 165.3, 139.1, 135.8, 130.9, 130.0, 129.0, 128.8, 128.6, 128.5, 127.5, 126.9, 125.9, 123.6, 97.5, 21.3 ppm; ν_{max}(KBr)/cm⁻¹ 3056, 2921, 1681, 1573, 1455, 1262, 837, 765; MS (EI) *m/z* 77, 105, 149, 252, 314, 357; HRMS-ESI (*m/z*): calcd for C₂₃H₁₉NNaOS, [M+Na]⁺: 380.1080, found 380.1077.



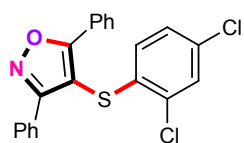
4-((3,4-Dimethoxyphenyl)thio)-3,5-diphenylisoxazole (**4l**): Yield: 80% (62.2 mg) as a yellow solid; mp = 106.7 - 108.2 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.26 - 8.09 (m, 2H), 7.84 (d, J = 7.2 Hz, 2H), 7.57 - 7.46 (m, 3H), 7.45 - 7.36 (m, 3H), 6.67 (q, J = 8.6 Hz, 2H), 6.60 (s, 1H), 3.78 (s, 3H), 3.65 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.9, 165.0, 149.5, 148.1, 130.9, 130.0, 128.8, 128.7, 128.5, 128.4, 127.6, 127.2, 126.9, 120.0, 112.1, 111.1, 103.7, 56.0, 55.8 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3061, 2934, 1649, 1571, 1495, 1446, 1245, 862, 758; MS (EI) m/z 77, 105, 181, 284, 389; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{19}\text{NNaO}_3\text{S}$, $[\text{M}+\text{Na}]^+$: 412.0978, found 412.0971.



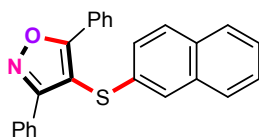
4-((3,4-Difluorophenyl)thio)-3,5-diphenylisoxazole (**4m**): Yield: 71% (51.8 mg) as a yellow solid; mp = 89.0 - 90.5 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.10 (dd, J = 7.2, 2.4 Hz, 2H), 7.79 (dd, J = 7.6, 1.6 Hz, 2H), 7.51 - 7.46 (m, 3H), 7.45 - 7.37 (m, 3H), 6.98 (dd, J = 18.0, 8.4 Hz, 1H), 6.92 - 6.84 (m, 1H), 6.83 - 6.76 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.4, 164.8, 151.1 (dd, J = 175.1, 13.0 Hz), 148.6 (dd, J = 171.8, 13.1 Hz), 132.4 (dd, J = 5.5, 3.8 Hz), 131.3, 130.2, 128.9, 128.6, 128.5, 127.9, 127.5, 126.8, 122.4 (dd, J = 6.1, 3.8 Hz), 118.2 (d, J = 18.3 Hz), 115.6 (d, J = 19.7 Hz), 101.7 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3059, 2925, 1604, 1593, 1495, 1272, 770, 695; MS (EI) m/z 77, 105, 157, 260, 365; HRMS-ESI (m/z): calcd for $\text{C}_{21}\text{H}_{13}\text{F}_2\text{NNaOS}$, $[\text{M}+\text{Na}]^+$: 388.0578, found 388.0577.



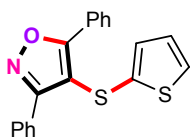
4-((3,4-Dichlorophenyl)thio)-3,5-diphenylisoxazole (**4n**): Yield: 76% (60.3 mg) as a yellow solid; mp = 128.1 - 129.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.19 - 7.98 (m, 2H), 7.77 (d, *J* = 7.6 Hz, 2H), 7.56 - 7.43 (m, 3H), 7.45 - 7.37 (m, 3H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.15 (s, 1H), 6.87 (d, *J* = 8.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 172.7, 164.9, 136.4, 133.5, 131.3, 131.0, 130.3, 130.2, 129.0, 128.7, 128.4, 127.9, 127.5, 126.7, 125.1, 100.8 ppm; ν_{max}(KBr)/cm⁻¹ 3055, 2928, 1549, 1446, 1267, 756, 679; MS (EI) m/z 77, 105, 189, 231, 397; HRMS-ESI (m/z): calcd for C₂₁H₁₃Cl₂NNaOS, [M+Na]⁺: 419.9987, found 419.9986.



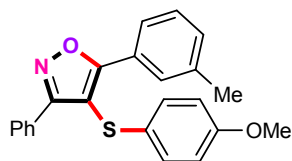
4-((2,4-Dichlorophenyl)thio)-3,5-diphenylisoxazole (**4o**): Yield: 70% (55.6 mg) as a yellow solid; mp = 130.5 - 132.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.15 - 7.97 (m, 2H), 7.78 (d, *J* = 7.6 Hz, 2H), 7.54 - 7.36 (m, 6H), 7.33 (s, 1H), 7.00 (d, *J* = 8.6 Hz, 1H), 6.74 (d, *J* = 8.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 164.9, 134.1, 131.9, 131.6, 131.3, 130.3, 129.7, 129.0, 128.7, 128.3, 127.9, 127.8, 127.4, 127.0, 126.6, 100.3 ppm; ν_{max}(KBr)/cm⁻¹ 3066, 2928, 1606, 1555, 1449, 1259, 800, 699; MS (EI) m/z 77, 105, 189, 362, 397; HRMS-ESI (m/z): calcd for C₂₁H₁₃Cl₂NNaOS, [M+Na]⁺: 419.9987, found 419.9984.



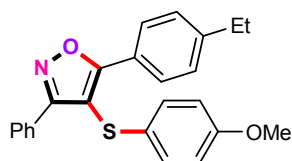
4-(Naphthalen-2-ylthio)-3,5-diphenylisoxazole (**4p**): Yield: 70% (53.1 mg) as a yellow solid; mp = 102.4 - 103.8 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.18 - 8.08 (m, 2H), 7.82 (d, J = 7.4 Hz, 2H), 7.72 (dd, J = 12.4, 8.4 Hz, 2H), 7.61 (d, J = 7.6 Hz, 1H), 7.52 - 7.32 (m, 9H), 7.25 (d, J = 9.2 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.7, 165.3, 133.9, 133.8, 131.7, 131.1, 130.1, 129.1, 128.9, 128.6, 128.5, 128.2, 127.8, 127.5, 127.1, 127.0, 126.8, 125.7, 124.2, 123.7, 101.6 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3056, 2926, 1632, 1556, 1453, 1266, 747, 696; MS (EI) m/z 77, 105, 180, 220, 347, 379; HRMS-ESI (m/z): calcd for $\text{C}_{25}\text{H}_{17}\text{NNaOS}$, $[\text{M}+\text{Na}]^+$: 402.0923, found 402.0924.



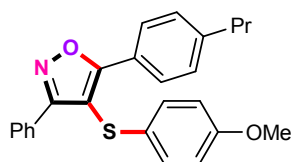
3,5-Diphenyl-4-(thiophen-2-ylthio)isoxazole (**4q**): Yield: 68% (45.6 mg) as a yellow solid; mp = 98.4 - 99.5 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.33 - 8.15 (m, 2H), 7.98 - 7.82 (m, 2H), 7.61 - 7.48 (m, 3H), 7.47 - 7.37 (m, 3H), 7.11 (d, J = 5.2 Hz, 1H), 6.86 - 6.71 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.2, 164.6, 133.9, 131.0, 130.8, 130.0, 128.9, 128.8, 128.6, 128.4, 127.8, 127.3, 126.9, 125.9, 105.7 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3059, 2922, 1639, 1550, 1450, 764, 687; MS (EI) m/z 77, 105, 127, 230, 307, 335; HRMS-ESI (m/z): calcd for $\text{C}_{19}\text{H}_{13}\text{NNaOS}_2$, $[\text{M}+\text{Na}]^+$: 358.0331, found 358.0336.



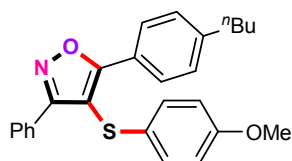
4-((4-Methoxyphenyl)thio)-3-phenyl-5-(*m*-tolyl)isoxazole (**5a**): Yield: 86% (64.2 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.06 - 7.93 (m, 2H), 7.82 (d, $J = 7.2$ Hz, 2H), 7.41 (q, $J = 6.0$ Hz, 3H), 7.35 (t, $J = 7.6$ Hz, 1H), 7.29 (d, $J = 7.6$ Hz, 1H), 7.02 (d, $J = 8.4$ Hz, 2H), 6.73 (d, $J = 8.4$ Hz, 2H), 3.71 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.9, 165.0, 158.5, 138.5, 131.7, 129.9, 128.8, 128.7, 128.7, 128.5, 128.4, 128.1, 127.1, 126.7, 124.7, 115.0, 103.6, 55.3, 21.5 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3060, 2928, 1606, 1570, 1478, 1255, 749; MS (EI) m/z 91, 119, 151, 210, 254, 373; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{19}\text{NNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 396.1029, found 396.1036.



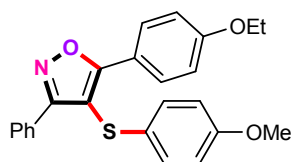
5-(4-Ethylphenyl)-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5b**): Yield: 82% (63.5 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.09 (d, $J = 8.0$ Hz, 2H), 7.81 (d, $J = 7.2$ Hz, 2H), 7.48 - 7.35 (m, 3H), 7.30 (d, $J = 8.0$ Hz, 2H), 7.02 (d, $J = 8.4$ Hz, 2H), 6.73 (d, $J = 8.4$ Hz, 2H), 3.71 (s, 3H), 2.69 (q, $J = 7.6$ Hz, 2H), 1.26 (t, $J = 7.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.1, 165.0, 158.4, 147.5, 129.9, 128.6, 128.6, 128.5, 128.3, 127.5, 126.8, 124.6, 115.0, 102.9, 55.3, 28.9, 15.2 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3063, 2954, 1585, 1488, 1245, 764, 695; MS (EI) m/z 105, 151, 210, 254, 387; HRMS-ESI (m/z): calcd for $\text{C}_{24}\text{H}_{21}\text{NNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 410.1185, found 410.1191.



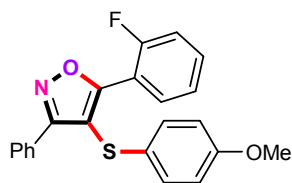
4-((4-Methoxyphenyl)thio)-3-phenyl-5-(4-propylphenyl)isoxazole (**5c**): Yield: 85% (68.2 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.08 (d, $J = 8.0$ Hz, 2H), 7.81 (d, $J = 7.0$ Hz, 2H), 7.48 - 7.35 (m, 3H), 7.28 (d, $J = 8.0$ Hz, 2H), 7.02 (d, $J = 8.4$ Hz, 2H), 6.73 (d, $J = 8.4$ Hz, 2H), 3.72 (s, 3H), 2.63 (t, $J = 7.6$ Hz, 2H), 1.91 - 1.58 (m, 2H), 0.95 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.1, 165.0, 158.4, 146.0, 134.4, 129.9, 128.9, 128.6, 128.5, 128.5, 127.4, 126.8, 124.6, 115.0, 102.8, 55.3, 38.0, 24.2, 13.8 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3062, 2945, 1588, 1492, 1410, 1246, 752, 695; MS (EI) m/z 77, 105, 207, 281, 357, 401; HRMS-ESI (m/z): calcd for $\text{C}_{25}\text{H}_{23}\text{NNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 424.1342, found 424.1346.



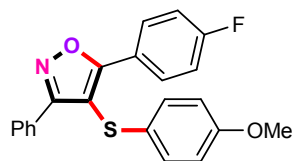
5-(4-Butylphenyl)-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5d**): Yield: 81% (67.2 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.08 (d, $J = 8.0$ Hz, 2H), 7.81 (d, $J = 7.0$ Hz, 2H), 7.47 - 7.36 (m, 3H), 7.28 (d, $J = 8.0$ Hz, 2H), 7.02 (d, $J = 8.4$ Hz, 2H), 6.73 (d, $J = 8.4$ Hz, 2H), 3.71 (s, 3H), 2.65 (t, $J = 7.6$ Hz, 2H), 1.63 (dd, $J = 15.2, 7.8$ Hz, 2H), 1.36 (dq, $J = 14.4, 7.2$ Hz, 2H), 0.93 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.1, 165.0, 158.4, 146.3, 129.9, 128.9, 128.6, 128.5, 128.5, 127.4, 126.8, 124.6, 115.0, 102.8, 55.3, 35.7, 33.3, 22.4, 13.9 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3048, 2935, 1605, 1476, 1248, 752, 689; MS (EI) m/z 77, 91, 161, 254, 372, 415; HRMS-ESI (m/z): calcd for $\text{C}_{26}\text{H}_{25}\text{NNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 438.1498, found 438.1502.



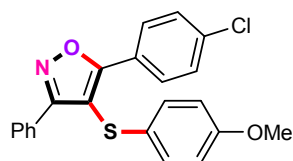
5-(4-Ethoxyphenyl)-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5e**): Yield: 76% (51.1 mg) as a yellow solid; mp = 101.2 - 102.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.13 (d, *J* = 8.8 Hz, 2H), 7.89 - 7.75 (m, 2H), 7.49 - 7.35 (m, 3H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 4.08 (q, *J* = 7.0 Hz, 2H), 3.72 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 171.9, 165.0, 161.0, 158.4, 129.8, 129.1, 128.6, 128.5, 128.4, 126.9, 119.7, 115.0, 114.7, 101.7, 63.7, 55.3, 14.7 ppm; ν_{max}(KBr)/cm⁻¹ 3046, 2929, 1603, 1495, 1251, 752, 696; MS (EI) m/z 77, 105, 151, 207, 296, 387, 403; HRMS-ESI (m/z): calcd for C₂₄H₂₁NNaO₃S, [M+Na]⁺: 426.1134, found 426.1139.



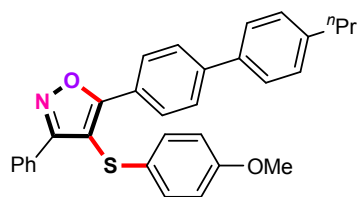
5-(2-Fluorophenyl)-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5f**): Yield: 73% (55.0 mg) as a yellow solid; mp = 94.5 - 96.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 7.2 Hz, 2H), 7.70 (t, *J* = 7.2 Hz, 1H), 7.50 (dd, *J* = 13.6, 7.2 Hz, 1H), 7.45 - 7.33 (m, 3H), 7.26 (d, *J* = 5.2 Hz, 1H), 7.21 (d, *J* = 9.4 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.68 (d, *J* = 8.4 Hz, 2H), 3.70 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.9, 163.8, 160.0 (d, *J* = 254.9 Hz), 158.7, 132.7 (d, *J* = 8.4 Hz), 131.0, 129.9, 129.7, 128.5, 128.5, 126.1, 124.2 (d, *J* = 3.7 Hz), 116.5 (d, *J* = 21.2 Hz), 115.6 (d, *J* = 13.5 Hz), 114.8, 107.7, 55.3 ppm; ν_{max}(KBr)/cm⁻¹ 3285, 2925, 1642, 1473, 1287, 753, 681; MS (EI) m/z 77, 105, 151, 210, 254, 377; HRMS-ESI (m/z): calcd for C₂₂H₁₆FNNaO₂S, [M+Na]⁺: 400.0778, found 400.0784.



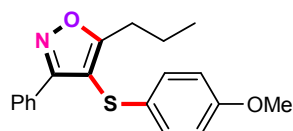
5-(4-Fluorophenyl)-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5g**): Yield: 78% (58.8 mg) as a yellow solid; mp = 86.1 - 87.7 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.27 - 8.09 (m, 2H), 7.81 (d, J = 7.2 Hz, 2H), 7.54 - 7.37 (m, 3H), 7.17 (t, J = 8.4 Hz, 2H), 7.00 (d, J = 8.4 Hz, 2H), 6.74 (d, J = 8.4 Hz, 2H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.8, 165.1, 164.2 (d, J = 252.7 Hz), 158.6, 130.0, 129.7 (d, J = 8.6 Hz), 128.7, 128.6, 128.5, 128.2, 126.2, 123.5 (d, J = 3.4 Hz), 116.1 (d, J = 21.9 Hz), 115.1, 103.4, 55.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3280, 2922, 1641, 1488, 1269, 754, 676; MS (EI) m/z 95, 151, 254, 377; HRMS-ESI (m/z): calcd for $\text{C}_{22}\text{H}_{16}\text{FNNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 400.0778, found 400.0783.



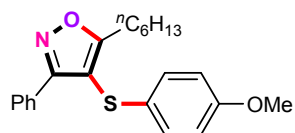
5-(4-Chlorophenyl)-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5h**): Yield: 77% (60.5 mg) as a yellow solid; mp = 105.0 - 106.8 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.13 (d, J = 8.4 Hz, 2H), 7.80 (d, J = 6.4 Hz, 2H), 7.56 - 7.34 (m, 5H), 6.99 (d, J = 8.8 Hz, 2H), 6.73 (d, J = 8.8 Hz, 2H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.5, 165.1, 158.6, 137.1, 130.0, 129.2, 128.8, 128.7, 128.6, 128.5, 128.2, 126.1, 125.6, 115.1, 104.2, 55.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3067, 2925, 1589, 1482, 1247, 744, 692; MS (EI) m/z 77, 151, 254, 350, 393; HRMS-ESI (m/z): calcd for $\text{C}_{22}\text{H}_{16}\text{ClNaO}_2\text{S}$, $[\text{M}+\text{Na}]^+$: 416.0482, found 416.0487.



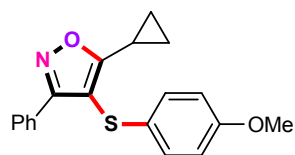
4-((4-Methoxyphenyl)thio)-3-phenyl-5-(4'-propyl-[1,1'-biphenyl]-4-yl)isoxazole (**5i**): Yield: 71% (67.7 mg) as a yellow solid; mp = 116.3 - 117.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.25 (d, *J* = 8.4 Hz, 2H), 7.82 (dd, *J* = 7.2, 1.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.49 - 7.36 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 3.71 (s, 3H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.88 - 1.60 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 171.6, 165.1, 158.5, 143.5, 142.8, 137.3, 129.9, 129.1, 128.7, 128.7, 128.5, 128.4, 127.8, 127.2, 127.0, 126.6, 125.7, 115.1, 103.5, 55.3, 37.7, 24.5, 13.9 ppm; ν_{max}(KBr)/cm⁻¹ 3066, 2941, 1587, 1484, 1253, 753, 688; MS (EI) *m/z* 77, 151, 207, 292, 381, 429, 477; HRMS-ESI (*m/z*): calcd for C₃₁H₂₇NNaO₂S, [M+Na]⁺: 500.1655, found 500.1660.



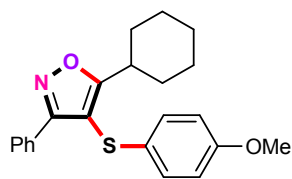
4-((4-Methoxyphenyl)thio)-3-phenyl-5-propylisoxazole (**5j**): Yield: 78% (50.7 mg) as a yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 7.86 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.42 - 7.38 (m, 3H), 7.00 (d, *J* = 8.8 Hz, 2H), 6.75 (d, *J* = 8.8 Hz, 2H), 3.73 (s, 3H), 2.89 (t, *J* = 7.6 Hz, 2H), 2.11 - 1.63 (m, 2H), 0.98 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 178.2, 163.1, 158.4, 134.4, 129.8, 128.8, 128.5, 128.3, 127.0, 114.9, 104.2, 55.3, 28.0, 20.9, 13.8 ppm; ν_{max}(KBr)/cm⁻¹ 3059, 2930, 1573, 1480, 1244, 756, 686; MS (EI) *m/z* 77, 151, 193, 254, 296, 325; HRMS-ESI (*m/z*): calcd for C₁₉H₂₀NO₂S, [M+H]⁺: 326.1209, found 326.1210.



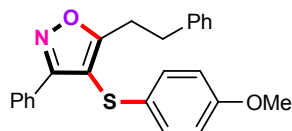
5-Hexyl-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5k**): Yield: 76% (55.8 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.87 (dd, $J = 7.6, 2.0$ Hz, 2H), 7.44 - 7.33 (m, 3H), 7.06 - 6.95 (m, 2H), 6.79 - 6.70 (m, 2H), 3.73 (s, 3H), 3.16 - 2.69 (m, 2H), 1.78 - 1.64 (m, 2H), 1.43 - 1.30 (m, 2H), 1.31 - 1.16 (m, 4H), 0.87 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.4, 163.1, 158.4, 129.8, 128.8, 128.6, 128.5, 128.3, 127.1, 114.9, 104.1, 55.3, 31.3, 28.9, 27.3, 26.1, 22.5, 14.0 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3060, 2931, 1567, 1483, 1416, 1267, 755, 684; MS (EI) m/z 77, 121, 151, 254, 296, 367; HRMS-ESI (m/z): calcd for $\text{C}_{22}\text{H}_{26}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 368.1679, found 368.1686.



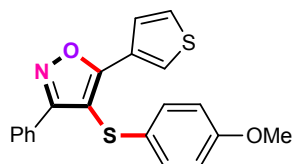
5-Cyclopropyl-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5l**): Yield: 65% (42.0 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 7.2$ Hz, 2H), 7.47 - 7.32 (m, 3H), 7.06 (d, $J = 8.2$ Hz, 2H), 6.76 (d, $J = 8.2$ Hz, 2H), 3.73 (s, 3H), 2.49 - 2.19 (m, 1H), 1.29 - 1.24 (m, 2H), 1.17 - 1.05 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.4, 163.5, 158.4, 129.9, 128.8, 128.5, 128.5, 128.3, 127.3, 114.9, 103.3, 55.4, 8.9, 8.2 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3056, 2933, 1576, 1481, 1250, 756, 694; MS (EI) m/z 69, 105, 151, 216, 254, 323; HRMS-ESI (m/z): calcd for $\text{C}_{19}\text{H}_{18}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 324.1053, found 324.1055.



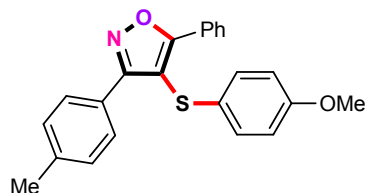
5-Cyclohexyl-4-((4-methoxyphenyl)thio)-3-phenylisoxazole (**5m**): Yield: 70% (51.1 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.87 (d, $J = 7.2$ Hz, 2H), 7.42 - 7.36 (m, 3H), 6.99 (d, $J = 8.4$ Hz, 2H), 6.74 (d, $J = 8.4$ Hz, 2H), 3.72 (s, 3H), 2.91 (d, $J = 7.4$ Hz, 2H), 2.30 (dt, $J = 15.4$, 7.6 Hz, 1H), 1.91 - 1.72 (m, 2H), 1.67 - 1.60 (m, 2H), 1.55 (dd, $J = 14.8$, 7.2 Hz, 2H), 1.44 - 1.07 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 178.1, 163.0, 158.4, 134.4, 129.8, 128.7, 128.5, 128.3, 127.1, 114.9, 104.2, 55.4, 38.6, 32.5, 31.8, 24.9 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3080, 2946, 1560, 1482, 1266, 756, 686; MS (EI) m/z 55, 77, 121, 193, 254, 296, 365; HRMS-ESI (m/z): calcd for $\text{C}_{22}\text{H}_{24}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 366.1522, found 366.1528.



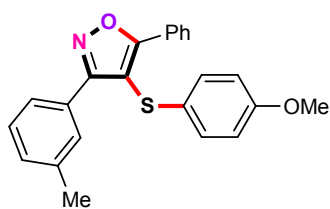
4-((4-Methoxyphenyl)thio)-5-phenethyl-3-phenylisoxazole (**5n**): Yield: 73% (56.5 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.83 (d, $J = 7.0$ Hz, 2H), 7.46 - 7.35 (m, 3H), 7.26 (dd, $J = 16.8$, 9.4 Hz, 3H), 7.17 (d, $J = 7.4$ Hz, 2H), 6.89 (d, $J = 8.0$ Hz, 2H), 6.70 (d, $J = 8.0$ Hz, 2H), 3.72 (s, 3H), 3.22 (t, $J = 7.8$ Hz, 2H), 3.04 (t, $J = 7.8$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 176.9, 163.1, 158.4, 140.0, 129.9, 129.0, 128.6, 128.5, 128.4, 128.3, 126.7, 126.5, 114.9, 104.9, 55.3, 33.3, 28.1 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3045, 2930, 1581, 1477, 1252, 752, 696; MS (EI) m/z 77, 121, 193, 296, 387; HRMS-ESI (m/z): calcd for $\text{C}_{24}\text{H}_{22}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 388.1366, found 388.1364.



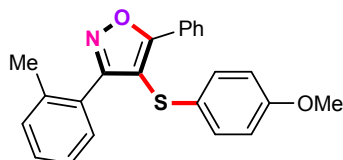
4-((4-Methoxyphenyl)thio)-3-phenyl-5-(thiophen-3-yl)isoxazole (**5o**): Yield: 66% (48.2 mg) as a yellow solid; mp = 87.6 - 89.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.94 (d, *J* = 3.8 Hz, 1H), 7.85 (d, *J* = 7.4 Hz, 2H), 7.52 (d, *J* = 5.0 Hz, 1H), 7.48 - 7.37 (m, 3H), 7.15 (t, *J* = 4.4 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 2H), 6.73 (d, *J* = 8.4 Hz, 2H), 3.71 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.2, 164.5, 158.6, 130.1, 130.0, 129.2, 128.9, 128.6, 128.5, 128.1, 127.9, 127.6, 126.0, 115.0, 102.4, 55.3 ppm; ν_{max}(KBr)/cm⁻¹ 3078, 2923, 1573, 1482, 1244, 754, 698; MS (EI) *m/z* 77, 111, 151, 186, 254, 365; HRMS-ESI (*m/z*): calcd for C₂₀H₁₆NO₂S₂, [M+H]⁺: 366.0617, found 366.0620.



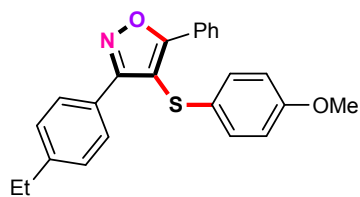
4-((4-Methoxyphenyl)thio)-5-phenyl-3-(*p*-tolyl)isoxazole (**6a**): Yield: 86% (64.2 mg) as a yellow solid; mp = 86.1 - 87.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.21 - 8.09 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.55 - 7.39 (m, 3H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 2H), 6.74 (d, *J* = 8.6 Hz, 2H), 3.71 (s, 3H), 2.37 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 171.8, 165.0, 158.4, 140.0, 130.8, 129.2, 128.8, 128.5, 128.5, 127.5, 127.2, 126.7, 125.4, 115.0, 103.4, 55.3, 21.4 ppm; ν_{max}(KBr)/cm⁻¹ 3051, 2928, 1579, 1483, 1246, 749, 681; MS (EI) *m/z* 77, 105, 151, 224, 268, 373; HRMS-ESI (*m/z*): calcd for C₂₃H₂₀NO₂S, [M+H]⁺: 374.1209, found 374.1210.



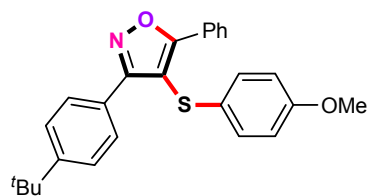
4-((4-Methoxyphenyl)thio)-5-phenyl-3-(m-tolyl)isoxazole (**6b**): Yield: 83% (61.9 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.24 - 8.06 (m, 2H), 7.60 (d, $J = 7.6$ Hz, 2H), 7.52 - 7.41 (m, 3H), 7.29 (d, $J = 7.6$ Hz, 1H), 7.23 (d, $J = 7.2$ Hz, 1H), 7.02 (d, $J = 8.8$ Hz, 2H), 6.73 (d, $J = 8.8$ Hz, 2H), 3.70 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.7, 165.2, 158.5, 138.1, 130.9, 130.7, 129.3, 128.9, 128.8, 128.4, 128.2, 127.5, 127.2, 126.7, 125.7, 115.0, 103.8, 55.3, 21.4 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3056, 2928, 1550, 1479, 1267, 755, 677; MS (EI) m/z 77, 105, 151, 207, 281, 373; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 374.1209, found 374.1211.



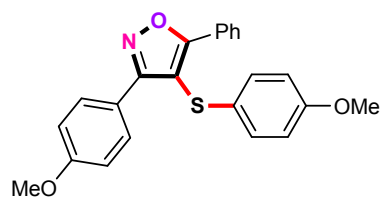
4-((4-Methoxyphenyl)thio)-5-phenyl-3-(o-tolyl)isoxazole (**6c**): Yield: 80% (59.7 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.37 - 8.26 (m, 2H), 7.61 - 7.49 (m, 3H), 7.35 (td, $J = 8.0, 4.0$ Hz, 1H), 7.28 (d, $J = 7.6$ Hz, 1H), 7.22 (d, $J = 4.4$ Hz, 2H), 6.95 (d, $J = 8.6$ Hz, 2H), 6.68 (d, $J = 8.6$ Hz, 2H), 3.74 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.8, 166.6, 158.9, 137.6, 130.8, 130.8, 130.3, 130.2, 129.5, 128.9, 127.9, 127.3, 125.6, 125.4, 114.6, 106.6, 55.3, 19.9 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3060, 2937, 1582, 1472, 1256, 752, 684; MS (EI) m/z 75, 105, 151, 224, 268, 373; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 374.1209, found 374.1213.



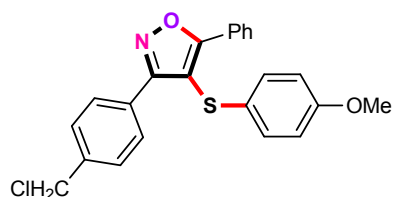
3-(4-Ethylphenyl)-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**6d**): Yield: 85% (65.7 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.16 (d, $J = 4.8$ Hz, 2H), 7.74 (d, $J = 7.6$ Hz, 2H), 7.53 - 7.41 (m, 3H), 7.24 (d, $J = 7.8$ Hz, 2H), 7.03 (d, $J = 7.8$ Hz, 2H), 6.74 (d, $J = 7.8$ Hz, 2H), 3.72 (s, 3H), 2.68 (q, $J = 7.6$ Hz, 2H), 1.25 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 171.8, 165.0, 158.4, 146.3, 130.8, 128.8, 128.6, 128.5, 128.0, 127.5, 127.2, 126.7, 125.6, 115.0, 103.4, 55.3, 28.8, 15.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3048, 2960, 1545, 1486, 1263, 754, 684; MS (EI) m/z 77, 105, 151, 282, 387; HRMS-ESI (m/z): calcd for $\text{C}_{24}\text{H}_{22}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 388.1366, found 388.1365.



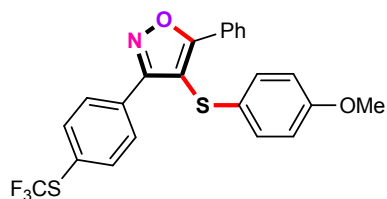
3-(4-(*tert*-Butyl)phenyl)-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**6e**): Yield: 77% (63.9 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.15 (d, $J = 8.0$ Hz, 2H), 7.86 (d, $J = 7.2$ Hz, 2H), 7.54 (d, $J = 8.0$ Hz, 2H), 7.51 - 7.40 (m, 3H), 7.07 (d, $J = 8.2$ Hz, 2H), 6.78 (d, $J = 8.2$ Hz, 2H), 3.76 (s, 3H), 1.38 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.1, 165.0, 158.4, 154.4, 129.9, 128.6, 128.5, 128.4, 127.3, 126.8, 125.8, 124.4, 115.0, 102.7, 55.3, 35.0, 31.1 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3057, 2952, 1586, 1483, 1416, 751, 683; MS (EI) m/z 77, 105, 281, 340, 374, 415; HRMS-ESI (m/z): calcd for $\text{C}_{26}\text{H}_{26}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 416.1679, found 416.1685.



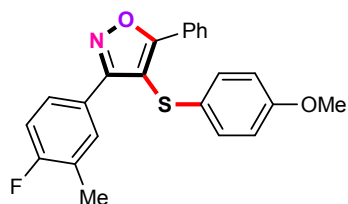
3-(4-Methoxyphenyl)-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**6f**): Yield: 80% (62.2 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.79 - 7.65 (m, 2H), 7.58 (d, $J = 8.2$ Hz, 2H), 7.47 - 7.35 (m, 4H), 7.01 (s, 1H), 6.90 (d, $J = 8.2$ Hz, 2H), 6.85 (d, $J = 8.2$ Hz, 1H), 4.02 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.7, 159.6, 152.7, 138.1, 137.2, 134.4, 129.6, 128.5, 128.4, 126.9, 126.7, 125.3, 118.2, 114.6, 113.9, 62.5, 55.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3065, 2948, 1587, 1495, 1446, 1235, 752, 680; MS (EI) m/z 77, 105, 135, 207, 312, 389; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_3\text{S}$, $[\text{M}+\text{H}]^+$: 390.1158, found 390.1155.



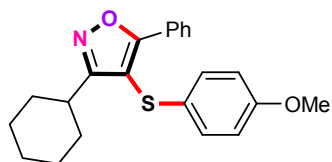
3-(4-(Chloromethyl)phenyl)-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**6g**): Yield: 62% (50.5 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.23 - 8.10 (m, 2H), 7.72 (d, $J = 8.0$ Hz, 2H), 7.21 (d, $J = 8.0$ Hz, 3H), 7.00 (d, $J = 8.0$ Hz, 2H), 6.86 - 6.66 (m, 4H), 3.97 (s, 2H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.8, 164.7, 159.4, 158.5, 140.3, 134.4, 130.9, 129.0, 128.8, 128.8, 128.6, 127.5, 115.0, 114.5, 103.7, 55.3, 41.1 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3060, 2925, 1587, 1485, 1254, 754, 679; MS (EI) m/z 77, 105, 199, 277, 355, 407; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{19}\text{ClNO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 408.0820, found 408.0823.



