

Electronic Supplementary Information

Direct Trifluoromethylselenolations of electron-rich aromatic(hetero) rings with N-trifluoromethylselenolating saccharin

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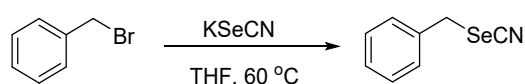
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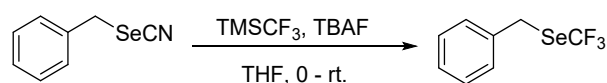
1) General

All reactions are performed in an air atmosphere unless otherwise stated. 400 MHz (for ^1H) or 500 MHz (for ^1H), 376 MHz (for ^{19}F) or 471 MHz (for ^{19}F), 101 MHz (for ^{13}C) or 126 MHz (for ^{13}C) spectrometer was recorded in Chloroform-*d* or DMSO-*d*₆. All chemical shifts were measured in ppm relative to TMS (0 ppm for ^1H NMR) as internal or external standard. The coupling constant is expressed in Hertz (Hz). We use the following abbreviations to explain multiplicity: s = singlet, d = two-state, t = triplet, q = four-state, m = multiplicity. The reaction was monitored by thin layer chromatography. Unless otherwise stated, yield refers to a substance purified by column chromatography using 200-300 mesh silica gel (Shanxi, China). Mass spectrometry experiments were performed on ESI instruments. Other reagents in the reaction were purchased from commercial sources and used without further purification.

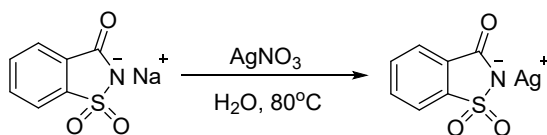
2) General Procedure for Synthesis of N-trifluoromethylselenolating saccharin



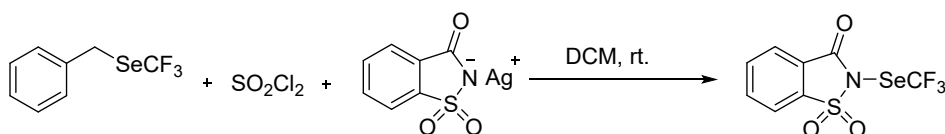
Potassium selenocyanate (12.60 g, 86.90 mmol, 1.1 equiv.), anhydrous tetrahydrofuran (60 mL) and benzyl bromide (9.47 mL, 79.53 mmol, 1.0 equiv.) were added to a dried round-bottom flask at 60 °C for 17 h. After the reaction was monitored by TLC, it was extracted 3 times with ether, and the organic layer was dried over anhydrous sodium sulfate, filtered, and concentrated to dryness to obtain a white solid with a yield of 95%. Without further purification, the product is directly used in the next reaction.^[1]



BnSeCN (12.00 g, 61.2 mmol, 1.0 equiv.) was added to a dried two-neck flask, vacuumed, filled with argon, and anhydrous tetrahydrofuran (123 mL) and TMSCF₃ (17.96 mL, 122.4 mmol, 2.0 equiv.) were added. The mixture was cooled to 0 °C, and 1 M TBAF (3.86 g, dissolved in 12.4 mL THF) was dropped to react for 10 min. The mixture was raised to room temperature for 7 h. After TLC monitoring reaction, *n*-pentane was extracted for 3 times, the organic layer was dried with anhydrous sodium sulfate, filtered and concentrated to dry, and the transparent liquid was obtained by column chromatography (PE) with a yield of 86%.^[2]



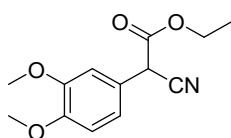
25.50 g (150 mmol) of silver nitrate was dissolved in 150 mL of water, heated to 80 °C and a solution of 37.06 g (153 mmol) of a sodium salt of saccharin in 150 mL of water was added dropwise with stirring. The white precipitate was filtered, washed with water and acetone, dried in air and 42.76 g (98%) of silver salt of saccharin was obtained as fine crystals. [3]



BnSeCF₃ (0.4780g, 2 mmol, 1.0 equiv.), SO₂Cl₂ (194 μL, 2.4 mmol, 1.2 equiv.), DCM (640 μL) were added into the reaction tube and vacuumized for 3 h at room temperature. Saccharin silver (1.16g, 4 mmol, 2.0 equiv.), DCM (4 mL) were added and reacted at room temperature for about 2 h. The color changed from yellow to colorless. The mixture was filtered (DCM rinsed), spun dry into solids, washed with n-pentane and pumped to obtain a white solid with a yield of 80%.

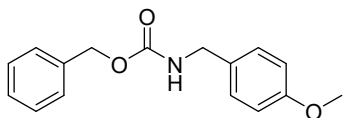
Amplification reaction: The reaction tube was vacuumized and filled with argon. BnSeCF₃ (7.17 g, 30 mmol, 3.0 equiv.), SO₂Cl₂ (2.91 mL, 36 mmol, 3.6 equiv.) and DCM (10 mL) were added to react at room temperature for 3 h. Saccharin silver (17.40 g, 60 mmol, 6.0 equiv.), DCM (50 mL) were added and reacted at room temperature for about 3 h. The color changed from yellow to colorless. The mixture was filtered (DCM rinsed), spun dry into solids, washed with n-pentane and pumped to obtain white solids with a yield of 82 %.

3) General Procedure for Preparation of 4a, 4b, 4c

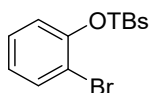


4ah, Add 60% sodium hydride (11.3 g, 282 mmol, 2.0 equiv.) to a three-neck flask, vacuum it, and fill it with nitrogen. 3, 4-dimethoxy phenylacetonitrile (25 g, 141 mmol, 1.0 equiv.) was dissolved in anhydrous tetrahydrofuran (120 mL), and solution was dropped into anhydrous tetrahydrofuran (270 mL) containing diethyl carbonate (34.2 mL, 282 mmol, 2.0 equiv.). The mixture is then added to the

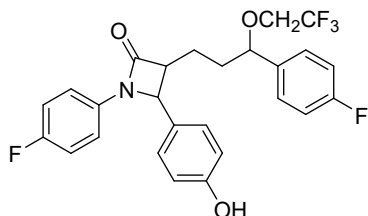
three-neck flask using a syringe. Under the condition of 80°C, reflux stirring for 5h, the reaction was cooled in ice bath, treated with cooling water, then extracted with ethyl acetate water layer, the organic layer was dried with anhydrous sodium sulfate, concentrated, column chromatography, the product 23.98 g, the yield of 68%.^[4]



4ai, (4-methoxyphenyl) methanamine (2 g, 14.6 mmol, 1.0 equiv.) is dissolved in THF (20 mL). NaOH (2M solution) (1.16g, 29.2mmol, 2.0 equiv.) was added and the reaction mixture was cooled to 0-5 °C. CBZ-Cl (2.74g, 16.0mmol, 1.1 equiv.) was added and stirred at room temperature for 3 h. The reaction was quenched with water and extracted with EtOAc. The organic layer was washed with brine, dried over sodium sulfate and concentrated to afford product (3.82 g, 96% yield).^[5]

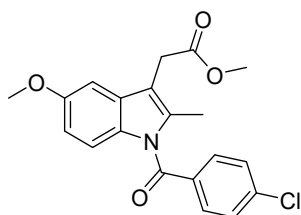


4ak, 2-bromophenol (2.5 mL, 23.5 mmol, 1.0 equiv.), imidazole (4 g, 59 mmol, 2.5 equiv.) and TBS-Cl (4.3 g, 57 mmol, 1.2 equiv.) were stirred overnight in DMF (25 mL). The reaction was treated with 150 mL water and extracted with 4 × 25 mL Et₂O. The organic phase was washed twice with saturated sodium chloride, dried with sodium sulfate and filtered. The solvent was evaporated and the crude product was filtered by silica gel to obtain 6.54 g bromo-2-[(tert-butyl)dimethylsiloxy]benzene (97%).^[6]

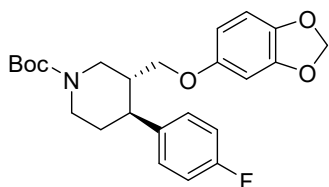


4cc, Ezetimibe (0.42 g, 1.03 mmol, 1.0 equiv.), N - trifluoromethylselenolating saccharin (0.41 g, 1.23 mmol, 1.2 equiv.) was added to trifluoroethanol (10 mL) and stirred at room temperature for 12 h. After the reaction was monitored by TLC, the organic layer was extracted with DCM, washed twice with sodium bicarb, dried with sodium sulfate, and condensed by rotary evaporation. The product was 0.32g

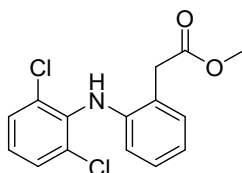
with a yield of 63%.



4cf, Indomethacin (2.0 g, 5.6 mmol, 1.0 equiv.), K_2CO_3 (2.48 g, 17.92 mmol, 3.2equiv.), and DMF (20 mL) were added to a round-bottom flask. Methane iodide (700 μ L, 11.2 mmol, 2.0 equiv.) was added and stirred at room temperature for 12 h. After the reaction, the crude product was diluted with water and ethyl acetate. The organic phase was washed with H_2O , saturated K_2CO_3 and salt water, dried on sodium sulfate, evaporated until dried, and the desired product (1.83 g, 88%) was obtained.^[7]



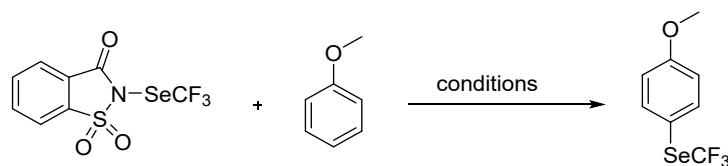
4cj, Paroxetine (1.0 g, 3.04 mmol, 1.0 equiv.) was added to 18 mL tetrahydrofuran: H_2O (1:1) to potassium carbonate (1.05 g, 7.6 mmol, 2.5 equiv.). Stir for about 5 minutes, add Boc_2O (840 mL, 3.65 mmol, 1.2 equiv.), and stir the reaction mixture at room temperature for 3 h. The organic phase and the aqueous phase were separated, the aqueous phase was extracted with ethyl acetate, the organic layer was dried with sodium sulfate, concentrated by rotary evaporation, and the product (1.11 g, 85%) was obtained by column chromatography.^[8]



4ck, 1-(2,6-Dichlorophenyl)-2-indolinone (3.0 g, 10.13 mmol, 1.0 equiv.), K_2CO_3 (4.48 g, 32.42 mmol, 3.2 equiv.), and DMF (30 mL) were added to a round-bottom flask. Methane iodide (1.3 mL, 20.26 mmol, 2.0 equiv.) was added and stirred at room temperature for 12 h. After the reaction, the crude product was diluted with water and ethyl acetate. The organic phase was washed with H_2O , saturated K_2CO_3 and salt water, dried on sodium sulfate, evaporated until dried, and the desired product (2.84 g,

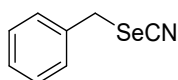
90%) was obtained.^[9]

4) General Procedure for Synthesis of 5a, 5b, 5c

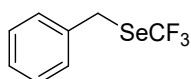


Taking template substrate anisole as an example, selenium reagent 3 (0.1188g, 0.36mm, 1.2eq.), anisole (33 μ L, 0.3mm, 1.0eq.), trifluoroethanol (2 mL) were added into the reaction tube, and the reaction was conducted overnight at room temperature. TLC monitored the reaction, and DCM was used to extract 3 times. The organic layer was dried with anhydrous sodium sulfate, filtered and concentrated to dry, and the transparent liquid was obtained by column chromatography (PE) with a yield of 91 %.

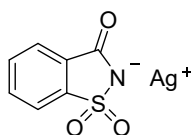
5) The spectral data of N-trifluoromethylselenolating saccharin



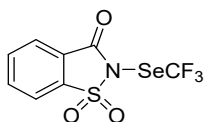
(Selenocyanatomethyl)benzene, white solid (95%), ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.32 (m, 5H), 4.29 (s, 2H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 135.53, 129.15, 129.02, 128.70, 102.09, 32.82.



Benzyl(trifluoromethyl)selane, colorless transparent oil (86%), ¹H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 7.16 (m, 5H), 4.17 (s, 2H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -34.46 (s, 3F); ¹³C NMR (101 MHz, Chloroform-*d*) δ 136.20, 129.15, 129.02, 127.92, 122.99 (q, *J* = 332.6 Hz), 29.26.

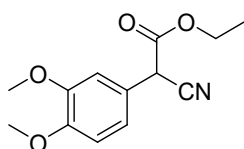


Saccharin silver, white solid (98%), ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.89-7.86 (m, 1H), 7.81 – 7.70 (m, 3H); ¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.63, 143.18, 133.06, 132.97, 132.01, 123.61, 120.20.

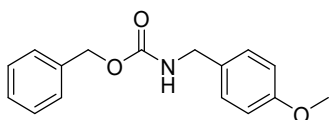


3, (N-trifluoromethylselenolating saccharin), white solid (82%), m.p. 46.3-46.6 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.15 (d, J = 7.6 Hz, 1H), 8.01 (d, J = 7.7 Hz, 1H), 7.96 (t, J = 7.5 Hz, 1H), 7.92-7.84 (m, 1H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -38.77 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.60, 138.62, 136.03, 134.85, 126.87, 126.50, 122.67 (q, J = 340.3 Hz), 122.00. HRMS-ESI (m/z) calcd for $\text{C}_8\text{H}_5\text{F}_3\text{NO}_3\text{SSe}$ (M+H): 331.9102, found: 331.9102. IR: ν 3095, 2970, 2692, 1750, 1717, 1592, 1458, 1333, 1221, 1174, 1161, 1139, 1088, 1076, 940, 900, 788, 749, 740, 674, 586, 570, 529, 506 cm^{-1} .

6) The spectral data of 4a, 4b, 4c

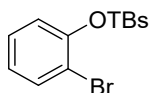


4ah, (ethyl 2-cyano-2-(3,4-dimethoxyphenyl)acetate), light yellow solid (68%), m.p. 50.3-50.6 °C. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.01-6.98 (m, 1H), 6.93 (t, J = 1.7 Hz, 1H), 6.87 (dd, J = 8.3, 1.4 Hz, 1H), 4.65 (s, 1H), 4.28-4.21 (m, 2H), 3.90 (d, J = 2.0 Hz, 3H), 3.88 (d, J = 1.9 Hz, 3H), 1.28 (tt, J = 7.1, 1.9 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.33, 149.84, 149.59, 122.21, 120.64, 115.99, 111.50, 110.67, 63.37, 56.14, 56.08, 43.42, 14.04. IR: ν 3012, 2986, 2962, 2932, 2838, 1723, 1593, 1514, 1455, 1438, 1421, 1369, 1344, 1314, 1266, 1240, 1195, 1180, 1141, 1030, 1020, 898, 860, 803, 766, 667, 621, 597, 585, 423 cm^{-1} .

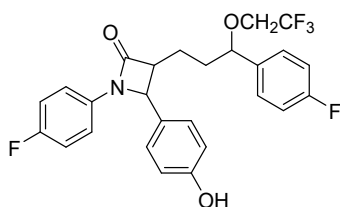


4ai, (benzyl (4-methoxybenzyl)carbamate), light yellow solid (96%), m.p. 78.0-78.7 °C. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.29 (m, 3H), 7.21 (d, J = 8.3 Hz, 1H), 6.89 – 6.82 (m, 1H), 5.13 (s, 1H), 4.32 (d, J = 5.9 Hz, 1H), 3.79 (s, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.11, 156.45, 136.62, 130.60, 129.04, 128.63, 128.24, 114.13, 66.89, 55.39, 44.72. IR: ν 3314, 3062, 3034, 3017, 2941, 2834, 1687, 1611, 1543, 1510, 1454, 1442, 1268, 1235, 1174, 1143, 1129, 1109, 1051, 1031, 1002, 919, 808,

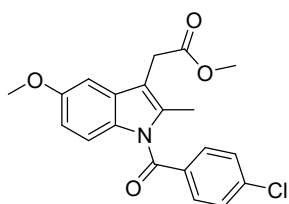
729, 692, 680, 574, 515, 444, 412 cm⁻¹.



4ak, ((2-bromophenoxy)(tert-butyl)dimethylsilane), colorless transparent oil (97%), ¹H NMR (400 MHz, Chloroform-*d*) δ 7.56-7.52 (m, 1H), 7.21-7.17 (m, 1H), 6.91 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.84 (td, *J* = 7.7, 1.5 Hz, 1H), 1.09 (s, 9H), 0.29 (s, 6H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 152.74, 133.56, 128.35, 122.49, 120.42, 115.54, 25.89, 18.49, -4.09. IR: ν 2958, 2930, 2895, 2886, 2858, 1583, 1475, 1440, 1283, 1252, 1047, 1030, 915, 837, 823, 807, 780, 750, 671, 440 cm⁻¹.

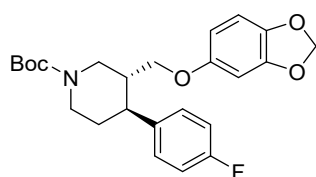


4cc, (1-(4-fluorophenyl)-3-(3-(4-fluorophenyl)-3-(2,2,2-trifluoroethoxy)propyl)-4-(4-hydroxyphenyl)azetidin-2-one), white solid (63%), m.p. 114.5-115.0 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.25 – 7.16 (m, 6H), 7.05 (td, *J* = 8.5, 4.9 Hz, 2H), 6.92 (td, *J* = 8.6, 3.4 Hz, 2H), 6.85 – 6.81 (m, 2H), 4.98 (s, 1H), 4.55 (dd, *J* = 15.7, 2.4 Hz, 1H), 4.47 – 4.35 (m, 1H), 3.60 (dddd, *J* = 27.8, 12.2, 9.4, 7.3 Hz, 2H), 3.05 (dd, *J* = 25.2, 6.7 Hz, 1H), 2.09 – 1.79 (m, 4H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -73.90 (s, 3F), -113.43 (s, 1F), -118.06 (s, 1F); ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.86, 157.98, 156.47, 135.93, 135.75, 133.82, 128.48, 128.40, 128.31, 127.47, 124.08 (q, *J* = 278.7, 273.6 Hz), 118.68, 118.60, 116.31, 116.08, 116.05, 116.02, 115.85, 115.81, 82.64, 82.56, 66.06, 65.89 (q, *J* = 34.4 Hz), 65.73, 61.20, 60.99, 60.28, 60.15, 35.77, 35.24, 25.21, 24.71. HRMS-ESI (*m/z*) calcd for C₂₆H₂₂F₅NNaO₃ (M+Na): 514.1412, found: 514.1412. IR: ν 2924, 1716, 1604, 1508, 1449, 1392, 1357, 1273, 1221, 1153, 1117, 1103, 968, 832, 669, 546, 515, 425 cm⁻¹.

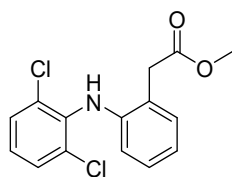


4cf, (methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate), light yellow solid

(88%), m.p. 59.9-60.4 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.63 (m, 2H), 7.51 – 7.41 (m, 2H), 6.96 (d, *J* = 2.6 Hz, 1H), 6.86 (d, *J* = 9.0 Hz, 1H), 6.67 (dd, *J* = 9.0, 2.6 Hz, 1H), 3.84 (s, 3H), 3.71 (s, 3H), 3.67 (s, 2H), 2.39 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 171.48, 168.43, 156.16, 139.39, 136.11, 134.01, 131.32, 130.90, 130.76, 129.25, 115.09, 112.62, 111.72, 101.39, 55.83, 52.30, 30.25, 13.46. IR: *ν* 3125, 3005, 2960, 2930, 2835, 1731, 1667, 1605, 1476, 1467, 1432, 1399, 363, 1323, 1291, 1234, 1214, 1190, 1167, 1153, 1085, 1072, 1036, 1025, 1014, 992, 914, 870, 845, 805, 752, 604, 482, 456, 441 cm⁻¹.

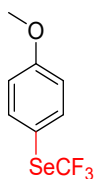


4cj, (tert-butyl-(3R,4S)-3-((benzo[d][1,3]dioxol-5-yloxy)methyl)-4-(4-fluorophenyl)piperidine-1-carboxylate), light yellow oil (85%), ¹H NMR (500 MHz, Chloroform-*d*) δ 7.17 – 7.11 (m, 2H), 7.01 – 6.94 (m, 2H), 6.62 (d, *J* = 8.5 Hz, 1H), 6.35 (d, *J* = 2.5 Hz, 1H), 6.13 (dd, *J* = 8.5, 2.5 Hz, 1H), 5.88 (s, 2H), 4.34 (d, *J* = 96.6 Hz, 2H), 3.60 (dd, *J* = 9.5, 2.9 Hz, 1H), 3.44 (dd, *J* = 9.4, 6.5 Hz, 1H), 2.84 – 2.75 (m, 2H), 2.67 (td, *J* = 11.9, 3.8 Hz, 1H), 2.04-1.99 (m, 1H), 1.85 – 1.76 (m, 1H), 1.74-1.66 (m, 1H), 1.49 (s, 9H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 154.94, 154.37, 148.28, 141.77, 128.93, 128.85, 115.74, 115.53, 107.96, 105.62, 101.23, 98.09, 79.80, 77.36, 68.88, 44.16, 28.59. IR: *ν* 3013, 2981, 2916, 2861, 1682, 1510, 1488, 1469, 1428, 1366, 1280, 1216, 1181, 1159, 1132, 1040, 937, 831, 750, 667, 534 cm⁻¹.

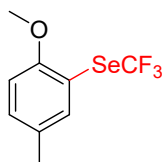


4ck, (methyl 2-((2,6-dichlorophenyl)amino)phenyl)acetate), light yellow solid (90%), m.p. 102.6-103.0 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 8.1 Hz, 2H), 7.23 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.13 (td, *J* = 7.8, 1.5 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.98 – 6.92 (m, 2H), 6.55 (d, *J* = 8.0 Hz, 1H), 3.82 (s, 2H), 3.75 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 172.77, 142.77, 137.83, 131.02, 129.62, 129.00, 128.13, 124.18, 124.17, 122.06, 118.20, 52.57, 38.62. IR: *ν* 3351, 2953, 1736, 1587, 1566, 1504, 1475, 1448, 1429, 1415, 1293, 1279, 1260, 1233, 1193, 1145, 1095, 1011, 842, 779, 749, 713, 658, 637, 604, 567, 504, 475, 444 cm⁻¹.

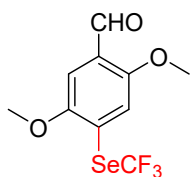
7) The spectral data of 5a, 5b, 5c



5aa, ((4-methoxyphenyl) (trifluoromethyl)selane), colorless transparent oil (91%), ^1H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.62 (m, 2H), 6.94 – 6.87 (m, 2H), 3.83 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.18 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.59, 139.10, 115.32, 122.65 (q, $J = 333.1$ Hz), 55.48. IR: ν 3364, 2965, 2943, 2929, 1592, 1492, 1458, 1442, 1293, 1252, 1089, 826, 736, 517, 427, 410 cm^{-1} .

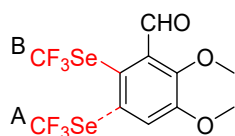


5ab, ((2-methoxy-5-methylphenyl)(trifluoromethyl)selane), colorless transparent oil (83%), ^1H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.47 (m, 1H), 7.25 – 7.17 (m, 1H), 6.86 (d, $J = 8.4$ Hz, 1H), 3.86 (s, 3H), 2.31 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.27 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.24, 137.93, 132.45, 131.23, 122.69 (q, $J = 333.2$ Hz), 111.38, 56.29, 20.36. HRMS-ESI (m/z) calcd for $\text{C}_9\text{H}_{10}\text{F}_3\text{OSe}$ ($\text{M}+\text{H}$): 270.9844, found: 270.9829. IR: ν 2966, 2944, 2927, 1602, 1491, 1463, 1440, 1279, 1253, 1119, 1090, 1053, 1025, 807, 735, 557, 452 cm^{-1} .

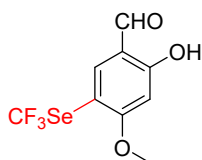


5ac, (2,5-dimethoxy-4-((trifluoromethyl)selanyl)benzaldehyde), white solid (89%), m.p. 93.9-94.3 $^{\circ}\text{C}$, ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 10.33 (s, 1H), 7.46 (s, 1H), 7.35 (s, 1H), 3.92 (s, 3H), 3.87 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.13 (s, 3F); ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 188.47, 155.54, 152.22, 125.71, 122.77 (q, $J = 333.6$ Hz), 121.30, 120.12, 108.94, 56.71. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_{10}\text{F}_3\text{O}_3\text{Se}$ ($\text{M}+\text{H}$): 314.9742, found: 314.9733. IR: ν 2973, 2941, 2885, 2852, 1726, 1683, 1676, 1601, 1479, 1463, 1377, 1278, 1214, 1095, 1048, 1020, 870, 737, 720, 670, 601, 462,

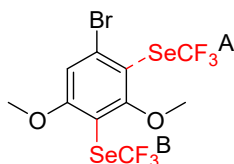
421 cm^{-1} .



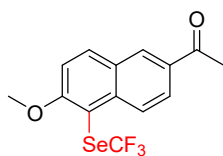
5ad, 97%, A:B = 5:4, A (2,3-dimethoxy-5-((trifluoromethyl)selanyl)benzaldehyde): light yellow solid, m.p. 52.0-52.4 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 10.47 (s, 1H), 7.41-7.38 (m, 1H), 7.17 (d, $J = 8.8$ Hz, 1H), 4.01 (s, 3H), 3.92 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.78 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.11, 154.45, 151.59, 128.17, 124.95, 123.46 (q, $J = 333.1$ Hz), 121.96, 119.34, 62.60, 56.37. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_{10}\text{F}_3\text{O}_3\text{Se}$ (M+H): 314.9742, found: 314.9732. IR: ν 2948, 2921, 2896, 2842, 1656, 1568, 1478, 1436, 1414, 1376, 1269, 1245, 1095, 1073, 990, 932, 806, 776, 733, 670, 587, 492, 420 cm^{-1} . B (2,3-dimethoxy-6-((trifluoromethyl)selanyl)benzaldehyde): light yellow oil, ^1H NMR (400 MHz, Chloroform-*d*) δ 10.40 (s, 1H), 7.78 (d, $J = 2.1$ Hz, 1H), 7.44 (d, $J = 2.1$ Hz, 1H), 4.04 (s, 3H), 3.94 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.00 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 188.94, 154.37, 153.41, 130.06, 128.40, 125.74, 124.08, 122.43 (q, $J = 337.1$ Hz), 120.77, 117.22, 62.41, 56.36. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_{10}\text{F}_3\text{O}_3\text{Se}$ (M+H): 314.9742, found: 314.9732. IR: ν 2941, 2900, 2841, 1686, 1659, 1569, 1479, 1435, 1414, 1377, 1303, 1264, 1243, 1092, 1073, 992, 930, 806, 775, 734, 670, 600, 587, 491 cm^{-1} .



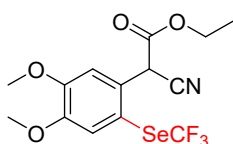
5ae, (2-hydroxy-4-methoxy-5-((trifluoromethyl)selanyl)benzaldehyde), white solid (91%), m.p. 73.9-74.4 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 11.68 (s, 1H), 9.74 (s, 1H), 7.89 (s, 1H), 6.52 (s, 1H), 3.96 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.18 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.18, 166.79, 166.61, 145.11, 122.35 (q, $J = 334.1$ Hz), 115.92, 100.06, 56.88. HRMS-ESI (m/z) calcd for $\text{C}_9\text{H}_8\text{F}_3\text{O}_3\text{Se}$ (M+H): 300.9585, found: 300.9577. IR: ν 3618, 2982, 2948, 2913, 2860, 1637, 1616, 1570, 1484, 1469, 1455, 1441, 1363, 1330, 1274, 1209, 1174, 1124, 1090, 1043, 987, 911, 853, 829, 784, 735, 685, 558, 469 cm^{-1} .



5af, (A: (2-bromo-4,6-dimethoxyphenyl)(trifluoromethyl)selane; B: (4-bromo-2,6-dimethoxyphenyl)(trifluoromethyl)selane), white solid (69%), m.p. 69.8-70.2 °C, A:B=10:1, ¹H NMR (400 MHz, Chloroform-*d*) δ 6.91 (d, *J* = 2.5 Hz, 1H), 6.45 (d, *J* = 2.6 Hz, 1H), 3.88 (s, 1H), 3.84 (s, 3H), 6.77 (s, 0.2H), 3.88 (s, 0.6H). (A:B=10:1); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -35.73 (s, 3F), -34.99. (A:B=10:1); ¹³C NMR (126 MHz, Chloroform-*d*) δ 163.52, 162.71, 134.48, 122.57 (q, *J* = 336.5 Hz), 110.52, 98.40, 56.74, 55.89, 161.53, 127.30, 122.57 (q, *J* = 336.5 Hz), 108.52, 106.95, 56.74. (A:B=10:1) HRMS-ESI (*m/z*) calcd for C₉H₉BrF₃O₂Se (M+H): 364.8898, found:364.8898. IR: *ν* 2979, 2951, 2921, 2850, 1574, 1560, 1452, 1424, 1401, 1363, 1301, 1277, 1216, 1089, 1078, 1037, 933, 833, 810, 735, 624, 575, 458 cm⁻¹.

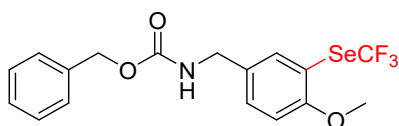


5ag, (1-(6-methoxy-5-((trifluoromethyl)selanyl)naphthalen-2-yl)ethan-1-one), white solid (96%), m.p. 119.7-120.3 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 8.54 (d, *J* = 9.0 Hz, 1H), 8.43 (d, *J* = 1.8 Hz, 1H), 8.17 – 8.09 (m, 2H), 7.43 (d, *J* = 9.1 Hz, 1H), 4.08 (s, 3H), 2.72 (s, 3H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -34.87 (s, 3F); ¹³C NMR (101 MHz, Chloroform-*d*) δ 197.66, 161.48, 139.44, 135.71, 133.00, 130.58, 128.49, 127.99, 126.30, 122.50 (q, *J* = 336.5 Hz), 113.70, 107.43, 57.05, 26.80. HRMS-ESI (*m/z*) calcd for C₁₄H₁₂F₃O₂Se (M+H): 348.9949, found: 348.9933. IR: *ν* 2980, 2951, 2920, 2849, 1673, 1619, 1588, 1574, 1561, 1454, 1401, 1361, 1275, 1216, 1117, 1086, 1052, 911, 834, 811, 735, 682, 575, 518, 419 cm⁻¹.

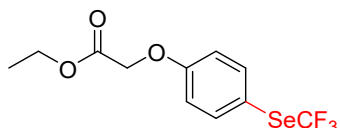


5ah, (ethyl 2-cyano-2-(4,5-dimethoxy-2-((trifluoromethyl)selanyl)phenyl)acetate), light yellow viscous oil (81%), ¹H NMR (400 MHz, Chloroform-*d*) δ 7.31 (s, 1H), 7.18 (s, 1H), 5.55 (s, 1H), 4.33 – 4.18 (m,

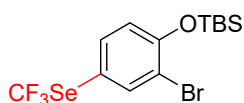
2H), 3.96 (s, 3H), 3.93 (s, 3H), 1.30 (t, $J = 7.2$ Hz, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.19 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.93, 152.05, 149.83, 128.78, 122.26 (q, $J = 334.4$ Hz), 121.33, 115.85, 114.64, 111.23, 63.71, 56.40, 56.35, 43.57, 29.79, 13.99. HRMS-ESI (m/z) calcd for $\text{C}_{14}\text{H}_{14}\text{F}_3\text{NNaO}_4\text{Se}$ ($\text{M}+\text{Na}$): 419.9932, found: 419.9925. IR: ν 2967, 2938, 2850, 1745, 1645, 1589, 1560, 1509, 1459, 1445, 1346, 1251, 1122, 1090, 1017, 974, 864, 737, 675, 409 cm^{-1} .



5ai, (benzyl (4-methoxy-3-((trifluoromethyl)selanyl)benzyl)carbamate), light yellow solid (51%), m.p. 67.5-67.8 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, $J = 2.3$ Hz, 1H), 7.39 – 7.31 (m, 6H), 6.91 (d, $J = 8.4$ Hz, 1H), 5.14 (s, 2H), 5.11 – 5.05 (m, 1H), 4.33 (d, $J = 6.0$ Hz, 2H), 3.88 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.07 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.62, 156.50, 136.55, 136.50, 132.00, 131.33, 128.65, 128.28, 128.22, 122.59 (q, $J = 333.3$ Hz), 111.53, 67.01, 56.30, 44.20. HRMS-ESI (m/z) calcd for $\text{C}_{17}\text{H}_{16}\text{F}_3\text{NNaO}_3\text{Se}$ ($\text{M}+\text{Na}$): 442.0140, found: 442.0129. IR: ν 3329, 2953, 2936, 2851, 1691, 1536, 1493, 1454, 1437, 1262, 1103, 1044, 1019, 974, 819, 750, 736, 698, 662, 596, 460, 408 cm^{-1} .

