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Ytterbium(III)-Catalyzed Three-Component Reactions: Synthesis of 4-Organoselenium-quinolines and Application in Copper-Free Sonogashira Cross-coupling Reactions

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I. General Information.

Materials and methods

All reactions were carried out under a nitrogen atmosphere; all compounds were characterized by ^{1}H NMR, ^{13}C NMR, ESI-MS. Copies of the ^{1}H, ^{13}C spectra can be found at the end of the Supporting Information. Nuclear Magnetic Resonance spectra were obtained using a Bruker DPX 300 (^{1}H at 300 MHz and ^{13}C at 75 MHz) instrument in $CDCl_3$ solvent. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for TMS (0.00 ppm). Data are reported as follows: chemical shift (δ), multiplicity, coupling constant (J) in Hertz and integrated intensity. Abbreviations to denote the multiplicity of a particular signal are: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sex (sextet) and m (multiplet). All ^{13}C NMR spectra are reported in ppm relative to deuterated-chloroform (77.23 ppm), unless otherwise stated, and all were obtained with ^{1}H decoupling. High-resolution mass spectra (HRMS) were recorded on a Shimadzu LCMS-IT-TOF ESI-TOF mass spectrometer. Reactions were monitored with the same mass spectrometer. Column chromatography was performed using silica gel (230−400 mesh). Thin Layer Chromatography (TLC) was performed using silica gel UV254, 0.20 mm thickness. FTIR data were obtained using an Agilent Technologies Cary 630. Melting points were obtained using a Buchi B-545 melting point apparatus.

Unless stated otherwise, commercial reagents were used without further purifcation. All reagents were weighed and handled in air at room temperature.

II. Experimental Details and Characterization Data

Synthesis of trimethylseleno alkynylsilane. A solution of ethynyltrimethylsilane (1 mmol) in THF was added to a 5 mL, two-necked, dry flask under nitrogen atmosphere. The solution was cooled to -78 °C for the dropwise addition of *n*-butyl lithium. The solution was held at that temperature for one hour. Then the arylselenyl bromide (1 mmol) was slowly transferred to the flask (arylselenyl bromide via syringe diluted in THF) then allowed to reach room temperature, maintaining stirring for approximately 4 hours at that same temperature. The reaction mixture was diluted with ethyl acetate and washed with water and a saturated NH_4Cl solution, the organic phase collected and

dried over $MgSO_4$, filtered and the solvent removed in vacuum. The crude mixture was purified by column chromatography.

*Trimethyl((phenylselanyl)ethynyl)silane (**a**)*. Orange oil (223 mg, 88%). IR υ_{max} cm^{-1}: 3062, 2959, 2900, 1579, 1479, 1441, 1251, 1069, 1024, 842, 761, 734, 689. ^1H NMR (300 MHz, $CDCl_3$) δ 7.52 – 7.41 (m, 2H), 7.26 – 7.14 (m, 3H), 0.20 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 129.49 (3C), 128.80 (2C), 127.00, 111.49, 84.63, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{11}H_{14}SeSi$ $(M + H)^+$: 255.0108, found: 254.9929.

*((Benzylselanyl)ethynyl)trimethylsilane (**b**)*. Yellow oil (227.80 mg, 85%). IR υ_{max} cm^{-1}: 3030, 2959, 2898, 2088, 1497, 1456, 1251, 1181, 840, 760, 698.^1H NMR (300 MHz, $CDCl_3$) δ 7.44 – 7.39 (m, 2H), 7.38 (d, *J* = 3.6 Hz, 3H), 4.12 (s, 2H), 0.31 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.43, 128.95 (2C), 128.41 (2C), 127.42, 109.19, 86.78, 32.78, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{12}H_{16}SeSi$ $(M + H)^+$: 269.0265, found: 269.0085.

*(((4-methoxyphenyl)selanyl)ethynyl)trimethylsilane (**c**)*. Orange oil (235.70 mg, 83%). IR υ_{max} cm^{-1}: 2959, 2900, 2838, 2089, 1592, 1575, 1492, 1290, 1246, 1175, 1033, 843, 825, 760.^1H NMR (300 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.9 Hz, 2H), 6.66 (d, *J* = 8.9 Hz, 2H), 3.56 (s, 3H), 0.03 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.40, 131.52 (2C), 122.07, 115.32 (2C), 109.81, 85.77, 55.24, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{12}H_{16}OSeSi$ $(M + H)^+$: 285.0215, found: 285.0035.

*Trimethyl(((4-(trifluoromethyl)phenyl)selanyl)ethynyl)silane (**d**)*. Yellow oil (298.53 mg, 93%). IR υ_{max} cm^{-1}: 2963, 2095, 1603, 1402, 1322, 1166, 1123, 1106, 1074, 1015, 845, 825, 761.^1H NMR (300 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.6 Hz, 2H), 7.35 (d, *J* = 1.9 Hz, 2H), 0.06 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.23 (2C), 128.60 (2C), 126.47, 126.42, 126.36, 113.59, 82.81, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{12}H_{13}F_3SeSi$ $(M + H)^+$: 322.9983, found: 322.9803.

*Trimethyl((o-tolylselanyl)ethynyl)silane (**e**)*. Yellow oil (198.30 mg, 74%). IR υ_{max} cm^{-1}: 3285, 3062, 2959, 2091, 1592, 1572, 1467, 1460, 1382, 1251, 856, 842, 745.^1H NMR (300 MHz, $CDCl_3$) δ 7.71 (s, 2H), 7.07 (d, *J* = 62.7 Hz, 2H), 2.23 (s, 3H), 0.20 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.74, 133.16 (2C), 129.24, 127.55, 126.75, 111.48, 84.64, 22.20, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{12}H_{16}SeSi$ $(M + H)^+$: 269.0265, found: 268.9615.

*Trimethyl((naphthalen-2-ylselanyl)ethynyl)silane (**f**).* Brown solid (243.30 mg, 80%). Mp: 51-55 °C. IR υ_{max} cm^{-1}: 3054, 2959, 2898, 2089, 1622, 1585, 1501, 1249, 819, 741. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.55 – 7.50 (m, 2H), 0.40 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.98, 132.23, 130.33, 128.94, 127.82, 127.79, 127.57, 127.06, 126.67, 126.29, 126.07, 125.69, 111.73, 84.72, 0.00 ppm. HRMS (ESI) *m/z,* calcd for $C_{15}H_{16}SeSi$ $(M + H)^+$: 305.0265, found: 305.0101.

*(((6-methoxynaphthalen-2-yl)selanyl)ethynyl)trimethylsilane (**g**).* Yellow solid (267.20 mg, 80%). Mp: 58-62 °C. IR υ_{max} cm^{-1}: 2959, 2840, 2088, 1622, 1587, 1499, 1387, 1264, 1251, 1212, 1030, 840, 760. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.60 (s, 1H), 7.19 (d, *J* = 9.0 Hz, 2H), 7.14 (s, 1H), 3.94 (s, 3H), 0.31 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.91, 133.59, 129.62, 128.68, 127.90, 127.29 (2C), 122.47, 119.51, 111.16, 105.87, 85.00, 55.29, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{16}H_{18}OSeSi$ $(M + H)^+$: 335.0371, found: 335.0137.

*(((4-fluorophenyl)selanyl)ethynyl)trimethylsilane (**h**).* Yellow oil (208.70 mg, 77%). IR υ_{max} cm^{-1}: 2959, 2091, 1587, 1488, 1251, 1229, 1160, 1015, 843, 823, 761. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.06 (t, *J* = 8.5 Hz, 2H), 0.25 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.08, 131.30, 131.20, 122.78, 116.96, 116.67, 111.45, 84.49, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{11}H_{13}FSeSi$ $(M + H)^+$: 272.0015, found: 271.9843.

Synthesis of Seleno alkynyl. Into a 50 mL flask under nitrogen atmosphere containing a solution of the acetylenic selenide (1 mmol) in methanol (5 mL) was added potassium carbonate (1 mmol). Allowing the ambient temperature to react for one hour. The solution was then extracted with H_2O and ethyl acetate, the organic phase collected and dried over $MgSO_4$, and the solvent removed in vacuum. The reaction residue was impregnated on silica submitted to column chromatography using flash silica.

*Ethynyl(phenyl)selane (**3a**).* Yellow oil (161.11 mg, 89%). IR υ_{max} cm^{-1}: 3280, 3060, 2035, 1579, 1479, 1441, 1069, 1022, 734, 687. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 6.3 Hz, 2H), 7.29 – 7.23 (m, 3H), 3.14 (s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ

129.68 (3C), 129.54 (2C), 127.45, 91.73, 64.73 ppm. HRMS (ESI) *m/z,* calcd for C_8H_6Se $(M + H)^+$: 182.9714, found: 182.9534.

*Benzyl(ethynyl)selane (**3b**)*. Yellow oil (163.80 mg, 84%). IR υ_{max} cm^{-1}: 3278, 3028, 1495, 1454, 1181, 1069, 1032, 760. ^1H NMR (300 MHz, $CDCl_3$) δ 7.26 (d, *J* = 5.2 Hz, 3H), 7.22 (d, *J* = 3.2 Hz, 2H), 3.97 (s, 2H), 2.83 (s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.56, 129.09 (2C), 128.77 (2C), 127.77, 90.13, 66.28, 32.62 ppm. HRMS (ESI) *m/z,* calcd for C_9H_8Se $(M + H)^+$: 196.9870, found: 197.0153.

*Ethynyl(4-methoxyphenyl)selane (**3c**)*. Orange oil (187.79 mg, 89%). IR υ_{max} cm^{-1}: 3278, 2836, 2034, 1590, 1575, 1490, 1462, 1290, 1244, 1175, 1030, 823. ^1H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, *J* = 9.1 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H), 3.13 (s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 15 9.72, 132.44 (2C), 122.15, 115.47 (2C), 90.29, 65.88, 55.37 ppm. HRMS (ESI) *m/z,* calcd for C_9H_8OSe $(M + H)^+$: 212.9819, found: 212.9471.

*Ethynyl(o-tolyl)selane (**3d**)*.Yellow oil (185.25 mg, 95%). IR υ_{max} cm^{-1}: 3278, 3060, 2974, 2920, 1592, 1572, 1458, 1382, 1033, 745. ^1H NMR (300 MHz, $CDCl_3$) δ 7.90 (s, 2H), 7.29 (s, 1H), 7.17 (s, 2H), 3.26 (s, 1H), 2.46 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.95, 130.44 (2C), 130.03, 127.40, 126.95, 91.79, 64.63, 21.17 ppm. HRMS (ESI) *m/z,* calcd for C_9H_8Se $(M + H)^+$: 196.9870, found: 196.9658.

*Ethynyl(naphthalen-2-yl)selane (**3e**)*. White solid (161.70 mg, 70%). Mp: 116-119 ºC. IR υ_{max} cm^{-1}: 32,68 3052, 1571, 1499, 1352, 1343, 1132, 988, 890, 858, 821, 739, 691. ^1H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, *J* = 1.7 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 3.9 Hz, 3H), 3.12 (s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 134.09, 132.46, 129.24, 128.35, 127.97, 127.32, 126.89, 126.84, 126.39, 124.91, 92.14, 64.96 ppm. HRMS (ESI) *m/z,* calcd for $C_{12}H_8Se$ $(M + H)^+$: 232.9870, found: 233.0046.

*Ethynyl(6-methoxynaphthalen-2-yl)selane (**3f**)*. White solid (232.29 mg, 89%). Mp: 119-121 ºC. IR υ_{max} cm^{-1}: 3257, 2970, 2939, 2114, 1620, 1262, 1212, 1164, 1028, 884, 855, 817. ^1H NMR (300 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.61 (d, *J* = 3.6 Hz, 2H), 7.52 (s, 1H), 7.09 (d, *J* = 11.3 Hz, 2H), 3.84 (s, 3H), 3.10 (s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.07, 133.78, 129.61 (2C), 128.79, 128.03, 121.47, 119.61, 105.88, 90.97,

65.02, 55.35 ppm. HRMS (ESI) *m/z,* calcd for $C_{13}H_{10}OSe$ $(M + H)^+$: 262.9976, found: 262.9438.

*Ethynyl(4-(trifluoromethyl)phenyl)selane (**3g**).* Yellow oil (219.12 mg, 88%). IR υ_{max} cm^{-1}: 3300, 1603, 1402, 1322, 1164, 1104, 1074, 1015, 827, 691. ^1H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 5.6 Hz, 2H), 3.17 (s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.05 (2C), 128.84 (2C), 126.25 (2C), 122.13, 93.10, 63.08 ppm. HRMS (ESI) *m/z,* calcd for $C_9H_5F_3Se$ $(M + H)^+$: 250.9588, found: 250.9408.

*Ethynyl(4-fluorophenyl)selane (**3h**).* Orange oil (167.16 mg, 84%). IR υ_{max} cm^{-1}: 3296, 2855, 1883, 1585, 1486, 1223, 1158, 1015, 821. ^1H NMR (300 MHz, $CDCl_3$) δ 7.44 (d, *J* = 5.7 Hz, 2H), 6.98 (d, *J* = 9.1 Hz, 2H), 3.13(s, 1H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.15, 135.02, 134.92, 125.79, 116.72, 116.43, 91.17, 84.73 ppm. HRMS (ESI) *m/z,* calcd for C_8H_5FSe $(M + H)^+$: 200.9619, found: 200.9081.

Synthesis of Selenoquinolines. In a two-necked flask, 25 mL, under nitrogen flow and mounted heating apparatus (reflux condenser and silicone oil bath) was added *p*-anisidine (1 mmol), The catalyst, $Yb(OTf)_3$ (10 mol%), solvent CH_3CN (5 ml), ethylglyoxalate (1 mmol), acetylenic selenide (1.2 mmol). All reactions were carried out under nitrogen atmosphere. The reaction is quenched with extraction of ethyl acetate and $NaHCO_3$, the organic phase collected and dried over $MgSO_4$, and the solvent removed in vacuum. The organic residue was impregnated on silica column chromatographed using flash silica.

*Ethyl 6-methoxy-4-(phenylselanyl)quinoline-2-carboxylate (**4a**).* Yellow solid (367.03 mg, 69%). Mp: 118–123 ºC. IR υ_{max} cm^{-1}: 2987, 2972, 2929, 2836, 1709, 1620, 1501, 1225, 1022, 825, 745. ^1H NMR (300 MHz, $CDCl_3$) δ 8.18 (d, *J* = 9.3 Hz, 1H), 7.91 (d, *J* = 1.4 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 2H), 7.42 (d, *J* = 6.5 Hz, 4H), 7.31 (s, 1H), 4.44 (q, *J* = 7.0, 6.5 Hz, 2H), 3.92 (s, 3H), 1.39 (t, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.19, 159.64, 144.97, 144.00, 143.03, 135.57 (2C), 132.97, 130.06 (3C), 129.21, 126.80, 123.40, 123.11, 103.38, 62.03, 55.71, 14.26 ppm. HRMS (ESI) *m/z,* calcd for $C_{19}H_{17}NO_3Se$ $(M + H)^+$: 388.0453, found: 388.0273.

*Ethyl 4-(phenylselanyl)quinoline-2-carboxylate (**4b**):* Yellow solid (89.25 mg, 25%). Mp: 97–99 ºC. IR υ_{max} cm^{-1}: 3358, 3054, 2980, 2929, 2905, 1717, 1689, 1495, 1441,

1369, 1311, 1195, 1147, 1110, 1022. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.5 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.80 (s, 2H), 7.69 (d, *J* = 7.5 Hz, 3H), 7.47 (t, *J* = 6.9 Hz, 3H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.10, 147.55, 147.39, 146.97, 136.29 (2C), 131.42, 130.47, 130.18, 129.59, 128.64 (3C), 126.01, 125.16, 121.59, 62.19, 14.21 ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{15}NO_2Se$ $(M + H)^+$: 358.0347, found:357.9950.

*Ethyl 6-chloro-4-(phenylselanyl)quinoline-2-carboxylate (**4c**)*. Yellow solid (156.00 mg, 40%). Mp: 147–149 ºC. IR υ_{max} cm^{-1}: 3077, 3058, 2985, 2942, 2877, 1719, 1480, 1367, 1315, 1181, 832, 737, 693. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (d, *J* = 9.0 Hz, 1H), 8.12 (s, 1H), 7.80 (s, 1H), 7.70 (dd, *J* = 12.9, 8.7 Hz, 2H), 7.47 (q, *J* = 7.0, 6.6 Hz, 3H), 7.26 (s, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.78, 147.54, 146.63, 145.42, 136.26 (2C), 134.87, 132.90, 131.50 (2C), 130.27 (2C), 129.76, 129.53, 124.30, 122.50, 62.28, 14.18 ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{14}ClNO_2Se$ $(M + H)^+$: 391.9957, found: 392.0070.

*Ethyl 6-bromo-4-(phenylselanyl)quinoline-2-carboxylate (**4d**)*. Yellow solid (151.90 mg, 35%), Mp: 133–136 ºC, IR υ_{max} cm^{-1}: 3054, 2939, 2983, 1715, 1479, 1367, 1311, 1181, 830, 817, 739, 691. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.06 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 9.4 Hz, 1H), 7.72 (s, 1H), 7.60 (d, *J* = 6.0 Hz, 2H), 7.39 (q, *J* = 6.9, 5.9 Hz, 3H), 4.35 (q, *J* = 7.1 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.78, 147.63, 146.60, 145.62, 136.31(2C), 134.07, 132.93, 130.28(2C), 129.78, 127.63(2C), 125.73, 123.22, 122.43, 62.28, 14.18 ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{14}BrNO_2Se$ $(M + H)^+$: 435.9452, found: 435.8030.

*Ethyl 6-hydroxy-4-(phenylselanyl)quinoline-2-carboxylate (**4e**)*. Yellow solid (149.20 mg, 40%). Mp: 191–193 ºC. IR υ_{max} cm^{-1}: 2920, 2851, 1723, 1631, 1505, 1322, 1274, 1222, 1113, 1022, 829, 745, 689. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.1 Hz, 1H), 7.80 (s, 1H), 7.58 (d, *J* = 6.4 Hz, 2H), 7.48 – 7.32 (m, 4H), 7.26 (s, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.03, 157.68, 145.40, 143.74, 141.51, 135.90 (2C), 131.85, 130.87, 130.05(2C), 129.36, 126.22, 123.85, 122.08, 107.40, 62.18, 14.05 ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{15}NO_3Se$ $(M + H)^+$: 374.0296, found: 374.0500.

*Ethyl 8-chloro-4-(phenylselanyl)quinoline-2-carboxylate (**4f**)*. Yellow solid (117.00 mg, 30%). Mp: 144–146 ºC. IR υ_{max} cm^{-1}: 2982, 2926, 1728, 1689, 1594, 1525, 1441, 1369, 1298, 1194, 1156, 748, 735, 693. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.82 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.52 (dt, *J* = 27.0, 7.7 Hz, 4H), 4.42 (q, *J* = 7.2 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.84, 148.45, 147.72, 143.57, 136.32(2C), 135.49, 130.64, 130.29(2C), 129.91, 129.79, 128.29, 125.82, 124.17, 122.25, 62.23, 14.11 ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{14}ClNO_2Se$ $(M + H)^+$: 391.9957, found: 391.9300.

*Ethyl 6-methyl-4-(phenylselanyl)quinoline-2-carboxylate (**4g**)*. Yellow solid (204.05 mg, 55%). Mp: 119-121 ºC. IR υ_{max} cm^{-1}: 3058, 2926, 2983, 1737, 1493, 1441, 1216, 1240, 1175, 1112, 1032, 1024, 836, 819, 745, 689. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.6 Hz, 1H), 7.86 (s, 1H), 7.77 (s, 1H), 7.63 (dd, *J* = 19.2, 7.1 Hz, 3H), 7.44 (t, *J* = 6.8 Hz, 3H), 4.42 (q, *J* = 7.0 Hz, 2H), 2.57 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.16, 146.60, 146.23, 145.52, 139.13, 136.24 (2C), 132.77, 131.11, 130.11 (3C), 129.47, 128.81, 126.20, 124.08, 121.70, 62.03, 21.97, 14.22 ppm. HRMS (ESI) *m/z,* calcd for $C_{19}H_{17}NO_2Se$ $(M + H)^+$: 372.0504, found: 371.9020.

*Ethyl 6-chloro-4-((6-methoxynaphthalen-2-yl)selanyl)quinoline-2-carboxylate (**4h**)*. White solid (188.40 mg, 40%). Mp: 189-192 ºC. IR υ_{max} cm^{-1}: 2985, 2965, 1721, 1628, 1315, 1261, 1210, 1184, 1028, 858, 836. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 – 8.02 (m, 2H), 7.69 (dq, *J* = 15.8, 7.7, 6.7 Hz, 4H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.25 – 7.00 (m, 3H), 4.28 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.82, 158.90, 147.55, 147.23, 145.37, 136.48, 134.93, 134.80, 132.97, 132.88, 131.47, 129.78, 129.48, 129.39, 128.80, 124.25, 122.25, 119.86, 119.66, 105.93, 62.21, 55.42, 14.08 ppm. HRMS (ESI) *m/z,* calcd for $C_{23}H_{18}ClNO_3Se$ $(M + H)^+$: 472.0219, found: 471.9740.

*6-methoxy-2-phenyl-4-(phenylselanyl)quinoline (**5b**)*. White solid (195.50 mg, 50%). Mp: 107-110 ºC. IR υ_{max} cm^{-1}: 3060, 2928, 2853, 1620, 1564, 1495, 1458, 1441, 1229, 1032, 823, 743, 693. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.1 Hz, 1H), 7.92 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 9.4 Hz, 3H), 7.47 – 7.32 (m, 8H), 3.91 (s, 3H) ppm.^{13}C NMR (75 MHz, $CDCl_3$) δ 158.01, 154.28, 143.86, 142.89, 139.30, 135.14 (3C), 131.82,

129.93 (2C), 128.76 (3C), 127.72 (3C), 127.19, 122.60, 121.62, 103.82, 55.62 ppm. HRMS (ESI) *m/z,* calcd for $C_{22}H_{17}NOSe$ $(M + H)^+$: 392.0545, found:392.0760.

*4-(6-methoxy-4-(phenylselanyl)quinolin-2-yl)phenol (**5c**).* Orange solid (244.20 mg, 60%). Mp: 196-199 ºC. IR υ_{max} cm^{-1}: 3010, 2932, 1607, 1572, 1499, 1238, 1181, 1035, 834, 745, 694. ^1H NMR (300 MHz, $CDCl_3$) δ 7.25 (s, 1H), 7.21 (d, *J* = 8.3 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 6.79 (s, 2H), 6.78 – 6.74 (m, 3H), 6.73 (s, 2H), 6.61 (d, *J* = 8.9 Hz, 2H), 3.74 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.10, 152.30, 142.45, 131.38, 130.75, 129.05 (2C), 128.40 (2C), 115.51(2C), 115.40 (2C), 115.15 (2C), 115.01(2C), 114.77(2C), 114.48 (2C), 55.90 ppm. HRMS (ESI) *m/z,* calcd for $C_{22}H_{17}NO_2Se(M + H)^+$: 408.0504, found: 407.9070.

*6-methoxy-2-(4-methoxyphenyl)-4-(phenylselanyl)quinolone (**5d**).* Yellow solid (273.65 mg, 65%) Mp: 90-93 ºC. IR υ_{max} cm^{-1}: 2952, 2916, 2838, 1609, 1512, 1493, 1452, 1441, 1251, 1229, 1175, 1032, 823, 743, 734, 691. ^1H NMR (300 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 40.4, 8.8 Hz, 1H), 7.61 (d, *J* = 6.6 Hz, 1H), 7.41 – 7.24 (m, 4H), 6.94 (d, *J* = 8.5 Hz, 1H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 6.58 (d, *J* = 8.0 Hz, 2H), 3.77 (s, 3H), 3.72 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.62, 158.86, 157.80, 142.64, 135.01 (2C), 131.78 (2C), 129.92 (2C), 128.83 (5C), 128.50, 122.43, 121.38, 114.17, 104.06 (2C), 55.29 (2C) ppm. HRMS (ESI) *m/z,* calcd for C23H19NO2Se (M + H)+: 422.0660, found: 422.0140.

*6-methoxy-4-(phenylselanyl)-2-(thiophen-2-yl)quinoline (**5e**).* Yellow solid (198.50 mg, 50%). Mp: 109-112 ºC. IR υ_{max} cm^{-1}: 2929, 2833, 1620, 1564, 1495, 1441, 1236, 1220, 1164, 1033, 825, 747, 694, 681, 674. ^1H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 9.1 Hz, 1H), 7.64 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.53 (s, 1H), 7.46 – 7.30 (m, 6H), 7.28 (d, *J* = 2.9 Hz, 1H), 7.05 (d, *J* = 3.8 Hz, 1H), 3.89 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.87, 149.48, 144.98, 143.60, 142.79, 135.29 (2C), 131.40, 129.95 (4C), 128.92, 127.97, 127.91, 125.04, 122.54, 119.98, 104.02, 55.60 ppm. HRMS (ESI) *m/z,* calcd for $C_{20}H_{15}NOSSe$ $(M + H)^+$: 398.0119, found: 397.8650.

*2-(furan-2-yl)-6-methoxy-4-(phenylselanyl)quinoline (**5f**).* Yellow oil (205.74 mg, 54%). IR υ_{max} cm^{-1}: 2933, 2833, 1620, 1512, 1233, 1033, 1013, 819, 737. ^1H NMR (300 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.2 Hz, 1H), 7.61 (d, *J* = 11.0 Hz, 3H), 7.50 (s, 1H), 7.38 (d, *J* = 7.1 Hz, 5H), 7.29 (s, 1H), 6.93 (d, *J* = 3.4 Hz, 1H), 3.87 (s, 3H) ppm. ^{13}C NMR

(75 MHz, $CDCl_3$) δ 157.97 (2C), 153.33, 143.72 (2C), 141.81, 135.11 (2C), 131.50, 129.92 (2C), 128.81, 128.13, 127.67, 122.63, 120.07, 112.05, 106.88, 104.18, 55.55 ppm. HRMS (ESI) *m/z,* calcd for $C_{20}H_{15}NO_2Se$ $(M + H)^+$: 382.0347, found: 381.9290.

2-(2,5-dimethoxyphenyl)-6-methoxy-4-(phenylselanyl)quinoline ***(5g)****.* Yellow oil (161.58 mg, 58%). IR υ_{max} cm^{-1}: 3058, 2998, 2935, 2833, 1620, 1570, 1495, 1462, 1434, 1262, 1227, 1208, 1179, 1024, 827, 735, 693. ^1H NMR (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 9.1 Hz, 1H), 7.73 (s, 1H), 7.72 – 7.61 (m, 2H), 7.45 (d, *J* = 3.0 Hz, 1H), 7.43 – 7.25 (m, 5H), 6.93 – 6.81 (m, 2H), 3.93 (s, 3H), 3.83 (s, 3H), 3.58 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.00, 154.07, 153.38, 151.50, 143.90, 141.41, 135.64 (2C), 131.78, 129.76 (2C), 0128.71, 127.87, 127.65, 125.51, 122.06, 116.40, 116.03, 114.85, 113.07, 103.71, 56.07, 55.86, 55.61 ppm. HRMS (ESI) *m/z,* calcd for $C_{24}H_{21}NO_3Se$ $(M + H)^+$: 452.0766, found: 452.0350.

2-(2,6-dichlorophenyl)-6-methoxy-4-(phenylselanyl)quinoline ***(5h)****.* Yellow solid (297.70 mg, 65%). Mp: 132-136 ºC. IR υ_{max} cm^{-1}: 2970, 2937, 1620, 1560, 1493, 1428, 1404, 1229, 1032, 827, 789, 754, 739, 698, 668. ^1H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 10.0 Hz, 1H), 7.59 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.42 – 7.30 (m, 8H), 7.22 (d, *J* = 4.1 Hz, 1H), 3.90 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.61, 152.49, 143.52, 142.78, 138.37, 135.05 (2C), 134.79, 131.84, 129.89 (2C), 129.84, 128.78, 128.45, 128.21 (3C), 127.66, 125.02, 122.75, 103.88, 55.68 ppm. HRMS (ESI) *m/z,* calcd for $C_{22}H_{15}C_{l2}NOSe$ $(M + H)^+$: 459.9775, found: 459.8510.

2-(2,6-dimethylphenyl)-6-methoxy-4-(phenylselanyl)quinoline ***(5i)****.* Yellow solid (188.55 mg, 45%). Mp: 125-127 ºC. IR υ_{max} cm^{-1}: 3058, 2918, 2853, 1620, 1570, 1492, 1477, 1441, 1231, 1166, 1028, 925, 834, 775, 739, 693, 681.^1H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, *J* = 10.0 Hz, 1H), 7.60 (d, *J* = 5.1 Hz, 2H), 7.45 – 7.28 (m, 5H), 7.19 – 6.97 (m, 4H), 3.93 (s, 3H), 2.01 (s, 6H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.18, 157.00, 143.76, 142.91, 140.31, 136.00, 135.31, 131.67, 129.92(2C), 128.93, 127.95, 127.72, 127.68(3C), 125.07, 125.03, 122.45, 103.84, 103.80, 55.68, 20.29(2C) ppm. HRMS (ESI) *m/z,* calcd for $C_{24}H_{21}NOSe$ $(M + H)^+$: 420.0867, found: 420.0410.

4-(6-methoxy-4-((4-methoxyphenyl)selanyl)quinolin-2-yl)phenol ***(5j)****.* Yellow solid (174.80 mg, 40%). Mp: 187-191 ºC. IR υ_{max} cm^{-1}: 3358, 2961, 2920, 2840, 1572, 1493, 1443, 1251, 1229, 1173, 1030, 825. ^1H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.1 Hz,

1H), 7.61 (d, *J* = 8.3 Hz, 4H), 7.37 (s, 1H), 7.34 – 7.21 (m, 2H), 7.04 (d, *J* = 8.3 Hz, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.71 (d, *J* = 6.1 Hz, 2H), 3.93 (s, 3H), 3.84 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.83, 157.81, 157.53, 154.76, 138.15(2C), 130.83, 129.07(2C), 128.54(2C), 122.70, 120.10, 116.72, 115.99, 115.94(2C), 115.51, 115.28, 114.86, 103.62, 55.78(2C) ppm. HRMS (ESI) *m/z,* calcd for $C_{23}H_{19}NO_3Se$ $(M + H)^+$: 438.0609, found: 438.0930.

*6-methoxy-2-(2-nitrophenyl)-4-(phenylselanyl)quinoline (**5k**)*. Orange oil (152.60 mg, 35%). IR υ_{max} cm^{-1}: 2931, 2834, 1713, 1609, 1510, 1344, 1238, 1181, 1035, 823, 743. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 9.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.67 – 7.55 (m, 4H), 7.47 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.39 (d, *J* = 5.5 Hz, 4H), 7.33 (s, 1H), 7.22 (s, 1H), 3.92 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.11, 159.37, 144.84, 143.79, 143.55, 140.70, 134.50 (3C), 132.63, 132.46, 130.31, 129.20, 128.61 (2C), 128.17, 125.47, 124.21, 123.66, 122.92, 103.12, 55.70 ppm. HRMS (ESI) *m/z,* calcd for $C_{22}H_{16}N_2O_3Se$ $(M + H)^+$: 437.0405, found: 436.9470.

*Ethyl 4-(benzylselanyl)-6-methoxyquinoline-2-carboxylate (**6b**)*. Yellow solid (240.60 mg, 60%). Mp: 95-99 ºC. IR υ_{max} cm^{-1}: 3438, 2931, 2838, 1706, 1618, 1497, 1322, 1274, 1227, 1117, 1020, 825, 698. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.16 (d, *J* = 9.1 Hz, 1H), 7.41 (s, 1H), 7.34 (d, *J* = 7.1 Hz, 2H), 7.26 (d, *J* = 7.7 Hz, 4H), 4.53 (q, *J* = 7.1 Hz, 2H), 4.35 (s, 2H), 3.90 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.35, 159.59, 144.77, 142.96, 142.85, 132.97, 131.01, 129.08 (2C), 128.72 (2C), 127.52, 123.28, 122.82, 103.63, 62.12, 55.64, 31.18, 14.43. HRMS (ESI) *m/z,* calcd for $C_{20}H_{19}NO_3Se$ $(M + H)^+$: 402.0609, found: 402.0209.

*Ethyl 6-methoxy-4-((4-methoxyphenyl)selanyl)quinoline-2-carboxylate (**6c**)*. Orange solid (200.16 mg, 48%). Mp: 139-143 ºC. IR υ_{max} cm^{-1}: 2961, 2937, 2838, 1709, 1512, 1492, 1229, 1248, 1171, 1108, 1026, 825. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 9.3 Hz, 1H), 7.68 (s, 1H), 7.51 (d, *J* = 7.7 Hz, 2H), 7.36 – 7.29 (m, 1H), 7.17 (d, *J* = 2.8 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.86 (s, 3H), 3.76 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.29, 160.89, 159.49, 145.75, 144.95, 142.78, 138.12 (3C), 132.86, 130.01, 123.23, 121.60, 115.86 (2C), 102.98, 61.93, 55.70, 55.34, 14.23 ppm. HRMS (ESI) *m/z,* calcd for $C_{20}H_{19}NO_4Se$ $(M + H)^+$: 418.0558, found: 418.0900.

Ethyl 6-methoxy-4-(o-tolylselanyl)quinoline-2-carboxylate ***(6d)***. Yellow solid (180.45 mg, 45%). Mp: 92-96 ºC. IR υ_{max} cm^{-1}: 2985, 2959, 2937, 2838, 1711, 1680, 1620, 1505, 1469, 1216, 1182, 1168, 1032, 823, 750. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 9.3 Hz, 1H), 7.64 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.35 – 7.28 (m, 3H), 7.21 (s, 1H), 7.11 (s, 1H), 4.34 (q, *J* = 7.3 Hz, 2H), 3.85 (s, 3H), 2 .35 (s, 3H), 1.29 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.19, 159.60, 145.02, 143.83, 143.00, 142.21, 137.02, 132.97, 130.95, 130.47, 129.99, 127.43, 127.39, 123.31, 122.20, 103.29, 61.95, 55.69, 22.70, 14.23 ppm. HRMS (ESI) *m/z,* calcd. for $C_{20}H_{19}NO_3Se$ $(M + H)^+$: 402.0609, found: 402.0170.

Ethyl 6-methoxy-4-(naphthalen-2-ylselanyl)quinoline-2-carboxylate ***(6e)***. Orange solid (174.80 mg, 40%). Mp: 124-128 ºC. IR υ_{max} cm^{-1}: 3105, 3052, 2987, 1739, 1706, 1613, 1469, 1372, 1220, 1195, 1104, 1020, 830, 814, 747. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.2 Hz, 2H), 7.88 (s, 1H), 7.77 – 7.67 (m, 3H), 7.52 – 7.42 (m, 3H), 7.34 – 7.25 (m, 2H), 4.29 (q, *J* = 7.1 Hz, 2H), 3.80 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.15, 159.72, 145.03, 143.10, 135.14, 134.14, 133.12, 132.97, 131.62, 130.57, 129.66, 127.92, 127.67, 127.12, 126.87, 124.22, 123.52, 123.43, 114.33, 103.54, 61.98, 55.70, 14.16 ppm. HRMS (ESI) *m/z,* calcd. for $C_{23}H_{19}NO_3Se$, $(M + H)^+$: 438.0609 found: 438.0140.

Ethyl 6-methoxy-4-((6-methoxynaphthalen-2-yl)selanyl)quinoline-2-carboxylate ***(6f)***. Yellow solid (210.15 mg, 45%). Mp: 169-172 ºC. IR υ_{max} cm^{-1}: 2920, 2853, 1706, 1620, 1512, 1499, 1264, 1227, 1212, 1108, 1024, 827. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 – 8.02 (m, 2H), 7.81 (s, 1H), 7.65 (dd, *J* = 11.8, 8.8 Hz, 2H), 7.51 (d, *J* = 10.2 Hz, 1H), 7.33 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.26 (d, *J* = 2.3 Hz, 1H), 7.11 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.07 (s, 1H), 4.28 (t, *J* = 7.1 Hz, 2H), 3.85 (s, 6H), 1.22 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.19, 159.62, 158.71, 144.98, 144.69, 142.96, 135.66, 134.67, 132.88, 132.67, 130.38, 129.72, 129.27, 128.57, 123.36, 122.77, 120.71, 119.74, 105.91, 103.35, 61.94, 55.70, 55.39, 14.15 ppm. HRMS (ESI) *m/z,* calcd for $C_{24}H_{21}NO_4Se$ $(M + H)^+$: 468.0715, found: 467.9210.

Ethyl 6-methoxy-4-((4-(trifluoromethyl)phenyl)selanyl)quinoline-2-carboxylate ***(6g)***. Yellow solid (204.75 mg, 45%). Mp: 132-135 ºC. IR υ_{max} cm^{-1}: 2972, 2836, 1736, 1682, 1618, 1501, 1324, 1223, 1164, 1026, 1017, 840, 823. ^{1}H NMR (300 MHz, $CDCl_3$) δ

8.13 (d, *J* = 9.2 Hz, 1H), 8.04 (s, 1H), 7.58 – 7.45 (m, 4H), 7.36 (dd, *J* = 9.3, 2.7 Hz, 1H), 7.26 (d, *J* = 2.7 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.95, 160.09, 145.12, 143.45, 140.86, 133.82 (4C), 133.18 (2C), 130.93, 126.58, 126.52, 125.47, 123.68, 103.89, 62.17, 55.68, 14.23 ppm. HRMS (ESI) *m/z,* calcd for $C_{20}H_{16}F_3NO_3Se$ $(M + H)^+$: 456.0327, found: 455.9150.

*Ethyl 4-((4-fluorophenyl)selanyl)-6-methoxyquinoline-2-carboxylate (**6h**).* Yellow solid (121.50 mg, 30%). Mp: 162-165 ºC. IR υ_{max} cm^{-1}: 2976, 2939, 2840, 1732, 1616, 1581, 1486, 1462, 1223, 1216, 1112, 1024, 843, 830, 817. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18 (d, *J* = 9.4 Hz, 1H), 7.82 (s, 1H), 7.72 – 7.57 (m, 2H), 7.43 (d, *J* = 9.4 Hz, 1H), 7.26 (s, 1H), 7.13 (t, *J* = 7.6 Hz, 2H), 4.45 (q, *J* = 7.0 Hz, 2H), 3.96 (s, 3H), 1.40 (t, *J* = 7.0 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.17, 161.91, 159.68, 144.98, 144.24, 142.96, 138.17, 138.09, 138.06, 133.00, 130.14, 123.41, 122.41, 117.61, 117.32, 103.10, 62.09, 55.72, 14.26 ppm. HRMS (ESI) *m/z,* calcd for $C_{19}H_{16}FNO_3Se$ $(M + H)^+$: 406.0359, found: 405.9900.

Synthesis of Derivatives of Sonogashira Reaction. In a two-necked flask, under nitrogen flow and mounted heating apparatus (reflux condenser and silicone oil bath) were added the oxazoline compounds (20 mol%), palladium chloride (10 mol%) and the solvent the compound 6-methoxy-4- (phenylselenyl) quinoline-2-carboxylate (1 mmol) was added after 15 minutes, then the compound 2-methylbut-3-yn-ol (2 mmol) and the base (2 mmol). The solution was stirred at 80 ºC until the total consumption of the starting material (TLC) (24 hours). To the mixture was added saturated NH_4Cl solution and then extracted with ethyl acetate three times. The organic phase was dried with $MgSO_4$, the solvent was evaporated under reduced pressure. The product was purified by column chromatography on silica.

*Ethyl 4-(3-hydroxy-3-methylbut-1-yn-1-yl)-6-methoxyquinoline-2-carboxylate (**8a**).* Orange solid (234.75 mg, 75%). Mp: 138-141 ºC. IR υ_{max} cm^{-1}. 3367, 3326, 2980, 2929, 1717, 1620, 1479, 1372, 1272, 1227, 1112, 1017, 830. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (t, *J* = 4.6 Hz, 2H), 7.40 (s, 1H), 7.19 (s, 1H), 4.47 (q, *J* = 6.9 Hz, 2H), 3.91 (s, 3H), 1.67 (s, 6H), 1.41 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.11, 160.10, 145.16, 143.69, 132.75 (2C), 130.43, 128.57, 124.07, 123.44 (2C), 103.19,

65.82, 62.14, 55.53, 31.44 (2C), 14.37 ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{19}NO_4$ $(M + H)^+$: 314.1393, found: 314.1213.

*Ethyl 6-methoxy-4-((trimethylsilyl)ethynyl)quinoline-2-carboxylate (**8b**)*. Orange oil (147.15 mg, 45%). IR υ_{max} cm^{-1}: 2957, 2928, 2853, 1717, 1620, 1477, 1223, 1106, 1024, 845, 836. ^1H NMR (300 MHz, $CDCl_3$) δ 8.27 – 8.15 (m, 2H), 7.56 (s, 1H), 7.26 (s, 1H), 4.54 (q, *J* = 7.2 Hz, 2H), 3.99 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 0.36 (s, 9H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.29, 160.32, 145.31, 143.90, 135.75, 132.91, 128.79, 124.32, 123.79, 103.47, 100.41 (2C), 62.34, 55.69, 14.57, 0.00 (3C) ppm. HRMS (ESI) *m/z,* calcd for $C_{18}H_{21}NO_3Si$ $(M + H)^+$: 328.1370, found: 328.0970.

*Ethyl 4-(3-hydroxyprop-1-yn-1-yl)-6-methoxyquinoline-2-carboxylate (**8c**)*. Orange solid (151.05 mg, 53%). Mp: 130-133 ºC. IR υ_{max} cm^{-1}: 3324, 2976, 2933, 2851, 1711, 1620, 1477, 1439, 1371, 1223, 1110, 1022, 834, 730, 694.^1H NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 5.8 Hz, 2H), 7.44 (s, 1H), 7.26 (s, 1H), 4.68 (s, 2H), 4.53 (q, *J* = 7.1 Hz, 2H), 3.97 (s, 3H), 3.59 (s, 1H), 1.48 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.01, 160.11, 144.84, 134.50, 132.46, 129.20, 128.61, 124.21, 123.66, 103.12, 97.93, 66.90, 62.19, 55.70, 51.44, 14.35 ppm. HRMS (ESI) *m/z,* calcd for $C_{16}H_{15}NO_4$ $(M + H)^+$: 286.1080, found: 286.1150.

*Ethyl 4-(4-hydroxybut-1-yn-1-yl)-6-methoxyquinoline-2-carboxylate (**8d**)*. Orange solid (170.43 mg, 57%). Mp: 101-105 ºC. IR υ_{max} cm^{-1}: 3328, 2931, 2885, 2227, 1719, 1620, 1477, 1371, 1220, 1110, 1032, 845. ^1H NMR (300 MHz, $CDCl_3$) δ 8.15 (d, *J* = 9.0 Hz, 1H), 7.98 (s, 1H), 7.35 (d, *J* = 9.5 Hz, 2H), 4.52 (q, *J* = 7.0 Hz, 2H), 3.91 (s, 3H), 3.74 (t, *J* = 6.3 Hz, 2H), 2.51 (t, *J* = 6.3 Hz, 2H), 1.48 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.98, 159.86, 144.58, 143.31, 132.15, 130.57, 129.49, 123.77, 123.49, 103.15, 98.53, 62.10, 60.84, 60.62, 55.58, 23.49, 14.32 ppm. HRMS (ESI) *m/z,* calcd for $C_{17}H_{17}NO_4$ $(M + H)^+$: 300.1237, found: 300.087.