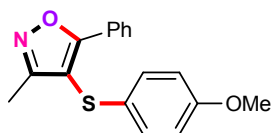
4-((4-Methoxyphenyl)thio)-5-phenyl-3-(4-((trifluoromethyl)thio)phenyl)isoxazole (**6h**): Yield: 67% (61.5 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.24 - 8.07 (m, 2H), 7.87 (d, $J = 8.0$ Hz, 2H), 7.68 (d, $J = 8.0$ Hz, 2H), 7.56 - 7.43 (m, 3H), 7.00 (d, $J = 8.8$ Hz, 2H), 6.72 (d, $J = 8.8$ Hz, 2H), 3.72 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.0, 163.8, 158.7, 136.1, 132.7, 131.1, 130.9, 129.6, 129.0, 128.9, 127.5, 127.7 (q, $J = 258.7$ Hz), 115.1, 104.0, 55.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3056, 2930, 1590, 1491, 1251, 754, 687; MS (EI) m/z 77, 105, 151, 310, 354, 459; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{17}\text{F}_3\text{NO}_2\text{S}_2$, $[\text{M}+\text{H}]^+$: 460.0647, found 460.0642.



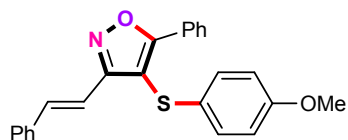
3-(4-Fluoro-3-methylphenyl)-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**6i**): Yield: 75% (58.7 mg) as a yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.09 (d, $J = 4.4$ Hz, 2H), 7.56 (d, $J = 6.8$ Hz, 2H), 7.47 - 7.37 (m, 3H), 7.00 - 6.90 (m, 3H), 6.67 (d, $J = 7.8$ Hz, 2H), 3.65 (s, 3H), 2.19 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 171.8, 164.3, 162.4 (d, $J = 248.8$ Hz), 158.6, 134.4, 132.0 (d, $J = 5.6$ Hz), 130.9, 128.8 (d, $J = 5.0$ Hz), 127.9 (d, $J = 8.6$ Hz), 127.5, 127.1, 126.4, 125.2 (d, $J = 17.7$ Hz), 124.1 (d, $J = 3.7$ Hz), 115.2 (d, $J = 23.0$ Hz), 115.0, 103.6, 55.4, 14.5 (d, $J = 2.9$ Hz) ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3067, 2928, 1579, 1481, 1249, 759, 690; MS (EI) m/z 77, 105, 151, 242, 286, 391; HRMS-ESI (m/z): calcd for $\text{C}_{23}\text{H}_{19}\text{FNO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 392.1115, found 392.1112.



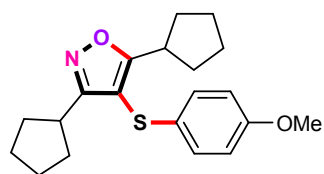
3-Cyclohexyl-4-((4-methoxyphenyl)thio)-5-phenylisoxazole (**6k**): Yield: 71% (51.8 mg) as a yellow solid; mp = 102.5 - 103.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.19 - 8.05 (m, 2H), 7.51 - 7.34 (m, 3H), 7.06 (d, *J* = 8.6 Hz, 2H), 6.78 (d, *J* = 8.6 Hz, 2H), 3.73 (s, 3H), 2.84 - 2.70 (m, 1H), 1.93 - 1.84 (m, 2H), 1.83 - 1.74 (m, 2H), 1.72 - 1.66 (m, 1H), 1.58 (dd, *J* = 11.6, 7.2 Hz, 2H), 1.33 - 1.23 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.7, 170.2, 158.5, 130.6, 128.7, 128.6, 127.4, 127.3, 126.6, 115.0, 103.4, 55.4, 35.6, 31.4, 26.3, 25.9 ppm; ν_{\max} (KBr)/cm⁻¹ 3058, 2936, 1579, 1480, 1258, 755, 688; MS (EI) *m/z* 77, 105, 153, 260, 297, 365; HRMS-ESI (*m/z*): calcd for C₂₂H₂₄NO₂S, [M+H]⁺: 366.1522, found 366.1516.



4-((4-Methoxyphenyl)thio)-3-methyl-5-phenylisoxazole (**6l**): Yield: 78% (46.3 mg) as a yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 8.26 - 8.00 (m, 2H), 7.56 - 7.41 (m, 3H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 3.74 (s, 3H), 2.22 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 163.8, 158.6, 130.7, 129.0, 128.8, 127.3, 127.2, 125.9, 115.0, 104.8, 55.4, 10.3 ppm; ν_{\max} (KBr)/cm⁻¹ 3060, 2928, 1557, 1481, 1250, 756, 683; MS (EI) *m/z* 77, 105, 151, 192, 297; HRMS-ESI (*m/z*): calcd for C₁₇H₁₆NO₂S, [M+H]⁺: 298.0896, found 298.0889.

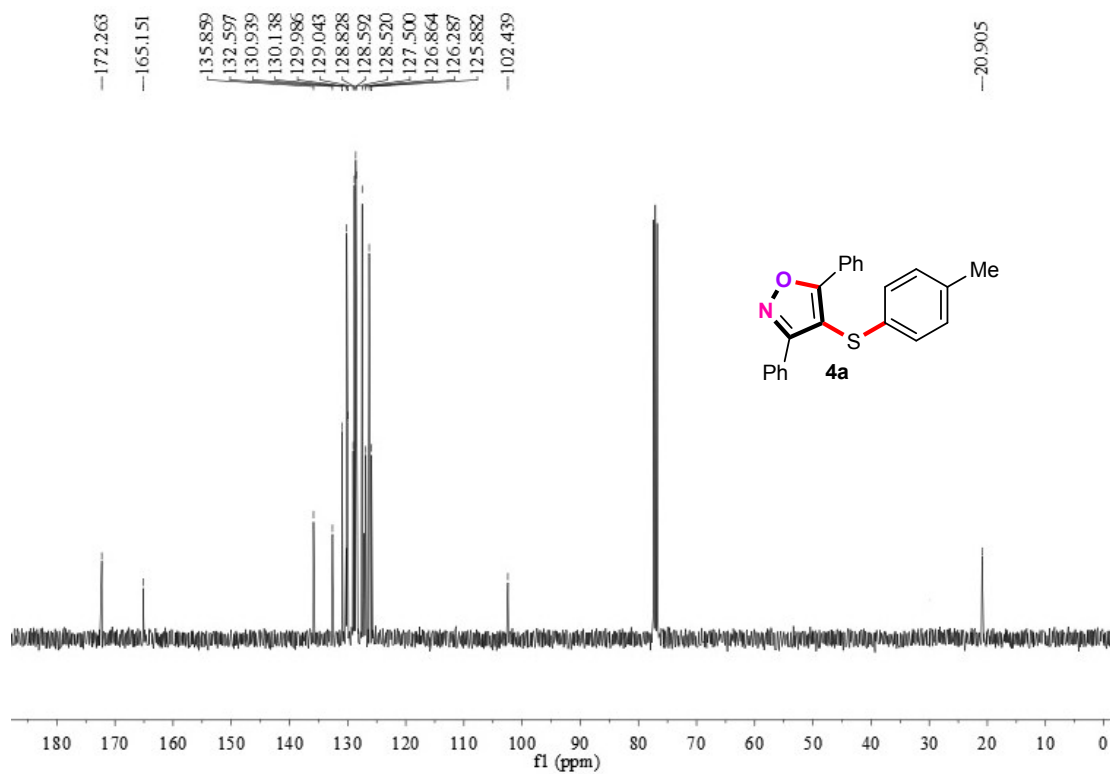
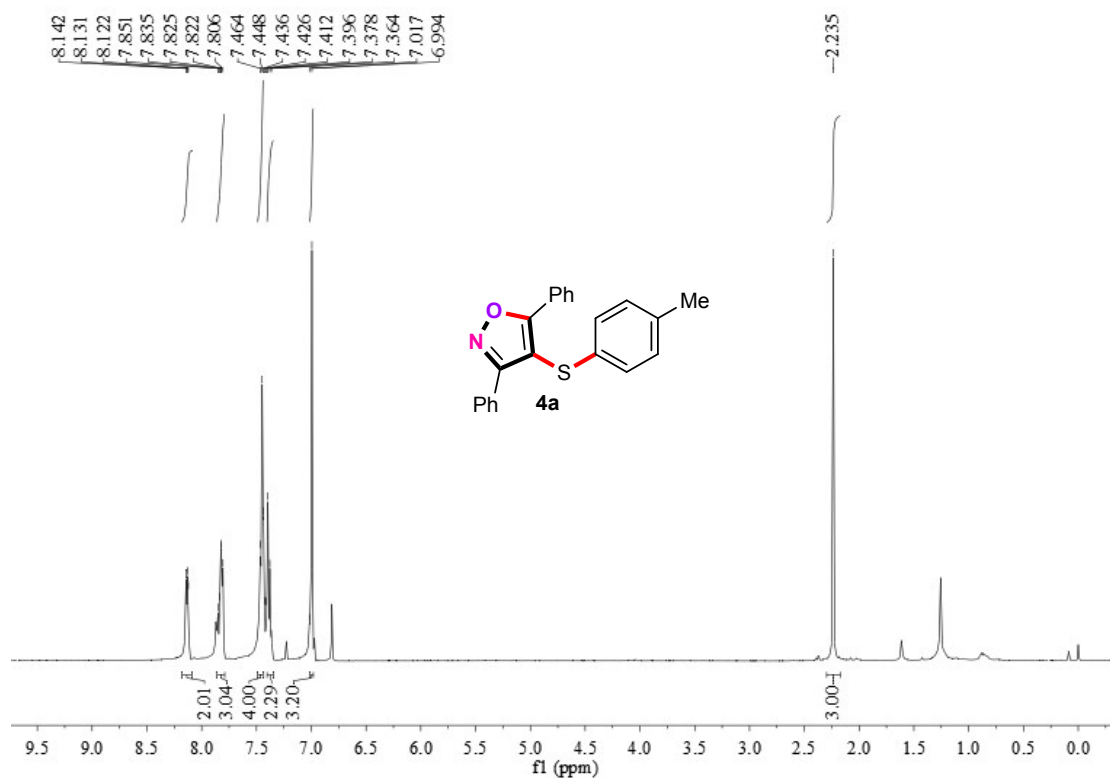


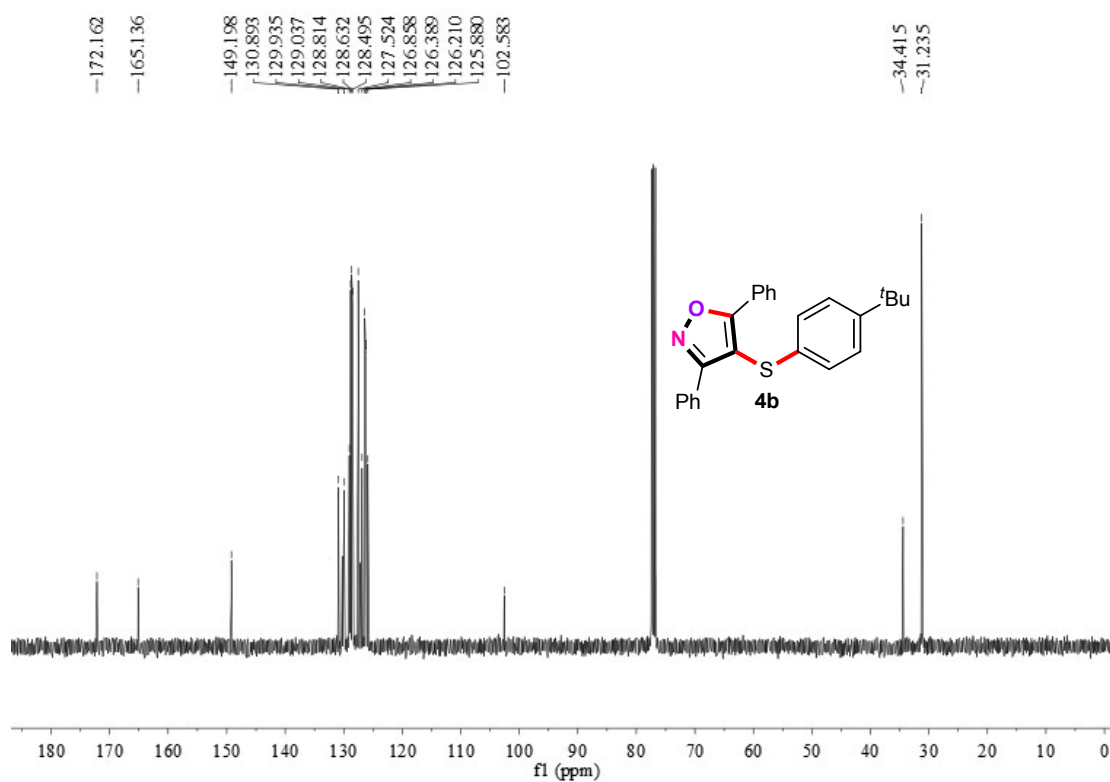
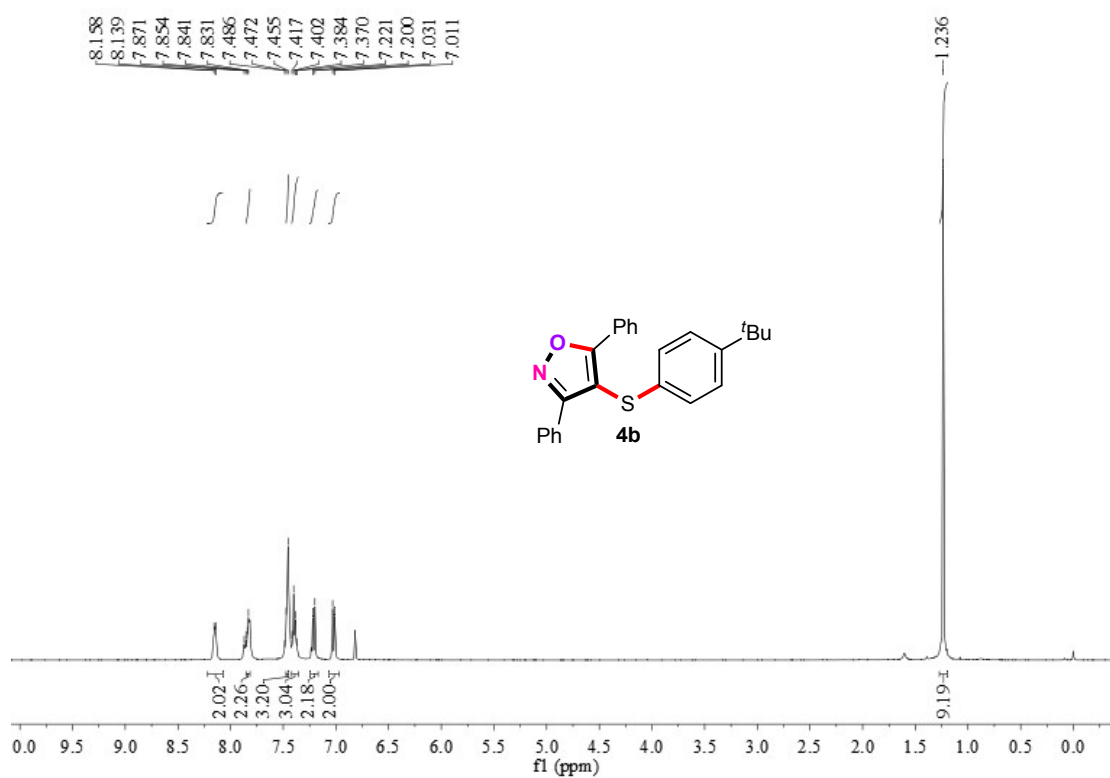
(*E*)-4-((4-Methoxyphenyl)thio)-5-phenyl-3-styrylisoxazole (**6m**): Yield: 70% (53.9 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.27 - 8.07 (m, 2H), 7.74 (d, $J = 16.6$ Hz, 1H), 7.56 - 7.43 (m, 5H), 7.32 (dt, $J = 20.0, 7.2$ Hz, 3H), 7.14 (d, $J = 8.4$ Hz, 2H), 7.02 (d, $J = 16.6$ Hz, 1H), 6.79 (d, $J = 8.4$ Hz, 2H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.1, 162.6, 158.6, 136.5, 136.1, 130.8, 128.9, 128.8, 128.7, 128.6, 127.4, 127.2, 127.1, 126.2, 115.2, 113.9, 103.9, 55.3 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3066, 2928, 1581, 1515, 1477, 1418, 1256, 753, 668; MS (EI) m/z 77, 105, 151, 280, 341, 385; HRMS-ESI (m/z): calcd for $\text{C}_{24}\text{H}_{20}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 386.1209, found 386.1203.

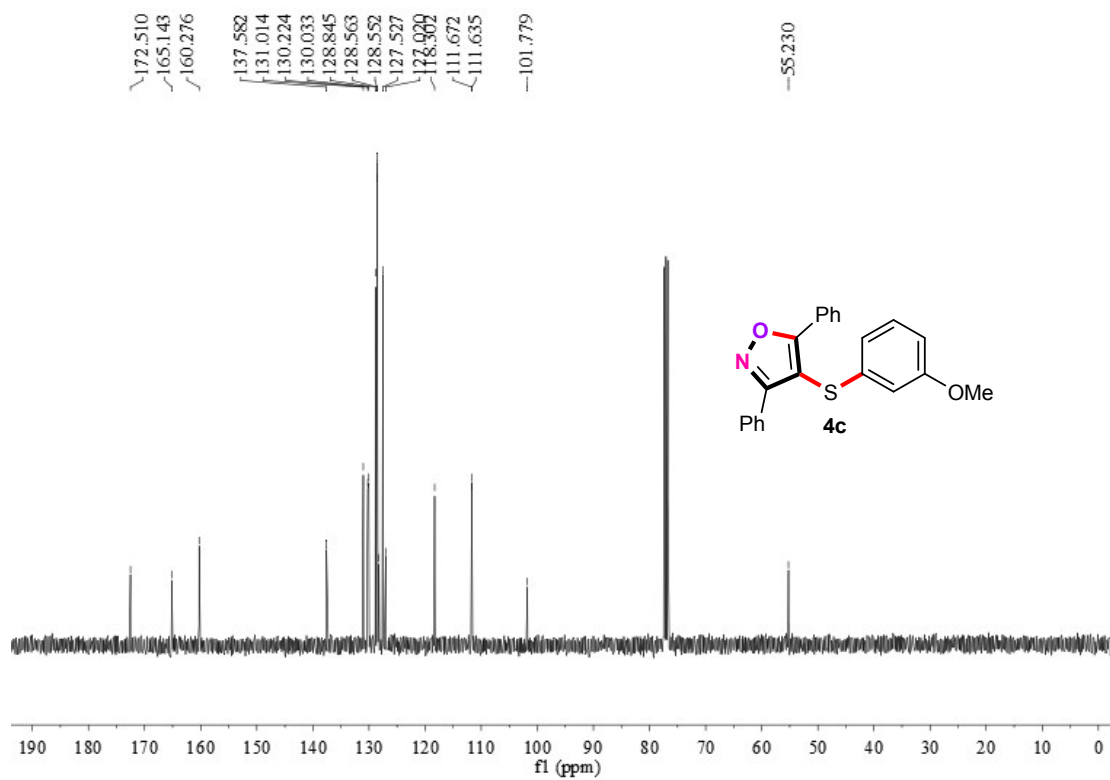
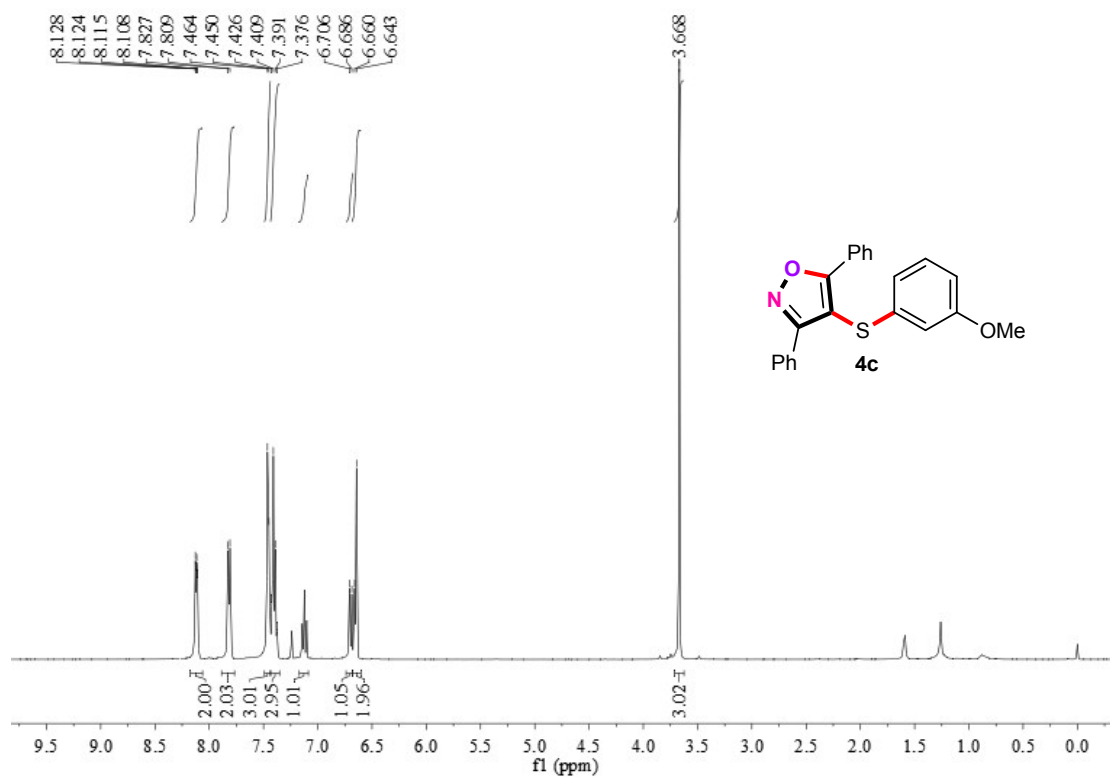


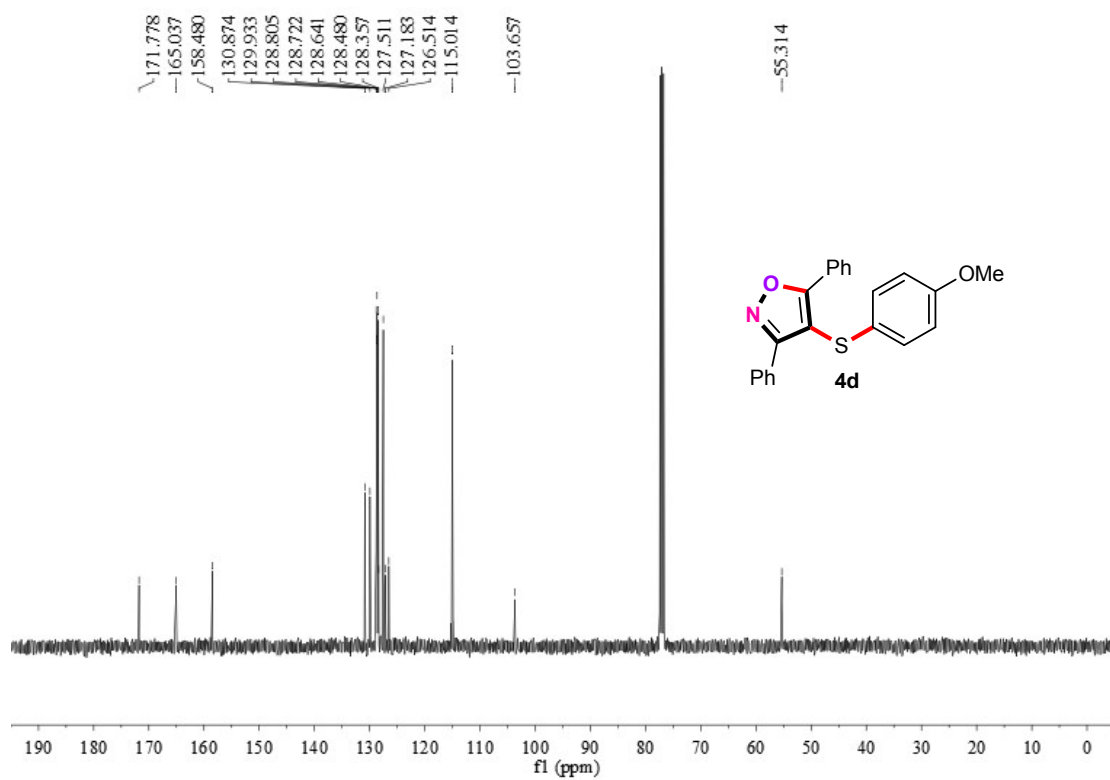
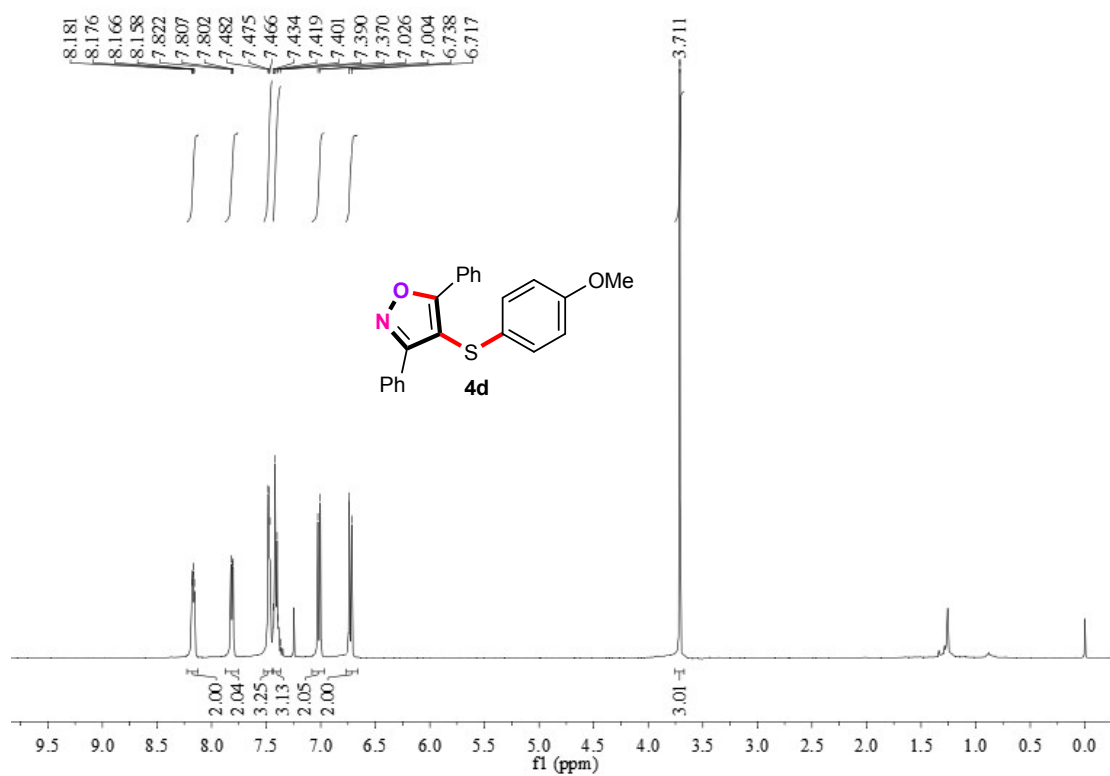
3,5-Dicyclopentyl-4-((4-methoxyphenyl)thio)isoxazole (**7**): Yield: 76% (52.1 mg) as a yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.03 (d, $J = 8.4$ Hz, 2H), 6.79 (d, $J = 8.6$ Hz, 2H), 3.77 (s, 3H), 3.02 (dd, $J = 16.0, 7.6$ Hz, 1H), 2.85 - 2.55 (m, 1H), 1.89 - 1.74 (m, 8H), 1.71 - 1.60 (m, 4H), 1.57 - 1.47 (m, 2H), 1.32 - 1.18 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.9, 169.2, 158.3, 128.6, 127.5, 114.8, 102.3, 55.4, 36.2, 35.6, 31.3, 30.6, 26.3, 26.0, 25.9, 25.6 ppm; $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 3048, 2931, 1583, 1478, 1248, 1170, 817, 756; MS (EI) m/z 77, 105, 151, 290, 343; HRMS-ESI (m/z): calcd for $\text{C}_{20}\text{H}_{26}\text{NO}_2\text{S}$, $[\text{M}+\text{H}]^+$: 344.1679, found 344.1674.

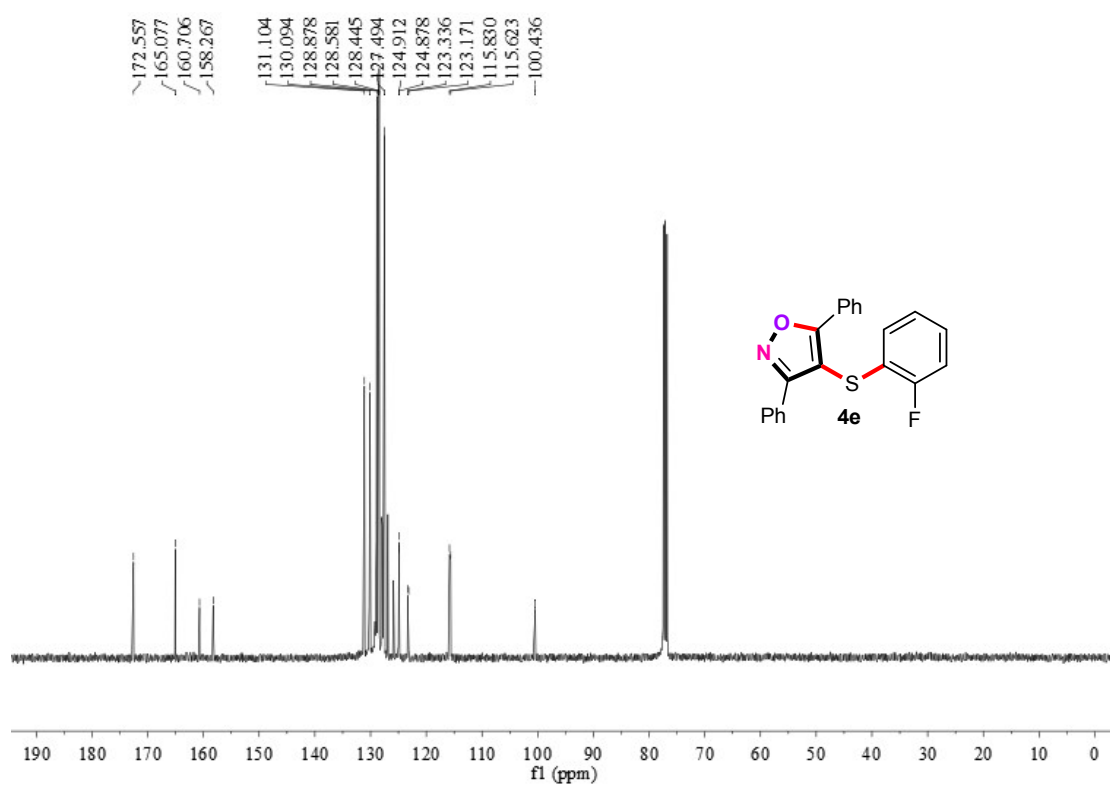
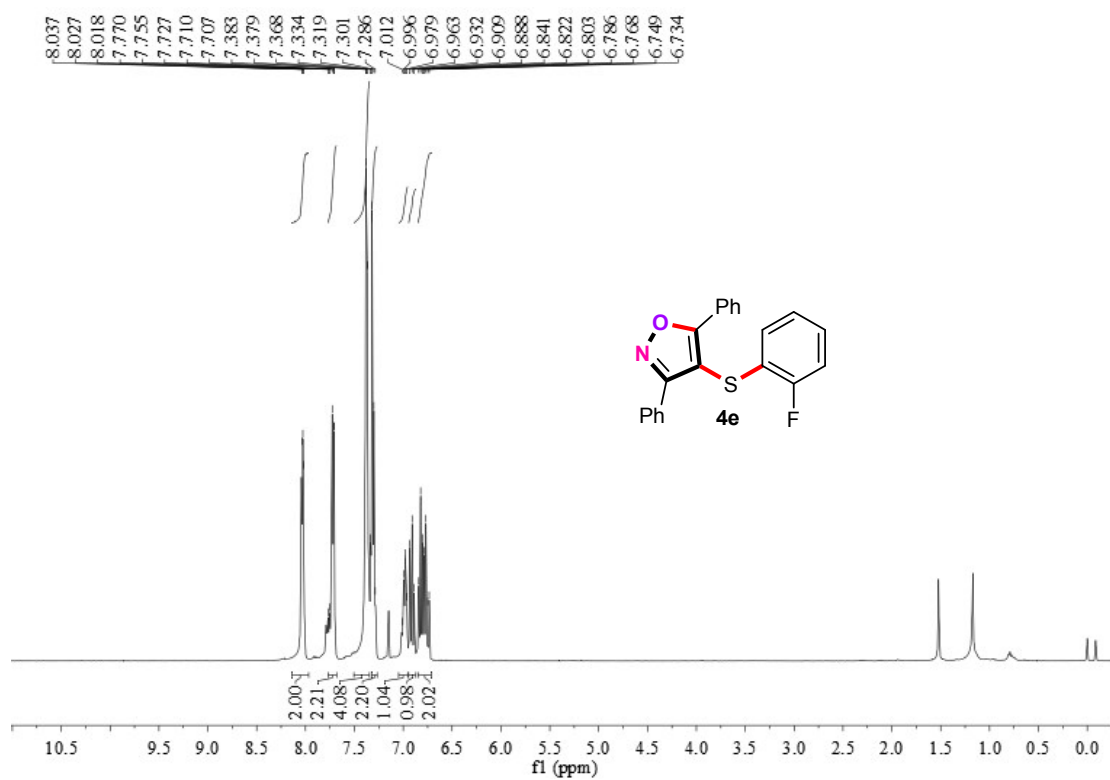
¹H and ¹³C NMR spectra of compounds 4