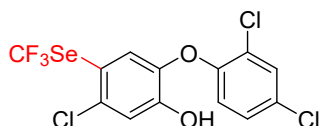


5aj, (ethyl 2-(4-((trifluoromethyl)selanyl)phenoxy)acetate), white solid (95%), m.p. 53.9-54.2 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.59 (m, 2H), 7.00 – 6.85 (m, 2H), 4.64 (s, 2H), 4.28 (q, $J = 7.1$ Hz, 2H), 1.30 (t, $J = 7.1$ Hz, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.94 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.47, 159.75, 139.10, 122.57 (q, $J = 333.0$ Hz), 115.93, 114.26, 65.35, 61.70, 14.24. IR: ν 2982, 2951, 2921, 2850, 1740, 1673, 1620, 1587, 1574, 1561, 1472, 1454, 1401, 1275, 1216, 1088, 1077, 911, 834, 810, 735, 575, 419 cm^{-1} .

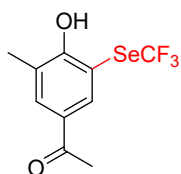


5ak, ((2-bromo-4-((trifluoromethyl)selanyl)phenoxy)(tert-butyl)dimethylsilane), colorless transparent oil

(72%), ^1H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, $J = 2.1$ Hz, 1H), 7.53 (dd, $J = 8.4, 2.2$ Hz, 1H), 6.86 (d, $J = 8.4$ Hz, 1H), 1.05 (s, 9H), 0.28 (s, 6H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.69 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.06, 142.00, 137.64, 122.55 (q, $J = 334.5$ Hz), 120.88, 116.31, HRMS-ESI (m/z) calcd for $\text{C}_{13}\text{H}_{19}\text{BrF}_3\text{OSeSi}$ ($\text{M}+\text{H}$): 434.9500, found: 434.9500. IR: ν 3294, 2958, 2931, 2888, 2859, 1720, 1657, 1530, 1476, 1296, 1258, 1234, 1130, 1094, 1044, 911, 841, 806, 782, 738, 680, 593, 506, 477 cm^{-1} .



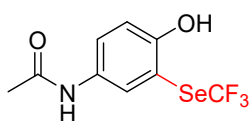
5al, (5-chloro-2-(2,4-dichlorophenoxy)-4-((trifluoromethyl)selanyl)phenol), light brown solid (87%), m.p. 70.2-70.8 $^{\circ}\text{C}$, ^1H NMR (400 MHz, DMSO- d_6) δ 11.07 (s, 1H), 7.74 (d, $J = 2.5$ Hz, 1H), 7.48 (s, 1H), 7.37 (dd, $J = 8.8, 2.5$ Hz, 1H), 7.26 (s, 1H), 6.81 (d, $J = 8.8$ Hz, 1H); ^{19}F NMR (376 MHz, DMSO- d_6) δ -36.41 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.70, 149.56, 142.69, 136.32, 131.13, 128.68, 126.76, 126.73, 122.43 (q, $J = 334.1$ Hz), 121.50, 118.11, 113.26. HRMS-ESI (m/z) calcd for $\text{C}_{13}\text{H}_6\text{Cl}_3\text{F}_3\text{NaO}_2\text{Se}$ ($\text{M}+\text{Na}$): 458.8443, found: 458.8443. IR: ν 3513, 1576, 1471, 1394, 1319, 1253, 1201, 1088, 945, 869, 839, 802, 756, 737, 705, 666, 571, 428 cm^{-1} .



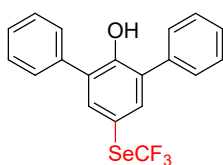
5am, (1-(4-hydroxy-3-methyl-5-((trifluoromethyl)selanyl)phenyl)ethan-1-one), white solid (81%), m.p. 79.7-80.0 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.15 (d, $J = 2.2$ Hz, 1H), 7.94 – 7.86 (m, 1H), 6.72 (s, 1H), 2.56 (s, 3H), 2.36 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.34 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.94, 159.49, 137.57, 135.12, 130.61, 125.76, 121.69 (q, $J = 335.2$ Hz), 108.72, 26.30, 16.87. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_{10}\text{F}_3\text{O}_2\text{Se}$ ($\text{M}+\text{H}$): 298.9793, found: 298.9780. IR: ν 3342, 2980, 2953, 2920, 2852, 1668, 1619, 1588, 1575, 1560, 1473, 1454, 1401, 1359, 1275, 1228, 1117, 1080, 976, 834, 811, 735, 624, 562, 424 cm^{-1} .



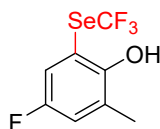
5an, (1-((trifluoromethyl)selanyl)naphthalen-2-yl)phenylacetamide, white solid (93%), m.p. 87.2-87.7 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.31 (d, $J = 8.5$ Hz, 1H), 7.94 (d, $J = 8.9$ Hz, 1H), 7.83 – 7.78 (m, 1H), 7.60 (ddd, $J = 8.4, 6.9, 1.3$ Hz, 1H), 7.44-7.40 (m, 1H), 7.34 (d, $J = 8.9$ Hz, 1H), 6.84 (s, 1H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.64 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.32, 135.97, 134.70, 129.52, 128.65, 128.43, 126.63, 124.29, 122.03 (q, $J = 337.0$ Hz), 120.35, 116.88, 103.80. HRMS-ESI (m/z) calcd for $\text{C}_{11}\text{H}_7\text{F}_3\text{NaOSe}$ (M+Na): 314.9506, found: 314.9506. IR: ν 3421, 2966, 2922, 2851, 1616, 1592, 1565, 1508, 1562, 1382, 1347, 1196, 1119, 1093, 928, 867, 823, 769, 751, 736, 644, 541, 507, 416 cm^{-1} .



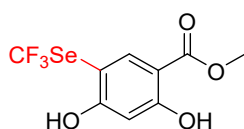
5ao, (N-(4-hydroxy-3-((trifluoromethyl)selanyl)phenyl)phenyl)acetamide), white solid (53%), m.p. 153.4-153.9 °C, ^1H NMR (400 MHz, DMSO- d_6) δ 10.14 (s, 1H), 9.86 (s, 1H), 7.89 (d, $J = 2.5$ Hz, 1H), 7.48 (dd, $J = 8.8, 2.6$ Hz, 1H), 6.92 (d, $J = 8.8$ Hz, 1H), 1.99 (s, 3H); ^{19}F NMR (376 MHz, DMSO- d_6) δ -34.99 (s, 3F); ^{13}C NMR (101 MHz, DMSO- d_6) δ 167.91, 153.65, 131.97, 127.80, 127.62, 124.48, 123.42, 122.83 (q, $J = 335.0$ Hz), 121.17, 115.75, 108.97, 23.80. HRMS-ESI (m/z) calcd for $\text{C}_9\text{H}_9\text{F}_3\text{NO}_2\text{Se}$ (M+H): 299.9745, found: 299.9736. IR: ν 3406, 3295, 1719, 1658, 1593, 1531, 1483, 1337, 1260, 1229, 1202, 1153, 1135, 1094, 889, 841, 832, 805, 738, 594, 518, 508, 458 cm^{-1} .



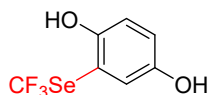
5ap, (5'-((trifluoromethyl)selanyl)-[1,1':3',1''-terphenyl]-2'-ol), white solid (90%), m.p. 72.9-73.6 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.66 (s, 2H), 7.59 – 7.47 (m, 8H), 7.46 – 7.40 (m, 2H), 5.66 (s, 1H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.75 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.61, 138.87, 136.22, 130.30, 129.40, 129.21, 128.4, 122.67 (q, $J = 333.2$ Hz). HRMS-ESI (m/z) calcd for $\text{C}_{19}\text{H}_{14}\text{F}_3\text{Ose}$ (M+H): 395.0157, found: 395.0105. IR: ν 3535, 2983, 2952, 2922, 2850, 1673, 1620, 1575, 1560, 1456, 1422, 1400, 1277, 1228, 1116, 1089, 1077, 835, 811, 781, 771, 736, 715, 697, 629, 583 cm^{-1} .



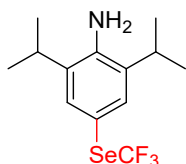
5aq, (4-fluoro-2-methyl-6-((trifluoromethyl)selanyl)phenol), light yellow oil (79%), ^1H NMR (400 MHz, Chloroform-*d*) δ 7.22 (dd, $J = 7.3, 3.1$ Hz, 1H), 7.03 (dd, $J = 8.7, 3.1$ Hz, 1H), 6.11 (s, 1H), 2.30 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.43 (s, 3F), -123.21 (s, 1F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.55 (d, $J = 242.5$ Hz), 151.94 (d, $J = 2.3$ Hz), 126.86 (d, $J = 7.3$ Hz), 121.98 (d, $J = 22.6$ Hz), 121.74 (q, $J = 335.4$ Hz), 121.46 (d, $J = 23.4$ Hz), 107.71 (d, $J = 8.4$ Hz), 17.08. HRMS-ESI (m/z) calcd for $\text{C}_8\text{H}_7\text{F}_4\text{OSe}$ (M+H): 274.9593, found: 274.9593. IR: ν 3535, 2979, 2947, 2923, 1673, 1589, 1559, 1470, 1422, 1401, 1277, 1228, 1083, 835, 812, 781, 767, 736, 698, 628, 583, 419 cm^{-1} .



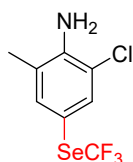
5ar, (methyl 2,4-dihydroxy-5-((trifluoromethyl)selanyl)benzoate), white solid (81%), m.p. 87.8-88.4 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 11.15 (s, 1H), 8.21 (s, 1H), 6.67 (s, 1H), 6.53 (s, 1H), 3.95 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.46 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.56, 166.58, 162.91, 141.99, 123.39, 121.72 (q, $J = 335.7$ Hz), 120.05, 107.76, 103.50, 100.33, 52.58. HRMS-ESI (m/z) calcd for $\text{C}_9\text{H}_7\text{F}_3\text{NaO}_4\text{Se}$ (M+Na): 338.9354, found: 338.9354. IR: ν 3335, 2953, 2924, 2853, 1670, 1613, 1587, 1443, 1410, 1349, 1321, 1265, 1229, 1195, 1134, 1088, 1023, 951, 835, 787, 736, 681, 597, 460, 444 cm^{-1} .



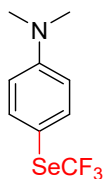
5as, (2-((trifluoromethyl)selanyl)benzene-1,4-diol), white solid (55%), m.p. 90.1-90.4 $^{\circ}\text{C}$, ^1H NMR (400 MHz, DMSO- d_6) δ 9.62 (s, 1H), 9.12 (s, 1H), 6.96 (d, $J = 2.7$ Hz, 1H), 6.82 (d, $J = 8.7$ Hz, 1H), 6.75 (dd, $J = 8.7, 2.9$ Hz, 1H); ^{19}F NMR (376 MHz, DMSO- d_6) δ -34.94 (s, 3F); ^{13}C NMR (126 MHz, DMSO- d_6) δ 150.40, 150.29, 122.87 (q, $J = 333.4$ Hz), 122.38, 119.10, 116.56, 109.32. HRMS-ESI (m/z) calcd for $\text{C}_7\text{H}_6\text{F}_3\text{O}_2\text{Se}$ (M+H): 258.9480, found: 258.9480. IR: ν 3421, 2980, 2954, 2930, 1457, 1423, 1298, 1156, 1145, 1134, 1082, 1070, 1050, 887, 789, 738, 473, 445 cm^{-1} .



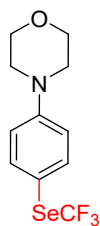
5at, (2,6-diisopropyl-4-((trifluoromethyl)selanyl)aniline), light yellow solid (99%), m.p. 74.1-74.5 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.37 (s, 2H), 2.96-2.86 (m, 2H), 1.29 (s, 6H), 1.27 (s, 6H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.51 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.68, 133.37, 132.53, 110.39, 119.50 (q, $J = 333.6$ Hz), 28.07, 22.31. HRMS-ESI (m/z) calcd for $\text{C}_{13}\text{H}_{19}\text{F}_3\text{NSe}$ (M+H): 326.0629, found: 326.0619. IR: ν 3364, 2965, 2924, 2870, 1620, 1510, 1456, 1241, 1089, 1010, 735, 696, 578, 539, 428 cm^{-1} .



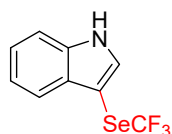
5au, (2-chloro-6-methyl-4-((trifluoromethyl)selanyl)aniline), light yellow solid (99%), m.p. 59.0-59.6 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.56 – 7.51 (m, 1H), 7.33 (d, $J = 1.9$ Hz, 1H), 4.26 (s, 2H), 2.20 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.39 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.45, 137.72, 135.81, 124.10, 123.96, 122.45 (q, $J = 333.6$ Hz), 120.79, 118.90, 108.85, 77.24, 17.72. HRMS-ESI (m/z) calcd for $\text{C}_8\text{H}_8\text{ClF}_3\text{NSe}$ (M+H): 289.9457, found: 289.9407. IR: ν 3486, 3385, 2980, 2919, 2861, 1614, 1558, 1473, 1444, 1398, 1082, 871, 835, 733, 724, 707, 575, 480, 460, 429 cm^{-1} .



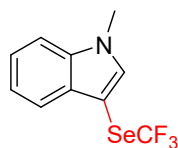
5av, (N,N-dimethyl-4-((trifluoromethyl)selanyl)aniline), light yellow solid (91%), m.p. 45.8-46.2 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.63 – 7.52 (m, 2H), 6.73 (d, $J = 8.4$ Hz, 2H), 3.01 (s, 6H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.71 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.71, 138.75, 124.41, 121.09, 112.73, 119.43 (q, $J = 333.9$ Hz), 107.16, 40.19. IR: ν 2921, 2898, 2824, 1590, 1507, 1442, 1368, 1228, 1198, 1125, 1090, 1078, 947, 807, 733, 510, 481 cm^{-1} .



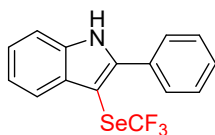
5aw, (4-(4-((trifluoromethyl)selanyl)phenyl)morpholine), light yellow solid (94%), m.p. 42.9-43.2 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.56 (m, 2H), 6.92 – 6.83 (m, 2H), 3.91 – 3.79 (m, 4H), 3.31 – 3.16 (m, 4H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.27 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.60, 138.70, 122.26 (q, $J = 333.5$ Hz), 115.74, 111.23, 66.76, 48.24. IR: ν 2960, 2902, 2865, 2835, 1587, 1500, 1447, 1413, 1380, 1343, 1305, 1286, 1262, 1092, 1049, 923, 834, 817, 734, 658, 552, 543, 527, 410 cm^{-1} .



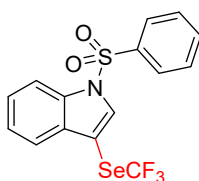
5axa, (3-((trifluoromethyl)selanyl)-1H-indole), light brown solid (89%), m.p. 60.3-60.8 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.56 (s, 1H), 7.79 – 7.75 (m, 1H), 7.53 (d, $J = 2.6$ Hz, 2H), 7.46 – 7.43 (m, 1H), 7.29 (td, $J = 5.0, 4.6, 2.0$ Hz, 2H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.63 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 136.16, 133.00, 130.14, 123.46, 121.62, 121.41 (q, $J = 335.2$ Hz), 120.18, 111.65, 93.32. IR: ν 3390, 2956, 2922, 2852, 1499, 1454, 1406, 1336, 1278, 1237, 1087, 1006, 982, 840, 746, 734, 620, 580, 540, 530, 447, 424 cm^{-1} .



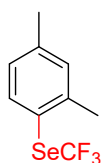
5axb, (3-((trifluoromethyl)selanyl)-1H-indole), white solid (98%), m.p. 66.0-66.5 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, $J = 7.7$ Hz, 1H), 7.42 – 7.36 (m, 2H), 7.32 (ddd, $J = 14.1, 6.4, 1.3$ Hz, 1H), 3.86 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -38.00 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.36, 137.20, 130.90, 122.95, 122.41 (q, $J = 335.6$ Hz), 121.23, 120.27, 109.86, 90.91, 33.29. IR: ν 3365, 2945, 2924, 2821, 1510, 1481, 1456, 1333, 1323, 1241, 1113, 1087, 1009, 818, 737, 696, 596, 577, 539, 524, 428 cm^{-1} .



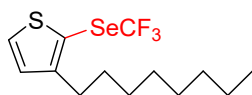
5axc, (2-phenyl-3-((trifluoromethyl)selanyl)-1H-indole), light yellow solid (98%), m.p. 96.3-97.0 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.63 (s, 1H), 7.87 – 7.79 (m, 1H), 7.77 – 7.73 (m, 2H), 7.53 – 7.45 (m, 4H), 7.32 – 7.29 (m, 2H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.63 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.18, 135.85, 132.22, 131.44, 129.28, 129.15, 128.84, 123.73, 122.49 (q, $J = 336.5$ Hz), 121.79, 120.76, 111.26. IR: ν 3363, 2965, 2923, 2859, 1716, 1483, 1455, 1444, 1396, 1346, 1324, 1296, 1224, 1115, 1087, 767, 749, 734, 694, 584, 568, 544, 428 cm^{-1} .



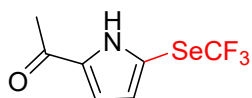
5axd, (1-(phenylsulfonyl)-3-((trifluoromethyl)selanyl)-1H-indole), white solid (83%), m.p. 152.0-152.7 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.99 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.96 – 7.89 (m, 3H), 7.70 – 7.65 (m, 1H), 7.61 – 7.55 (m, 1H), 7.48 (dd, $J = 8.5, 7.2$ Hz, 2H), 7.44 – 7.32 (m, 2H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.15 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.76, 134.94, 134.53, 134.07, 132.06, 129.67, 127.07, 125.91, 124.46, 123.00 (q, $J = 334.8$ Hz), 121.08, 113.62. HRMS-ESI (m/z) calcd for $\text{C}_{15}\text{H}_{11}\text{F}_3\text{NO}_2\text{SSe}$ ($\text{M}+\text{H}$): 405.9622, found: 405.9560. IR: ν 3130, 2957, 2923, 2852, 1517, 1472, 1424, 1366, 1265, 1174, 1117, 1087, 1036, 933, 841, 755, 745, 725, 682, 584, 569, 549, 425 cm^{-1} .



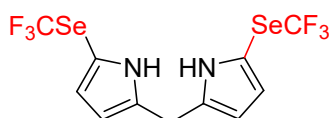
5ay, ((2,4-dimethylphenyl)(trifluoromethyl)selane), colorless transparent oil (84%), ^1H NMR (400 MHz, Chloroform-*d*) δ 7.64 (d, $J = 7.8$ Hz, 1H), 7.19 – 7.15 (m, 1H), 7.03 – 6.96 (m, 1H), 2.52 (s, 3H), 2.35 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.96 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.47, 141.59, 139.21, 131.68, 127.92, 122.85 (q, $J = 333.4$ Hz), 121.20, 23.42, 21.36. HRMS-ESI (m/z) calcd for $\text{C}_9\text{H}_{10}\text{F}_3\text{Se}$ ($\text{M}+\text{H}$): 254.9894, found: 254.9894. IR: ν 3423, 2967, 2923, 2851, 1617, 1593, 1565, 1507, 1462, 1437, 1382, 1347, 1196, 1118, 1082, 1028, 823, 769, 751, 737, 644, 543, 487, 416 cm^{-1} .



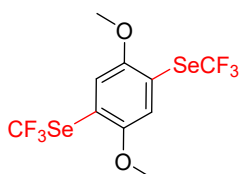
5aza, (3-octyl-2-((trifluoromethyl)selanyl)thiophene), colorless transparent oil (86%), $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (d, $J = 5.4$ Hz, 1H), 7.03 (d, $J = 5.4$ Hz, 1H), 2.85 – 2.73 (m, 2H), 1.58 (t, $J = 7.6$ Hz, 2H), 1.34 – 1.26 (m, 10H), 0.92 – 0.84 (m, 3H); $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -37.76 (s, 3F); $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 152.64, 132.97, 129.10, 122.05 (q, $J = 337.1$ Hz), 111.72, 32.01, 30.88, 30.23, 29.53, 29.50, 29.36, 22.82, 14.25. HRMS-ESI (m/z) calcd for $\text{C}_{13}\text{H}_{19}\text{F}_3\text{NaSSe}$ ($\text{M}+\text{Na}$): 367.0217, found: 367.0217. IR: ν 2969, 2924, 2858, 1745, 1658, 1588, 1552, 1502, 1464, 1378, 1338, 1301, 1252, 1229, 1138, 1085, 839, 736, 528 cm^{-1} .



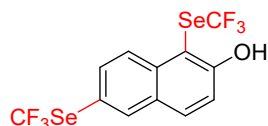
5azb, 1-(5-((trifluoromethyl)selanyl)-1H-pyrrol-2-yl)ethan-1-one, colorless solid, $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 10.36 (s, 1H), 7.30 (dd, $J = 3.0, 1.4$ Hz, 1H), 7.11 (dd, $J = 2.3, 1.4$ Hz, 1H), 2.47 (s, 3H); $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -38.16 (s, 3F); $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 188.43, 133.41, 132.14, 123.74, 122.07 (q, $J = 335.3$ Hz), 120.41, 100.25, 25.69. HRMS-ESI (m/z) calcd for $\text{C}_7\text{H}_6\text{F}_3\text{NNaOSe}$ ($\text{M}+\text{Na}$): 279.9464, found: 279.9460. IR: ν 3056, 2958, 1730, 1656, 1585, 1140, 1100, 829, 728, 530 cm^{-1} .



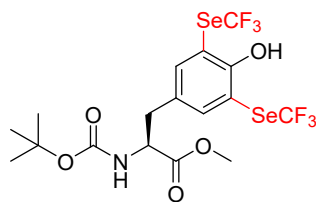
5azc, bis(5-((trifluoromethyl)selanyl)-1H-pyrrol-2-yl)methane, colorless solid, $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 8.72 (s, 2H), 6.84 (d, $J = 2.6$ Hz, 2H), 4.37 (s, 2H), 1.66 (s, 2H). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -37.54 (d, $J = 52.64$ Hz, 3F). $^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 139.89, 129.40, 122.23 (q, $J = 335.3$ Hz), 121.76 (q, $J = 335.3$ Hz), 110.34, 106.75, 100.13, 29.85, 24.62. HRMS-ESI (m/z) calcd for $\text{C}_{11}\text{H}_8\text{F}_6\text{N}_2\text{NaSe}_2$ ($\text{M}+\text{Na}$): 464.8820, found: 464.8822. IR: ν 3067, 2960, 2858, 1650, 1150, 1120, 834, 731 cm^{-1} .



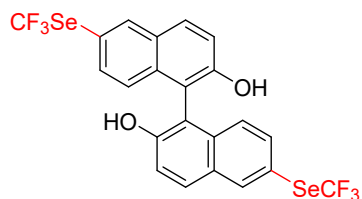
5ba, ((2,5-dimethoxy-1,4-phenylene)bis((trifluoromethyl)selane)), white solid (95%), m.p. 107.1-107.5 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.24 (s, 2H), 3.87 (s, 6H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.61 (s, 6F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.20, 122.61 (q, $J = 333.1$ Hz), 118.80, 115.89, 57.04. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_8\text{F}_6\text{NaO}_2\text{Se}_2$ ($\text{M}+\text{Na}$): 456.8651, found: 456.8645. IR: ν 2974, 2947, 2848, 1479, 1461, 1434, 1350, 1270, 1212, 1095, 1064, 1019, 867, 756, 736, 644, 523, 460 cm^{-1} .



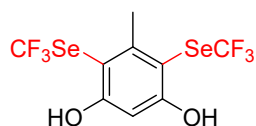
5bb, (1,6-bis((trifluoromethyl)selanyl)naphthalen-2-ol), light yellow solid (83%), m.p. 89.2-89.7 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.31 (d, $J = 8.8$ Hz, 1H), 8.23 (d, $J = 1.8$ Hz, 1H), 7.95 (d, $J = 8.9$ Hz, 1H), 7.87 (dd, $J = 8.8, 1.8$ Hz, 1H), 7.41 (d, $J = 8.9$ Hz, 1H), 6.95 (s, 1H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.45 (s, 3F), -35.89 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.69, 138.02, 136.76, 135.52, 134.80, 129.78, 128.06, 122.66 (q, $J = 333.2$ Hz), 121.92 (q, $J = 336.9$ Hz), 118.14, 118.04, 103.98. HRMS-ESI (m/z) calcd for $\text{C}_{12}\text{H}_7\text{F}_6\text{OSe}_2$ ($\text{M}+\text{H}$): 440.8726, found: 440.8726. IR: ν 3433, 2957, 2924, 2852, 1612, 1584, 1494, 1457, 1403, 1383, 1349, 1213, 1160, 1142, 1130, 1070, 930, 901, 822, 734, 664, 567, 525, 515, 414 cm^{-1} .



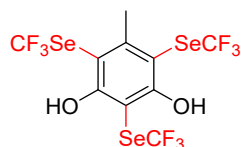
5bc, (methyl(S)-2-((tert-butoxycarbonyl)amino)-3-(4-hydroxy-3,5-is((trifluoromethyl)selanyl)phenyl)propanoate), white solid (38%), m.p. 113.0-113.4 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.56 (s, 2H), 6.66 (s, 1H), 5.05 (d, $J = 7.7$ Hz, 1H), 4.57 (d, $J = 6.9$ Hz, 1H), 3.72 (s, 3H), 3.17-3.01 (m, 2H), 1.44 (s, 9H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.08 (s, 6F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.73, 156.79, 155.03, 142.81, 130.61, 122.15 (q, $J = 334.4$ Hz), 109.90, 54.33, 52.55, 36.81, 28.36. HRMS-ESI (m/z) calcd for $\text{C}_{17}\text{H}_{19}\text{F}_6\text{NNaO}_5\text{Se}_2$ ($\text{M}+\text{Na}$): 613.9390, found: 613.9390. IR: ν 3420, 3350, 2992, 2956, 2920, 1732, 1682, 1525, 1450, 1317, 1280, 1149, 1128, 1086, 1066, 998, 854, 803, 762, 734, 637, 485, 462, 409 cm^{-1} .



5bd, (6,6'-bis((trifluoromethyl)selanyl)-[1,1'-binaphthalene]-2,2'-diol), light yellow solid (93%), m.p. 80.4-80.8 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.34 (d, $J = 1.8$ Hz, 2H), 8.02 (d, $J = 9.0$ Hz, 2H), 7.60 (dd, $J = 8.7, 1.8$ Hz, 2H), 7.46 (d, $J = 9.0$ Hz, 2H), 7.12 (d, $J = 8.7$ Hz, 2H), 5.13 (s, 2H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.91 (s, 6F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.39, 138.20, 134.93, 134.05, 132.13, 129.89, 125.47, 122.67 (q, $J = 334.2$ Hz), 119.17, 117.99, 110.58. HRMS-ESI (m/z) calcd for $\text{C}_{22}\text{H}_{13}\text{F}_6\text{O}_2\text{Se}_2$ ($\text{M}+\text{H}$): 582.9145, found: 582.9145. IR: ν 3495, 2953, 2928, 2857, 1705, 1611, 1585, 1492, 1464, 1381, 1346, 1273, 1217, 1120, 1089, 1068, 966, 930, 892, 816, 753, 737, 673, 556, 422 cm^{-1} .

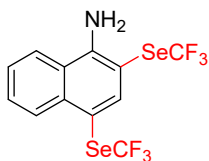


5be, (5-methyl-4,6-bis((trifluoromethyl)selanyl)benzene-1,3-diol), white solid (71%), m.p. 57.9-58.5 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 6.78 (s, 2H), 6.75 (s, 1H), 2.92 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.72 (s, 6F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.93, 152.46, 123.59, 121.92 (q, $J = 336.6$ Hz), 120.24, 104.48, 99.88, 26.53. HRMS-ESI (m/z) calcd for $\text{C}_9\text{H}_7\text{F}_6\text{O}_2\text{Se}_2$ ($\text{M}+\text{H}$): 420.8675, found: 420.8675. IR: ν 3431, 3084, 2953, 2923, 2853, 1589, 1562, 1435, 1415, 1338, 1308, 1234, 1149, 1122, 1074, 856, 736, 600, 488 cm^{-1} .

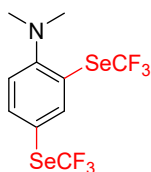


5bf, (5-methyl-2,4,6-tris((trifluoromethyl)selanyl)benzene-1,3-diol), white solid (95%), m.p. 71.0-72.0 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 7.38 (s, 2H), 2.98 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.84 (s, 3F), -35.52 (s, 6F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.94, 156.83, 122.08 (q, $J = 336.2$ Hz), 121.93 (q, $J = 336.4$ Hz), 104.04, 94.70, 27.26. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_5\text{F}_9\text{NaO}_2\text{Se}_3$ ($\text{M}+\text{Na}$): 590.7534, found: 590.7534. IR: ν 3411, 3357, 2968, 2929, 1552, 1535, 1419,

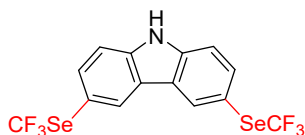
1368, 1338, 1306, 1107, 1070, 1007, 752, 737, 668, 636, 583, 529 cm^{-1} .



5bg, (2,4-bis((trifluoromethyl)selanyl)naphthalen-1-amine), light yellow solid (94%), m.p. 99.4-99.9 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.49 (d, $J = 8.5$ Hz, 1H), 8.26 (s, 1H), 7.86 (dt, $J = 8.4, 0.8$ Hz, 1H), 7.72-7.67 (m, 1H), 7.60-7.56 (m, 1H), 5.46 (s, 2H).; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.48 (s, 3F), -36.73 (s, 3F); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.16, 148.11, 137.53, 129.41, 129.39, 126.58, 123.91, 122.96, 122.58 (q, $J = 336.0$ Hz), 122.53 (q, $J = 336.0$ Hz), 121.19, 110.09, 100.28. HRMS-ESI (m/z) calcd for $\text{C}_{12}\text{H}_8\text{F}_6\text{NSe}_2$ ($\text{M}+\text{H}$): 439.8886, found: 439.8835. IR: ν 3523, 3400, 2952, 2923, 1612, 1558, 1498, 1424, 1381, 1363, 1156, 1146, 1087, 1038, 777, 754, 734, 667, 528, 419 cm^{-1} .

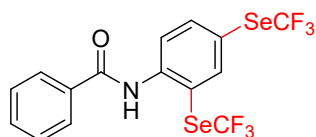


5bh, (N,N-dimethyl-2,4-bis((trifluoromethyl)selanyl)aniline), light yellow oil (90%), ^1H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, $J = 1.9$ Hz, 1H), 7.67 (dd, $J = 8.3, 2.0$ Hz, 1H), 7.17 (d, $J = 8.3$ Hz, 1H), 2.78 (s, 6H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.56 (s, 3F), -36.40 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.45, 141.27, 138.16, 123.08 (q, $J = 333.3$ Hz), 122.40 (q, $J = 333.3$ Hz), 121.56, 120.88, 117.95, 110.85, 44.98. HRMS-ESI (m/z) calcd for $\text{C}_{10}\text{H}_{10}\text{F}_6\text{NSe}_2$ ($\text{M}+\text{H}$): 417.9042, found: 417.9033. IR: ν 2991, 2948, 2870, 2837, 2793, 1572, 1477, 1454, 1434, 1378, 1321, 1266, 1120, 1088, 1042, 939, 825, 737, 674, 598, 577, 512, 460, 428 cm^{-1} .

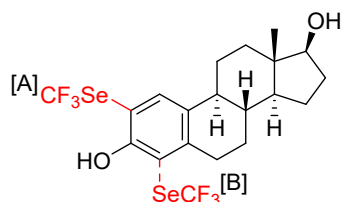


5bi, (3,6-bis((trifluoromethyl)selanyl)-9H-carbazole), light yellow solid (79%), m.p. 157.7-158.7 $^{\circ}\text{C}$, ^1H NMR (400 MHz, Chloroform-*d*) δ 8.50 (d, $J = 1.9$ Hz, 2H), 8.36 (s, 1H), 7.83 (dd, $J = 8.5, 1.7$ Hz, 2H), 7.48 (d, $J = 8.4$ Hz, 2H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -37.03 (s, 6F); ^{13}C NMR (101 MHz,

Chloroform-*d*) δ 140.60, 135.59, 130.50, 124.44, 123.87, 121.12, 112.89, 112.01. 140.60, 135.59, 130.50, 124.44, 123.87, 121.12, 112.89, 122.78 (q, $J = 333.3$ Hz), 112.01. HRMS-ESI (m/z) calcd for $C_{14}H_8F_6NSe_2$ ($M+H$): 463.8886, found: 463.8886. IR: ν 3490, 2967, 2924, 2850, 1597, 1466, 1430, 1288, 1242, 1110, 1082, 1053, 886, 809, 732, 574, 524, 410 cm^{-1} .