*Ethyl 6-methoxy-4-((4-methoxyphenyl)ethynyl)quinoline-2-carboxylate (**8e**)*. Brown solid (223.82 mg, 62%). Mp: 101-105 ºC. IR υ_{max} cm^{-1}: 3451, 2931, 2836, 2201, 1709, 1607, 1512, 1223, 1110, 1018, 832.^1H NMR (300 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.21 (d, *J* = 9.1 Hz, 1H), 7.69 – 7.56 (m, 4H), 6.95 (d, *J* = 8.3 Hz, 2H), 4.55 (q, *J* = 7.1 Hz, 2H), 4.02 (s, 3H), 3.87 (s, 3H), 1.49 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.26, 160.61, 160.00, 145.26, 143.78, 135.51, 133.52, 132.73, 130.31, 130.04,

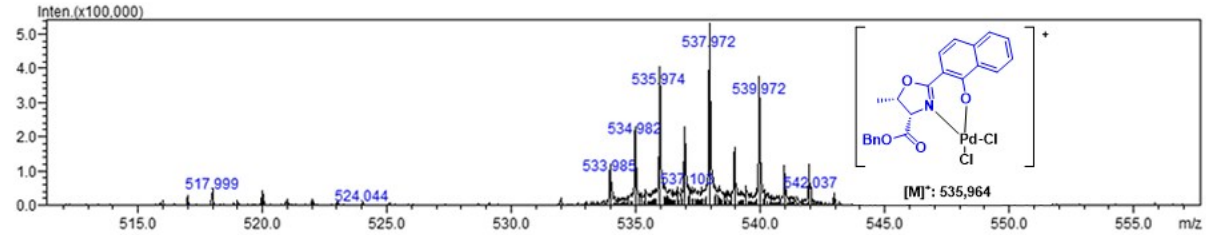
129.56, 123.72, 123.36, 114.34, 103.49, 99.68, 84.09, 76.59, 62.10, 55.61, 55.39, 14.39 ppm. HRMS (ESI) *m/z,* calcd for $C_{22}H_{19}NO_4$ $(M + H)^+$: 362.1393, found: 362.0950.

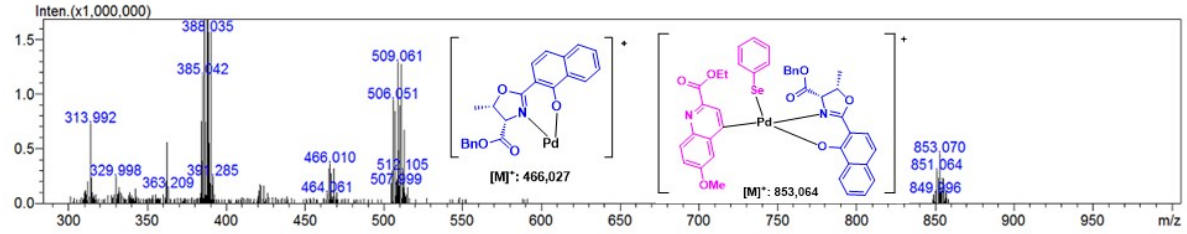
Ethyl 4-(hex-1-yn-1-yl)-6-methoxyquinoline-2-carboxylate ***(8f)***. Orange solid (171.05 mg, 55%). Mp: 52-55 ºC. IR υ_{max} cm^{-1}: 2963, 2931, 2231, 1734, 1715, 1618, 1479, 1216, 1108, 1022, 851, 840. ^1H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 7.0 Hz, 2H), 7.53 (d, *J* = 2.8 Hz, 1H), 7.42 (d, *J* = 9.3 Hz, 1H), 4.54 (q, *J* = 7.1 Hz, 2H), 3.98 (s, 3H), 2.62 (t, *J* = 6.8 Hz, 2H), 1.70 (q, *J* = 7.4, 7.0 Hz, 2H), 1.59 (q, *J* = 7.1 Hz, 2H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.00 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.28, 159.90, 145.17, 143.68, 132.61, 130.77, 130.13, 123.99, 123.38, 103.32, 101.39, 62.07 (2C), 55.55, 30.56, 22.05, 19.48, 14.38, 13.60 ppm. HRMS (ESI) *m/z,* calcd for $C_{19}H_{21}NO_3$ $(M + H)^+$: 312.3828, found: 312.1760.

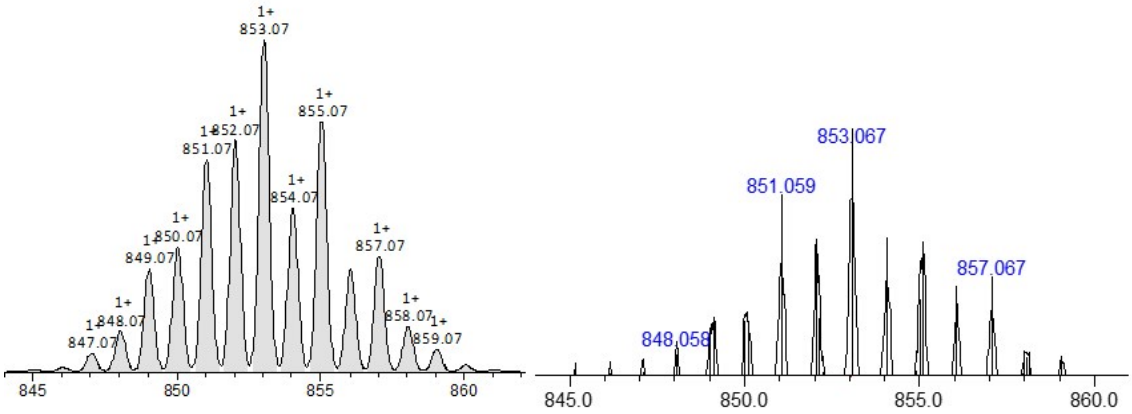
Ethyl 4-((4-aminophenyl)ethynyl)-6-methoxyquinoline-2-carboxylate ***(8g)***. Brown solid (221.44 mg, 64%). Mp: 154-159 ºC. IR υ_{max} cm^{-1}: 3373, 2929, 2197, 1700, 1605, 1510, 1480, 1270, 1225, 1112, 1018, 836, 829. ^1H NMR (300 MHz, $CDCl_3$) δ 8.26 (s, 1H), 8.19 (d, *J* = 9.1 Hz, 1H), 7.64 (d, *J* = 2.7 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.26 (s, 1H), 6.69 (d, *J* = 8.1 Hz, 2H), 4.55 (q, *J* = 7.1 Hz, 2H), 4.01 (s, 3H), 1.49 (t, *J* = 7.1 Hz, 3H) ppm.^{13}C NMR (75 MHz, $CDCl_3$) δ 165.33, 159.88, 147.90, 145.24, 143.75, 133.89, 133.49, 132.63, 130.29, 129.99, 123.42, 123.29, 114.74, 114.61, 111.10, 103.57, 100.95, 83.53, 62.06, 55.60, 14.39 ppm. HRMS (ESI) *m/z,* calcd for $C_{21}H_{18}N_2O_3$ $(M + H)^+$: 347.1396, found: 347.0980.

Ethyl 6-methoxy-4-((2-nitrophenyl)ethynyl)quinoline-2-carboxylate ***(8h)***. Brown solid (142.88 mg, 38%). Mp: 143-146 ºC. IR υ_{max} cm^{-1}: 2970, 2082, 1709, 1607, 1525, 1475, 1439, 1343, 1270, 1229, 1199, 1106, 1018, 856, 836, 788, 694. ^1H NMR (300 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.18 (t, *J* = 8.6 Hz, 2H), 7.85 (d, *J* = 8.9 Hz, 2H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 9.4 Hz, 1H), 4.56 (q, *J* = 6.8 Hz, 2H), 4.10 (s, 3H), 1.50 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.09, 160.74, 149.37, 144.85, 143.86, 135.29, 133.26, 132.53, 130.64, 129.78, 127.90, 125.00, 124.61, 124.38, 117.73, 103.31, 93.56, 92.38, 62.21, 56.30, 14.41 ppm. HRMS (ESI) *m/z,* calcd for $C_{21}H_{16}N_2O_5$ $(M + H)^+$: 377.1138, found: 377.0958.

III. Copies of high resultion (ESI-TOF) mass spectrometry spectra

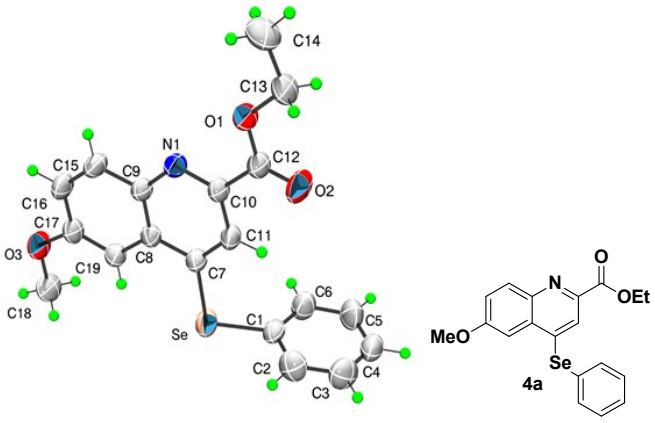


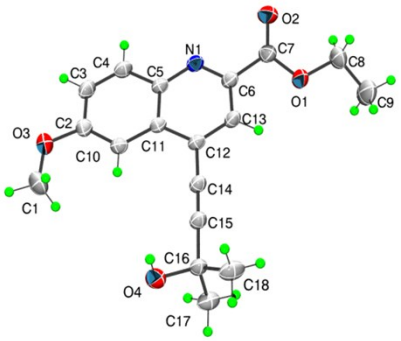


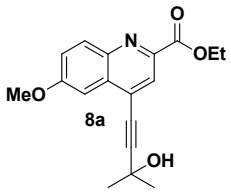


Simulated Experimental

IV. The X-ray crystal structure of 4a and 8a

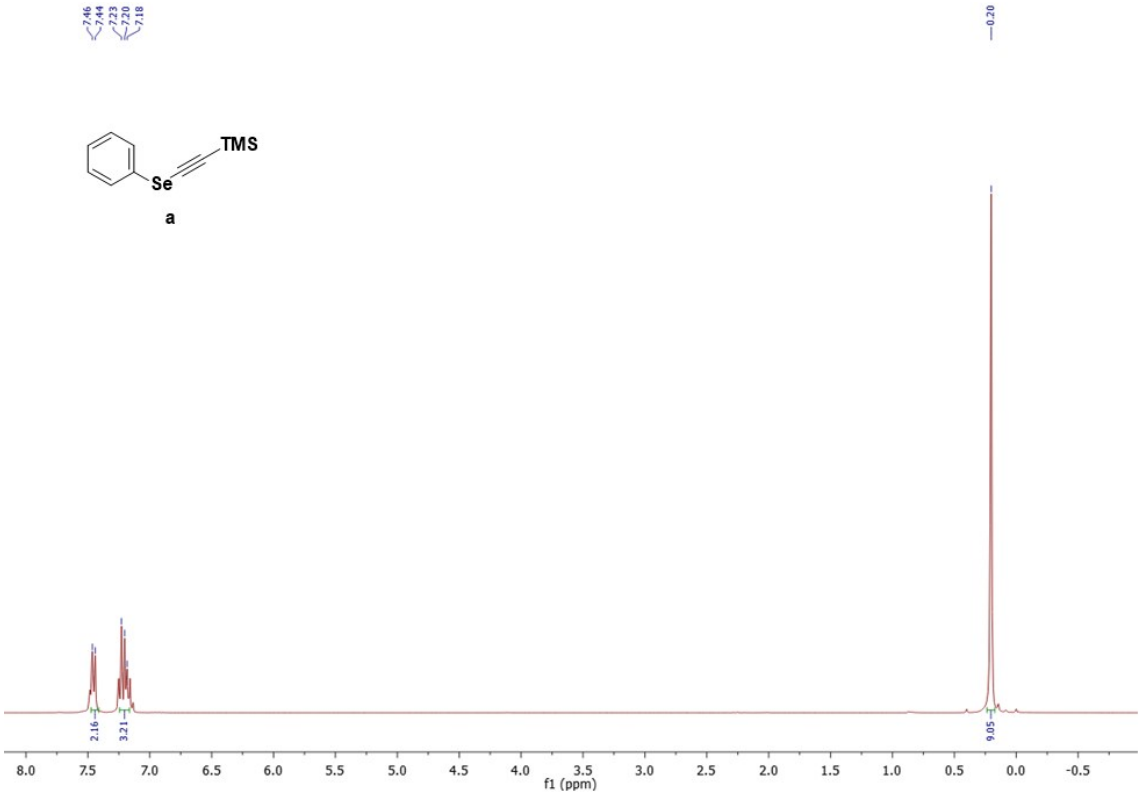


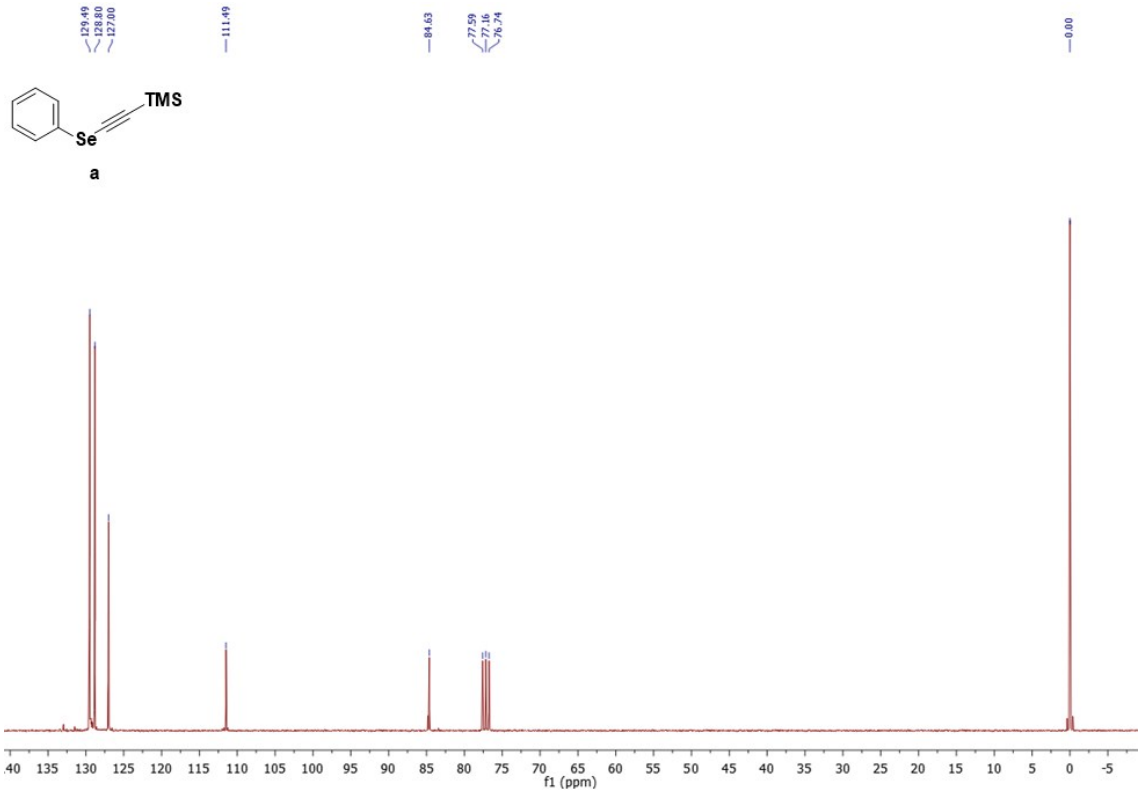

O2
N1
C7
C8
C4
C3
C5
C6
O1
C9
O3
C2
C13
C10
C11
C12
C14
C1
C15
C16
O4
C18
C17

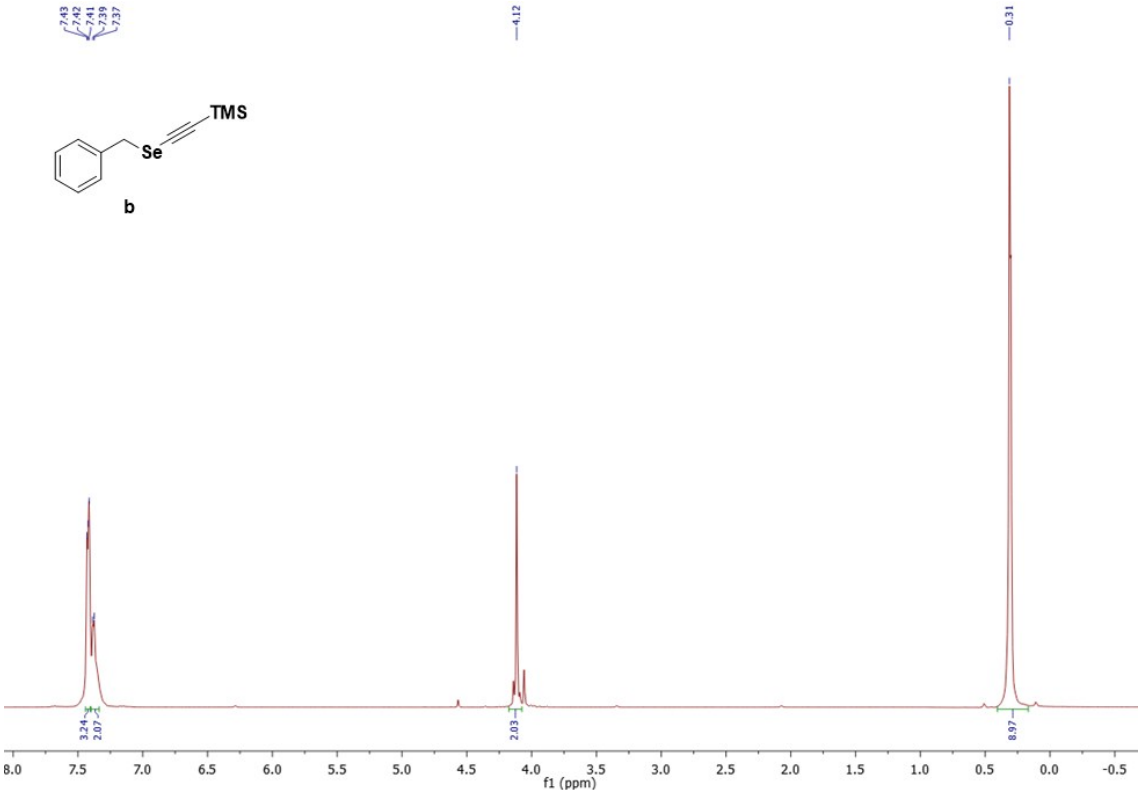

O
N
OEt
MeO
OH

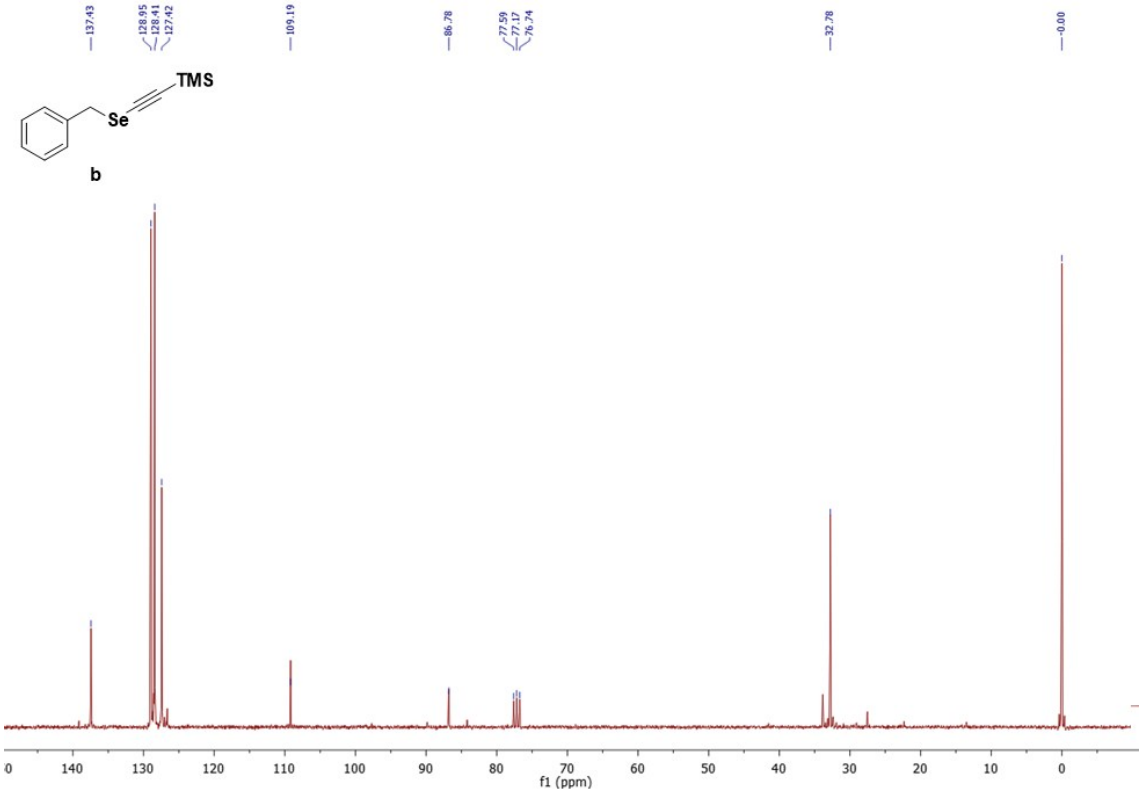
8a

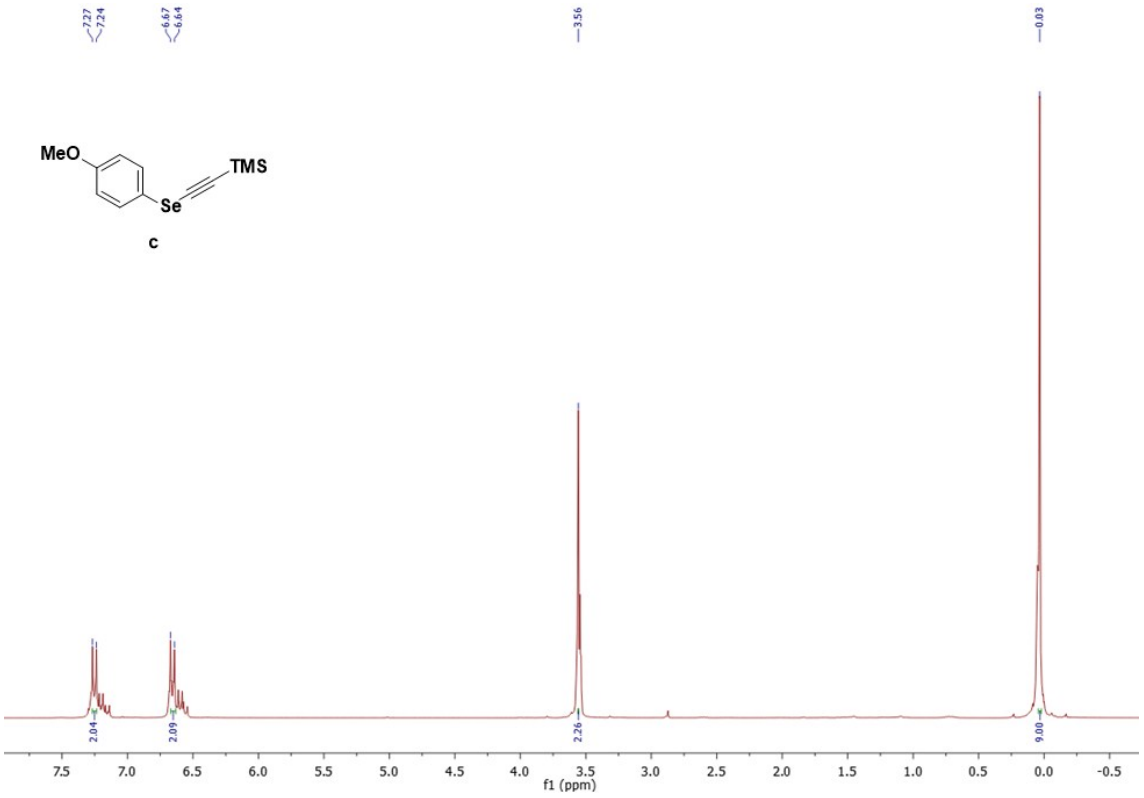
V. Copies of ^{1}H NMR and ^{13}C NMR Spectra of all compounds.

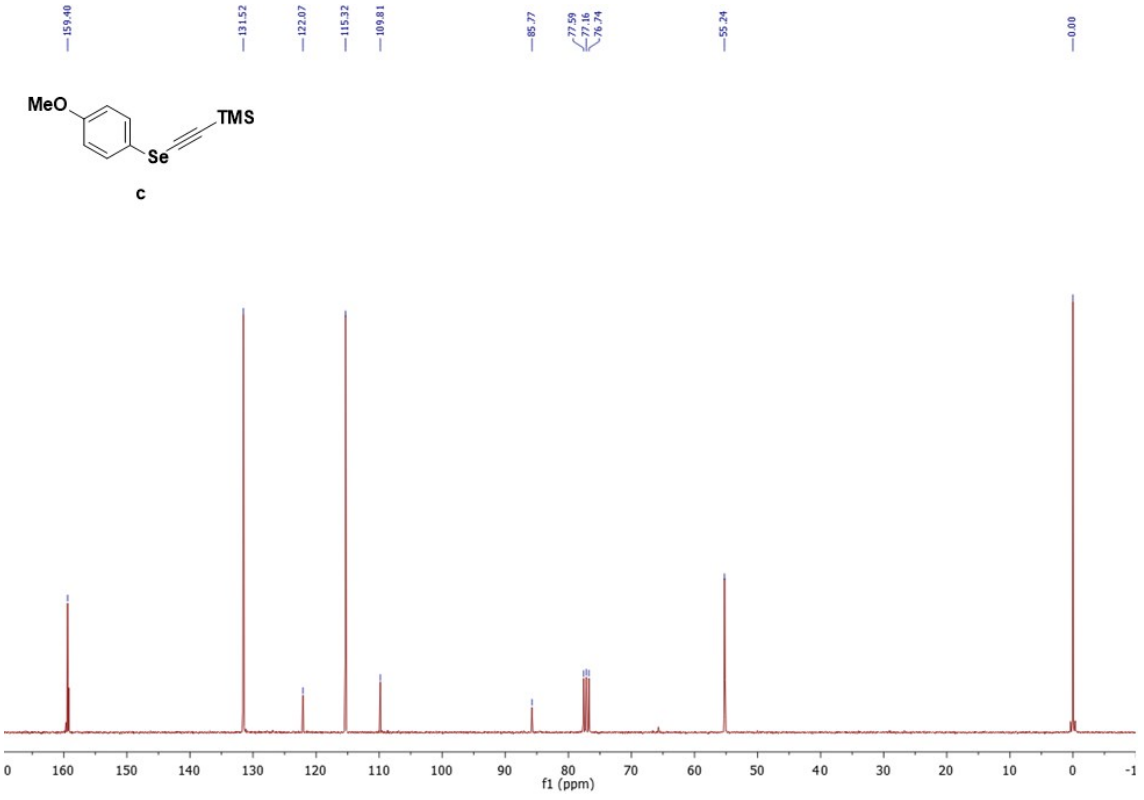


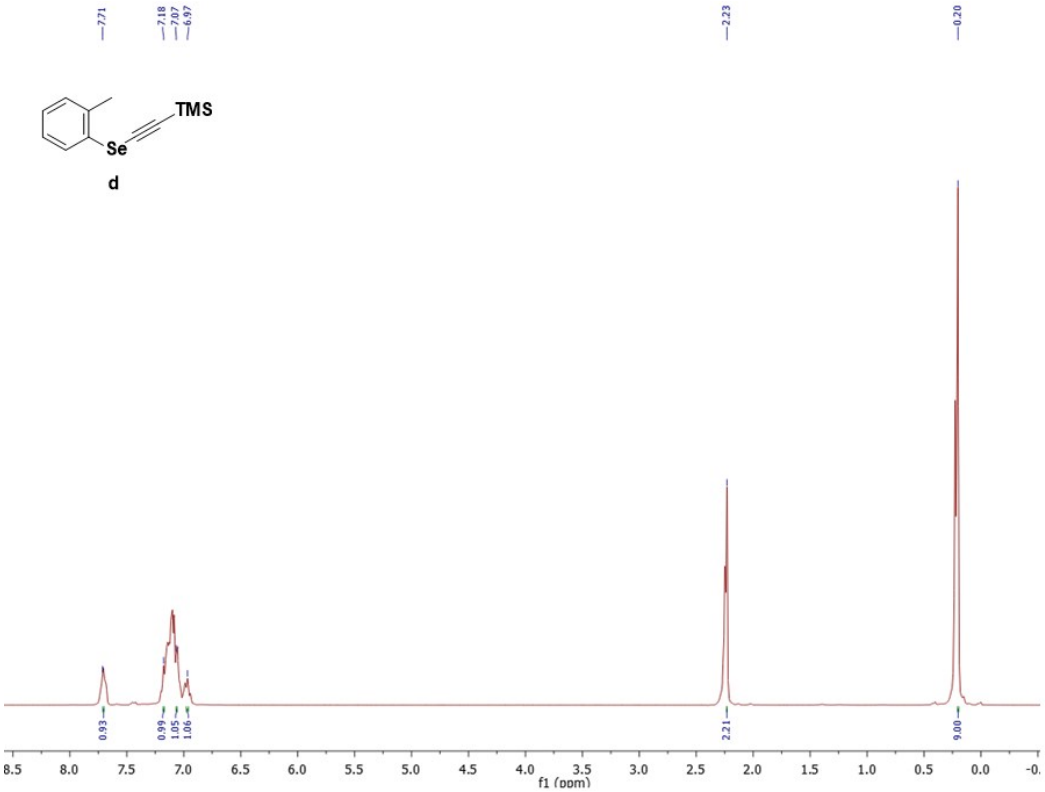


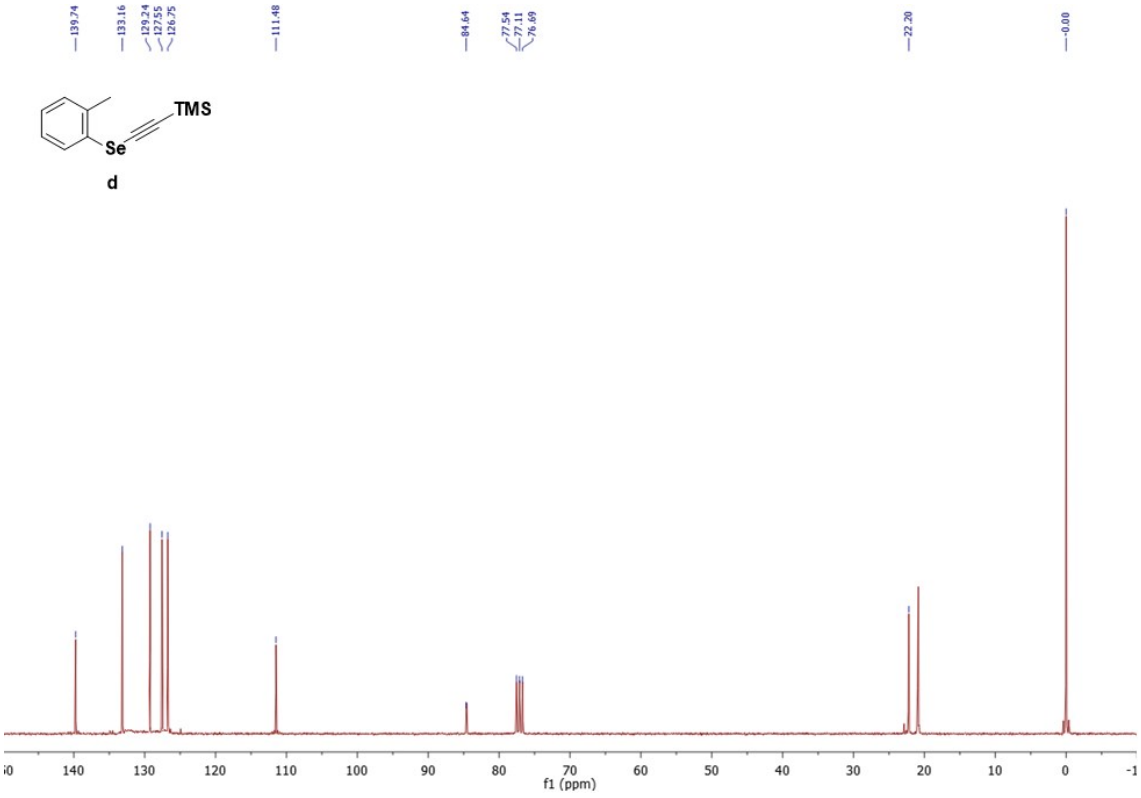

7.43
7.42
7.41
7.39
7.37
4.12
0.31
TMS
Se
b
3.24
2.07
2.03
8.97
f1 (ppm)

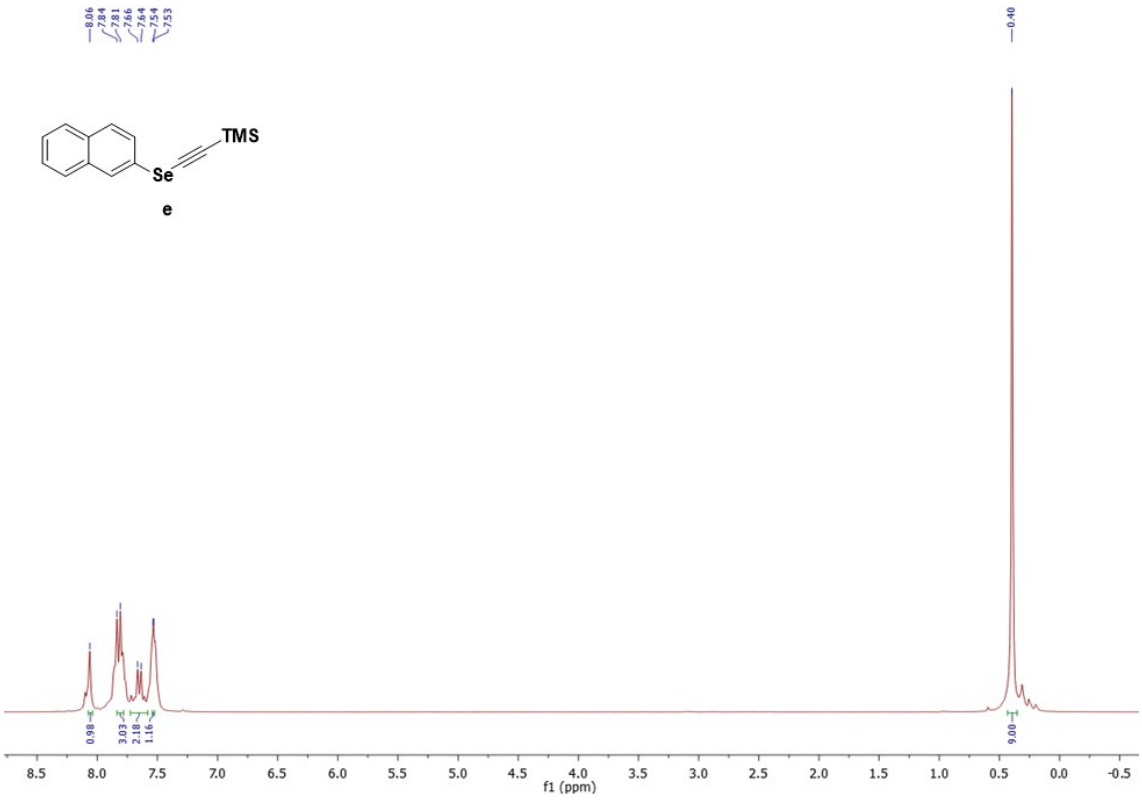

137.43
128.95
128.41
127.42
109.19
86.78
77.59
77.17
76.74
32.78
0.00
TMS
Se
b
f1 (ppm)

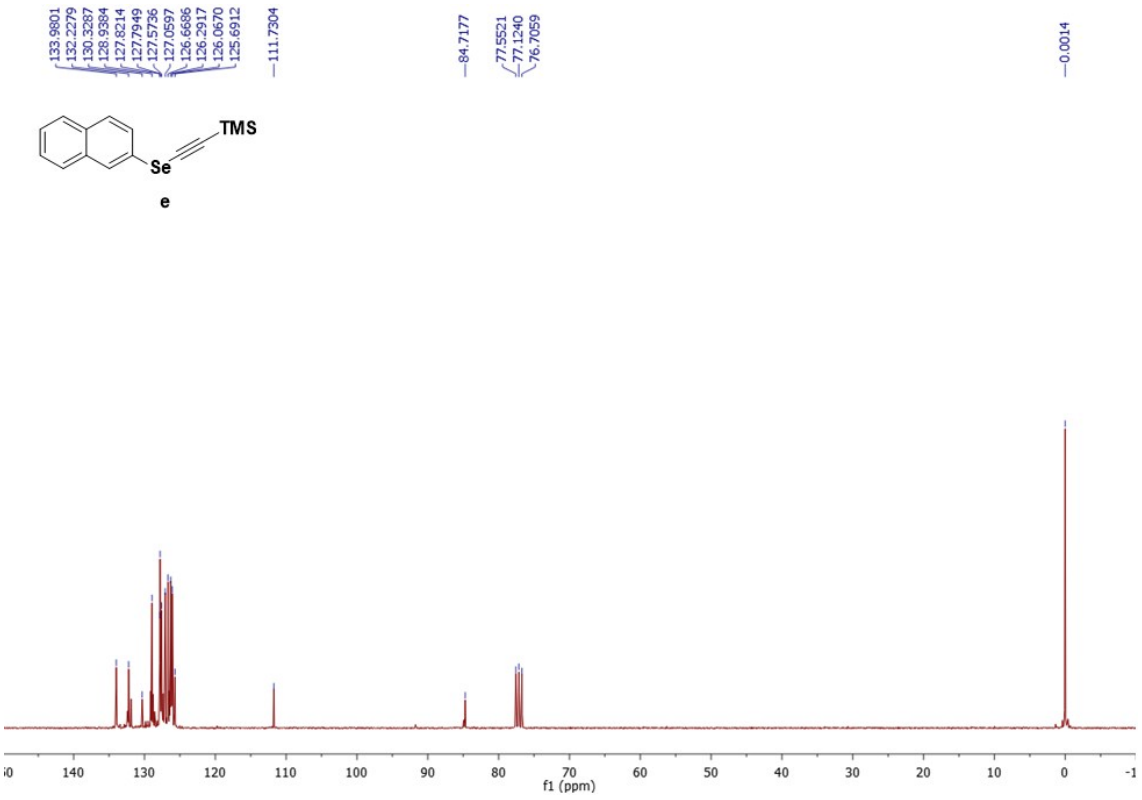

7.27
7.24
6.67
6.64
3.56
0.03
MeO
TMS
Se
c
2.04
2.09
2.26
9.00
f1 (ppm)

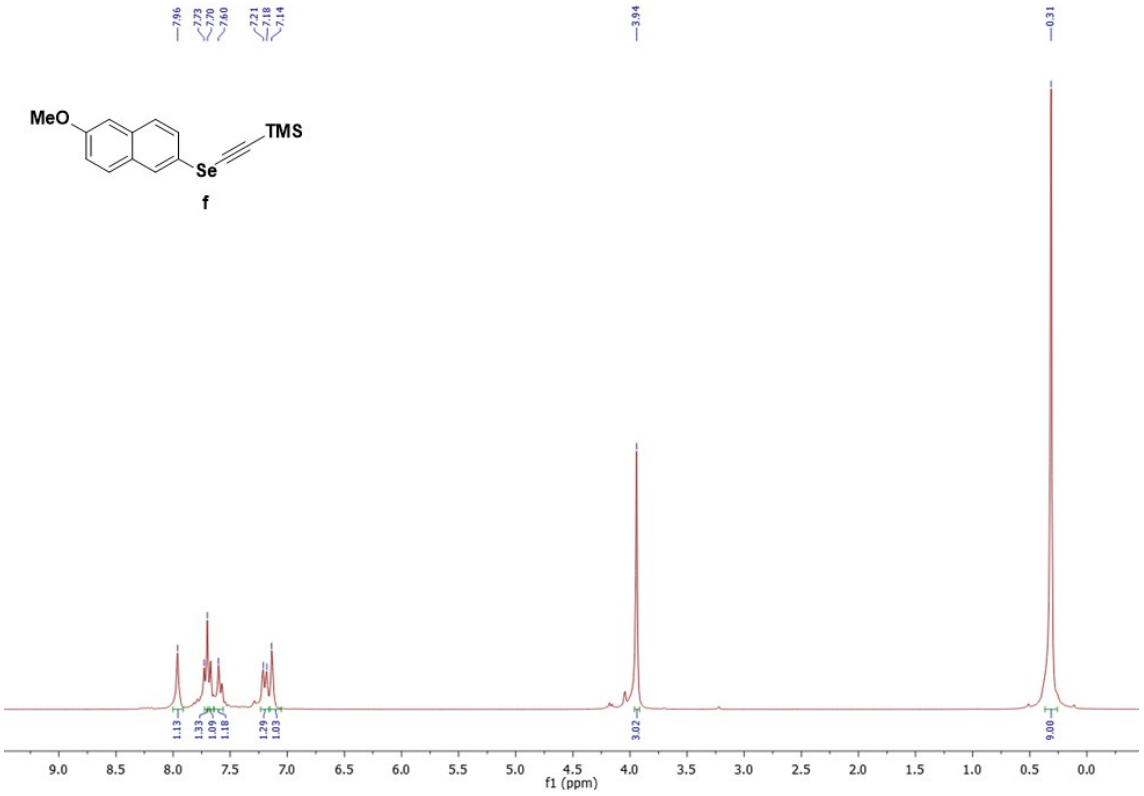

159.40
131.52
122.07
115.32
109.81
85.77
77.59
77.16
76.74
55.24
0.00
MeO
TMS
Se
c
f1 (ppm)