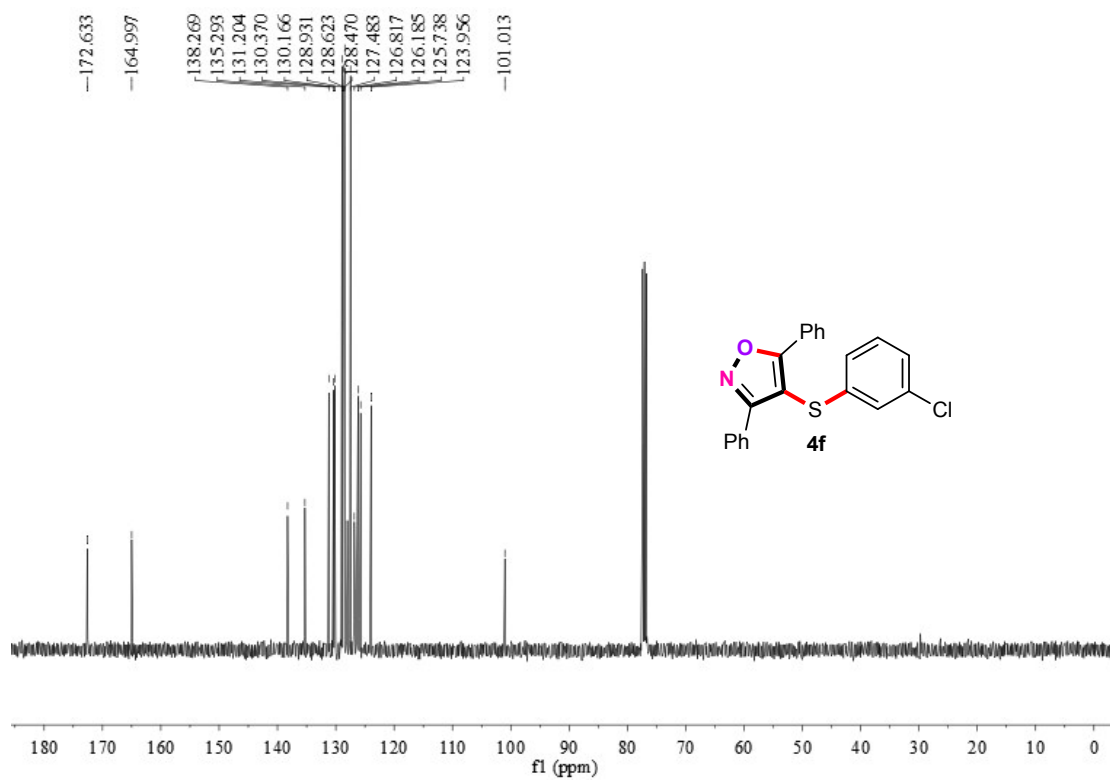
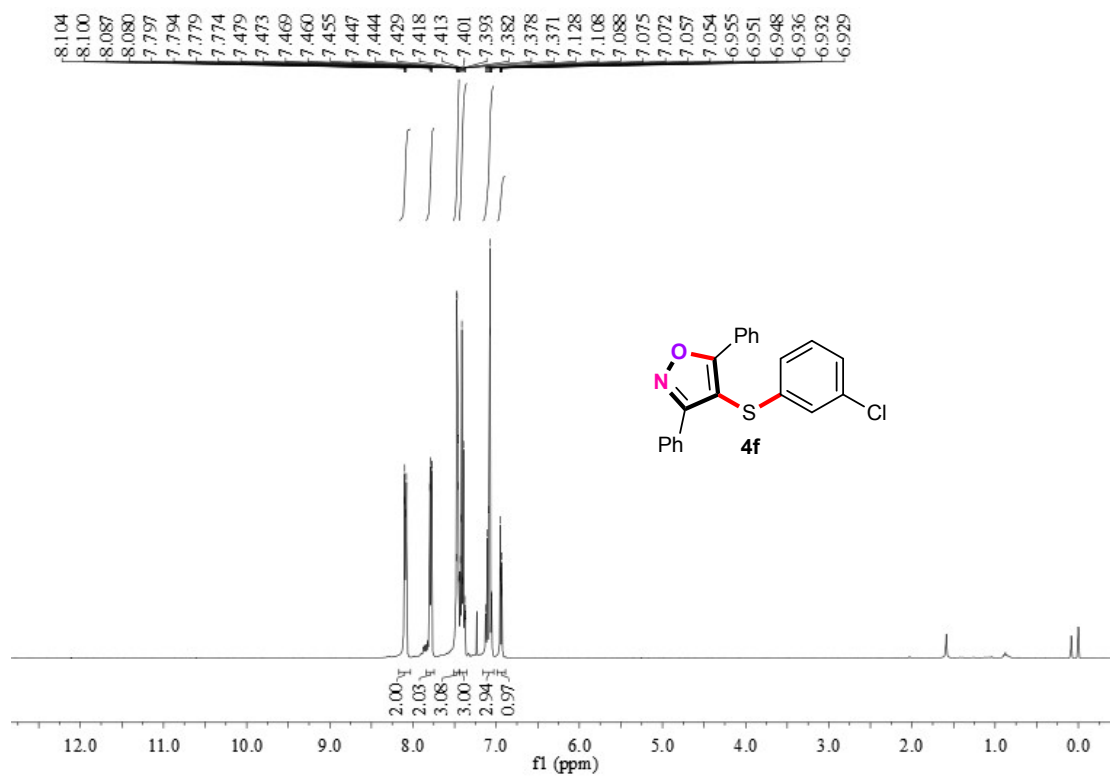


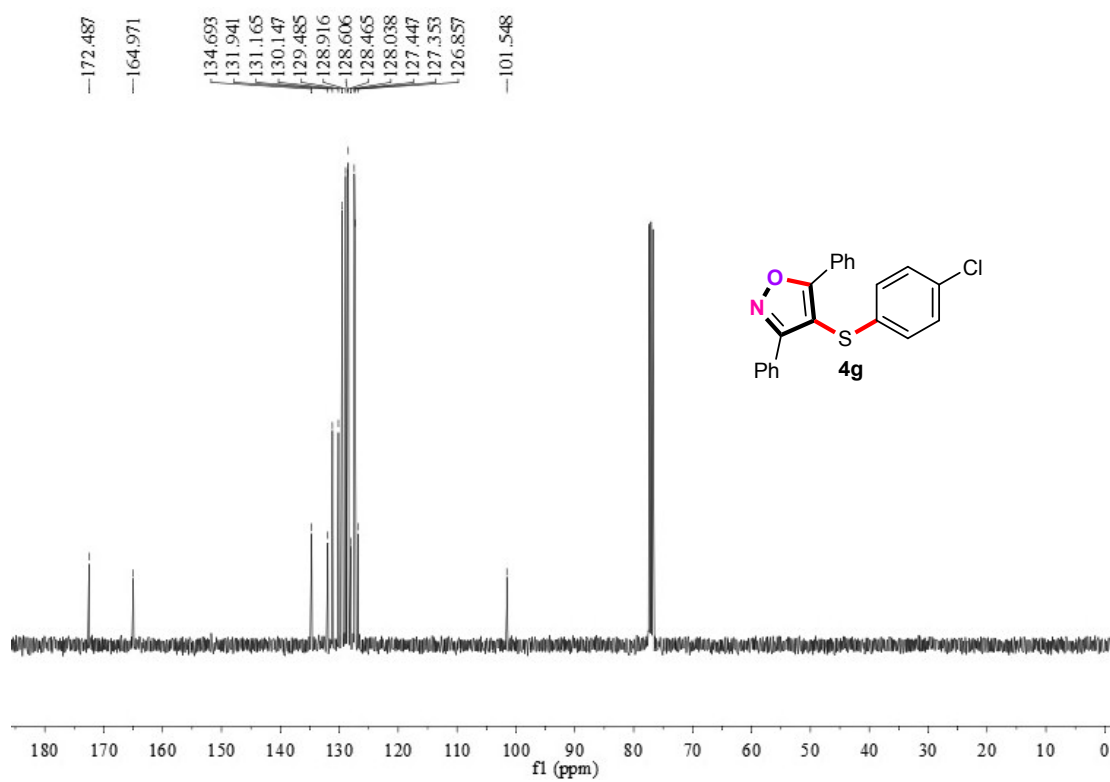
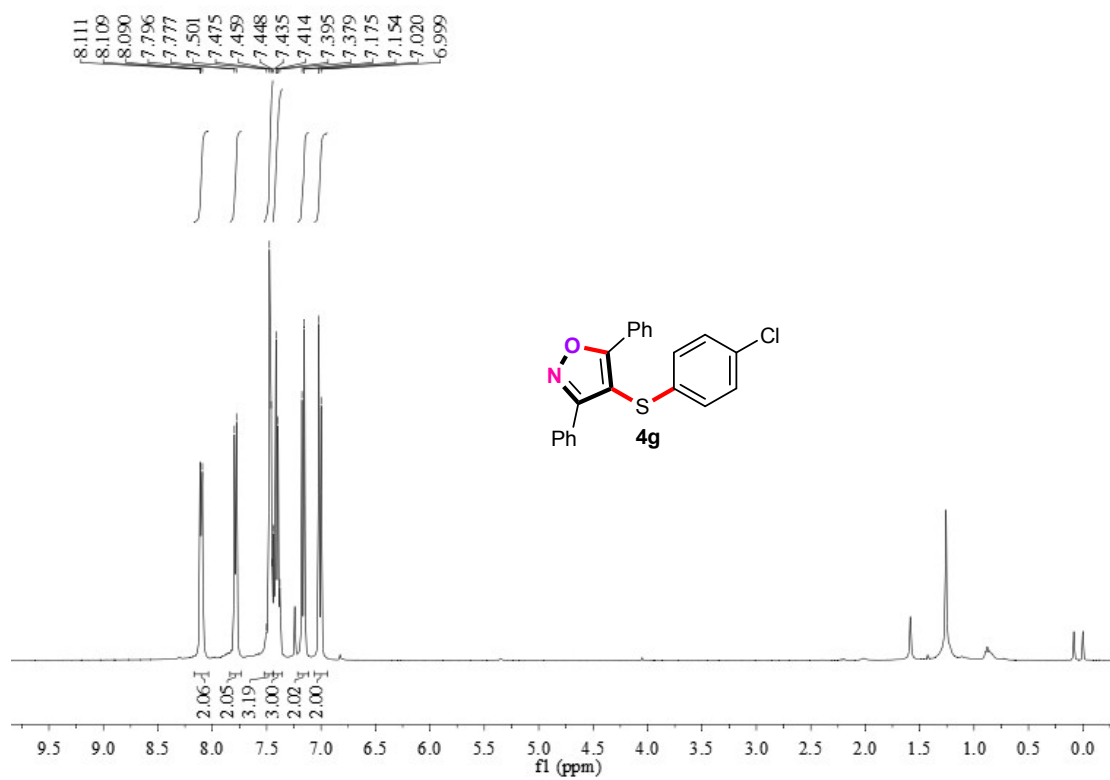


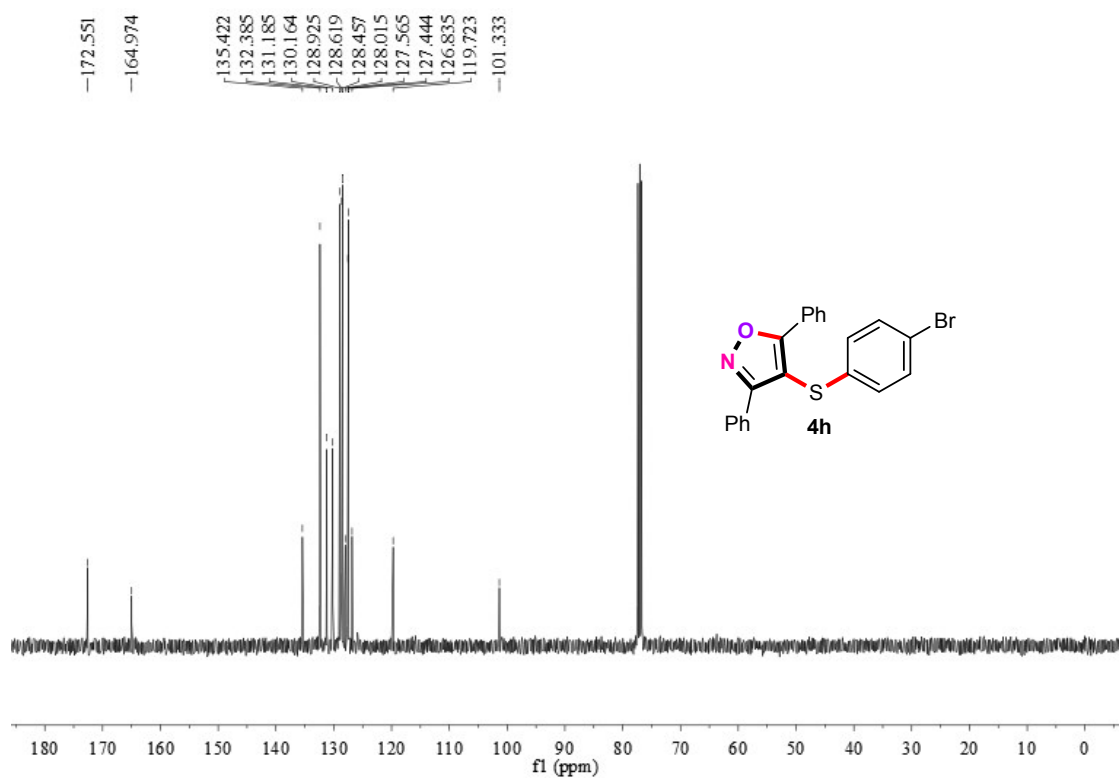
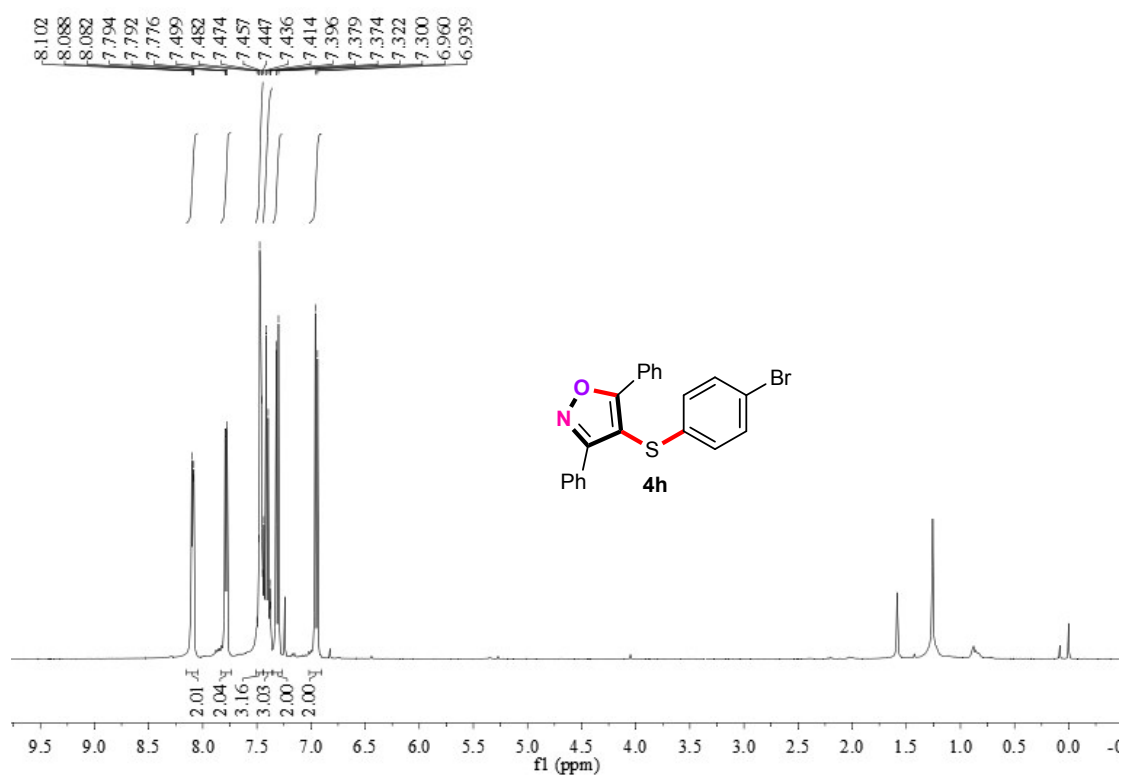


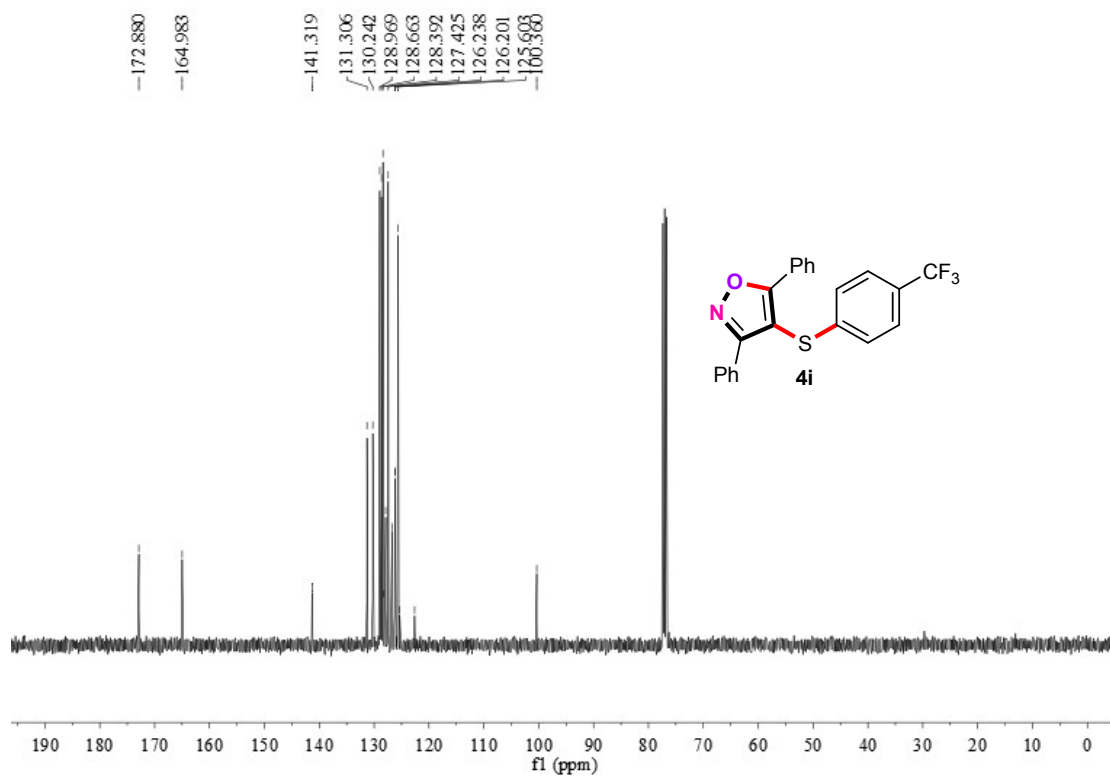
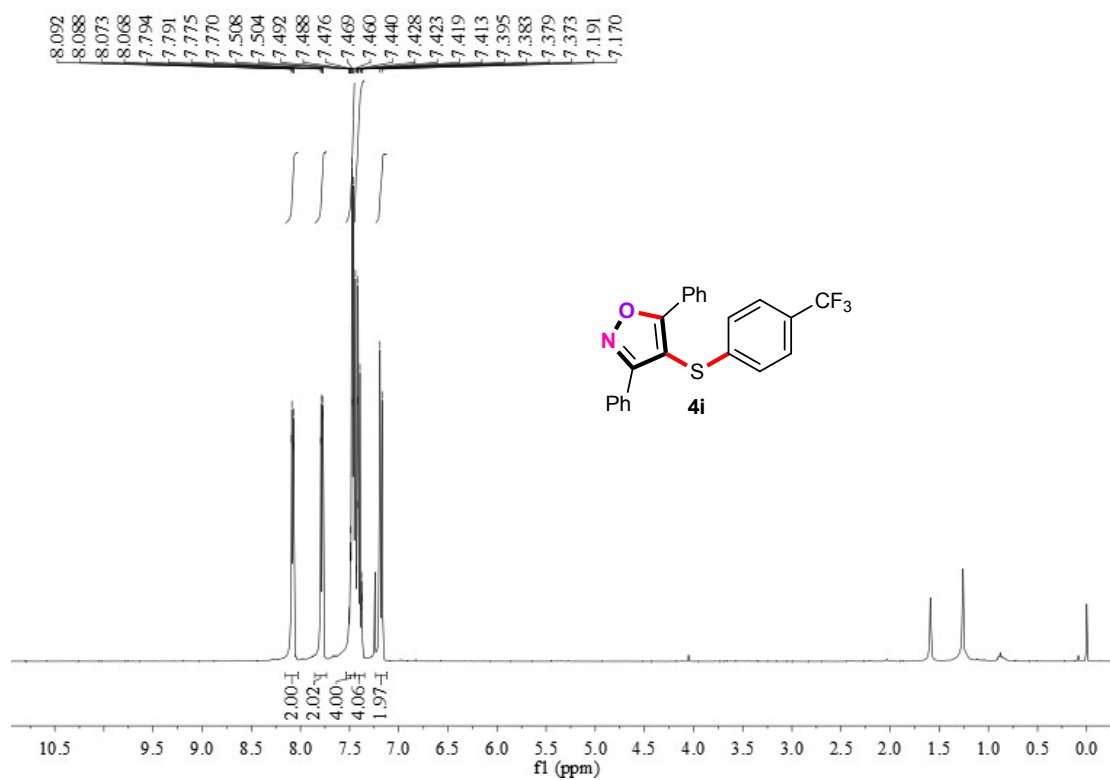


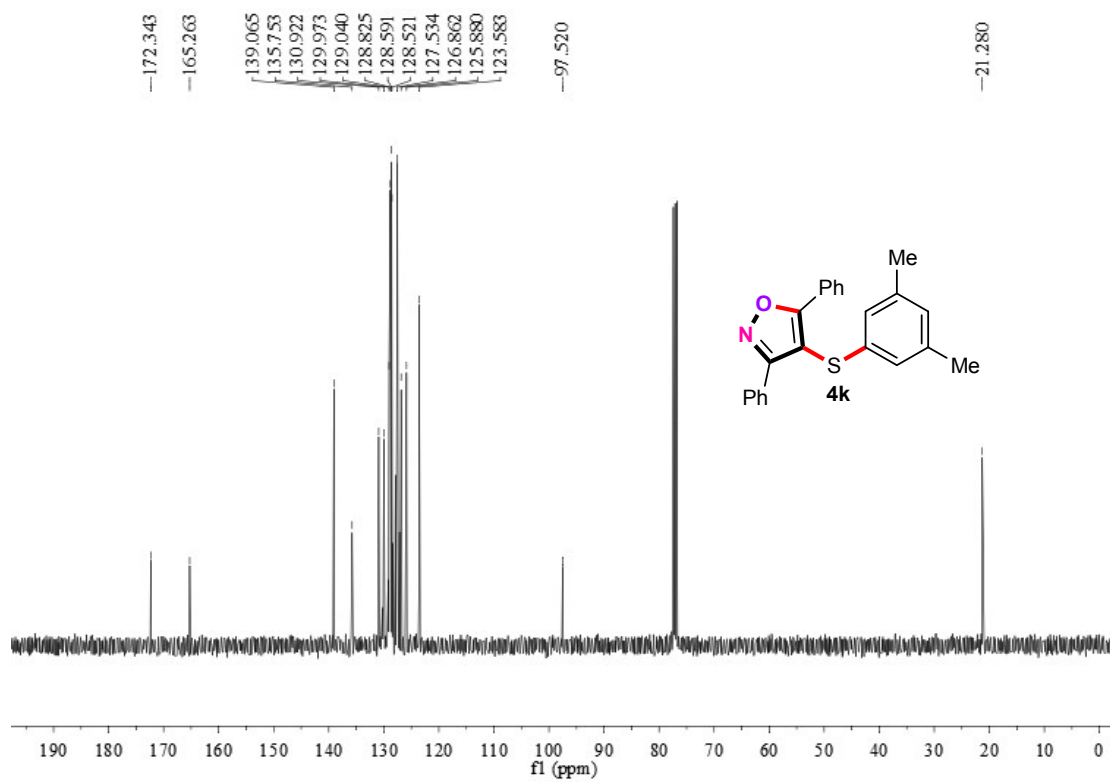
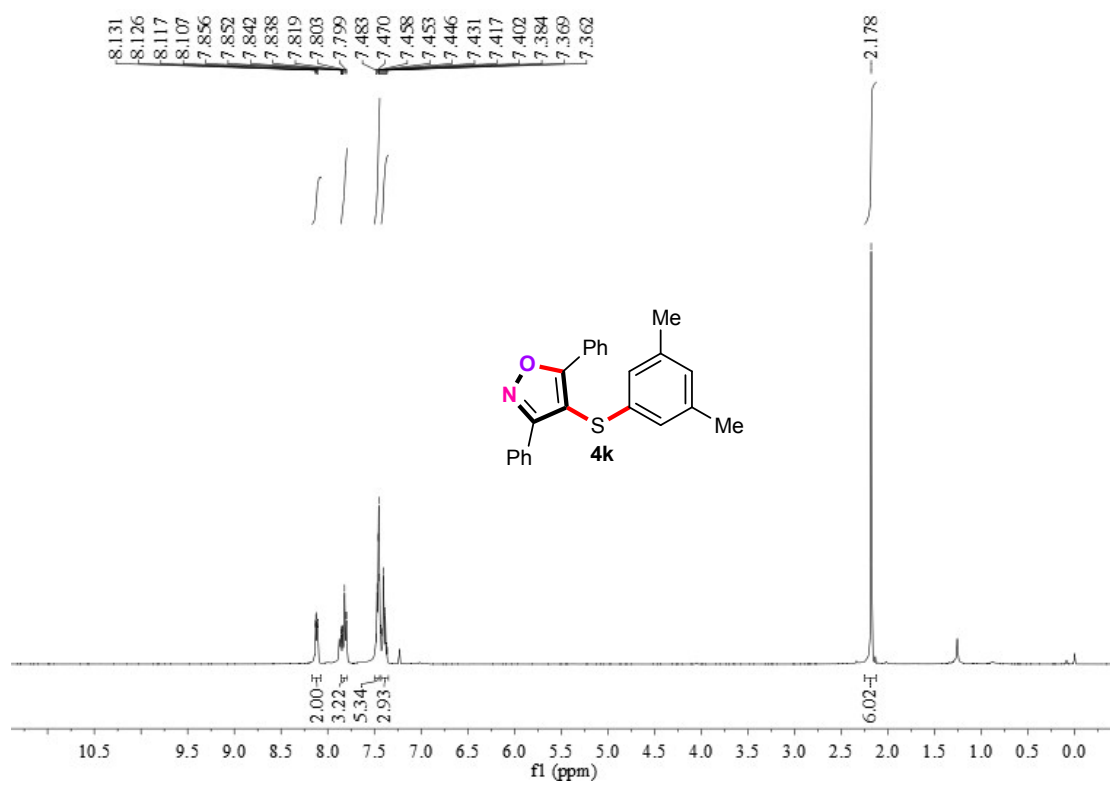


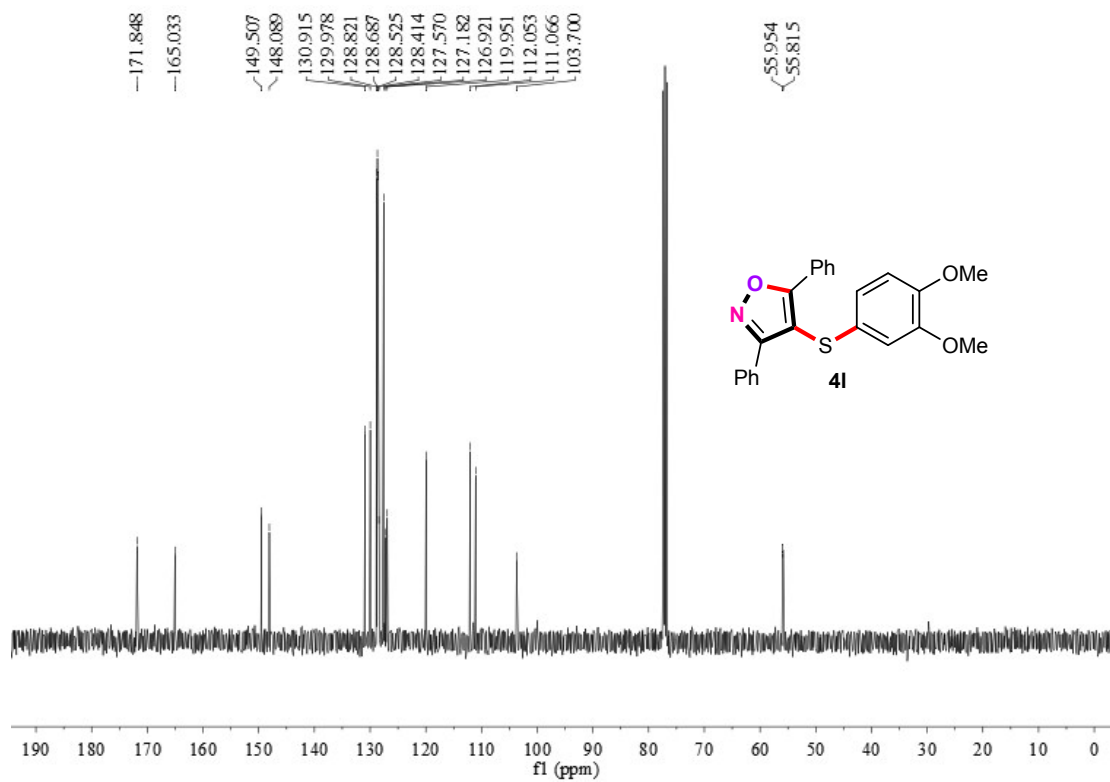
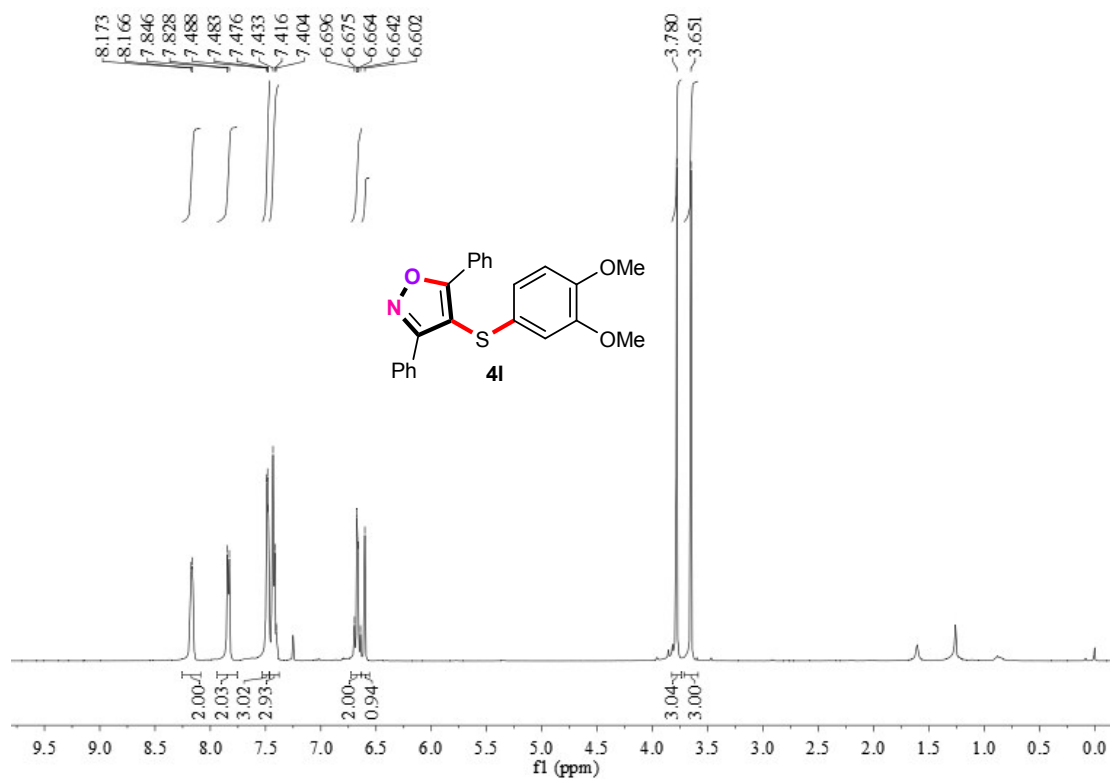


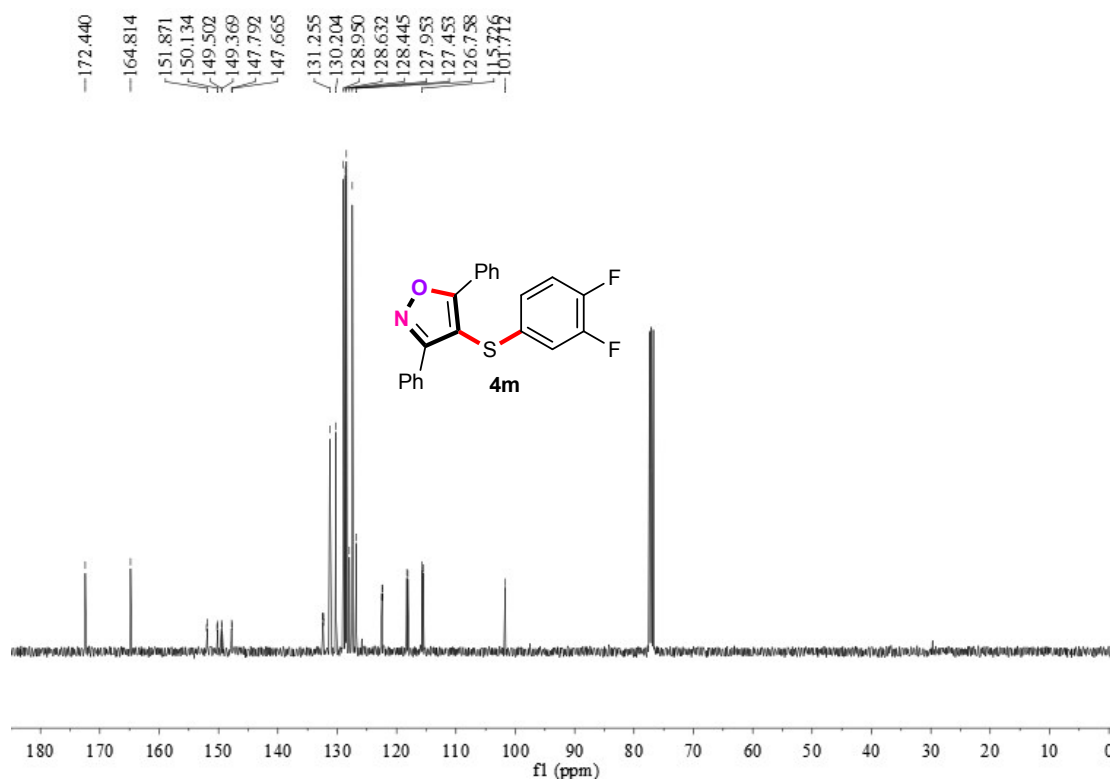
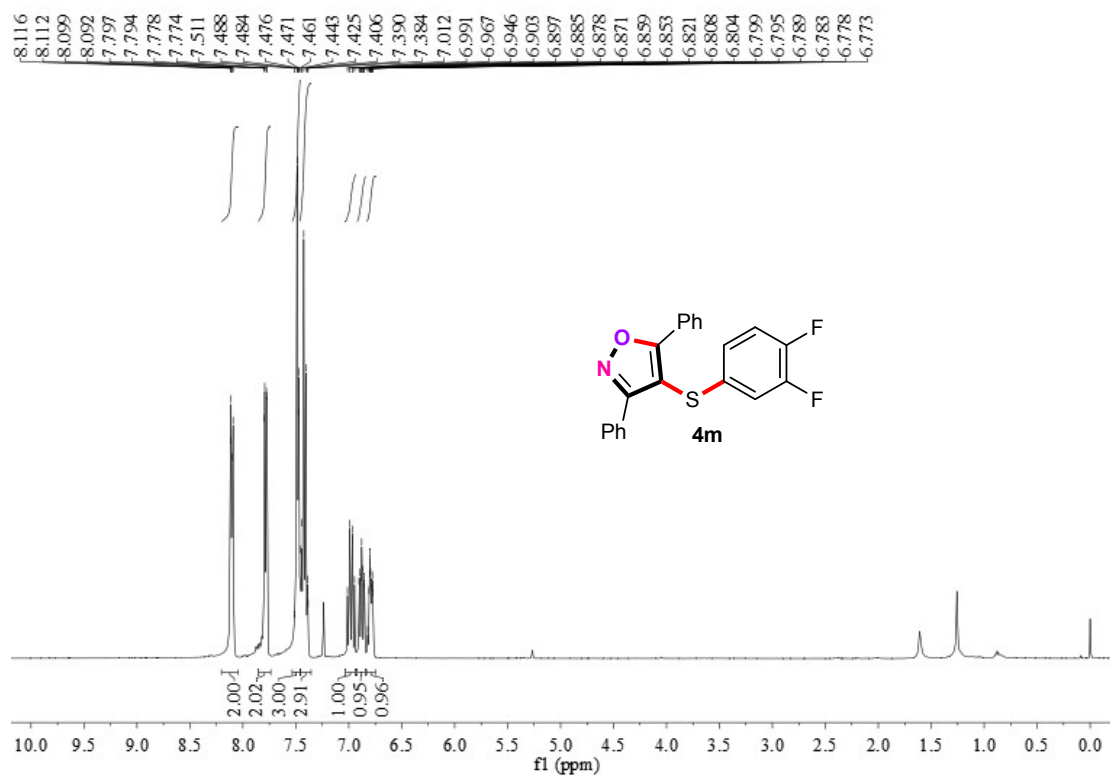