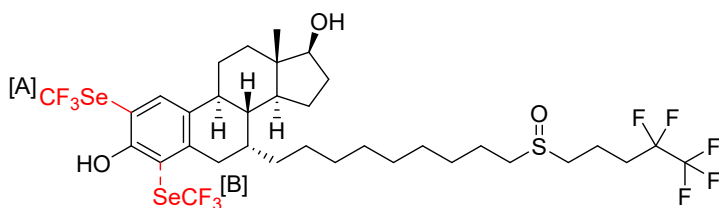


5bj, (N-(2,4-bis((trifluoromethyl)selanyl)phenyl)benzamide), white solid (66%), m.p. 140.0-140.9 °C, 1H NMR (400 MHz, Chloroform-*d*) δ 9.13 (s, 1H), 8.79 (d, $J = 8.7$ Hz, 1H), 8.22 (d, $J = 2.0$ Hz, 1H), 7.95-7.91 (m, 3H), 7.67 – 7.59 (m, 1H), 7.55 (dd, $J = 8.2, 6.6$ Hz, 2H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.87 (s, 3F), -36.28 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.46, 147.79, 142.87, 142.00, 134.10, 132.80, 129.28, 127.21, 122.40 (q, $J = 333.2$ Hz), 122.01 (q, $J = 335.1$ Hz), 121.56, 117.39, 113.33. HRMS-ESI (m/z) calcd for $C_{15}H_9F_6NNaOSe_2$ ($M+Na$): 515.8811, found: 515.8811. IR: ν 3311, 1658, 1562, 1505, 1491, 1372, 1296, 1179, 1155, 1122, 1071, 901, 836, 798, 738, 709, 688, 631, 598, 562, 461 cm^{-1} .

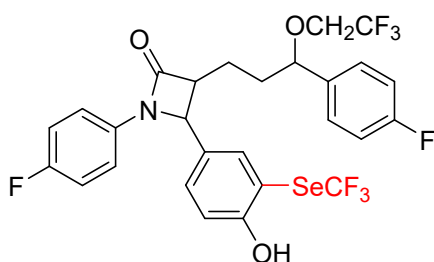


5ca, ([A]: (8R,9S,13S,14S,17S)-13-methyl-2-((trifluoromethyl)selanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol; [B]: (8R,9S,13S, 14S,17S)-13-methyl-4-((trifluoromethyl)selanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol), white solid (85%), m.p. 83.4-84.1 °C, [A]:[B] = 4:1, 1H NMR (400 MHz, Chloroform-*d*) δ 7.53 (s, 1H), 6.82 (s, 1H), 5.97 (s, 1H), 3.77 – 3.68 (m, 1H), 2.87 (dd, $J = 8.8, 4.3$ Hz, 2H), 2.34 – 2.25 (m, 2H), 2.22-2.08 (m, 3H), 2.02 – 1.83 (m, 3H), 1.75-1.66 (m, 2H), 1.57 – 1.15 (m, 16H), 0.80 – 0.77 (m, 4H). 7.39 (d, $J = 8.6$ Hz, 0.25H), 6.94 (d, $J = 8.6$ Hz, 0.25H), 6.35 (s, 0.25H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -34.39 (s, 3F). -36.03 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.97, 143.62, 135.91, 134.19, 122.07 (q, $J = 335.1$ Hz), 115.54, 112.80, 106.02, 81.90, 50.02, 44.26, 43.68, 43.27, 38.53, 38.08, 36.72, 36.60, 31.90, 30.51, 29.68, 27.42, 26.96, 26.55, 26.30, 23.16, 23.12, 11.16.

HRMS-ESI (m/z) calcd for C₁₉H₂₄F₃O₂Se (M+H): 421.0888, found: 421.0888. IR: ν 2920, 2870, 1597, 1469, 1407, 1340, 1263, 1207, 1125, 1092, 1054, 1010, 892, 870, 755, 737, 667 cm⁻¹.

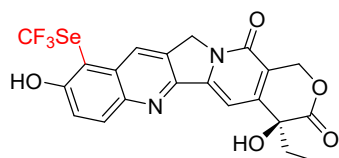


5cb, ([A]: (7R,8R,9S,13S,14S,17S)-13-methyl-7-(9-((4,4,5,5,5-pentafluoropentyl)sulfinyl)nonyl)-2-((trifluoromethyl)selanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol; [B]: (7R,8R,9S,13S,14S,17S)-13-methyl-7-(9-((4,4,5,5,5-pentafluoropentyl)sulfinyl)nonyl)-4-((trifluoromethyl)selanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol), lightyellow solid (66%), m.p. 73.1-73.4 °C, [A]:[B] = 2:1, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.53 (s, 1H), 7.39 (d, *J* = 8.6 Hz, 1H), 6.94 (d, *J* = 8.6 Hz, 1H), 6.79 (d, *J* = 3.3 Hz, 1H), 3.82 – 3.68 (m, 2H), 3.27 (d, *J* = 17.5 Hz, 1H), 2.92 – 2.65 (m, 9H), 2.37 – 2.14 (m, 11H), 1.92 (d, *J* = 12.4 Hz, 2H), 1.73 – 1.13 (m, 52H), 0.97 (dd, *J* = 17.8, 8.2 Hz, 2H), 0.78 (d, *J* = 1.3 Hz, 5H); ¹⁹F NMR (376MHz, Chloroform-*d*) δ -34.53, -35.93, -85.43, -118.11, -118.18; ¹³C NMR (101 MHz, Chloroform-*d*) δ 156.00, 155.24, 141.49, 136.41, 133.04, 131.43, 122.21 (q, *J* = 333.3 Hz), 122.06 (q, *J* = 333.7 Hz), 116.51, 113.01, 106.36, 81.88, 52.58, 52.50, 50.86, 46.46, 46.43, 43.40, 41.80, 41.78, 41.32, 38.46, 37.91, 37.86, 36.96, 36.84, 36.62, 34.70, 33.50, 33.14, 33.09, 30.54, 30.46, 29.92, 29.85, 29.75, 29.64, 29.58, 29.55, 29.43, 29.31, 29.22, 29.19, 29.16, 28.98, 28.82, 28.09, 27.96, 27.74, 27.58, 27.24, 25.82, 25.64, 25.49, 22.65, 14.73, 14.69, 11.17. HRMS-ESI (m/z) calcd for C₃₃H₄₆F₈NaO₃SSe (M+Na): 777.2097, found: 777.2092. IR: ν 2923, 2856, 1598, 1542, 1454, 1410, 1350, 1266, 1193, 1121, 1094, 1057, 1016, 984, 754, 737, 721, 525, 516, 462, 427, 409 cm⁻¹.

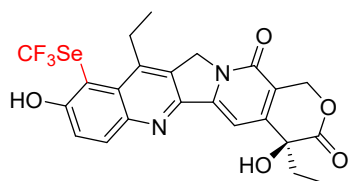


5cc, (1-(4-fluorophenyl)-3-(3-(4-fluorophenyl)-3-(2,2,2-trifluoroethoxy)propyl)-4-(4-hydroxy-3-((trifluoromethyl)selanyl)phenyl)azetidin-2-one), light yellow viscous oil (94%), ¹H NMR (400 MHz,

Chloroform-*d*) δ 7.62 (dd, $J = 5.1, 2.3$ Hz, 1H), 7.38 (ddd, $J = 8.4, 2.3, 1.1$ Hz, 1H), 7.26 – 7.17 (m, 4H), 7.11 (d, $J = 8.5$ Hz, 1H), 7.09 – 7.02 (m, 2H), 6.97 – 6.88 (m, 2H), 6.27 (s, 1H), 4.57 (dd, $J = 14.4, 2.4$ Hz, 1H), 4.42 (p, $J = 5.2$ Hz, 1H), 3.73 – 3.50 (m, 2H), 3.22 – 3.03 (m, 1H), 2.13 – 1.81 (m, 4H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.53 (d, $J = 4.1$ Hz, 3F), -73.94 (d, $J = 14.9$ Hz, 3F), -113.39 (d, $J = 6.3$ Hz, 1F), -117.70 (d, $J = 3.3$ Hz, 1F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.43, 167.35, 163.96, 161.51, 160.43, 158.01, 157.80, 136.49, 135.74, 133.55, 131.13, 131.10, 130.44, 130.38, 128.41, 128.34, 128.27, 124.00 (q, $J = 280.17$ Hz), 121.89 (q, $J = 336.1$ Hz), 118.60, 118.52, 116.94, 116.10, 115.98, 115.88, 115.77, 109.89, 82.60, 82.49, 65.99, 65.65, 60.47, 60.32, 60.23, 60.13, 35.69, 35.17, 25.16, 24.70. HRMS-ESI(*m/z*) calcd for $\text{C}_{27}\text{H}_{21}\text{F}_8\text{NNaO}_3\text{Se}$ ($\text{M}+\text{Na}$): 662.0451, found: 662.0443. IR: ν 2925, 1718, 1605, 1508, 1424, 1388, 1335, 1276, 1223, 1144, 1119, 1091, 1045, 969, 832, 738, 669, 565, 547, 516, 459, 427, 411 cm^{-1} .

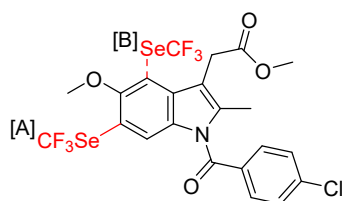


5cd, ((*S*)-4-ethyl-4,9-dihydroxy-10-((trifluoromethyl)selanyl)-1,12-dihydro-14H-pyrano[3',4':6,7]indolizino[1,2-b]quinoline-3,14(4H)-dione), light yellow solid (80%), m.p. 181.2-181.9 °C, ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 11.37 (s, 1H), 8.98 (s, 1H), 8.23 (d, $J = 9.2$ Hz, 1H), 7.69 (d, $J = 9.2$ Hz, 1H), 7.27 (s, 1H), 6.51 (s, 1H), 5.41 (s, 2H), 5.30 (s, 2H), 1.99 – 1.75 (m, 2H), 0.88 (t, $J = 7.3$ Hz, 3H); ^{19}F NMR (376 MHz, $\text{DMSO-}d_6$) δ -34.88 (s, 3F); ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 172.59, 159.89, 156.71, 149.87, 149.66, 145.17, 143.69, 134.48, 132.19, 131.29, 129.72, 122.80 (q, $J = 335.5$ Hz), 122.16, 118.48, 103.10, 96.29, 72.38, 65.28, 50.48, 30.37, 7.78. HRMS-ESI (*m/z*) calcd for $\text{C}_{21}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_5\text{Se}$ ($\text{M}+\text{H}$): 513.0171, found: 513.0169. IR: ν 2970, 2925, 1747, 1656, 1581, 1556, 1476, 1381, 1330, 1242, 1144, 1097, 1049, 1004, 841, 756, 735, 727, 532, 429, 412 cm^{-1} .

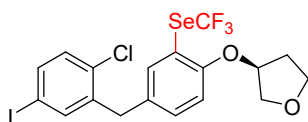


5ce, ((*S*)-4,11-diethyl-4,9-dihydroxy-10-((trifluoromethyl)selanyl)-1,12-dihydro-14H-pyrano[3',4':6,7]indolizino[1,2-b]quinoline-3,14(4H)-dione), yellow solid (77%), m.p. 189.1-189.6 °C, ^1H

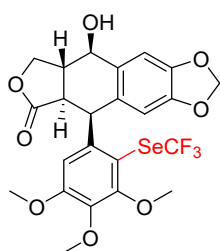
NMR (400 MHz, DMSO-*d*₆) δ 11.35 (s, 1H), 8.22 (d, *J* = 9.1 Hz, 1H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.24 (s, 1H), 6.52 (s, 1H), 5.42 (s, 2H), 5.33 (s, 2H), 3.68-3.59 (m, 2H), 1.91-1.80 (m, 2H), 1.33 (t, *J* = 7.4 Hz, 3H), 0.87 (t, *J* = 7.3 Hz, 3H); ¹⁹F NMR (376 MHz, DMSO-*d*₆) δ -35.75 (s, 3F); ¹³C NMR (101 MHz, DMSO-*d*₆) δ 172.59, 160.72, 156.76, 150.07, 148.66, 145.97, 145.42, 144.80, 136.35, 132.00, 130.25, 122.69 (q, *J* = 337.7 Hz), 121.16, 118.41, 100.66, 96.04, 72.43, 65.29, 50.25, 30.31, 24.97, 13.63, 7.78. HRMS-ESI (*m/z*) calcd for C₂₃H₂₀F₃N₂O₅Se (M+H): 541.0484, found: 541.0482. IR: ν 2980, 2886, 1744, 1656, 1587, 1553, 1502, 1465, 1378, 1303, 1229, 1139, 1080, 1048, 840, 750, 737, 726, 525, 460, 408 cm⁻¹.



5cf, 97%, [A]:[B] = 3:2, A(methyl-2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-6-((trifluoromethyl)selenyl)-1H-indol-3-yl)acetate): white solid, m.p. 124.8-125.3 °C, ¹H NMR (500 MHz, Chloroform-*d*) δ 7.69 – 7.65 (m, 2H), 7.52 – 7.47 (m, 2H), 7.29 (s, 1H), 7.01 (s, 1H), 3.93 (s, 3H), 3.72 (s, 3H), 3.69 (s, 2H), 2.42 (s, 3H); ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -35.96 (s, 3F); ¹³C NMR (126 MHz, Chloroform-*d*) δ 171.21, 168.12, 155.56, 139.91, 137.75, 133.31, 132.67, 131.31, 130.84, 129.39, 123.22, 122.55 (q, *J* = 334.8 Hz), 112.37, 108.19, 100.04, 56.62, 52.37, 30.17, 13.46. B(methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-4-((trifluoromethyl)selenyl)-1H-indol-3-yl)acetate): light yellow solid, m.p. 97.6-98.1 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 9.2 Hz, 2H), 6.80 (d, *J* = 9.1 Hz, 1H), 4.10 (s, 2H), 3.89 (s, 3H), 3.72 (s, 3H), 2.30 (s, 3H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -35.90 (s, 3F); ¹³C NMR (101 MHz, Chloroform-*d*) δ 171.97, 168.17, 157.39, 139.93, 138.60, 133.68, 133.11, 131.91, 131.48, 129.41, 122.29 (q, *J* = 335.2 Hz), 117.88, 113.30, 107.61, 101.40, 57.11, 52.26, 31.13, 29.82, 13.55. HRMS-ESI (*m/z*) calcd for C₂₁H₁₇ClF₃NNaO₄Se (M+Na): 541.9856, found: 541.9850. IR: ν 2957, 2923, 2851, 1734, 1678, 1591, 1460, 1427, 1392, 1355, 1314, 1278, 1197, 1158, 1128, 1068, 907, 845, 827, 787, 764, 738, 681, 624, 567, 482, 461, 408 cm⁻¹.



5cg, ((S)-3-(4-(2-chloro-5-iodobenzyl)-2-((trifluoromethyl)selanyl)phenoxy)tetrahydrofuran), light yellow viscous oil (97%), ¹H NMR (400 MHz, Chloroform-*d*) δ 7.52=7.46 (m, 3H), 7.15 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 4.98-4.94 (m, 1H), 4.05 (dd, *J* = 10.2, 4.8 Hz, 1H), 4.00 – 3.90 (m, 5H), 2.19-2.16 (m, 2H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -34.91 (s, 3F); ¹³C NMR (126 MHz, Chloroform-*d*) δ 155.71, 140.66, 139.58, 137.68, 137.01, 134.30, 132.28, 131.87, 131.42, 114.07, 113.15, 91.84, 78.68, 72.95, 67.28, 37.87, 33.14. HRMS-ESI (*m/z*) calcd for C₁₈H₁₆ClF₃IO₂Se (M+H): 562.8995, found: 562.8995. IR: *ν* 2967, 2921, 2867, 1618, 1598, 1484, 1460, 1335, 1276, 1252, 1133, 1084, 1048, 1014, 934, 897, 812, 795, 737, 638, 603, 531, 518 cm⁻¹.

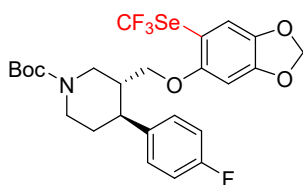


5ch, ((5*S*,5*aR*,8*aR*,9*R*)-9-hydroxy-5-(3,4,5-trimethoxy-2-((trifluoromethyl)selanyl) phenyl)-5,8,8*a*,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-*d*][1,3]dioxol-6(5*aH*)-one), white solid (96%), m.p. 182.1-182.4 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.14 (s, 1H), 6.18 (s, 1H), 6.09 (s, 1H), 5.99 (dd, *J* = 4.1, 1.0 Hz, 2H), 5.40 (d, *J* = 6.4 Hz, 1H), 4.62 (d, *J* = 9.8 Hz, 1H), 4.50 (dd, *J* = 8.3, 7.1 Hz, 1H), 4.12 (dd, *J* = 10.4, 8.4 Hz, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 3.60 (s, 4H), 3.39 – 3.33 (m, 2H), 2.79 – 2.65 (m, 1H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -36.48 (s, 3F); ¹³C NMR (101 MHz, Chloroform-*d*) δ 174.41, 155.54, 155.38, 148.08, 147.75, 141.71, 140.82, 132.91, 131.47, 123.23 (q, *J* = 334.6 Hz), 115.46, 110.19, 109.87, 105.72, 101.58, 71.86, 71.37, 61.41, 61.00, 56.21, 44.11, 43.40, 41.26. HRMS-ESI (*m/z*) calcd for C₂₃H₂₁F₃NaO₈Se (M+Na): 585.0246, found: 585.0246. IR: *ν* 2987, 2970, 2912, 1764, 1579, 1559, 1480, 1385, 1327, 1304, 1233, 1172, 1085, 1047, 1005, 933, 878, 863, 770, 736, 695, 665, 566, 517, 429, 409 cm⁻¹.

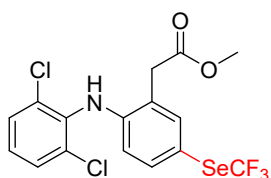


5ci, ((S)-N-(1,2,3,10-tetramethoxy-9-oxo-4-((trifluoromethyl)selanyl)-5,6,7,9-tetrahydrobenzo[*a*]heptalen

-7-yl)acetamide), light yellow solid (54%), m.p. 130.9-131.4 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 8.64 (d, *J* = 6.0 Hz, 1H), 7.62 (s, 1H), 7.29 (s, 1H), 6.88 (d, *J* = 10.9 Hz, 1H), 4.52 (dt, *J* = 11.5, 5.6 Hz, 1H), 4.02 (s, 3H), 3.97 (s, 3H), 3.95 (s, 3H), 3.66 (s, 3H), 3.53 (d, *J* = 7.8 Hz, 1H), 2.33 – 2.25 (m, 2H), 1.96 (s, 3H), 1.92 – 1.82 (m, 1H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -35.05 (s, 3F); ¹³C NMR (101 MHz, Chloroform-*d*) δ 179.63, 170.57, 164.52, 156.13, 154.30, 152.35, 145.90, 140.19, 136.28, 135.97, 130.05, 129.81, 122.20 (q, *J* = 334.5 Hz), 112.98, 112.77, 61.65, 61.43, 61.34, 56.66, 52.79, 35.01, 29.75, 22.75. HRMS-ESI (m/z) calcd for C₂₃H₂₅F₃NO₆Se (M+H): 548.0794, found: 548.0786. IR: *ν* 3276, 2980, 2944, 2921, 1646, 1618, 1587, 1563, 1542, 1457, 1406, 1346, 1249, 1120, 1090, 1052, 1016, 976, 952, 834, 736, 674, 607, 519, 506, 461, 426, 411 cm⁻¹.

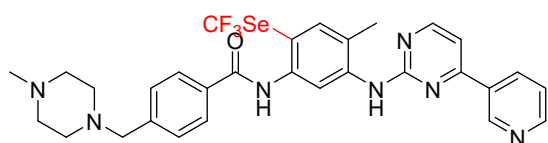


5cj, (tert-butyl(3R,4S)-4-(4-fluorophenyl)-3-(((6-((trifluoromethyl)selanyl)benzo[d][1,3]dioxol-5-yl)oxy)-methyl)piperidine-1-carboxylate), white solid (97%), m.p. 54.4-54.9 °C, ¹H NMR (500 MHz, Chloroform-*d*) δ 7.18 – 7.10 (m, 3H), 6.97 (t, *J* = 8.7 Hz, 2H), 6.28 (s, 1H), 5.93 (s, 2H), 4.43 (d, *J* = 13.4 Hz, 1H), 3.65 (dd, *J* = 9.2, 2.6 Hz, 1H), 3.60 – 3.45 (m, 1H), 2.88 (d, *J* = 65.0 Hz, 3H), 2.03 (d, *J* = 8.6 Hz, 1H), 1.85-1.80 (m, 1H), 1.76-1.67 (m, 1H), 1.50 (s, 9H); ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -36.01 (s, 3F), -116.16 (s, 1F); ¹³C NMR (126 MHz, Chloroform-*d*) δ 155.30, 154.97, 151.17, 141.92, 139.22, 139.19, 128.94, 128.88, 122.60 (q, *J* = 334.3 Hz), 117.25, 115.77, 115.60, 102.08, 101.89, 95.67, 79.85, 42.16, 34.02, 28.62. HRMS-ESI (m/z) calcd for C₂₅H₂₇F₄NNaO₅Se (M+Na): 600.0883, found: 600.0873. IR: *ν* 2981, 2920, 1683, 1606, 1509, 1465, 1422, 1386, 1366, 1280, 1225, 1186, 1160, 1123, 1092, 1038, 934, 866, 832, 752, 737, 668, 567, 538, 410 cm⁻¹.

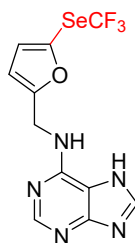


5ck, (methyl 2-(2-((2,6-dichlorophenyl)amino)-5-((trifluoromethyl)selanyl)phenyl) acetate), white solid (99%), m.p. 84.6-85.0 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 2.1 Hz, 1H), 7.47 (dd, *J* =

8.4, 2.1 Hz, 1H), 7.39 (s, 1H), 7.37 (s, 1H), 7.20 (s, 1H), 7.06 (t, $J = 8.1$ Hz, 1H), 6.47 (d, $J = 8.3$ Hz, 1H), 3.80 (s, 2H), 3.78 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -36.82 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.31, 145.17, 139.98, 137.42, 136.61, 130.59, 129.10, 125.42, 124.34, 122.58 (q, $J = 333.5$ Hz), 118.08, 113.42, 52.78, 38.45. HRMS-ESI (m/z) calcd for $\text{C}_{16}\text{H}_{12}\text{Cl}_2\text{F}_3\text{NNaO}_2\text{Se}$ ($\text{M}+\text{Na}$): 479.9255, found: 479.9252. IR: ν 3375, 2964, 2922, 2858, 1783, 1741, 1687, 1656, 1597, 1526, 1494, 1457, 1438, 1384, 1338, 1290, 1248, 1183, 1145, 1087, 1062, 889, 748, 691, 673, 591, 577, 530, 505, 410 cm^{-1} .

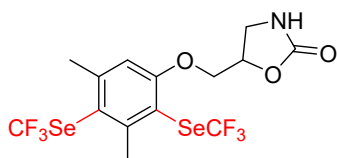


5cl, (N-(4-methyl-5-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)-2-((trifluoromethyl) selanyl)phenyl)-4-((4-methylpiperazin-1-yl)methyl)benzamide), light yellow solid (61%), m.p. 202.3-202.7 °C, ^1H NMR (400 MHz, Chloroform-*d*) δ 9.81 9.75 (s, 1H), 9.23 (d, $J = 2.4$ Hz, 1H), 9.00 (s, 1H), 8.76 (dt, $J = 8.0, 2.0$ Hz, 1H), 8.69 (dd, $J = 4.8, 1.7$ Hz, 1H), 8.55 (d, $J = 5.2$ Hz, 1H), 7.96 – 7.85 (m, 2H), 7.60 (s, 1H), 7.48 (d, $J = 8.1$ Hz, 2H), 7.42 (dd, $J = 8.0, 4.8$ Hz, 1H), 7.25 (d, $J = 5.2$ Hz, 2H), 3.58 (s, 2H), 2.52 (s, 8H), 2.33 (s, 3H), 2.32 (s, 3H); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -35.87 (s, 3F); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.82, 163.02, 160.03, 159.23, 151.65, 148.57, 142.97, 141.86, 140.71, 139.75, 135.76, 132.57, 129.61, 127.10, 123.99, 123.01, 122.19 (q, $J = 335.7$ Hz), 111.49, 109.29, 104.97, 62.50, 55.07, 52.94, 45.90, 17.50. HRMS-ESI (m/z) calcd for $\text{C}_{30}\text{H}_{31}\text{F}_3\text{N}_7\text{OSe}$ ($\text{M}+\text{H}$): 642.1702, found: 642.1702. IR: ν 3434, 2951, 2928, 2795, 1654, 1569, 1514, 1498, 1441, 1413, 1395, 1318, 1124, 1096, 1008, 904, 878, 861, 796, 755, 735, 700, 685, 583, 459 cm^{-1} .



5cm, (N-((5-((trifluoromethyl)selanyl)furan-2-yl)methyl)-7H-purin-6-amine), light brown solid (98%), m.p. 190.9-191.3 °C, ^1H NMR (400 MHz, DMSO-*d*₆) δ 12.96 (s, 1H), 8.22 (s, 2H), 8.15 (s, 1H), 7.01 (d, $J = 3.3$ Hz, 1H), 6.41 (d, $J = 3.3$ Hz, 1H), 4.76 (s, 2H); ^{19}F NMR (376 MHz, DMSO-*d*₆) δ -37.03 (s, 3F); ^{13}C NMR (101

MHz, DMSO-*d*₆) δ 160.17, 152.20, 139.55, 130.35, 125.77, 122.18 (q, *J* = 338.0 Hz), 109.70. HRMS-ESI (*m/z*) calcd for C₁₁H₉F₃N₅OSe (M+H): 363.9919, found: 363.9908. IR: ν 3271, 2969, 2937, 1746, 1618, 1590, 1455, 1404, 1301, 1252, 1137, 1086, 1013, 934, 897, 795, 737, 723, 662, 637, 519, 469, 409 cm⁻¹.



5cn, (5-((3,5-dimethyl-2,4-bis((trifluoromethyl)selanyl)phenoxy)methyl)oxazolidin-2-one), white solid (91%), m.p. 94.4-94.6 °C, ¹H NMR (400 MHz, Chloroform-*d*) δ 6.84 (s, 1H), 5.42 (s, 1H), 5.02 (dtd, *J* = 9.0, 5.4, 3.7 Hz, 1H), 4.28-4.10 (m, 2H), 3.90 – 3.80 (m, 1H), 3.76-3.72 (m, 1H), 2.98 (s, 3H), 2.66 (s, 3H); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -35.12 (s, 3F), -35.58 (s, 3F); ¹³C NMR (126 MHz, Chloroform-*d*) δ 160.64, 159.56, 152.92, 150.79, 122.84 (q, *J* = 334.5 Hz), 122.66 (q, *J* = 334.4 Hz), 121.33, 118.71, 111.90, 73.77, 68.82, 42.78, 27.21, 26.16. HRMS-ESI (*m/z*) calcd for C₁₄H₁₃F₆NNaO₃Se₂ (M+Na): 539.9022, found: 539.9020. IR: ν 3270, 3170, 2979, 2911, 1780, 1751, 1562, 1544, 1450, 1372, 1313, 1246, 1213, 1141, 1079, 1041, 928, 840, 757, 736, 667, 763, 406 cm⁻¹.