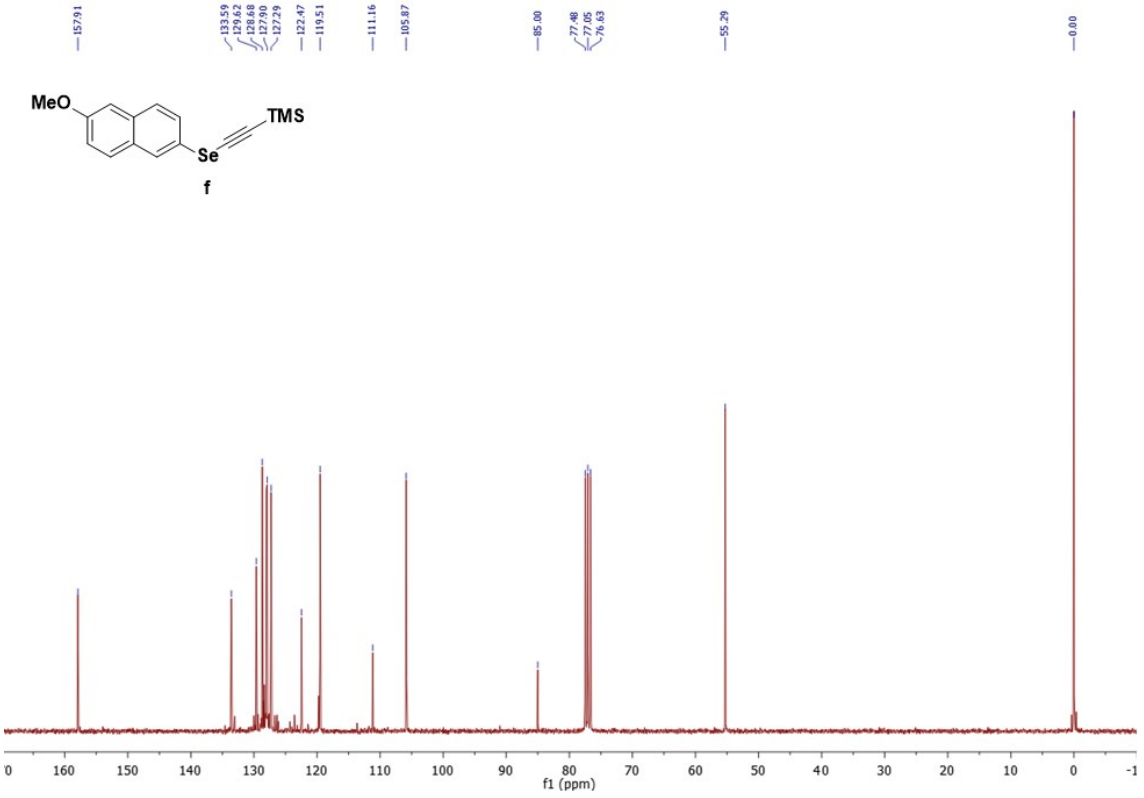

7.71
7.18
7.07
6.97
2.23
0.20
TMS
Se
d
0.93
0.99
1.05
1.06
2.21
9.00
f1 (ppm)

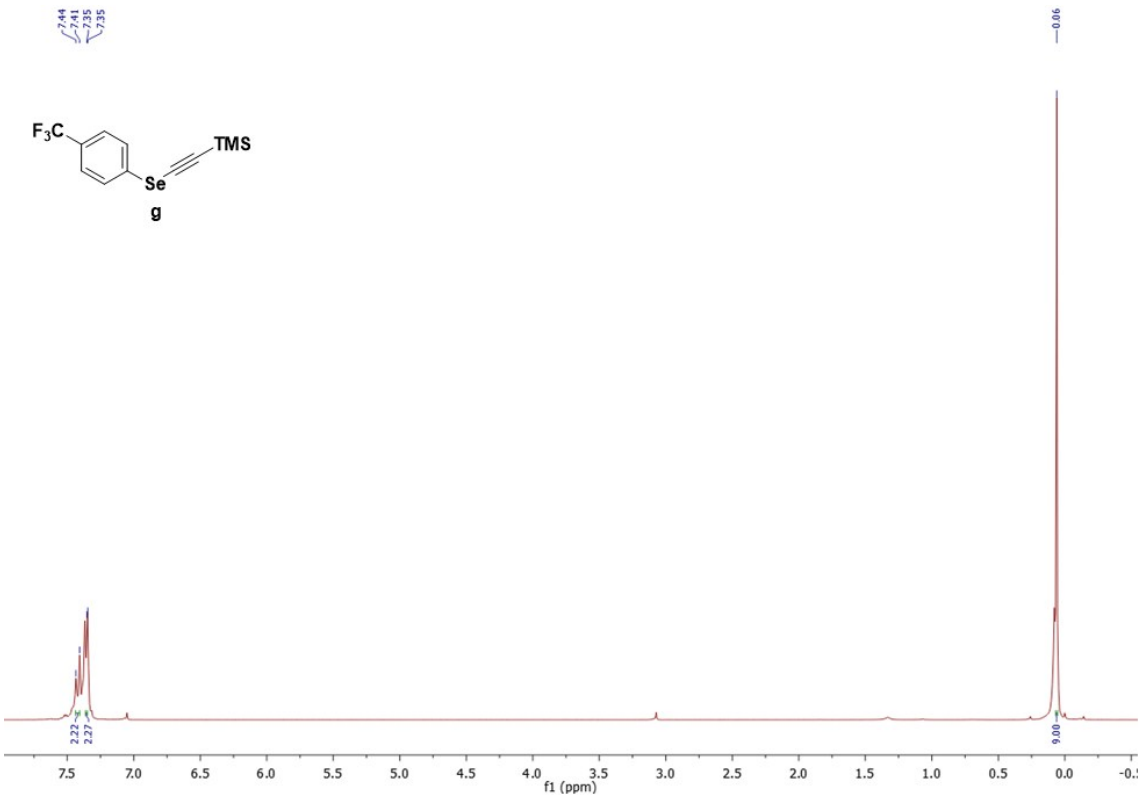

139.74
133.16
129.24
127.55
126.75
111.48
84.64
77.54
77.11
76.69
22.20
0.00
TMS
Se
d
f1 (ppm)

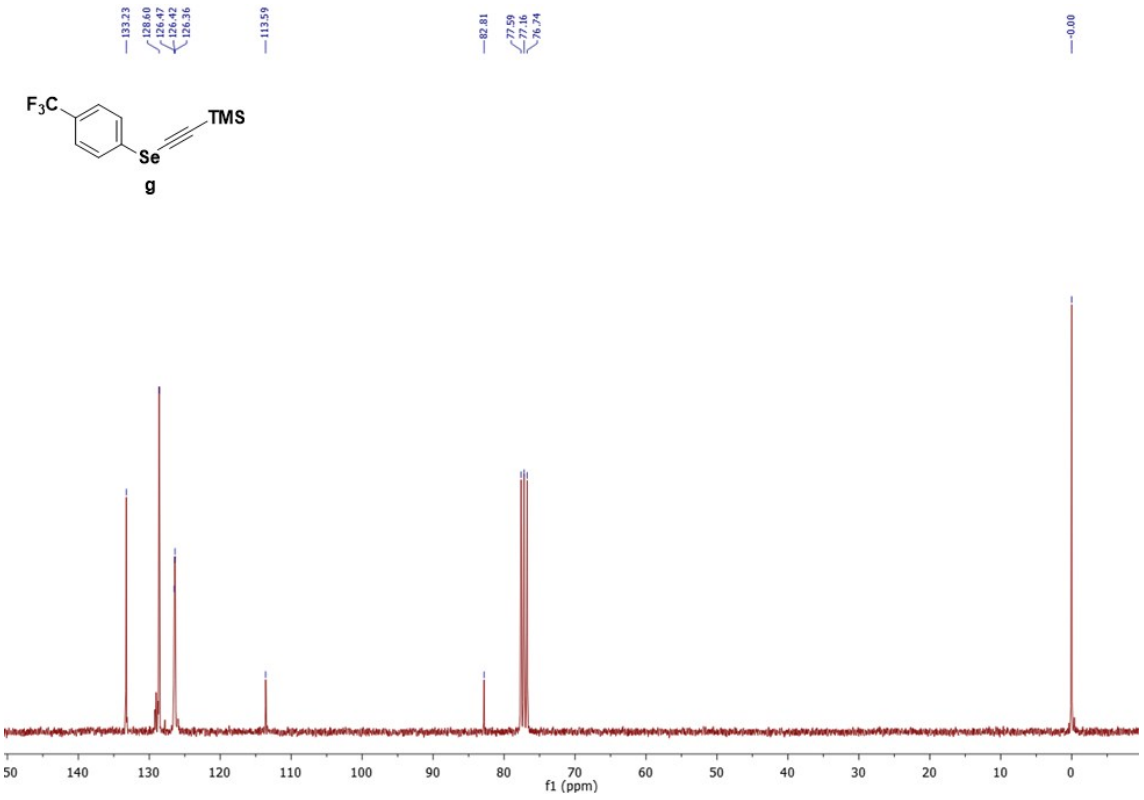

8.06
7.84
7.81
7.66
7.64
7.54
7.53
0.40
TMS
Se
e
0.98
3.03
2.18
1.16
9.00
f1 (ppm)

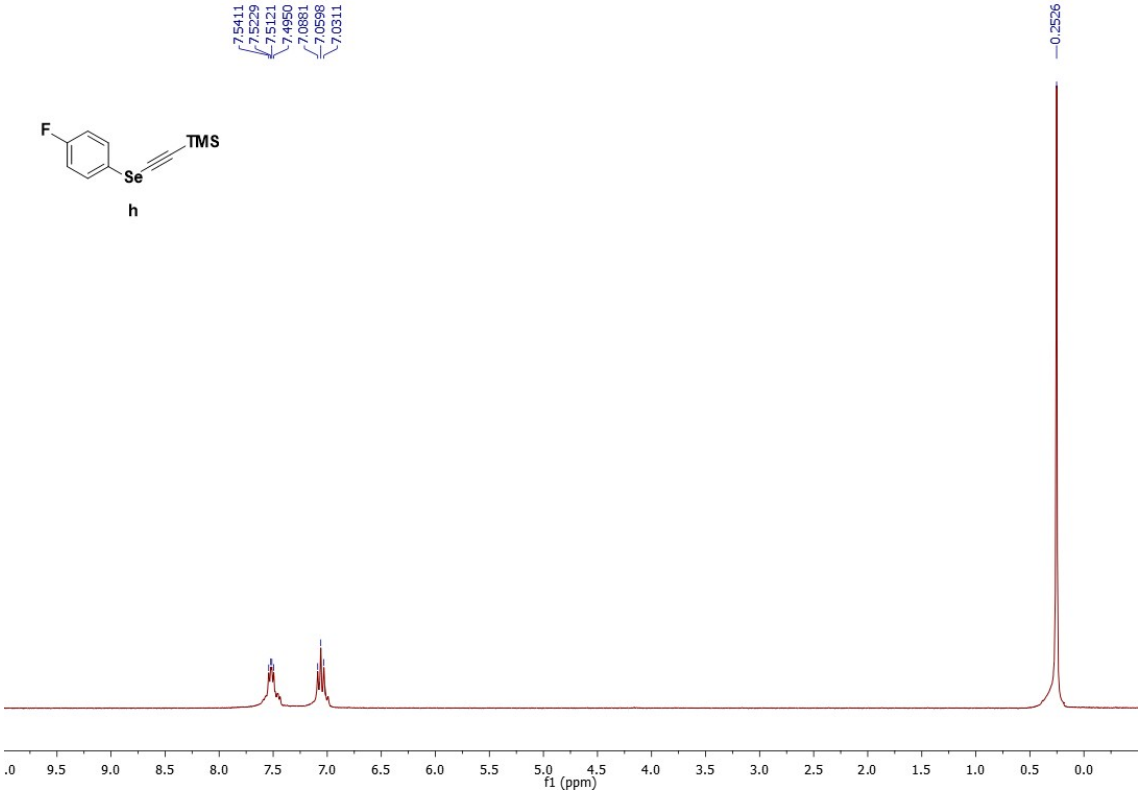

133.9801
132.2279
130.3287
128.9384
127.8214
127.7949
127.5736
127.0597
126.6686
126.2917
126.0670
125.6912
111.7304
84.7177
77.5521
77.1240
76.7059
0.0014
TMS
Se
e
f1 (ppm)

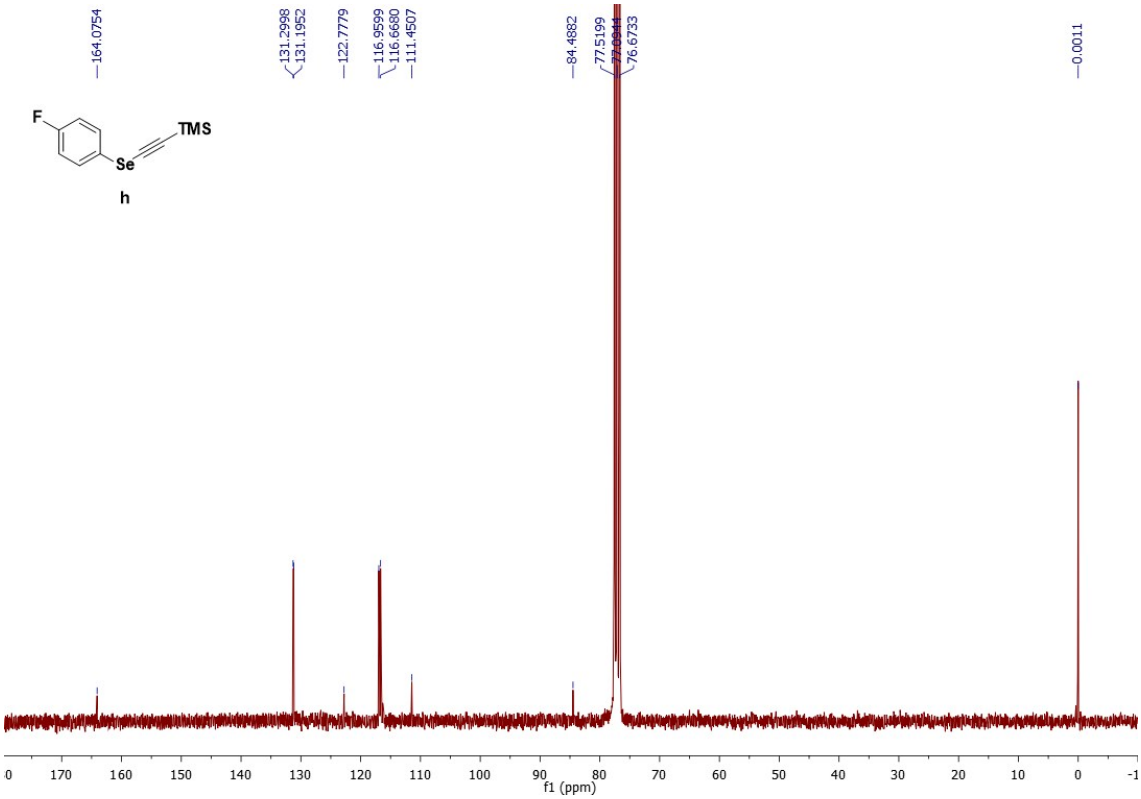

7.96
7.73
7.70
7.60
7.21
7.18
7.14
3.94
0.31
MeO
TMS
Se
f
1.13
1.33
1.08
1.18
1.29
1.03
3.02
9.00
f1 (ppm)


157.91
133.59
129.62
128.68
127.90
127.29
122.47
119.51
111.16
105.87
85.00
77.48
77.05
76.63
55.29
0.00
MeO
TMS
Se
f
f1 (ppm)


7.44
7.41
7.35
7.35
0.06
F3C
TMS
Se
g
2.22
2.27
9.00
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)


133.23
128.60
126.47
126.42
126.36
113.59
82.81
77.59
77.16
76.74
0.00
F3C
TMS
Se
g
50
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.5411
7.5229
7.5121
7.4950
7.0881
7.0598
7.0311
0.2526
F
TMS
Se
h
f1 (ppm)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131.1952
122.7779
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116.6680
111.4507
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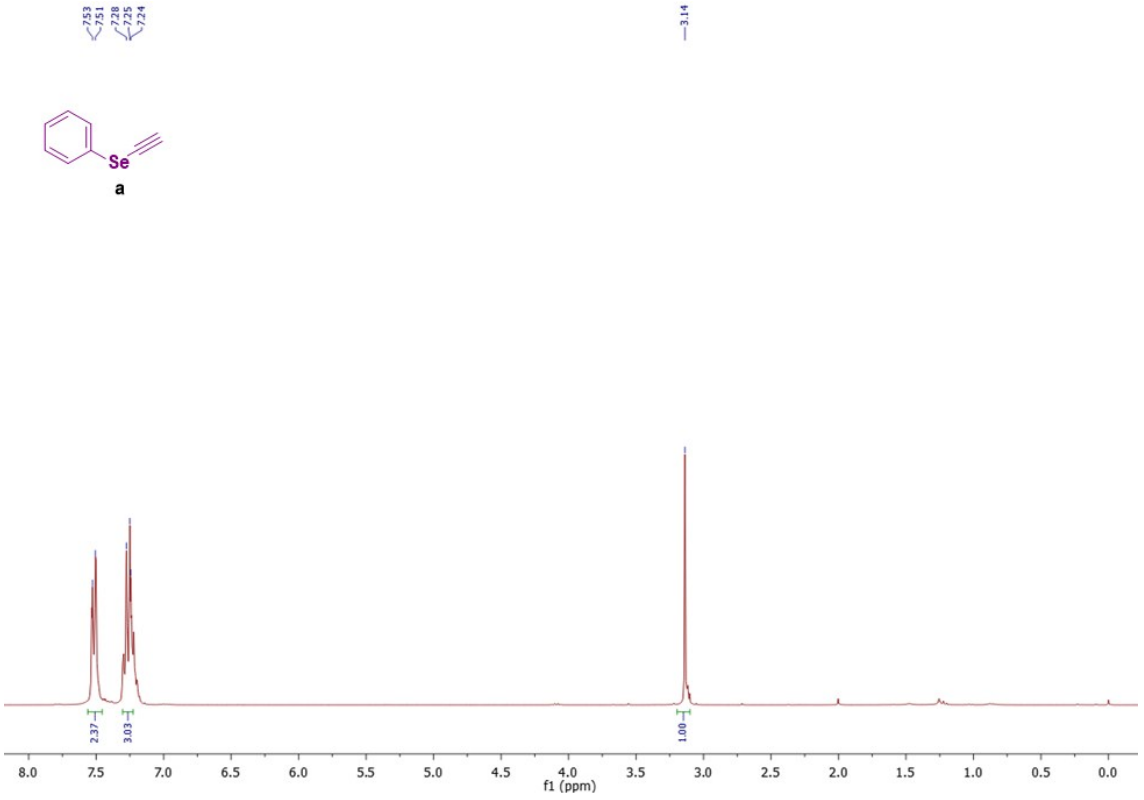
77.5199
76.6733
0.0011
F
TMS
Se
h
f1 (ppm)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7.25
7.24
3.14
Se
a
2.37
3.03
1.00
8.0
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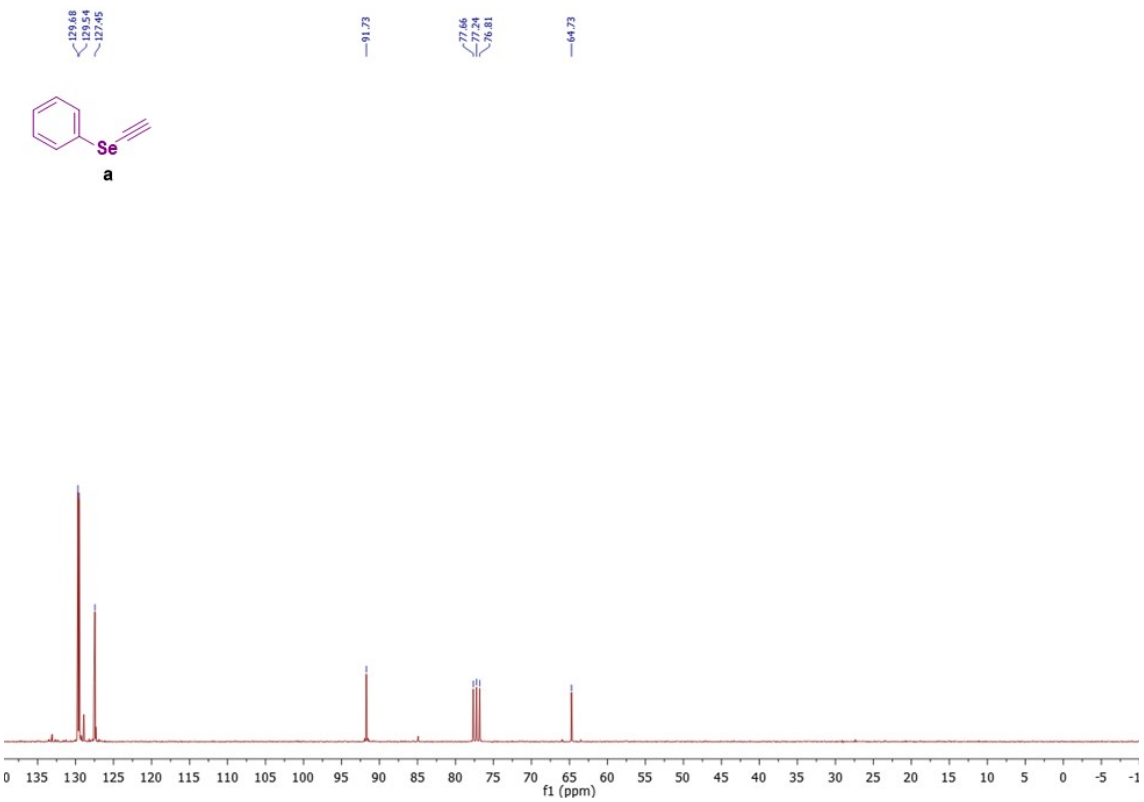
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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91.73
77.66
77.24
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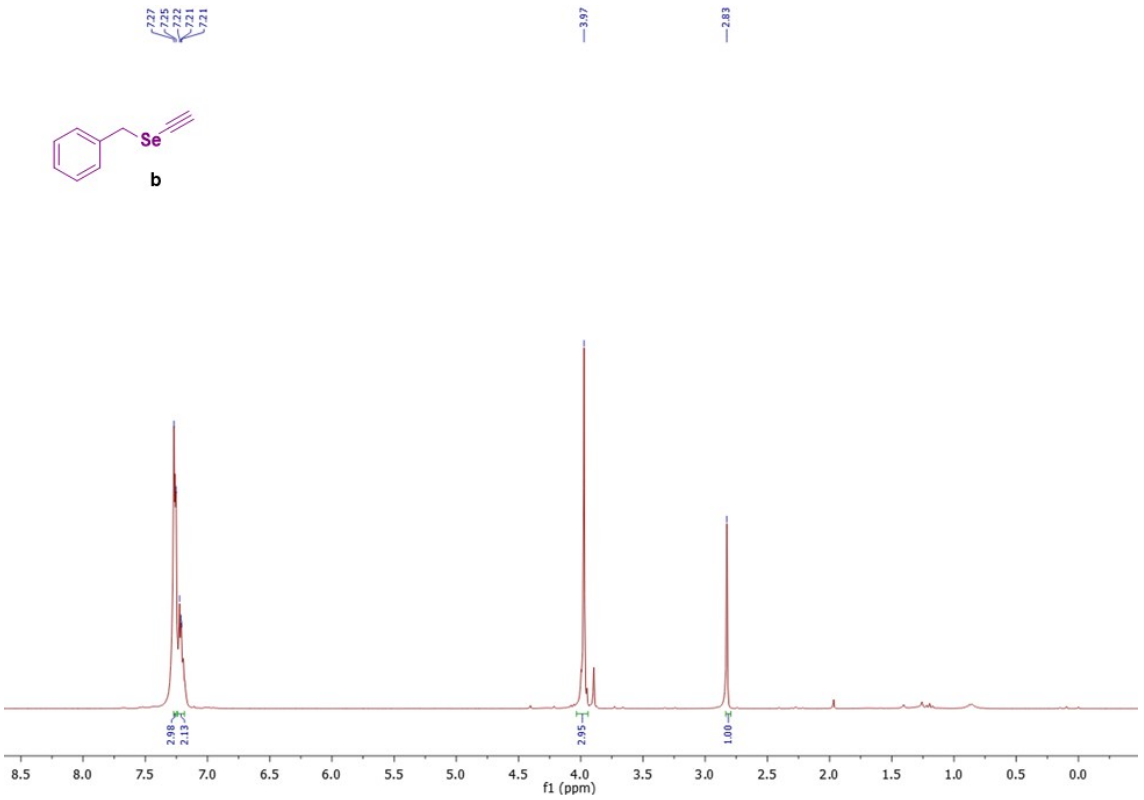
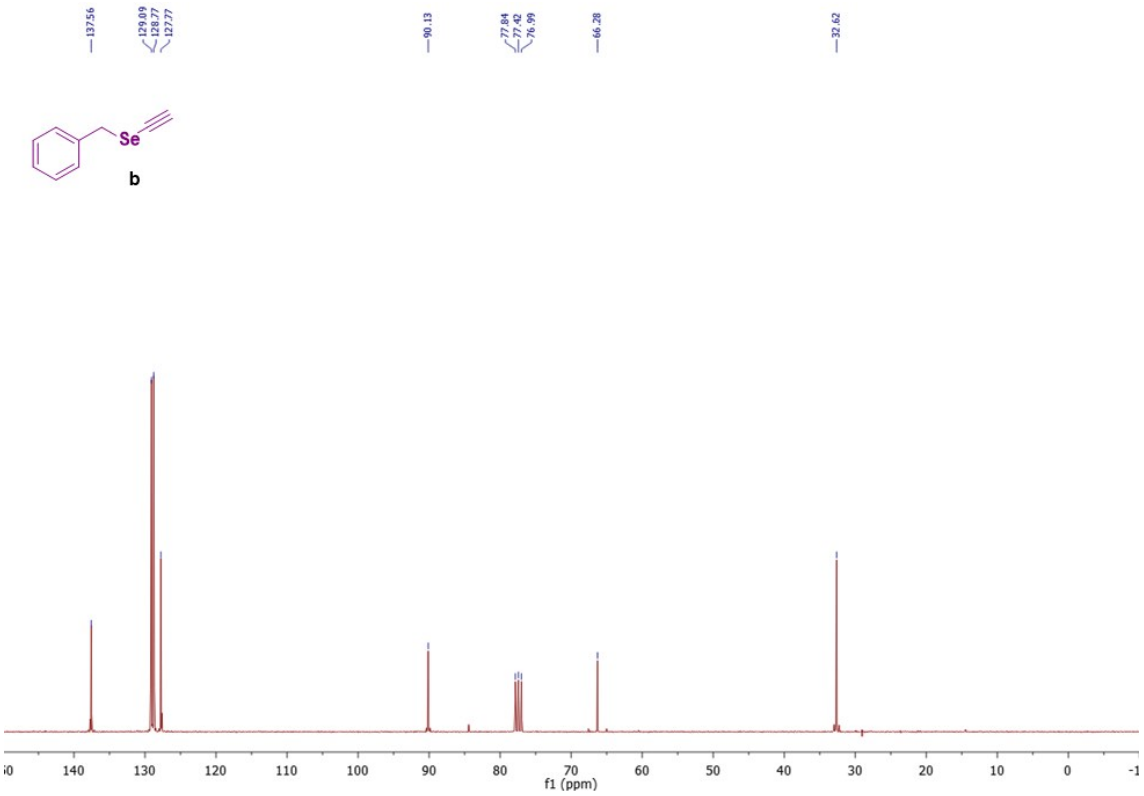
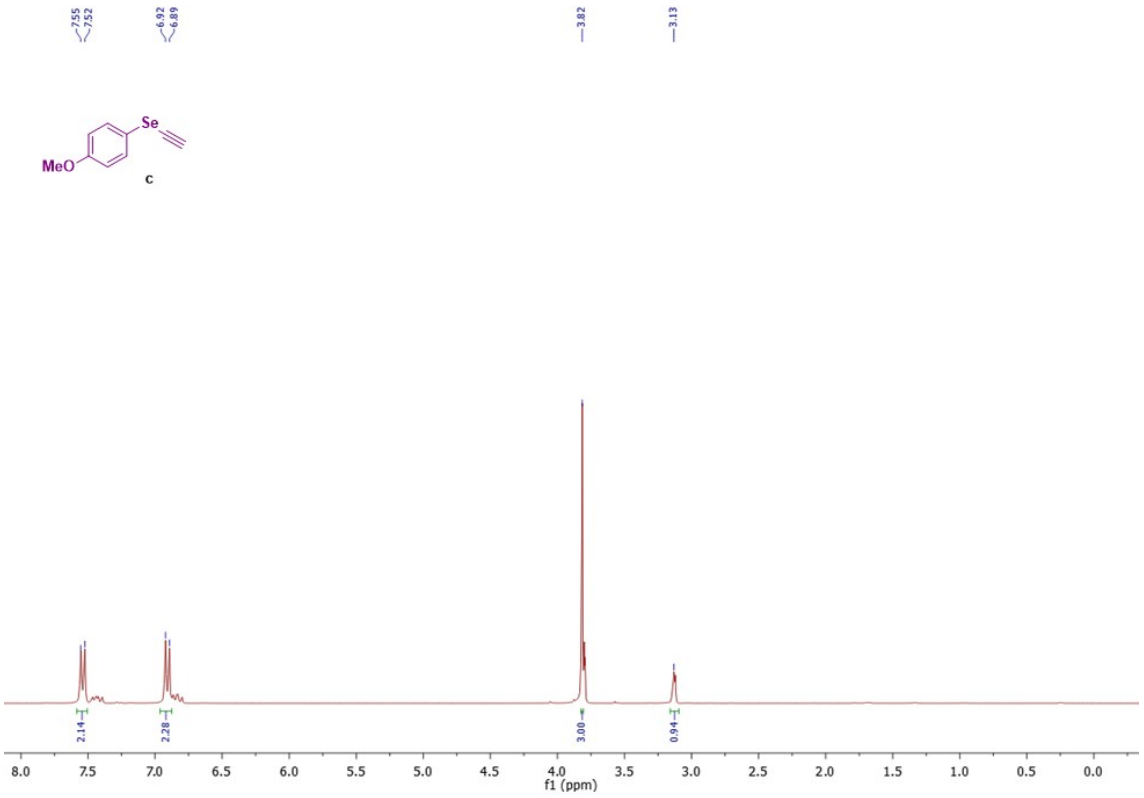
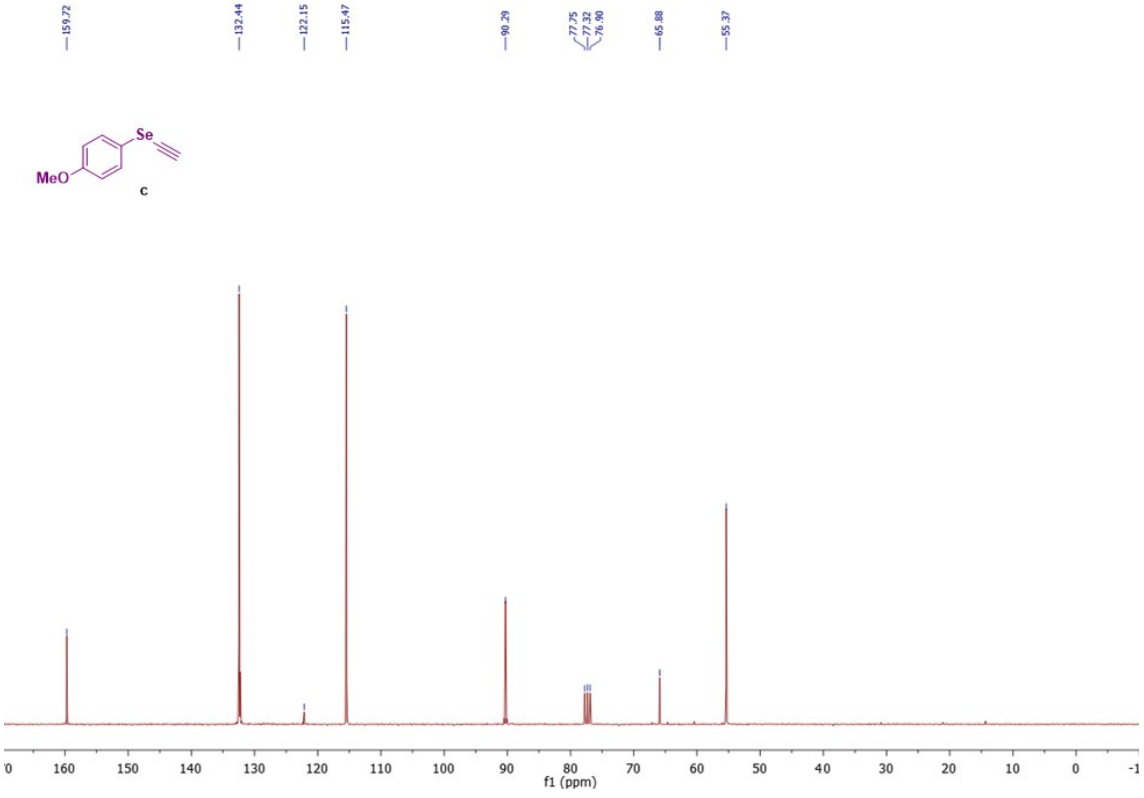
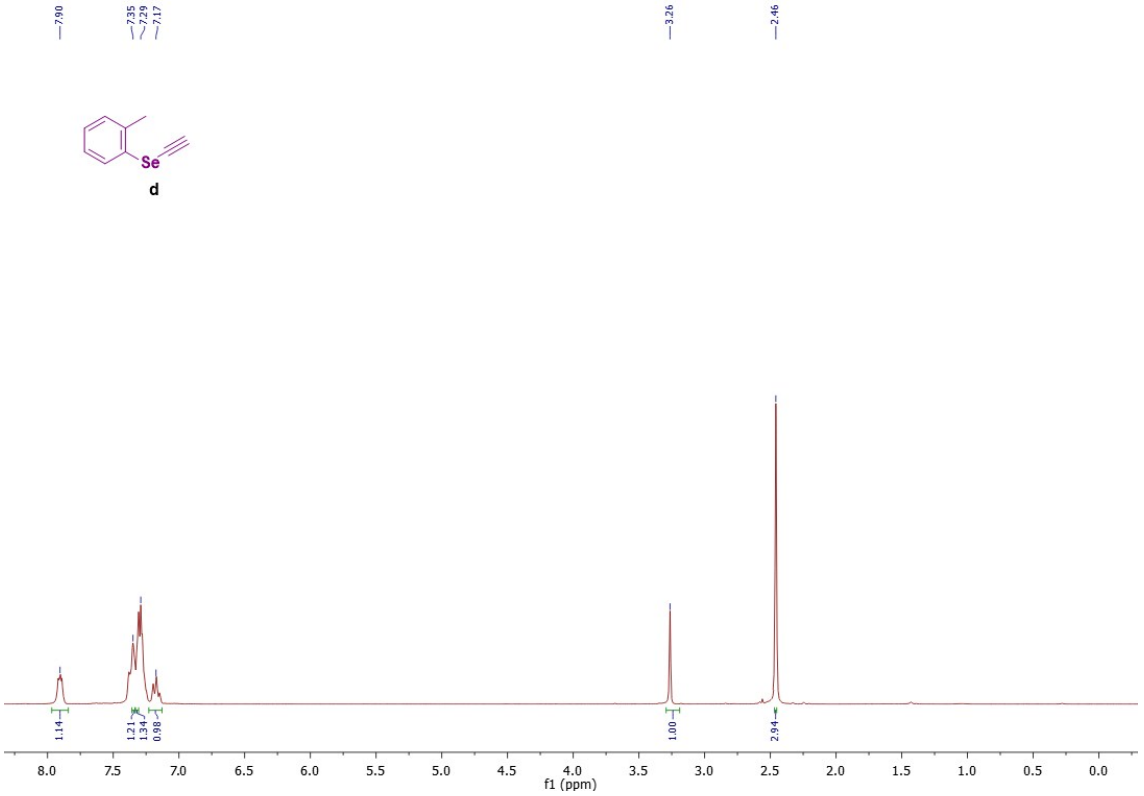
64.73
Se
a
0
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
f1 (ppm)

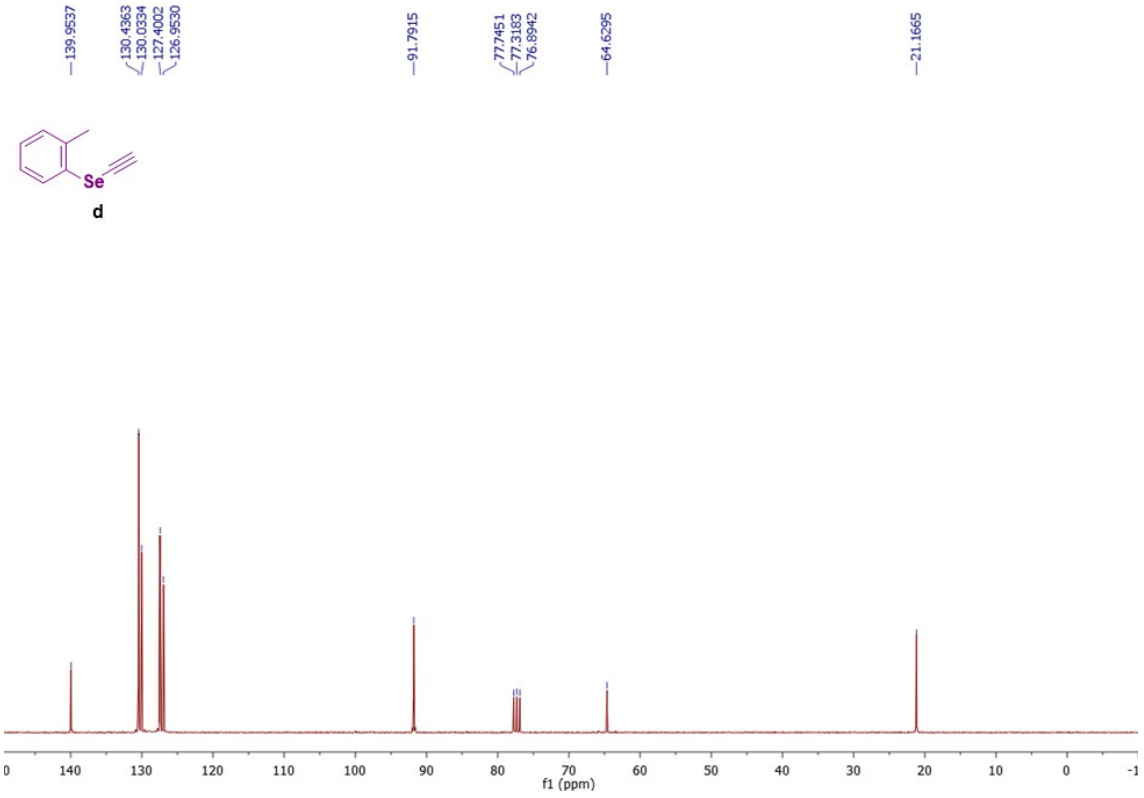

7.27
7.25
7.22
7.21
7.21
3.97
2.83
Se
b
2.98
2.13
2.95
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

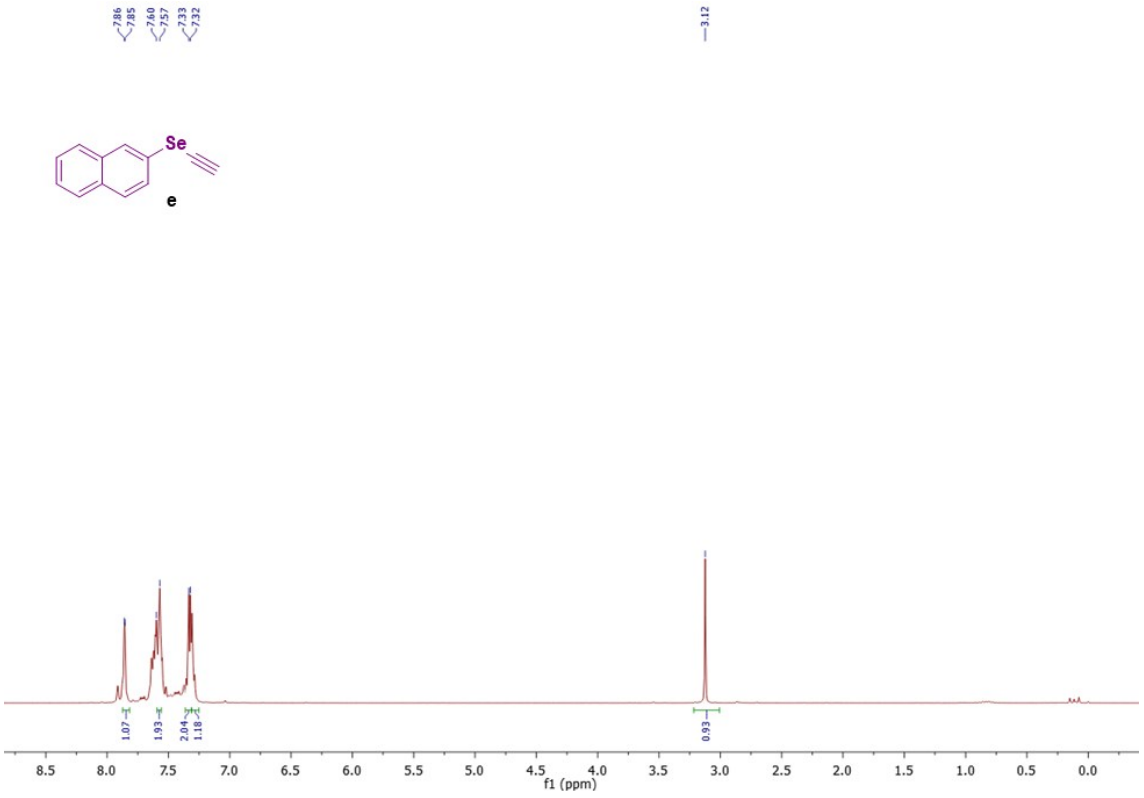

137.56
129.09
128.77
127.77
90.13
77.84
77.42
76.99
66.28
32.62
Se
b
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

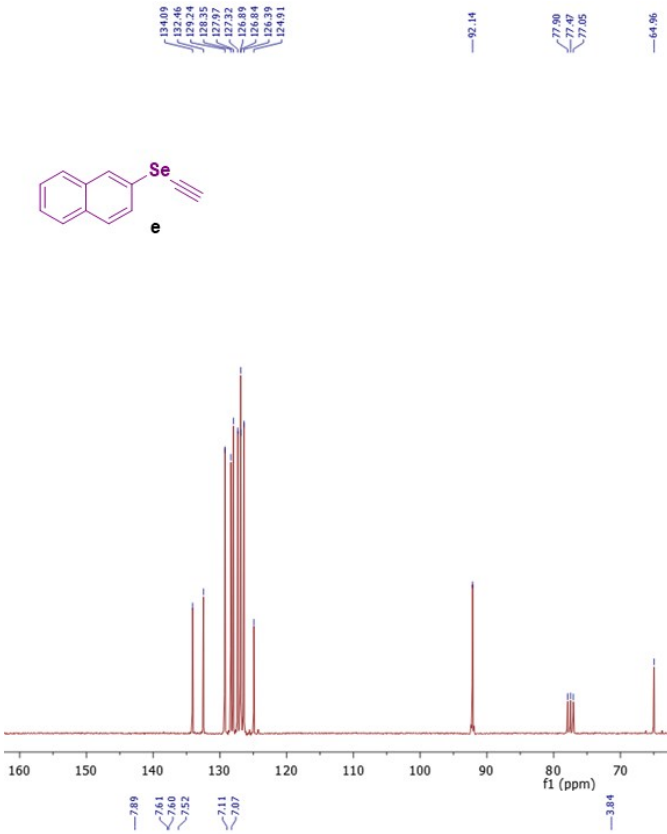

7.55
7.52
6.92
6.89
3.82
3.13
Se
MeO
c
2.14
2.28
3.00
0.94
f1 (ppm)