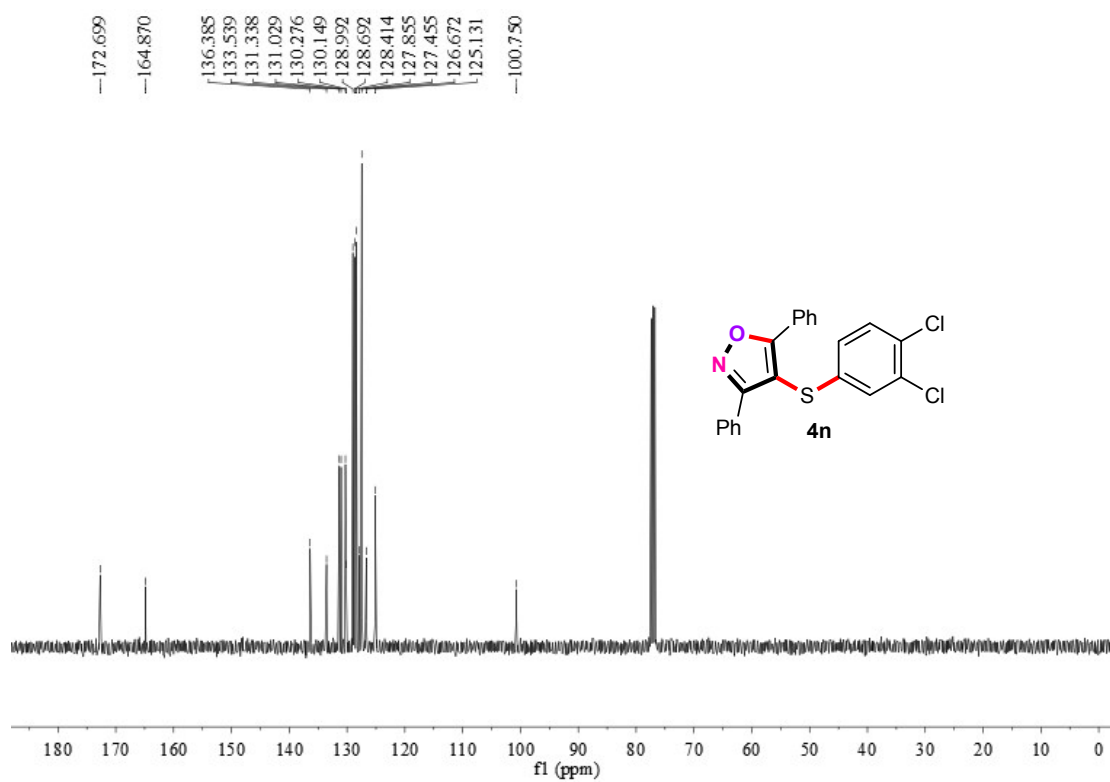
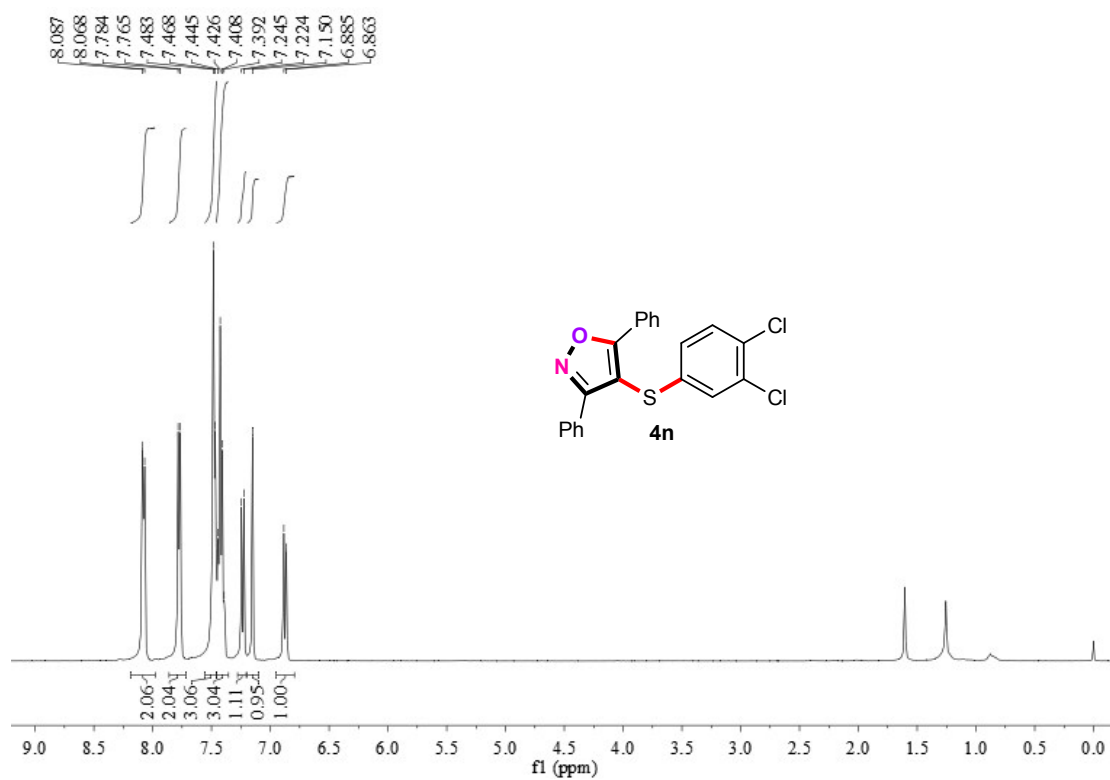


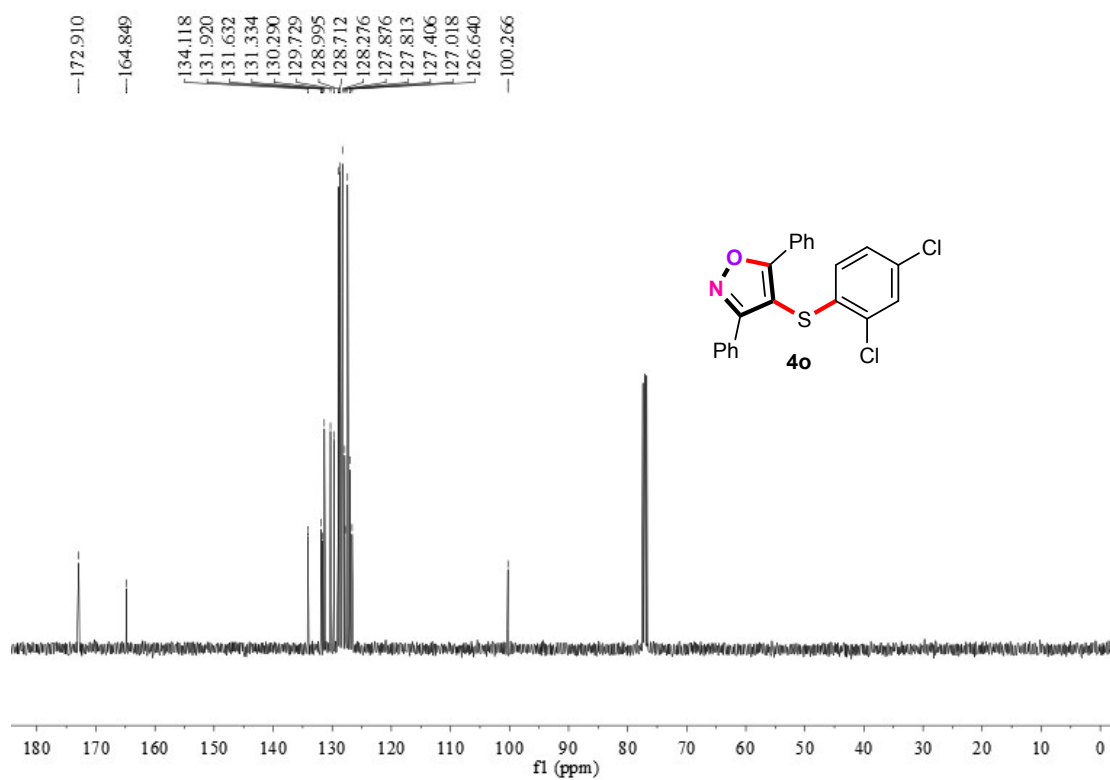
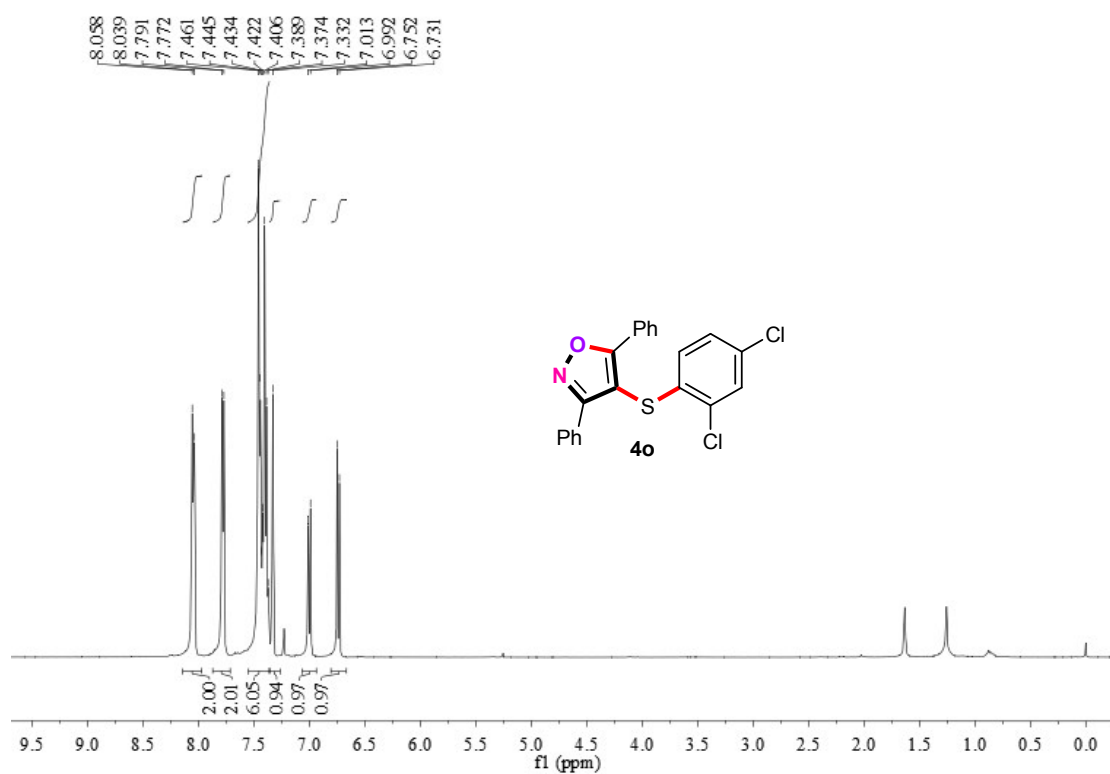


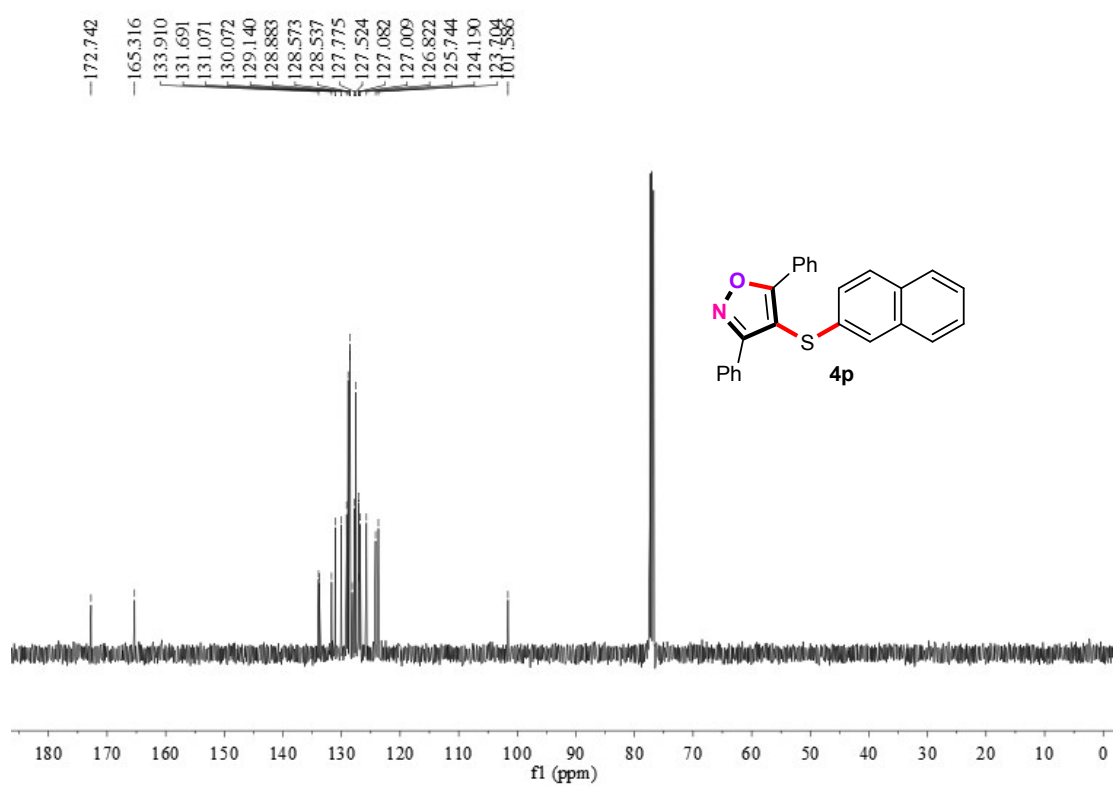
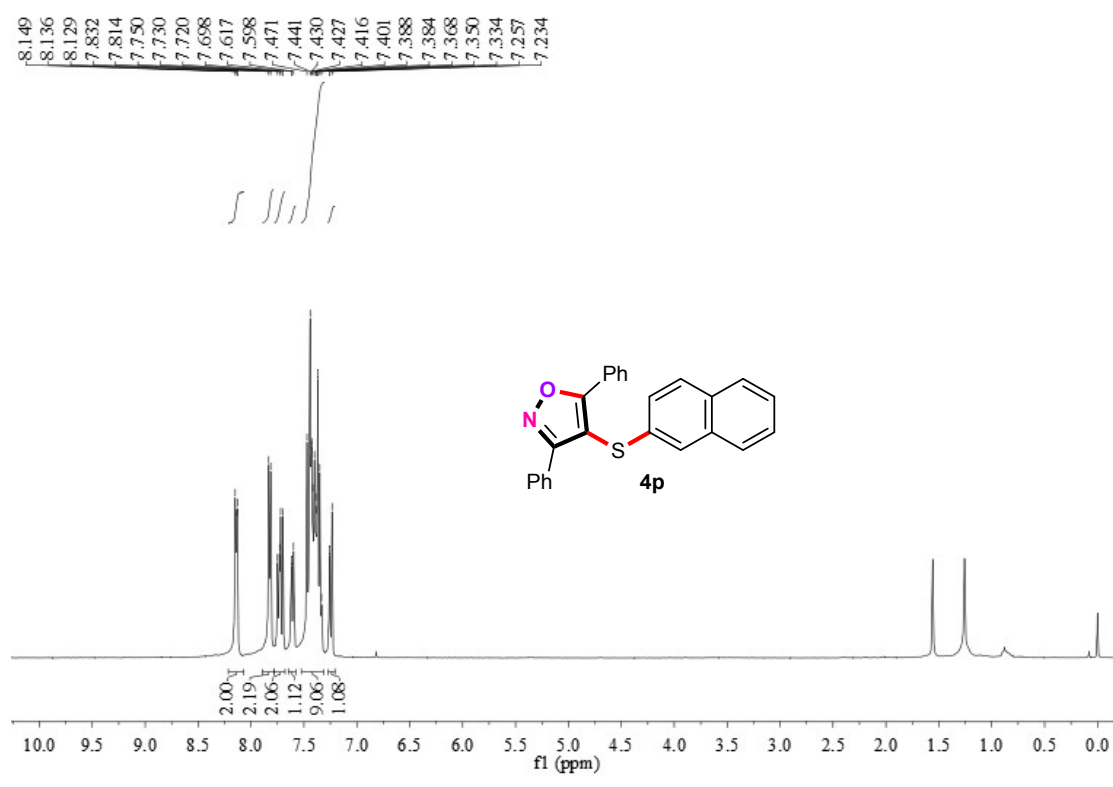


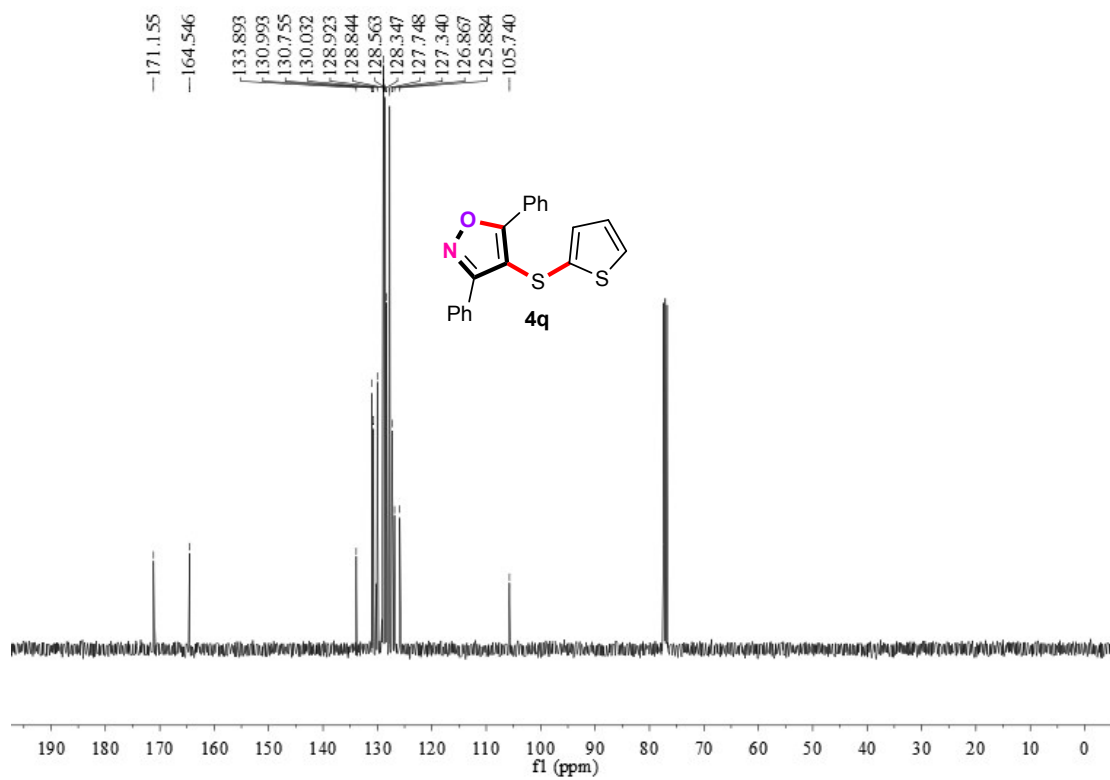
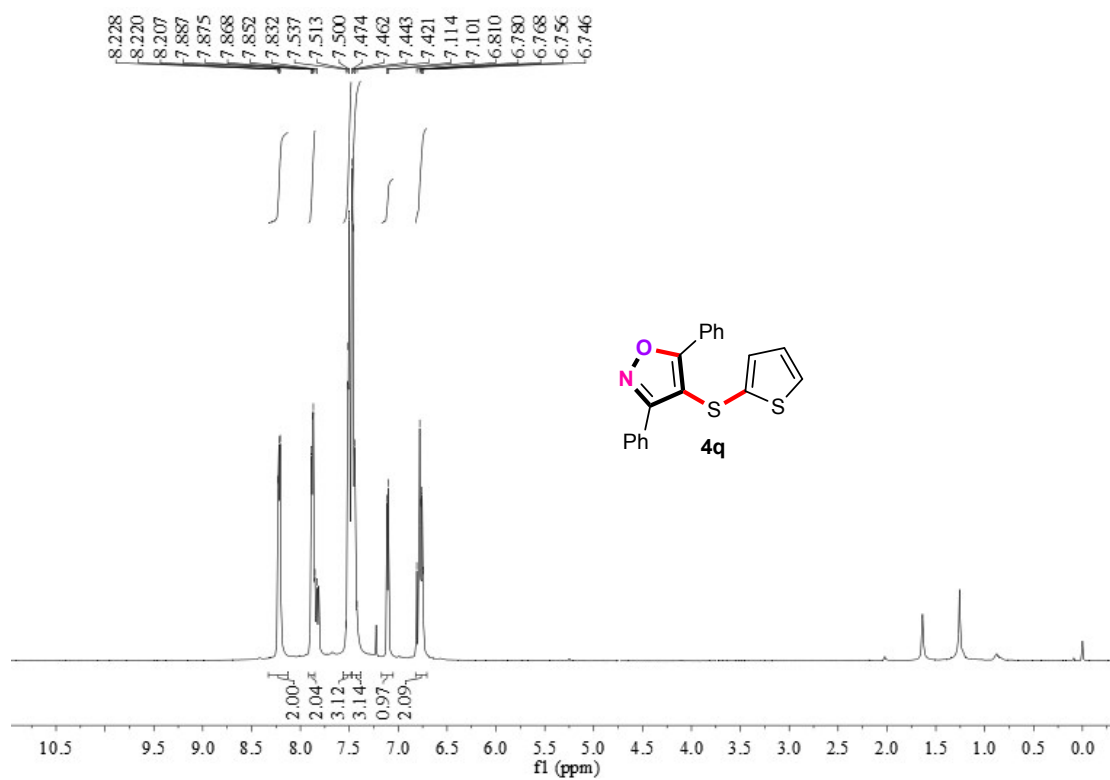




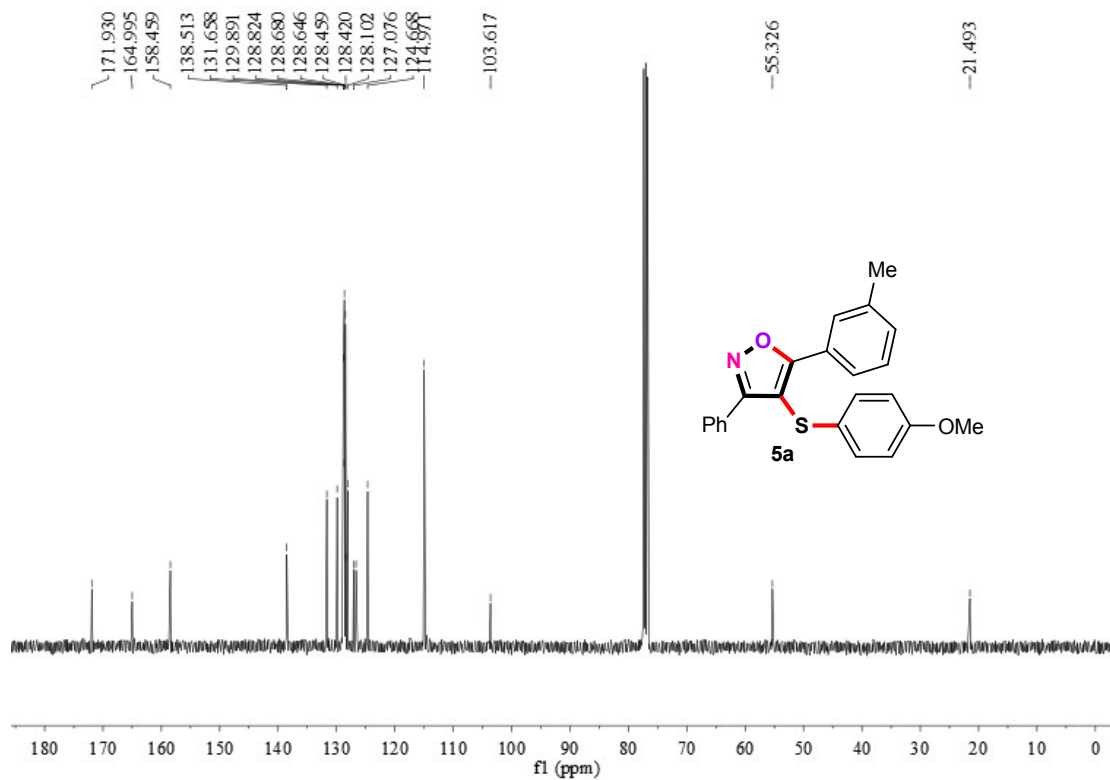
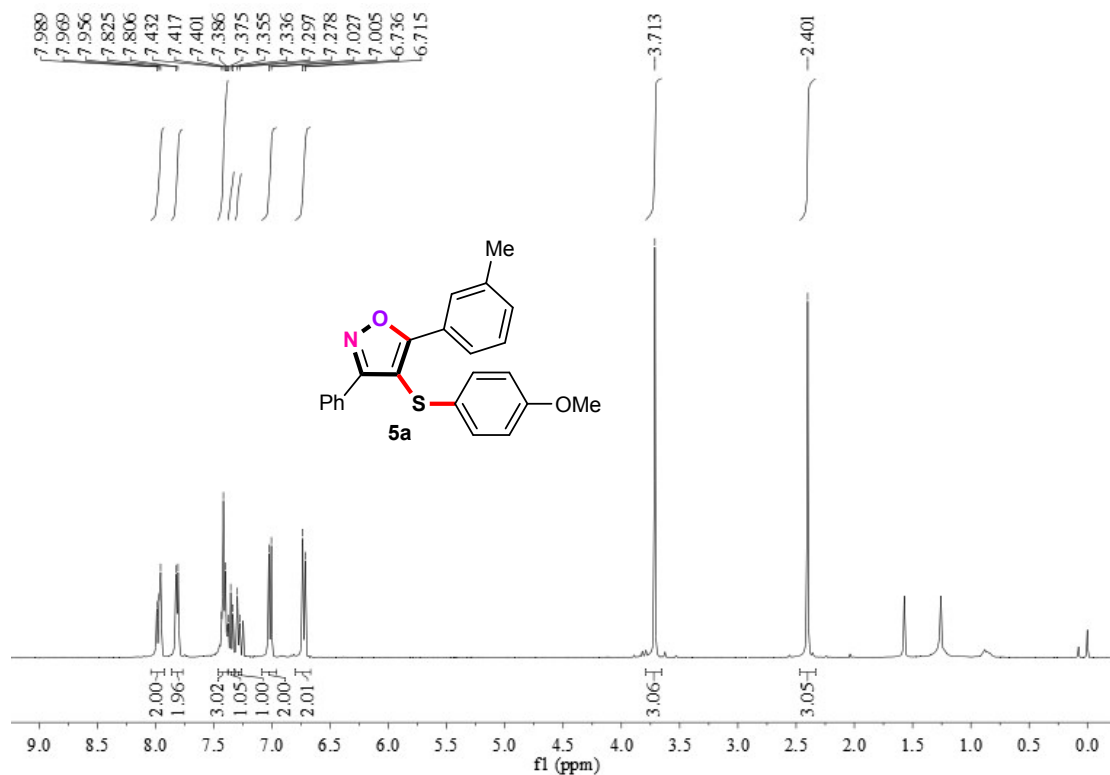


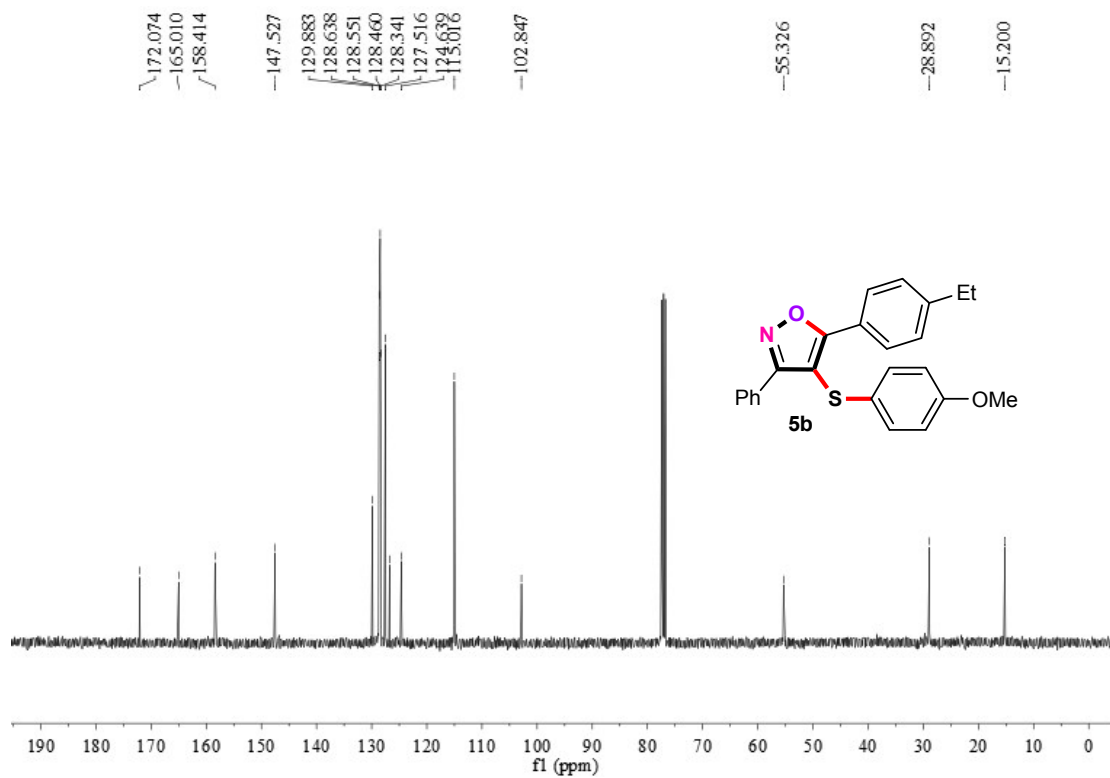
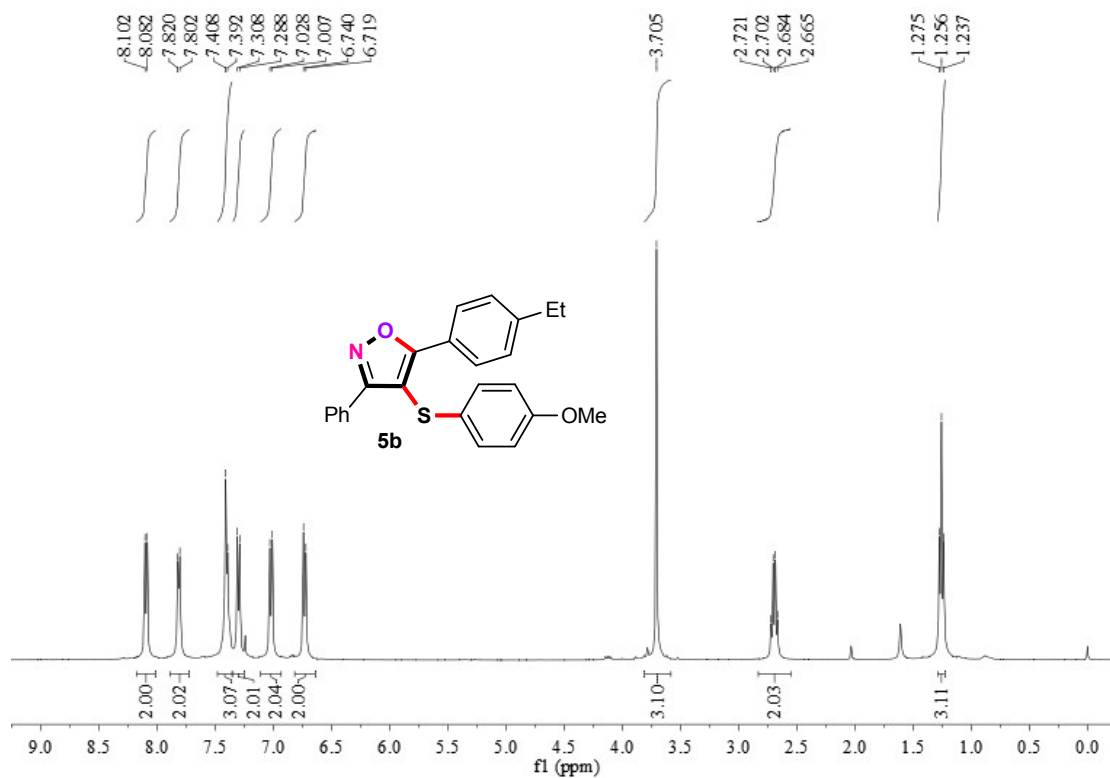