8) References

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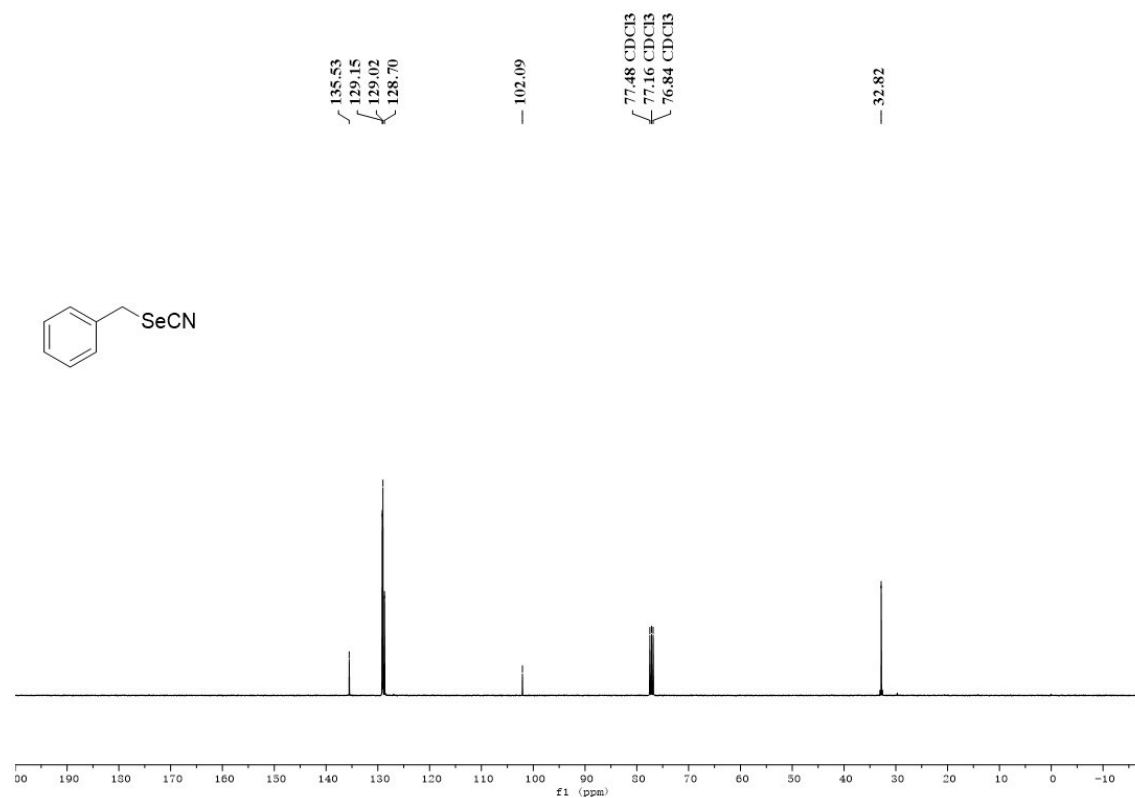
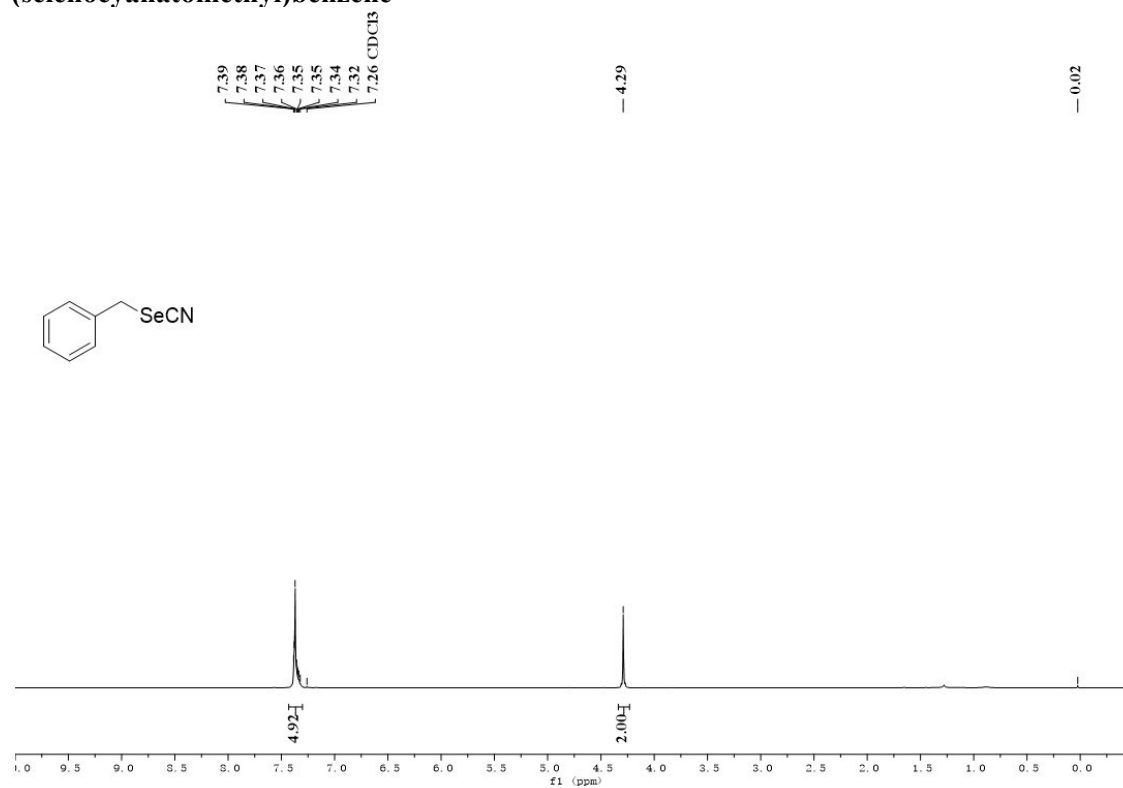
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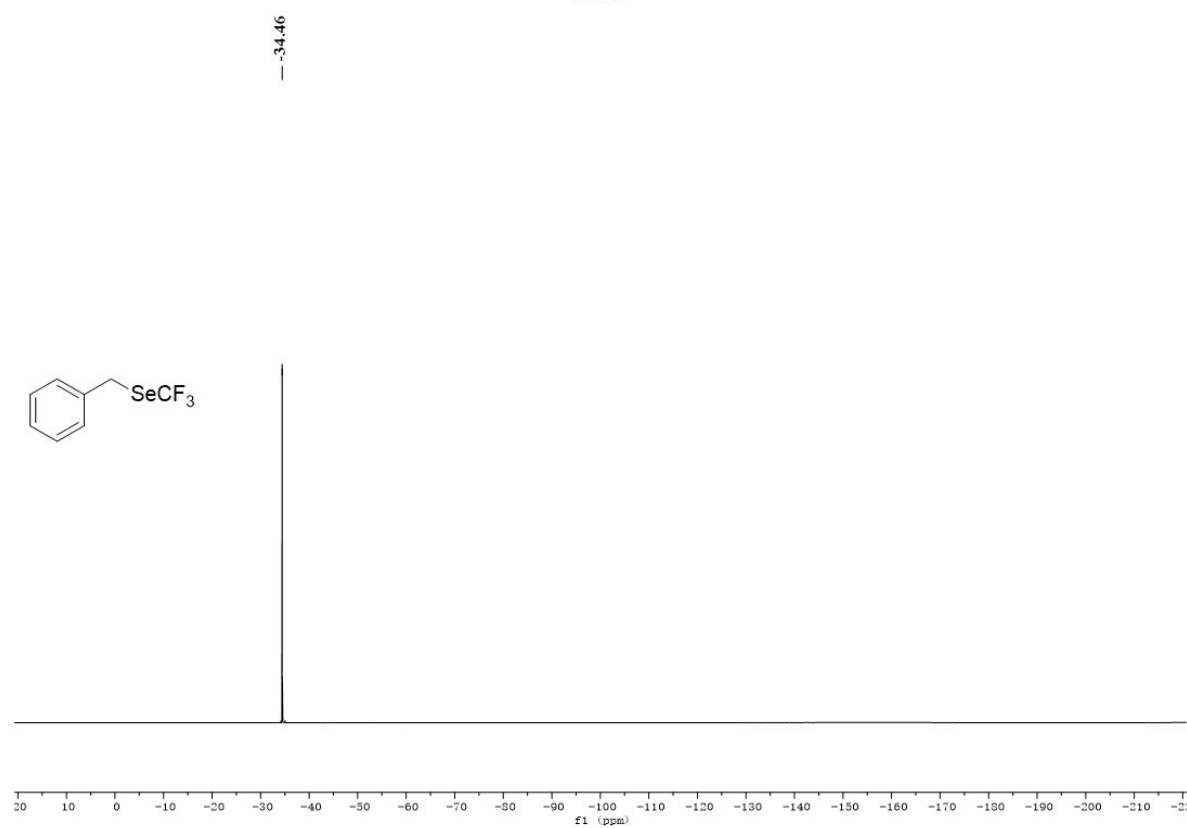
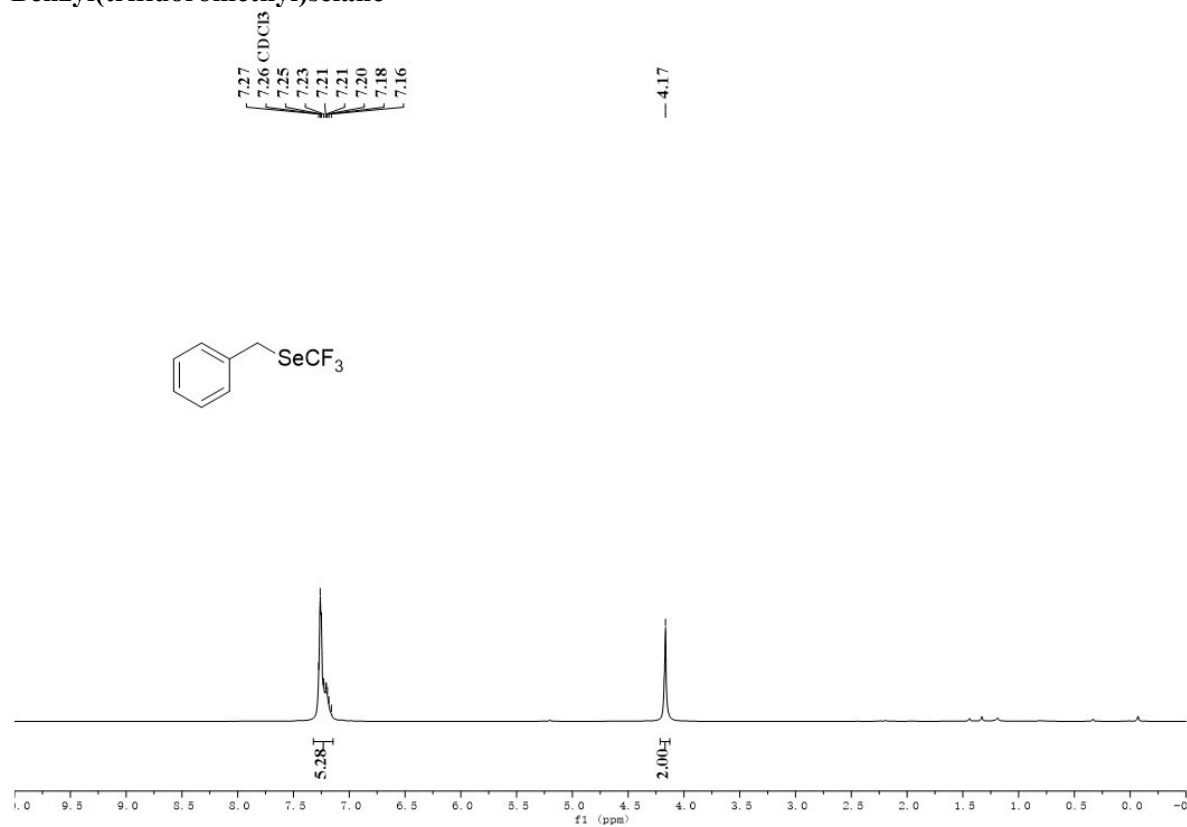
9) ^1H , ^{19}F & ^{13}C spectra

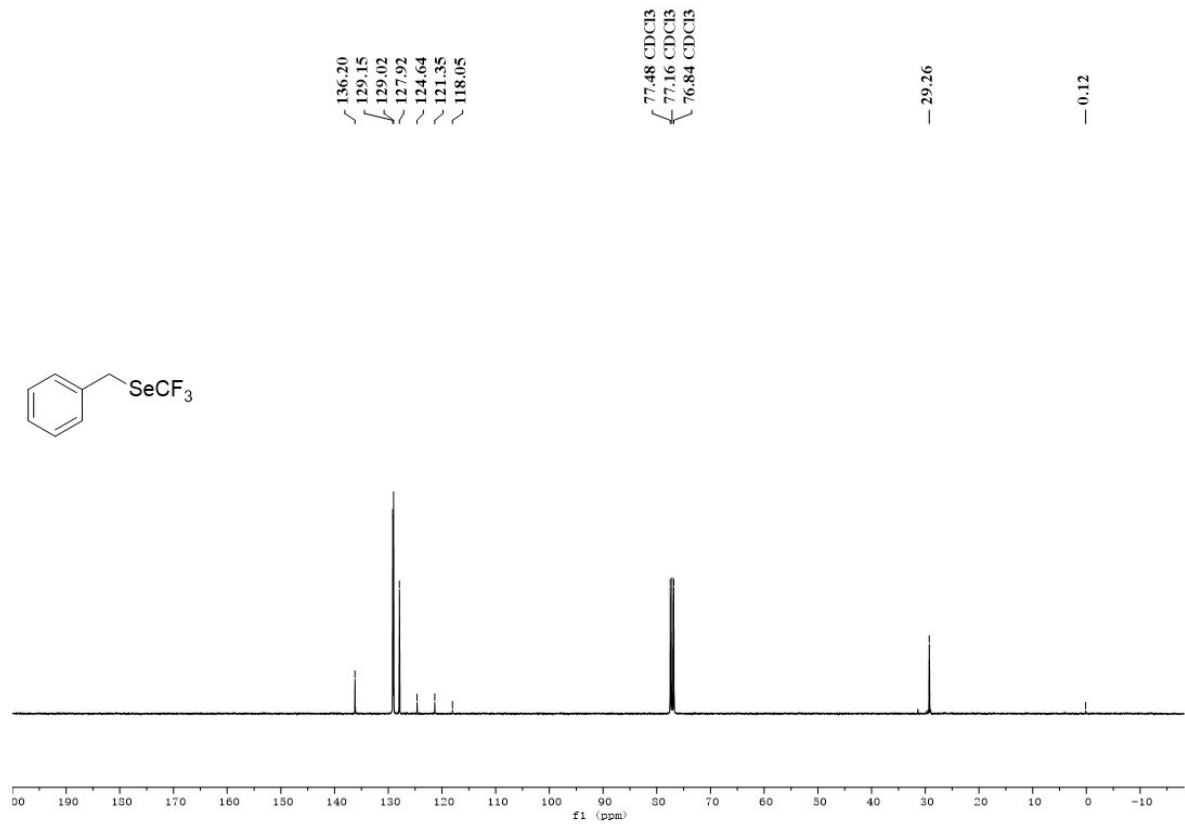
The single peak nearby 0.00 in the NMR spectra is the chemical shift of the internal standard.

(selenocyanatomethyl)benzene

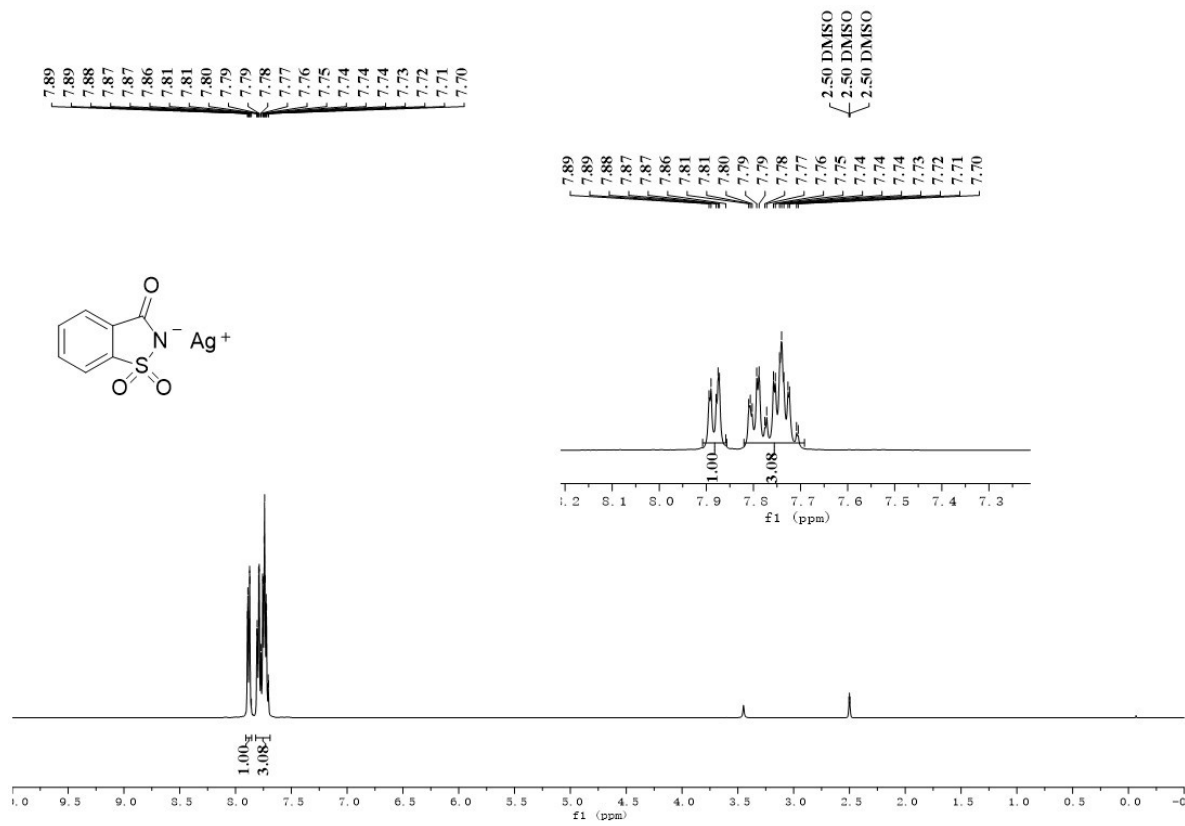


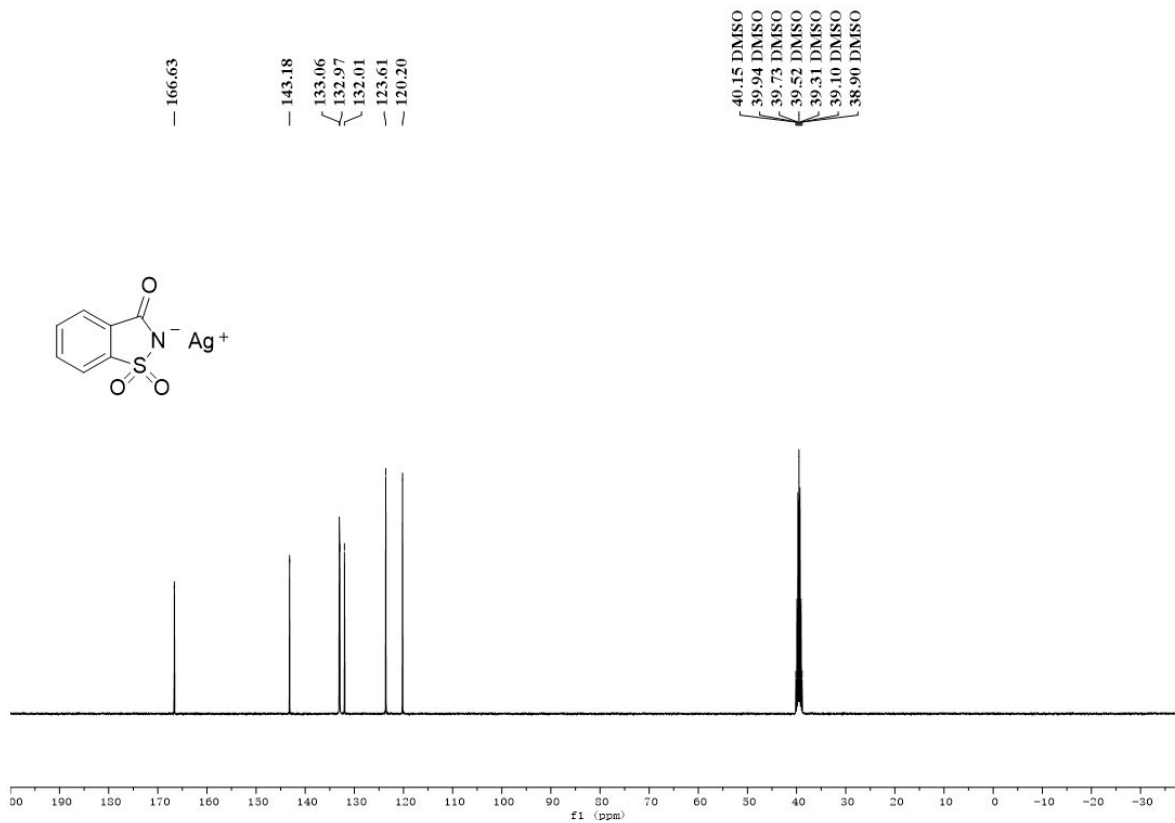
Benzyl(trifluoromethyl)selane



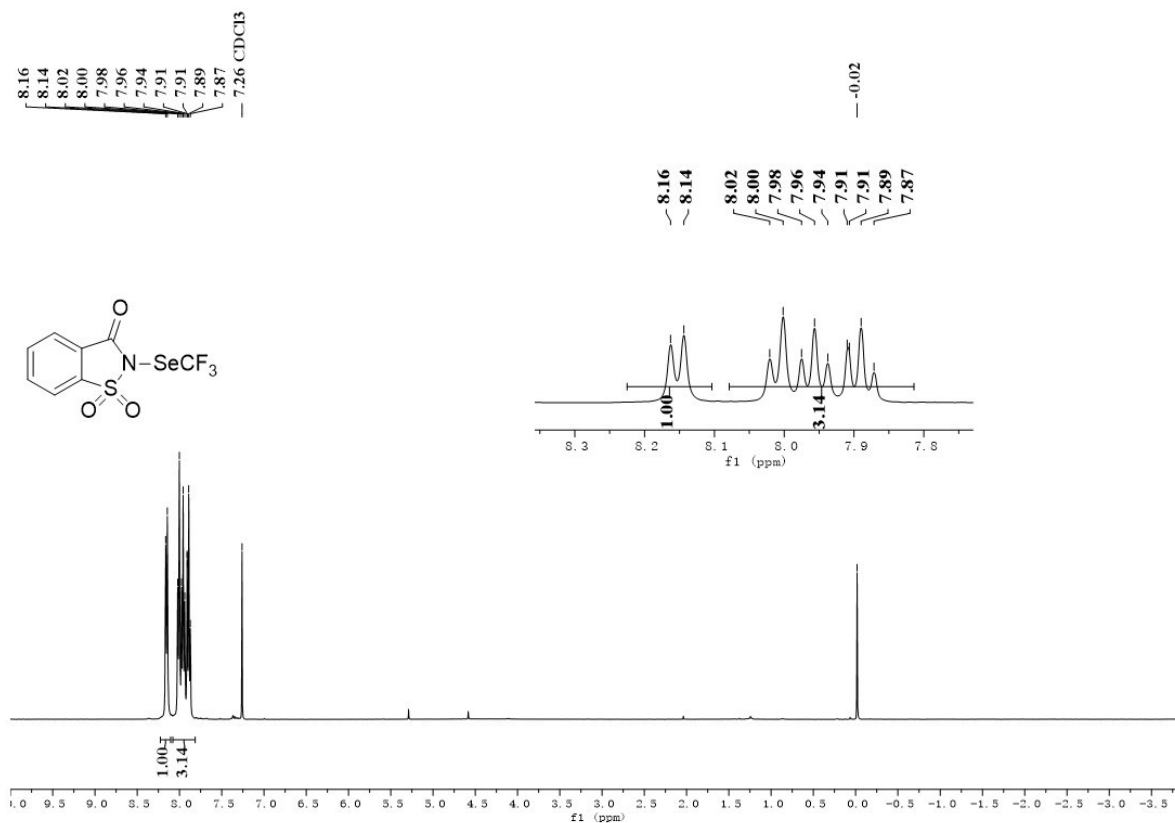


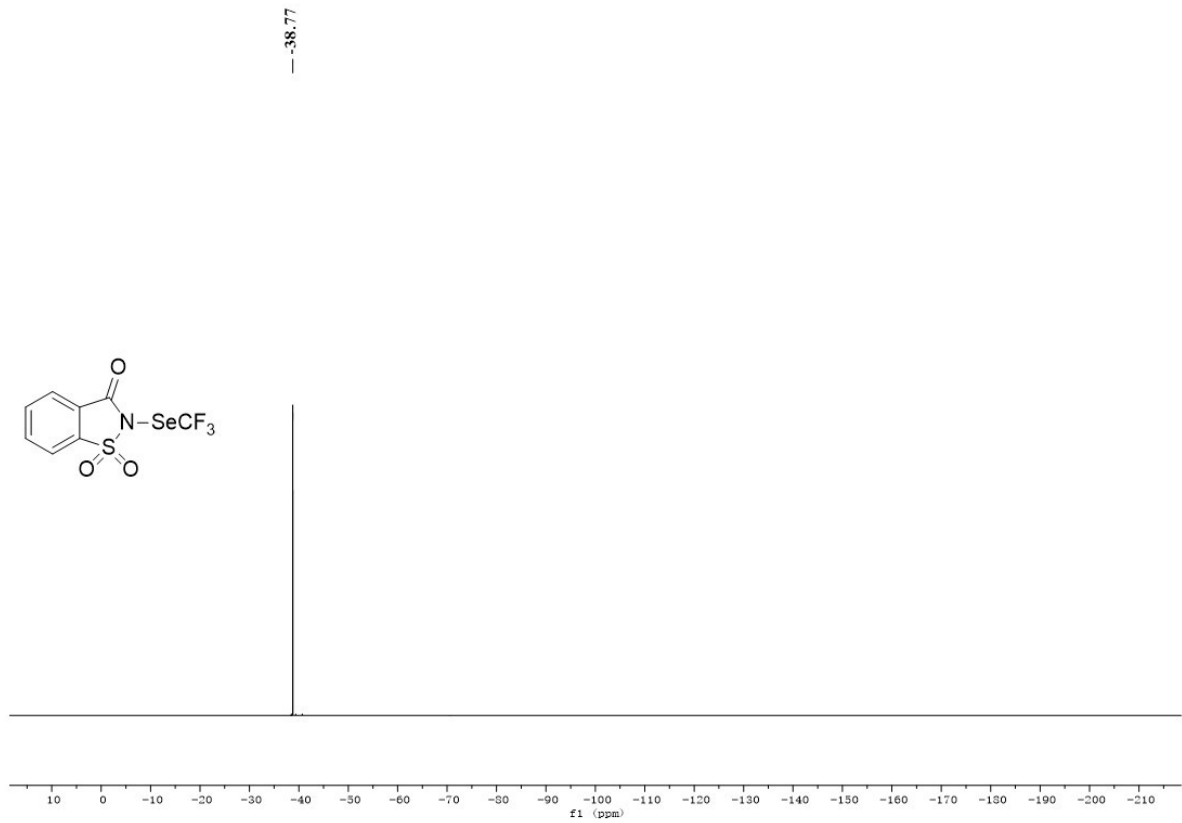
Saccharin silver





3 (N-trifluoromethylselenolating saccharin)



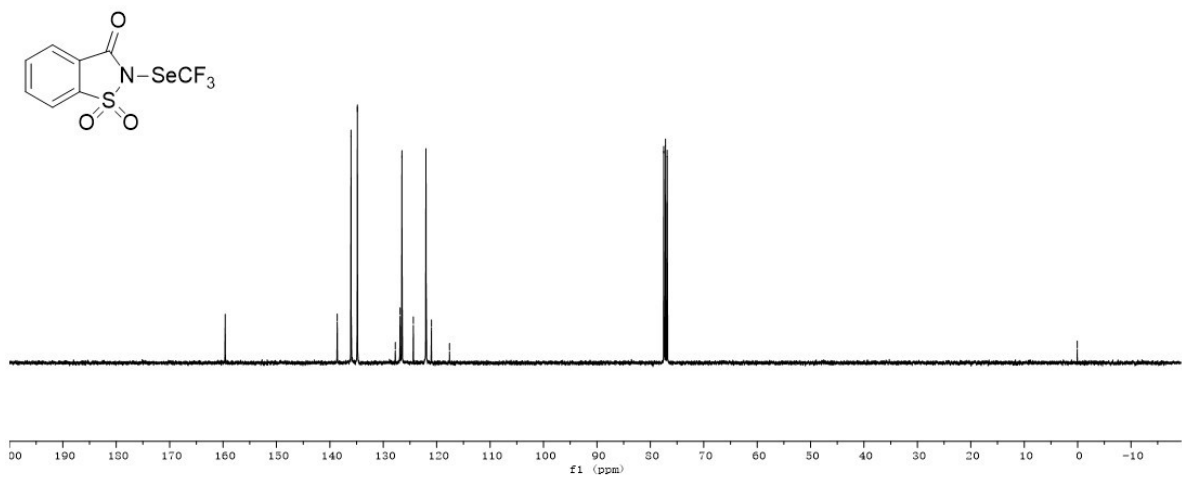


— 159.60

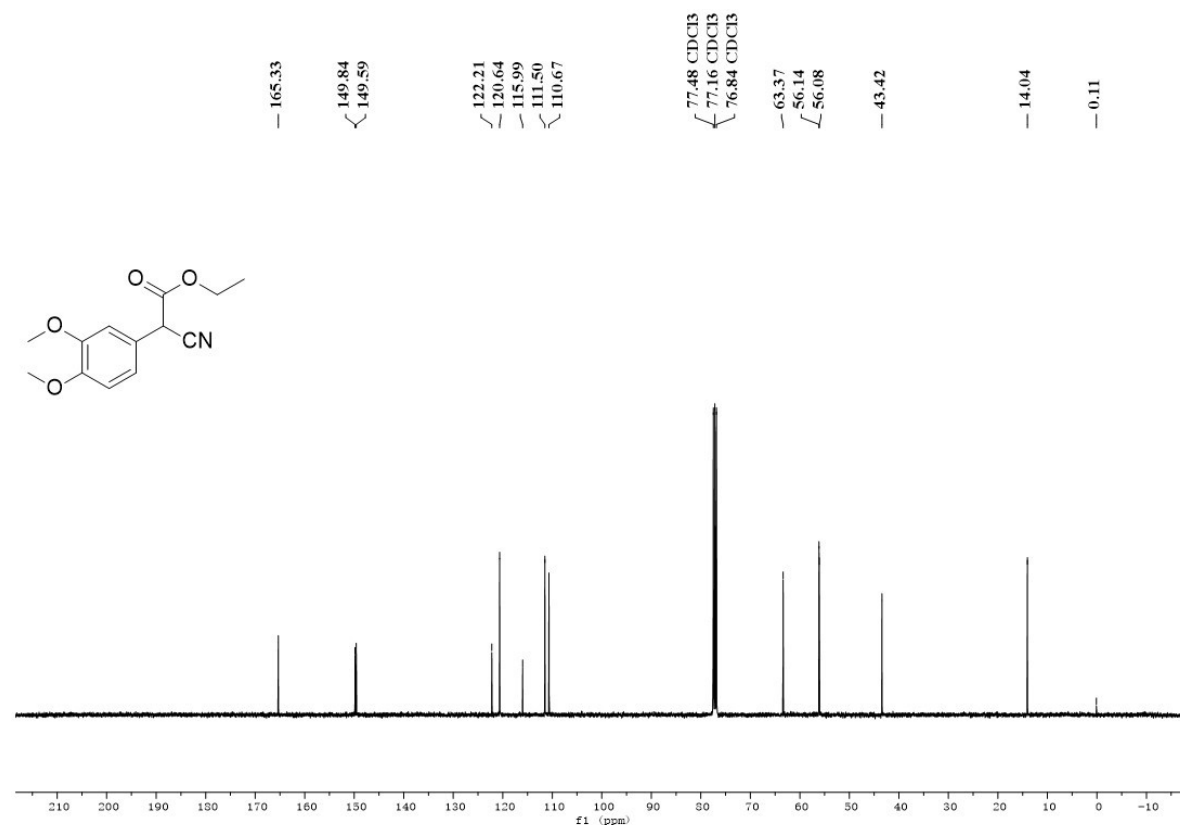
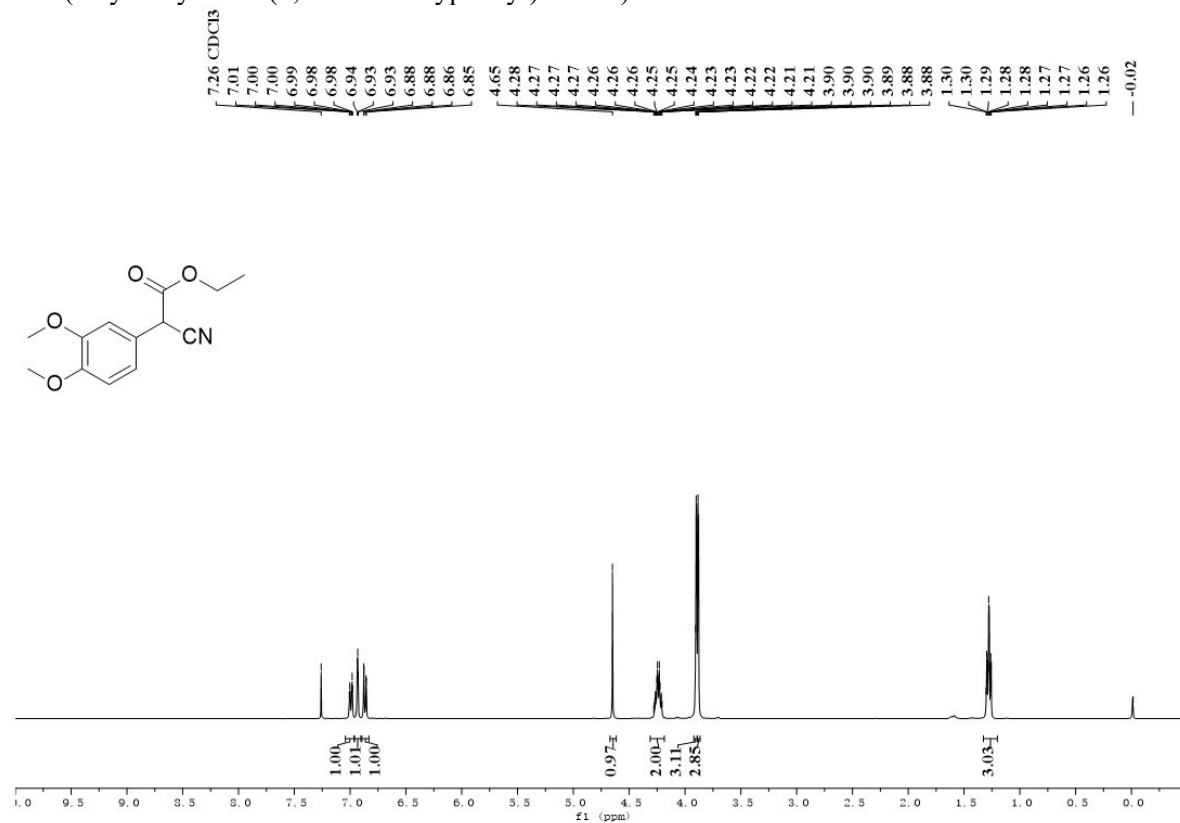
138.62
136.03
134.85
127.75
126.87
126.50
124.37
122.00
120.98
117.60