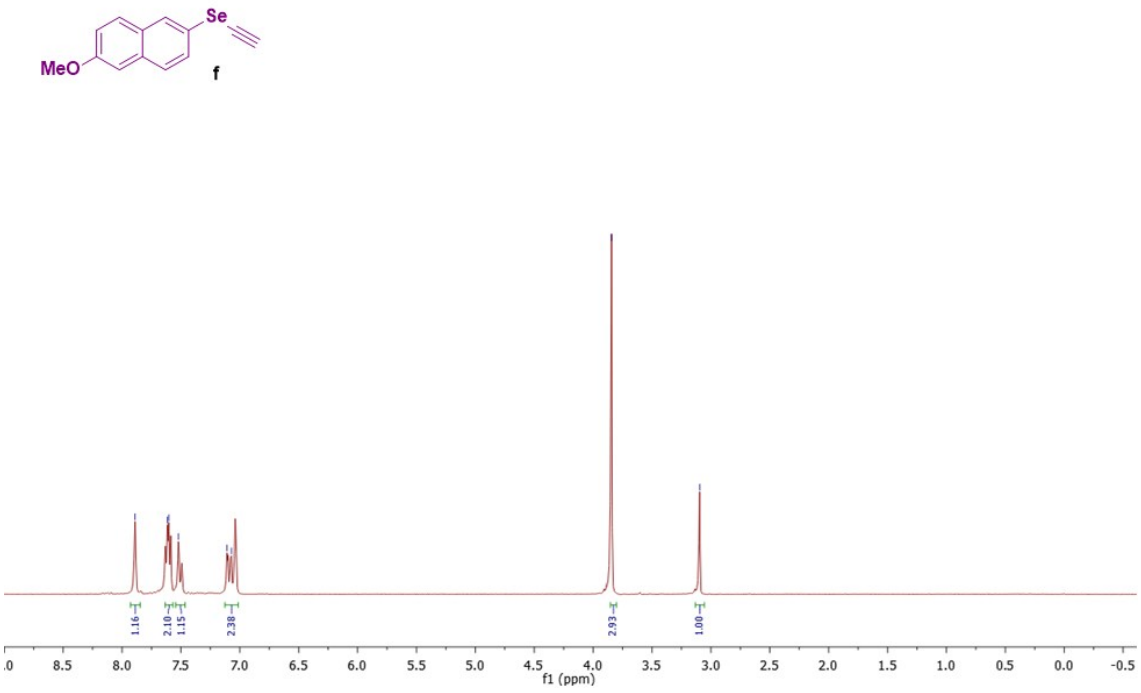

159.72
132.44
122.15
115.47
90.29
77.75
77.32
76.90
65.88
55.37
Se
MeO
c
f1 (ppm)

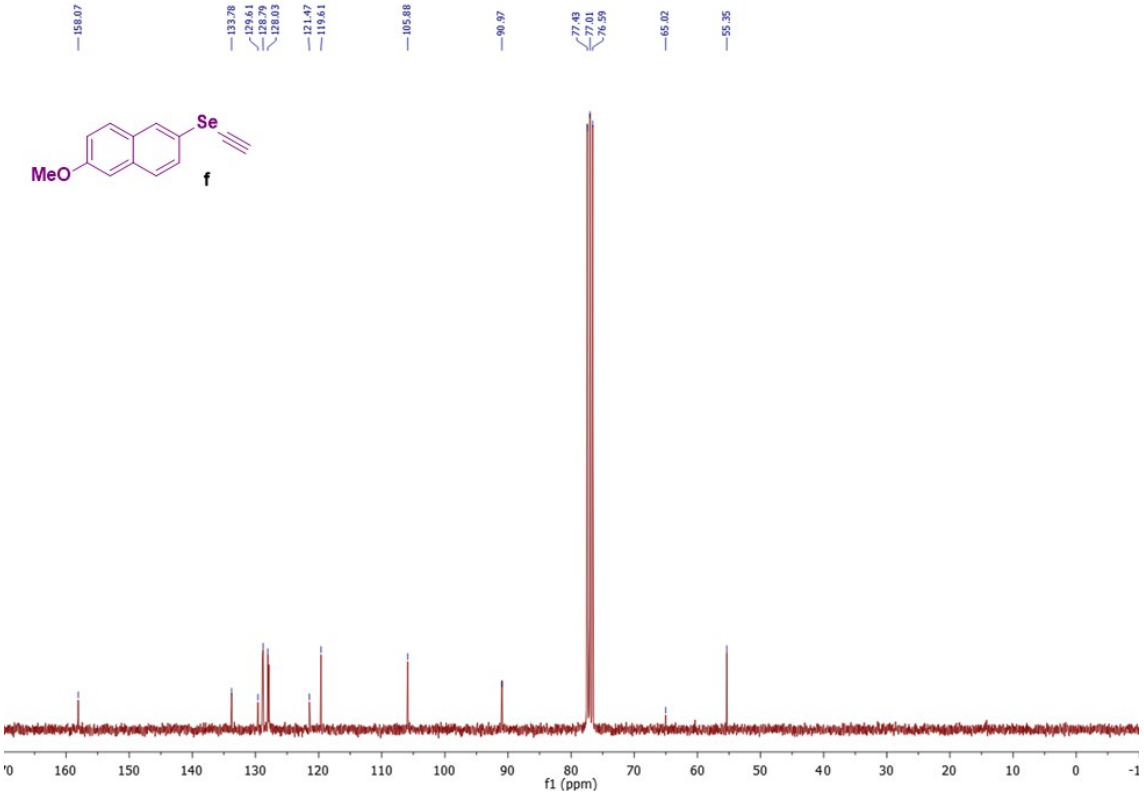

7.90
7.35
7.29
7.17
3.26
2.46
Se
d
1.14
1.21
1.34
0.98
1.00
2.94
f1 (ppm)

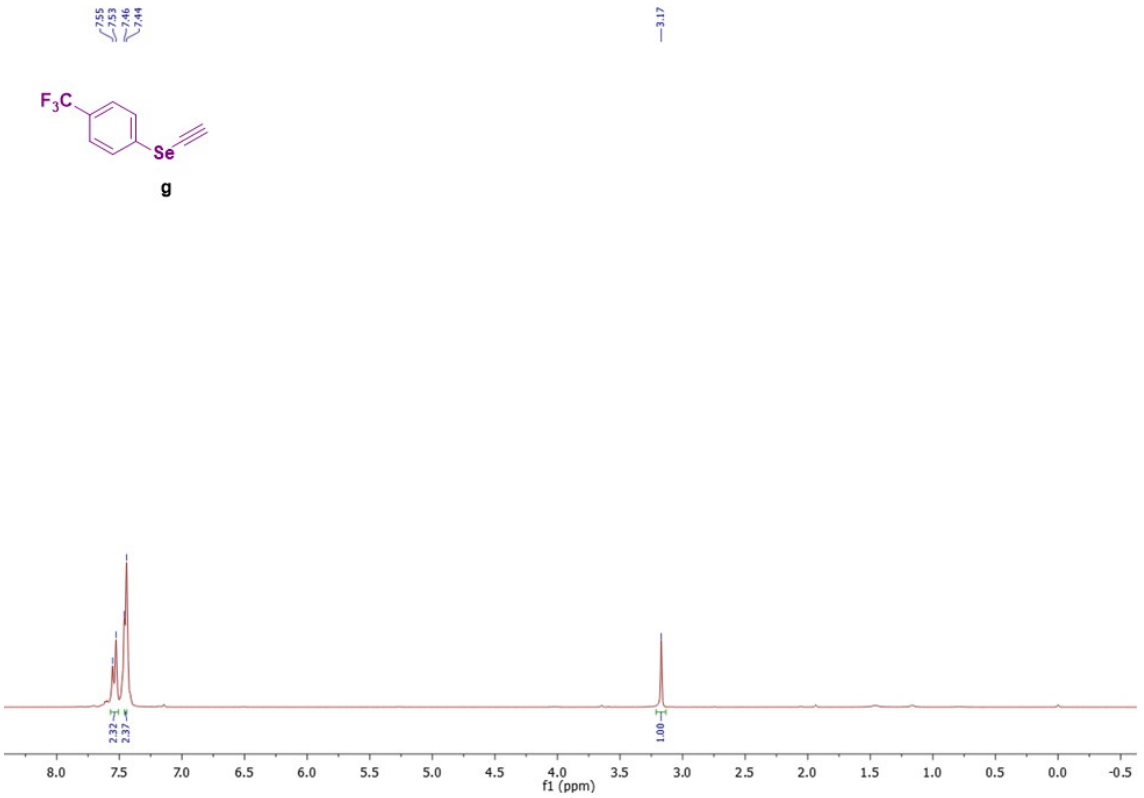

139.9537
130.4363
130.0334
127.4002
126.9530
91.7915
77.7451
77.3183
76.8942
64.6295
21.1665
Se
d
f1 (ppm)


7.86
7.85
7.60
7.57
7.33
7.32
3.12
Se
e
1.07
1.93
2.04
1.18
0.93
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)


134.09
132.46
129.24
128.35
127.97
127.32
126.89
126.84
126.39
124.91
92.14
77.90
77.47
77.05
64.96
Se
e
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
7.89
7.61
7.60
7.52
7.11
7.07
3.84
3.10

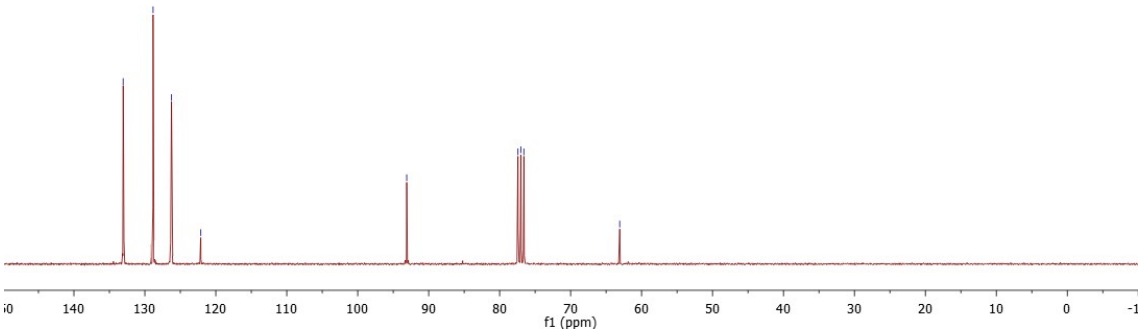

Se
MeO
f
1.16
2.10
1.15
2.38
2.93
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


158.07
133.78
129.61
128.79
128.03
121.47
119.61
105.88
90.97
77.48
77.01
76.59
65.02
55.35
Se
MeO
f
f1 (ppm)


7.55
7.53
7.46
7.44
3.17
F3C
Se
g
2.32
2.37
1.00
f1 (ppm)

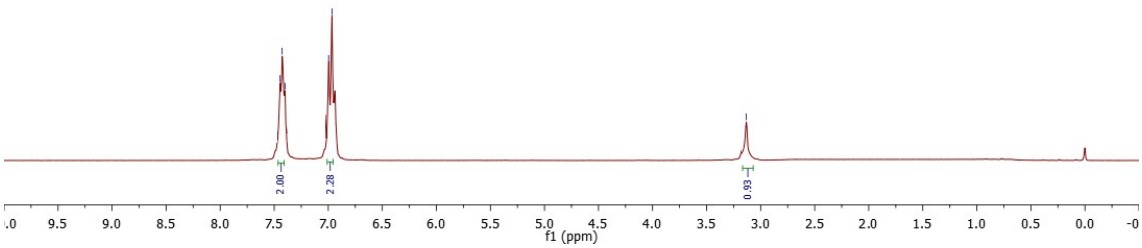

133.05
128.84
126.25
122.13
93.10
77.48
77.01
76.59
63.08
F3C
Se

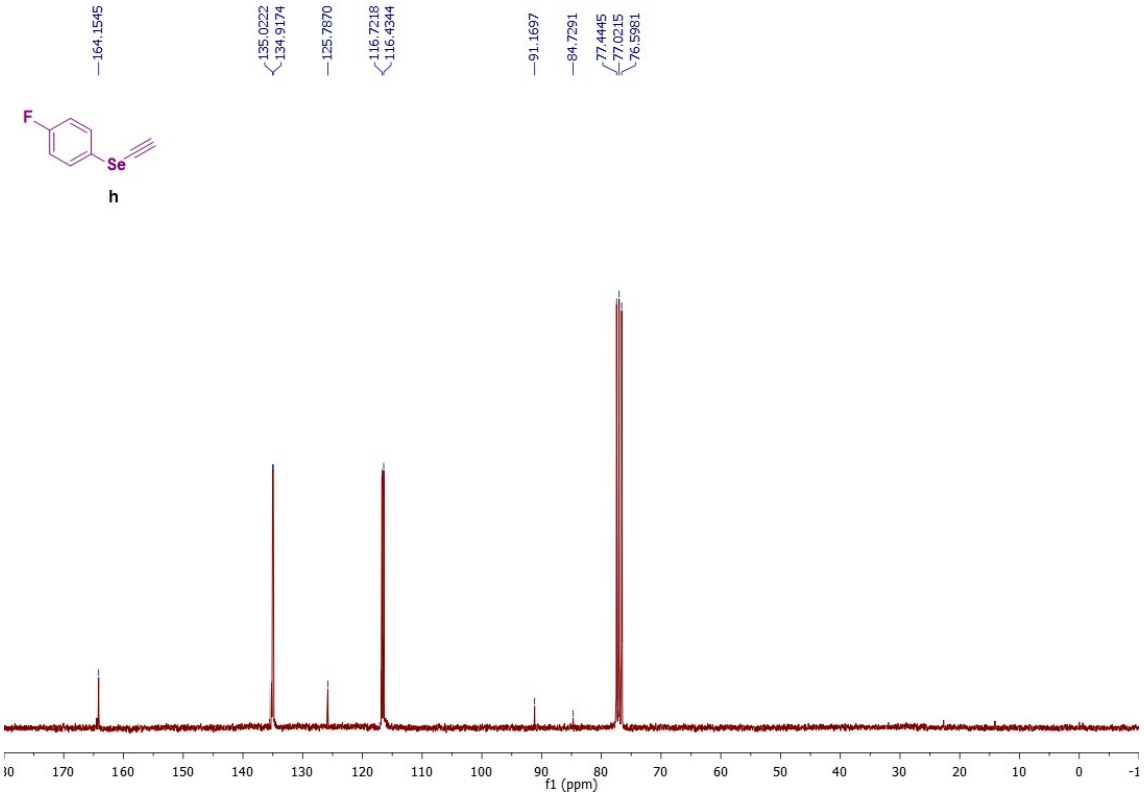
g

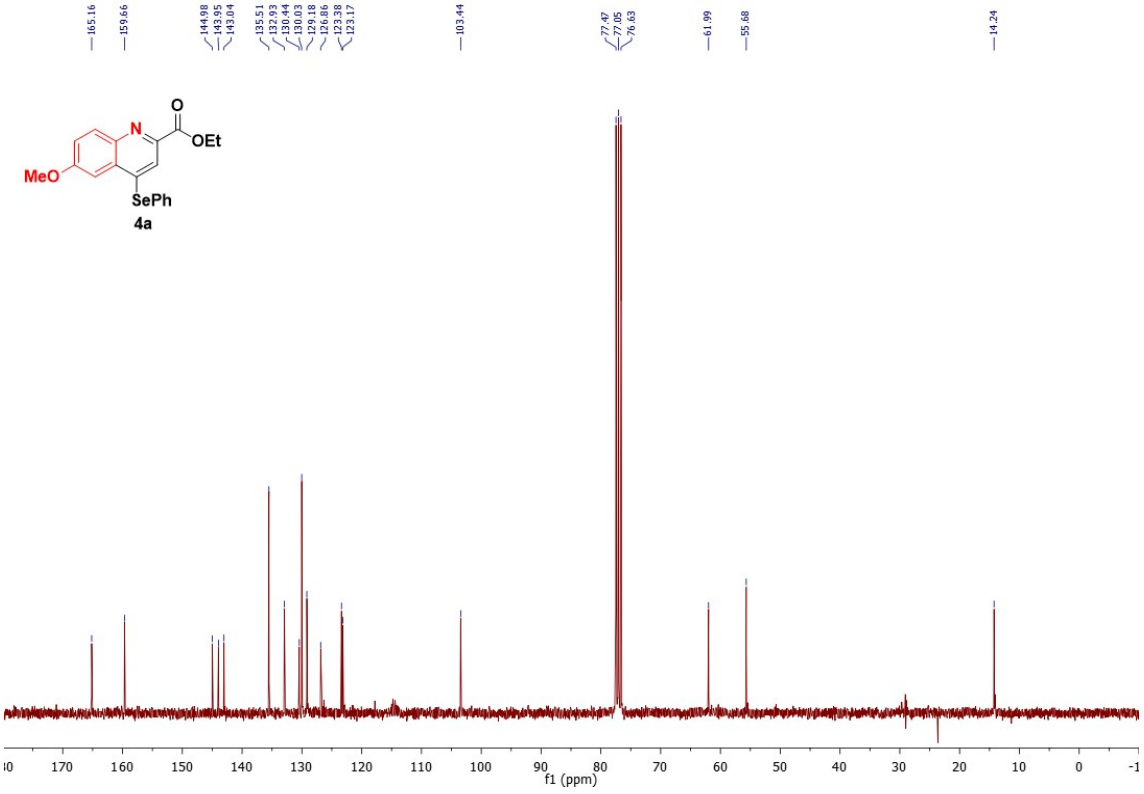

f1 (ppm)

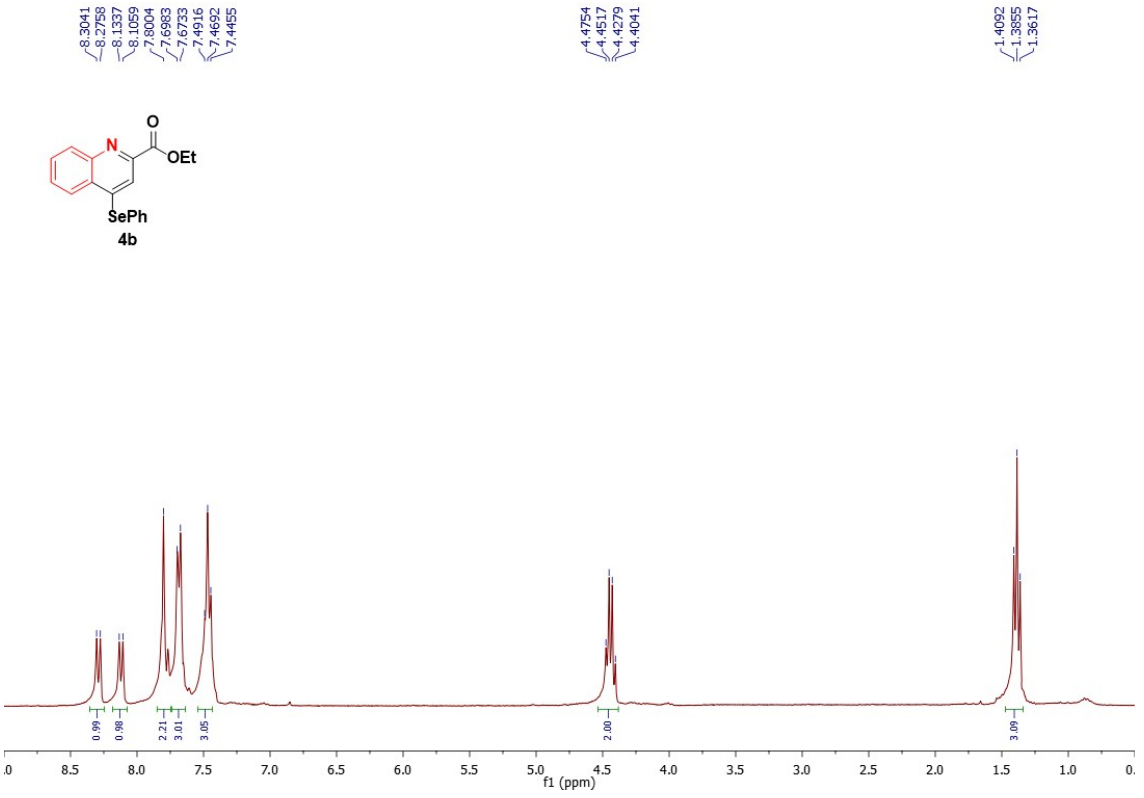

7.4455
7.4266
7.4003
6.9965
6.9662
3.1307
F
Se

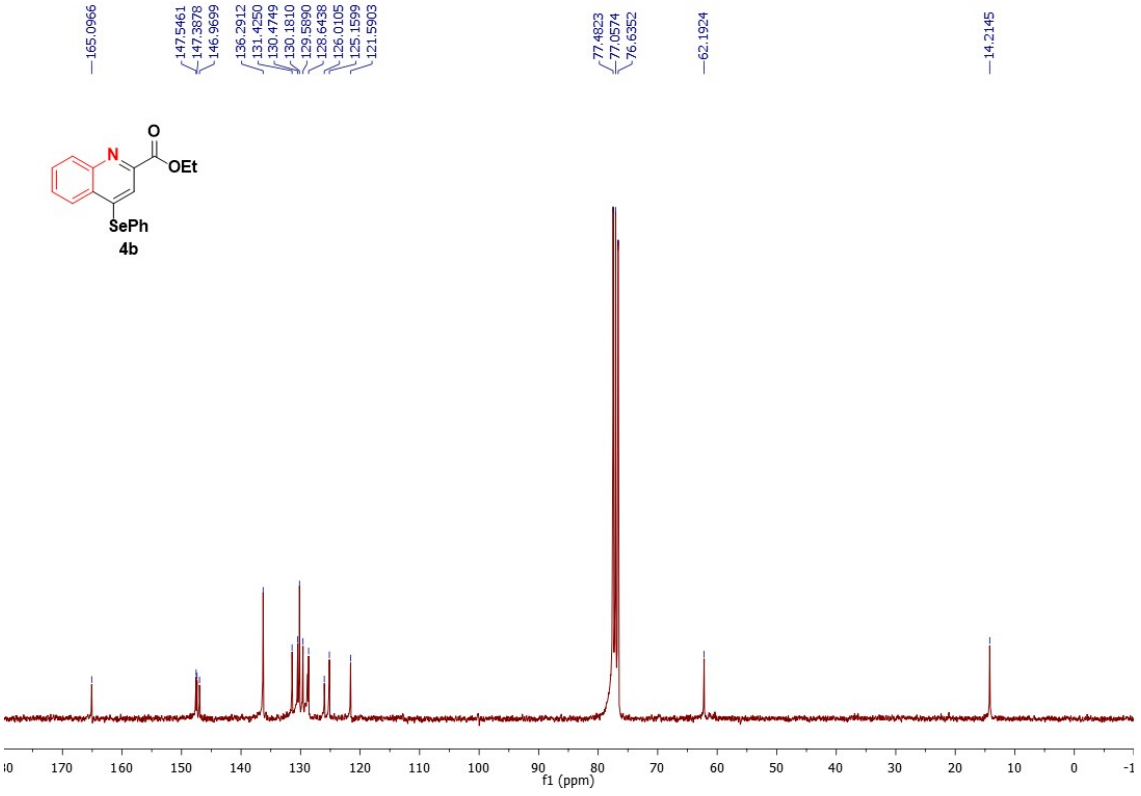
h

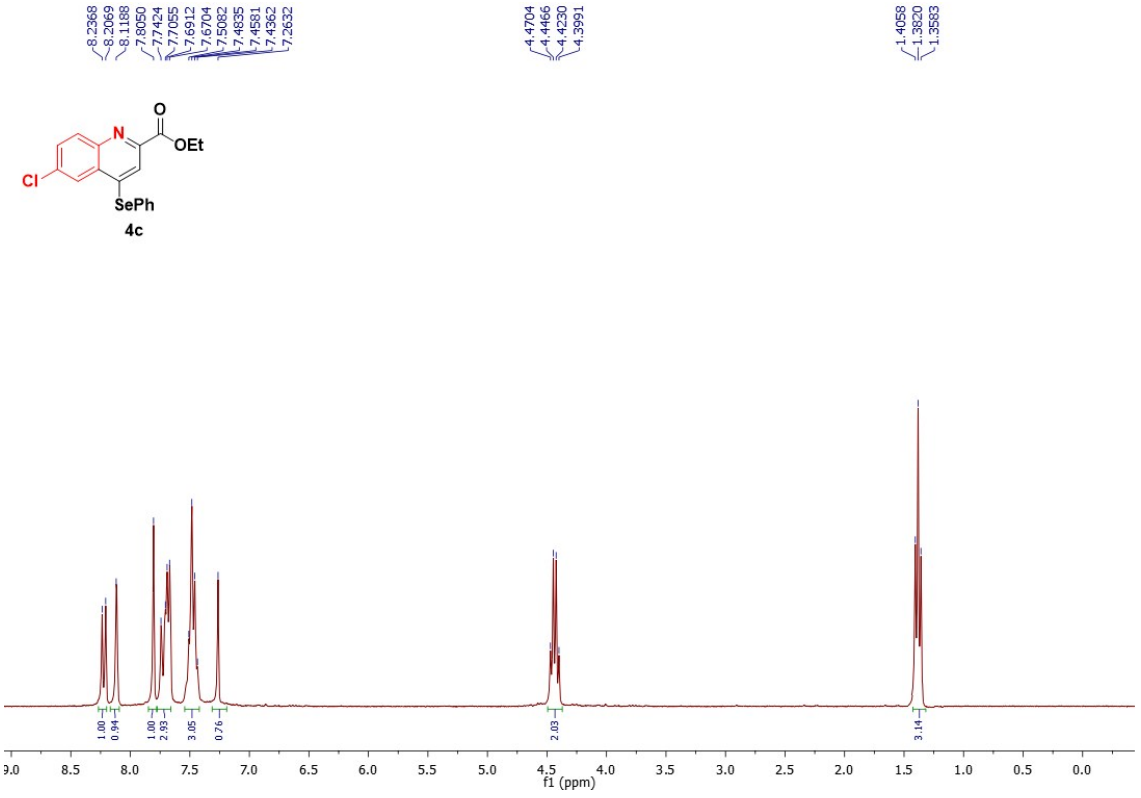

2.00
2.28
0.93
f1 (ppm)

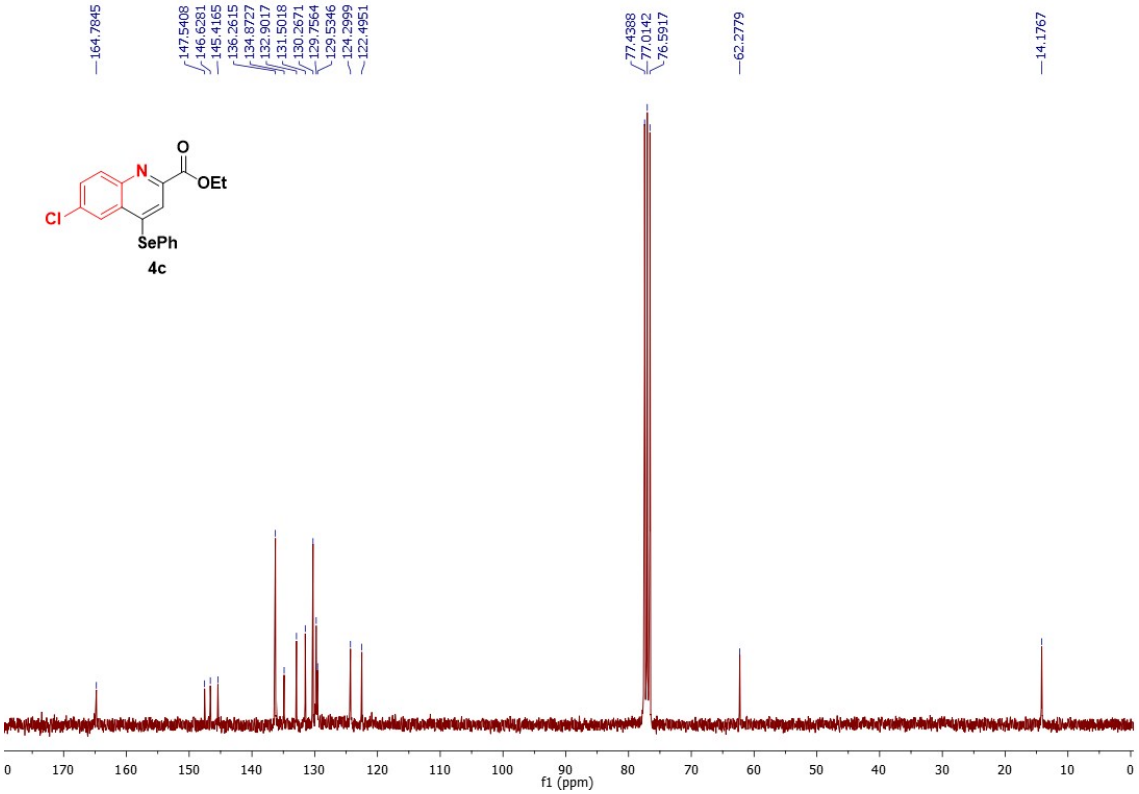

164.1545
135.0222
134.9174
125.7870
116.7218
116.4344
91.1697
84.7291
77.4445
77.0215
76.5981
F
Se
h
f1 (ppm)
8.1975
8.1666
7.9133
7.9086
7.6472
7.6221
7.4264
7.4048
7.3058
4.4778
4.4530
4.4291
4.4075
3.9244
1.4152
1.3917
1.3700
O
N
OEt
MeO
SePh
4a
1.29
1.00
2.16
4.28
1.08
2.27
3.29
3.20
f1 (ppm)


165.16
159.66
144.98
143.95
143.04
135.51
132.93
130.44
130.03
129.18
126.86
123.38
123.17
103.44
77.47
77.05
76.63
61.99
55.68
14.24
O
N
OEt
MeO
SePh
4a
f1 (ppm)


8.3041
8.2758
8.1337
8.1059
7.8004
7.6983
7.6733
7.4916
7.4692
7.4455
4.4754
4.4517
4.4279
4.4041
1.4092
1.3855
1.3617
O
N
OEt
SePh
4b
0.99
0.98
2.21
3.01
3.05
2.00
3.09
f1 (ppm)


165.0966
147.5461
147.3878
146.9699
136.2912
131.4250
130.4749
130.1810
129.5890
128.6438
126.0105
125.1599
121.5903
77.4823
77.0574
76.6352
62.1924
14.2145
O
N
OEt
SePh
4b
f1 (ppm)


8.2368
8.2069
8.1188
7.8050
7.7424
7.7055
7.6912
7.6704
7.5082
7.4835
7.4581
7.4362
7.2632
4.4704
4.4466
4.4230
4.3991
1.4058
1.3820
1.3583
O
N
OEt
Cl
SePh
4c
1.00
0.94
1.00
2.93
3.05
0.76
2.03
3.14
f1 (ppm)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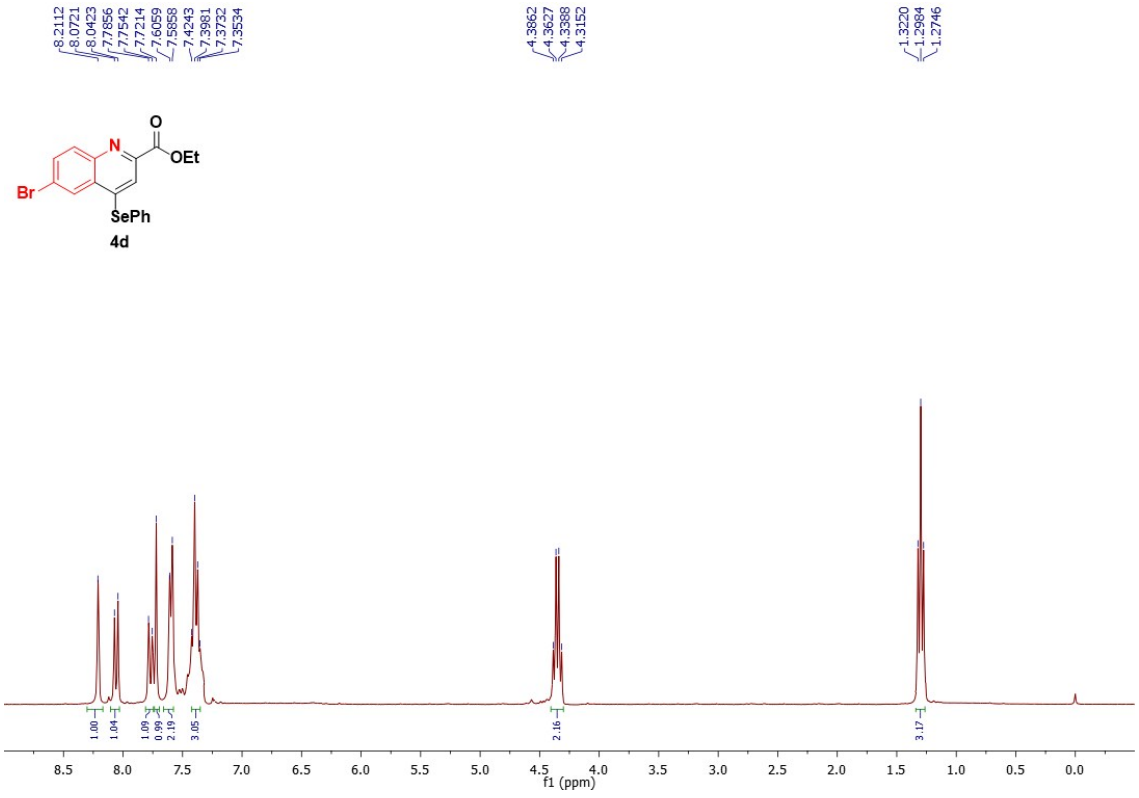
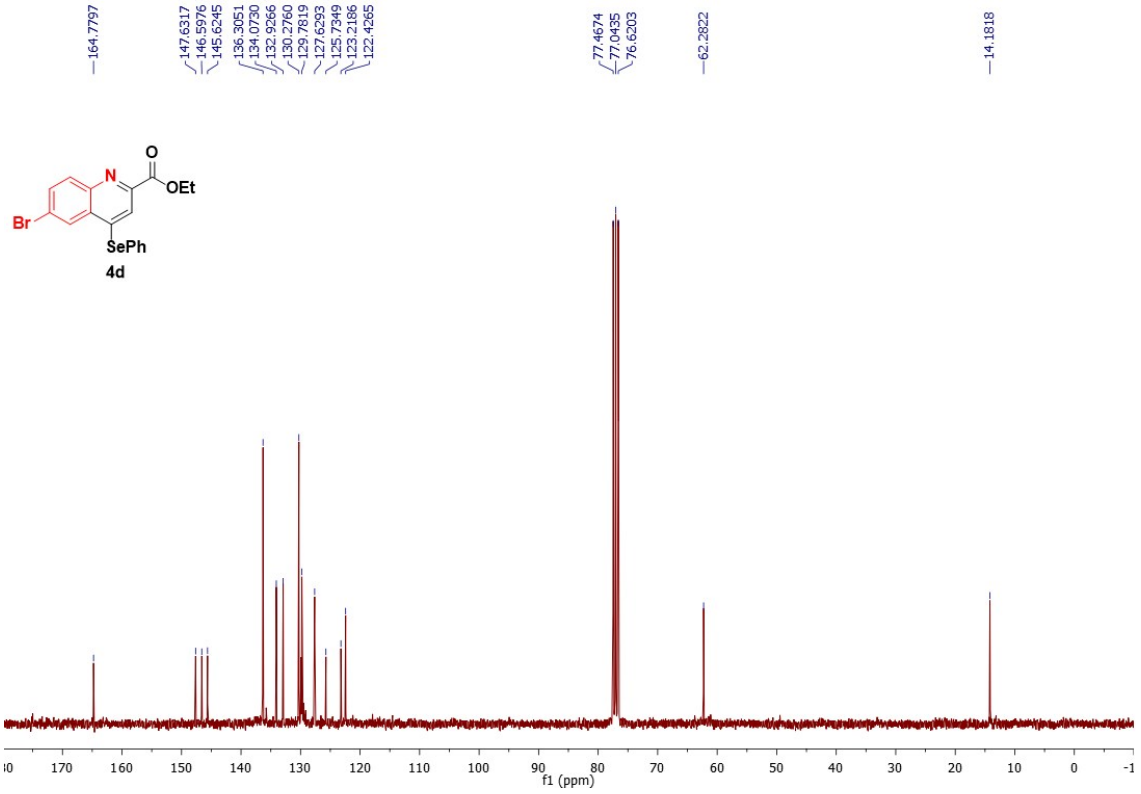
147.5408
146.6281
145.4165
136.2615
134.8727
132.9017
131.5018
130.2671
129.7564
129.5346
124.2999
122.4951
77.4388
77.0142
76.5917
62.2779
14.1767
O
N
OEt
Cl
SePh
4c
f1 (ppm)


8.2112
8.0721
8.0423
7.7856
7.7542
7.7214
7.6059
7.5858
7.4243
7.3981
7.3732
7.3534
4.3862
4.3627
4.3388
4.3152
1.3220
1.2984
1.2746
O
N
OEt
Br
SePh
4d
1.00
1.04
1.09
0.99
2.19
3.05
2.16
3.17
f1 (ppm)


164.7797
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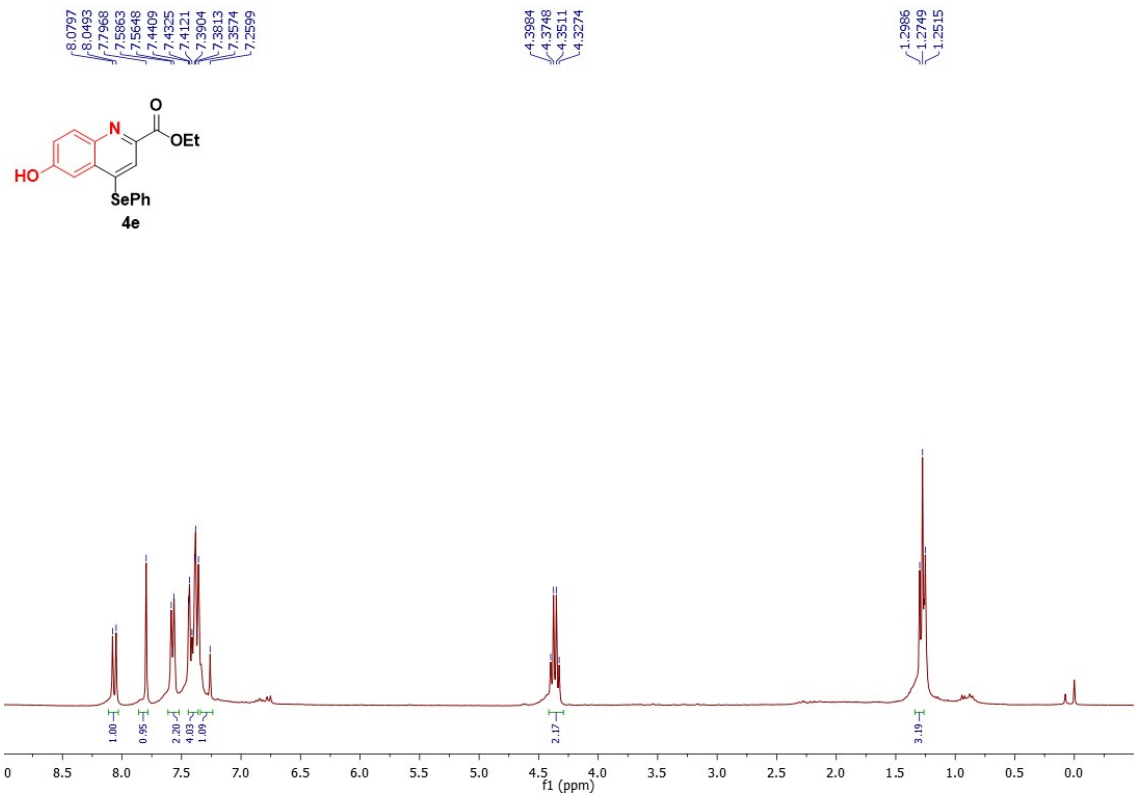
146.5976
145.6245
136.3051
134.0730
132.9266
130.2760
129.7819
127.6293
125.7349
123.2186
122.4265
77.4674
77.0435
76.6203
62.2822
14.1818
O
N
OEt
Br
SePh
4d
f1 (ppm)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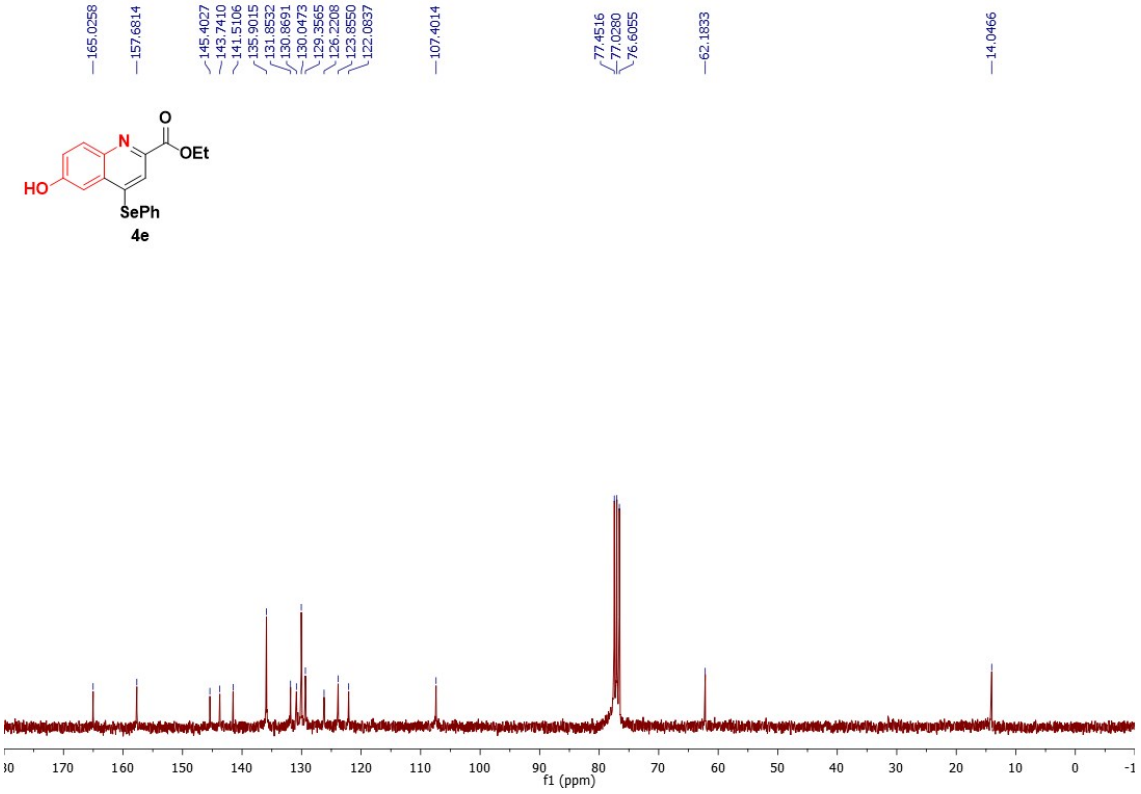
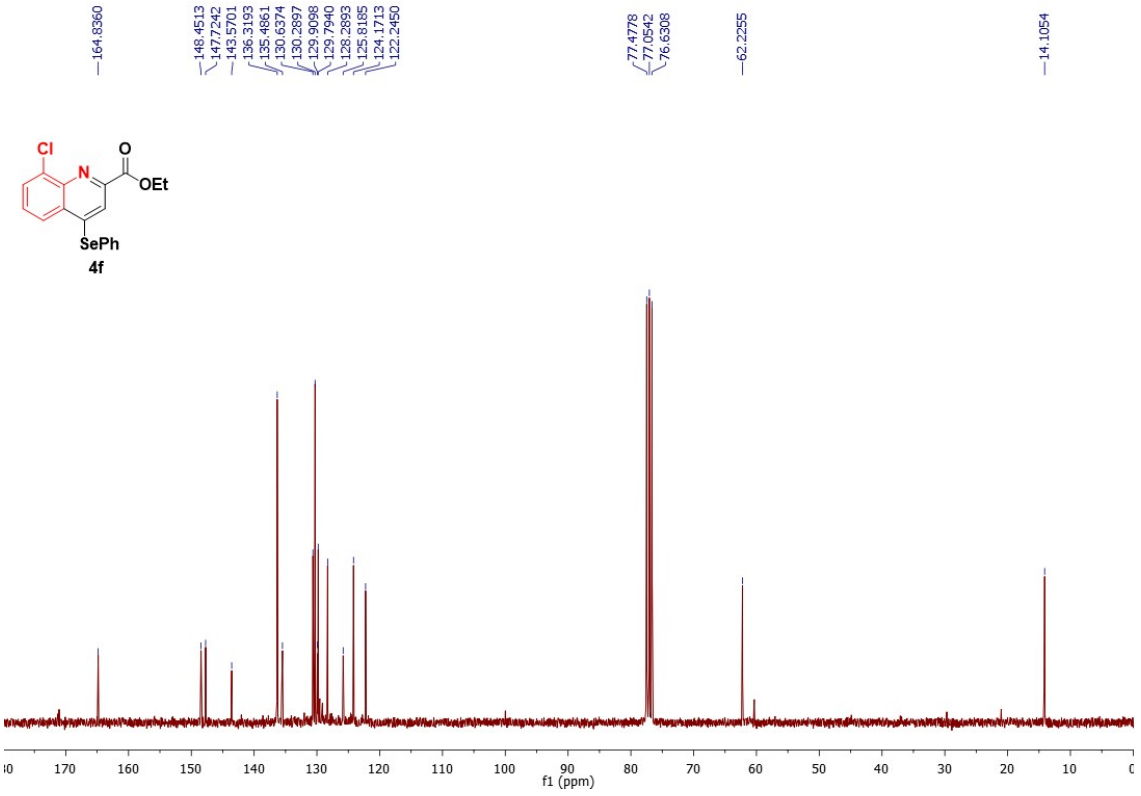
8.0493
7.7968
7.5863
7.5648
7.4409
7.4325
7.4121
7.3904
7.3813
7.3574
7.2599
4.3984
4.3748
4.3511
4.3274
1.2986
1.2749
1.2515
O
N
OEt
HO
SePh
4e
1.00
0.95
2.20
4.03
1.09
2.17
3.19
f1 (ppm)