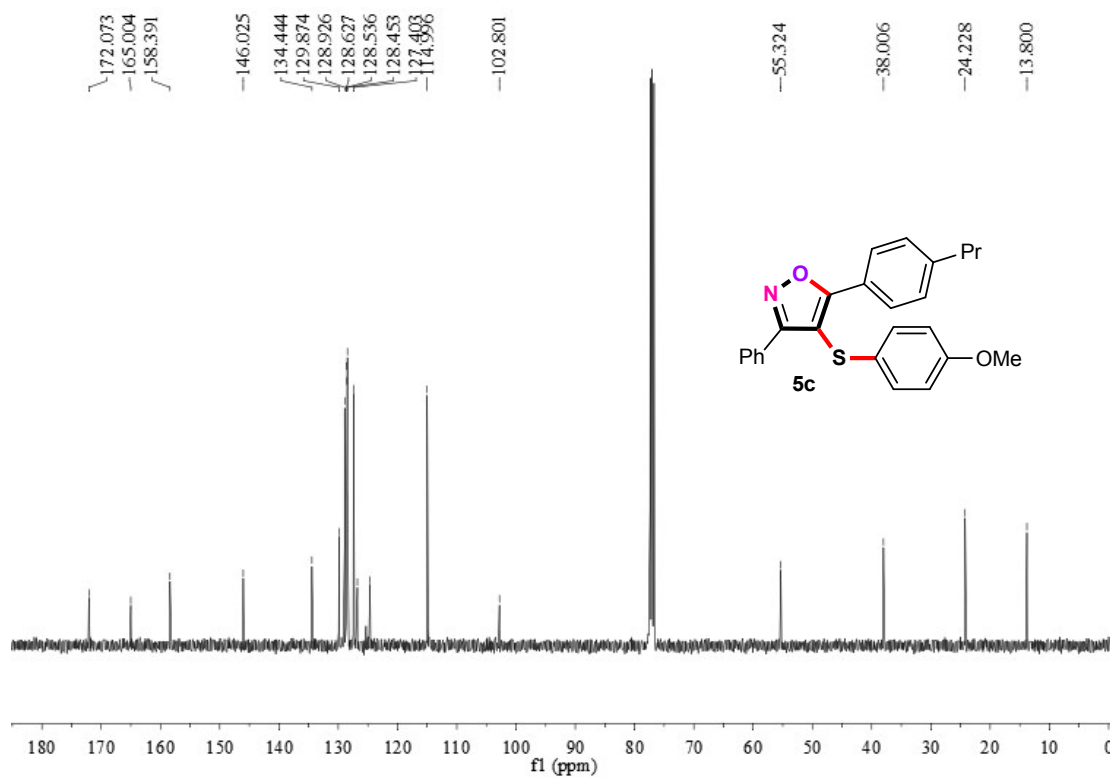
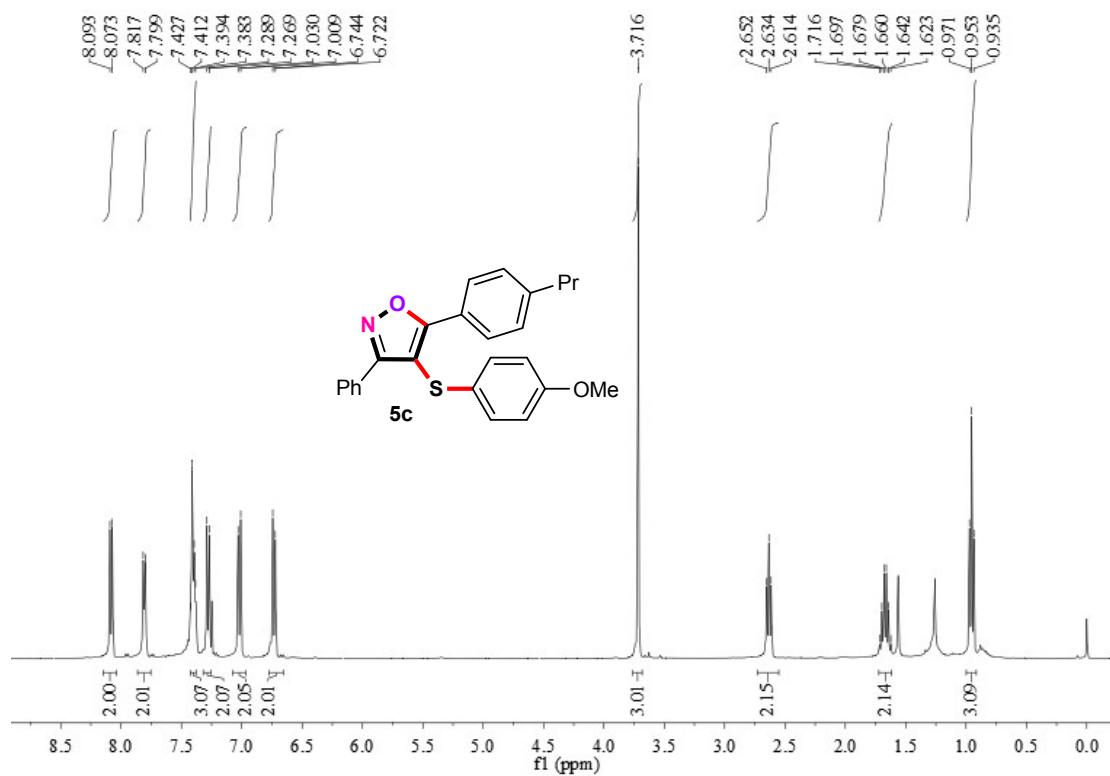


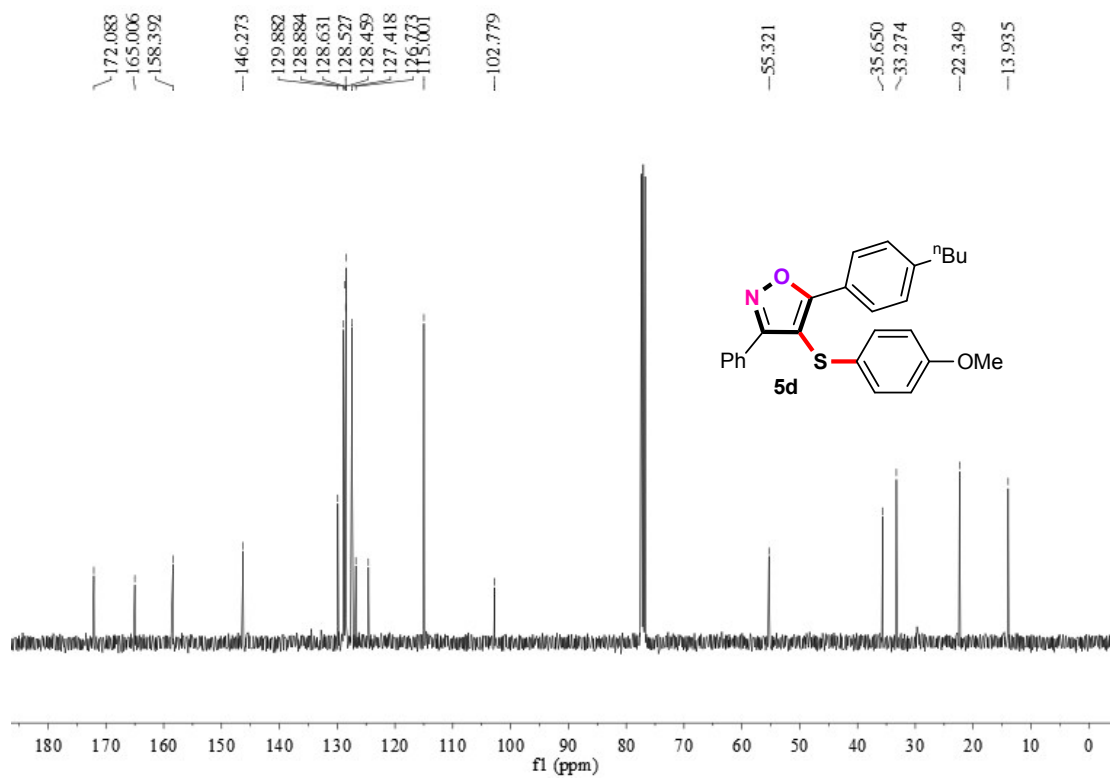
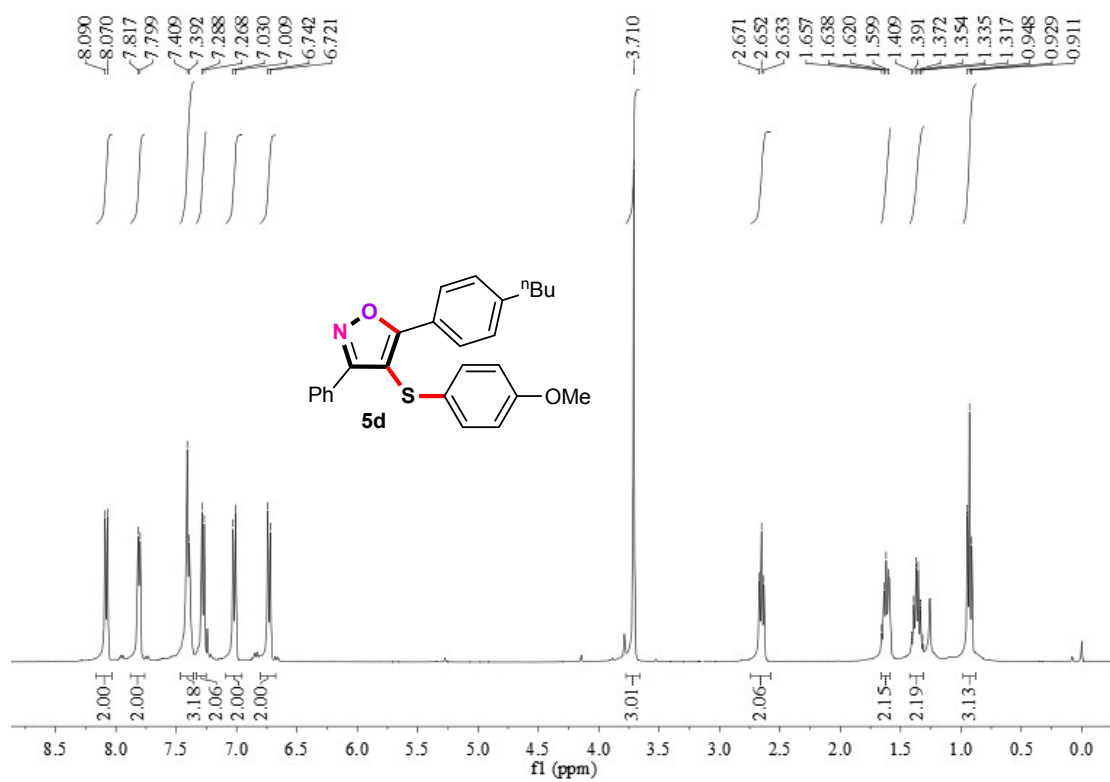


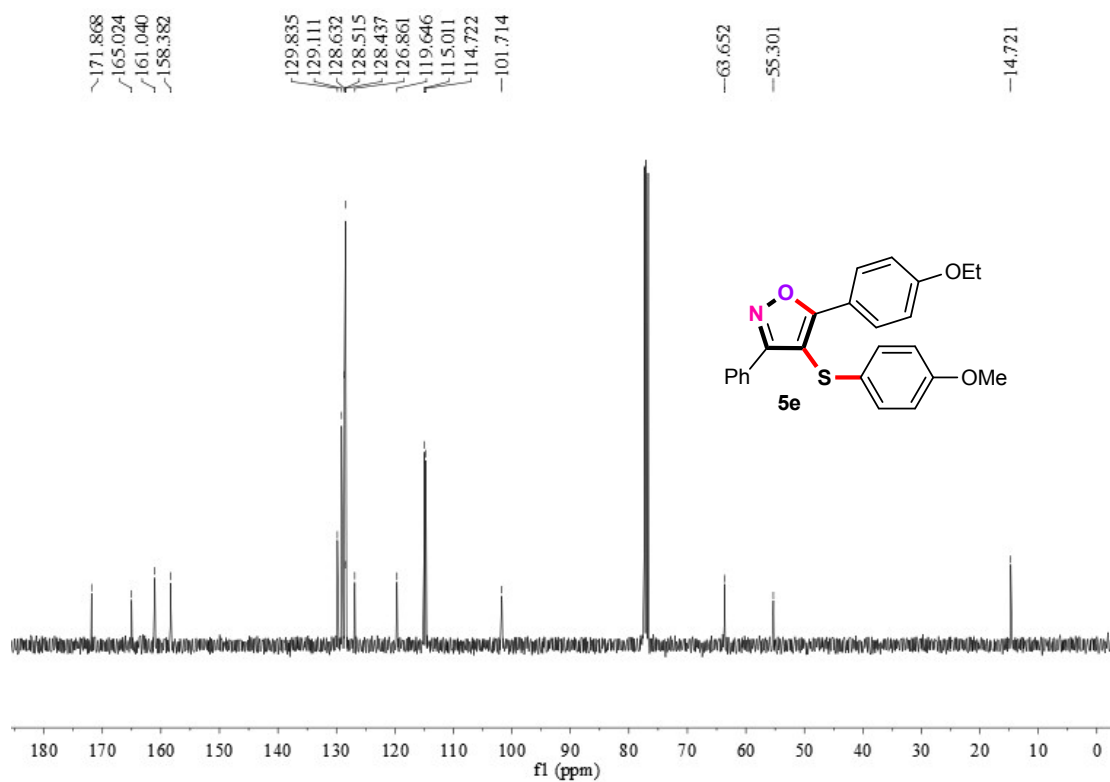
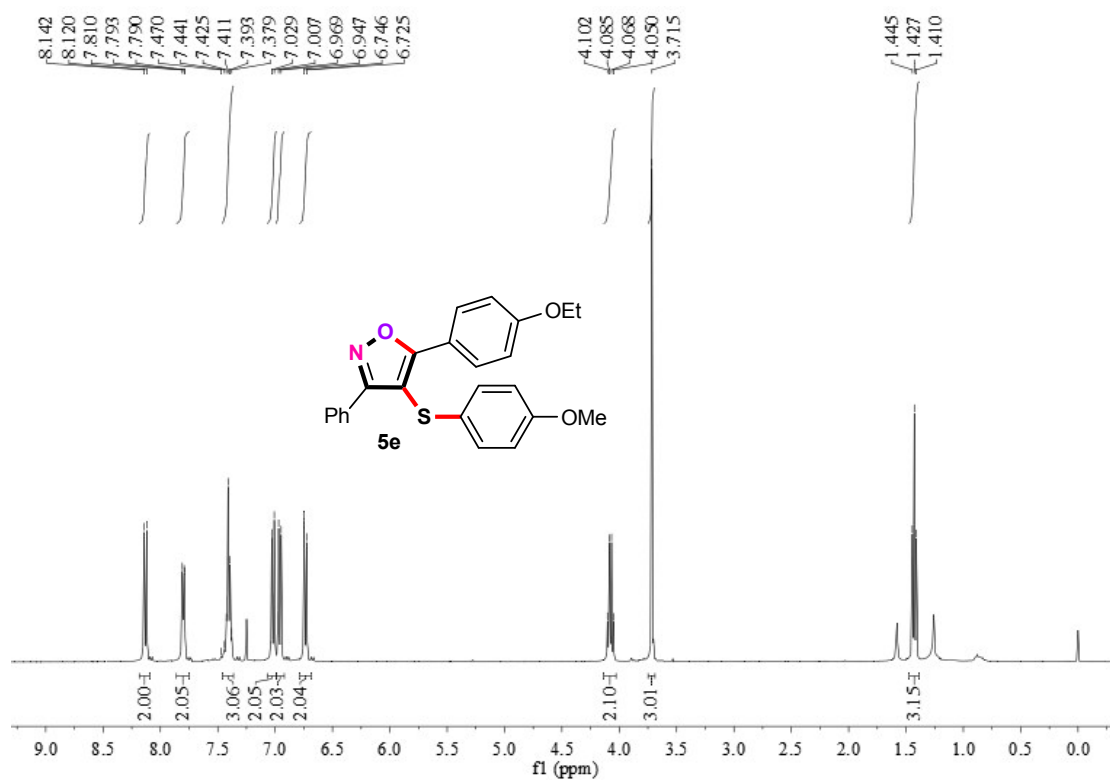
^1H and ^{13}C NMR spectra of compounds 5

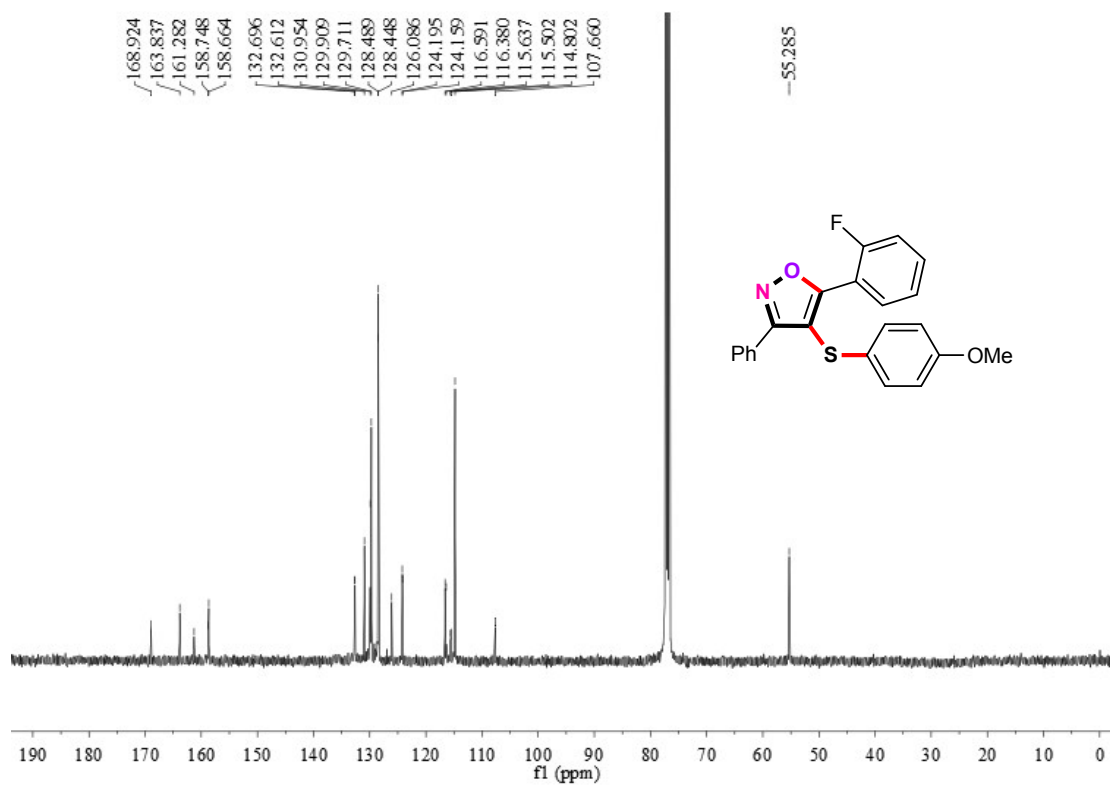
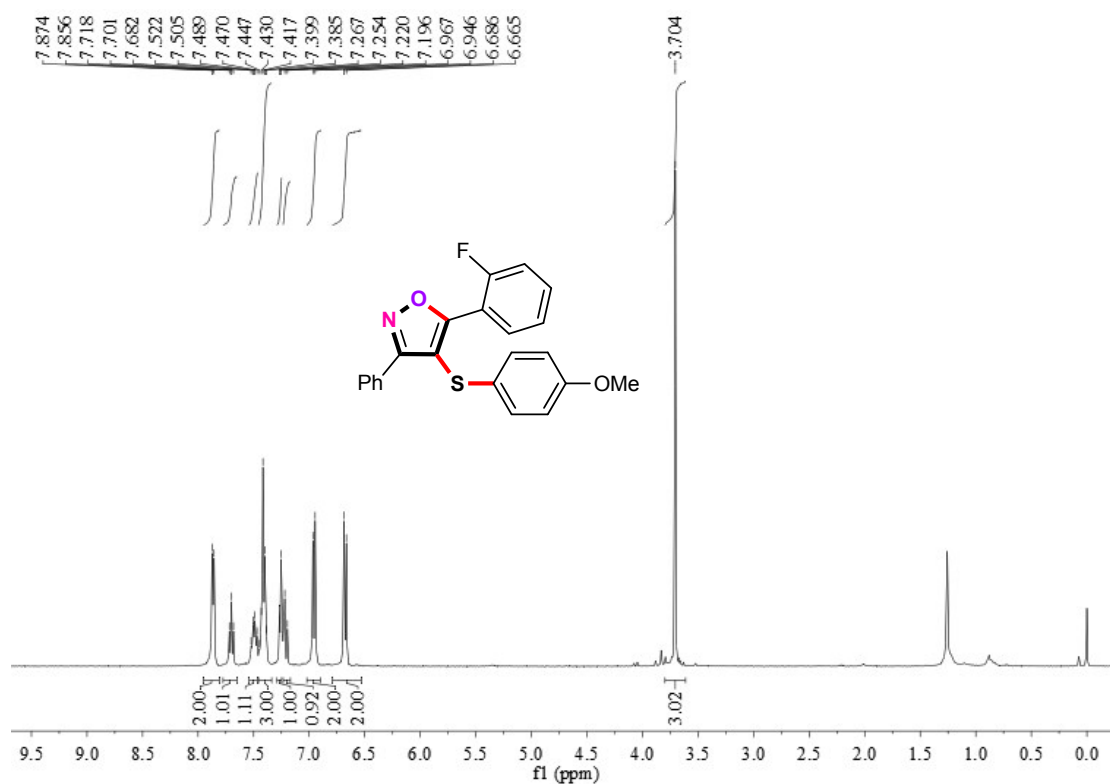


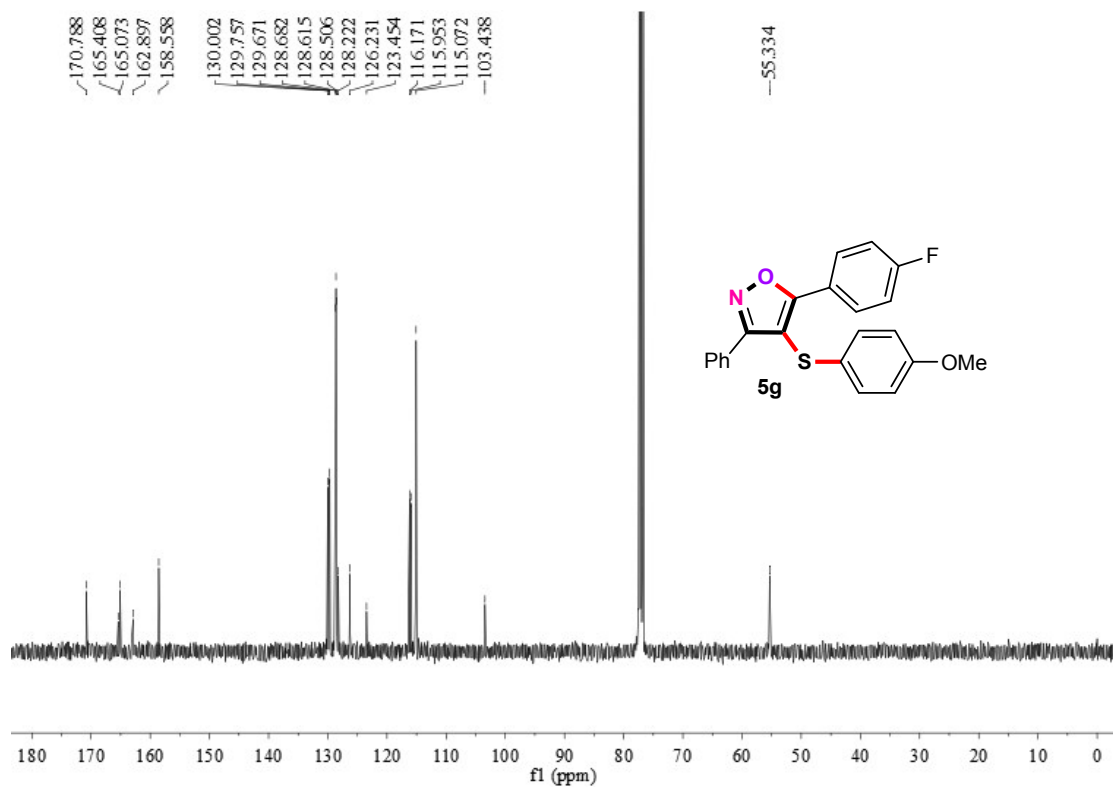
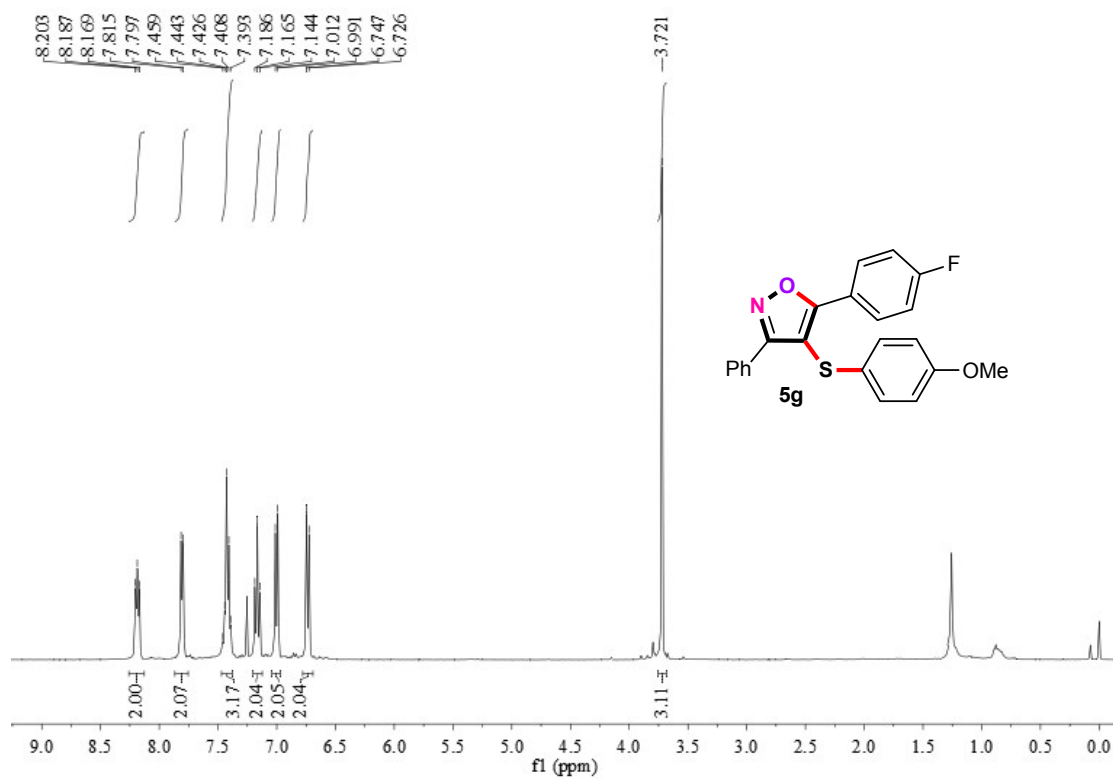


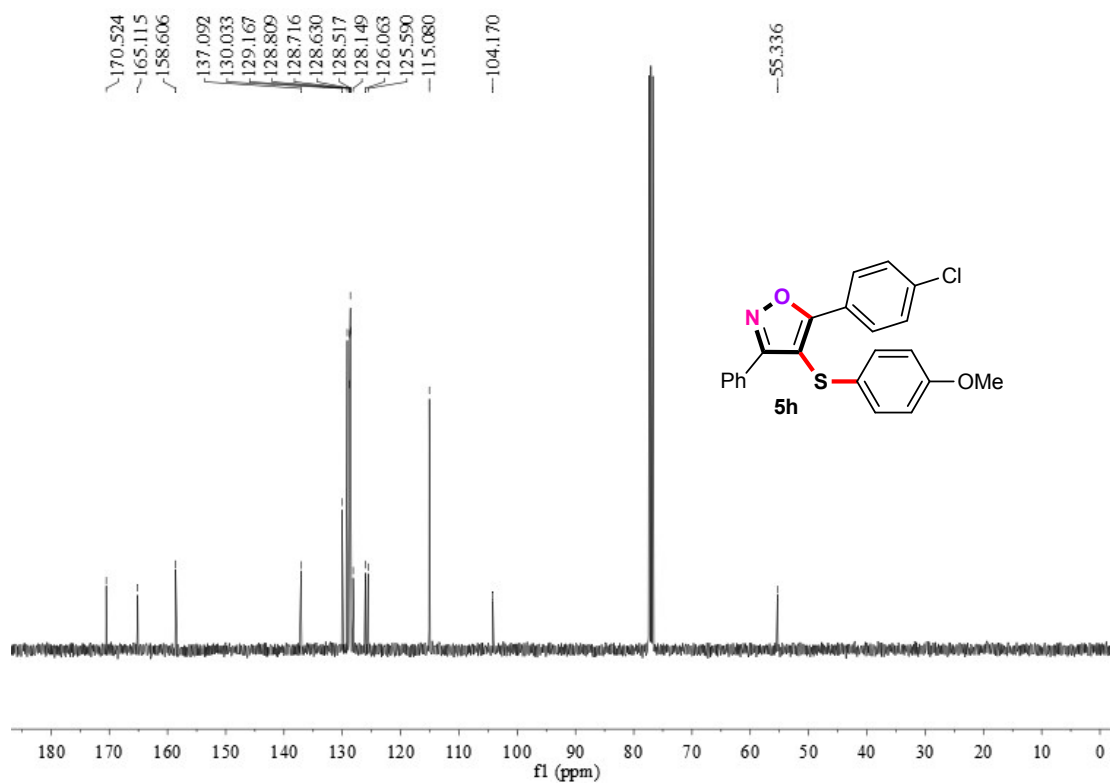
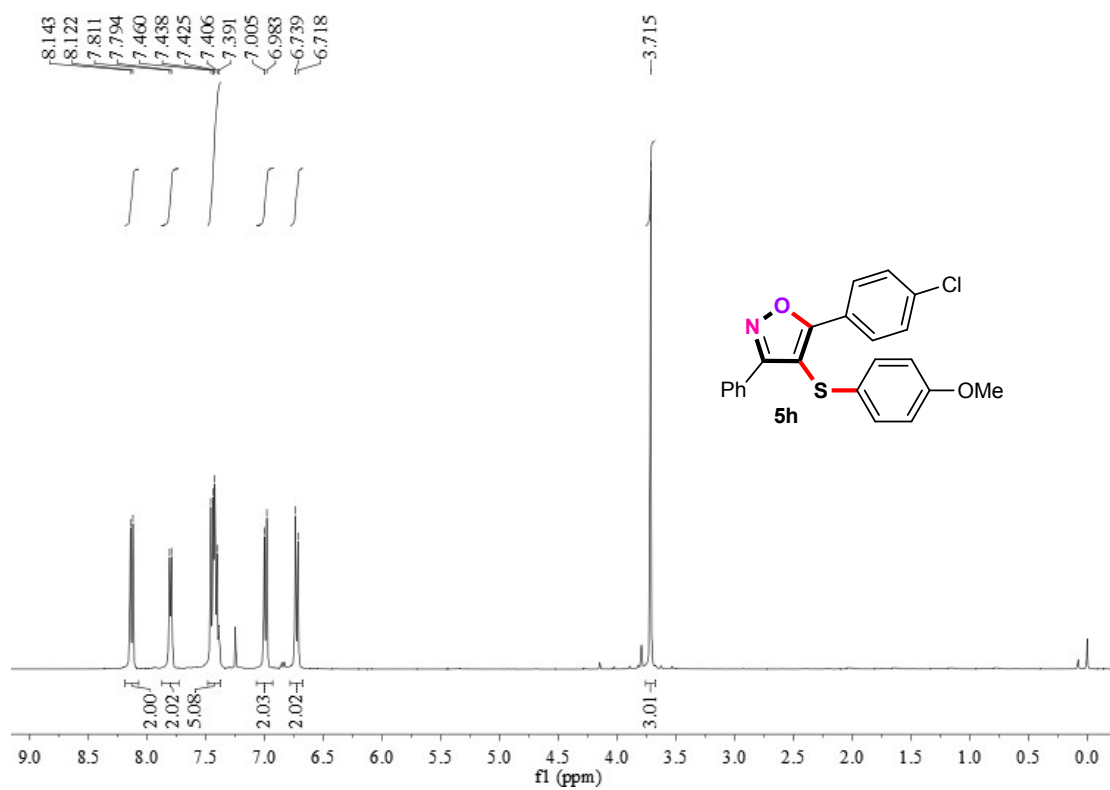