77.48 CDCl3
77.16 CDCl3
76.84 CDCl3

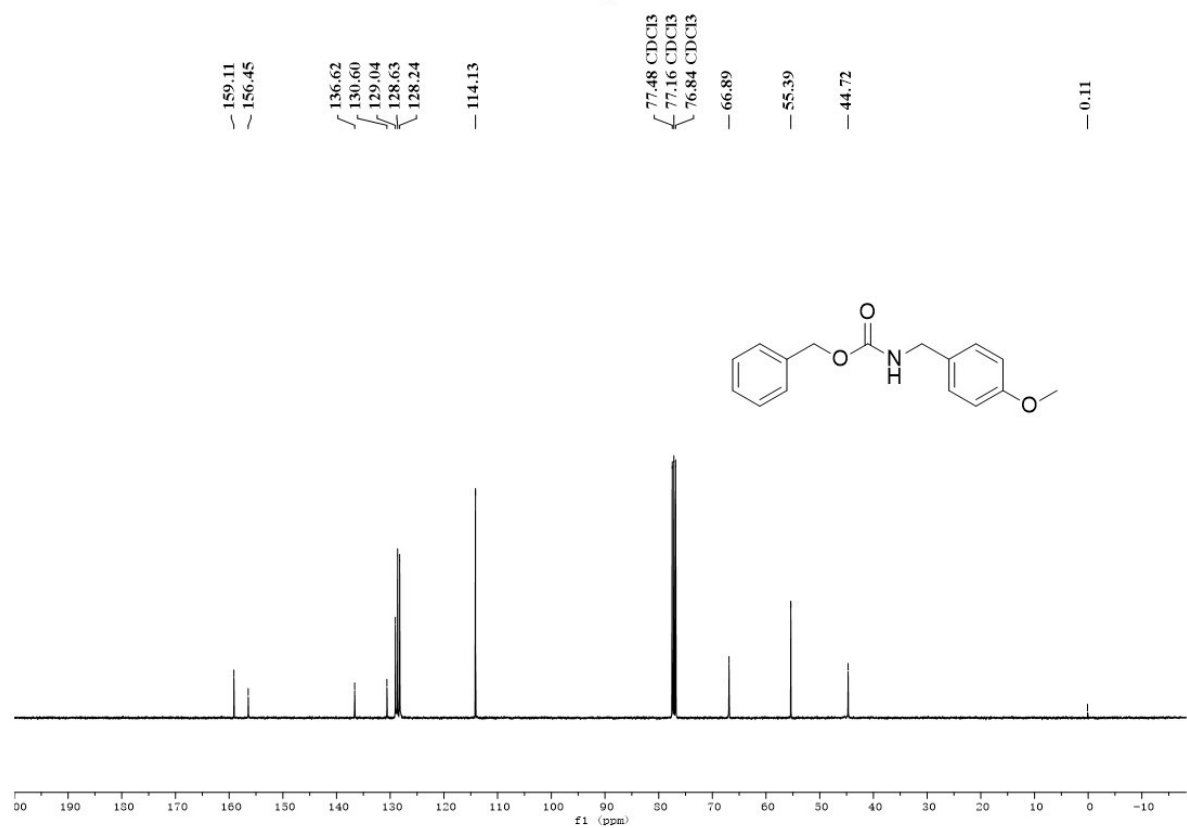
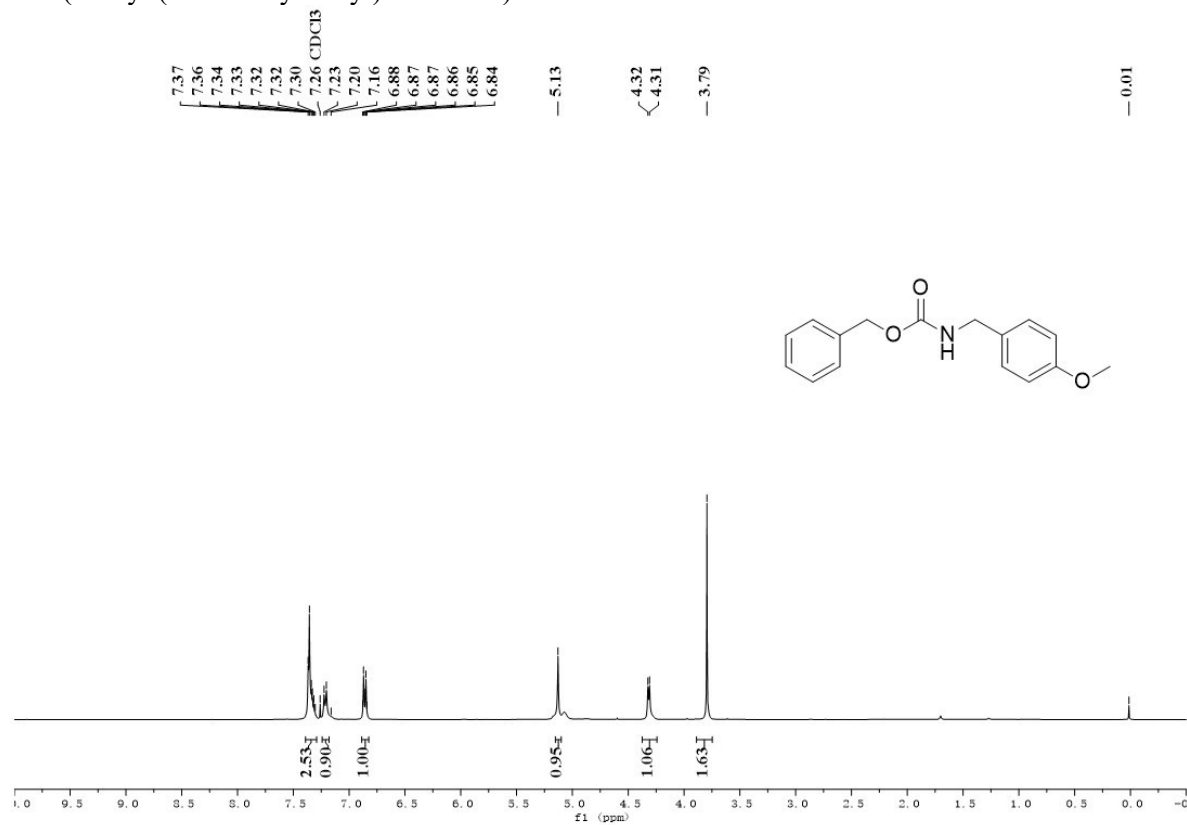
— 0.07



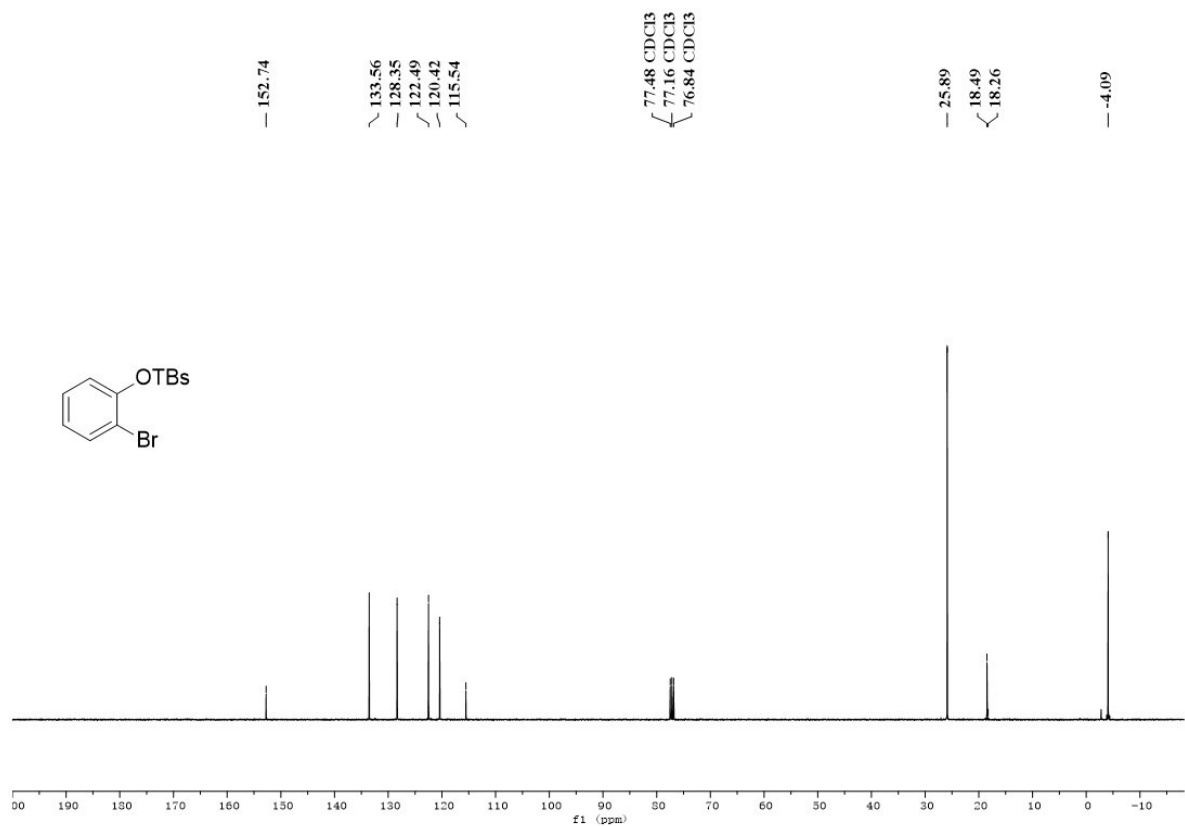
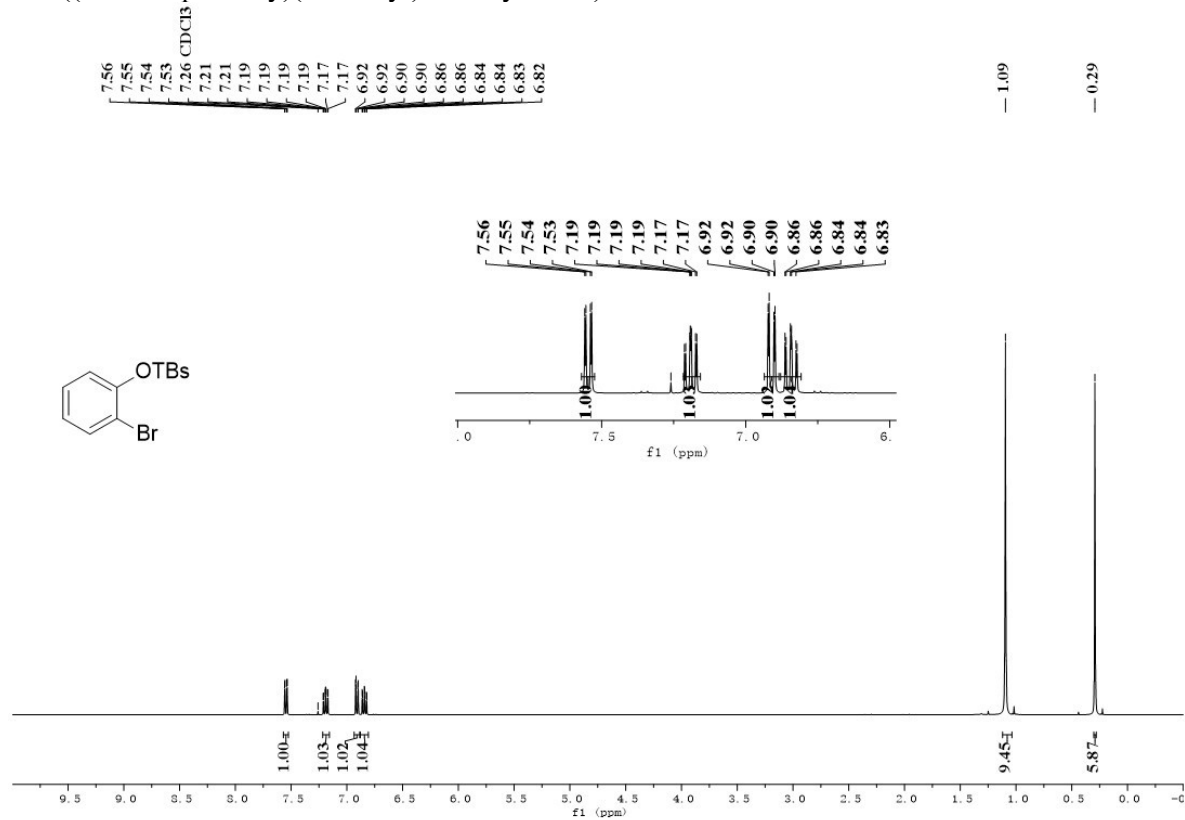
4ah (ethyl 2-cyano-2-(3,4-dimethoxyphenyl)acetate)



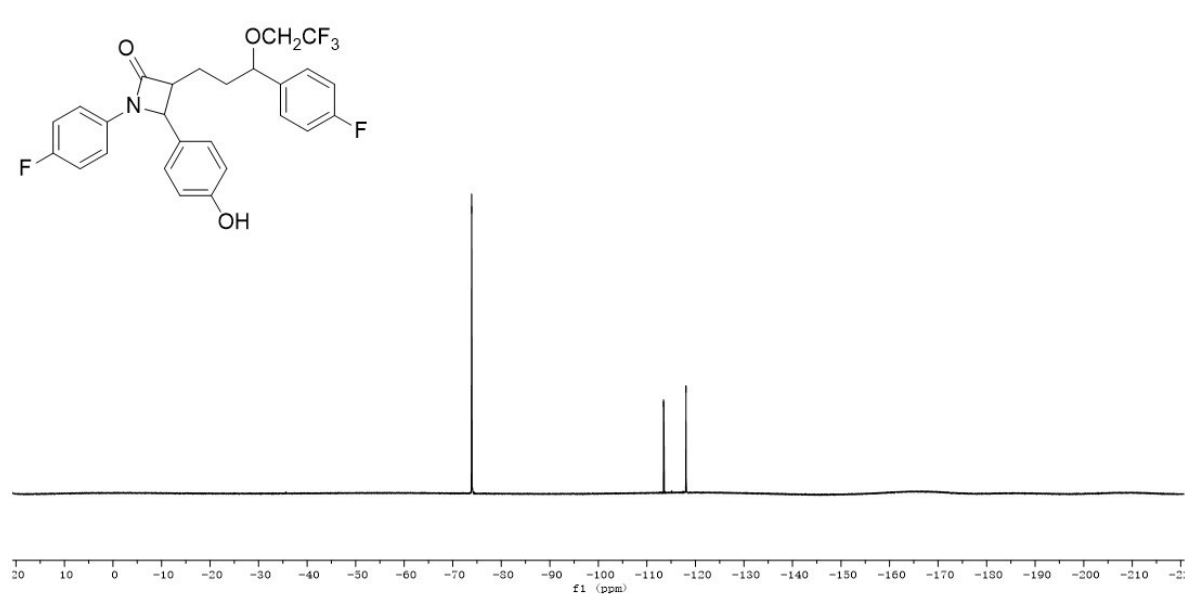
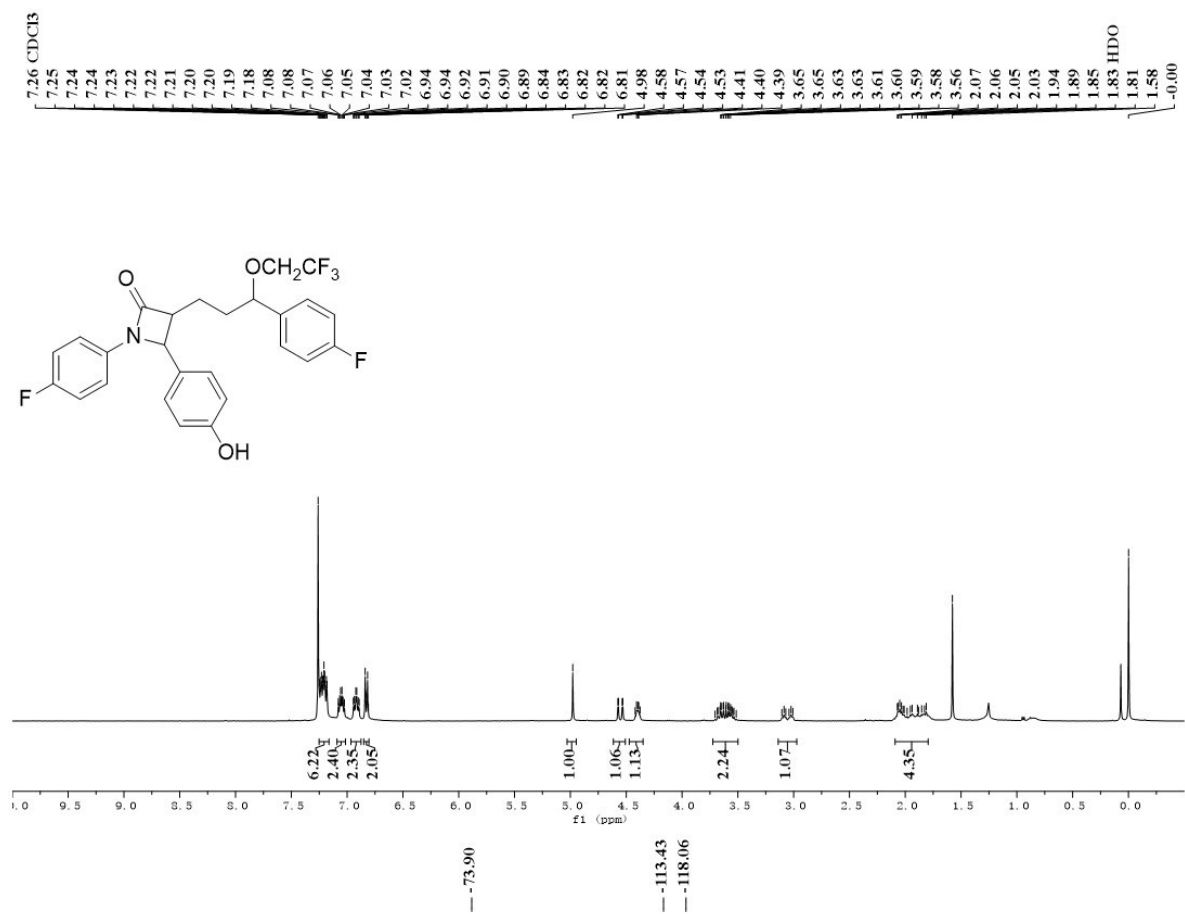
4ai (benzyl (4-methoxybenzyl)carbamate)

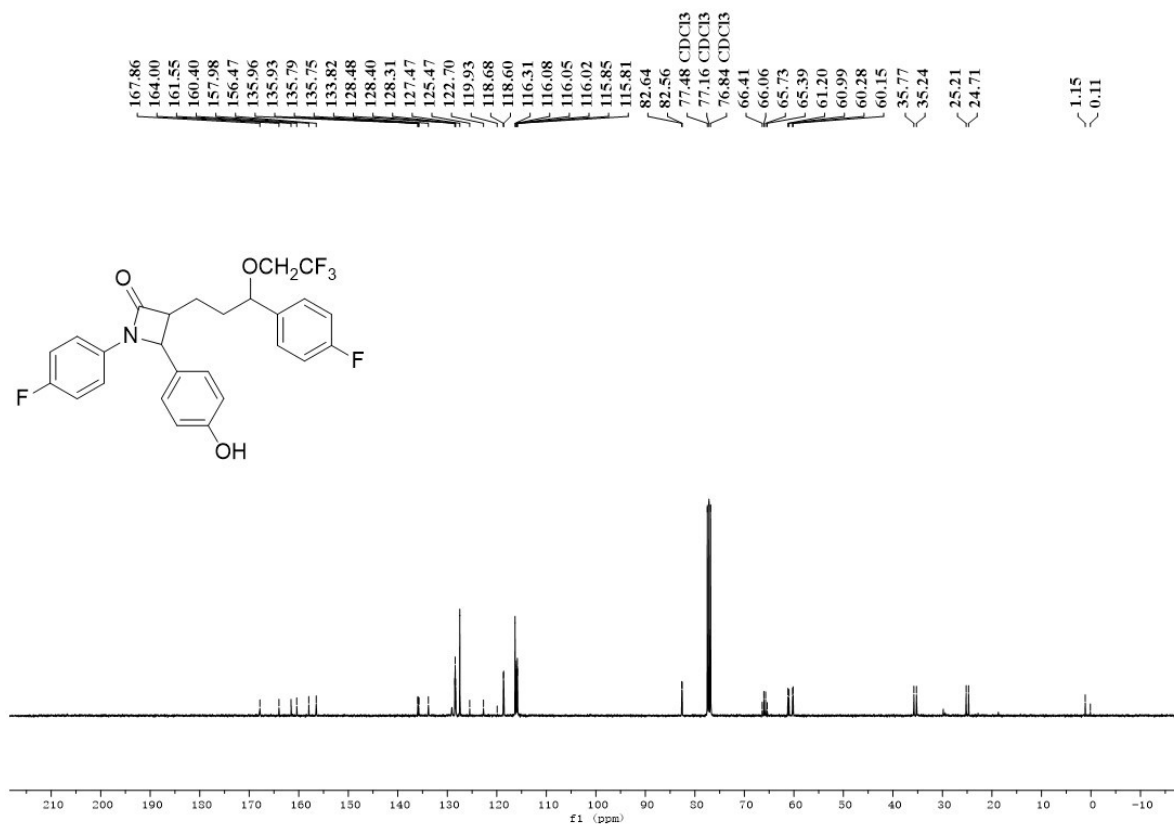


4ak ((2-bromophenoxy)(tert-butyl)dimethylsilane)

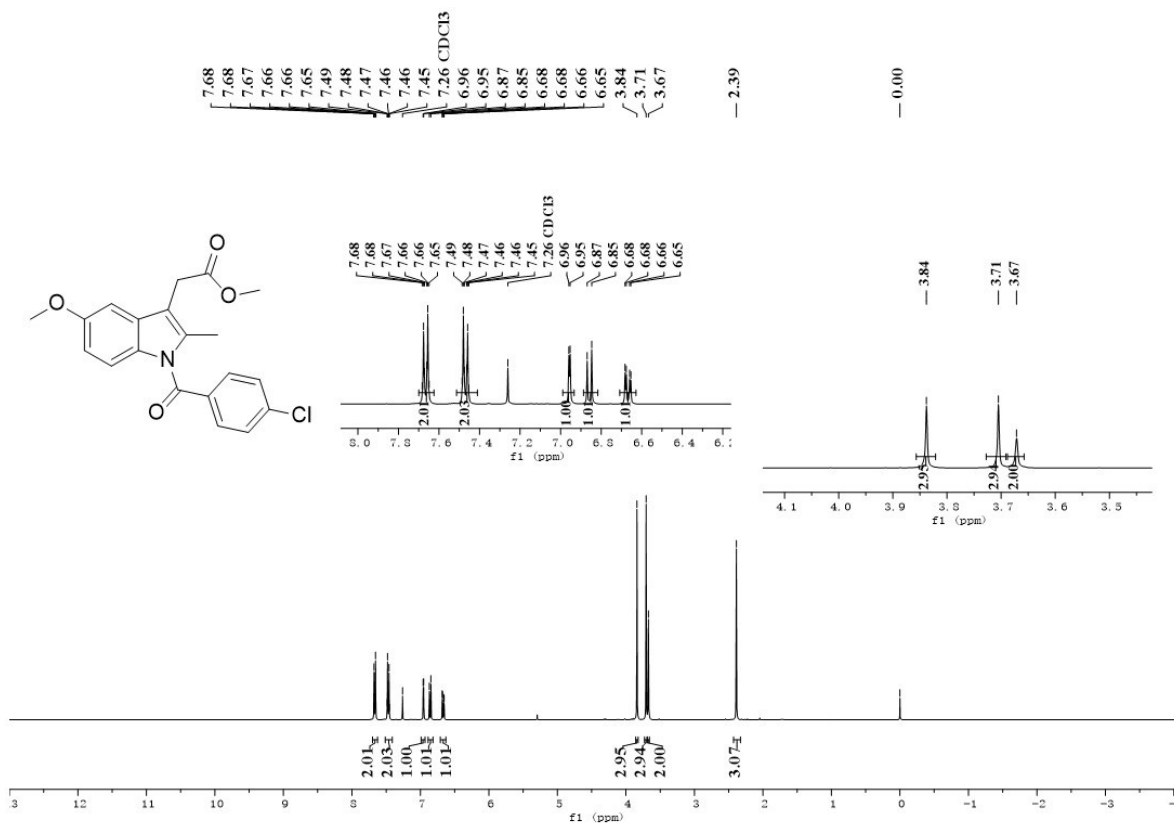


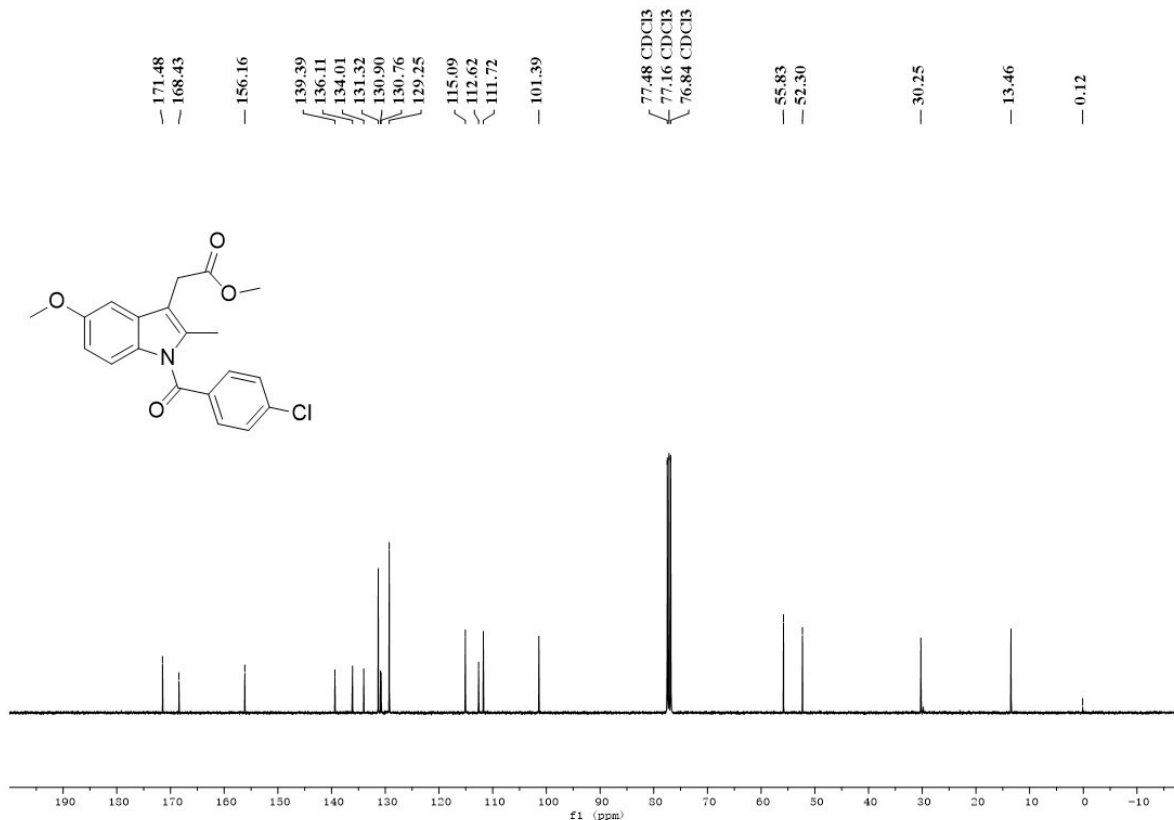
4cc (1-(4-fluorophenyl)-3-(3-(4-fluorophenyl)-3-(2,2,2-trifluoroethoxy)propyl)-4-(4-hydroxyphenyl)azetidin-2-one)



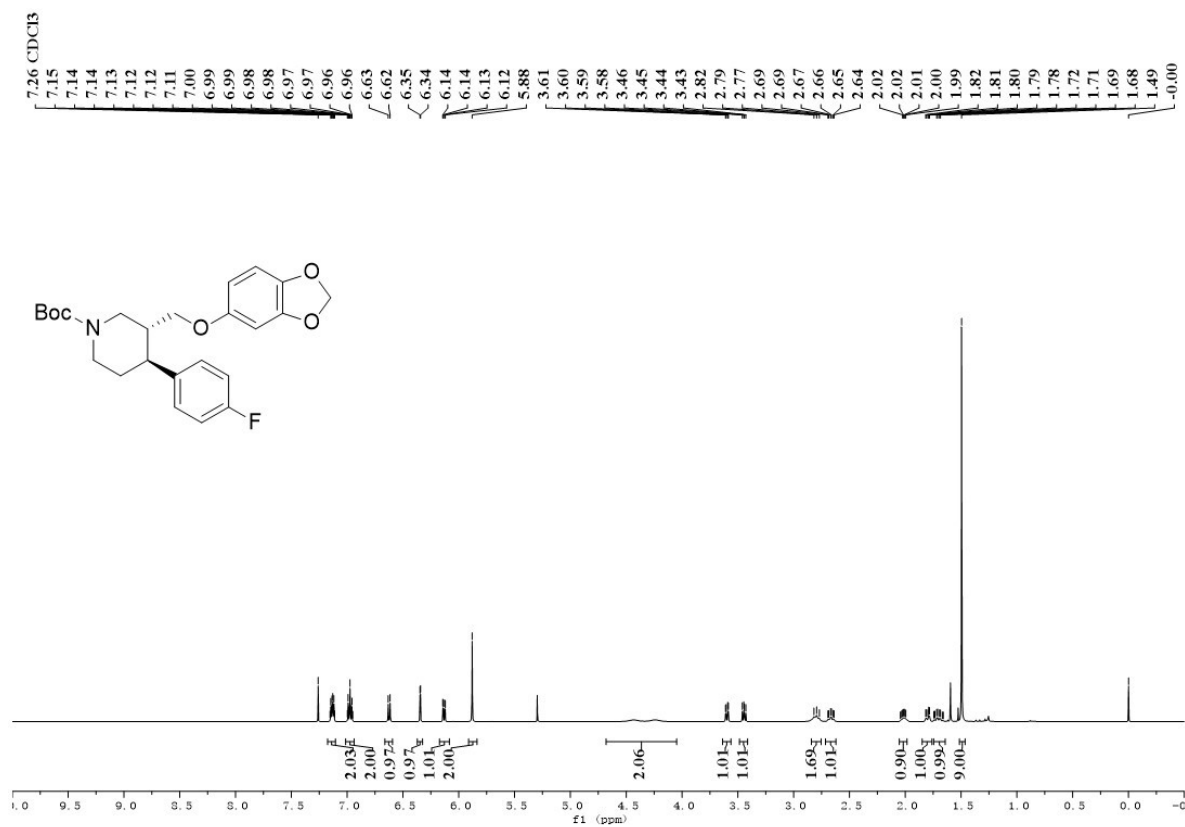


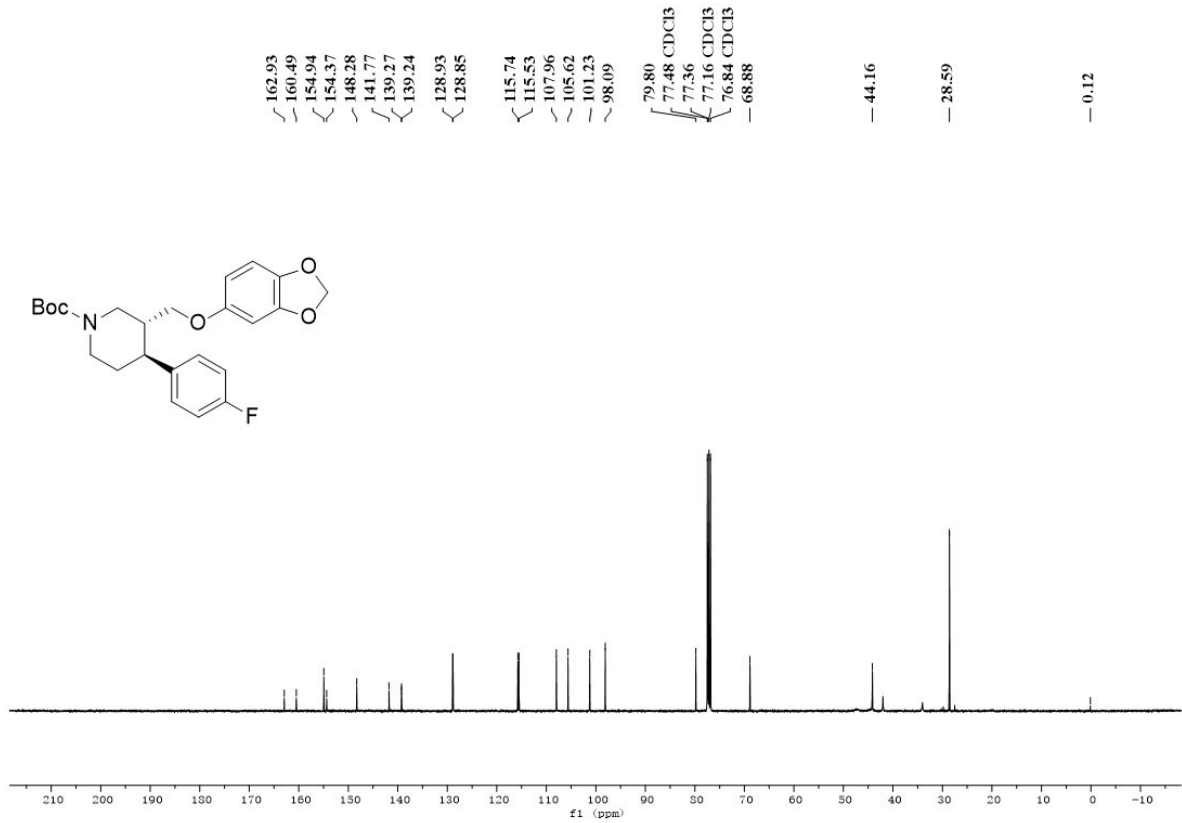
4c (methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate)