165.0258
157.6814
145.4027
143.7410
141.5106
135.9015
131.8532
130.8691
130.0473
129.3565
126.2208
123.8550
122.0837
107.4014
77.4516
77.0280
76.6055
62.1833
14.0466
O
N
OEt
HO
SePh
4e
f1 (ppm)
8.0457
8.0178
7.9115
7.8864
7.8163
7.6806
7.6546
7.5903
7.5638
7.5573
7.4955
7.4724
7.4474
4.4508
4.4269
4.4031
4.3792
1.4159
1.3924
1.3683
Cl
O
N
OEt
SePh
4f
0.98
1.08
1.02
2.04
4.24
2.00
3.15
f1 (ppm)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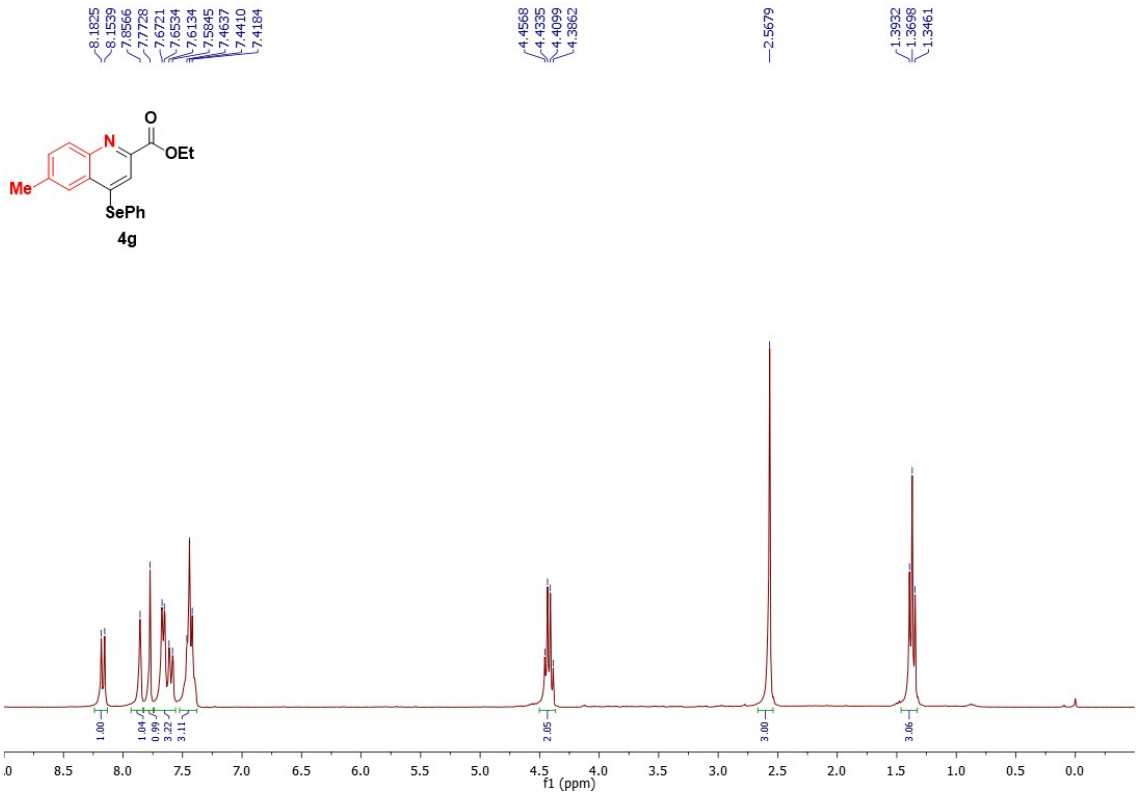
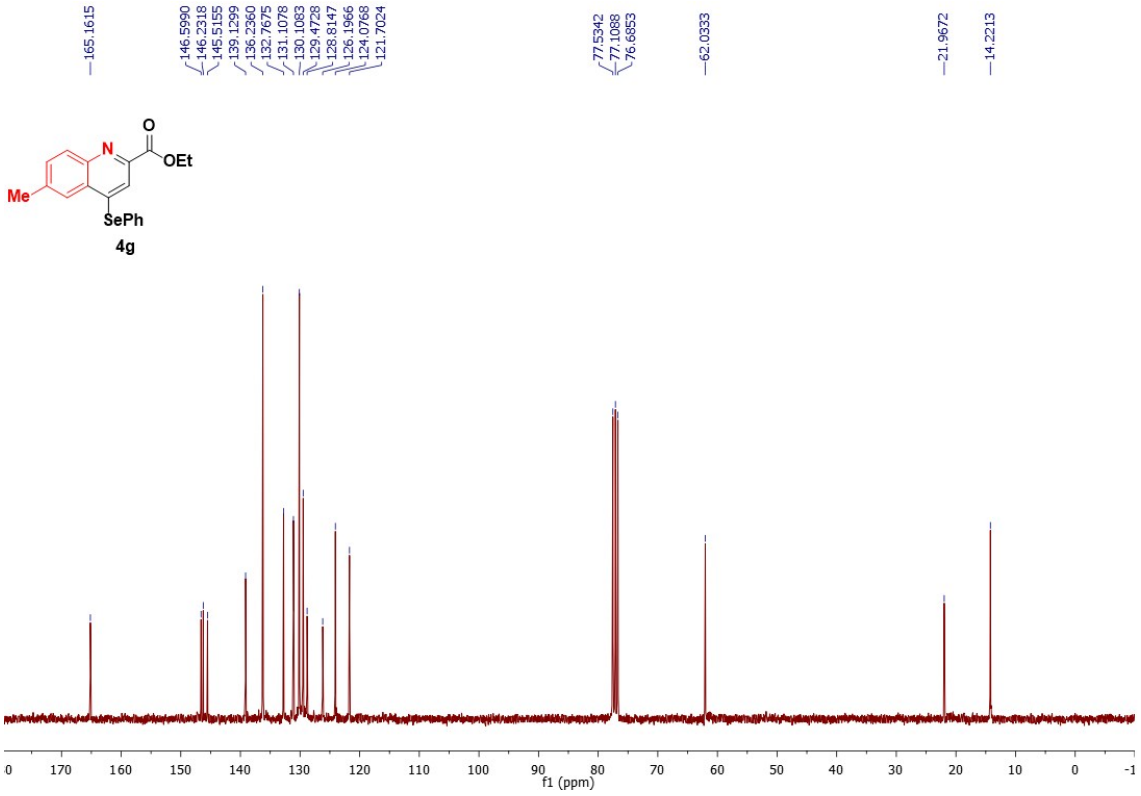
148.4513
147.7242
143.5701
136.3193
135.4861
130.6374
130.2897
129.9098
129.7940
128.2893
125.8185
124.1713
122.2450
77.4778
77.0542
76.6308
62.2255
14.1054
Cl
N
O
OEt
SePh
4f
f1 (ppm)


8.1825
8.1539
7.8566
7.7728
7.6721
7.6534
7.6134
7.5845
7.4637
7.4410
7.4184
4.4568
4.4335
4.4099
4.3862
2.5679
1.3932
1.3698
1.3461
N
O
OEt
Me
SePh
4g
1.00
1.04
0.99
3.22
3.11
2.05
3.00
3.06
f1 (ppm)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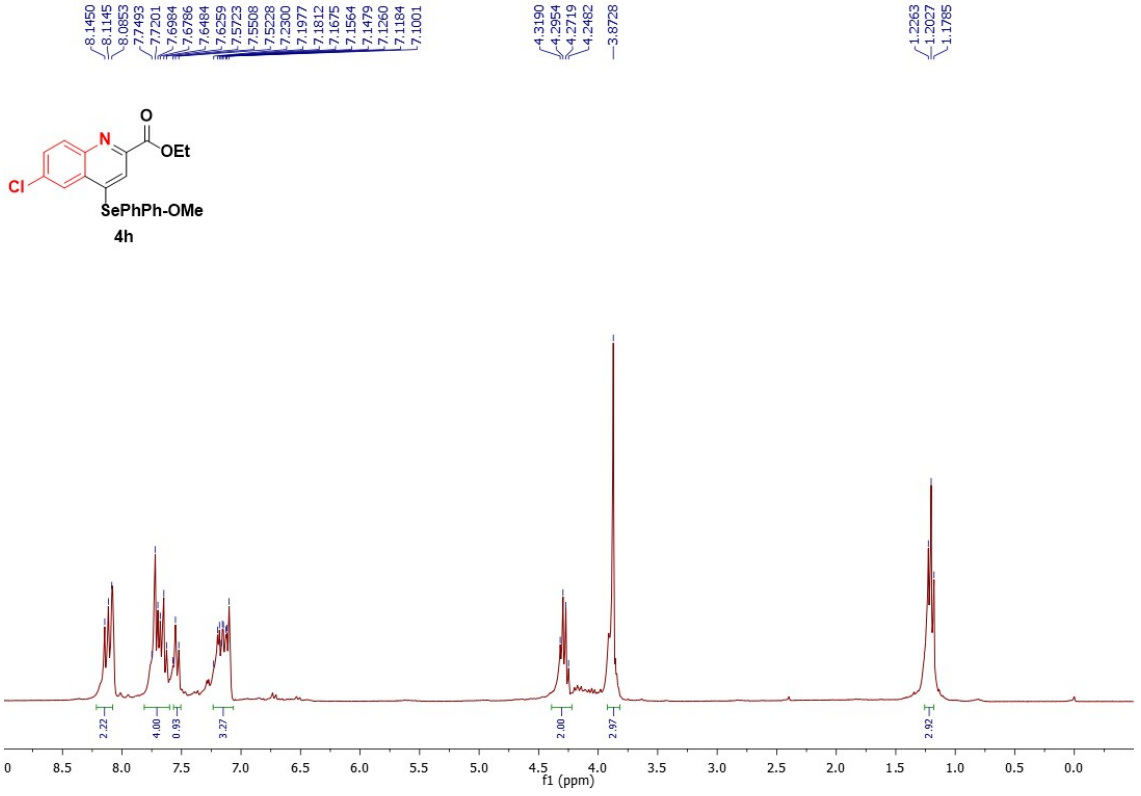
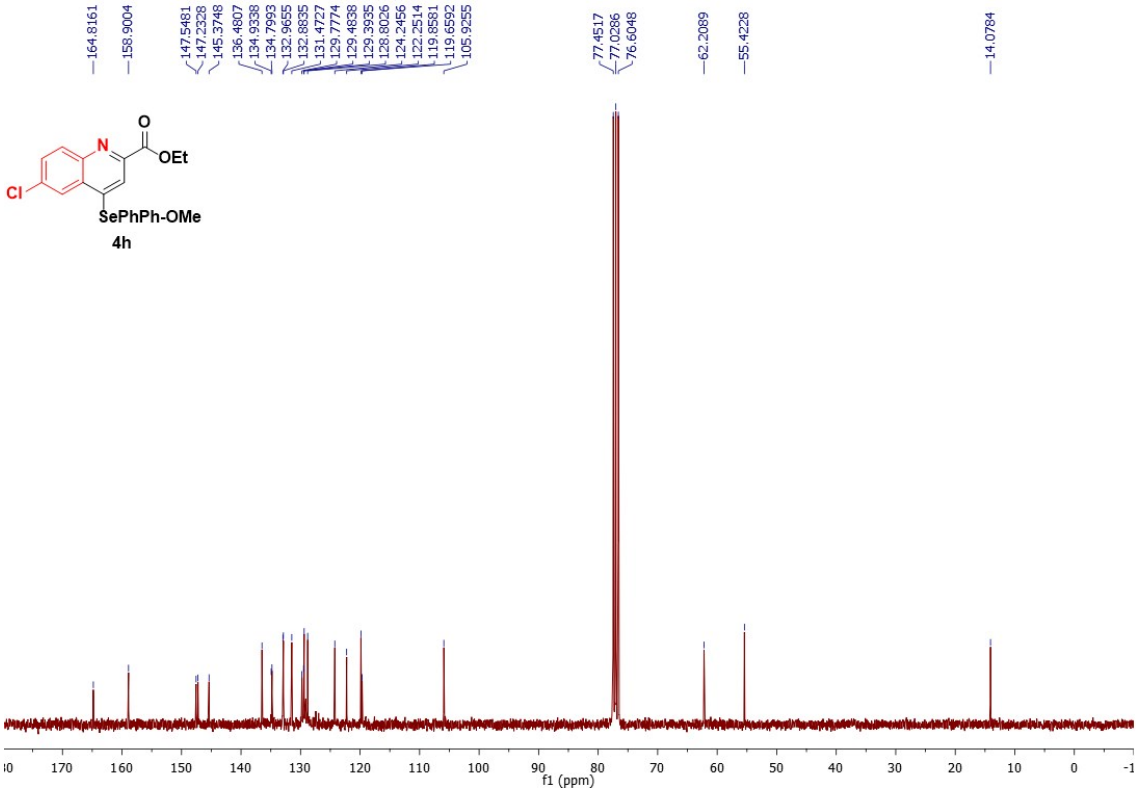
146.2318
145.5155
139.1299
136.2360
132.7675
131.1078
130.1083
129.4728
128.8147
126.1966
124.0768
121.7024
77.5342
77.1088
76.6853
62.0333
21.9672
14.2213
O
N
OEt
Me
SePh
4g
f1 (ppm)


8.1450
8.1145
8.0853
7.7493
7.7201
7.6984
7.6786
7.6484
7.6259
7.5723
7.5508
7.5228
7.2300
7.1977
7.1812
7.1675
7.1564
7.1479
7.1260
7.1184
7.1001
4.3190
4.2954
4.2719
4.2482
3.8728
1.2263
1.2027
1.1785
O
N
OEt
Cl
SePhPh-OMe
4h
2.22
4.00
0.93
3.27
2.00
2.97
2.92
f1 (ppm)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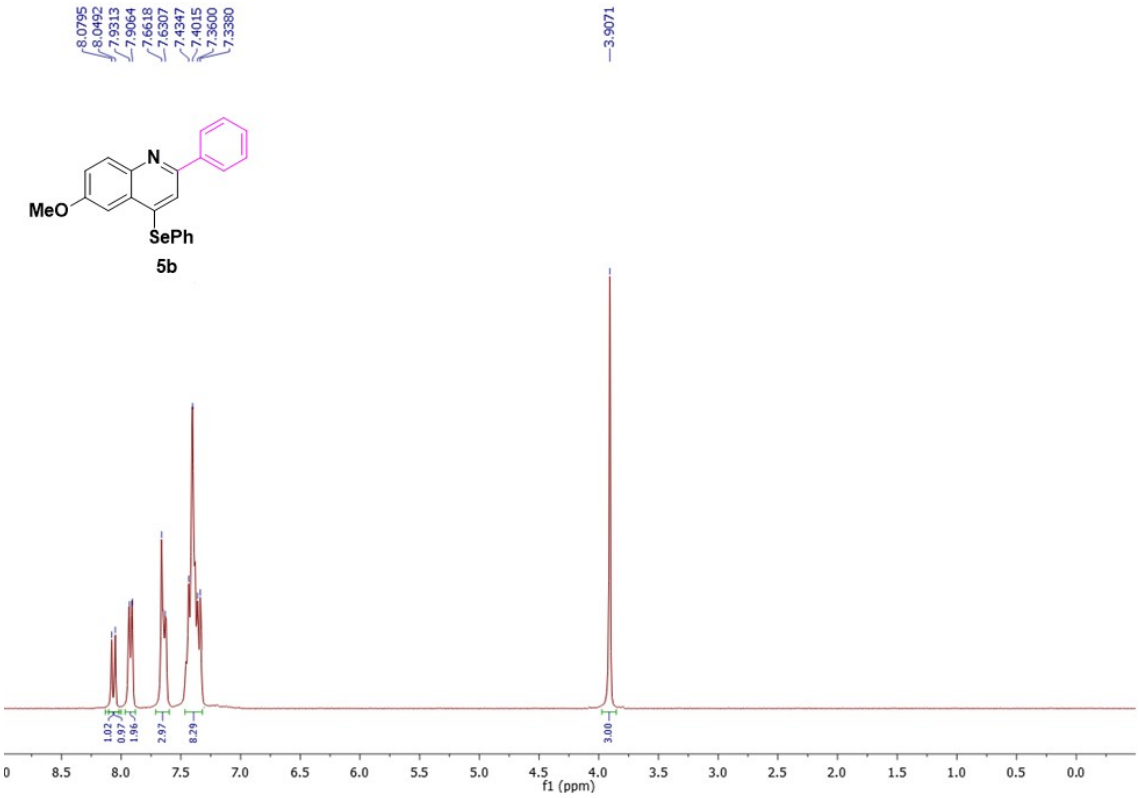
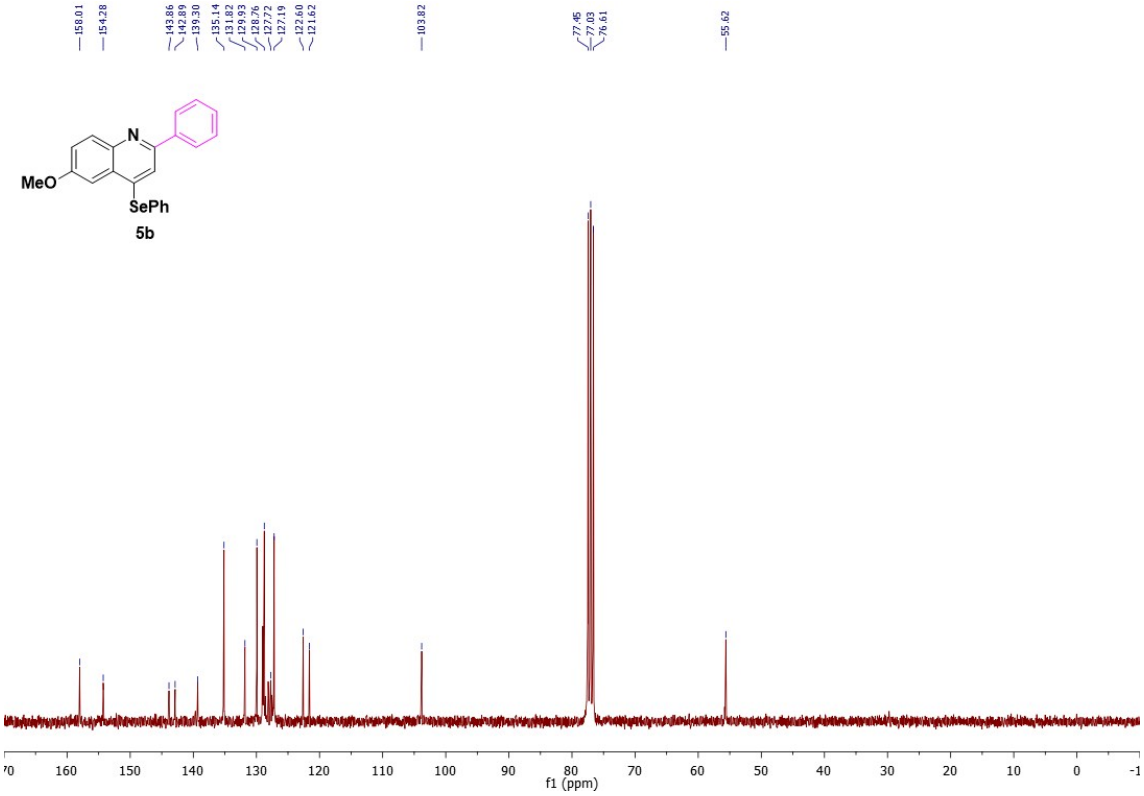
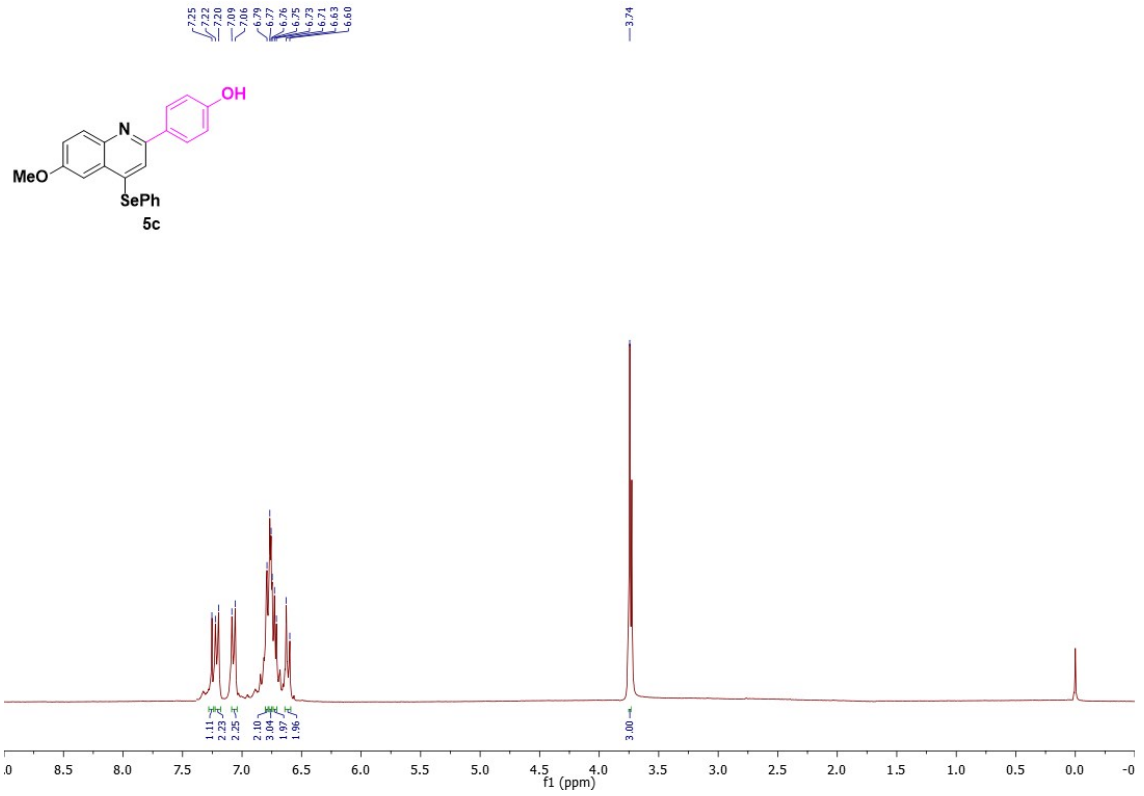
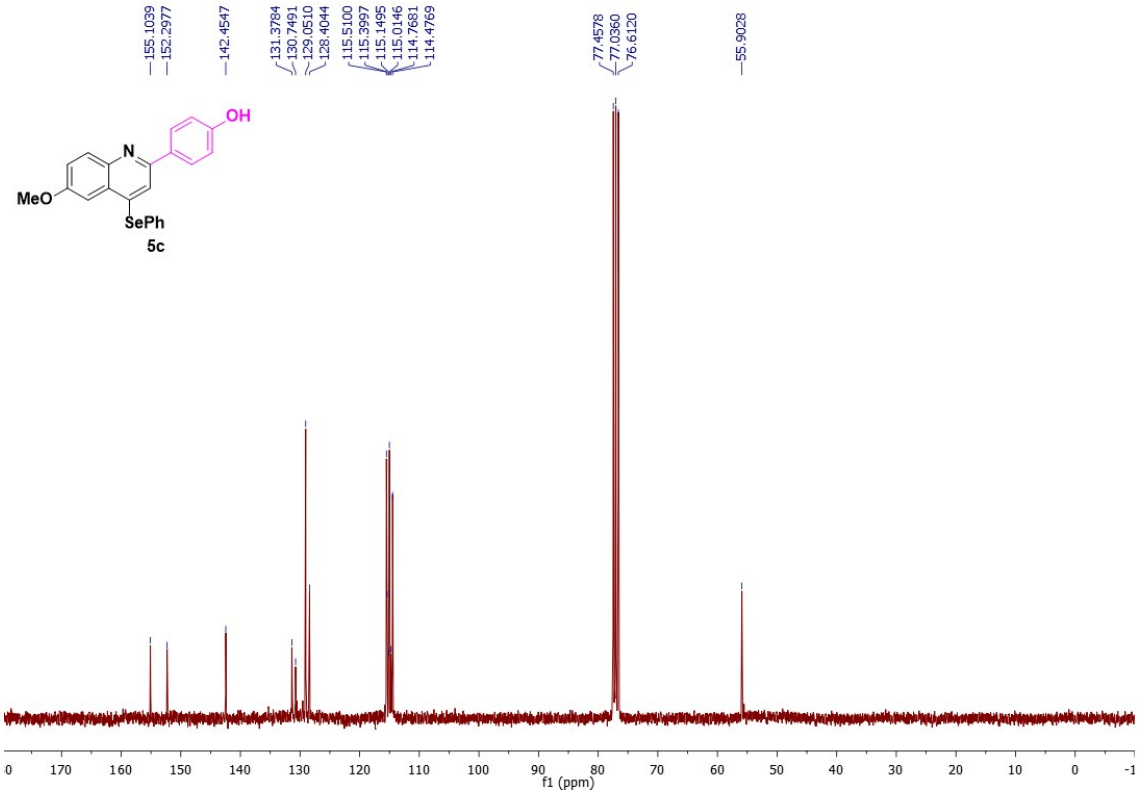
147.5481
147.2328
145.3748
136.4807
134.9338
134.7993
132.9655
132.8835
131.4727
129.7774
129.4838
129.3935
128.8026
124.2456
122.2514
119.8581
119.6592
105.9255
77.4517
77.0286
76.6048
62.2089
55.4228
14.0784
O
OEt
N
Cl
SePhPh-OMe
4h
f1 (ppm)


8.0795
8.0492
7.9313
7.9064
7.6618
7.6307
7.4347
7.4015
7.3600
7.3380
3.9071
N
MeO
SePh
5b
1.02
0.97
1.96
2.97
8.29
3.00
f1 (ppm)


158.01
154.28
143.86
142.89
139.30
135.14
131.82
129.93
128.76
127.72
127.19
122.60
121.62
103.82
77.45
77.03
76.61
55.62
MeO
SePh
5b
f1 (ppm)