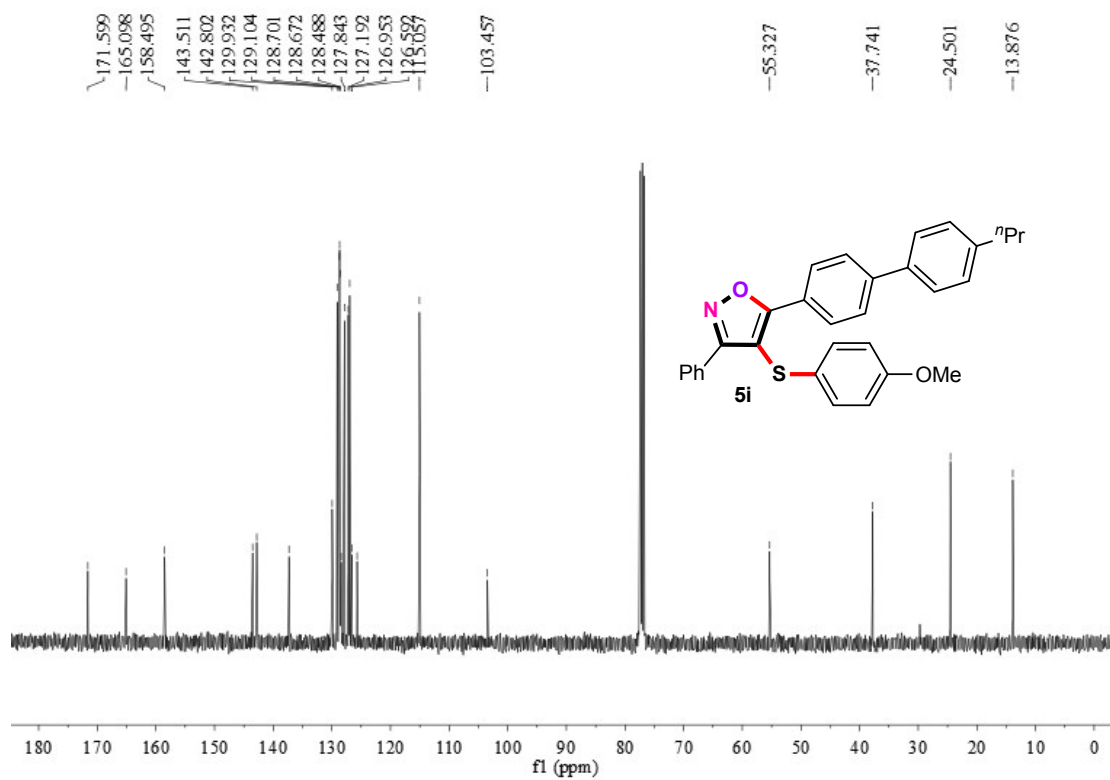
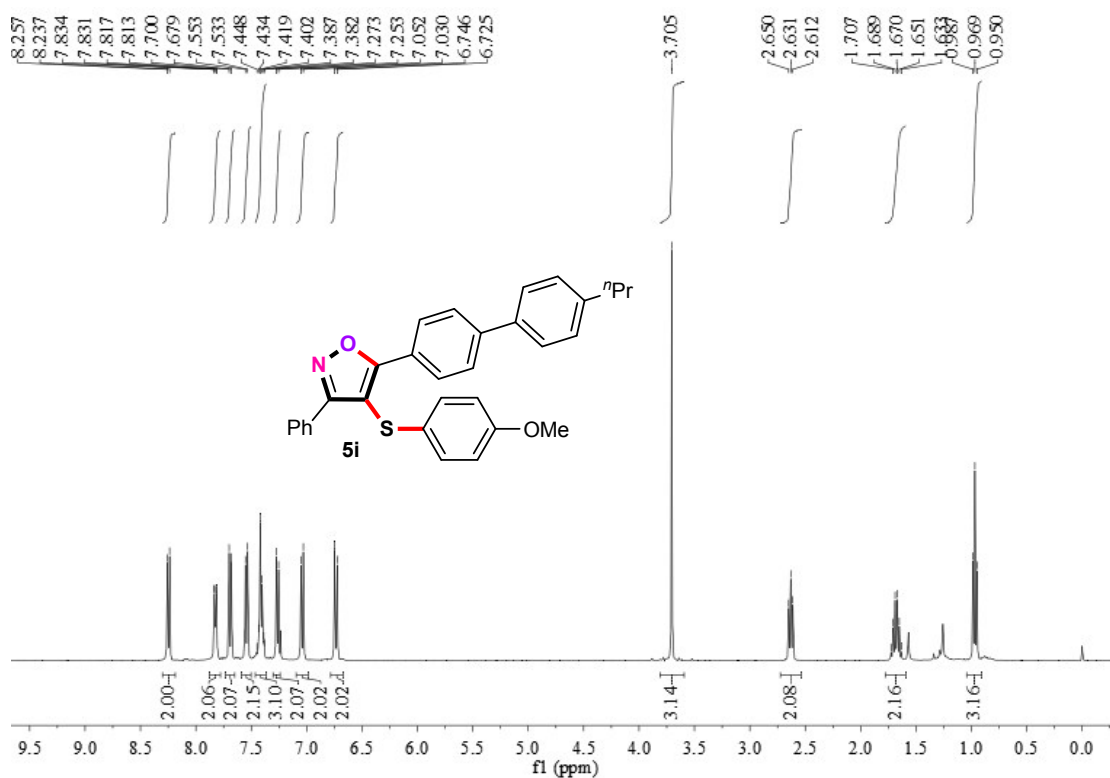


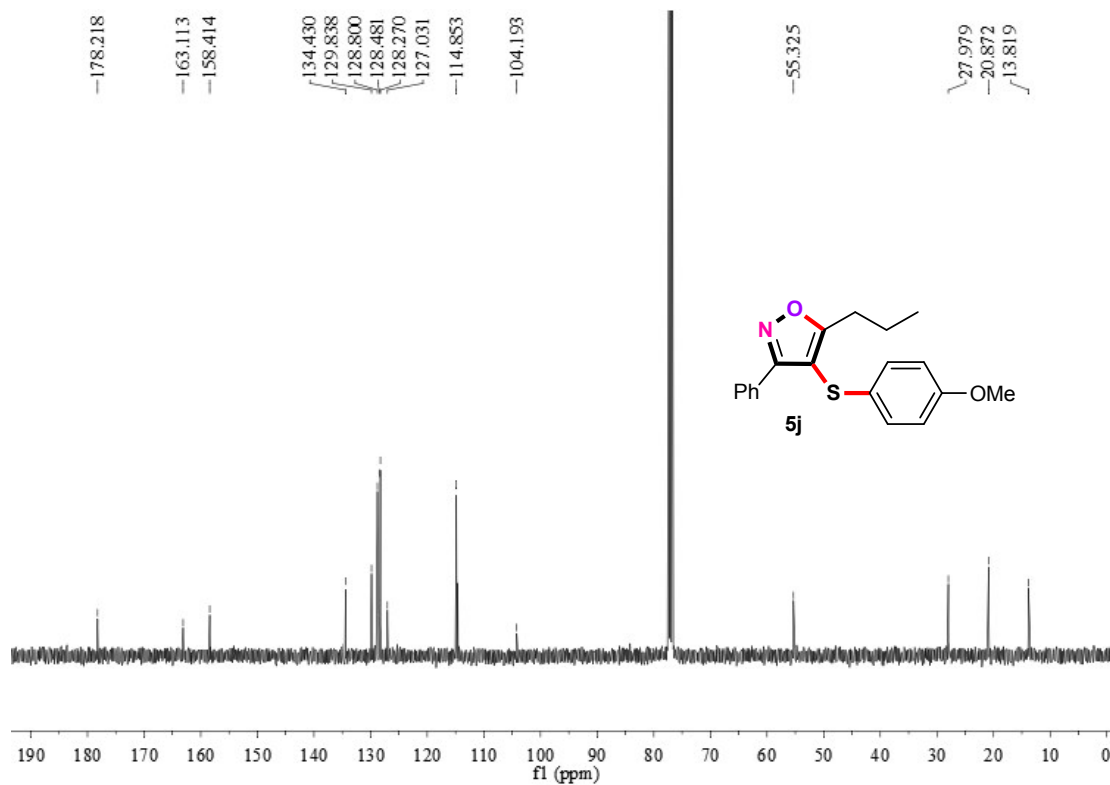
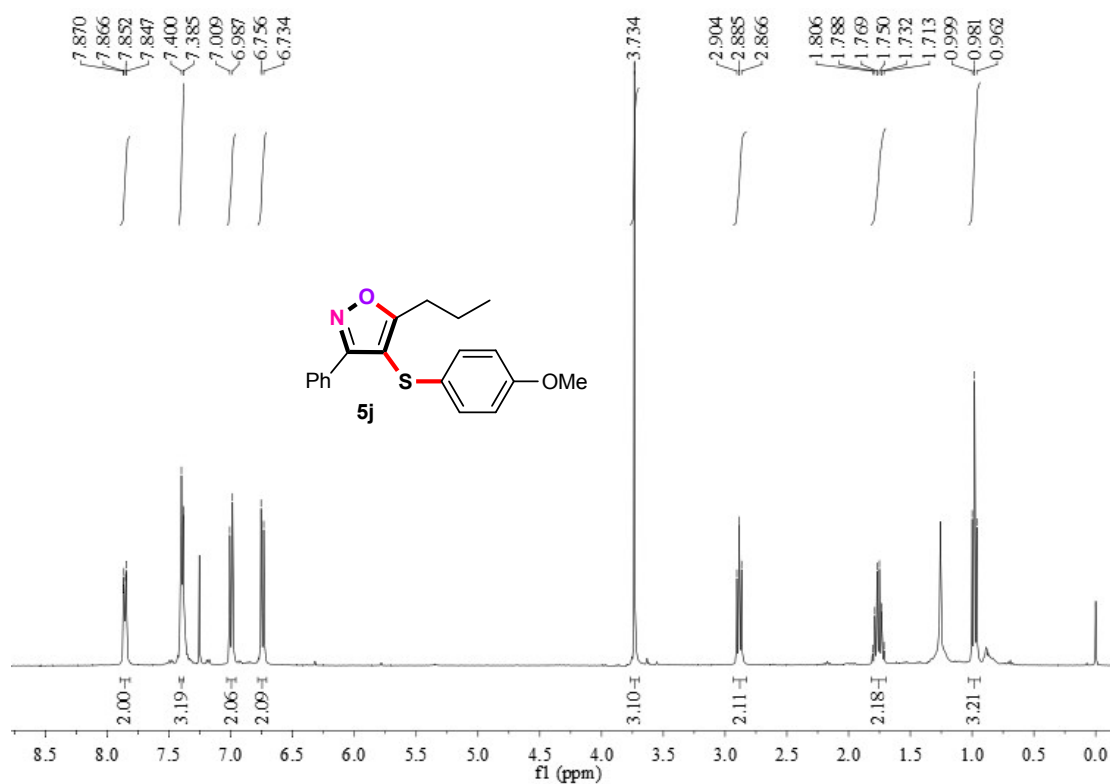


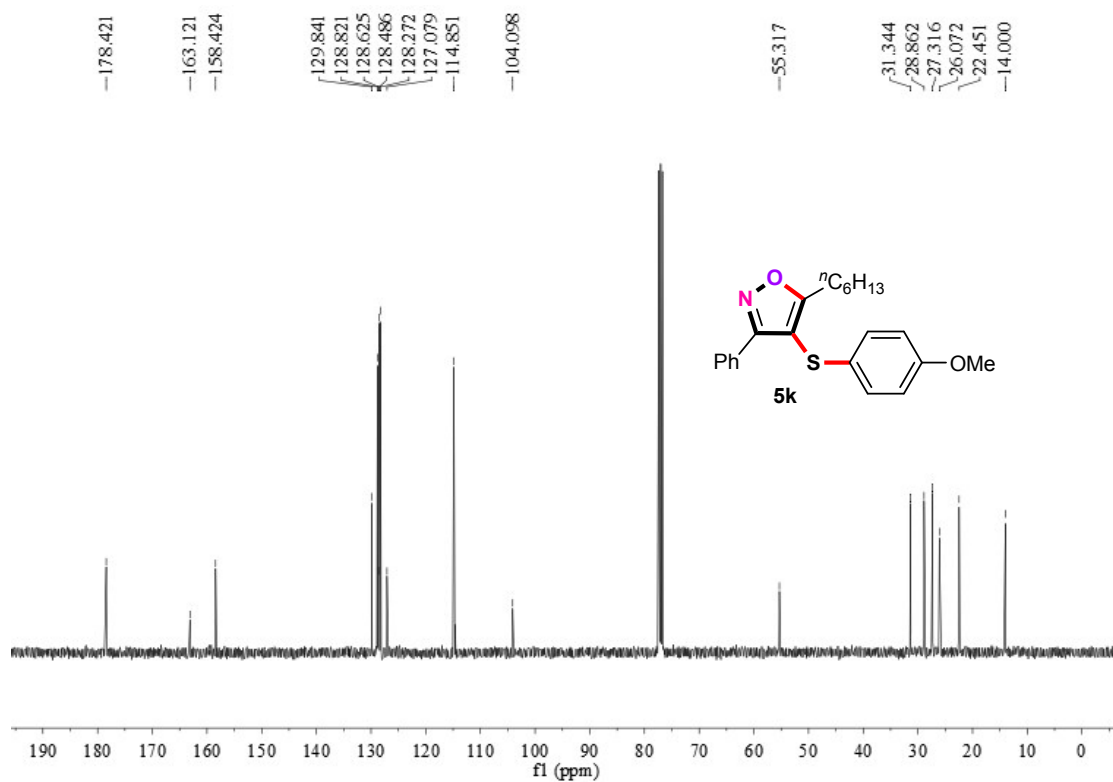
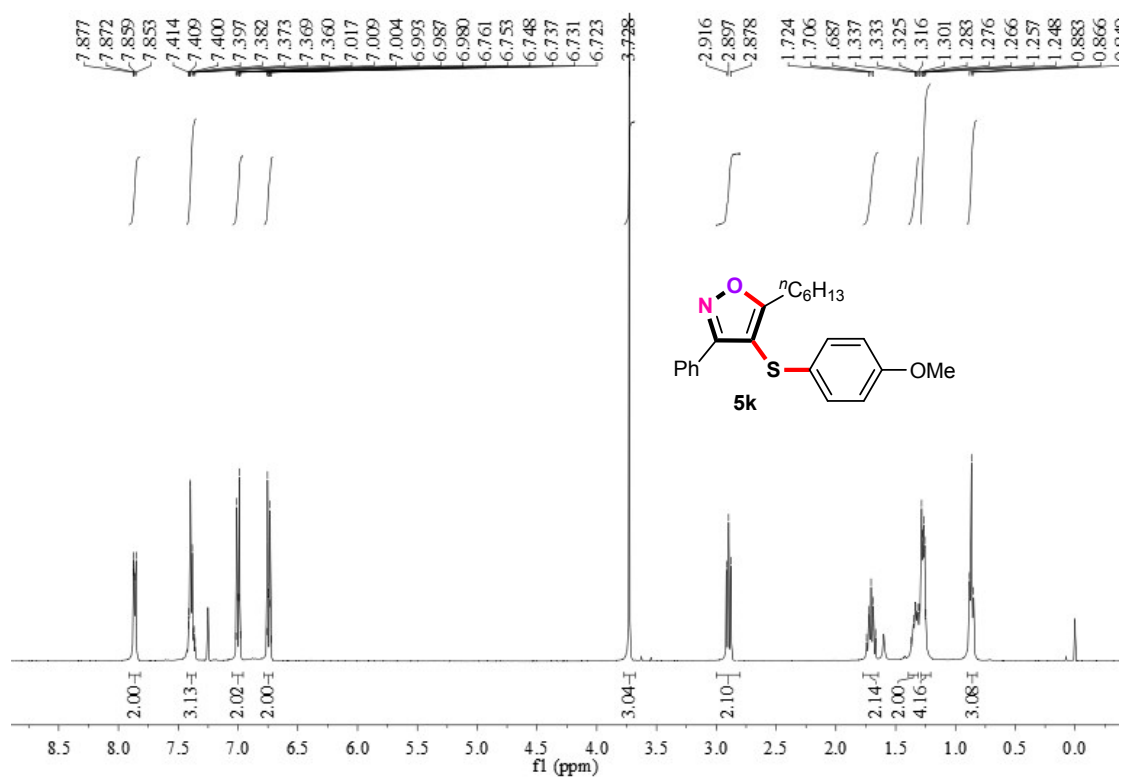


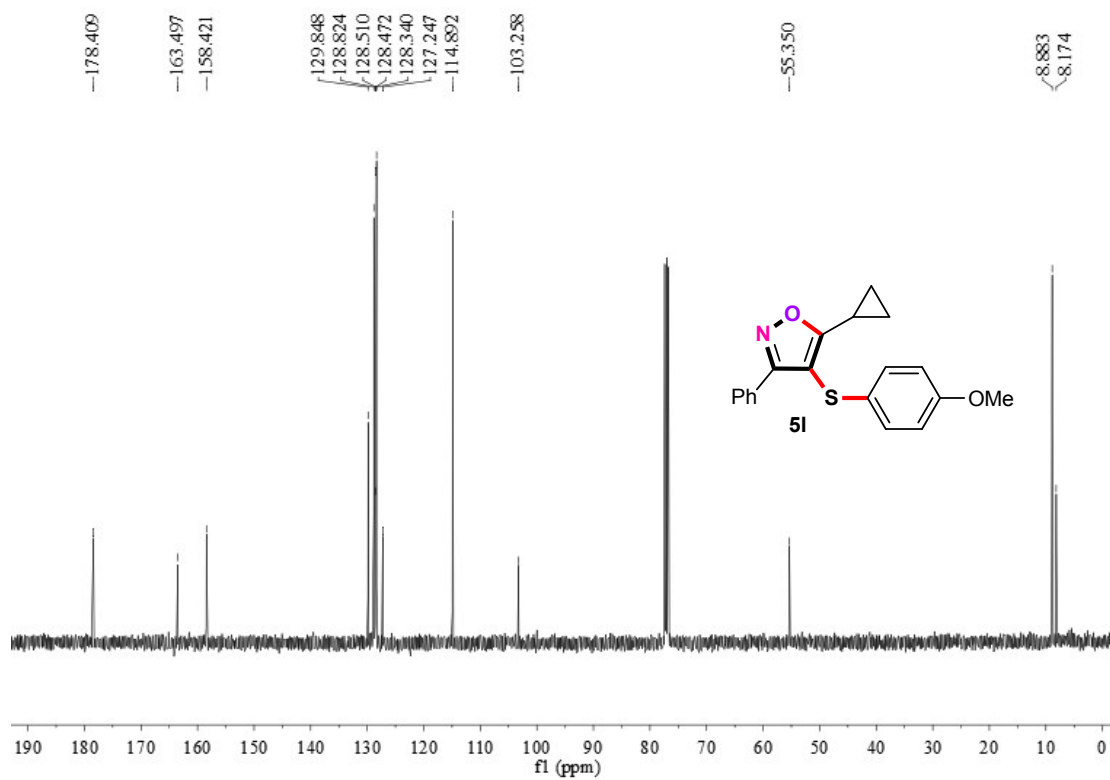
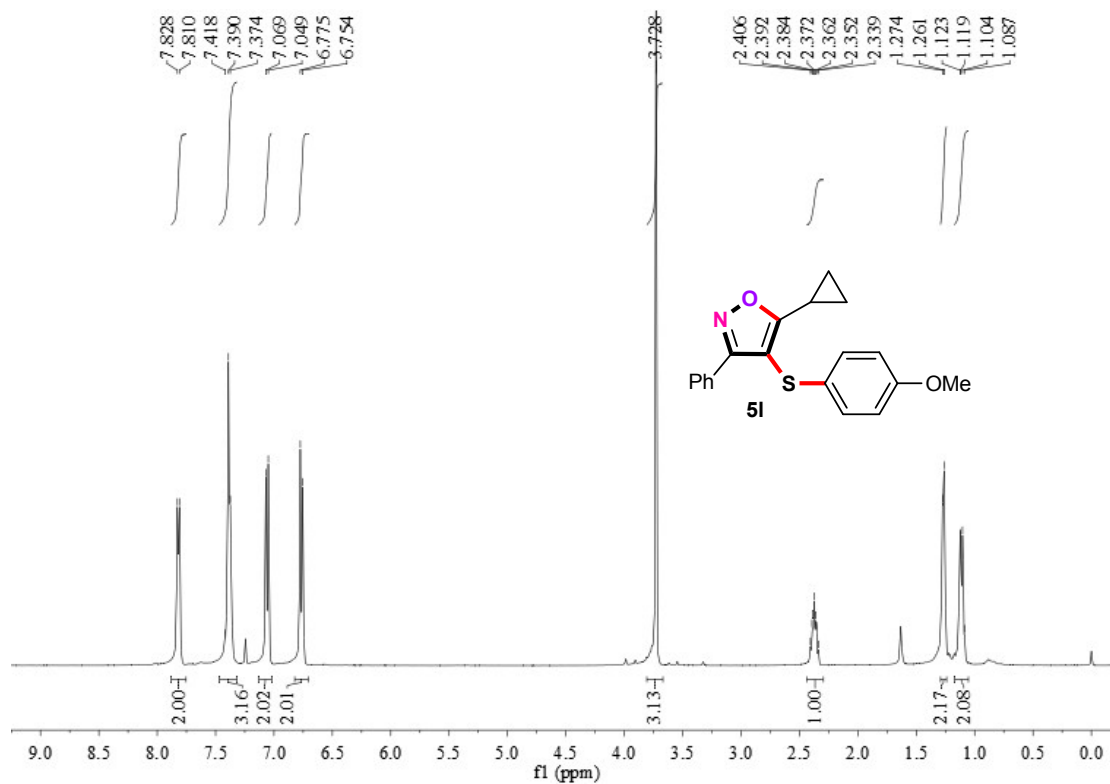


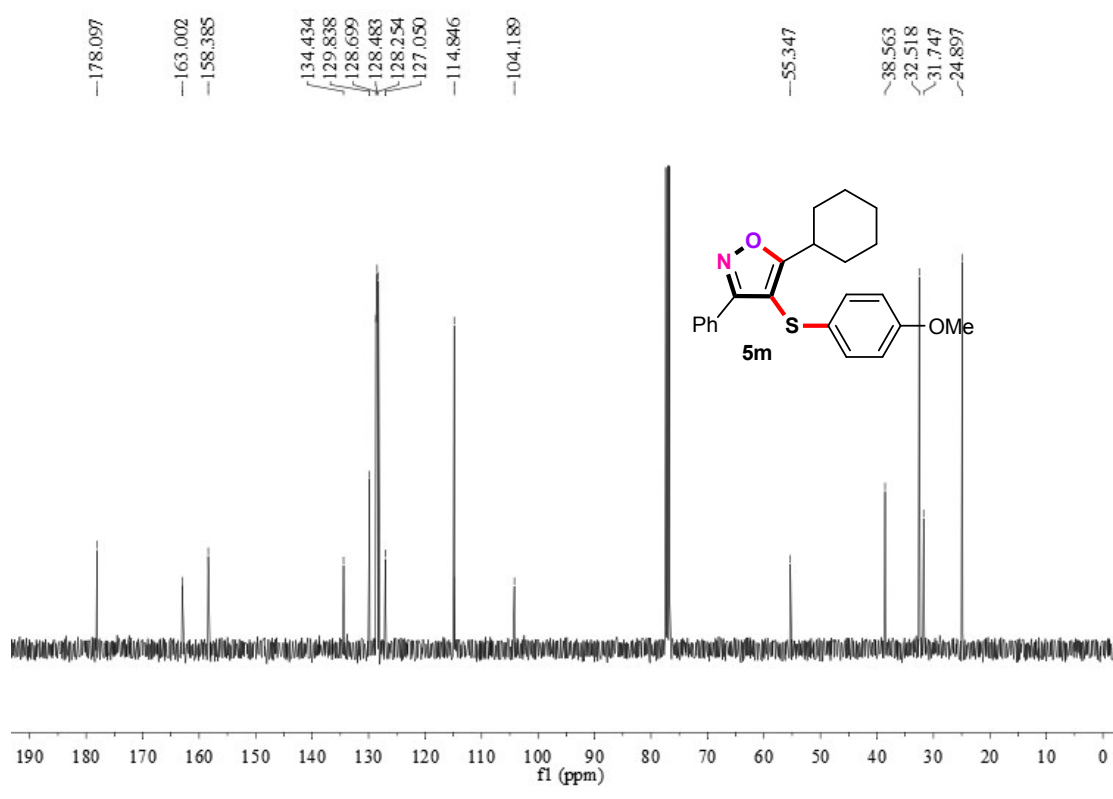
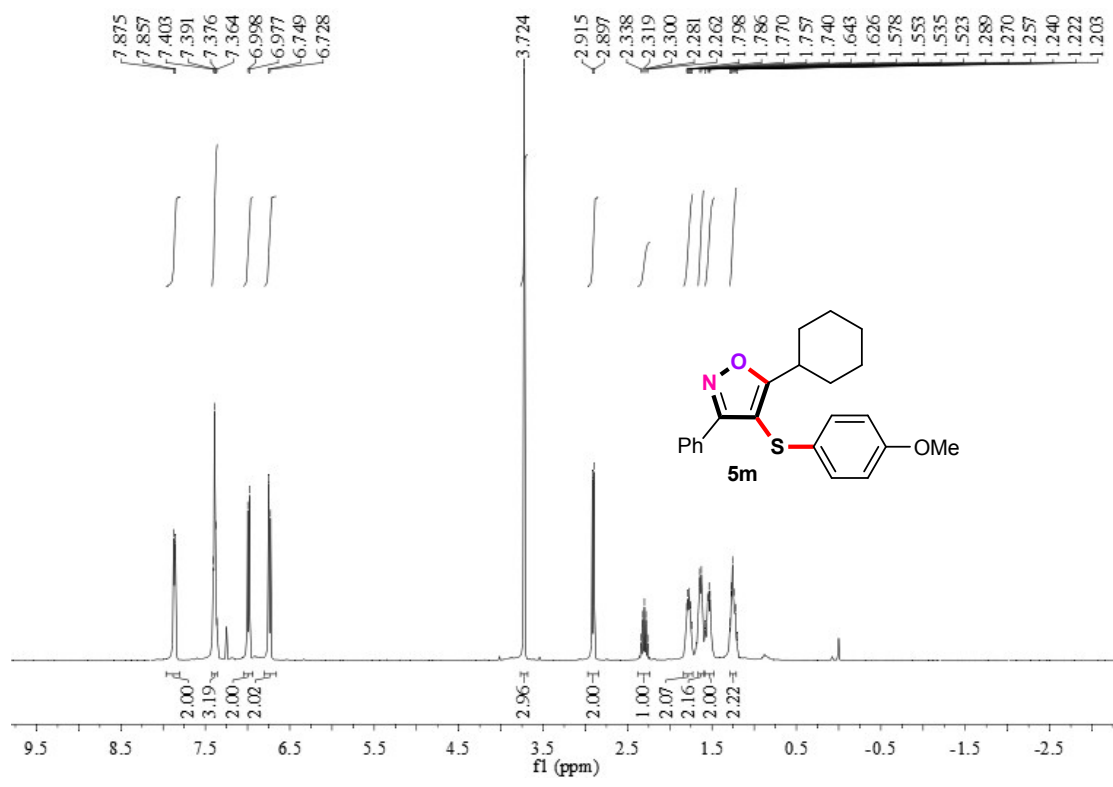


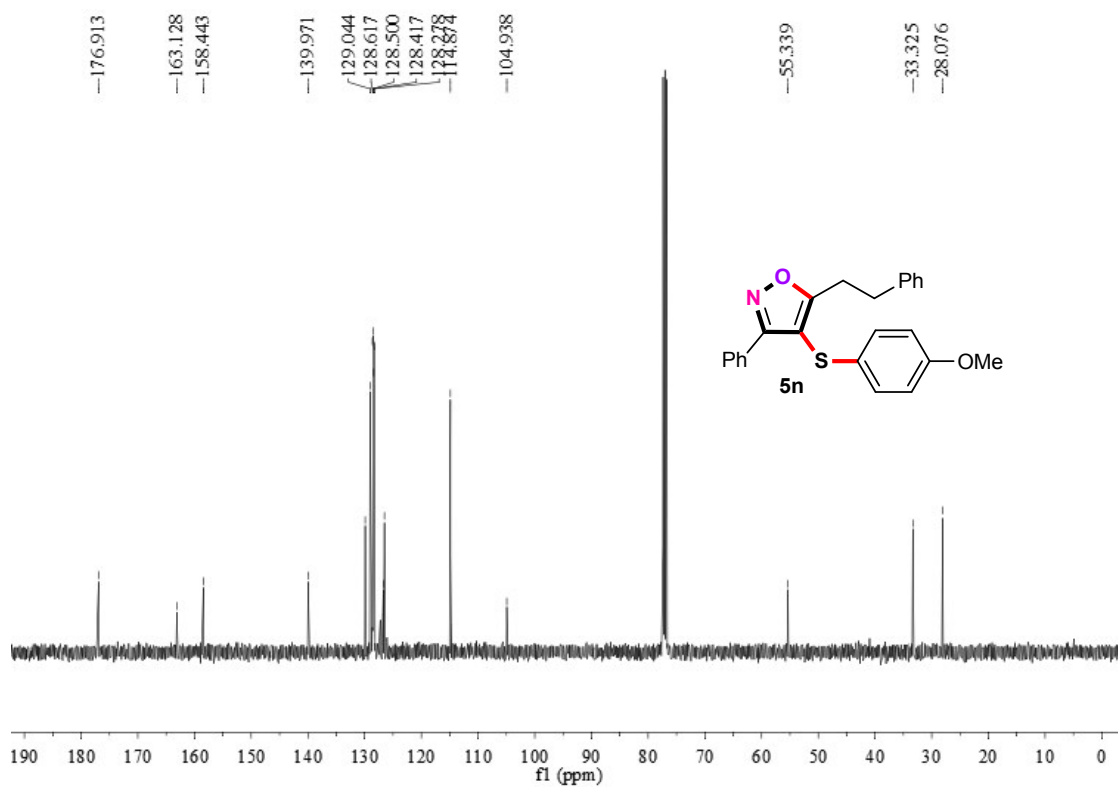
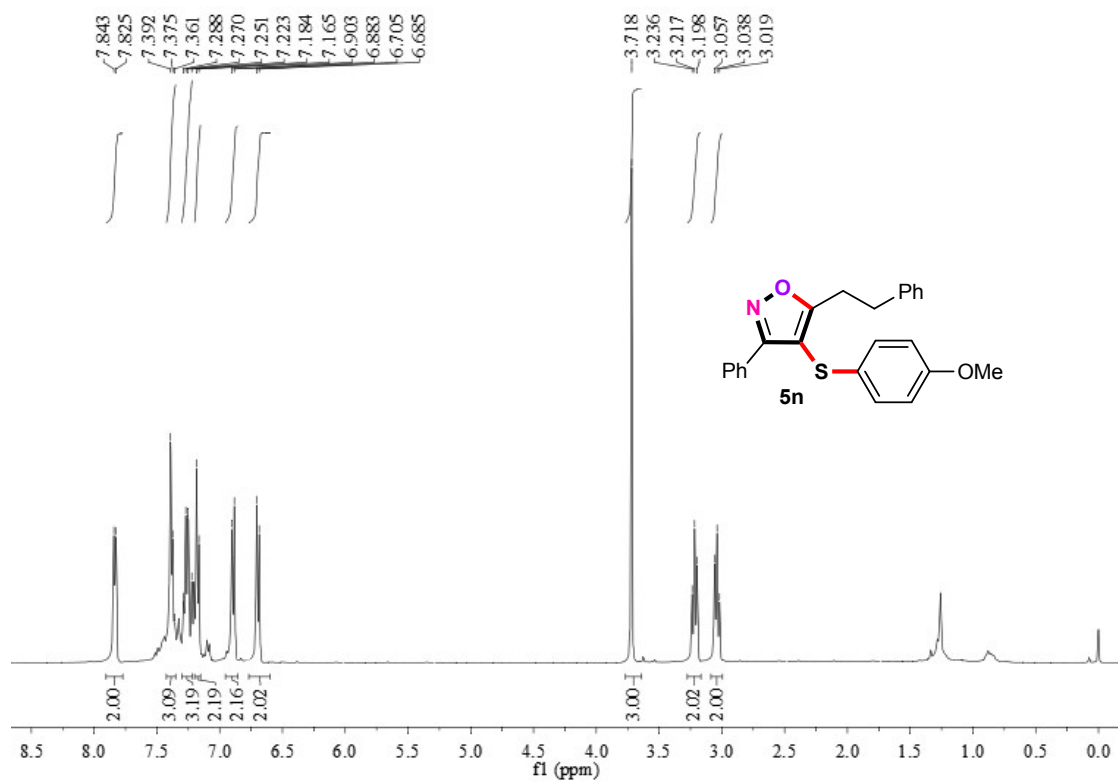