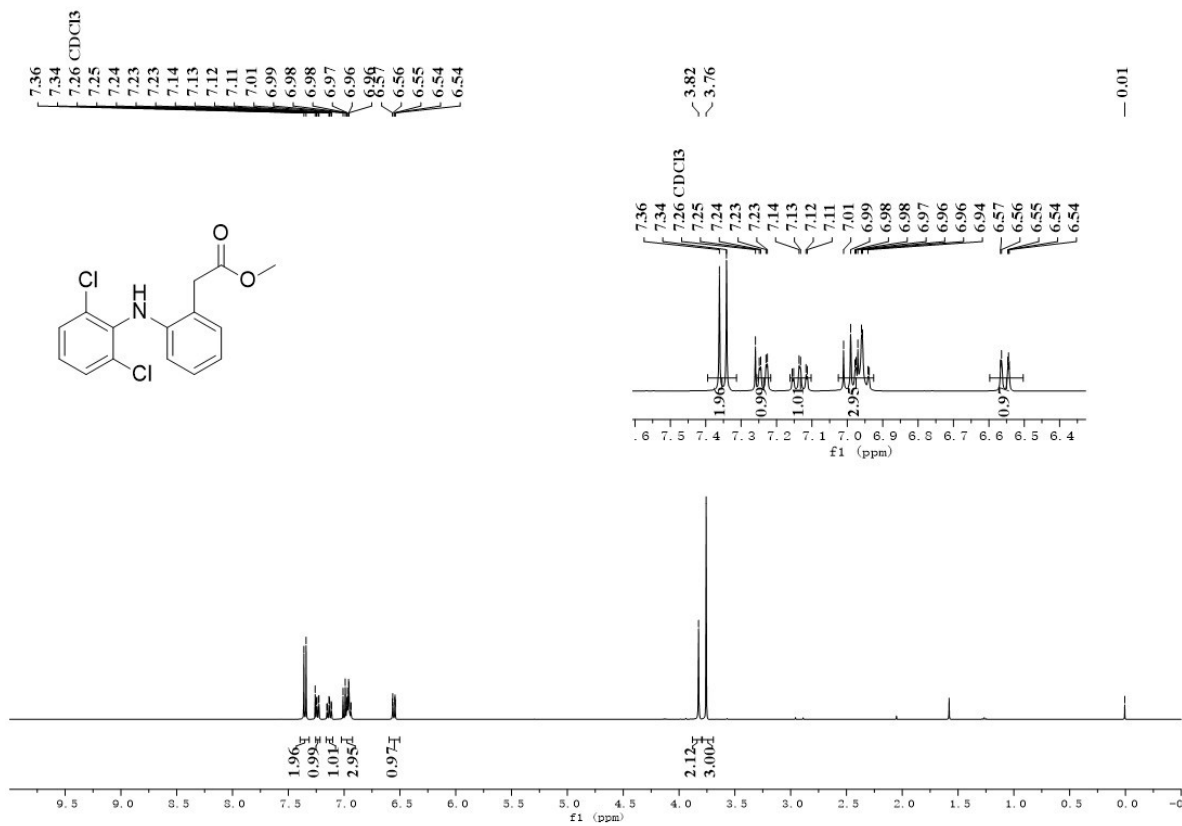


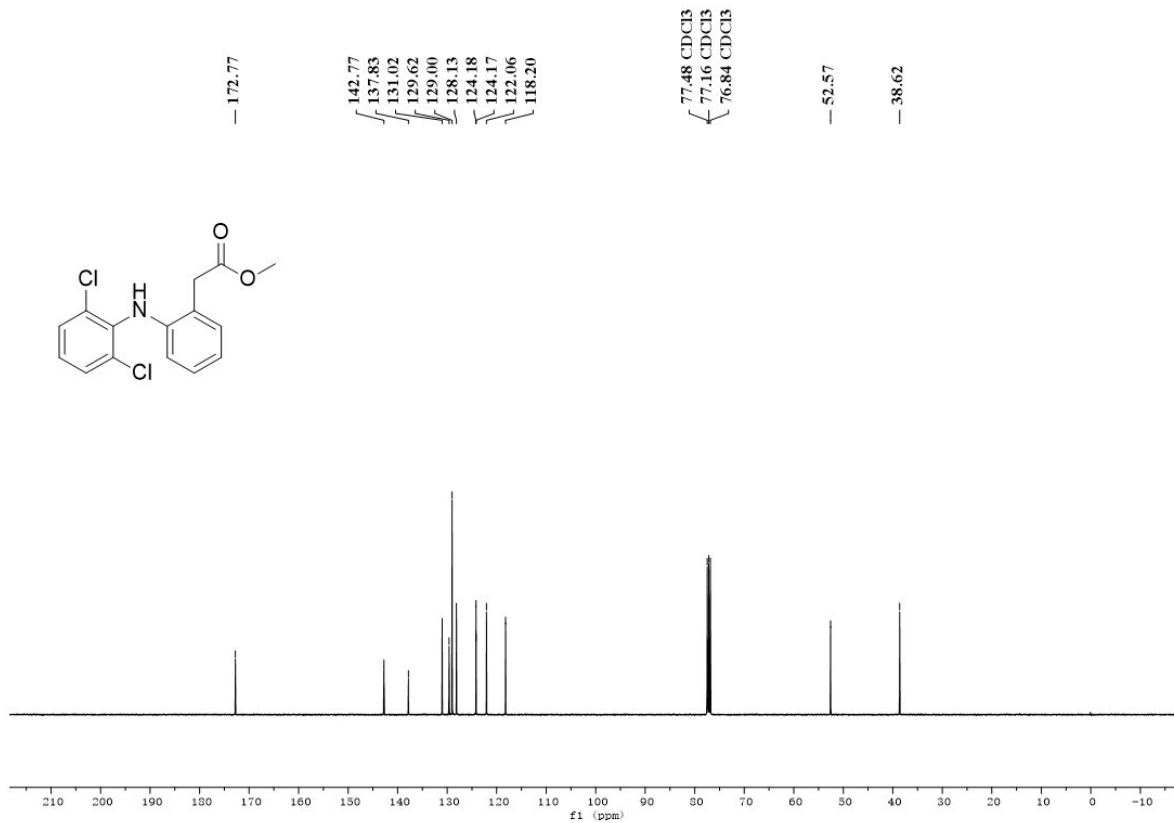
4cj (tert-butyl (3R,4S)-3-((benzo[d][1,3]dioxol-5-yloxy)methyl)-4-(4-fluorophenyl)piperidine-1-carboxylate)



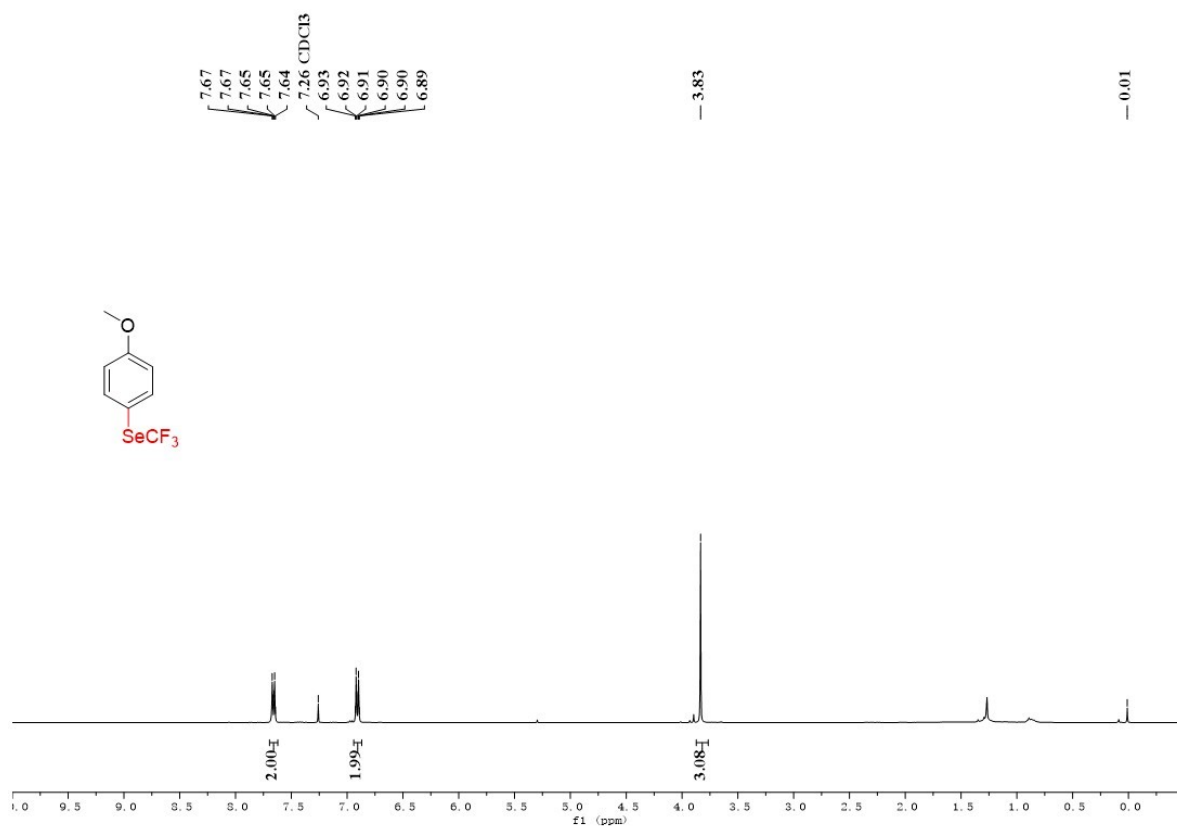


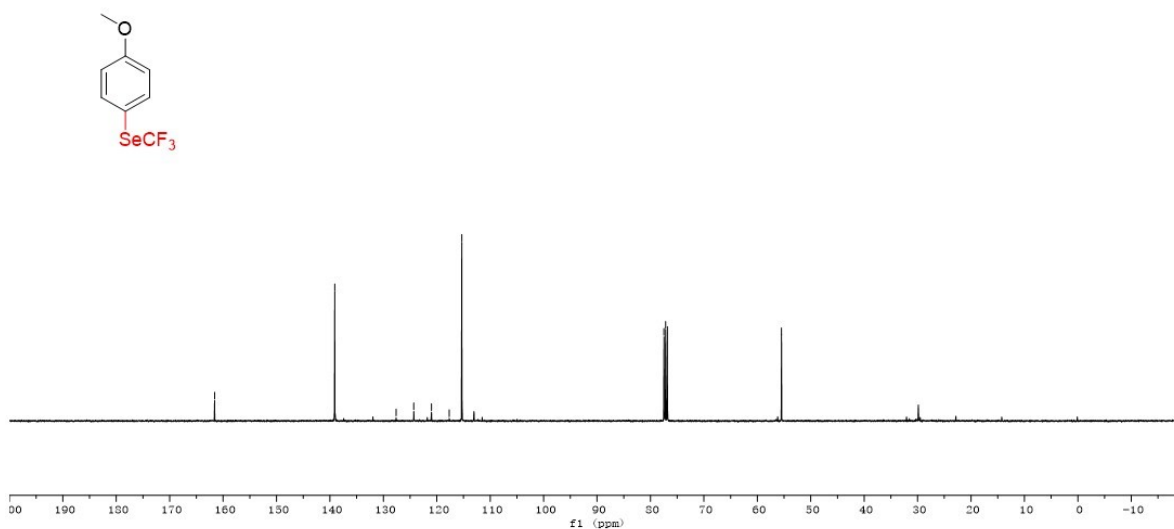
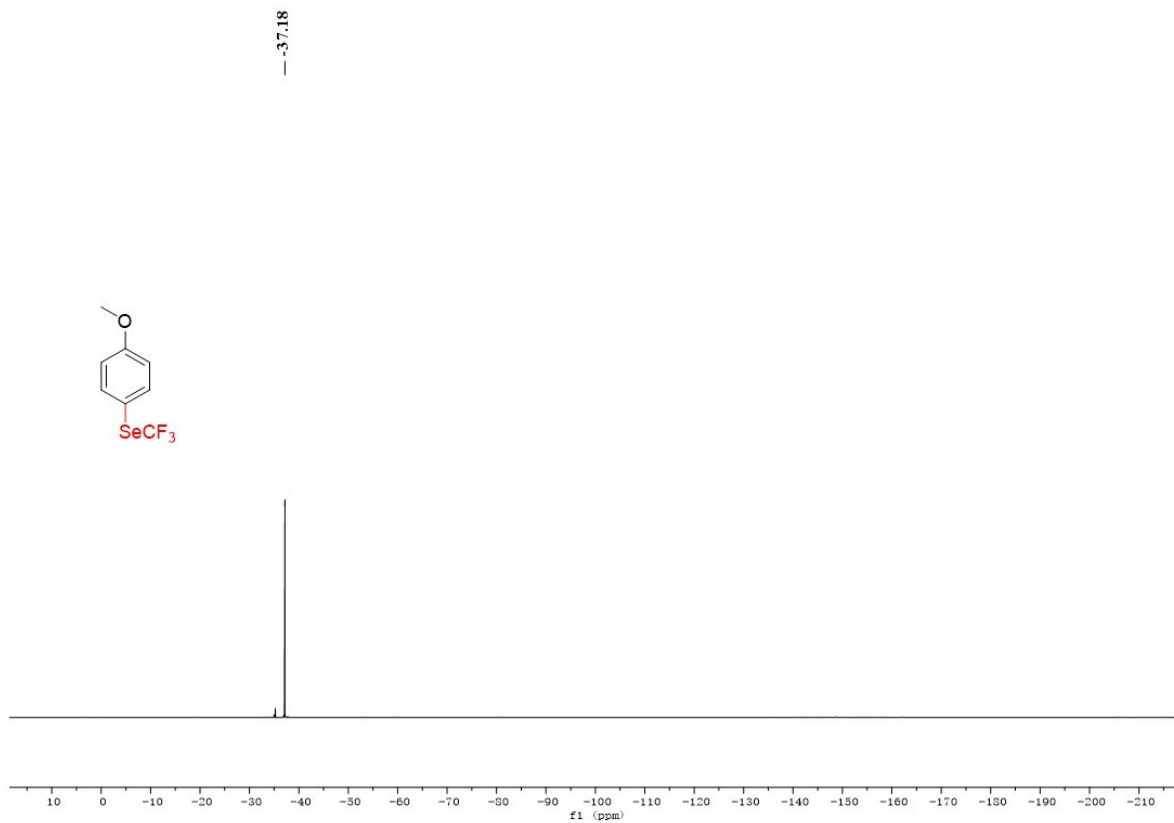
4ck (methyl 2-((2,6-dichlorophenyl)amino)phenyl)acetate)



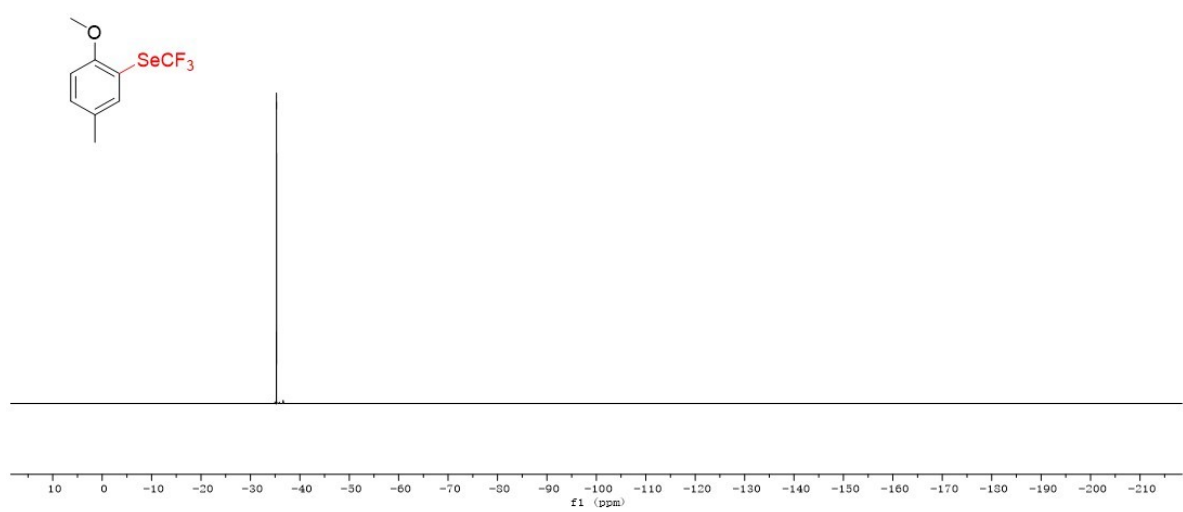
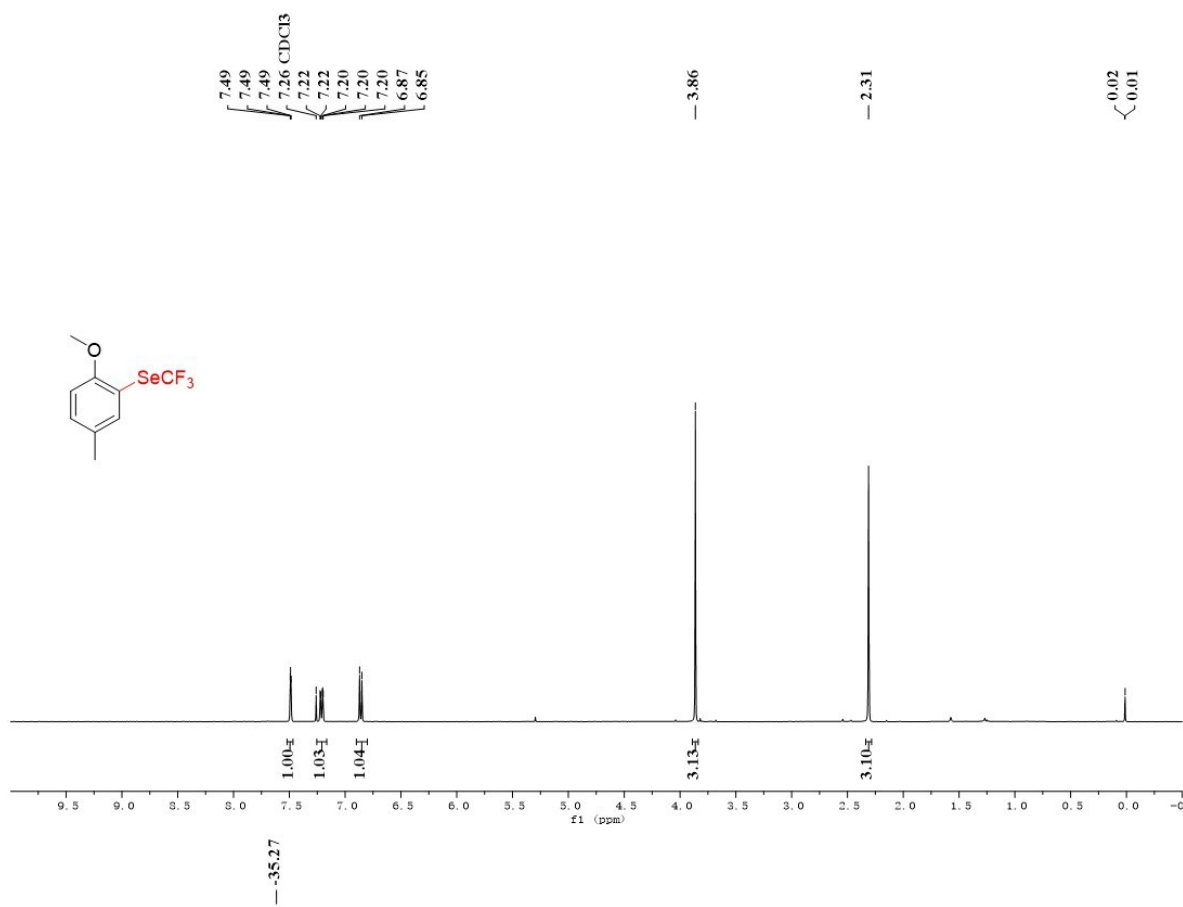


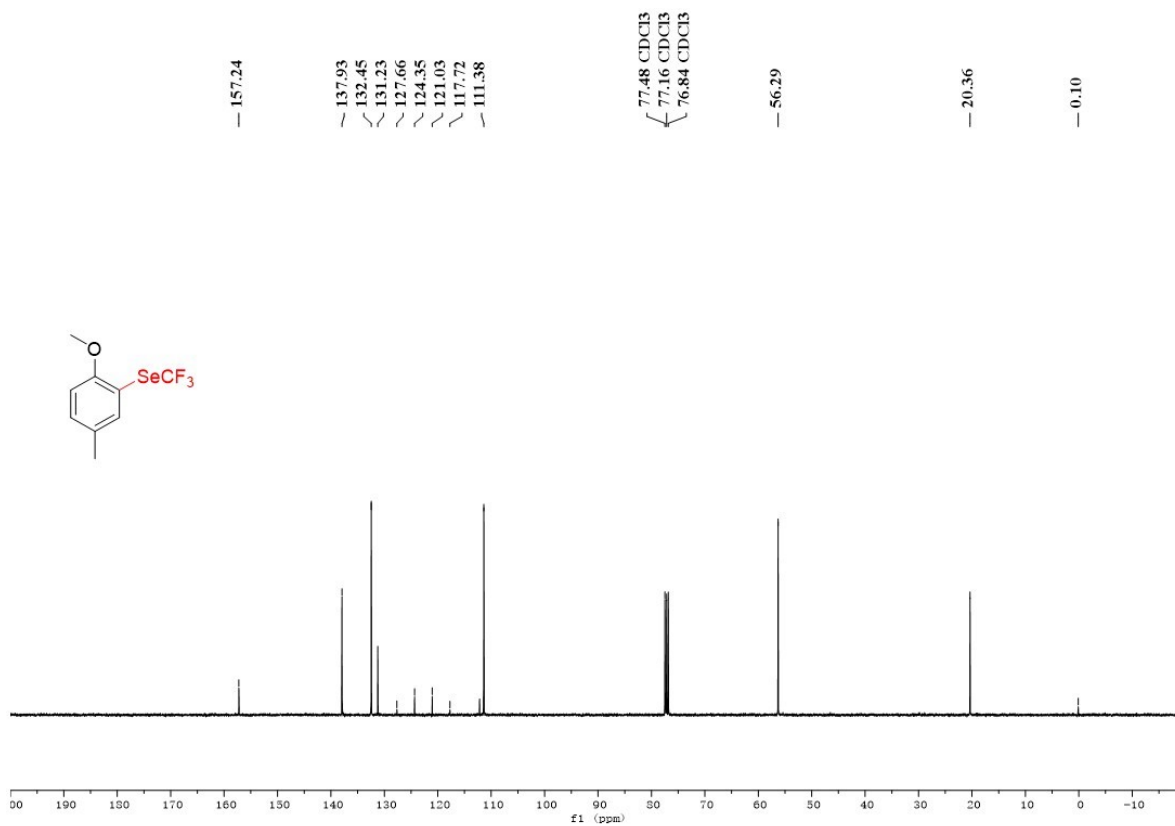
5aa ((4-methoxyphenyl)(trifluoromethyl)selane)



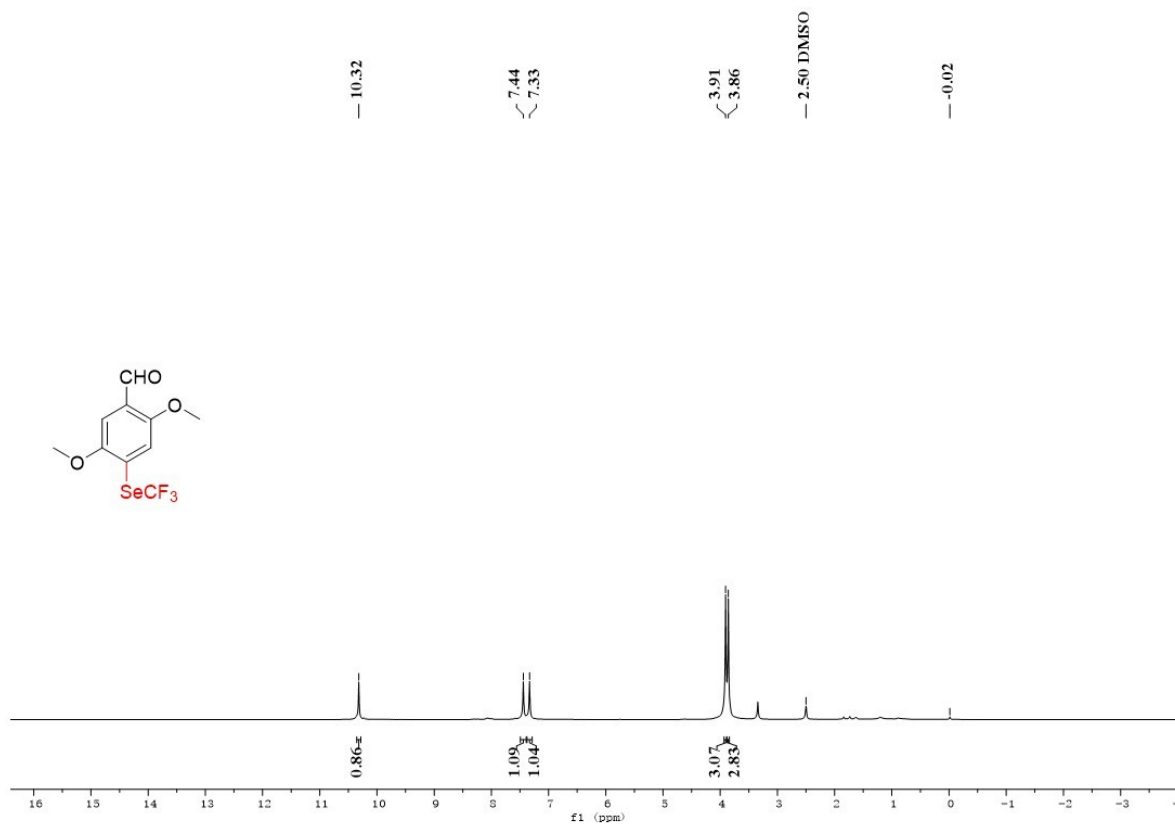


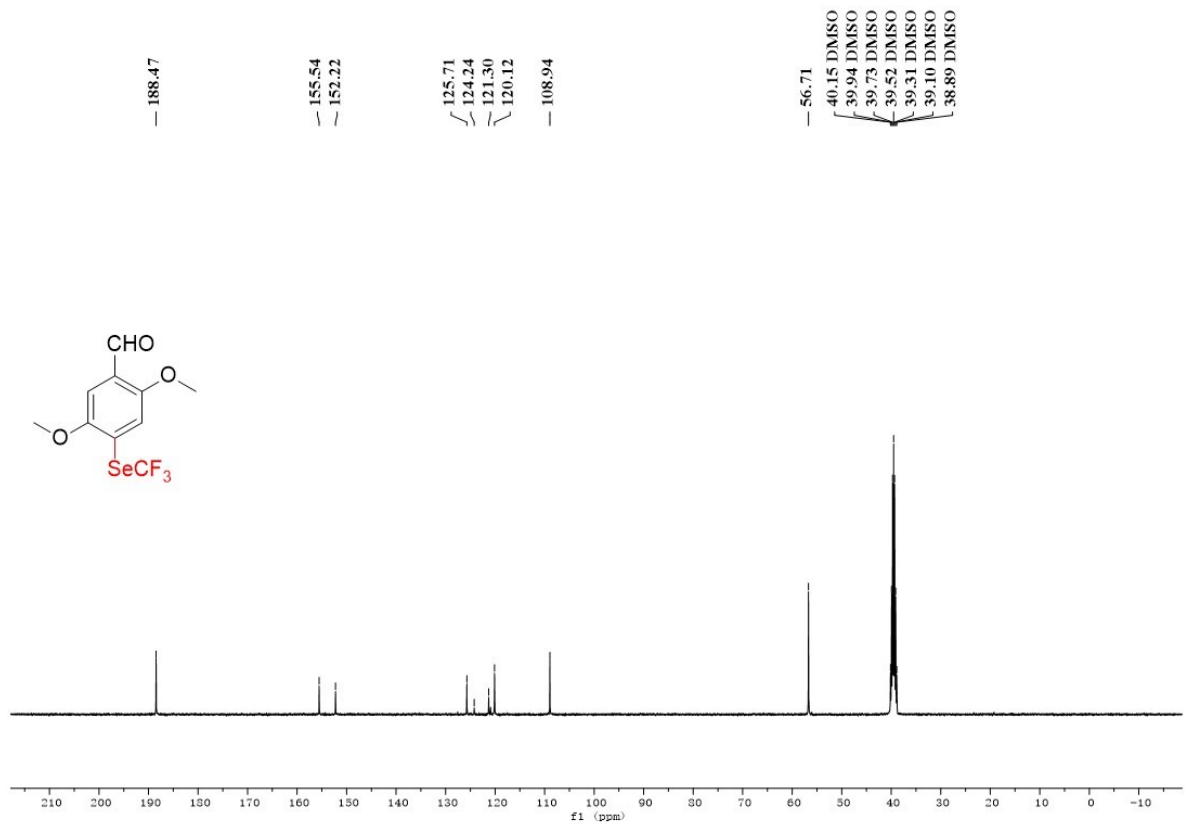
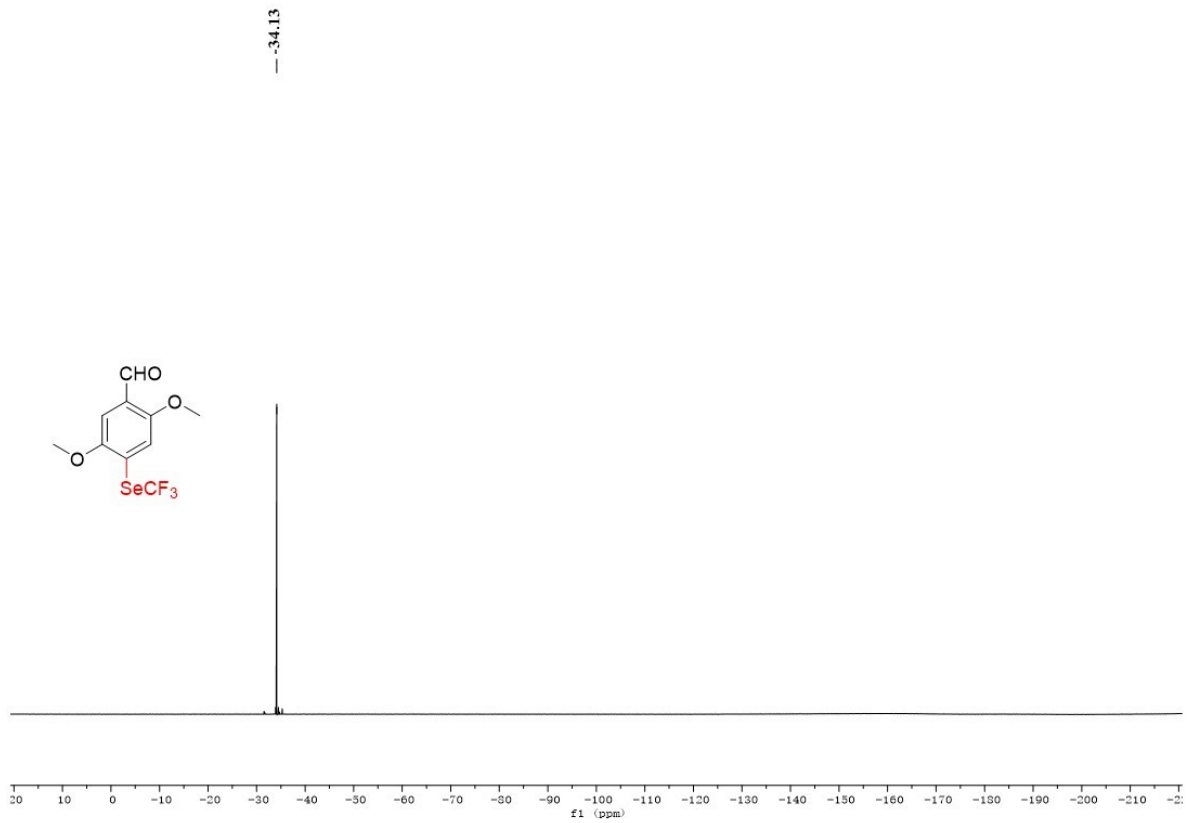
5ab ((2-methoxy-5-methylphenyl)(trifluoromethyl)selane)