7.25
7.22
7.20
7.09
7.06
6.79
6.77
6.76
6.75
6.73
6.71
6.63
6.60
3.74
OH
MeO
SePh
5c
1.11
2.23
2.25
2.10
3.04
1.97
1.90
3.00
f1 (ppm)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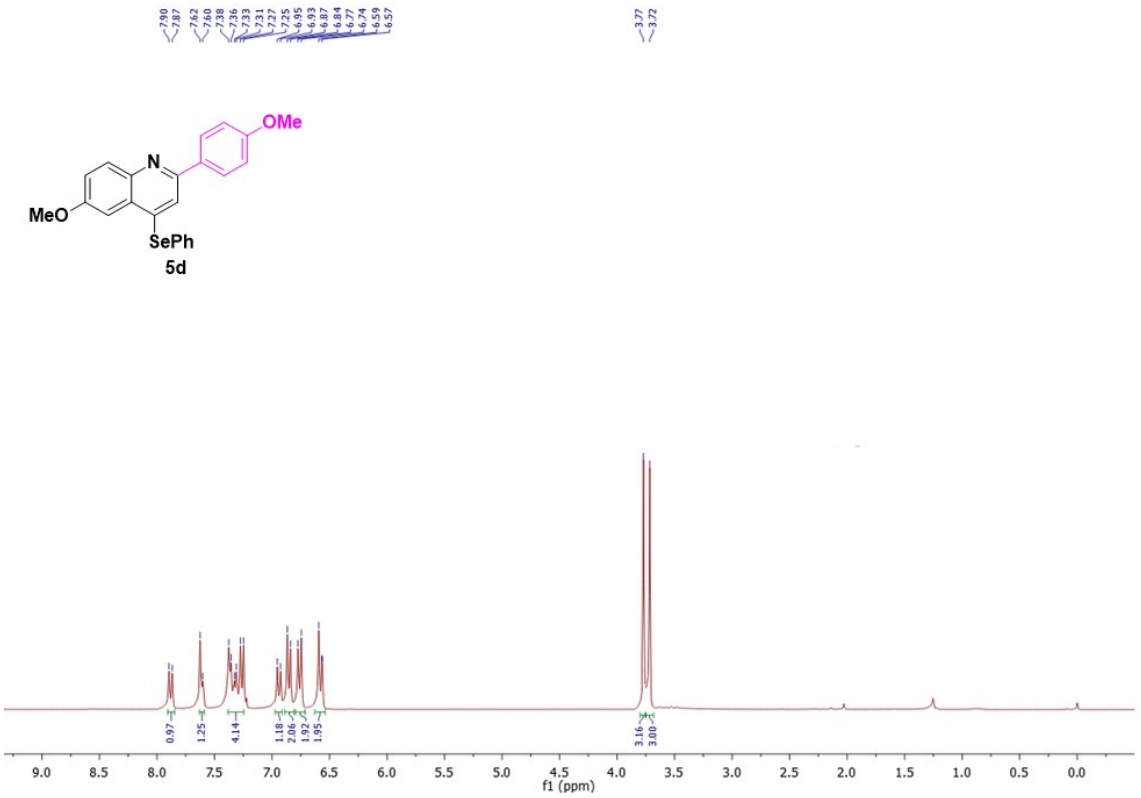
130.7491
129.0510
128.4044
115.5100
115.3997
115.1495
115.0146
114.7681
114.4769
77.4578
77.0360
76.6120
55.9028
OH
N
MeO
SePh
5c
f1 (ppm)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7.36
7.33
7.31
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7.25
6.95
6.93
6.87
6.84
6.77
6.74
6.59
6.57
3.77
3.72
OMe
N
MeO
SePh
5d
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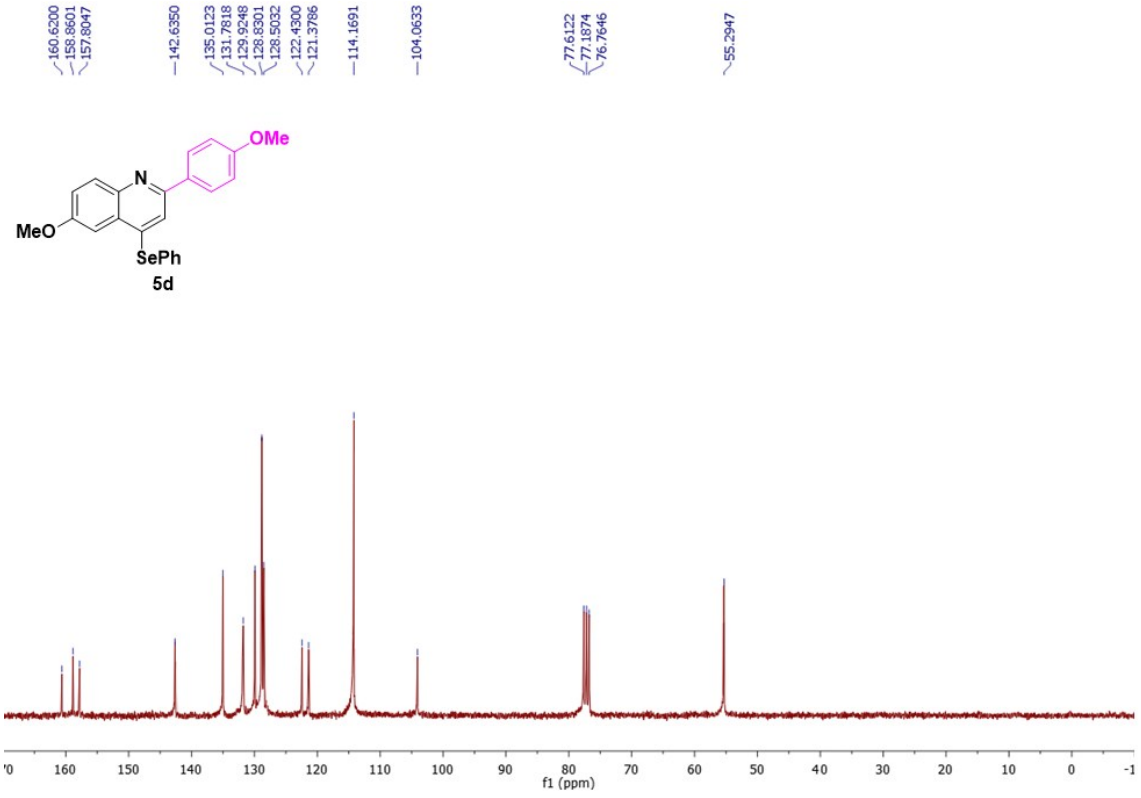
1.25
4.14
1.18
2.06
1.92
1.95
3.16
3.00
f1 (ppm)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129.9248
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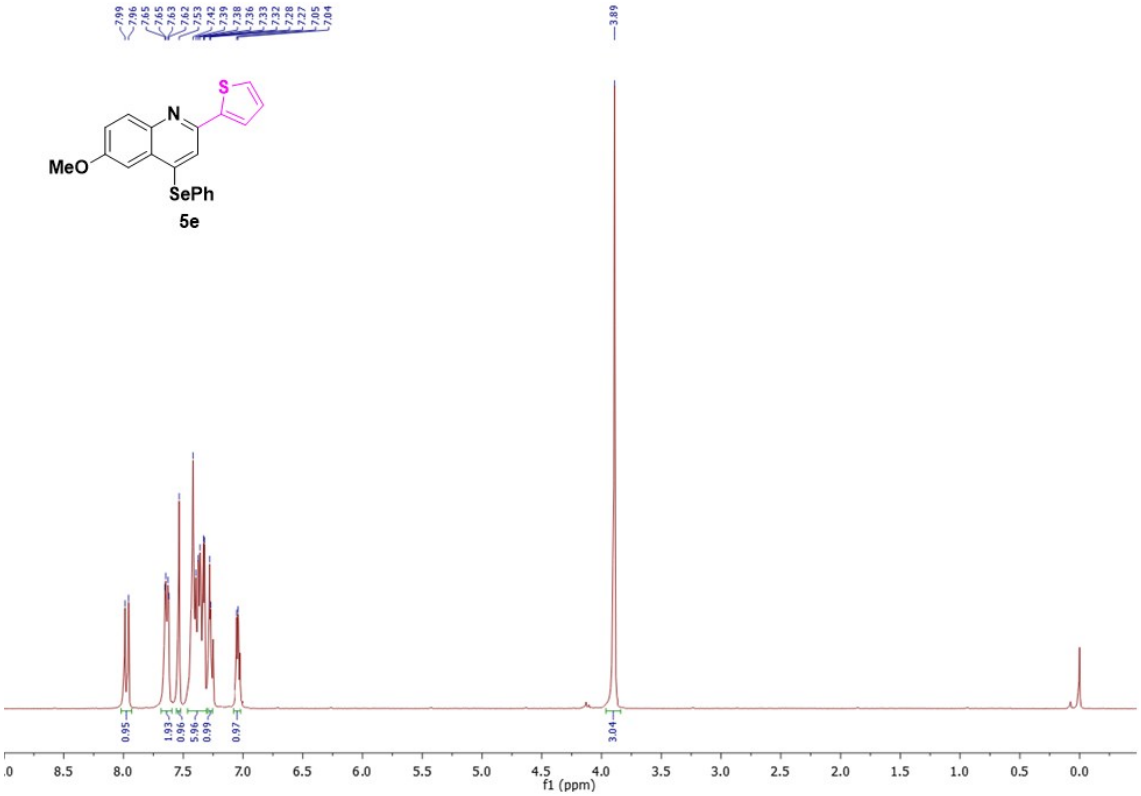
128.5032
122.4300
121.3786
114.1691
104.0633
77.6122
77.1874
76.7646
55.2947
OMe
N
MeO
SePh
5d
f1 (ppm)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7.42
7.39
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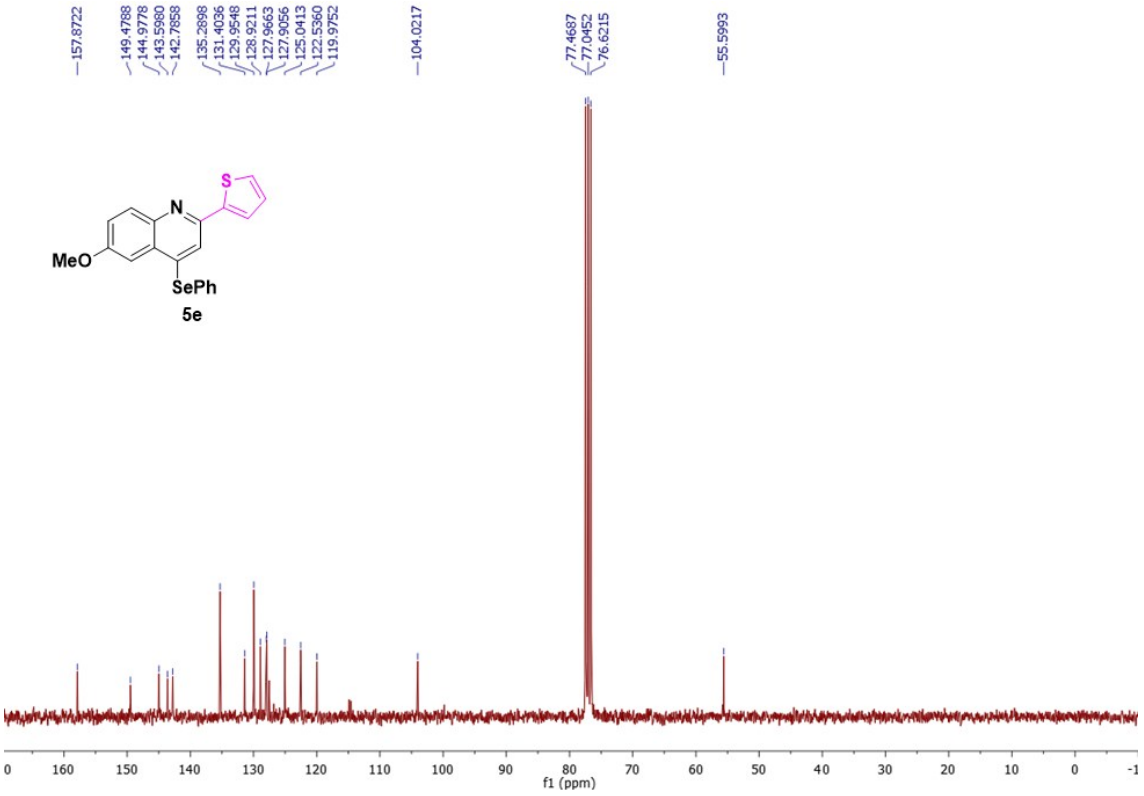
7.36
7.33
7.32
7.28
7.27
7.05
7.04
3.89
S
N
MeO
SePh
5e
0.95
1.93
0.96
5.96
0.99
0.97
3.04
f1 (ppm)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128.9211
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127.9056
125.0413
122.5360
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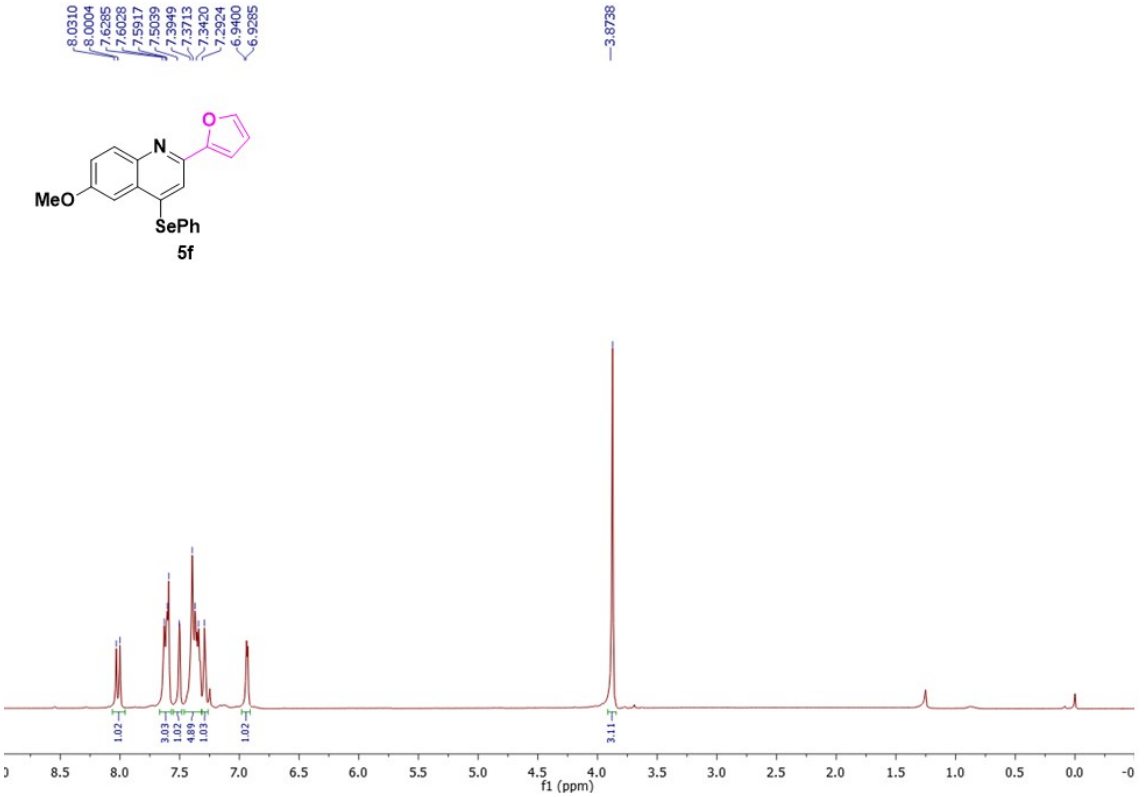
76.6215
55.5993
S
N
MeO
SePh
5e
f1 (ppm)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8.0004
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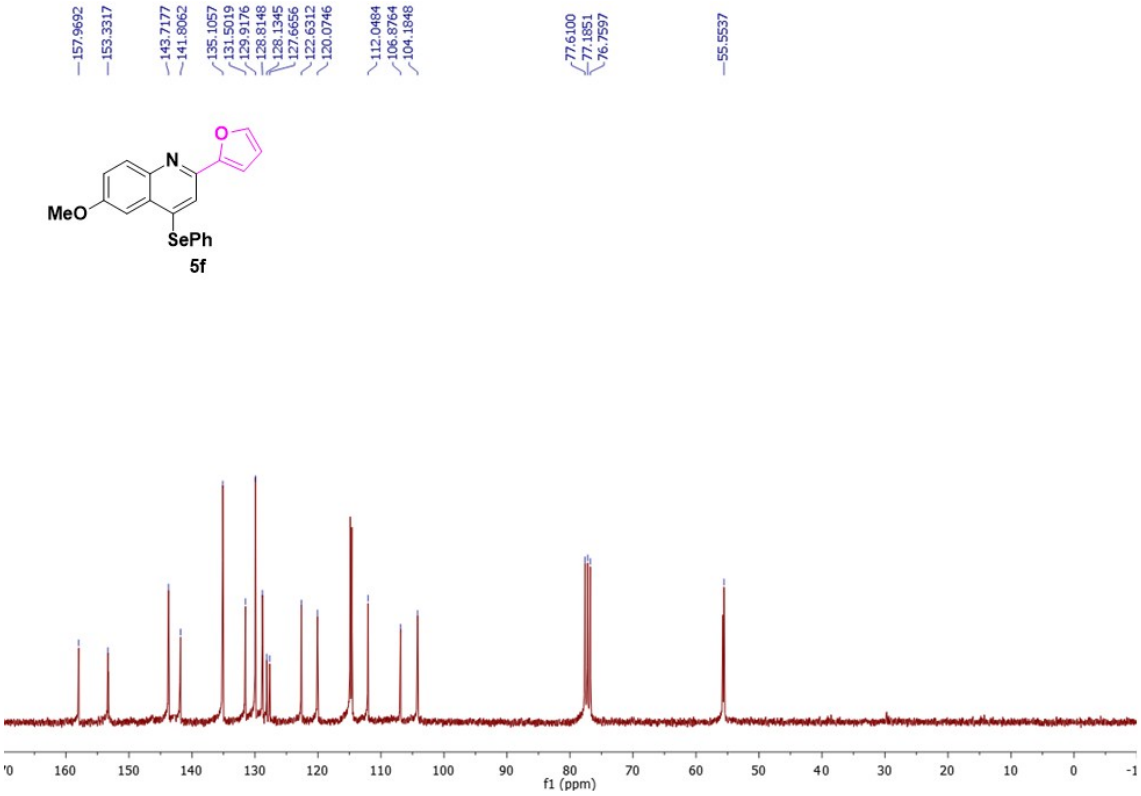
7.5917
7.5039
7.3949
7.3713
7.3420
7.2924
6.9400
6.9285
3.8738
O
N
MeO
SePh
5f
1.02
3.03
1.02
4.89
1.03
1.02
3.11
f1 (ppm)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128.1345
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122.6312
120.0746
112.0484
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76.7597
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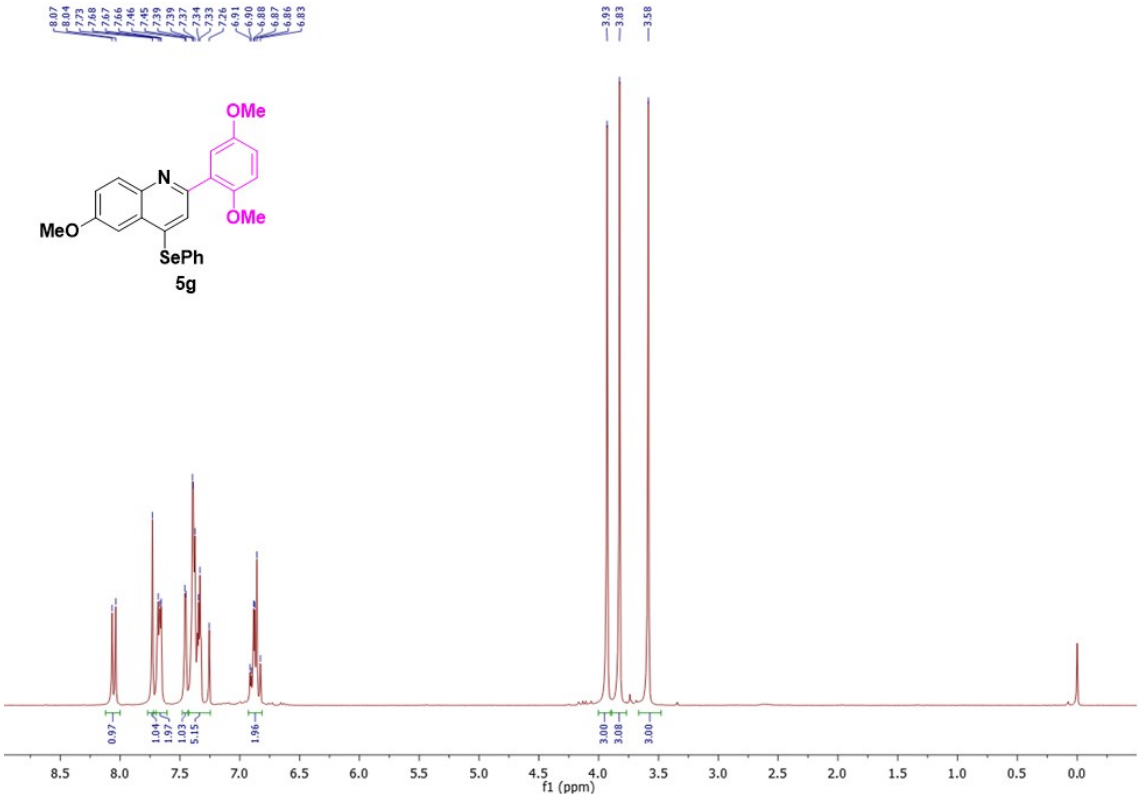
N
MeO
SePh
5f
f1 (ppm)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7.73
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7.67
7.66
7.46
7.45
7.39
7.39
7.37
7.34
7.33
7.26
6.91
6.90
6.88
6.87
6.86
6.83
3.93
3.83
3.58
OMe
OMe
N
MeO
SePh
5g
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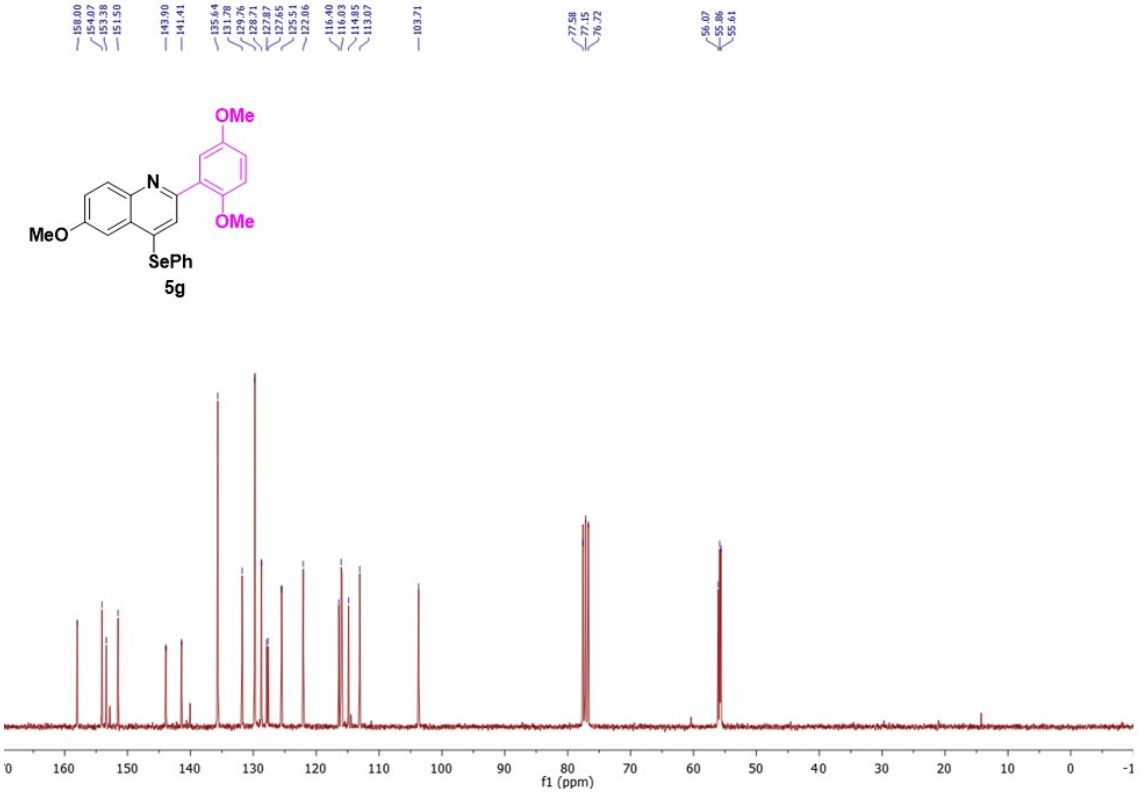
1.04
1.97
1.03
5.15
1.96
3.00
3.08
3.00
f1 (ppm)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135.64
131.78
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129.71
127.87
127.65
125.51
122.06
116.40
116.03
114.85
113.07
103.71
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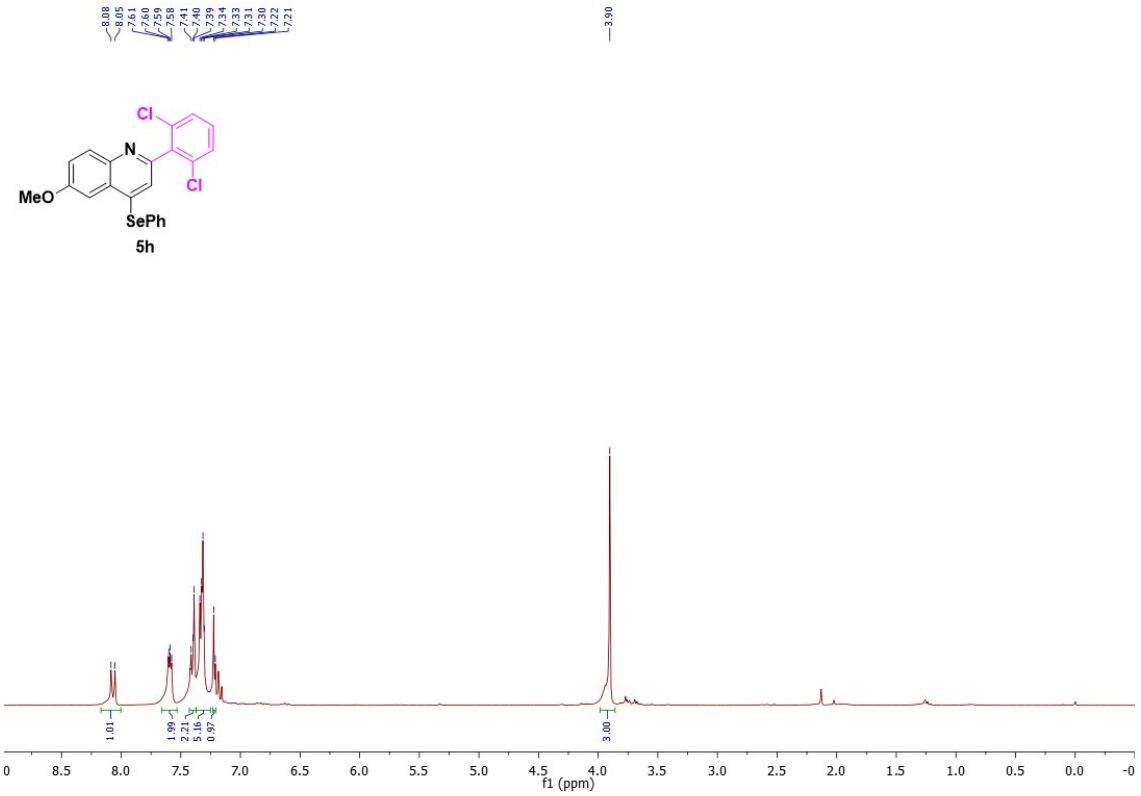
77.15
76.72
56.07
55.86
55.61
OMe
OMe
MeO
N
SePh
5g
f1 (ppm)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7.61
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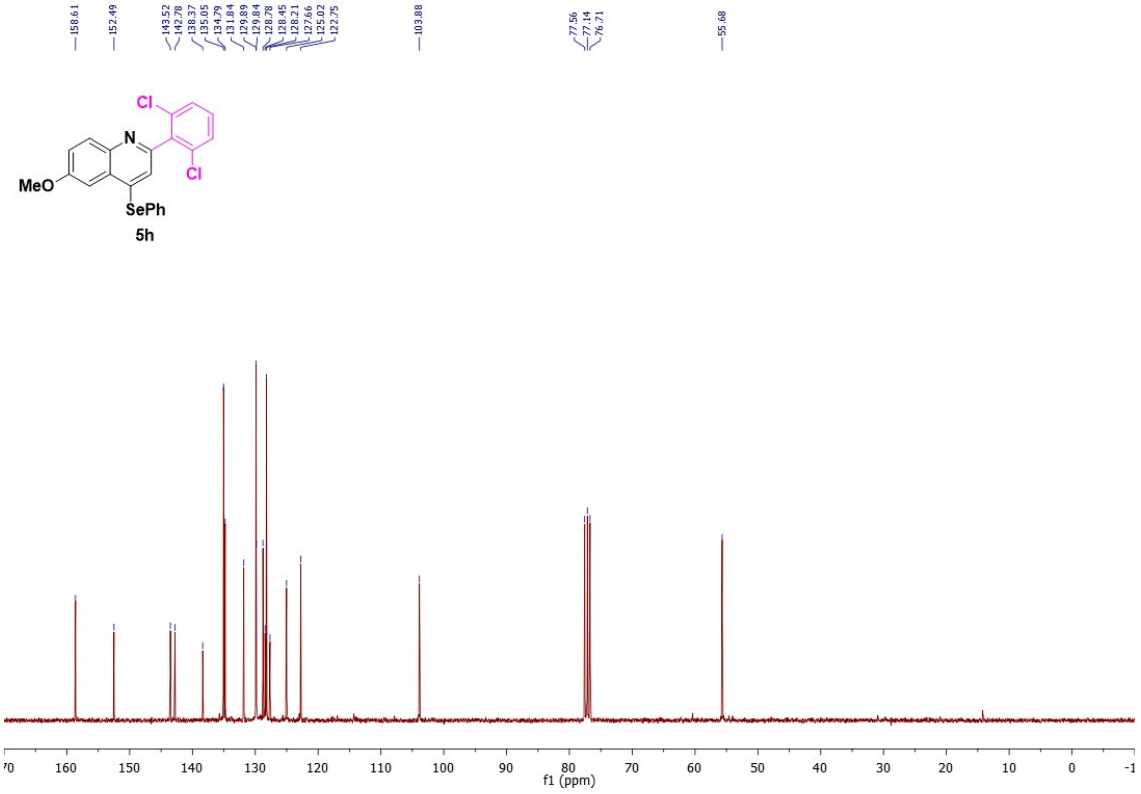
7.58
7.41
7.40
7.39
7.34
7.33
7.31
7.30
7.22
7.21
3.90
Cl
Cl
MeO
N
SePh
5h
1.01
1.99
2.21
5.16
0.97
3.00
f1 (ppm)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135.05
134.79
131.84
129.89
129.84
128.78
128.45
128.21
127.66
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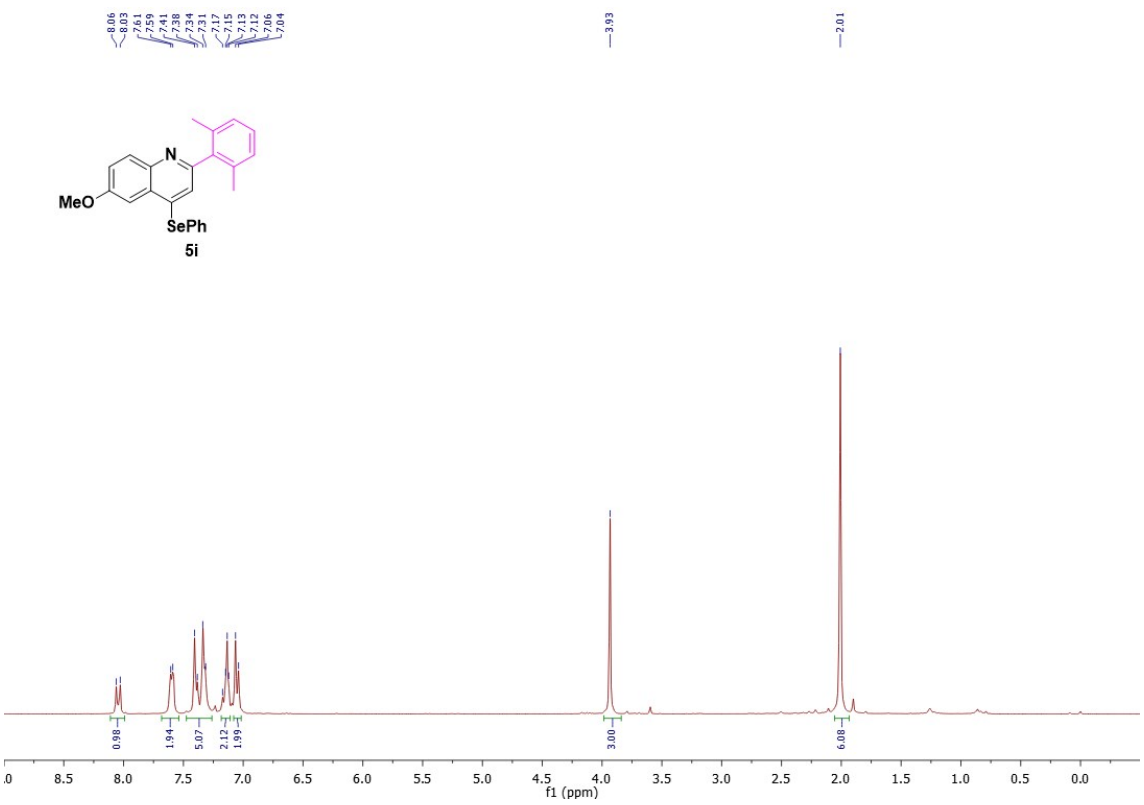
103.88
77.56
77.14
76.71
55.68
Cl
N
Cl
MeO
SePh
5h
f1 (ppm)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8.03
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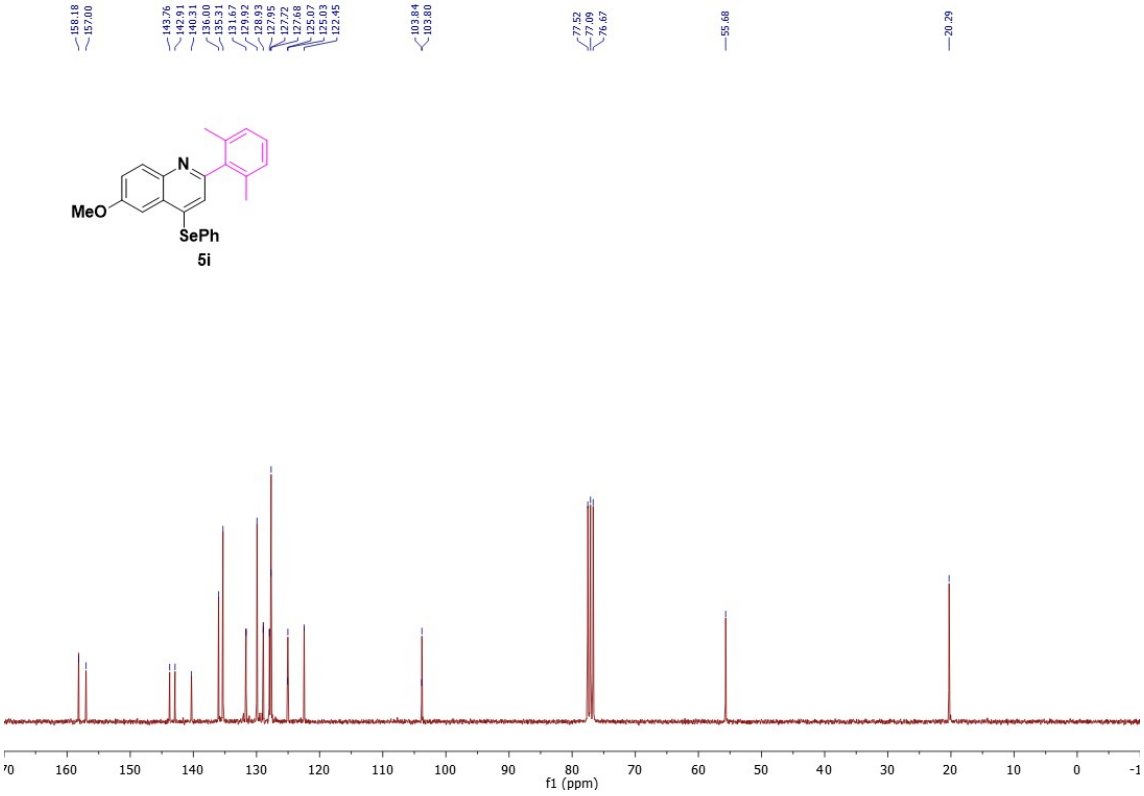
7.59
7.41
7.38
7.34
7.31
7.17
7.15
7.13
7.12
7.06
7.04
3.93
2.01
N
MeO
SePh
5i
0.98
1.94
5.07
2.12
1.99
3.00
6.08
f1 (ppm)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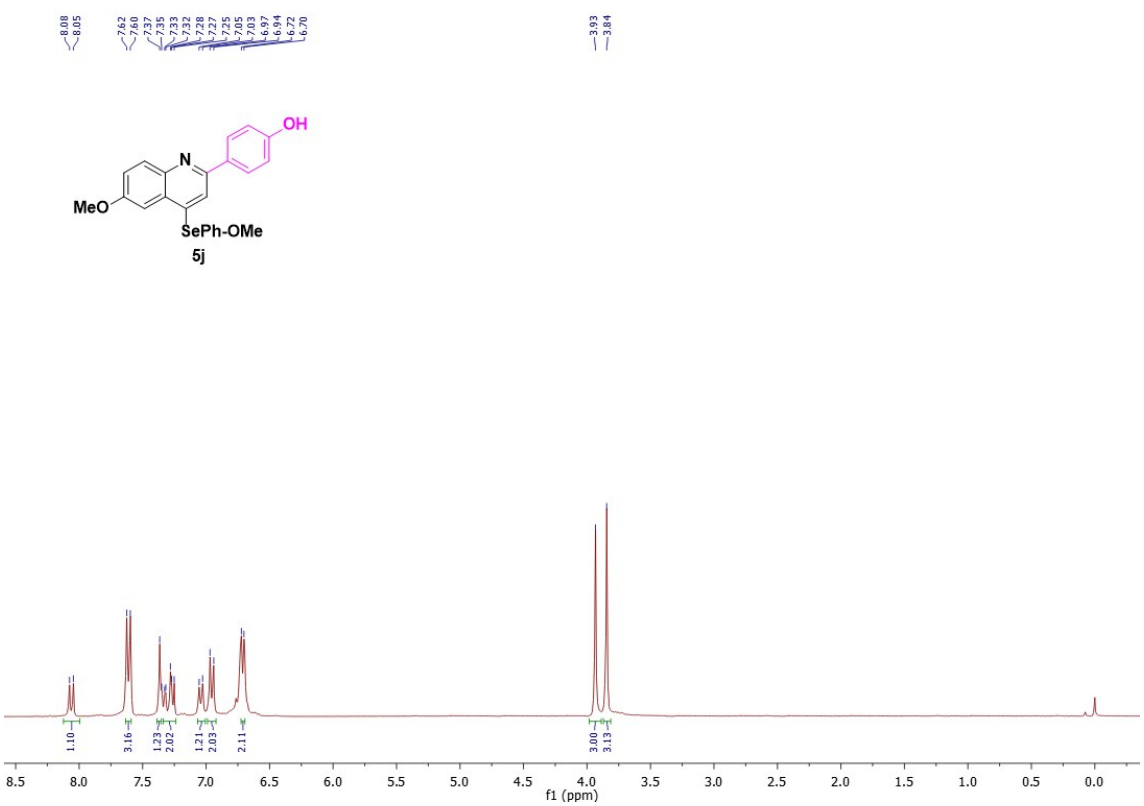
127.68
125.07
123.03
122.45
103.84
103.80
77.52
77.08
76.67
55.68
20.29
N
MeO
SePh
5i
f1 (ppm)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7.60
7.37
7.35
7.33
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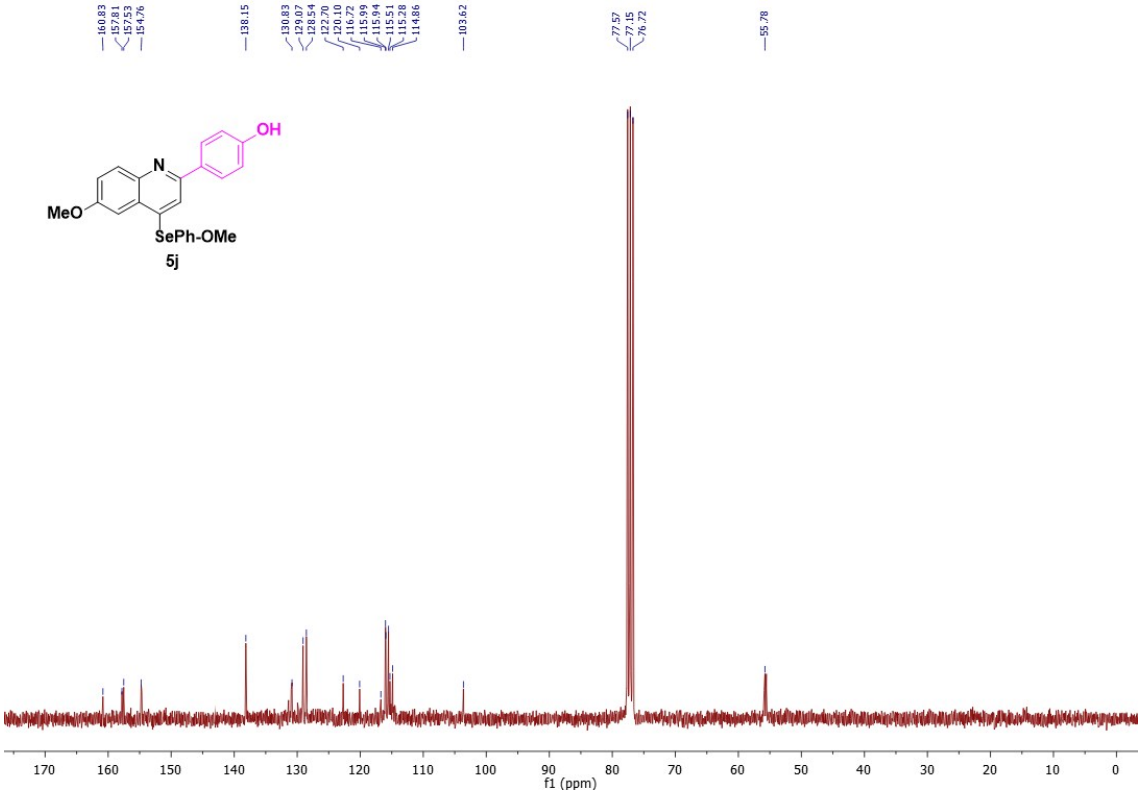
7.28
7.27
7.25
7.05
7.03
6.97
6.94
6.72
6.70
3.93
3.84
OH
N
MeO
SePh-OMe
5j
1.10
3.16
1.23
2.02
1.21
2.03
2.11
3.00
3.13
f1 (ppm)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128.54
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120.10
116.72
115.99
115.94
115.51
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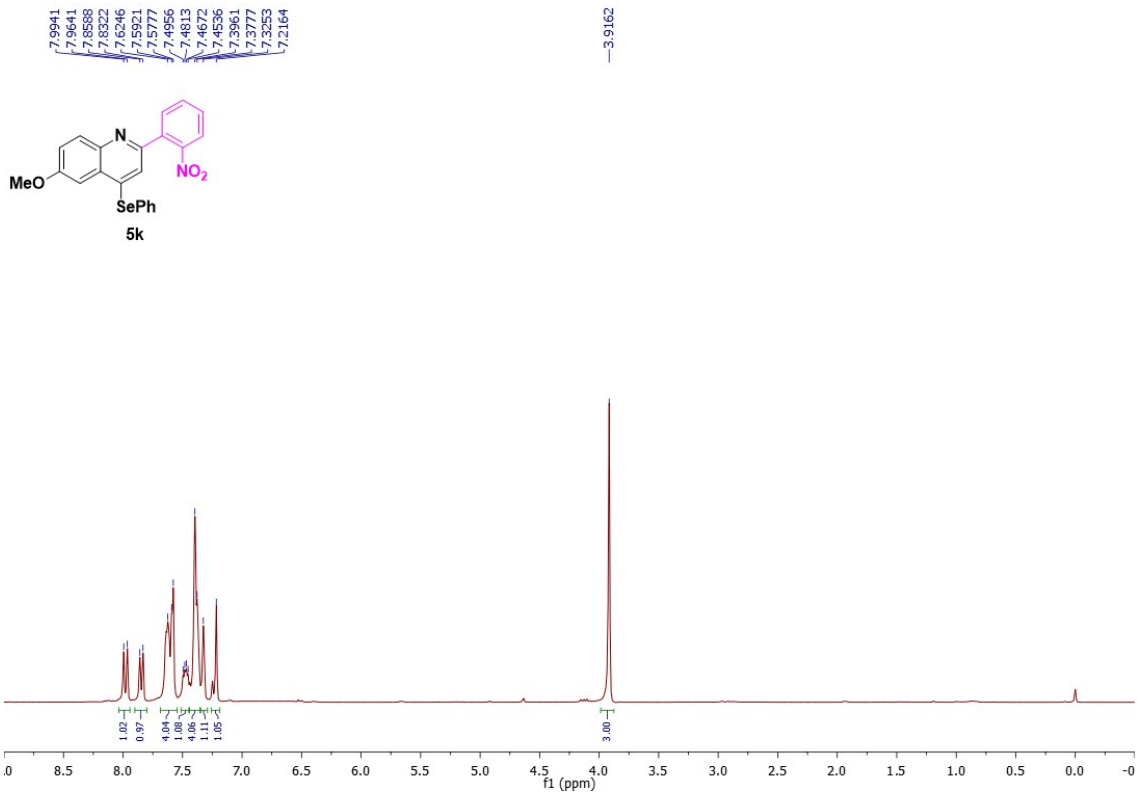
77.57
77.15
76.72
55.78
OH
N
MeO
SePh-OMe
5j
f1 (ppm)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7.4536
7.3961
7.3777
7.3253
7.2164
3.9162
N
NO2
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SePh
5k
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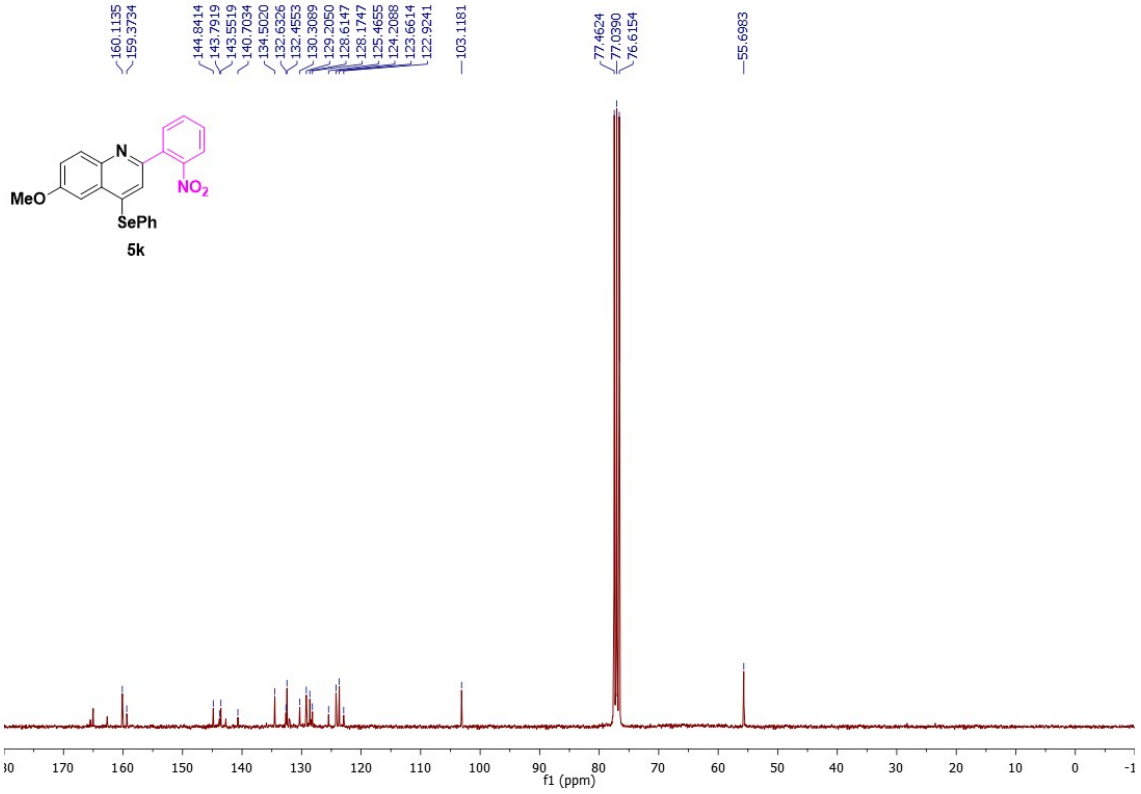
0.97
4.04
1.08
4.06
1.11
1.05
3.00
f1 (ppm)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128.6147
128.1747
125.4655
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123.6614
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MeO
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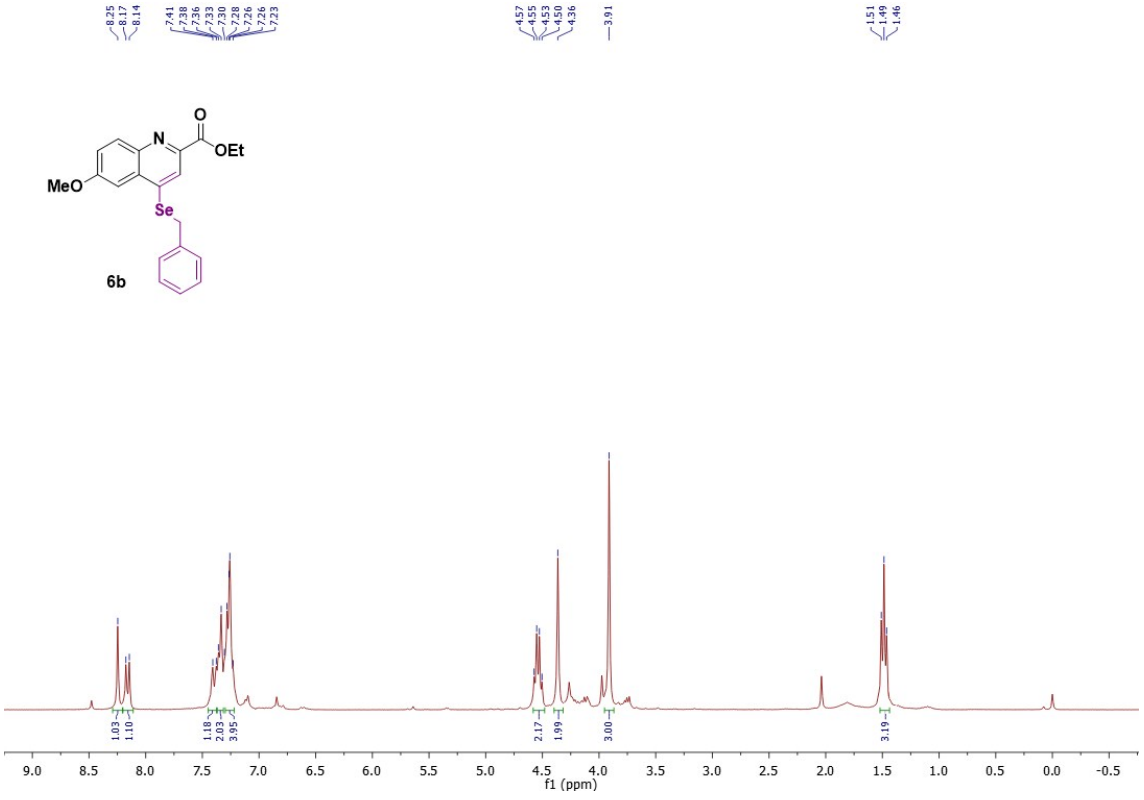
NO2
SePh
5k
f1 (ppm)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7.26
7.23
4.57
4.55
4.53
4.50
4.36
3.91
1.51
1.49
1.46
MeO
N
O
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Se
6b
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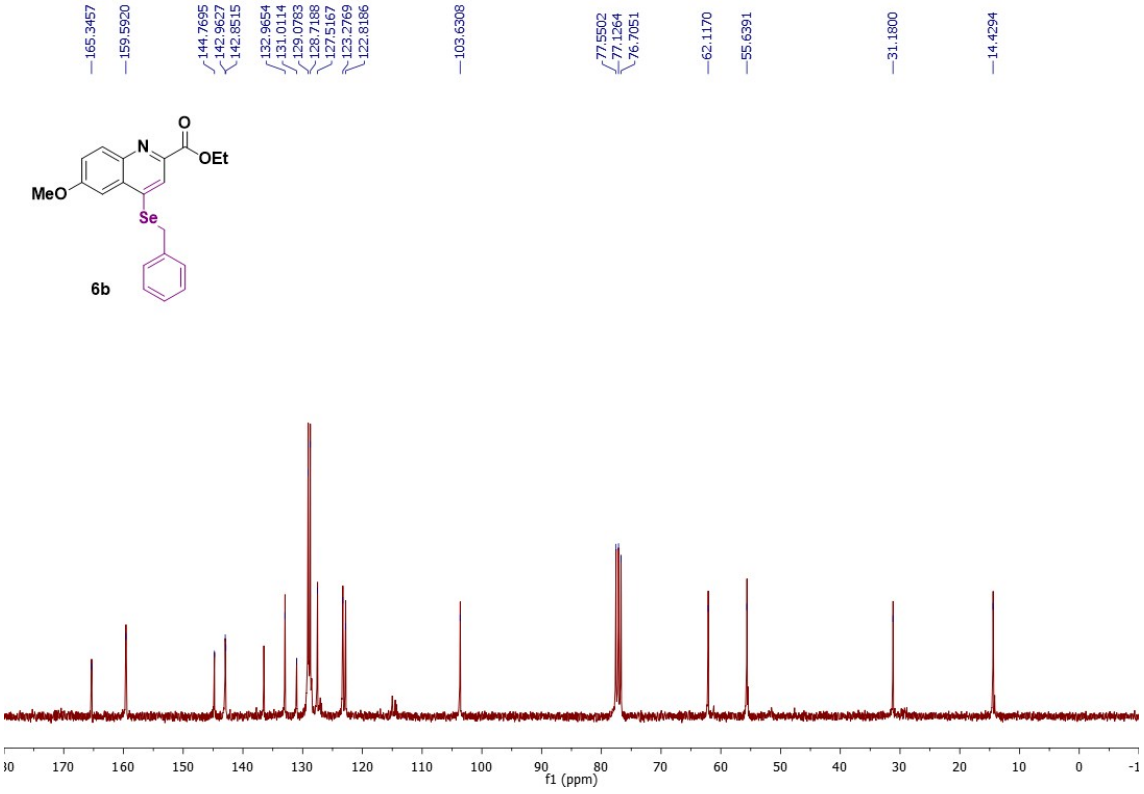
1.10
1.18
2.03
3.95
2.17
1.99
3.00
3.19
f1 (ppm)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103.6308
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31.1800
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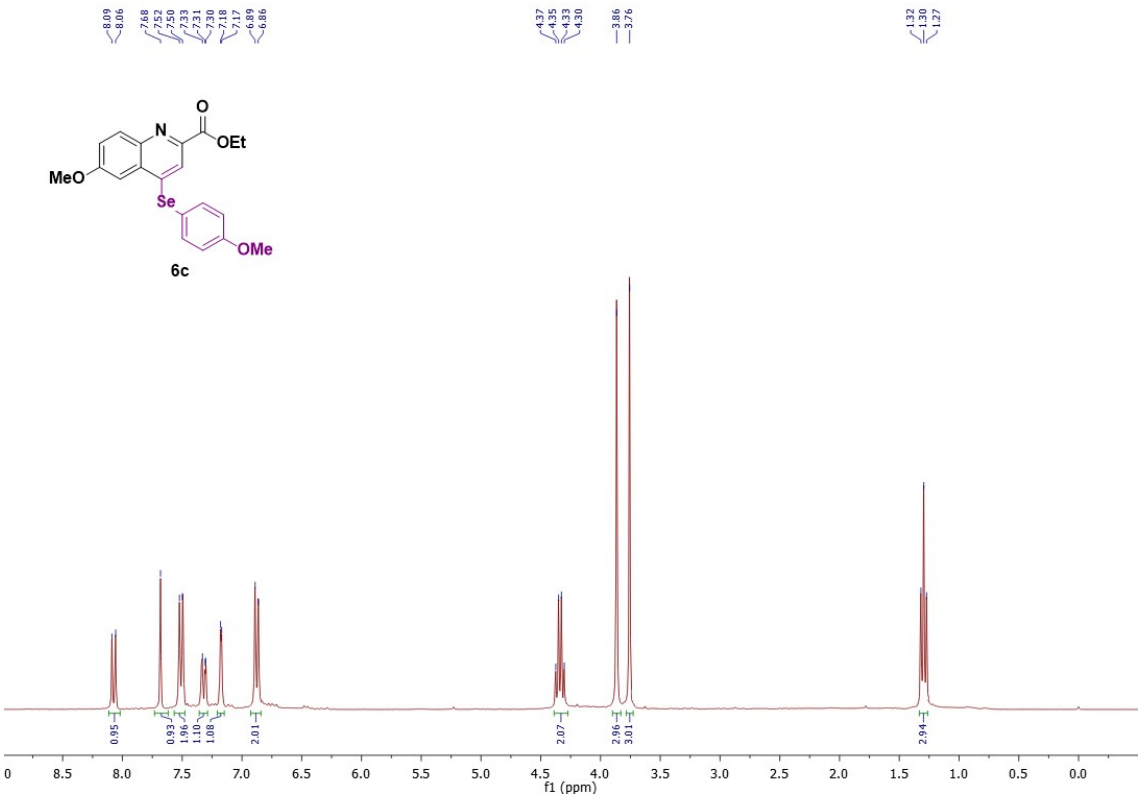
N
OEt
MeO
Se
6b
f1 (ppm)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7.31
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7.18
7.17
6.89
6.86
4.37
4.35
4.33
4.30
3.86
3.76
1.32
1.30
1.27
O
N
OEt
MeO
Se
OMe
6c
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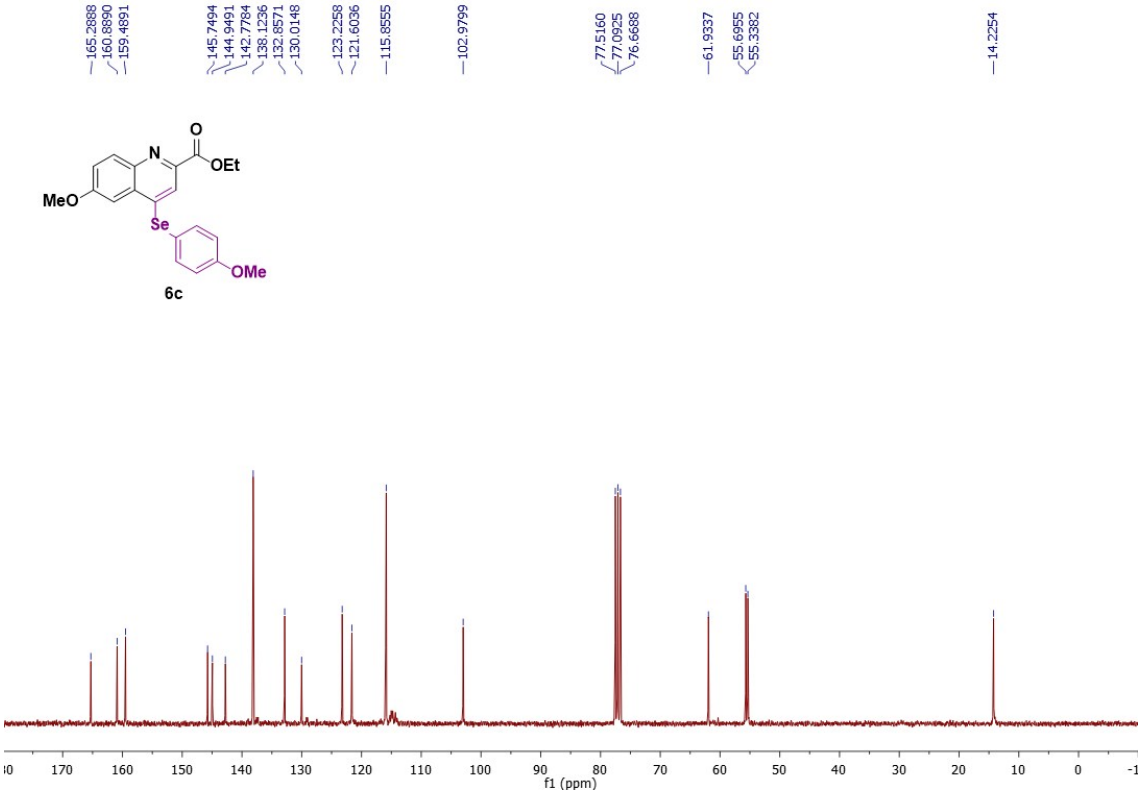
0.93
1.96
1.10
1.08
2.01
2.07
2.96
3.01
2.94
f1 (ppm)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115.8555
102.9799
77.5160
77.0925
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14.2254
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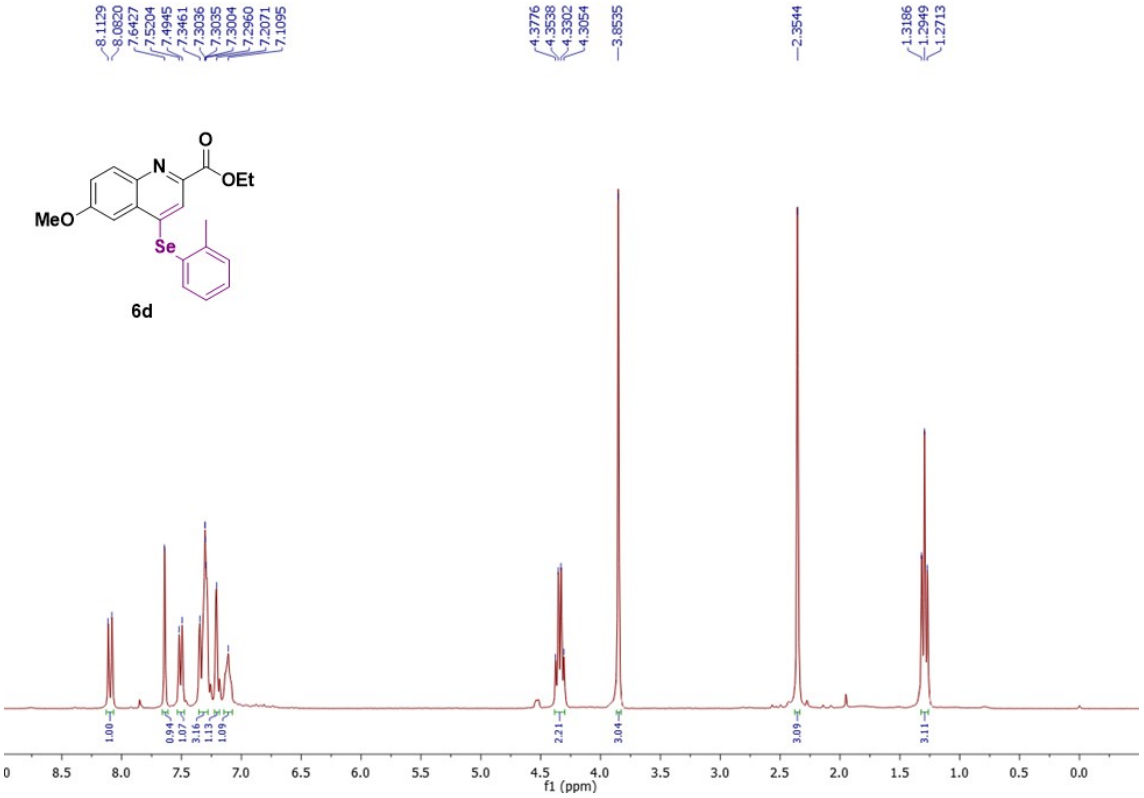
OEt
MeO
Se
OMe
6c
f1 (ppm)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7.1095
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4.3538
4.3302
4.3054
3.8535
2.3544
1.3186
1.2949
1.2713
O
N
OEt
MeO
Se
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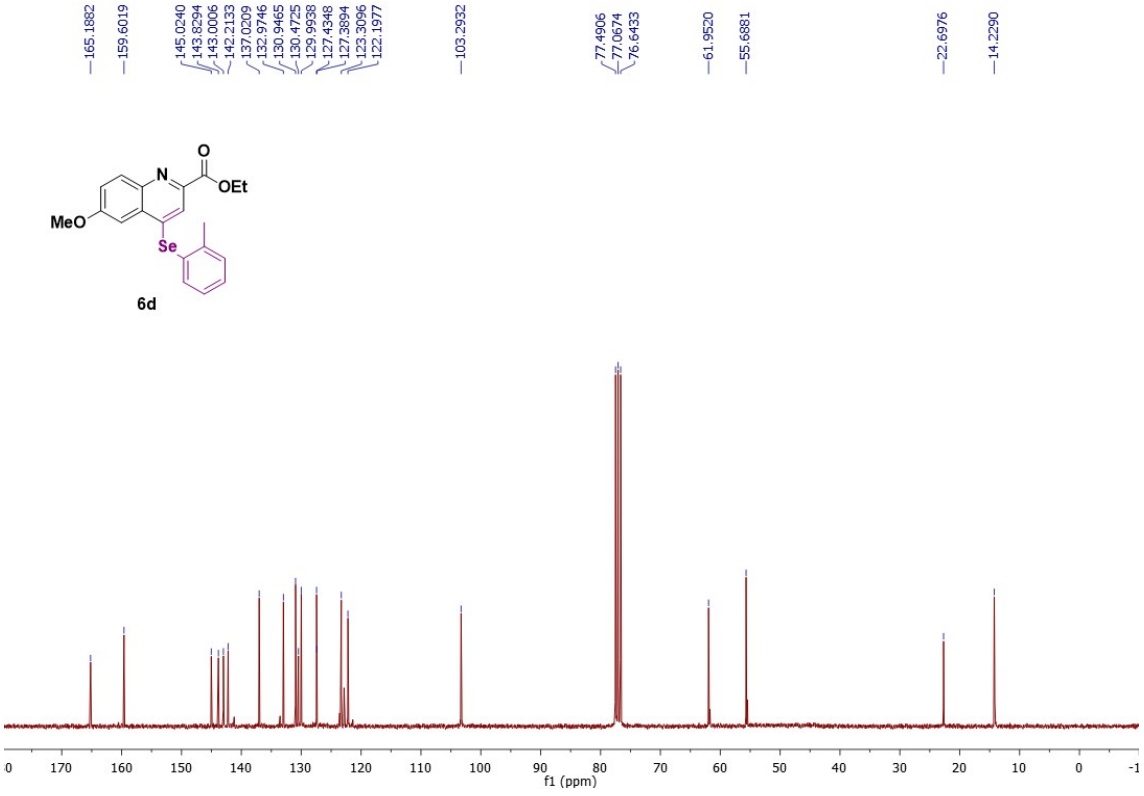
3.16
1.13
1.09
2.21
3.04
3.09
3.11
f1 (ppm)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127.3894
123.3096
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77.4906
77.0674
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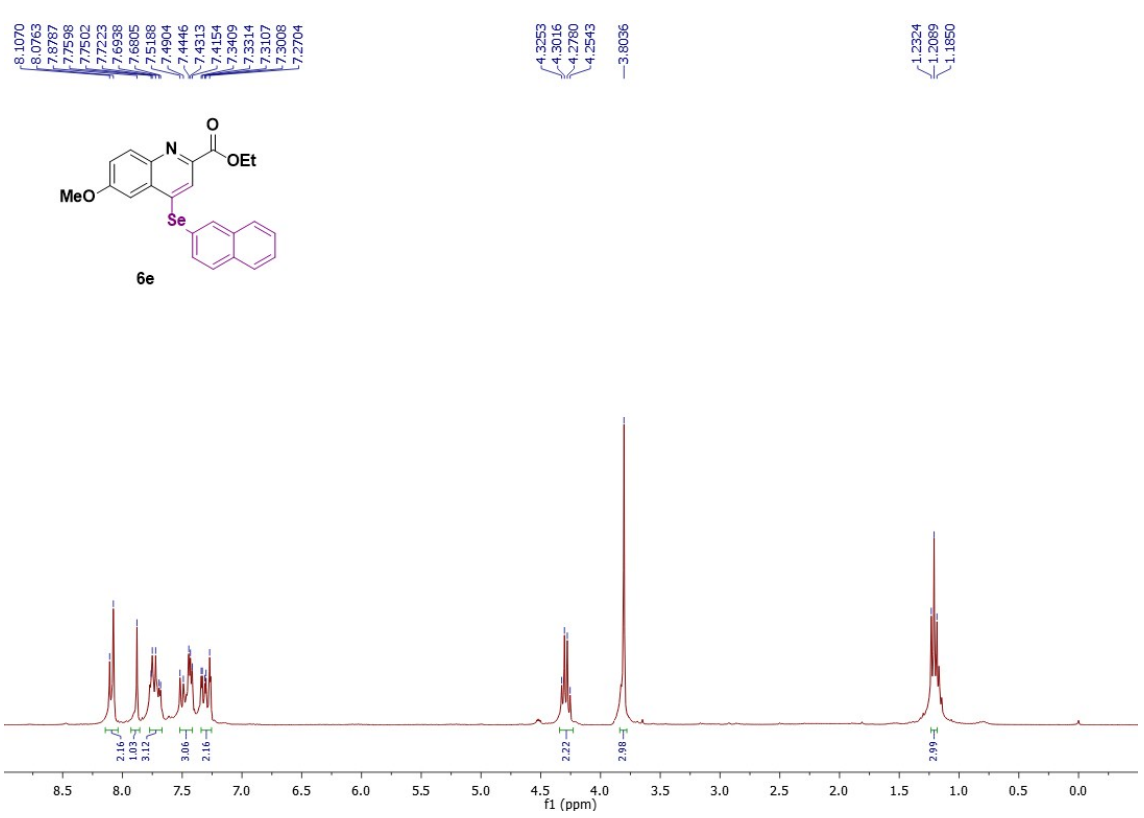
OEt
MeO
Se
6d
f1 (ppm)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4.2543
3.8036
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1.2089
1.1850
O
N
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Se
6e
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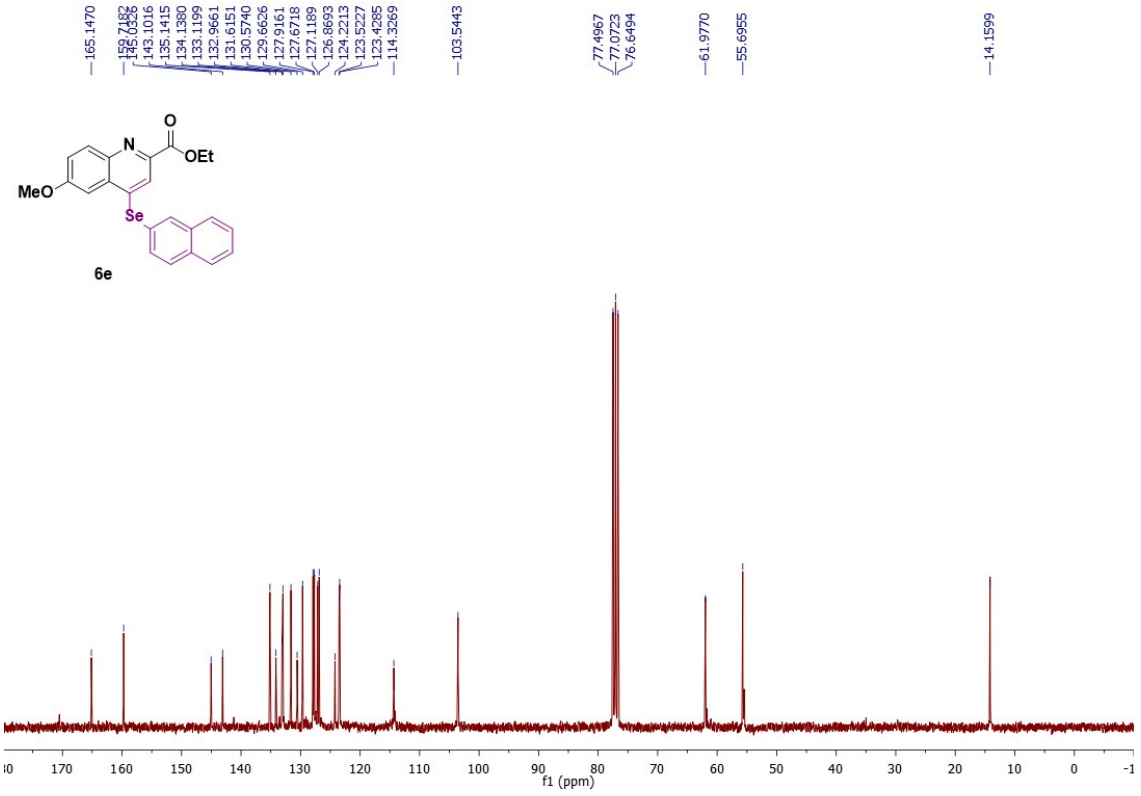
1.03
3.12
3.06
2.16
2.22
2.98
2.99
f1 (ppm)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124.2213
123.5227
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114.3269
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77.4967
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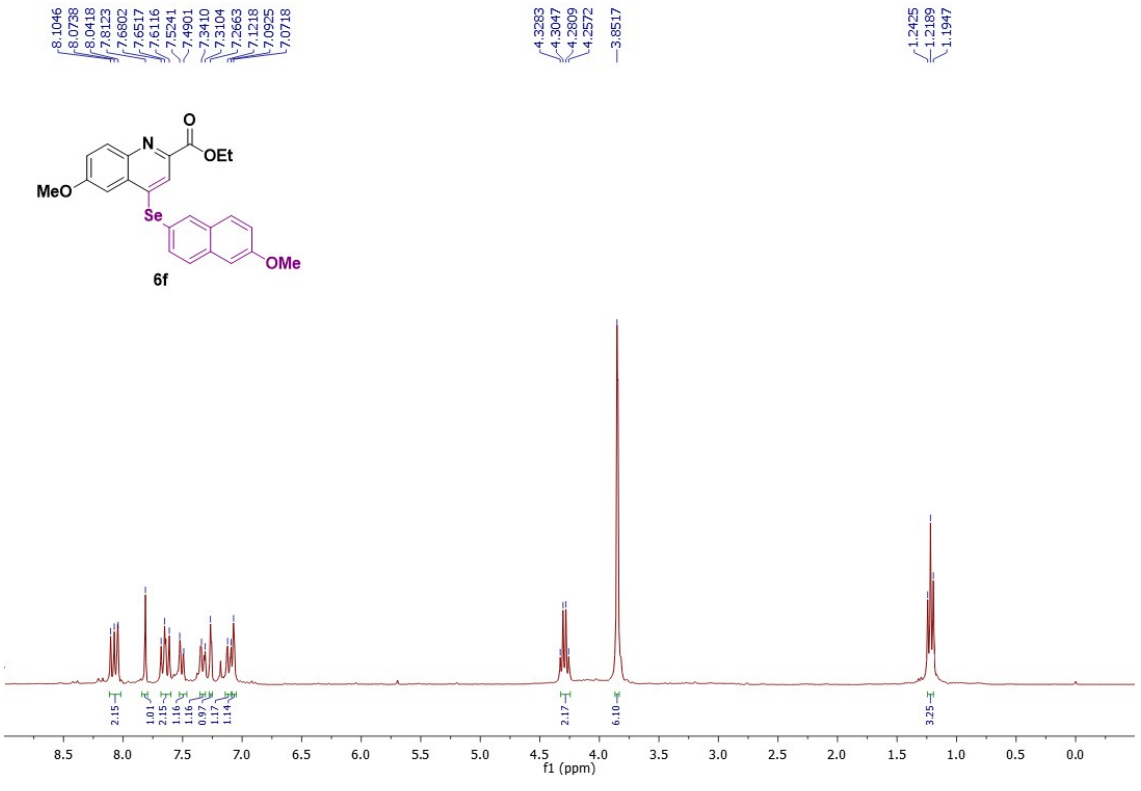
N
OEt
MeO
Se
6e
f1 (ppm)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7.3104
7.2663
7.1218
7.0925
7.0718
4.3283
4.3047
4.2809
4.2572
3.8517
1.2425
1.2189
1.1947
O
N
OEt
MeO
Se
OMe
6f
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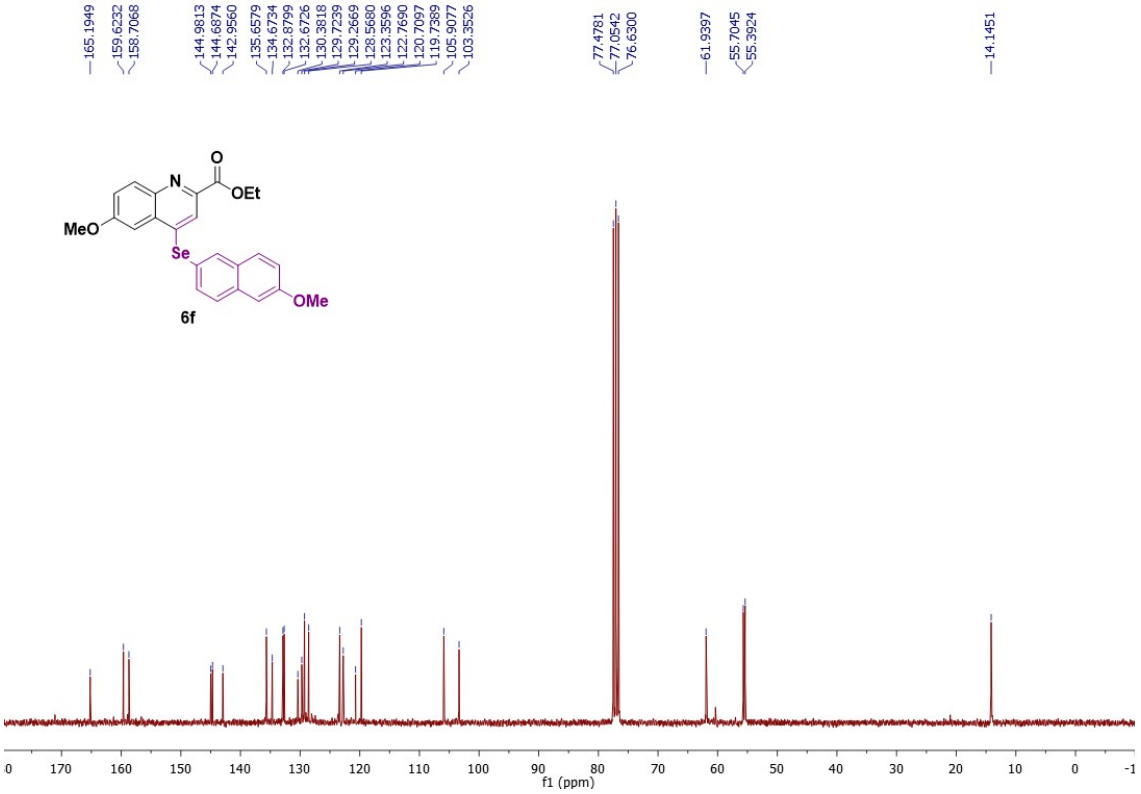
1.01
2.15
1.16
1.16
0.97
1.17
1.14
2.17
6.10
3.25
f1 (ppm)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119.7389
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103.3526
77.4781
77.0542
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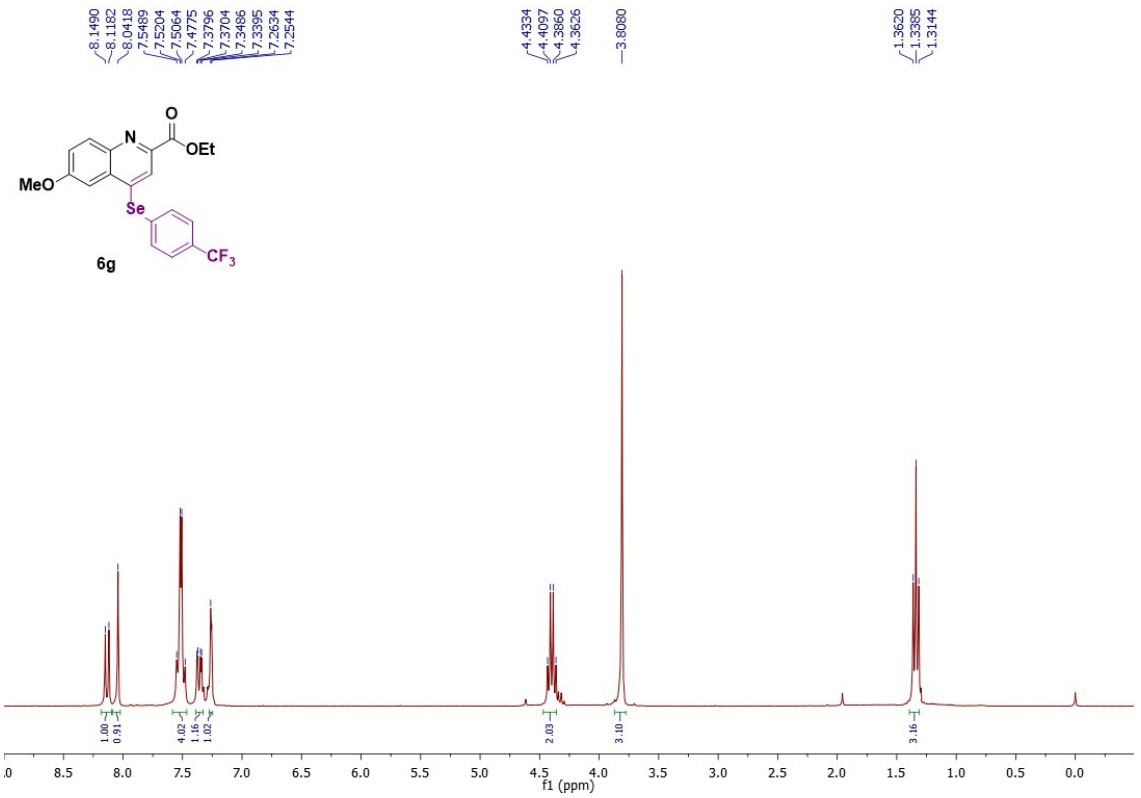
55.3924
14.1451
O
N
OEt
MeO
Se
OMe
6f
f1 (ppm)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7.2544
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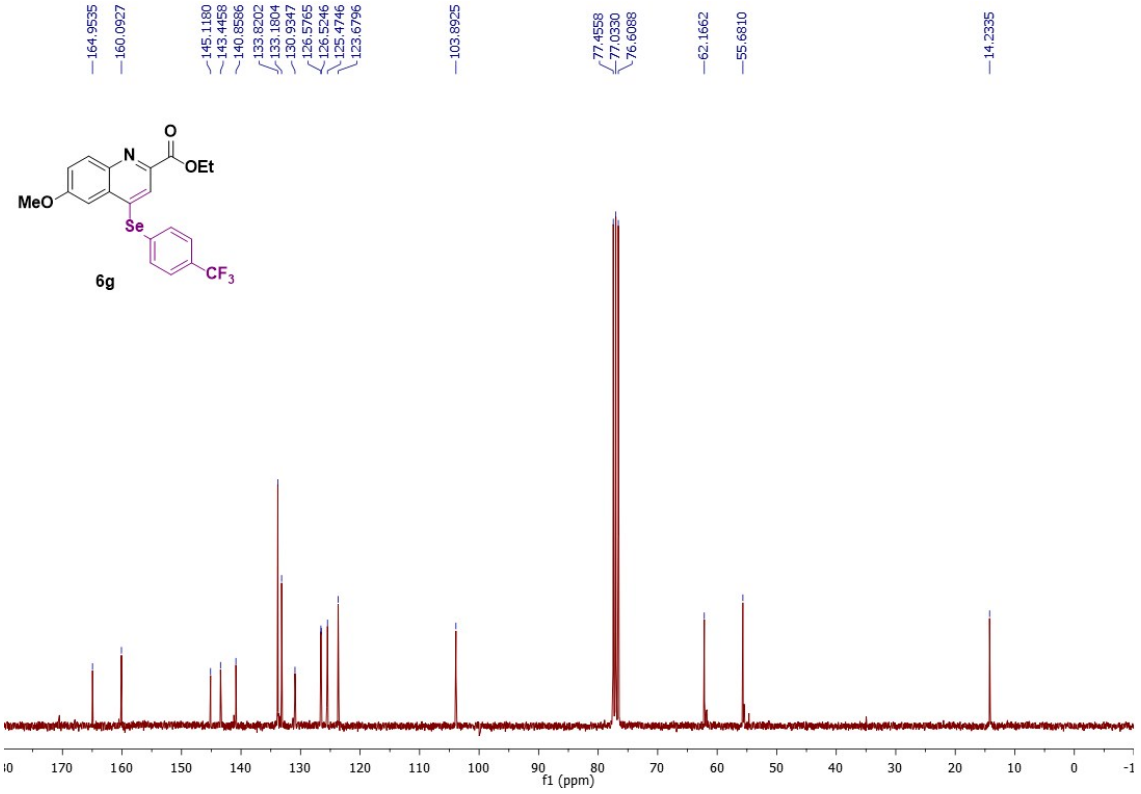
4.3626
3.8080
1.3620
1.3385
1.3144
O
N
OEt
MeO
Se
CF3
6g
1.00
0.91
4.02
1.16
1.02
2.03
3.10
3.16
f1 (ppm)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133.1804
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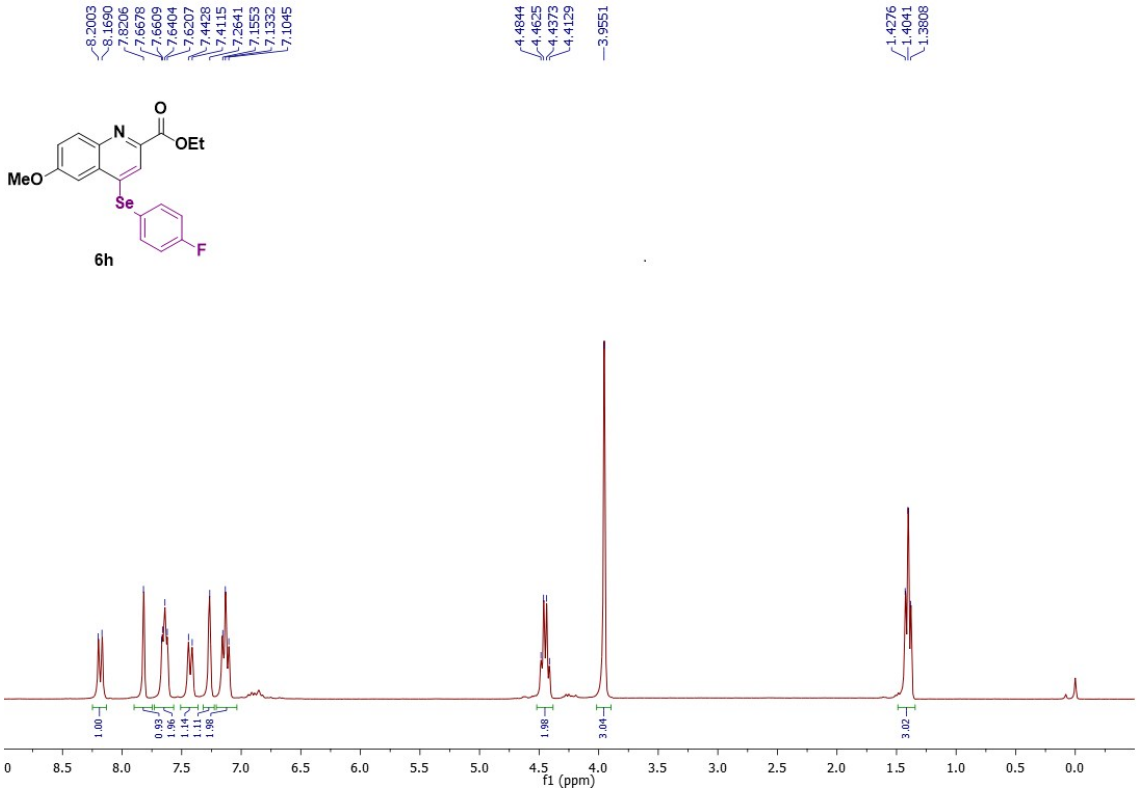
126.5246
125.4746
123.6796
103.8925
77.4558
77.0330
76.6088
62.1662
55.6810
14.2335
O
N
OEt
MeO
Se
CF3
6g
f1 (ppm)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7.6609
7.6404
7.6207
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7.4115
7.2641
7.1553
7.1332
7.1045
4.4844
4.4625
4.4373
4.4129
3.9551
1.4276
1.4041
1.3808
O
N
OEt
MeO
Se
F
6h
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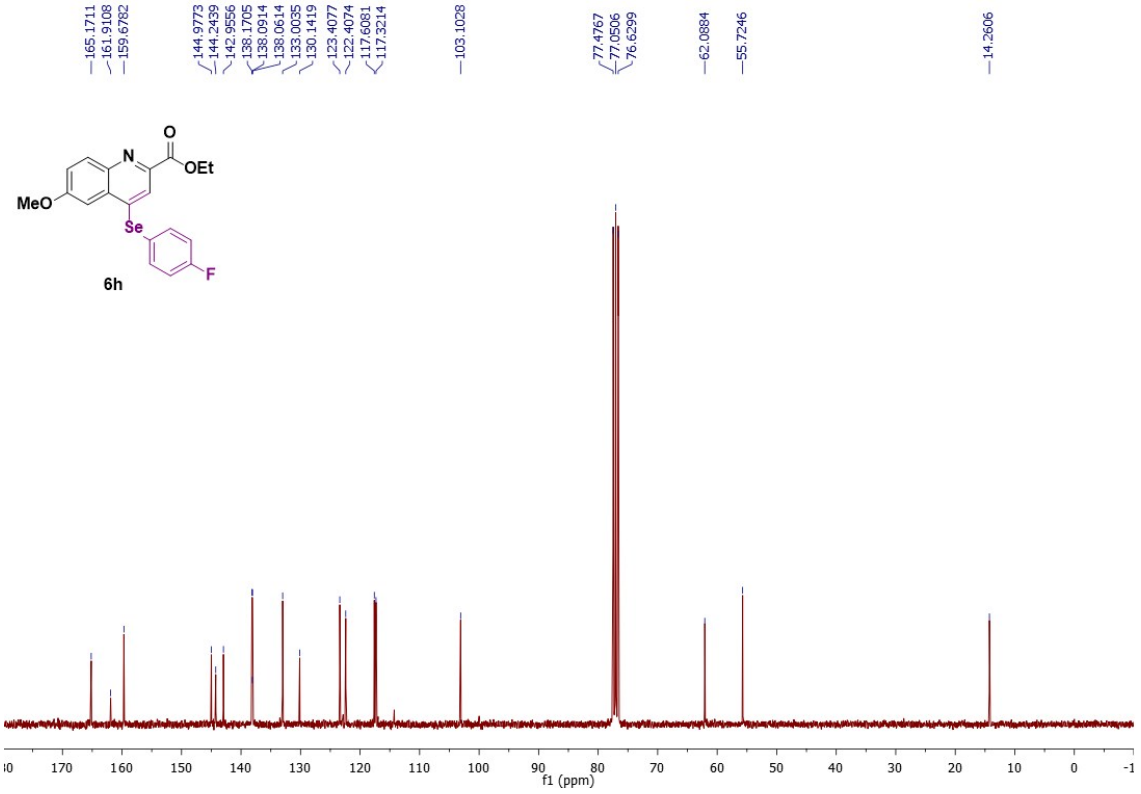
0.93
1.96
1.14
1.11
1.98
1.98
3.04
3.02
f1 (ppm)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138.1705
138.0914
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133.0035
130.1419
123.4077
122.4074
117.6081
117.3214
103.1028
77.4767
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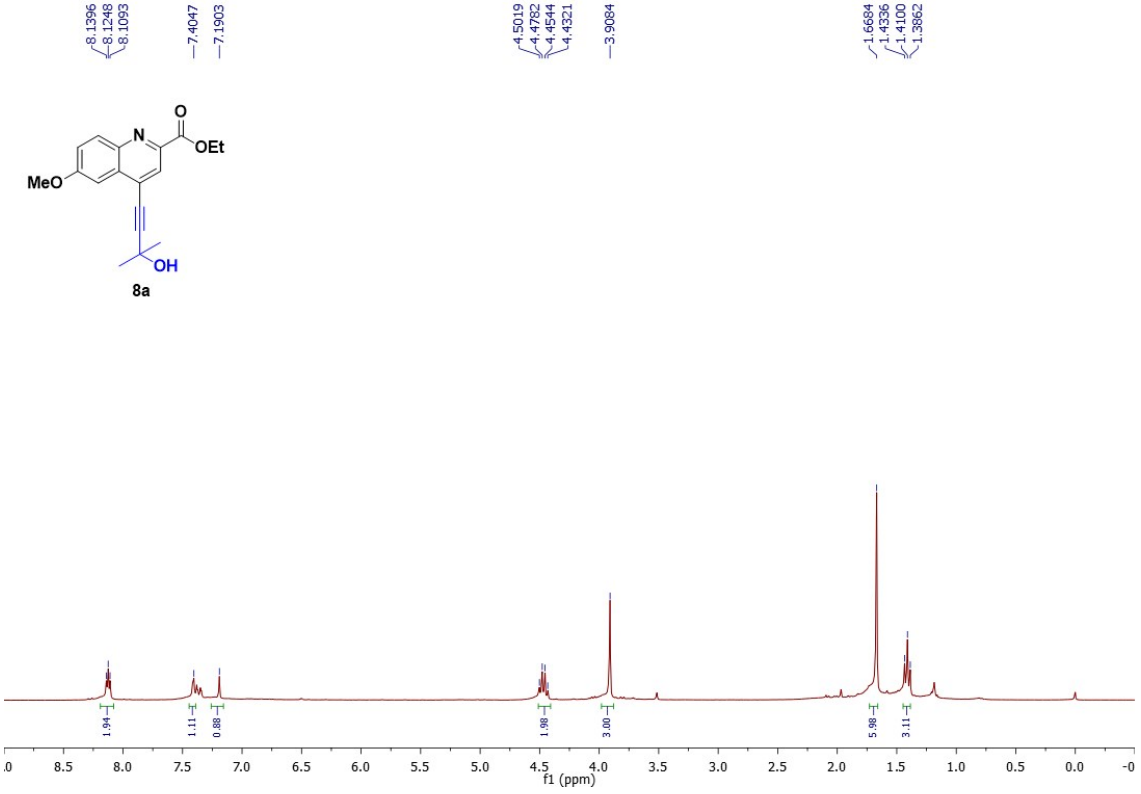
76.6299
62.0884
55.7246
14.2606
O
N
OEt
MeO
Se
F
6h
f1 (ppm)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8.1093
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7.1903
4.5019
4.4782
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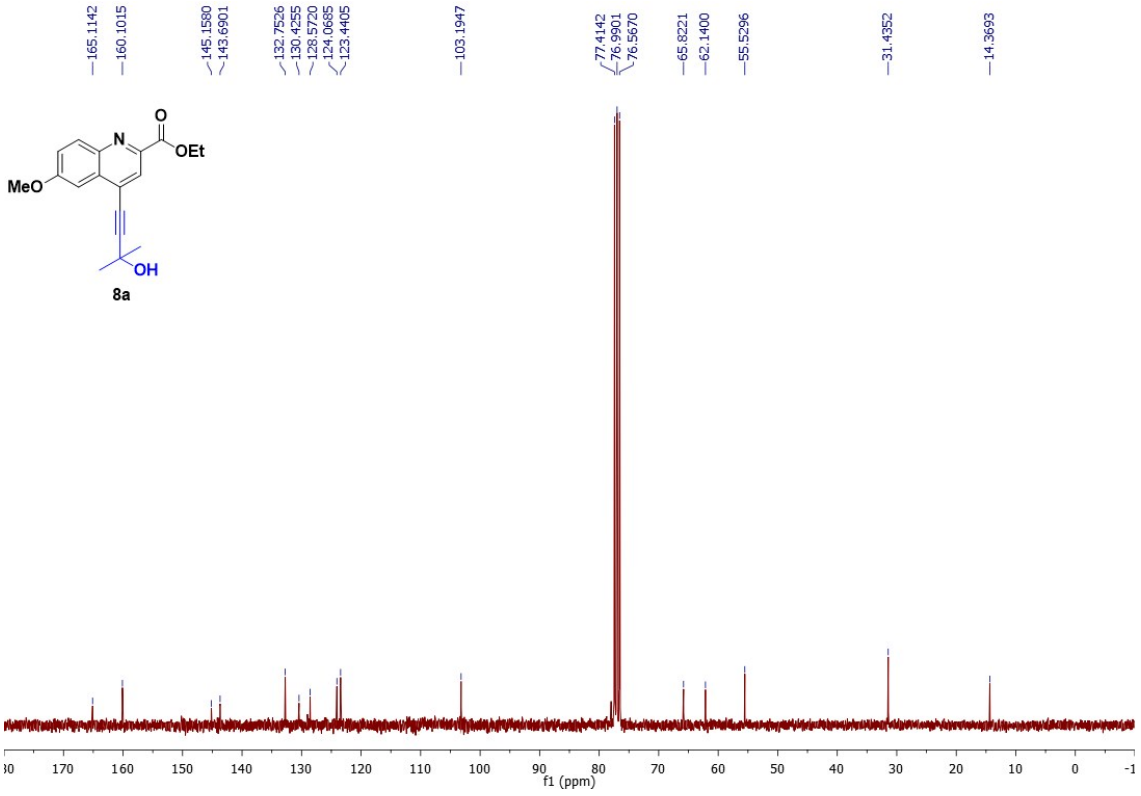
1.6684
1.4336
1.4100
1.3862
O
N
OEt
MeO
OH
8a
1.94
1.11
0.88
1.98
3.00
5.98
3.11
f1 (ppm)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128.5720
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123.4405
103.1947
77.4142
76.9901
76.5670
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55.5296
31.4352
14.3693
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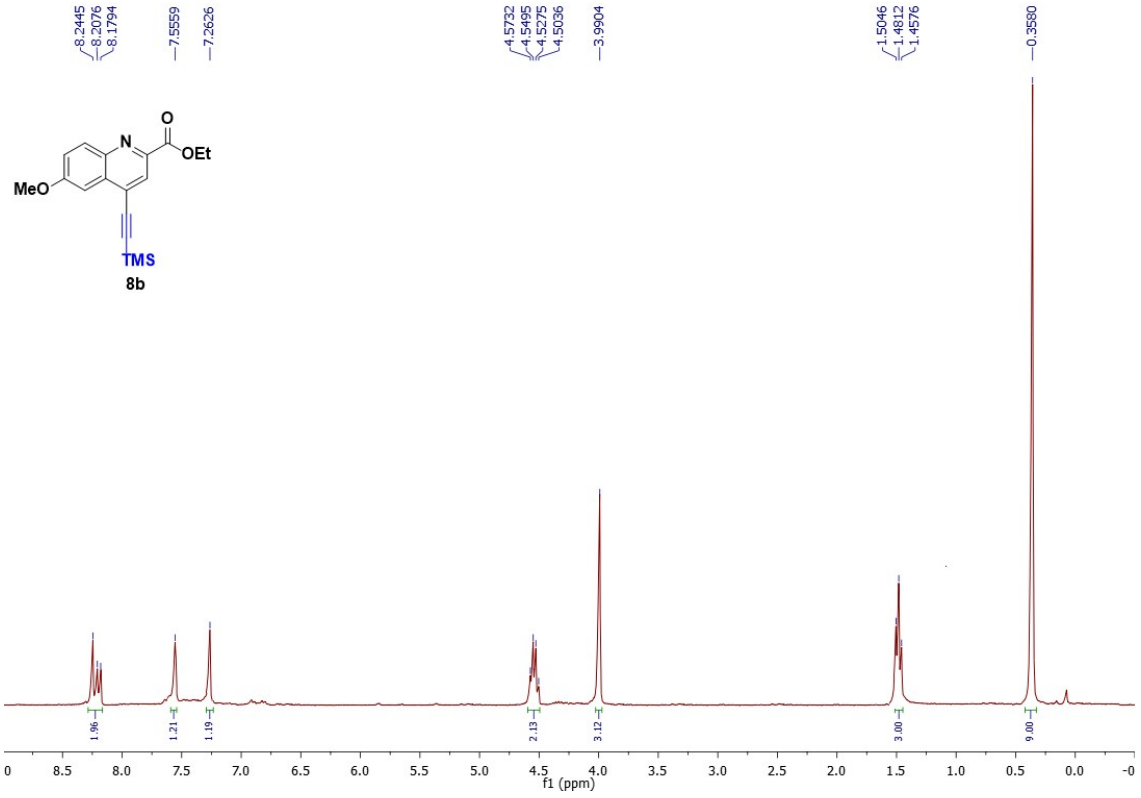
N
OEt
MeO
OH
8a
f1 (ppm)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7.2626
4.5732
4.5495
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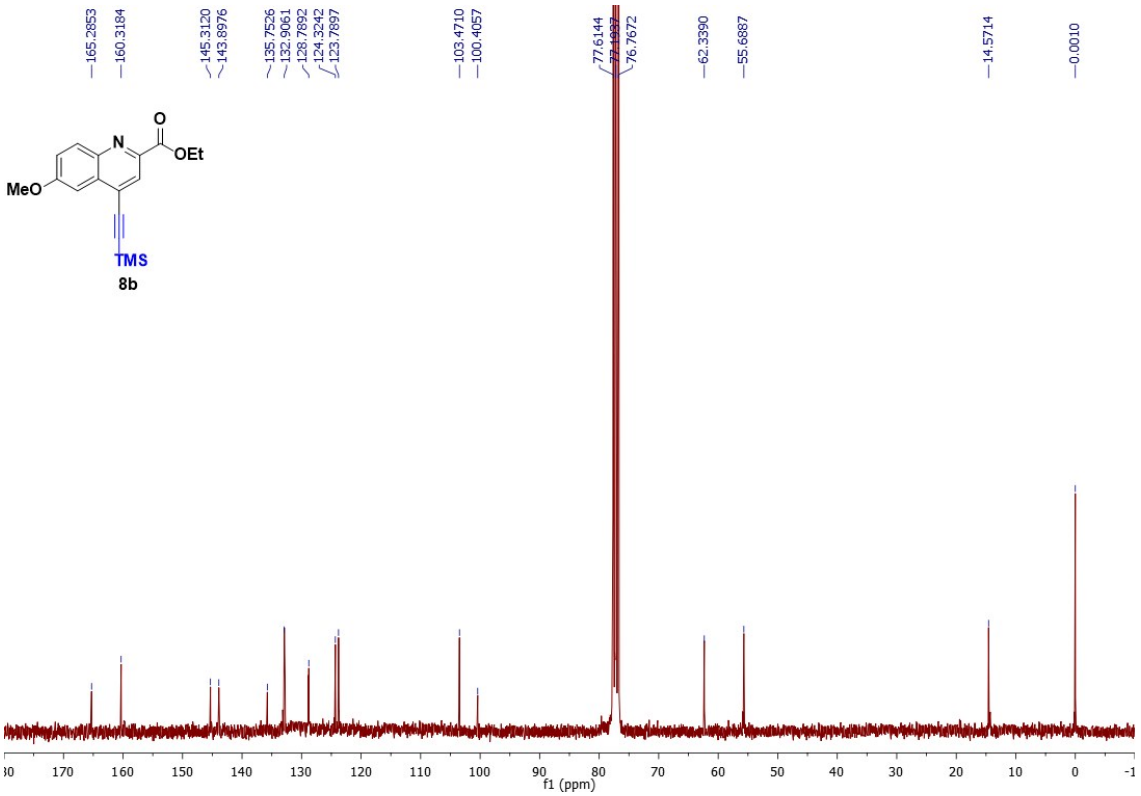
4.5036
3.9904
1.5046
1.4812
1.4576
0.3580
O
N
OEt
MeO
TMS
8b
1.96
1.21
1.19
2.13
3.12
3.00
9.00
f1 (ppm)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123.7897
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100.4057
77.6144
77.1933
76.7672
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55.6887
14.5714
0.0010
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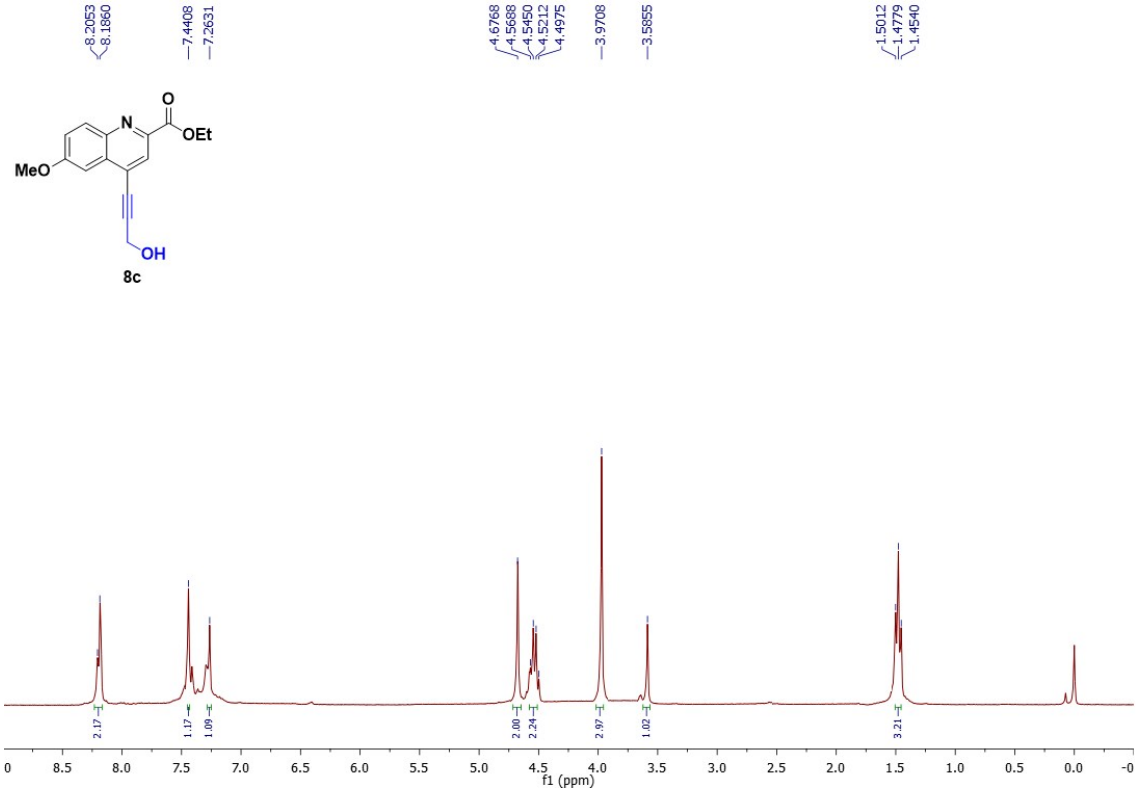
N
OEt
MeO
TMS
8b
f1 (ppm)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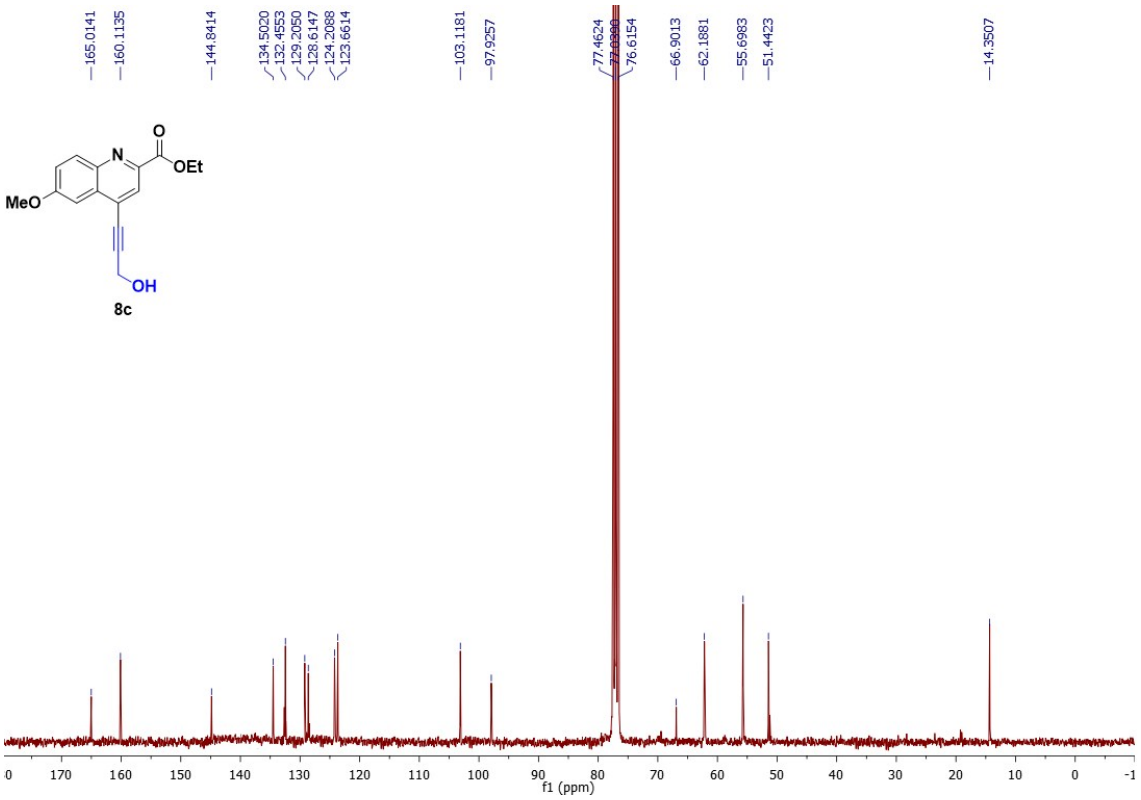
7.2631
4.6768
4.5688
4.5450
4.5212
4.4975
3.9708
3.5855
1.5012
1.4779
1.4540
O
N
OEt
MeO
OH
8c
2.17
1.17
1.09
2.00
2.24
2.97
1.02
3.21
f1 (ppm)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132.4553
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128.6147
124.2088
123.6614
103.1181
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77.4624
77.0390
76.6154
66.9013
62.1881
55.6983
51.4423
14.3507
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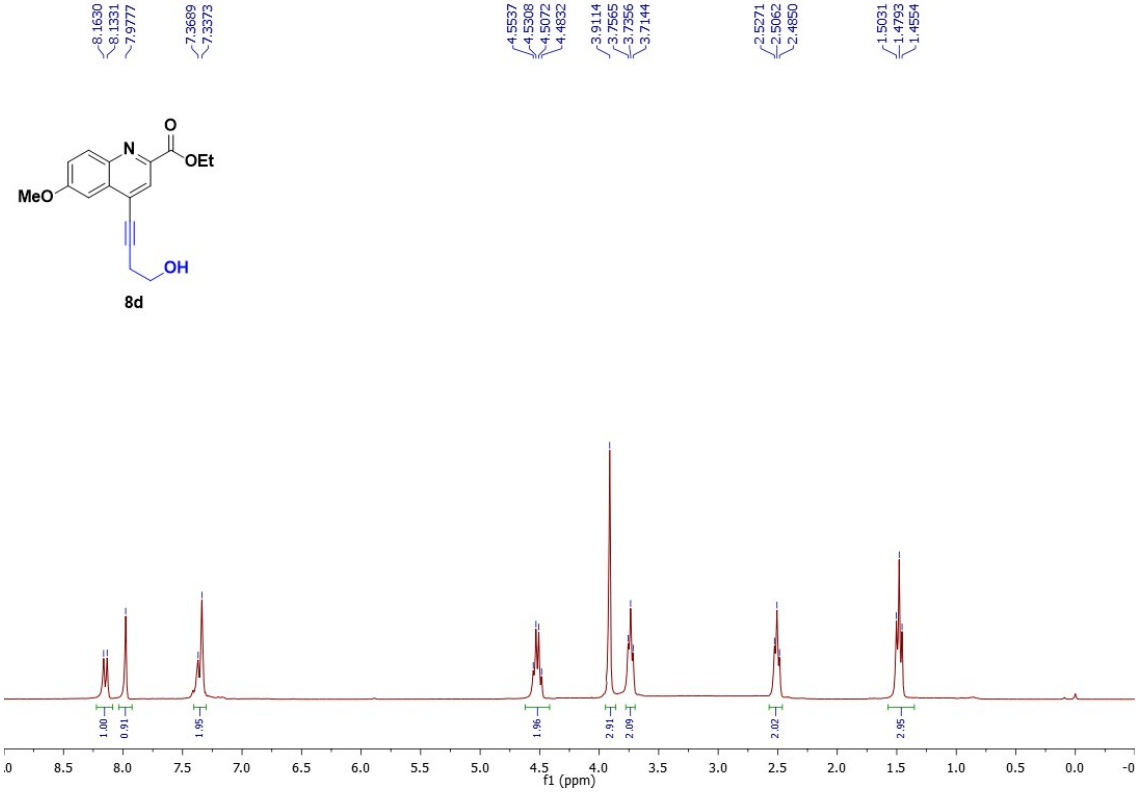
N
OEt
MeO
OH
f1 (ppm)