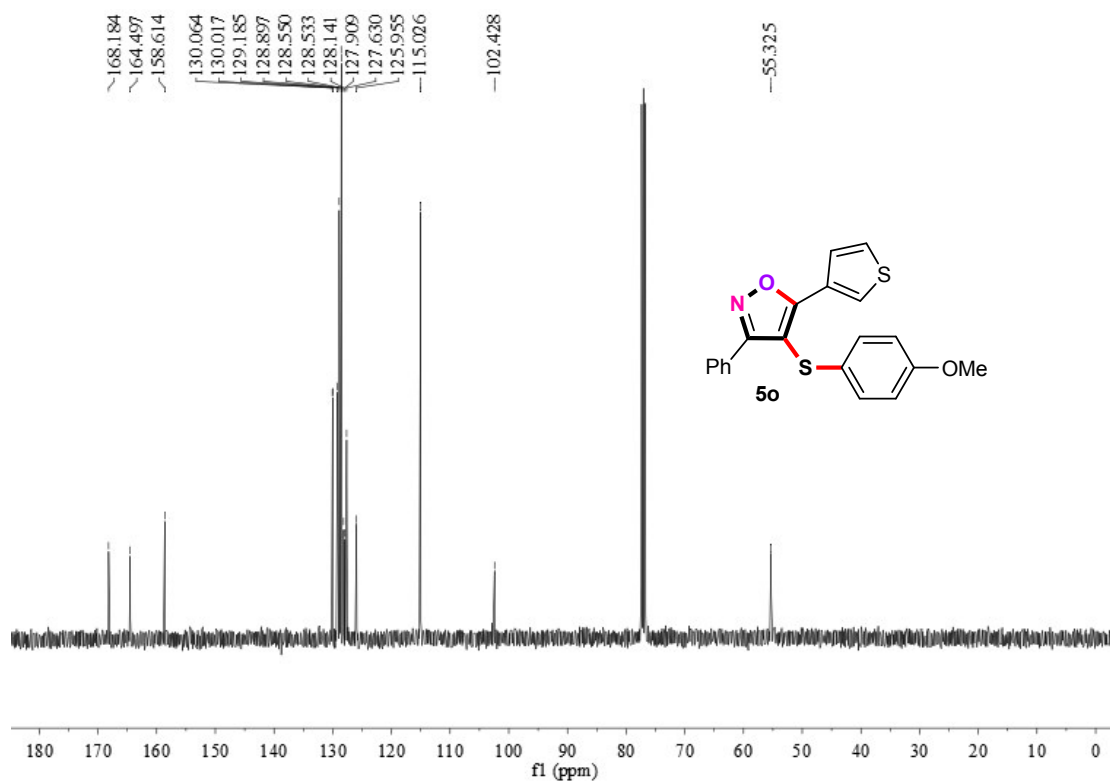
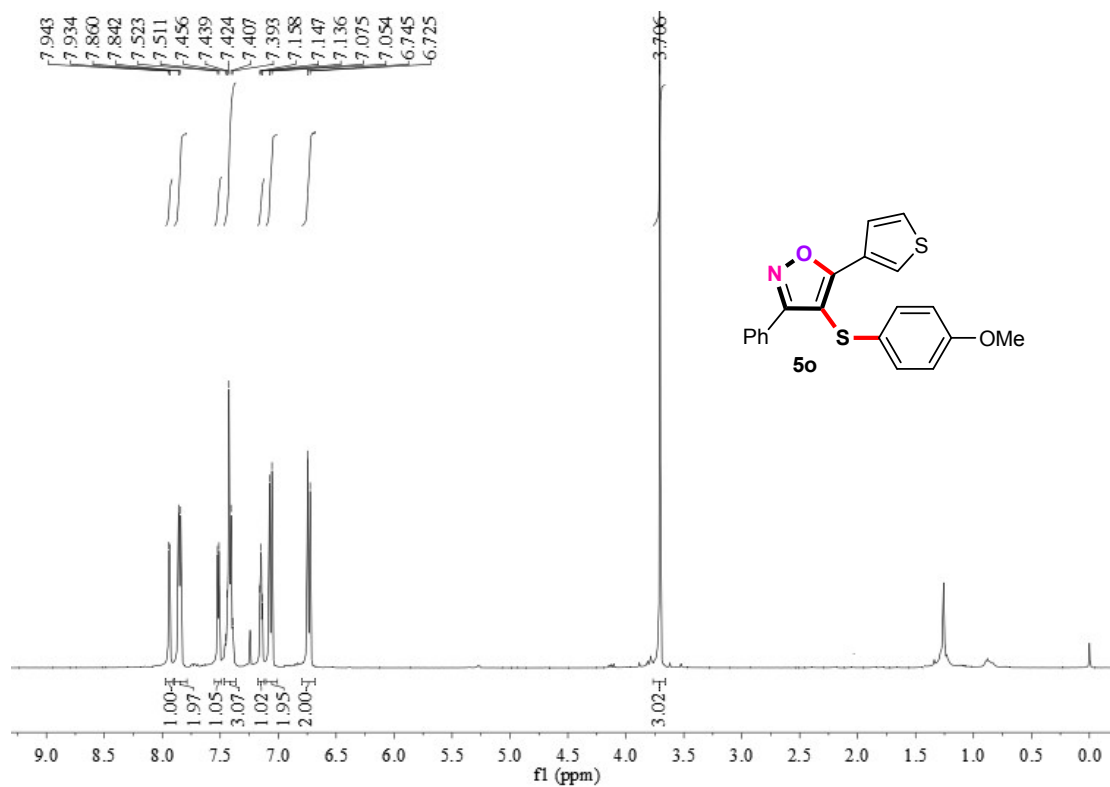




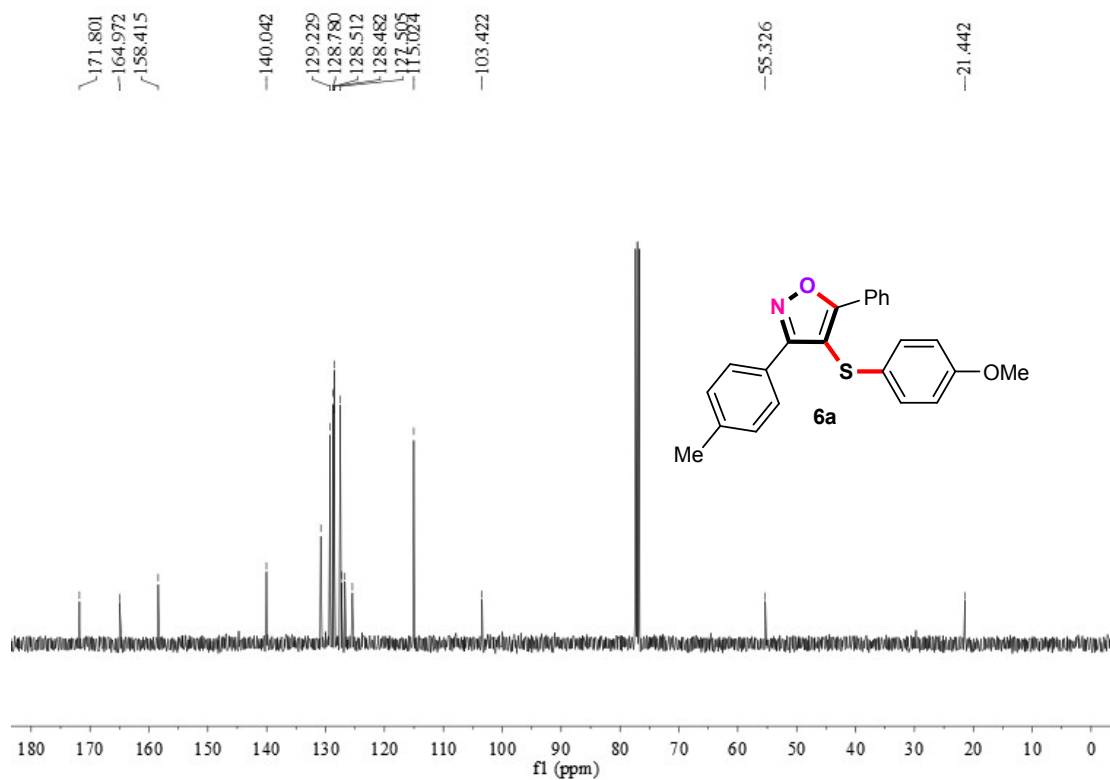
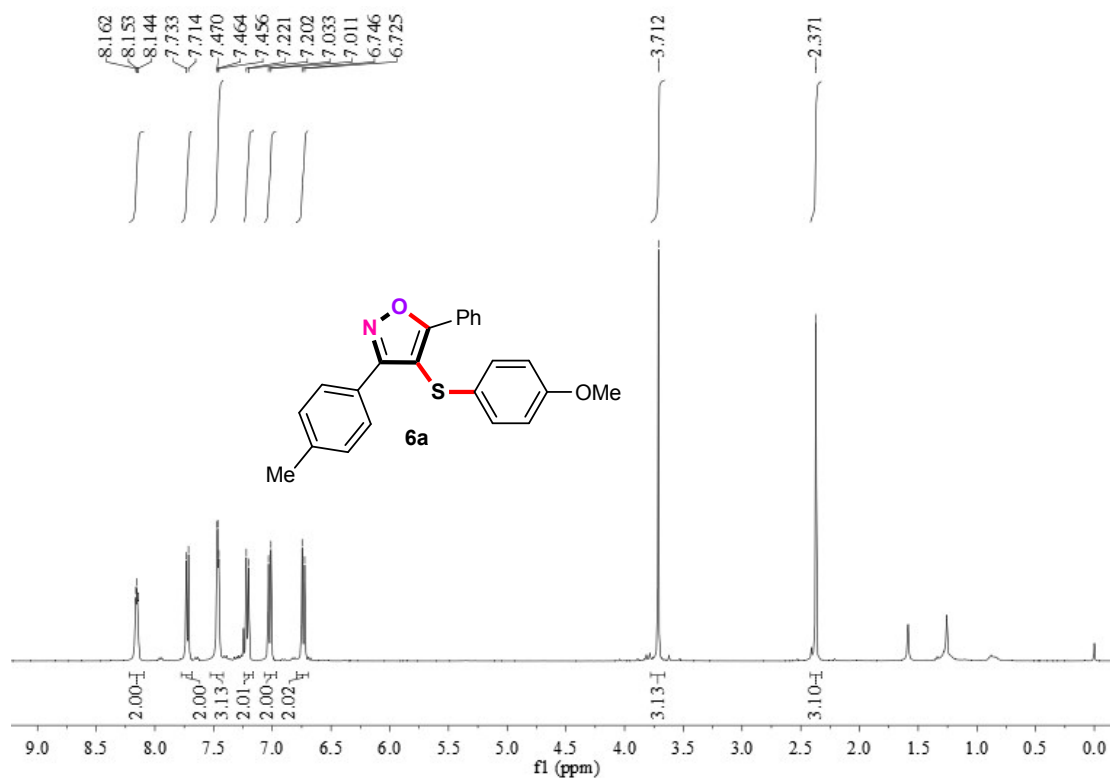


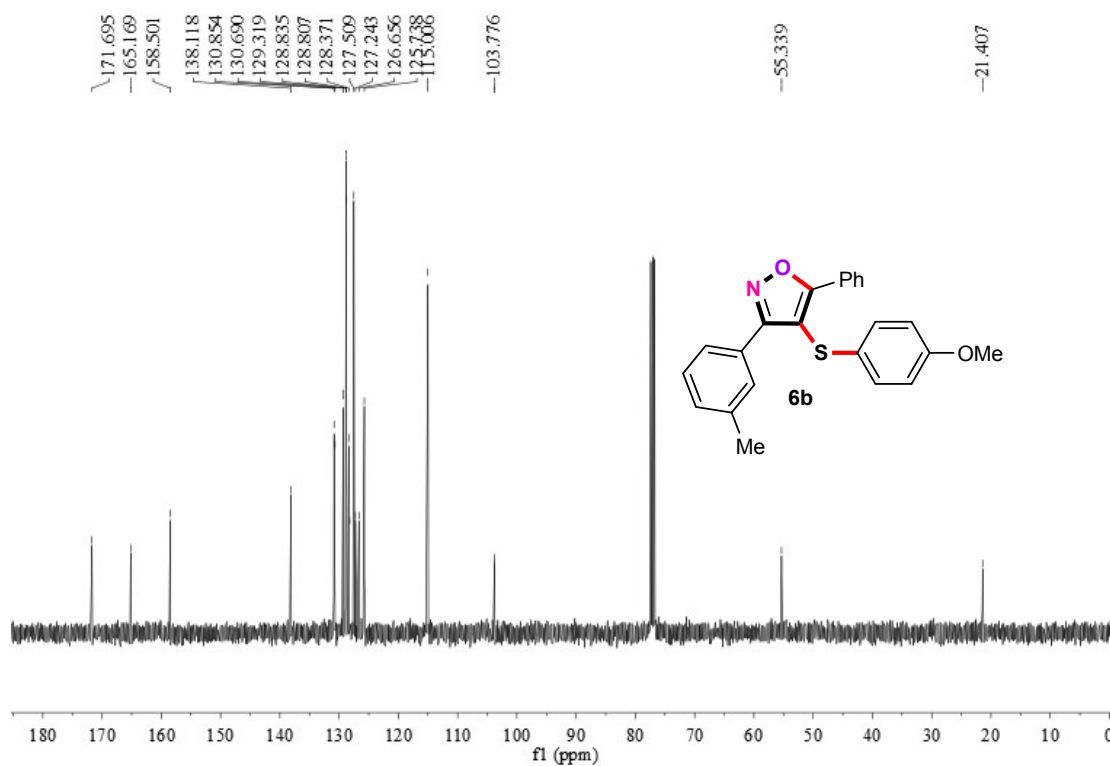
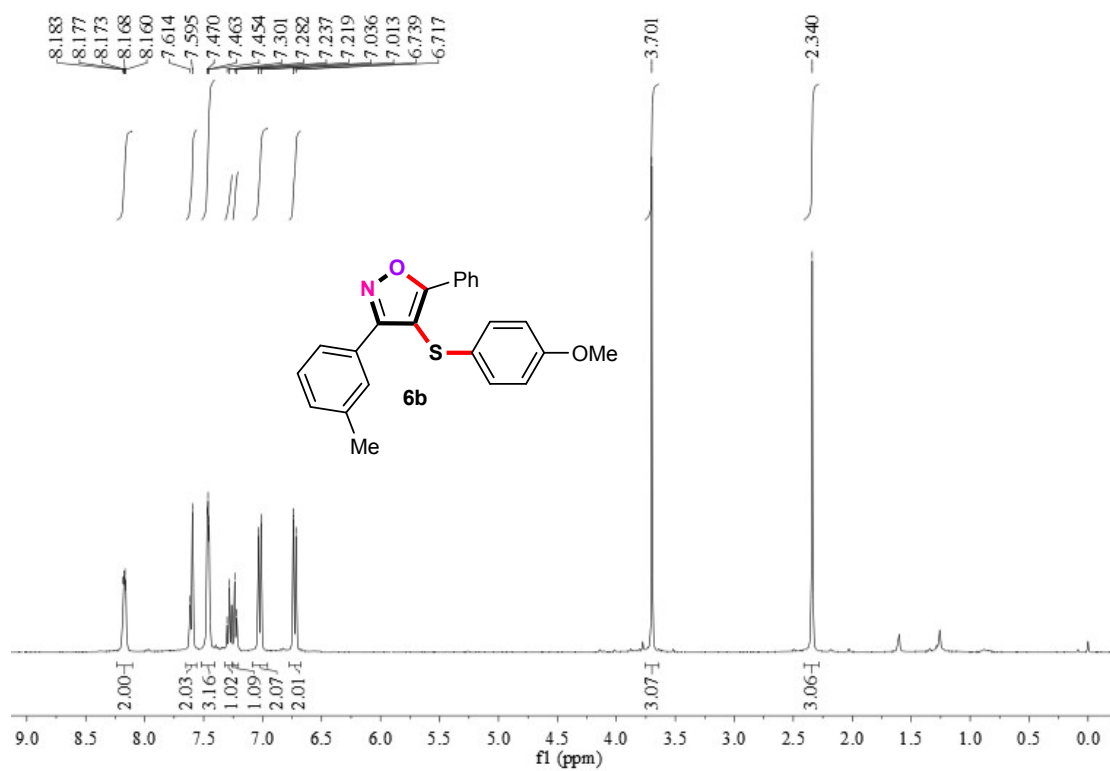


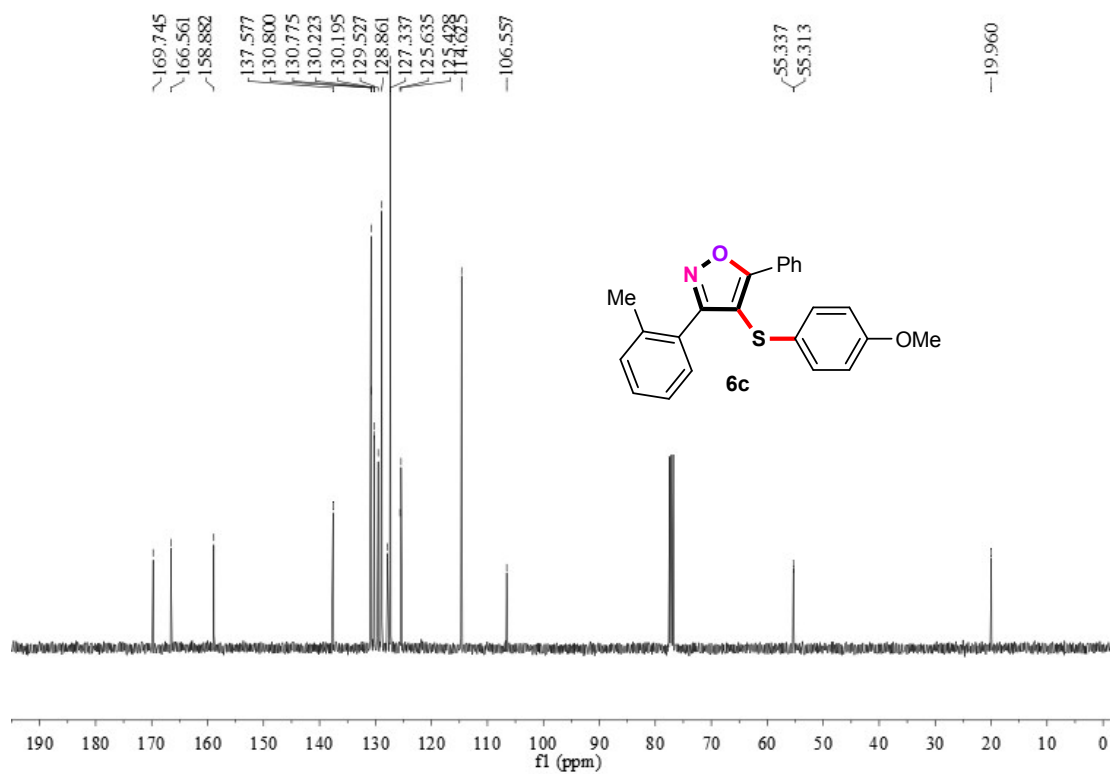
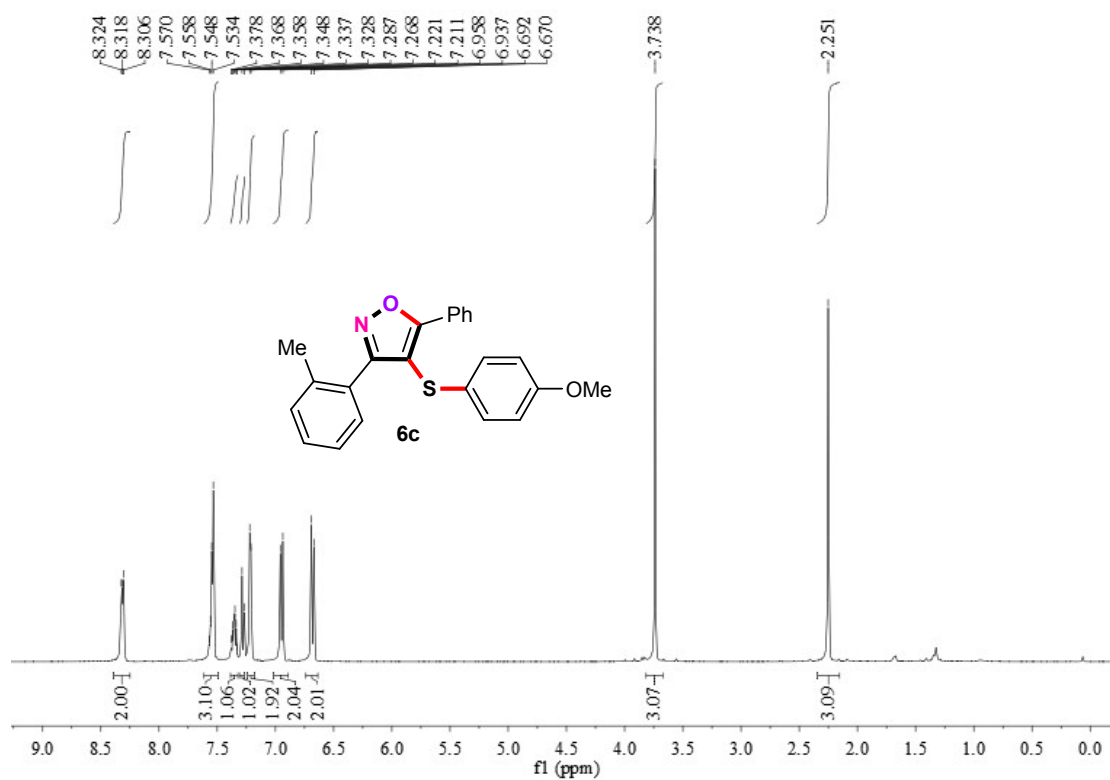


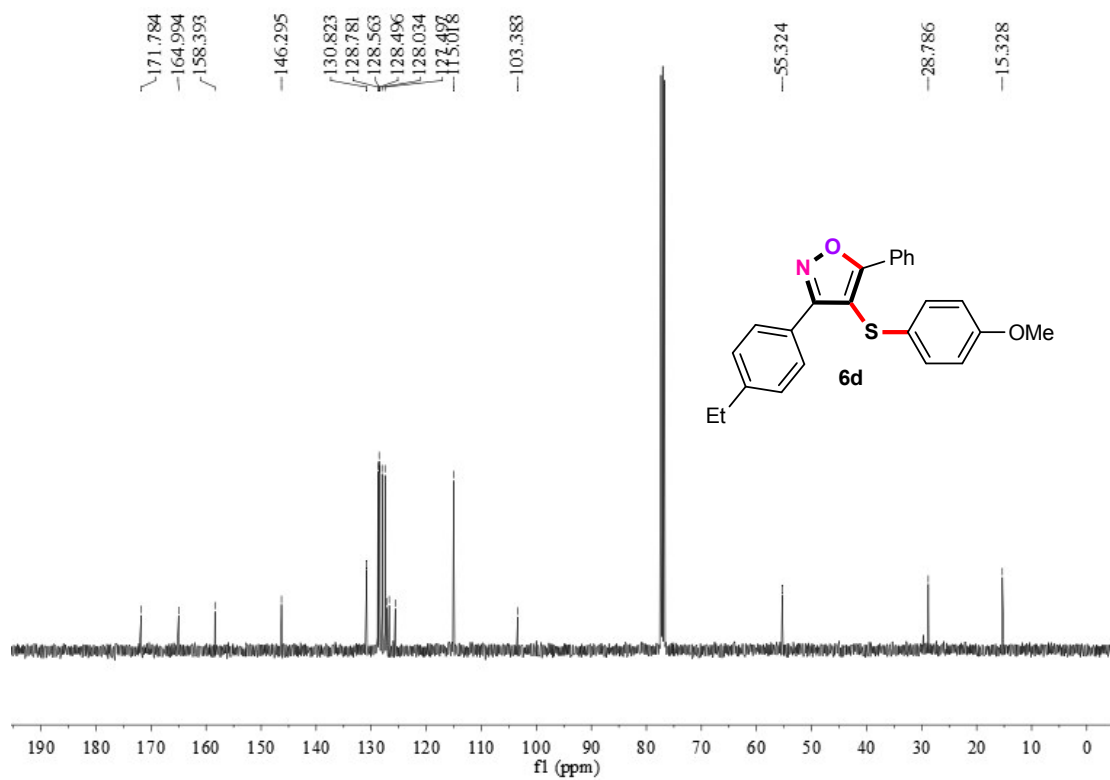
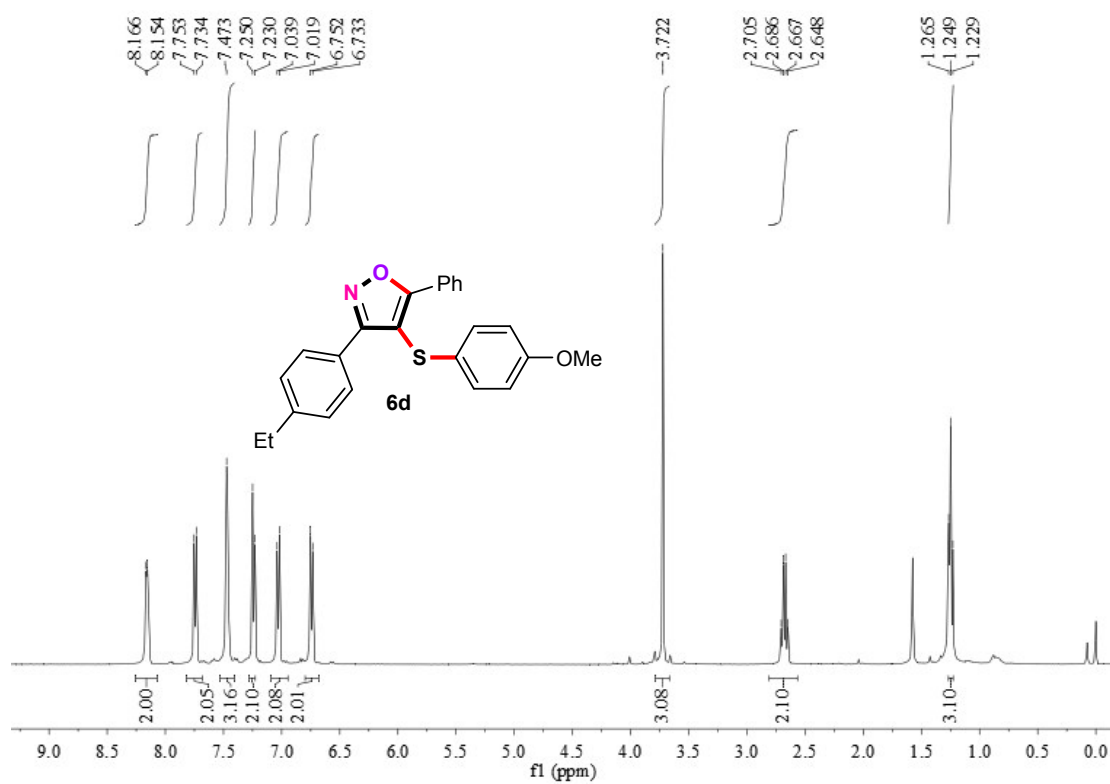


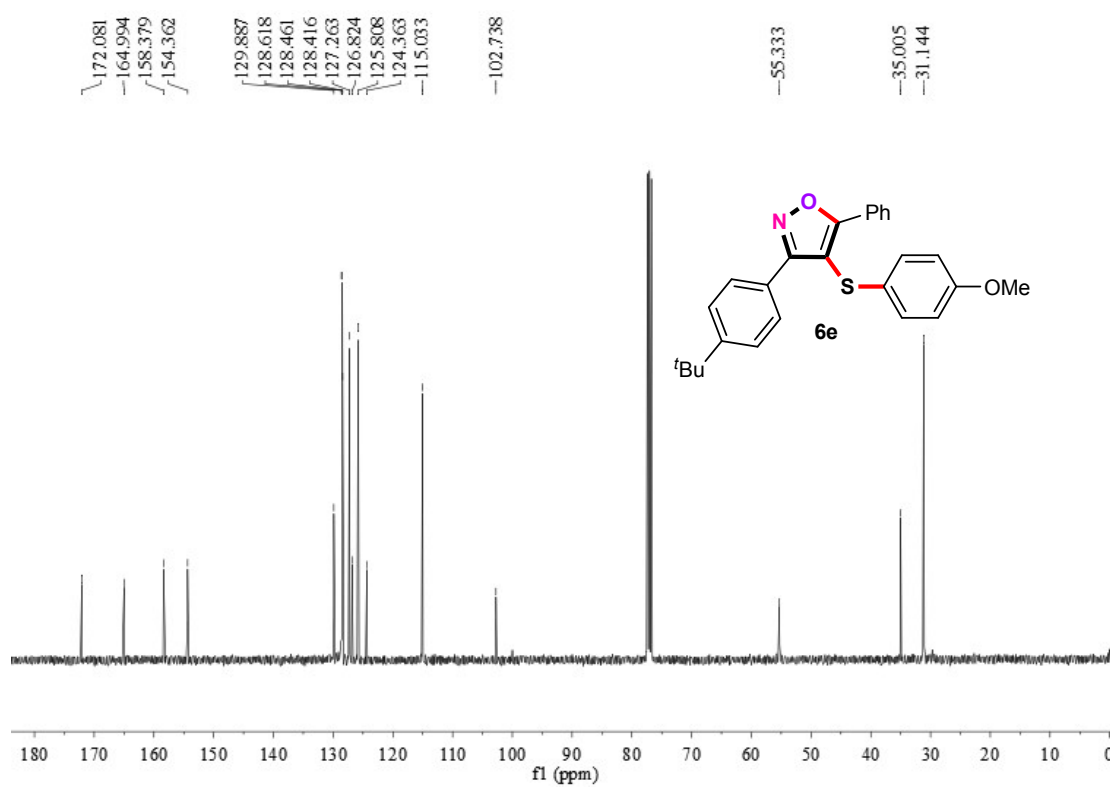
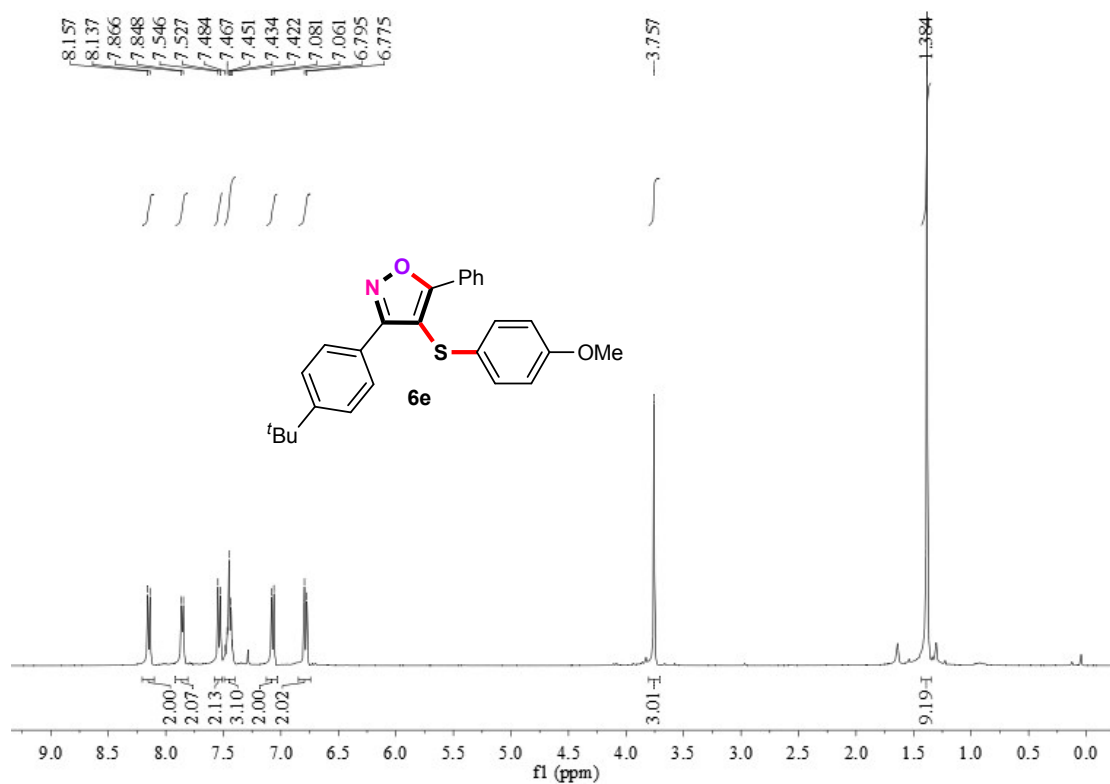
¹H and ¹³C NMR spectra of compounds 6

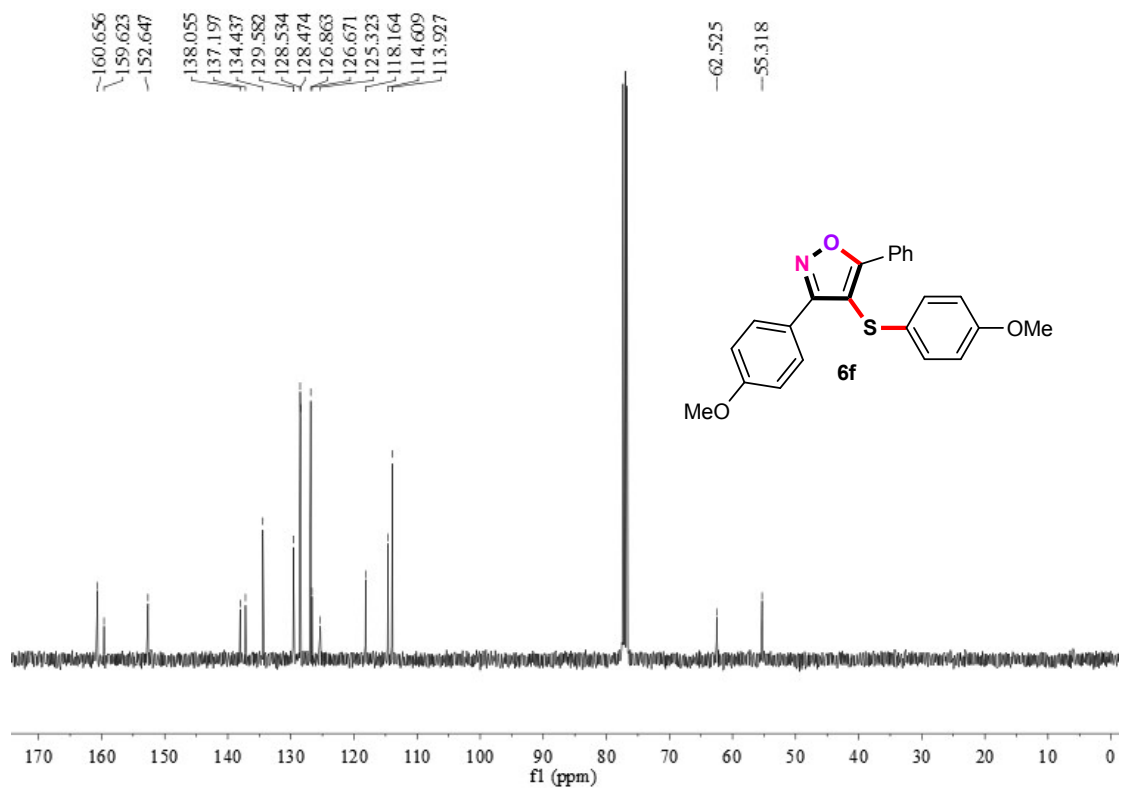
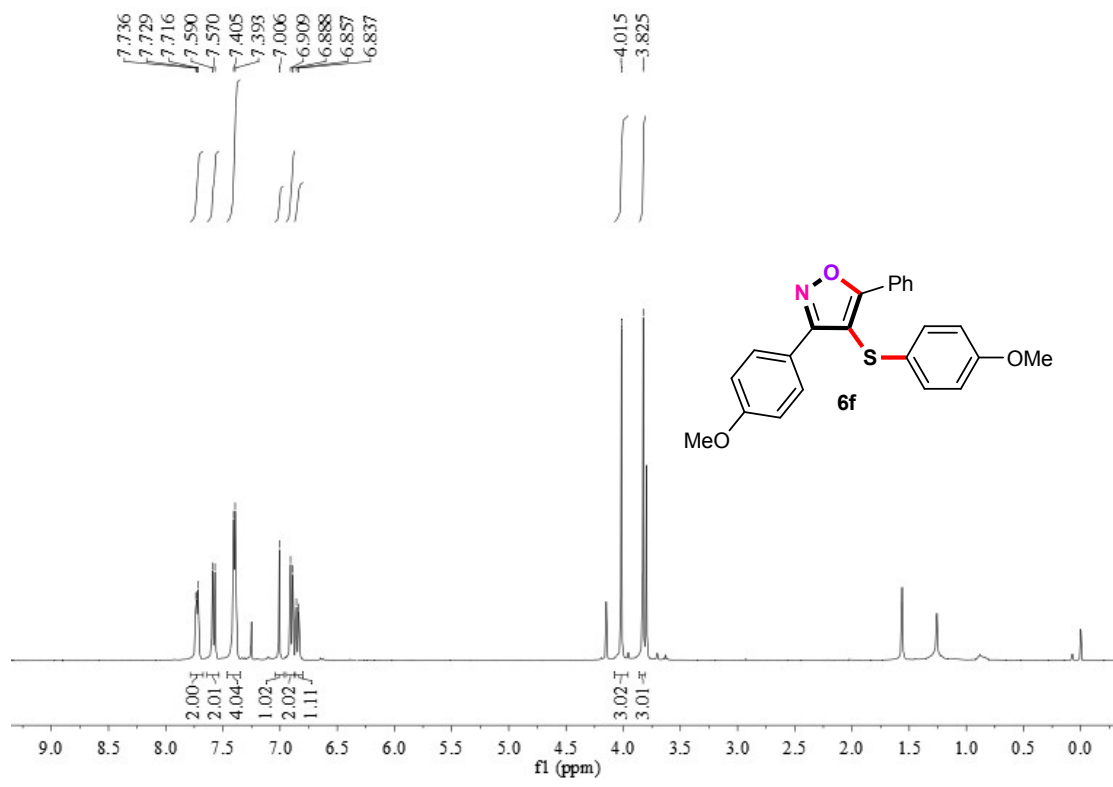