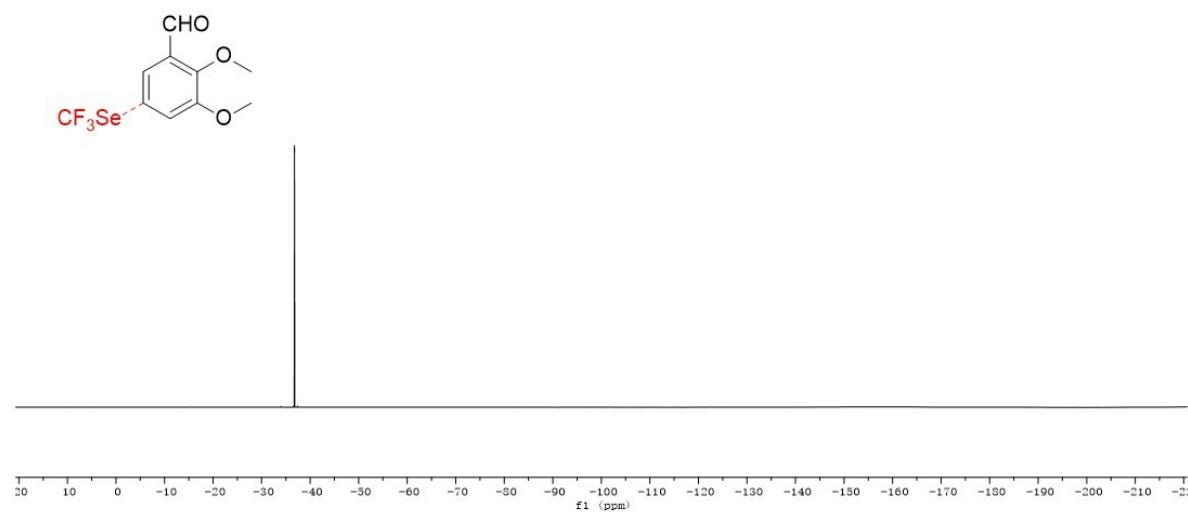
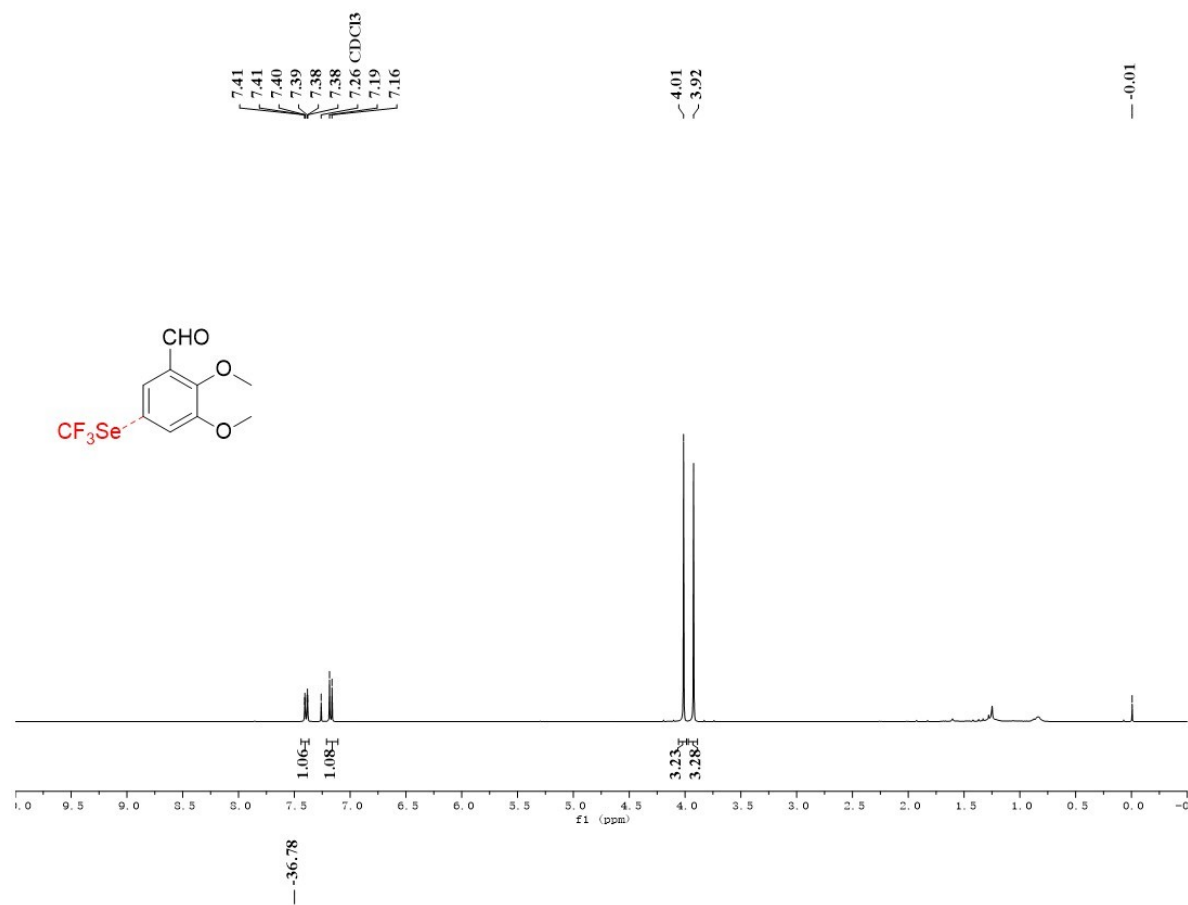
5ac (2,5-dimethoxy-4-((trifluoromethyl)selenyl)benzaldehyde)

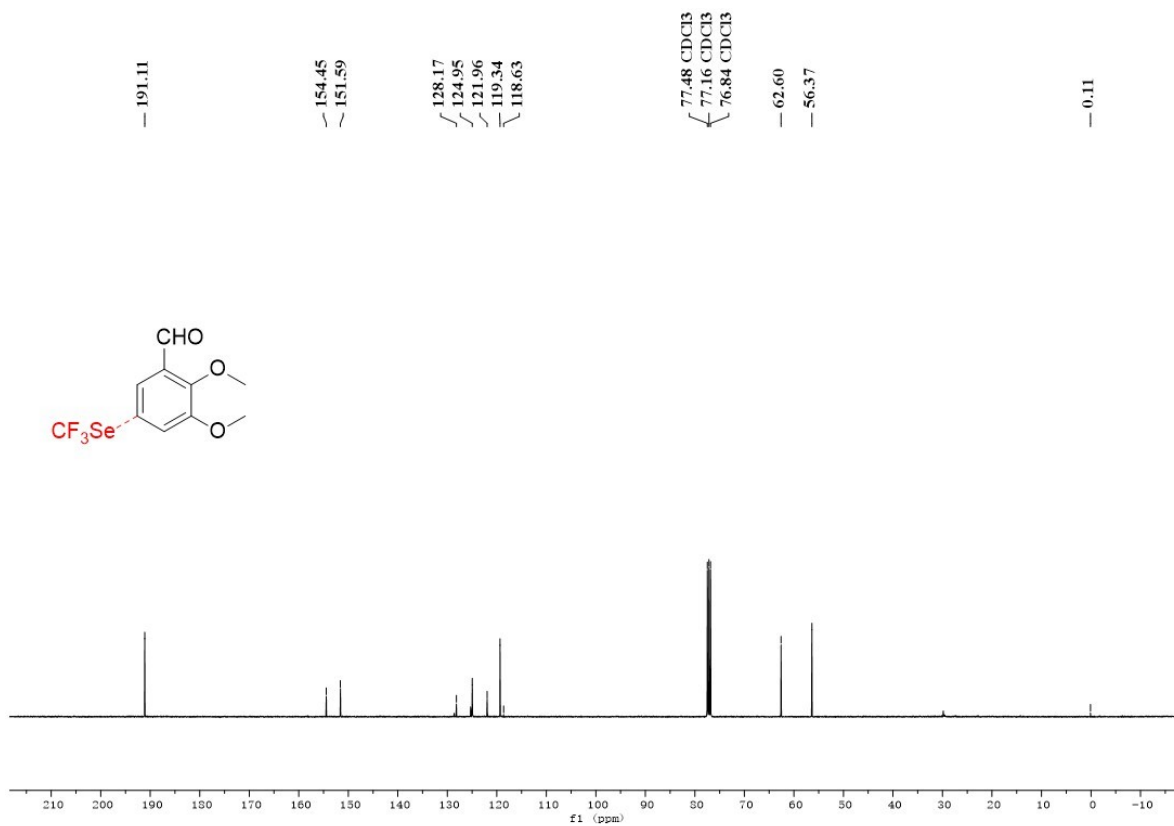




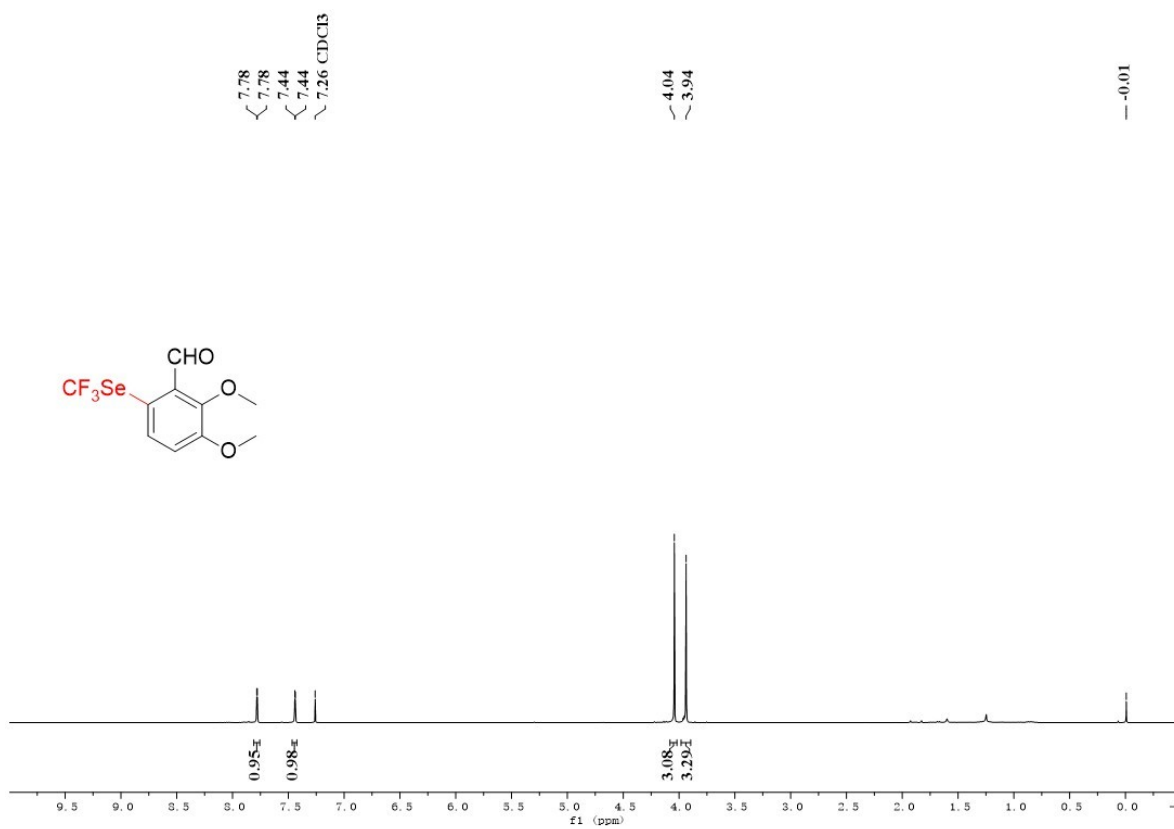
5ad, A:B = 5:4

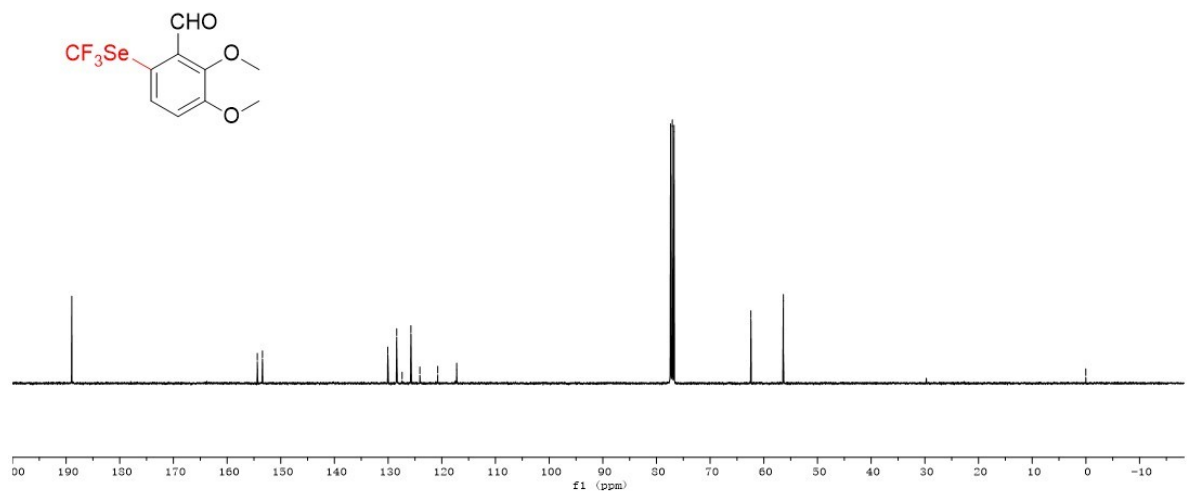
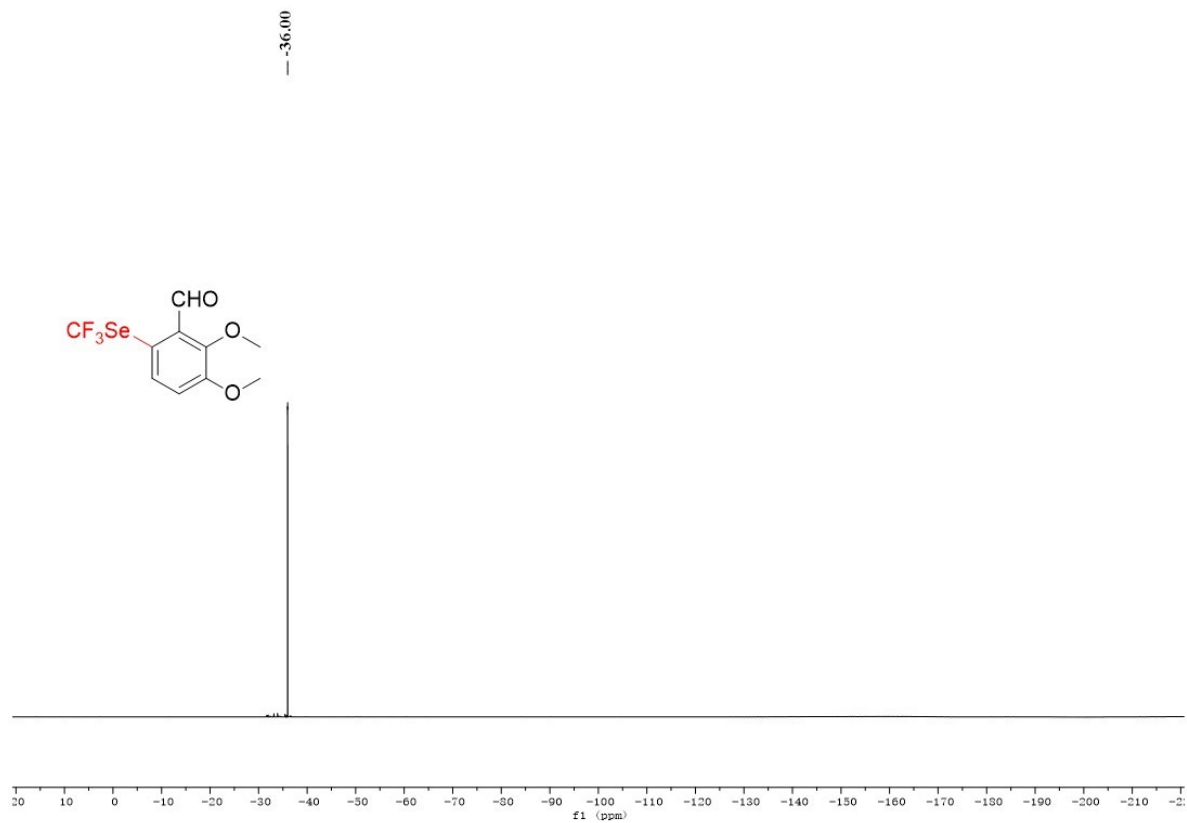
A (2,3-dimethoxy-5-((trifluoromethyl)selanyl)benzaldehyde)



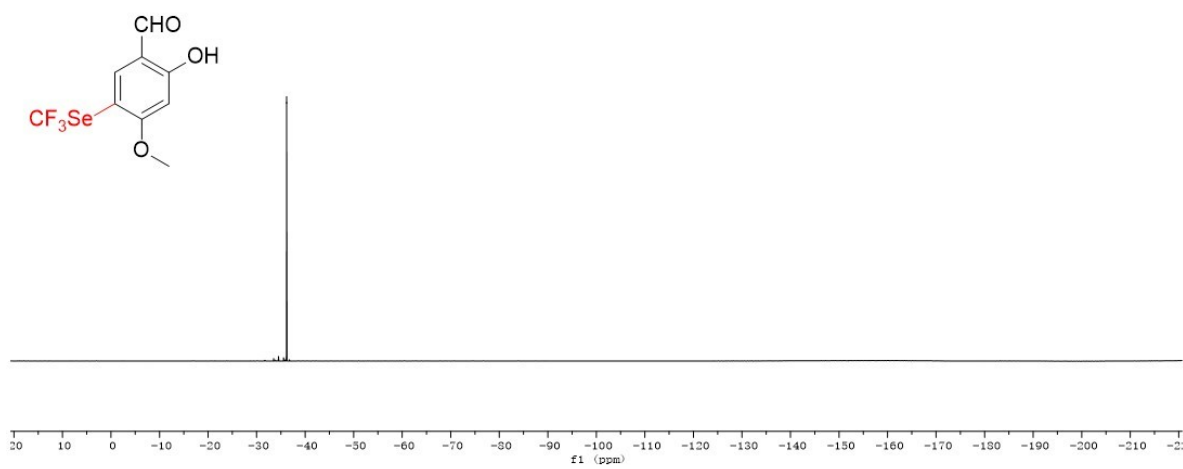
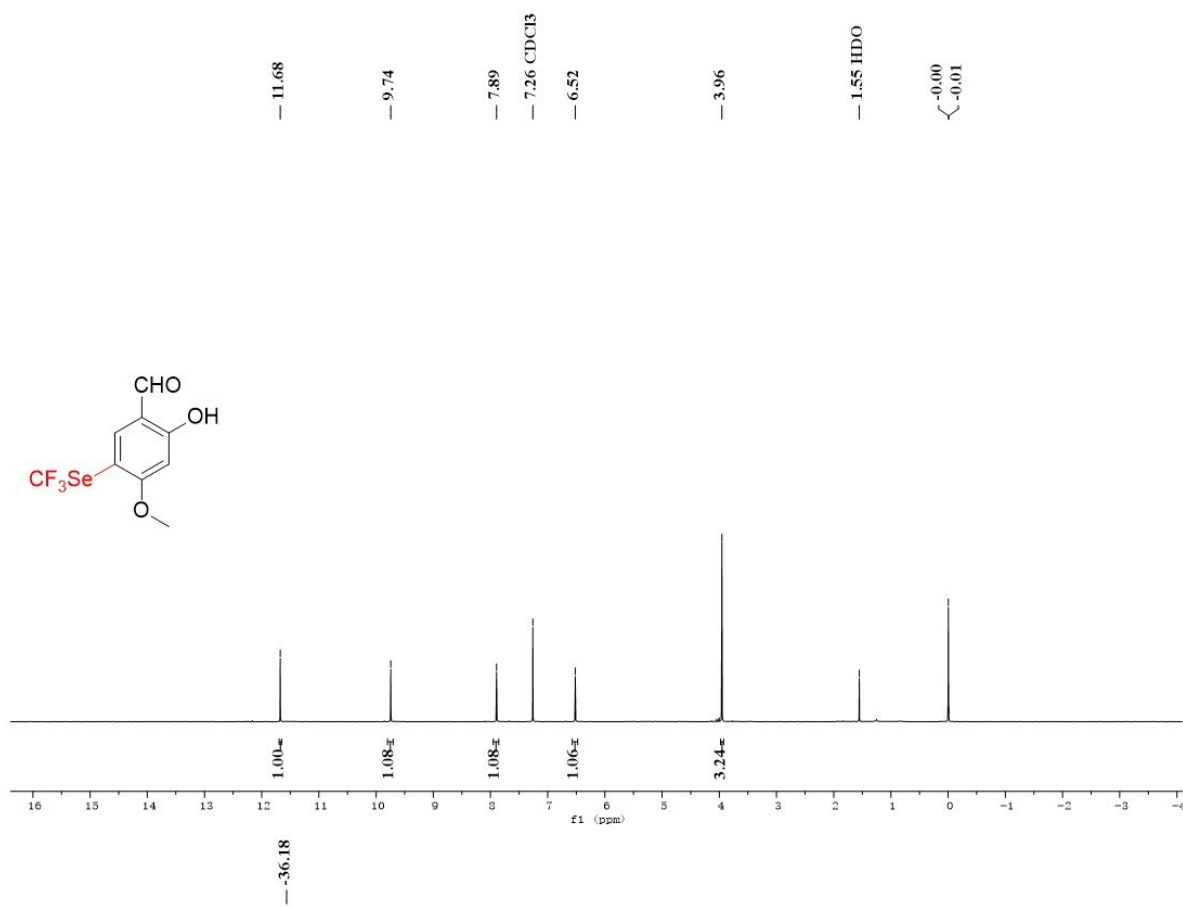


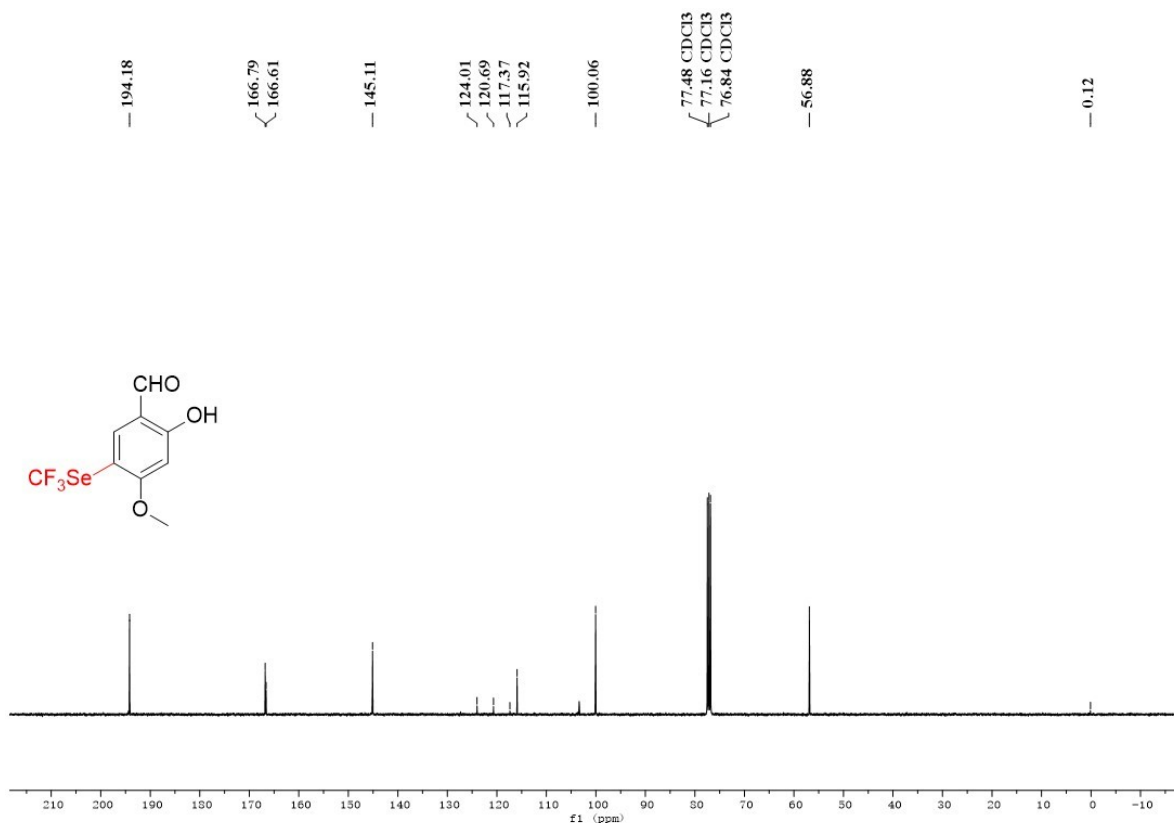
5ad B (2,3-dimethoxy-6-((trifluoromethyl)selenyl)benzaldehyde)



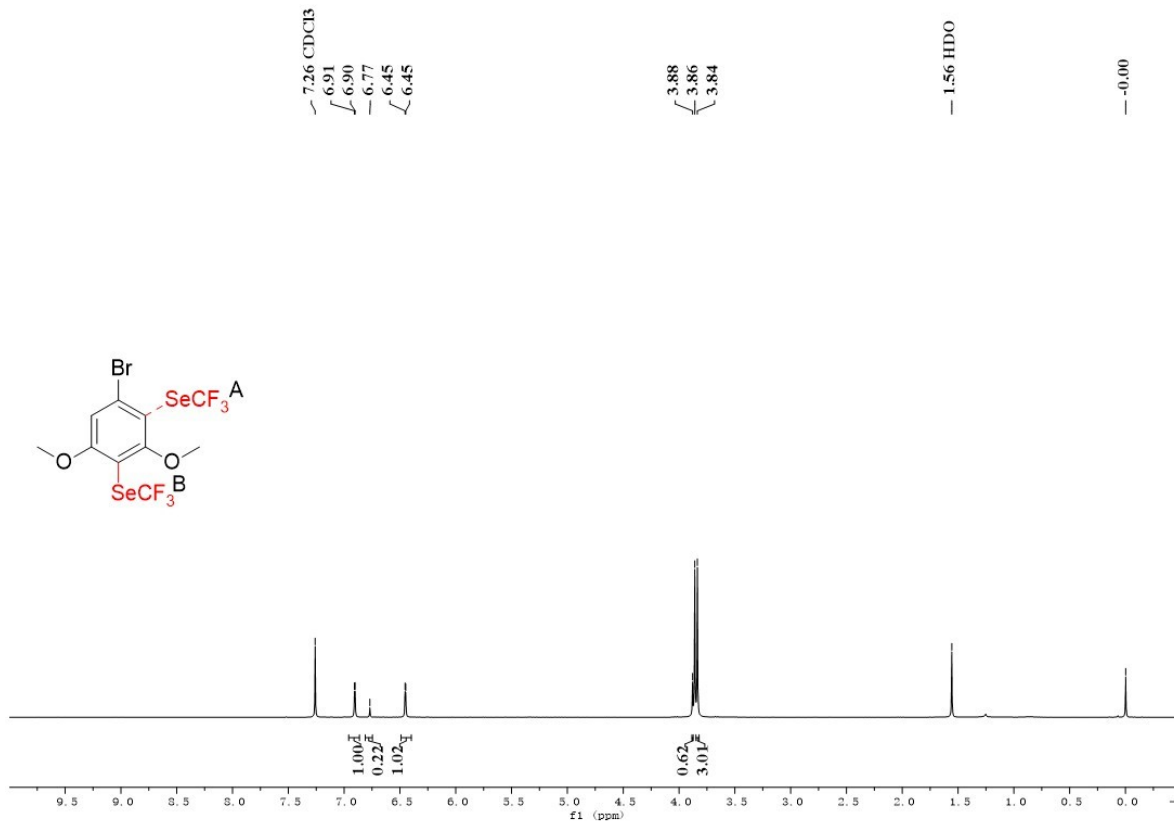


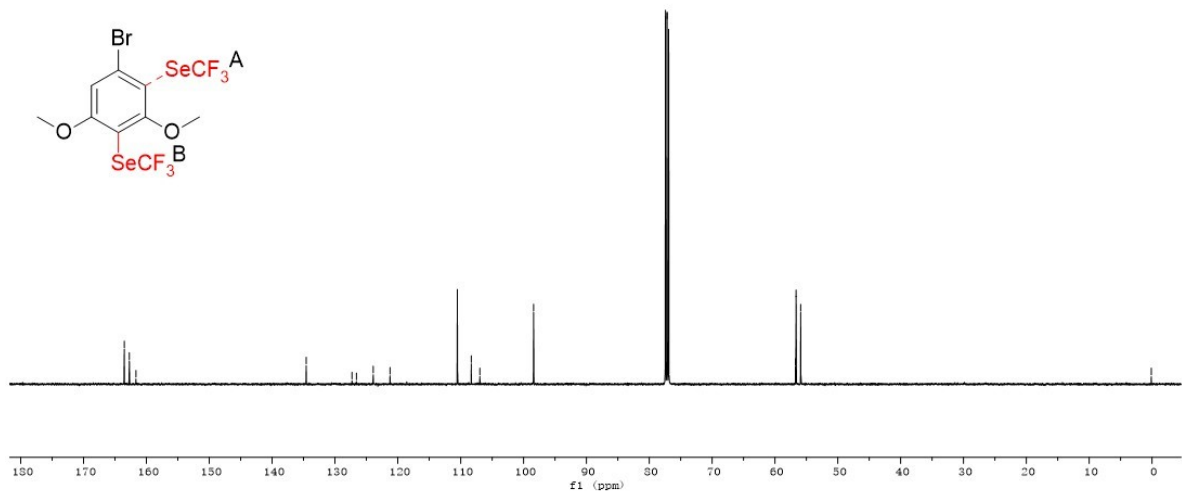
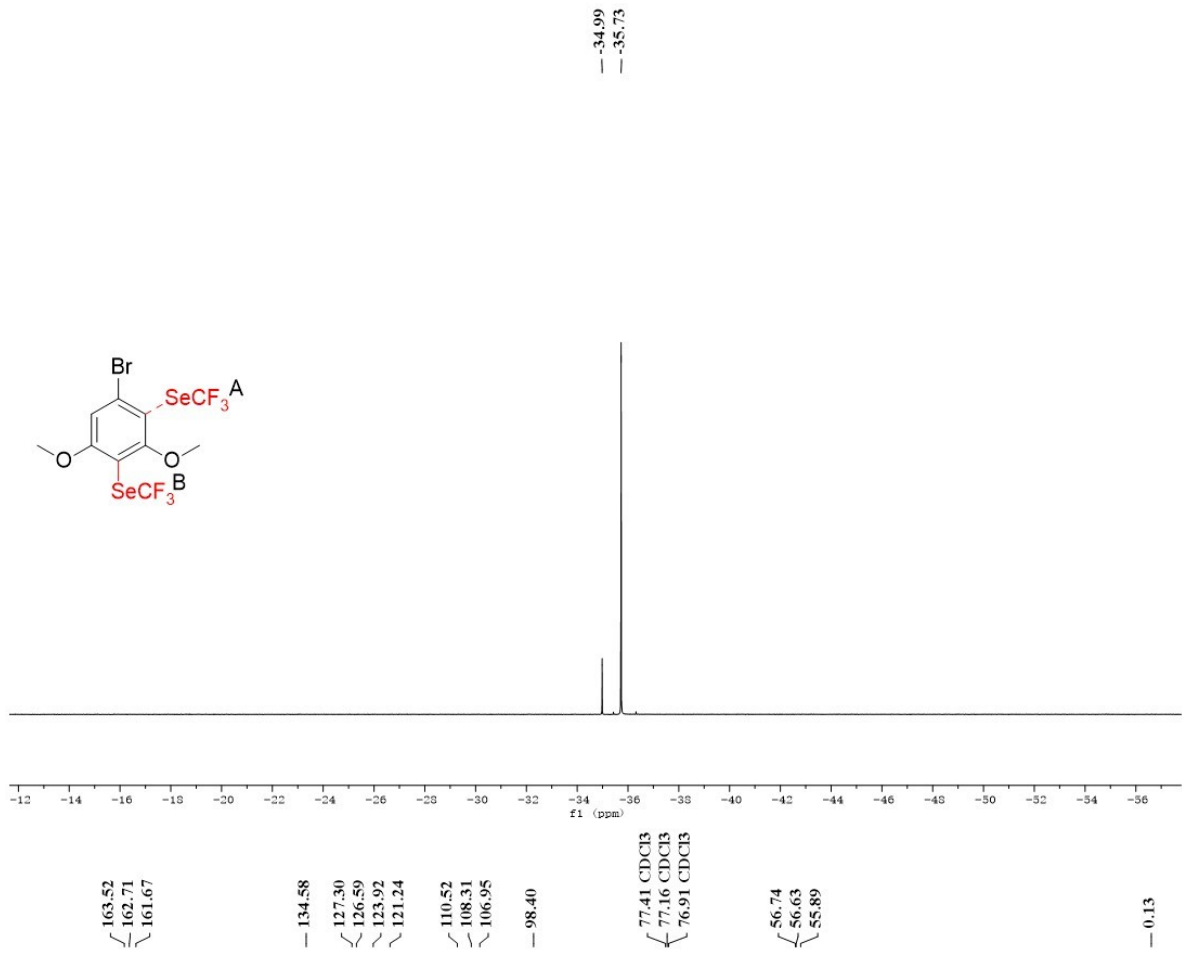
5ae (2-hydroxy-4-methoxy-5-((trifluoromethyl)selenanyl)benzaldehyde)