8c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4.5308
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4.4832
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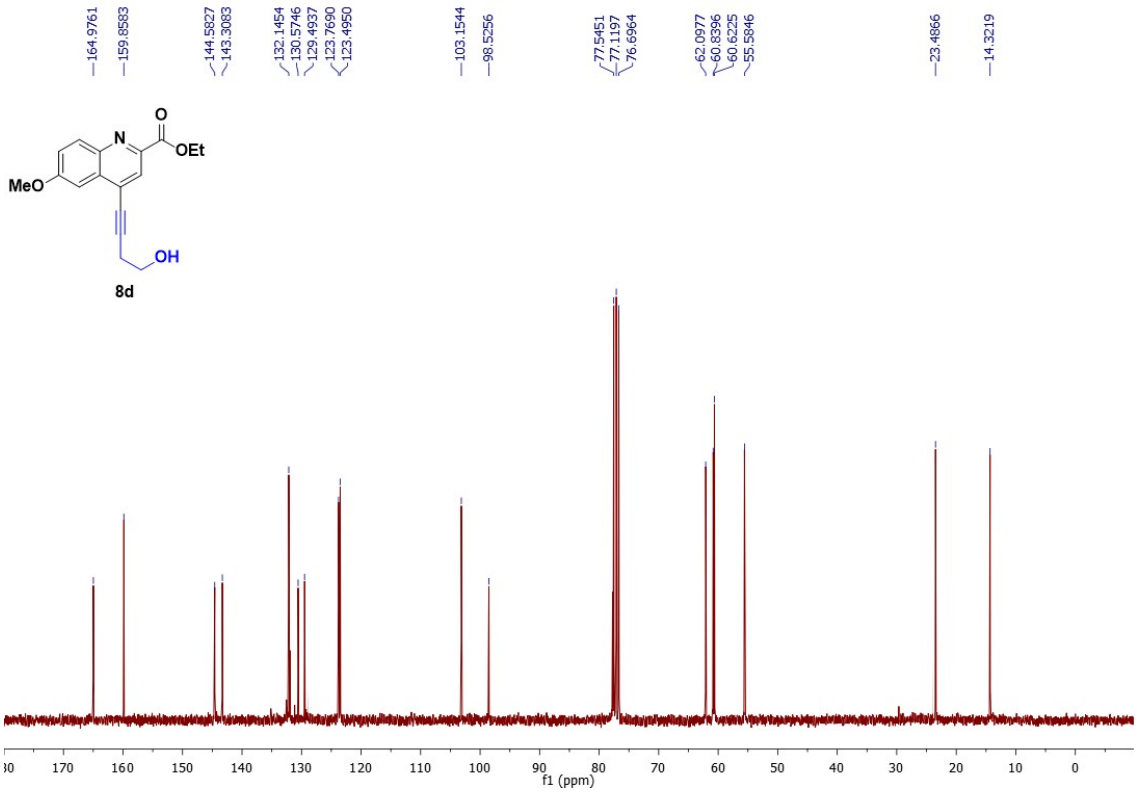
3.7565
3.7356
3.7144
2.5271
2.5062
2.4850
1.5031
1.4793
1.4554
O
N
OEt
MeO
OH
1.00
0.91
1.95
1.96
2.91
2.09
2.02
2.95
f1 (ppm)