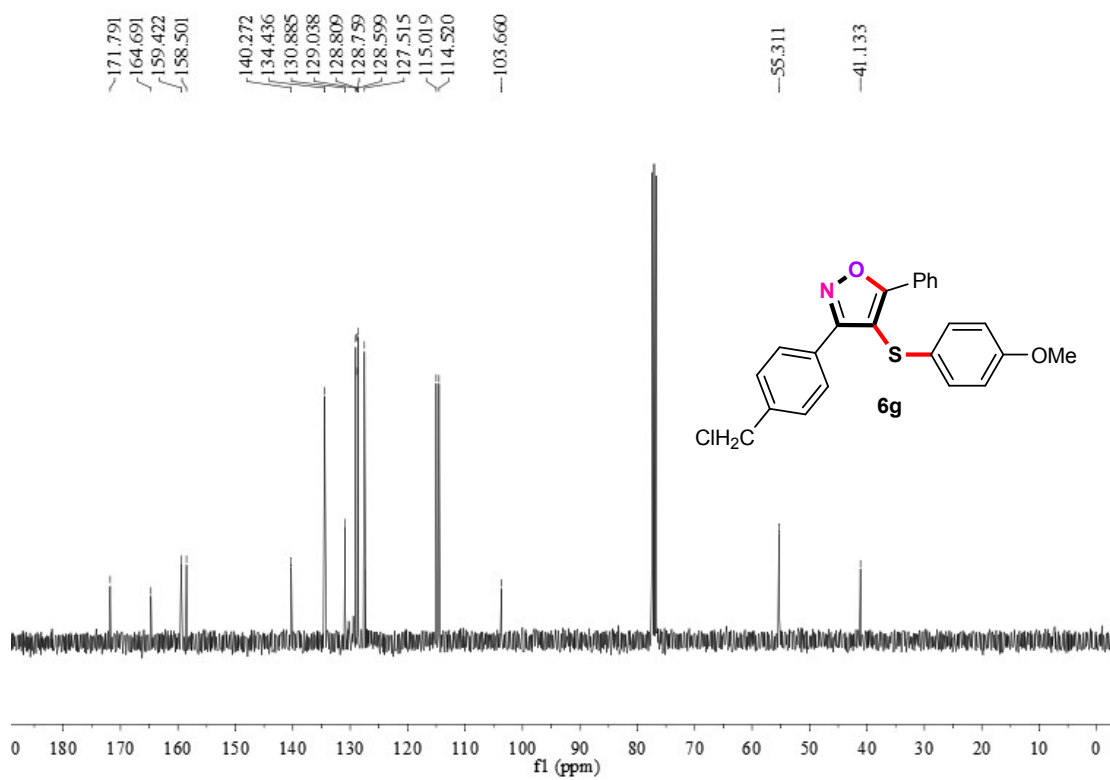
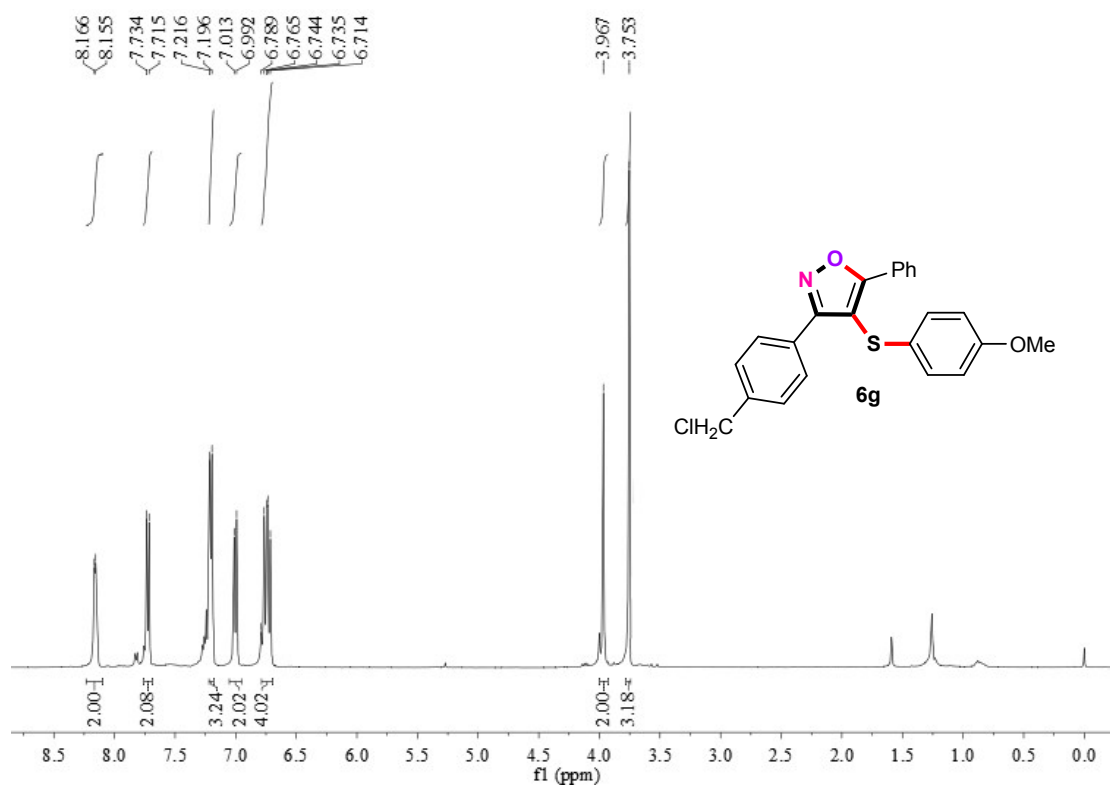


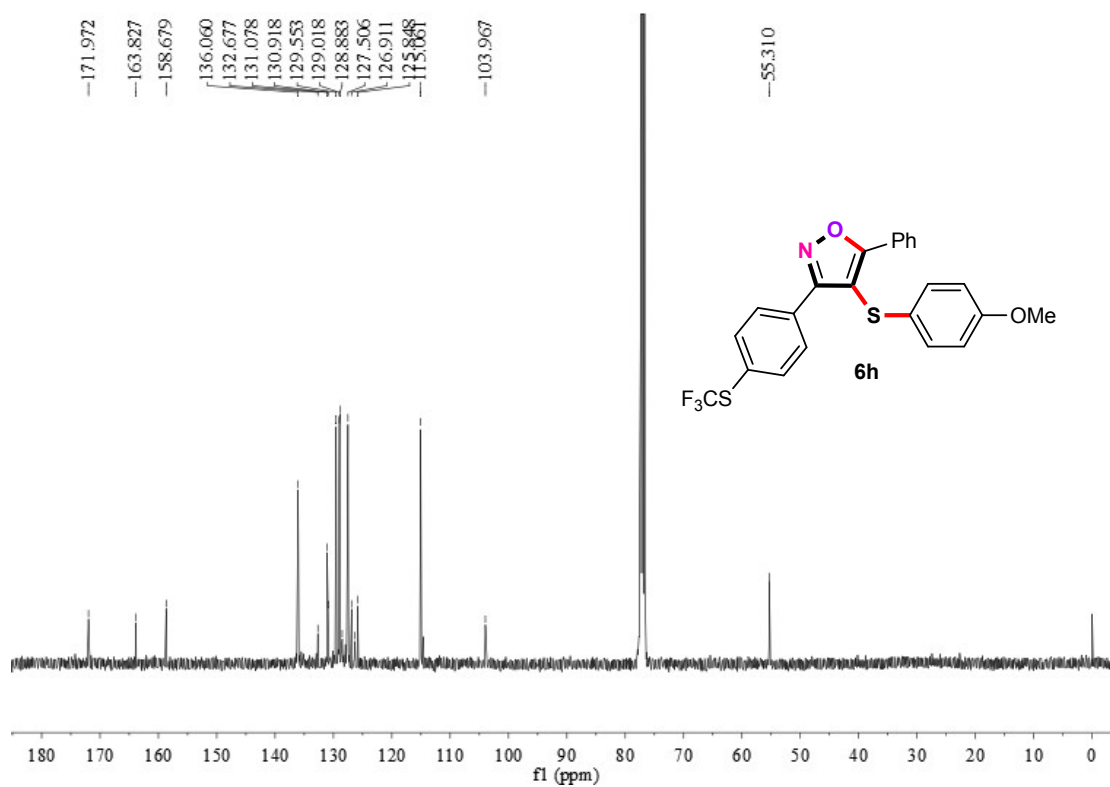
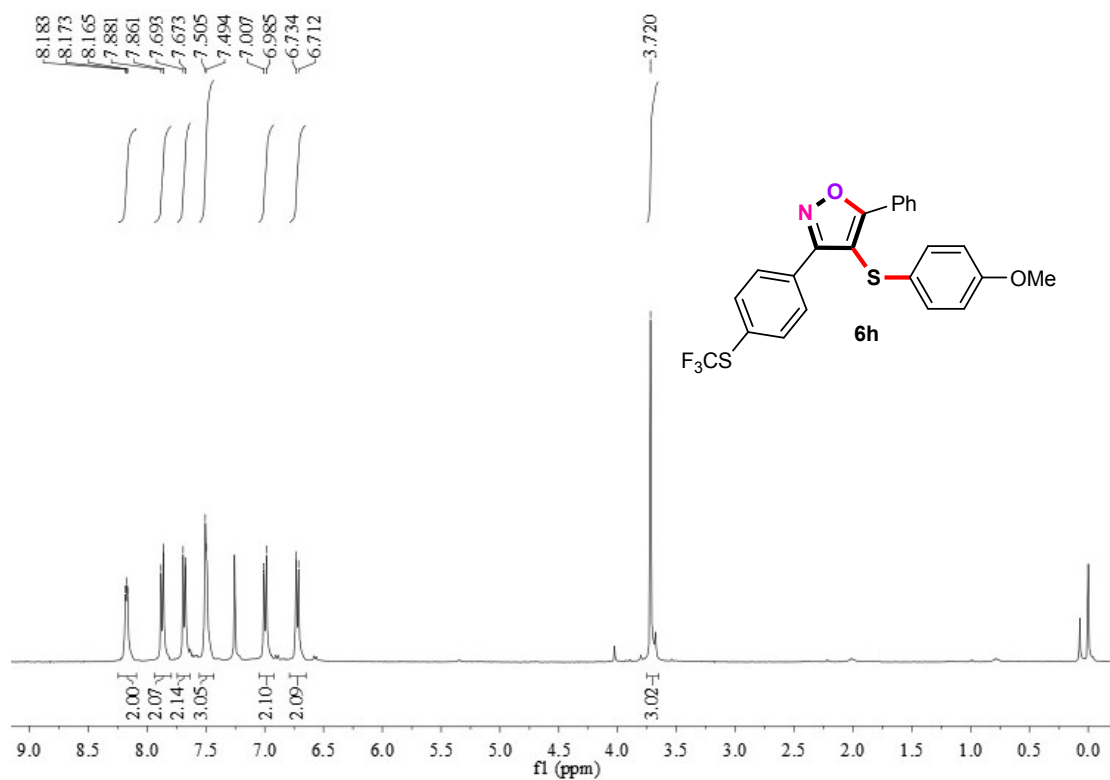


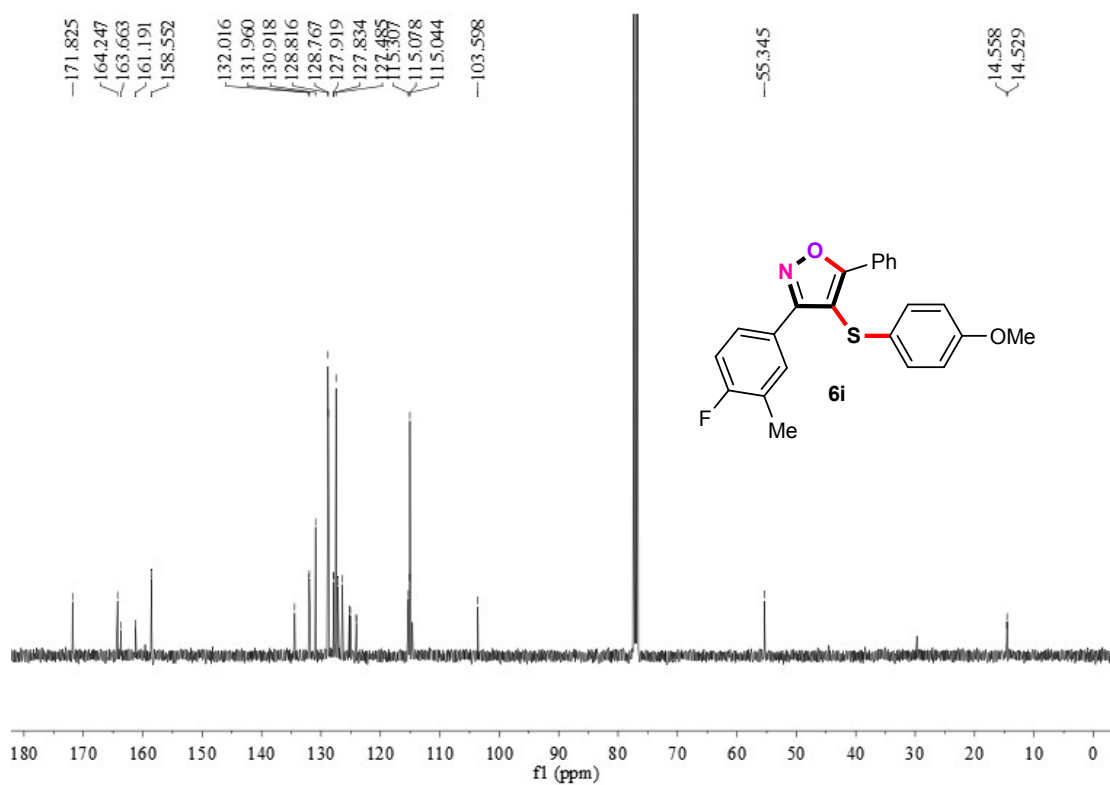
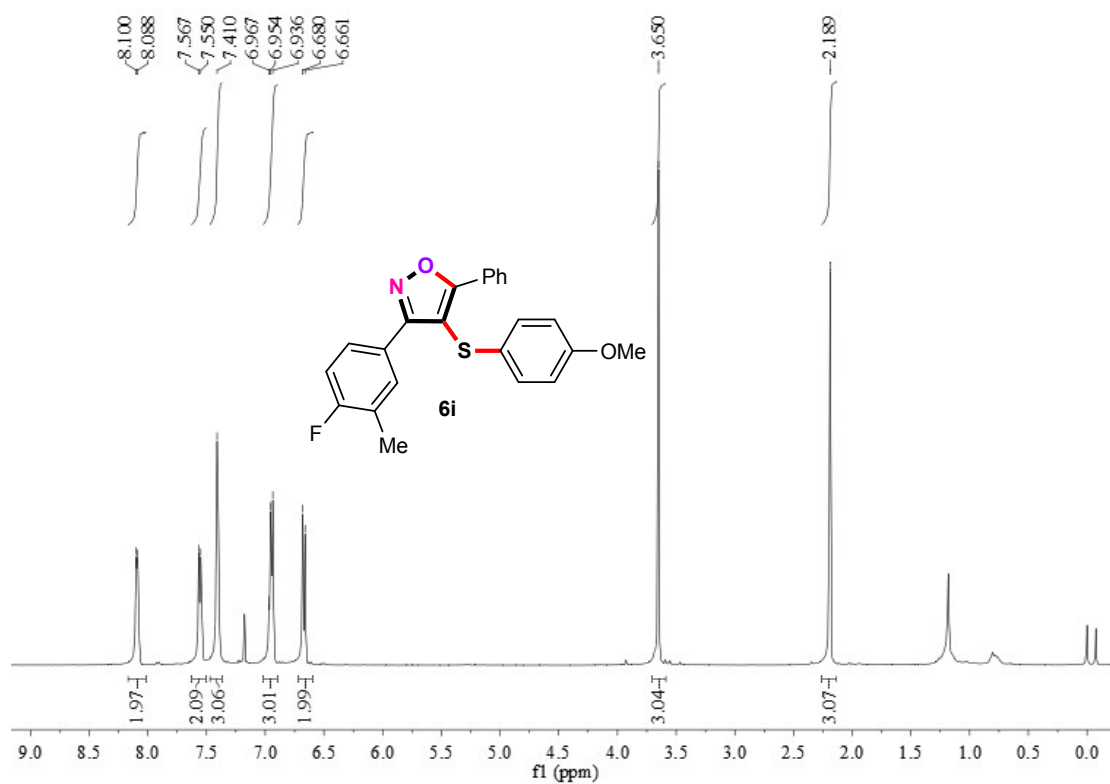


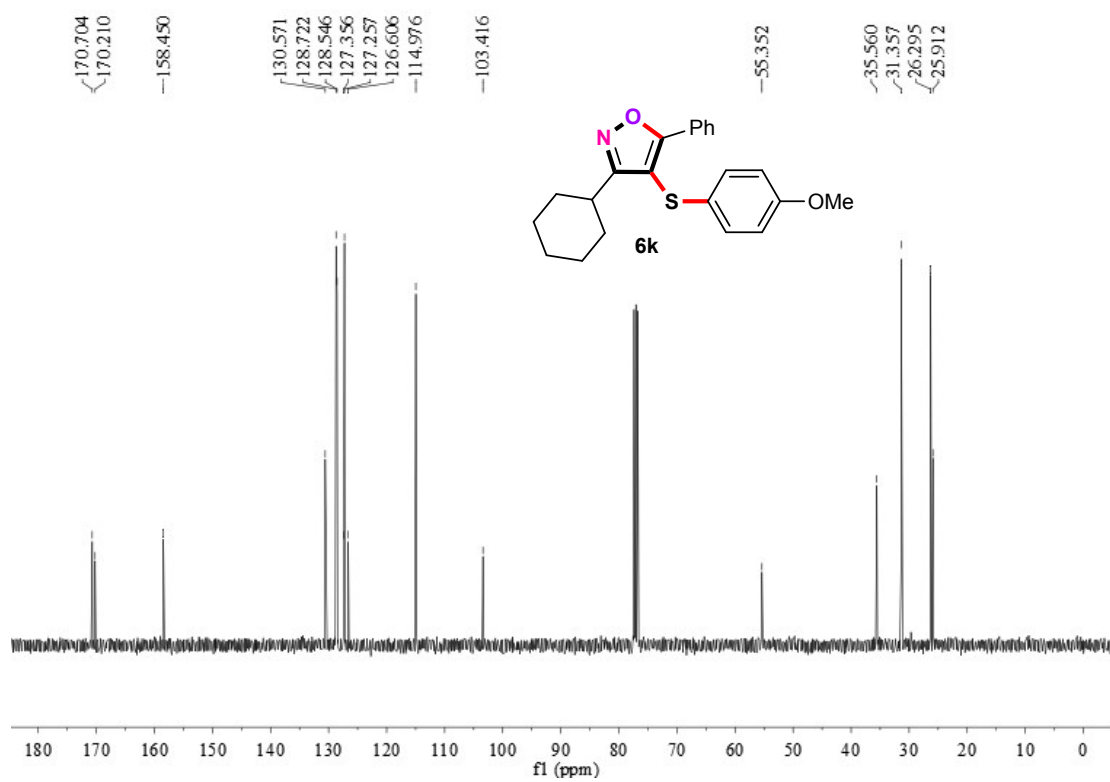
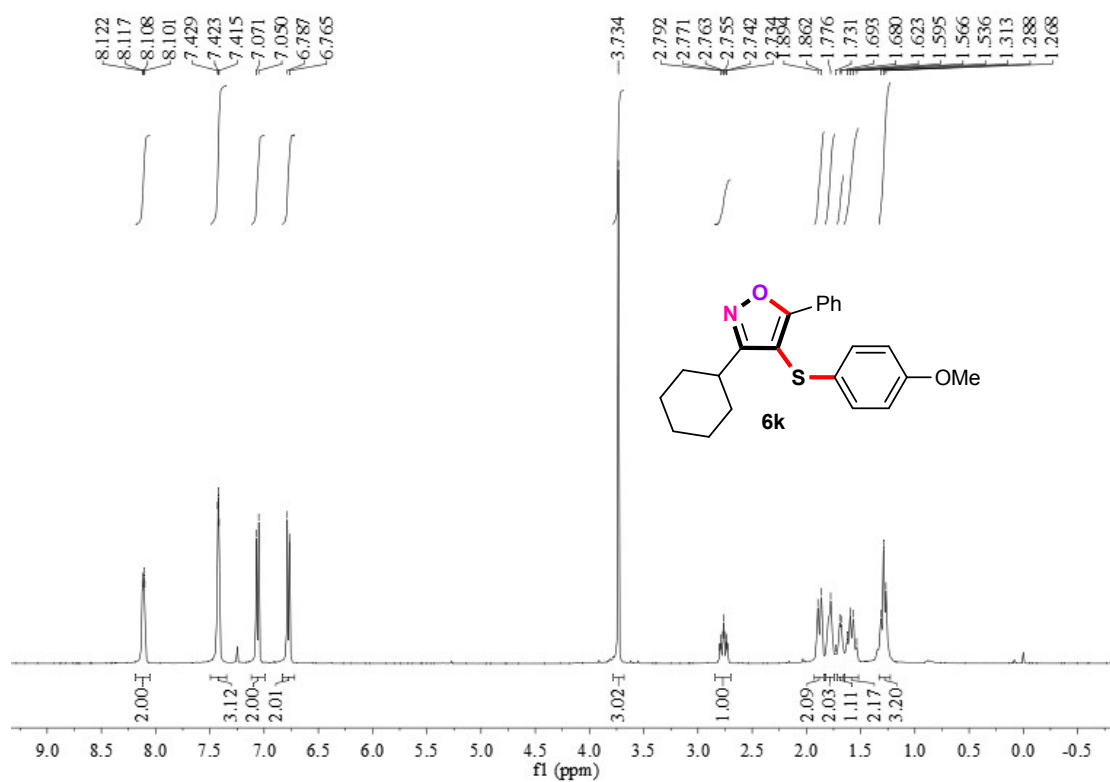


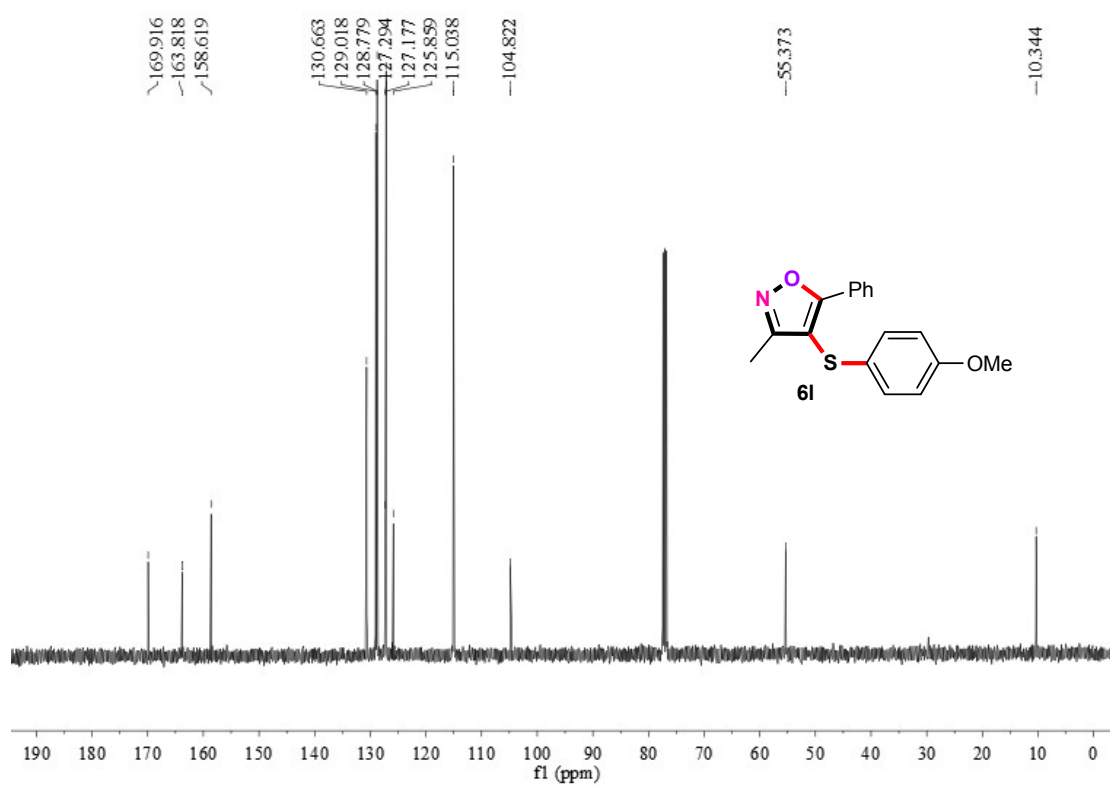
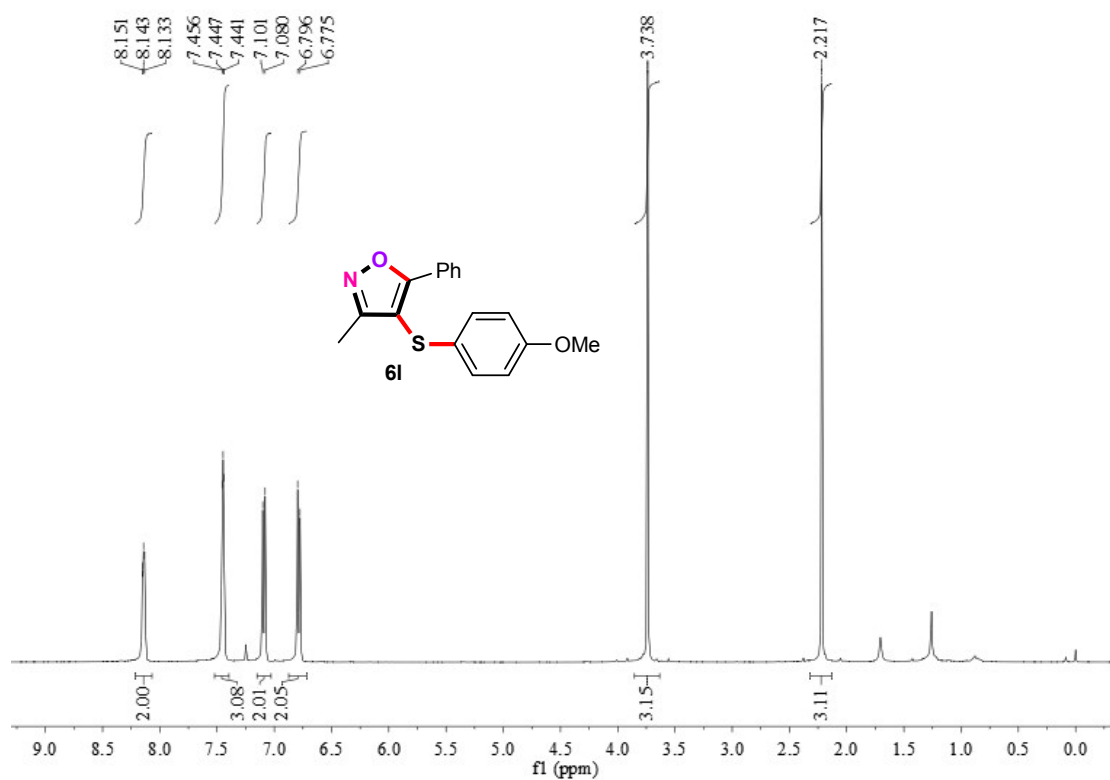


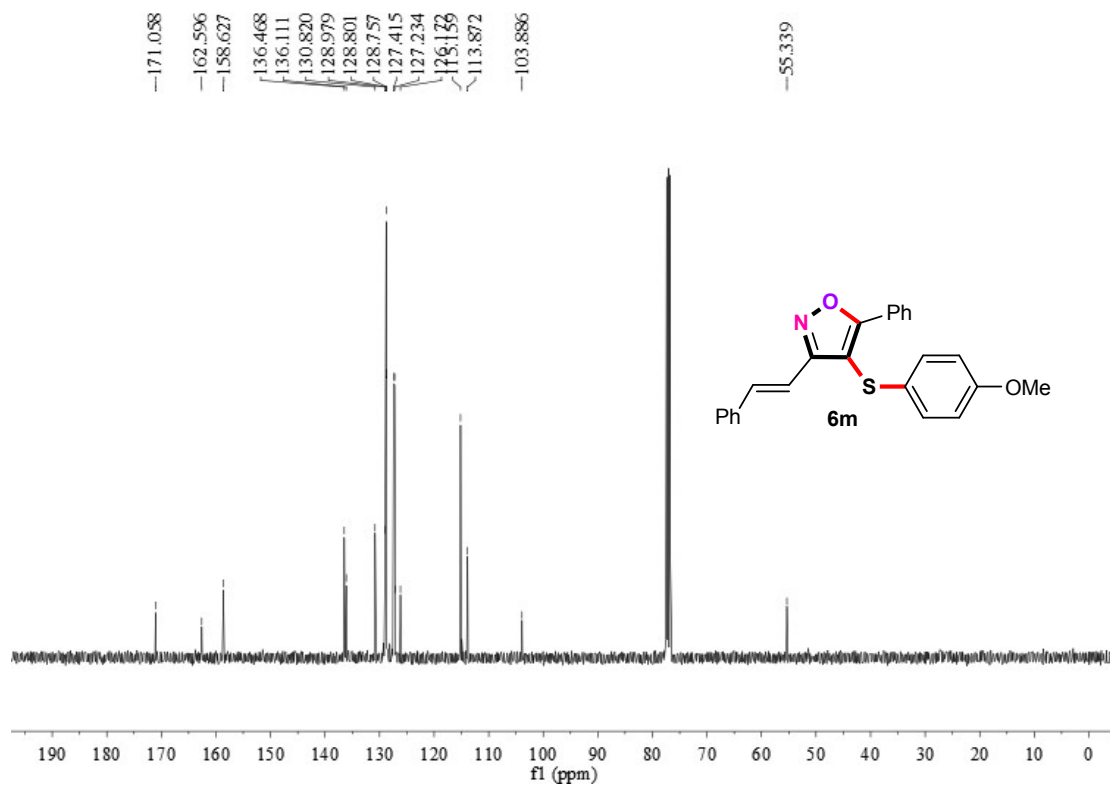
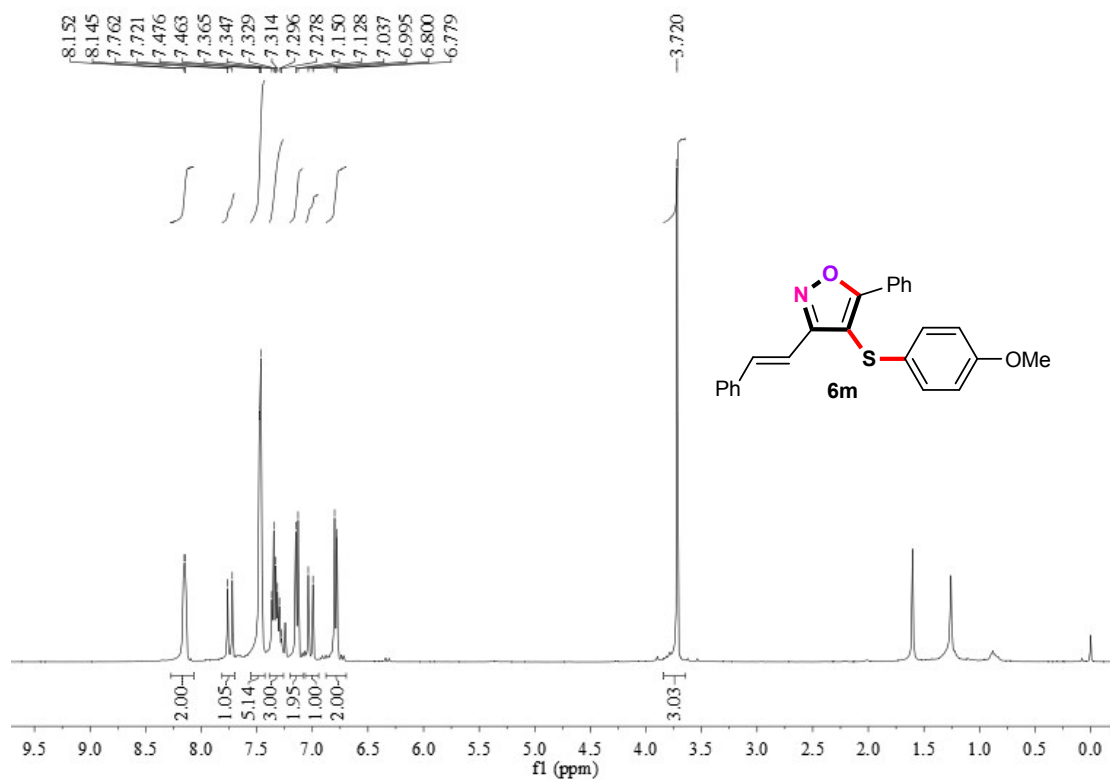












^1H and ^{13}C NMR spectra of compounds 7