8d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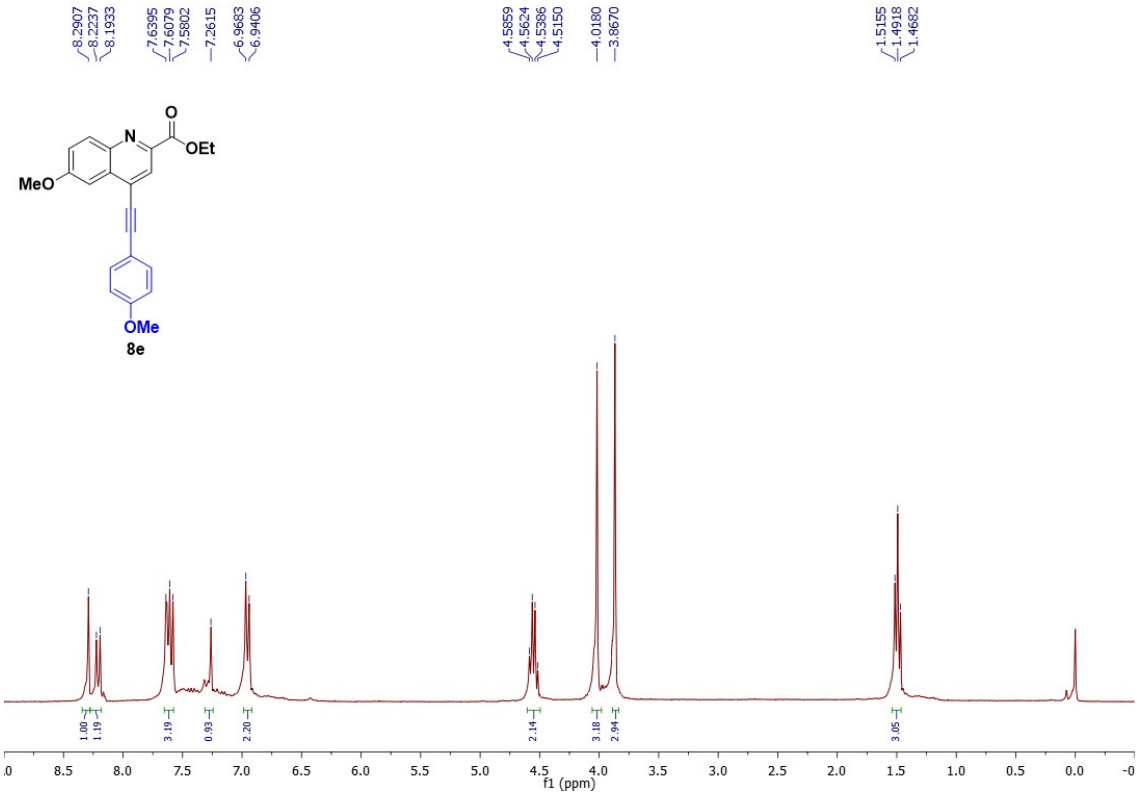
77.1197
76.6964
62.0977
60.8396
60.6225
55.5846
23.4866
14.3219
O
N
OEt
MeO
OH
8d
f1 (ppm)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8.1933
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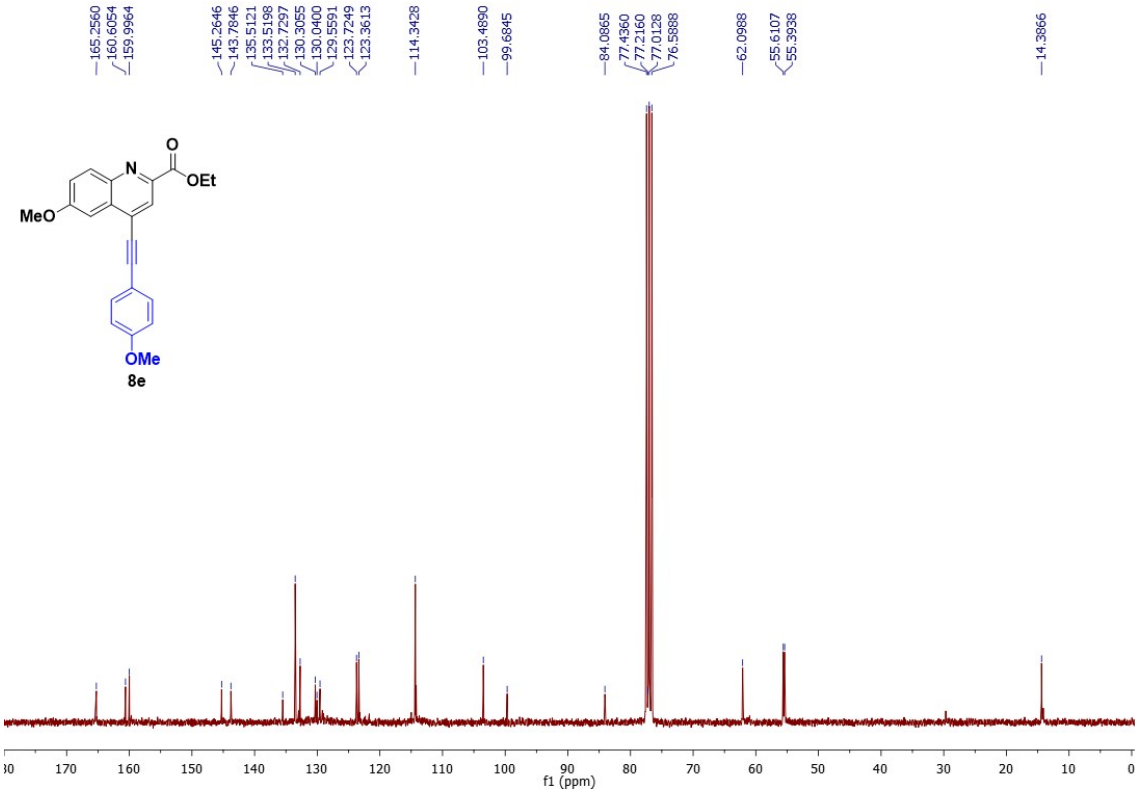
4.5624
4.5386
4.5150
4.0180
3.8670
1.5155
1.4918
1.4682
O
N
OEt
MeO
OMe
8e
1.00
1.19
3.19
0.93
2.20
2.14
3.18
2.94
3.05
f1 (ppm)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123.7249
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114.3428
103.4890
99.6845
84.0865
77.4360
77.2160
77.0128
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55.6107
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14.3866
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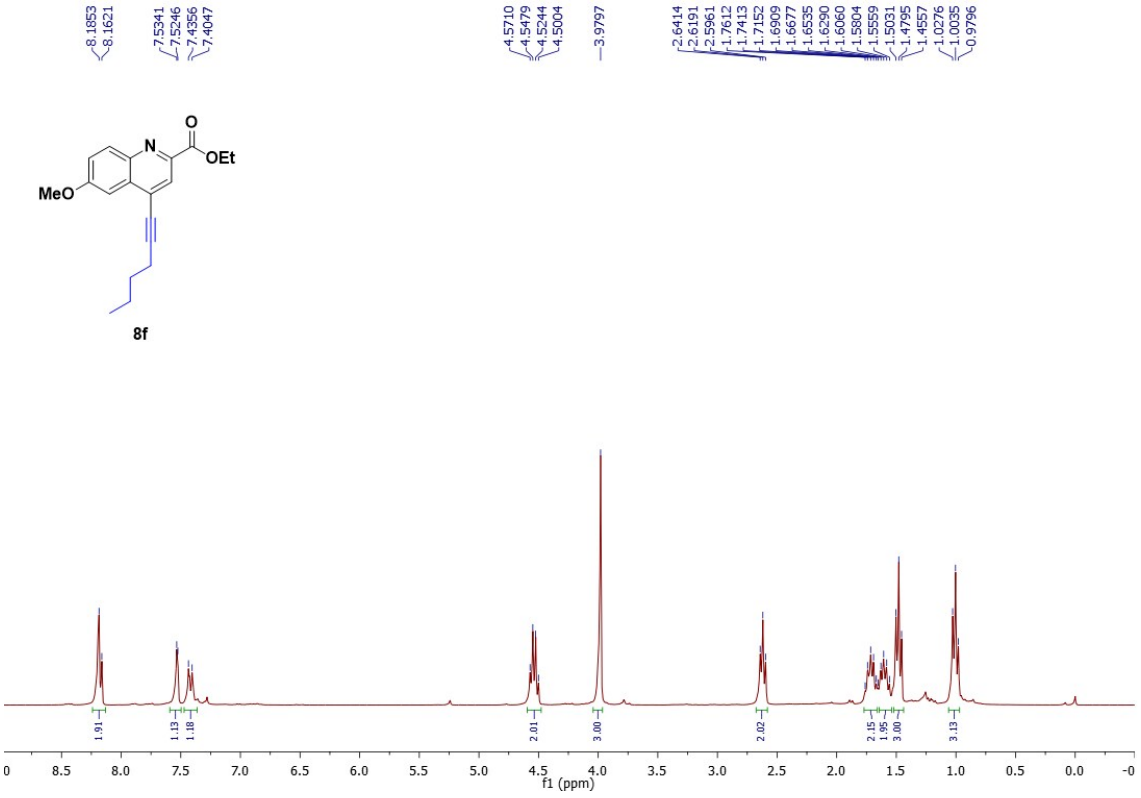
OEt
MeO
OMe
8e
f1 (ppm)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2.6414
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2.5961
1.7612
1.7413
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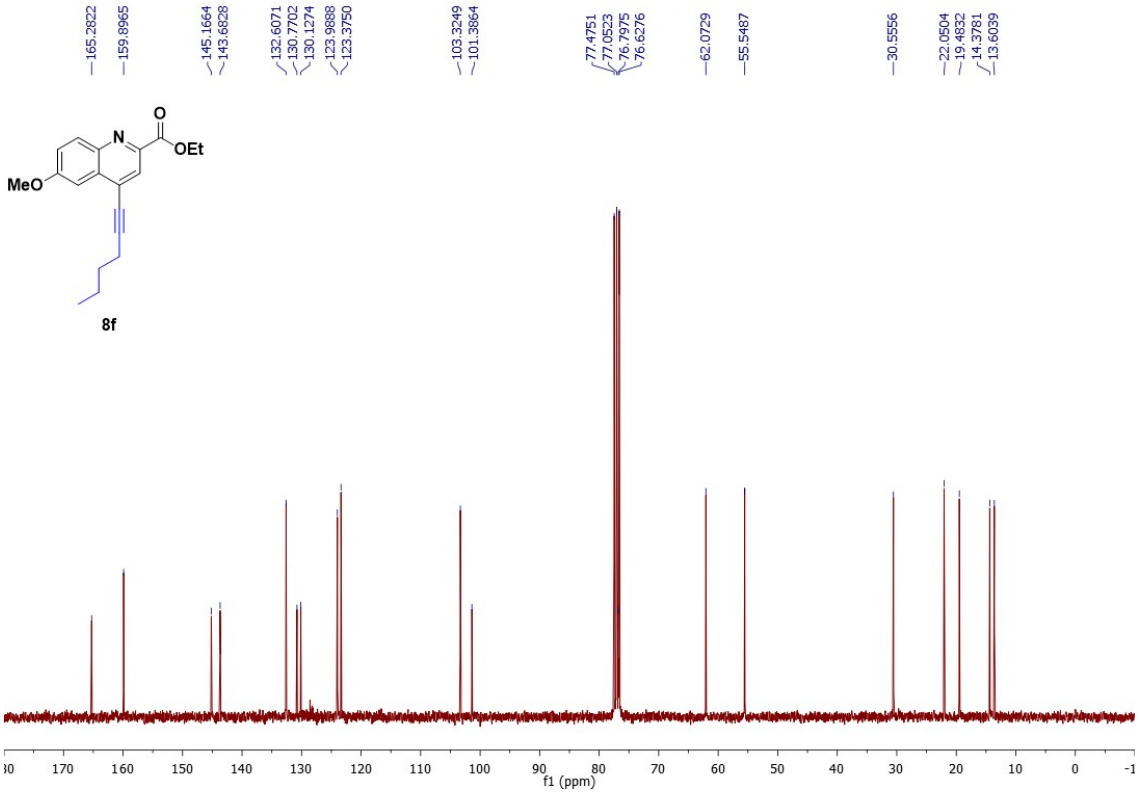
1.6909
1.6677
1.6535
1.6290
1.6060
1.5804
1.5559
1.5031
1.4795
1.4557
1.0276
1.0035
0.9796
O
N
OEt
MeO
8f
1.91
1.13
1.18
2.01
3.00
2.02
2.15
1.95
3.00
3.13
f1 (ppm)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77.4751
77.0523
76.7975
76.6276
62.0729
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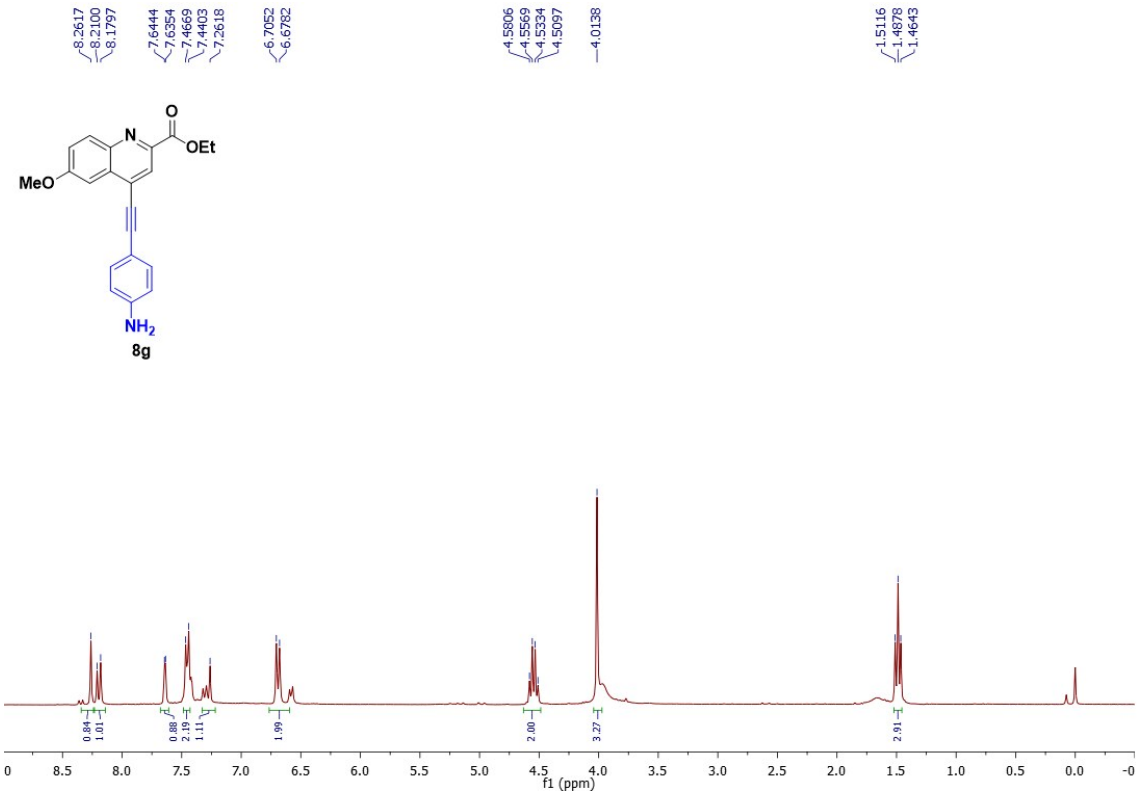
30.5556
22.0504
19.4832
14.3781
13.6039
O
N
OEt
MeO
8f
f1 (ppm)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4.5569
4.5334
4.5097
4.0138
1.5116
1.4878
1.4643
O
N
OEt
MeO
NH2
8g
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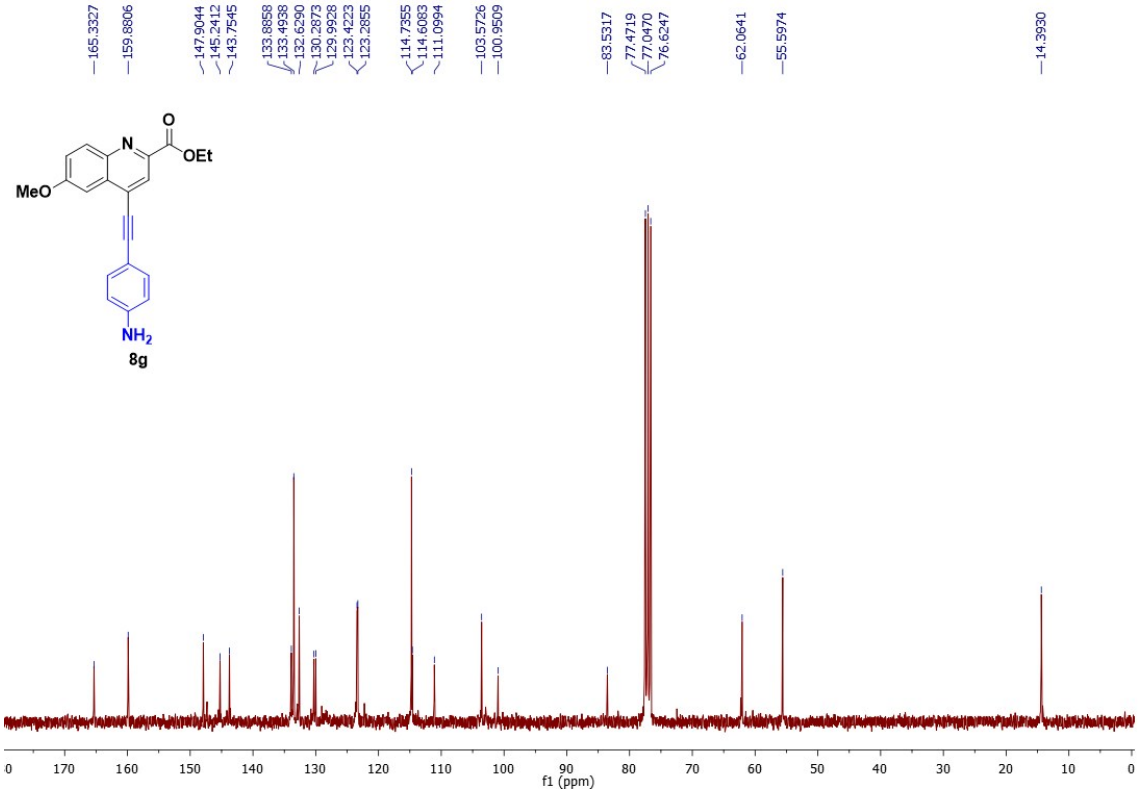
0.88
2.19
1.11
1.99
2.00
3.27
2.91
f1 (ppm)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100.9509
83.5317
77.4719
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62.0641
55.5974
14.3930
O
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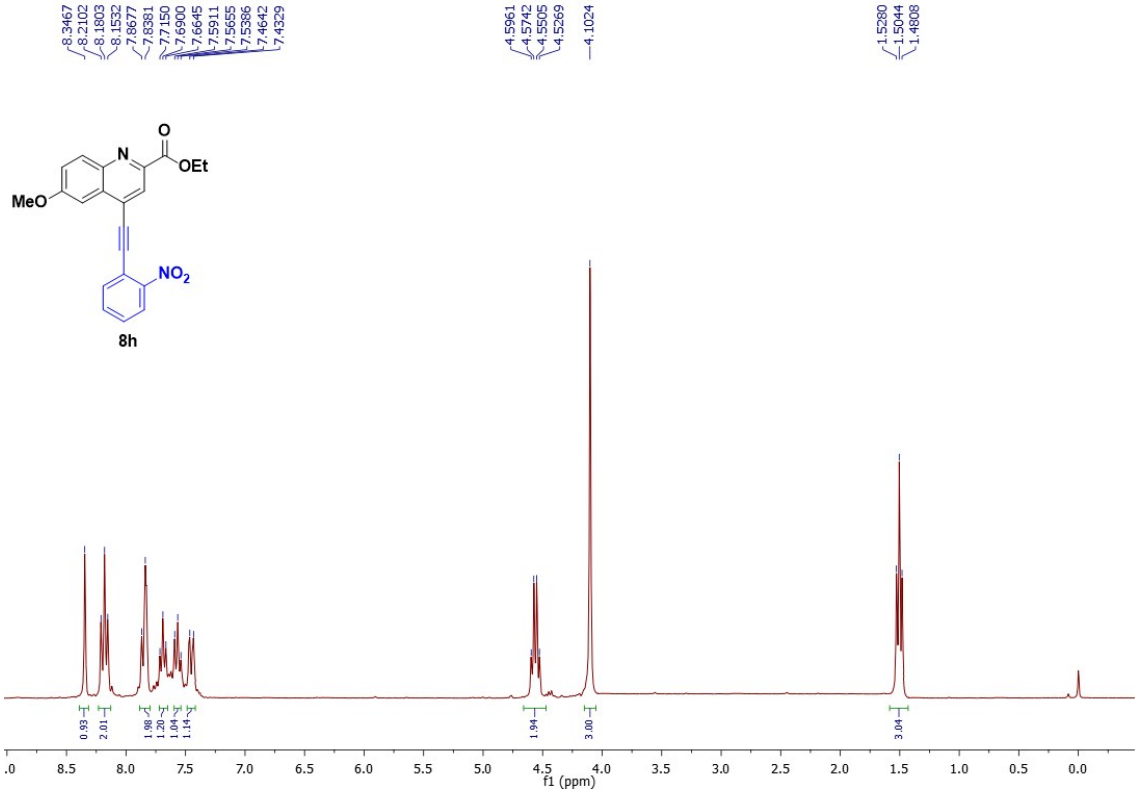
OEt
MeO
NH2
8g
f1 (ppm)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4.5742
4.5505
4.5269
4.1024
1.5280
1.5044
1.4808
O
N
OEt
MeO
NO2
8h
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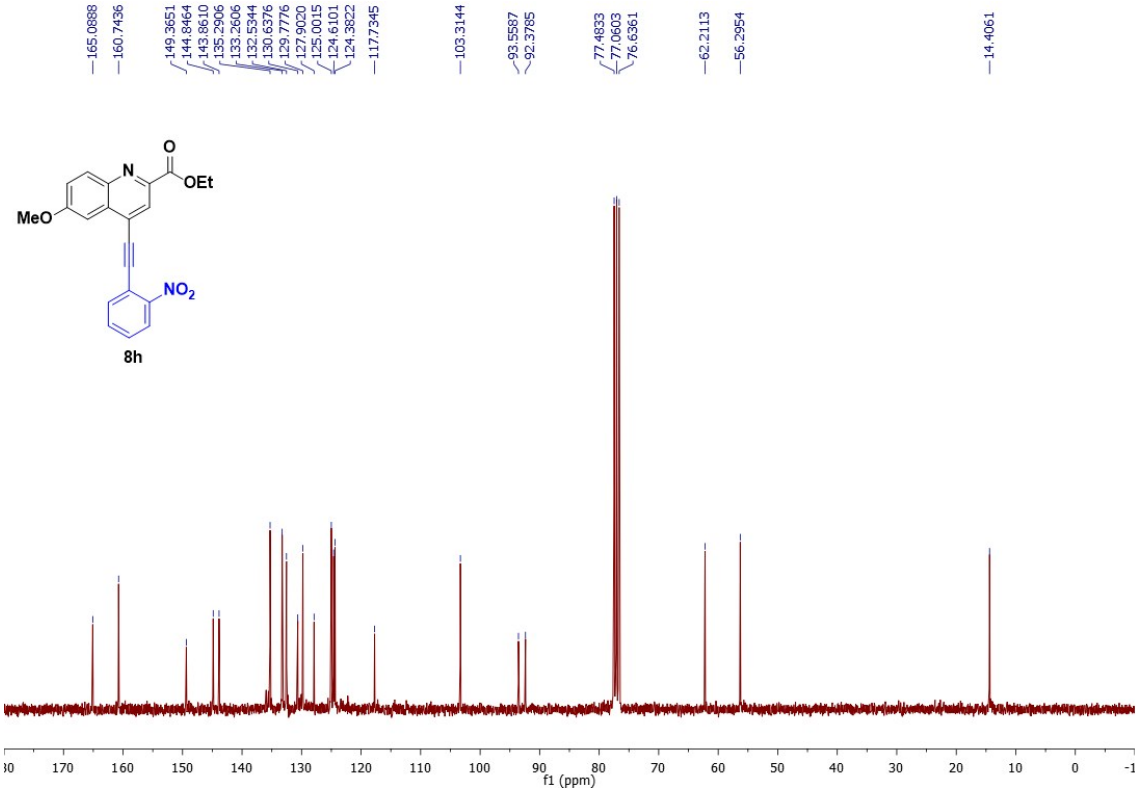
2.01
1.98
1.20
1.04
1.14
1.94
3.00
3.04
f1 (ppm)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125.0015
124.6101
124.3822
117.7345
103.3144
93.5587
92.3785
77.4833
77.0603
76.6361
62.2113
56.2954
14.4061
O
N
OEt
MeO
NO2
8h
f1 (ppm)