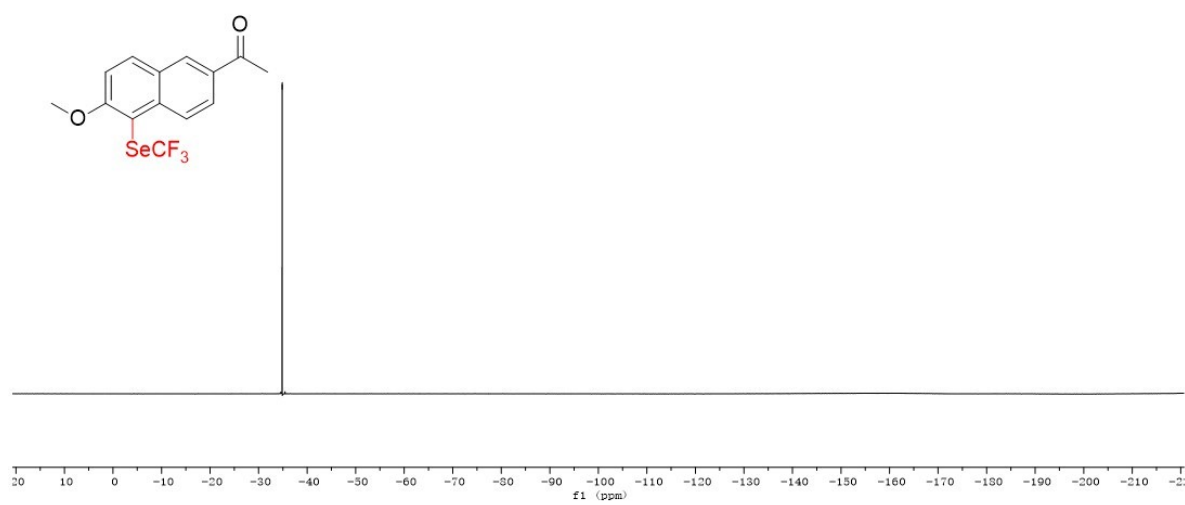
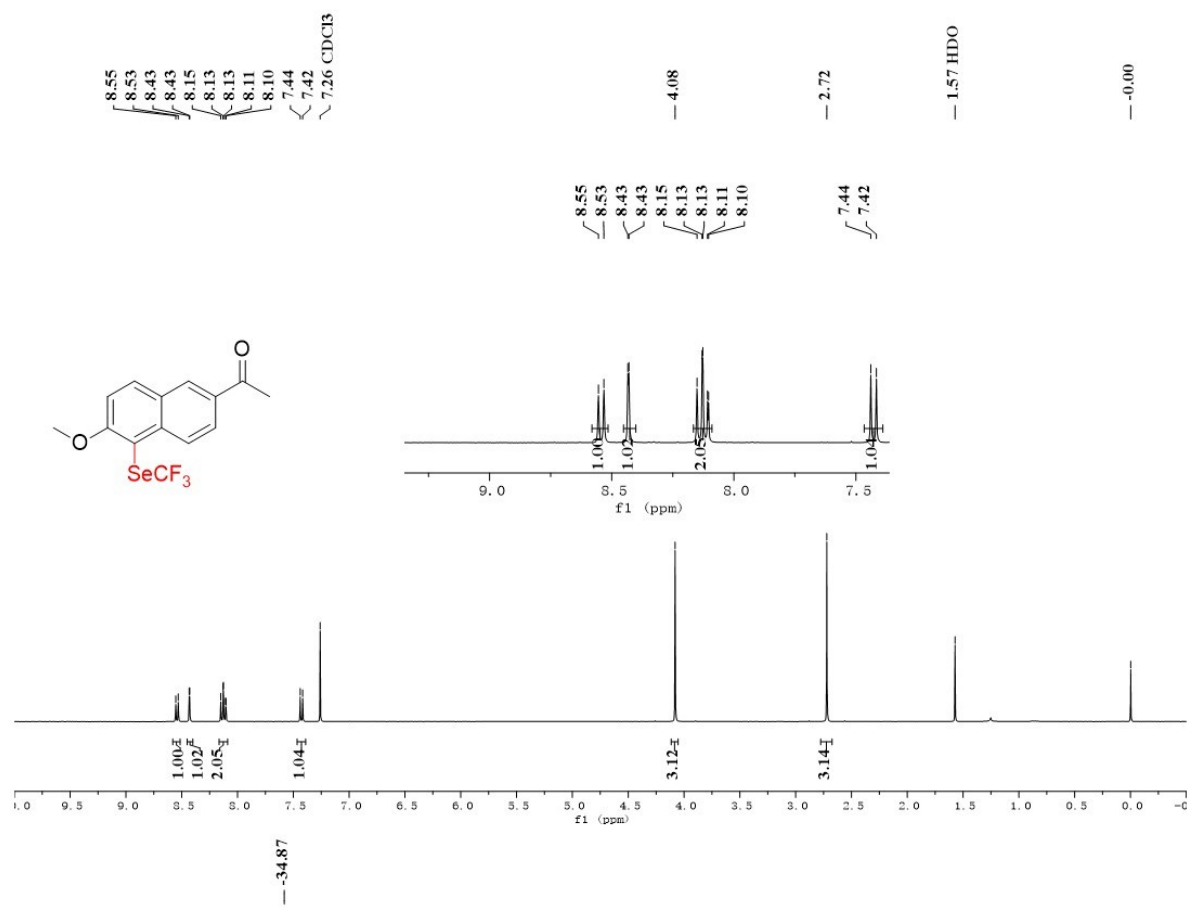


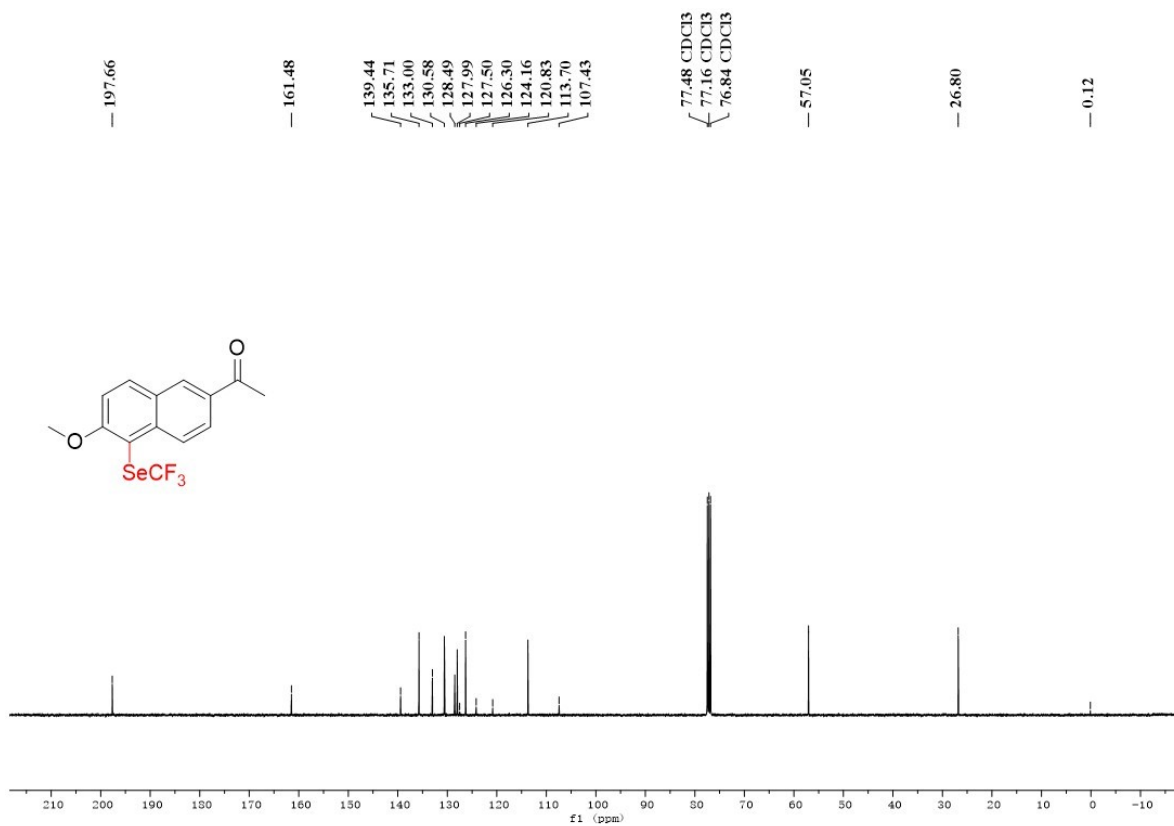
5af (A: (2-bromo-4,6-dimethoxyphenyl)(trifluoromethyl)selane; B: (4-bromo-2,6-dimethoxyphenyl)(trifluoromethyl)selane)



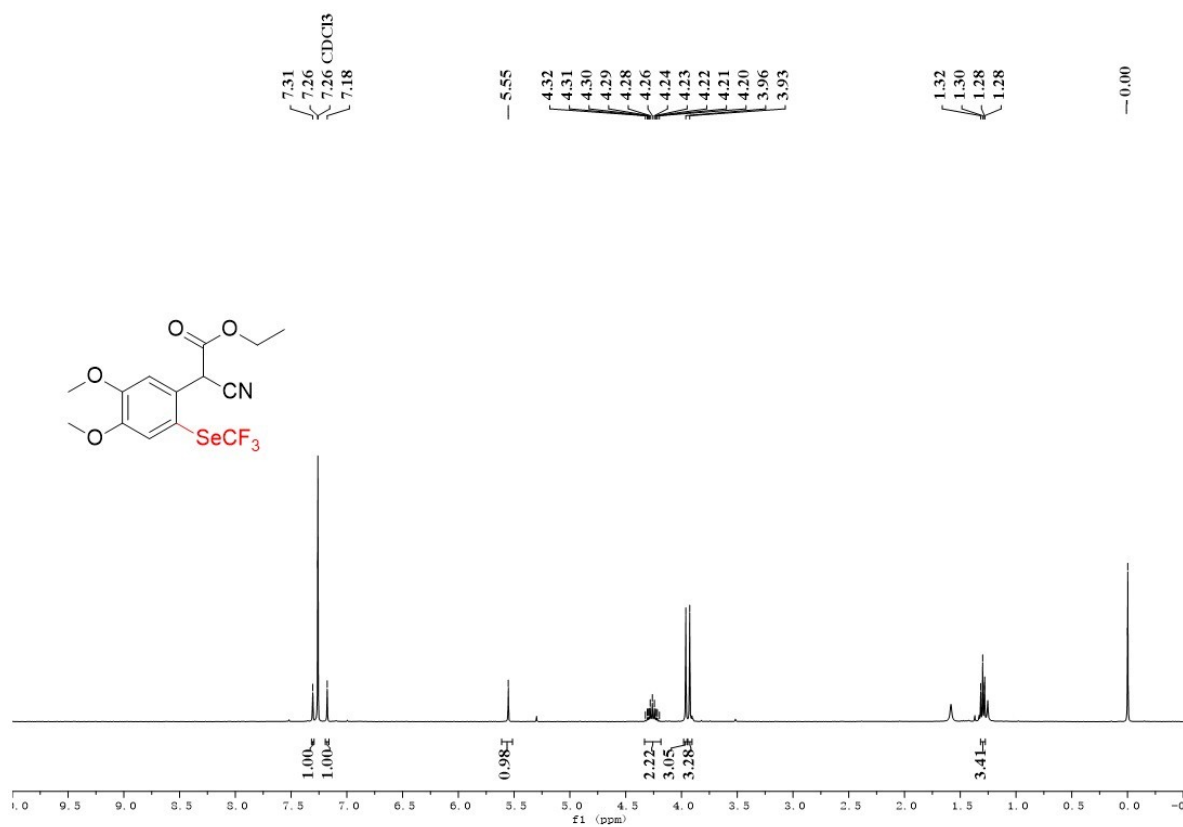


5ag (1-(6-methoxy-5-((trifluoromethyl)selanyl)naphthalen-2-yl)ethan-1-one)

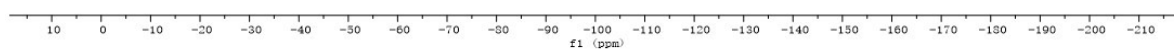




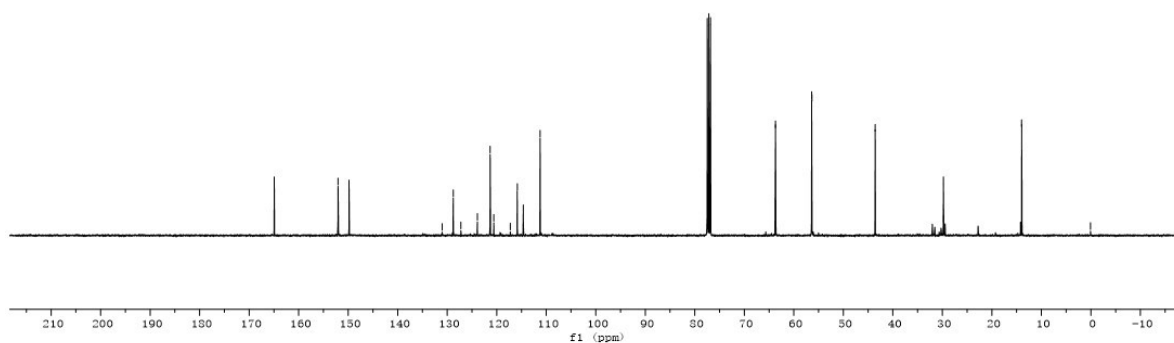
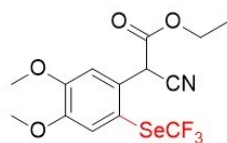
5ah (ethyl 2-cyano-2-(4,5-dimethoxy-2-((trifluoromethyl)selenanyl)phenyl)acetate)



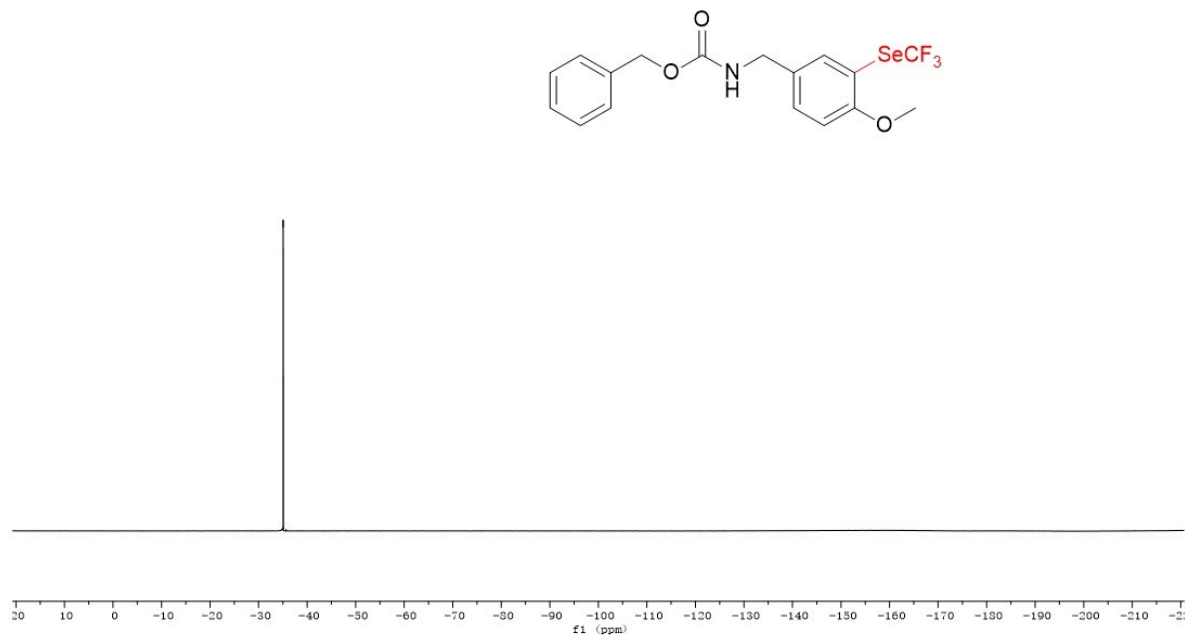
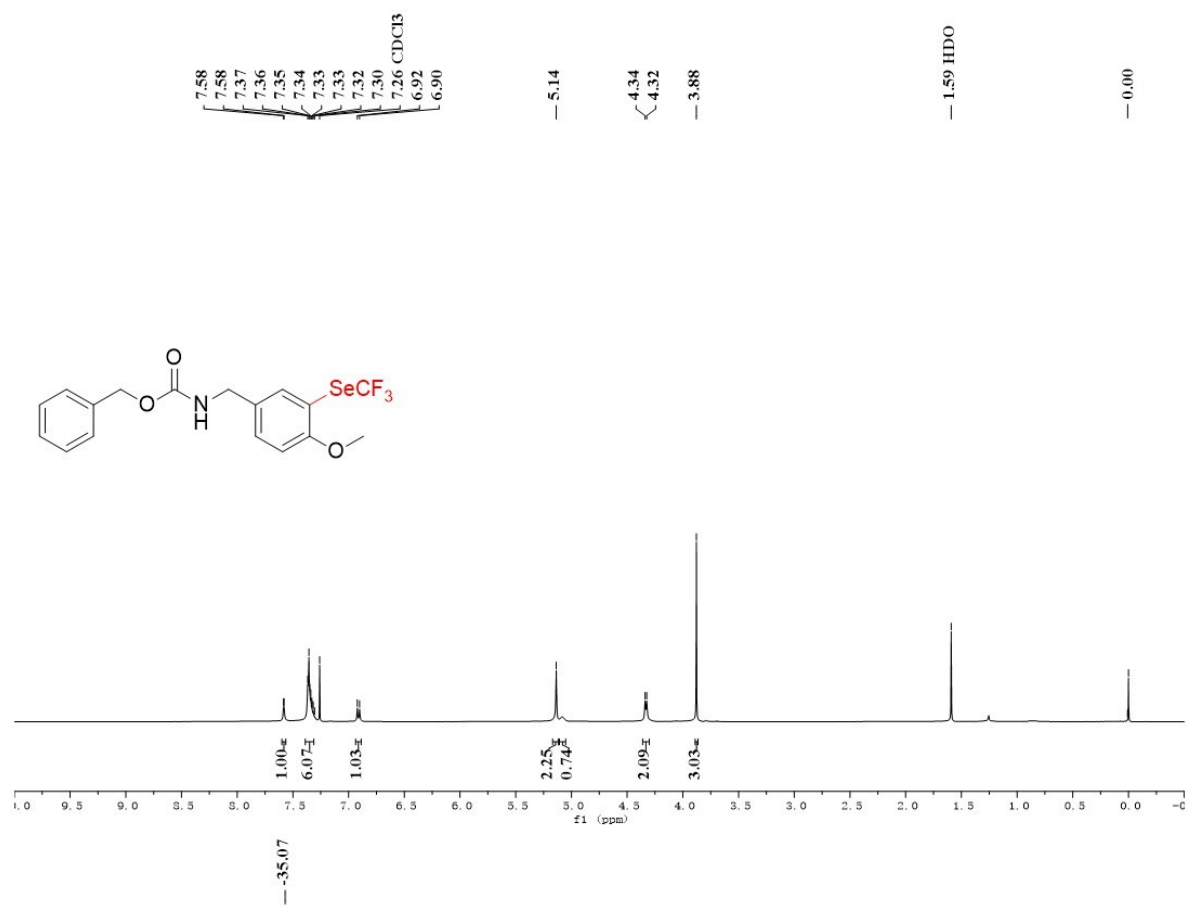
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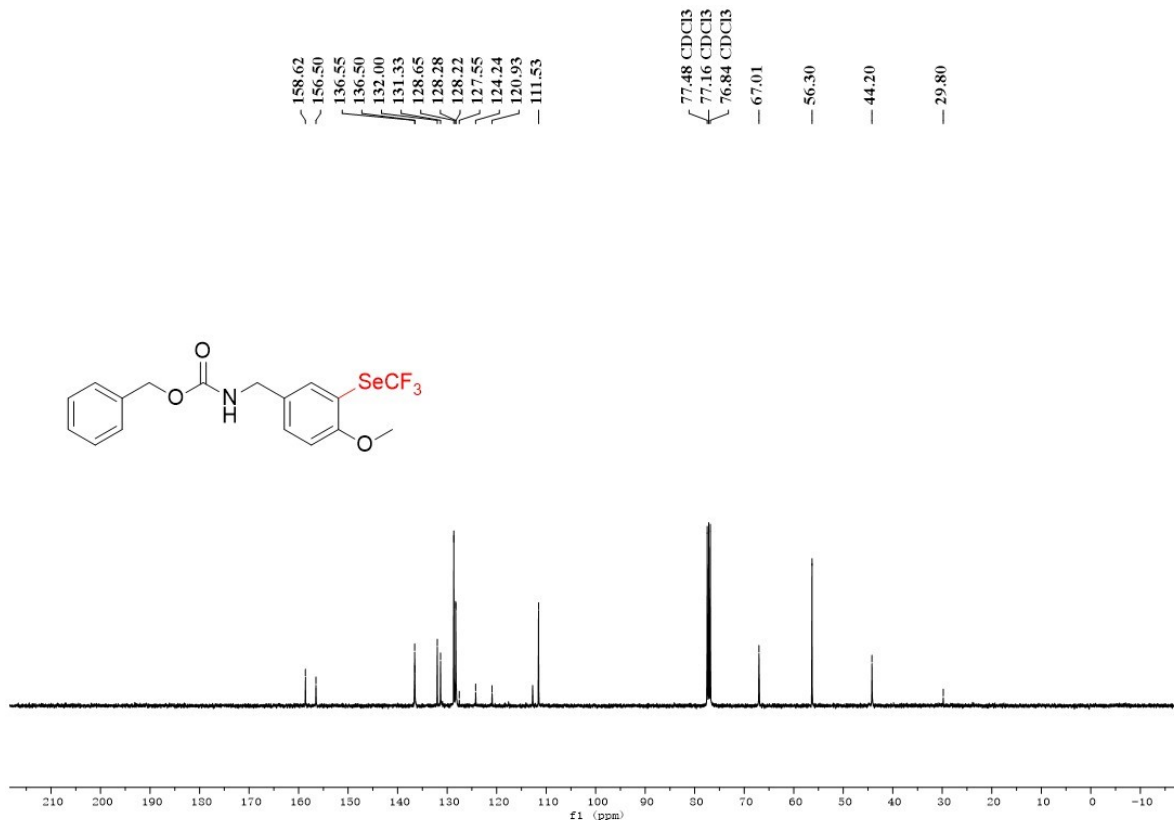


164.93
152.05
149.83
131.03
128.78
127.24
123.92
121.33
120.59
117.27
115.85
114.64
111.23
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
63.71
56.40
56.35
43.57
29.79
29.75
13.99
0.07

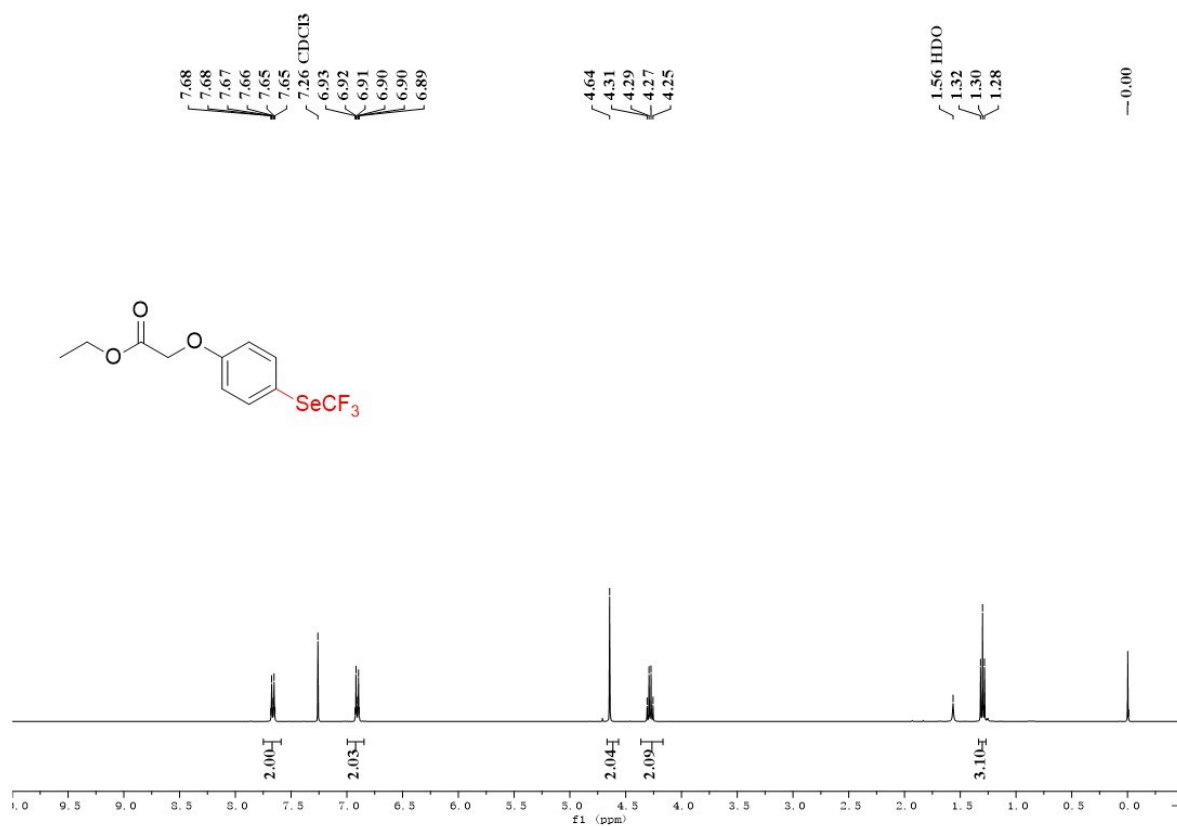


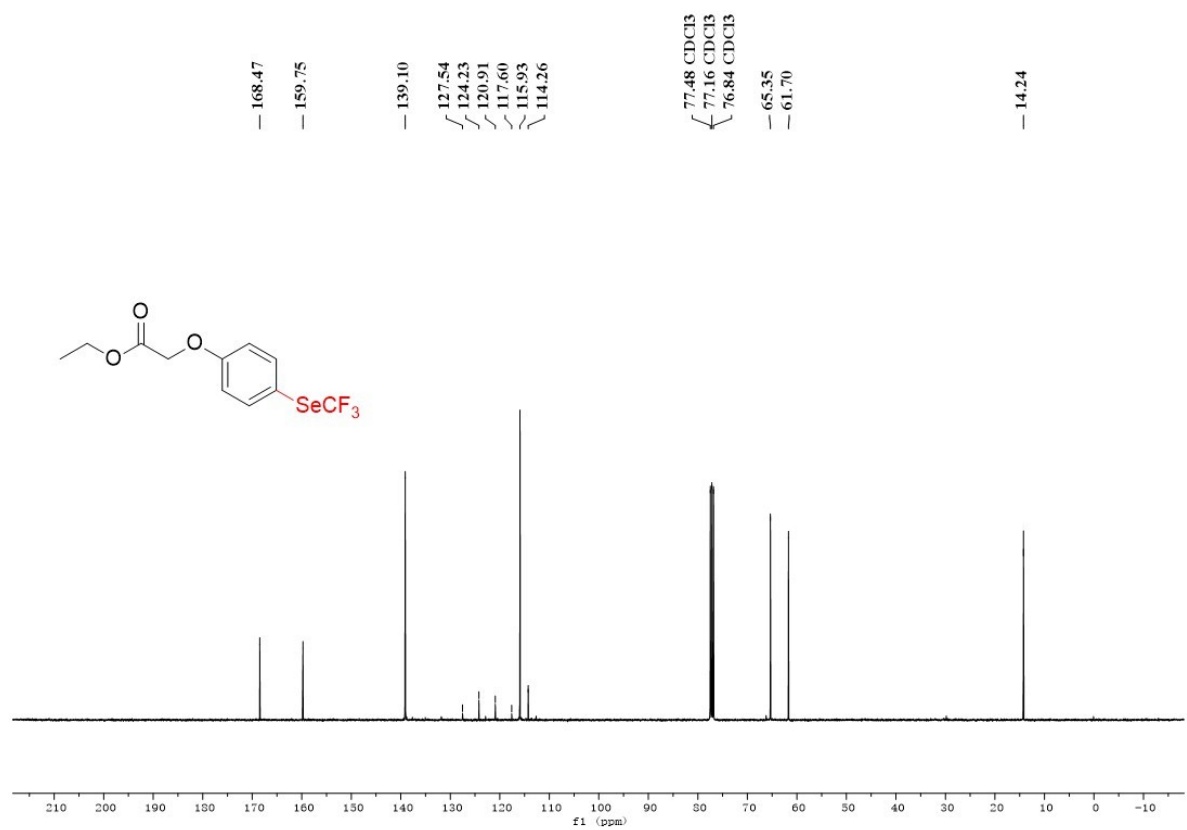
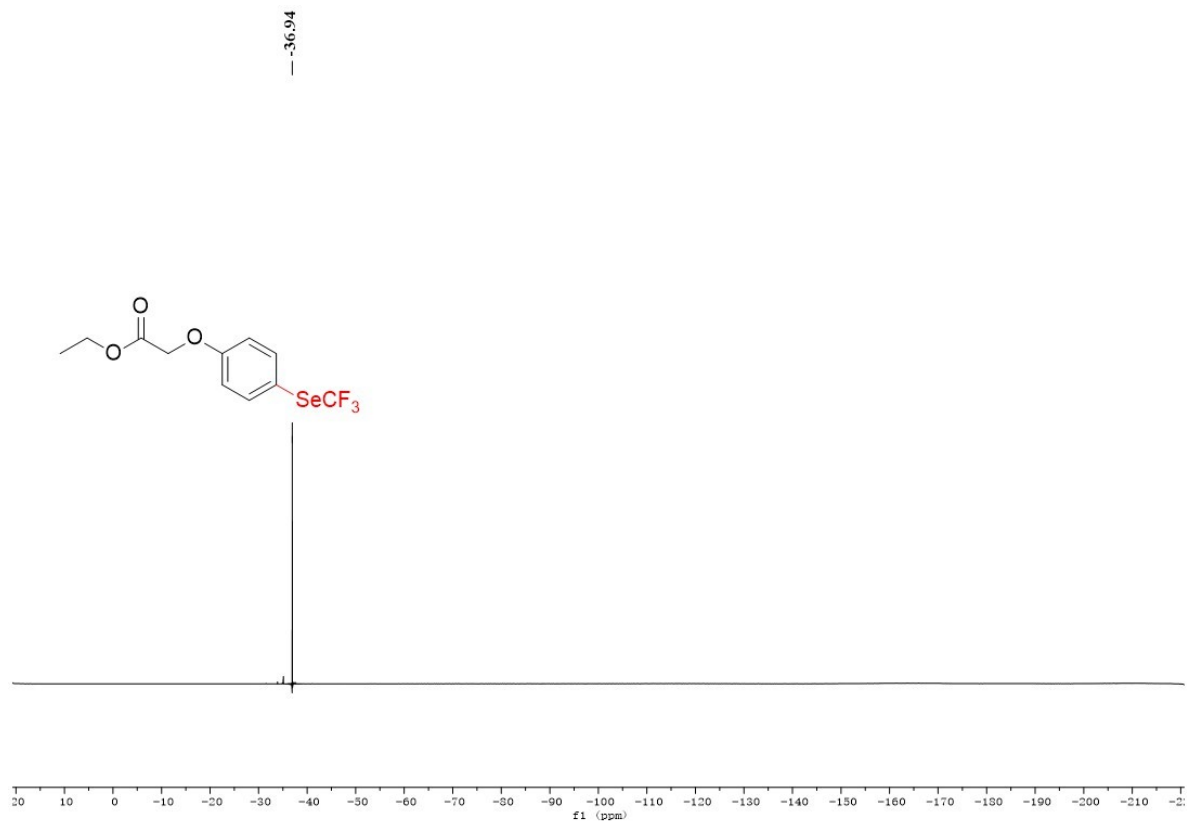
5ai (benzyl (4-methoxy-3-((trifluoromethyl)selanyl)benzyl)carbamate)



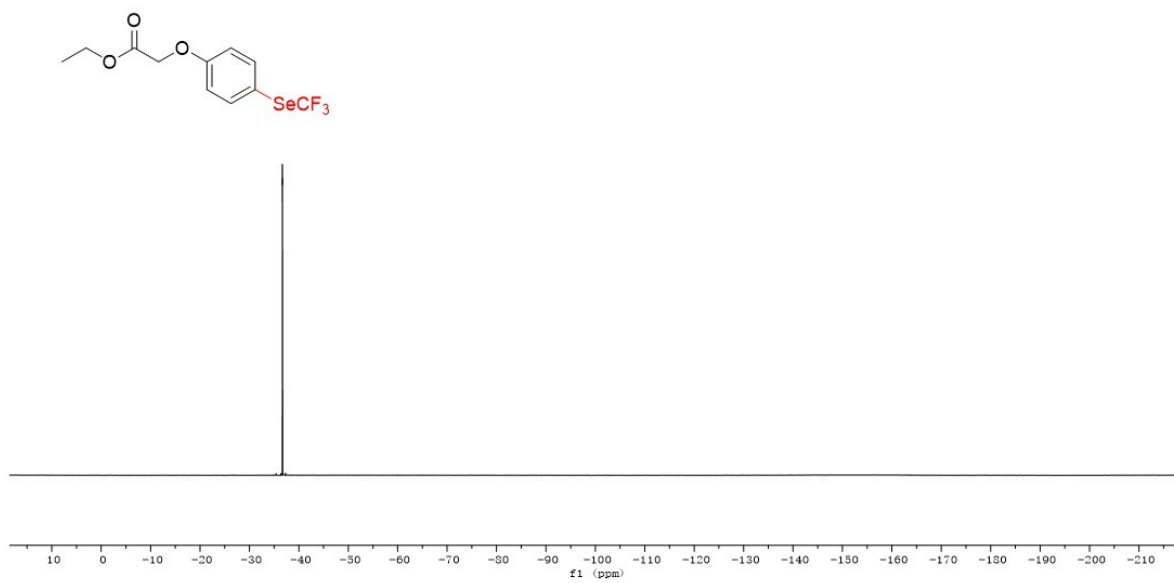
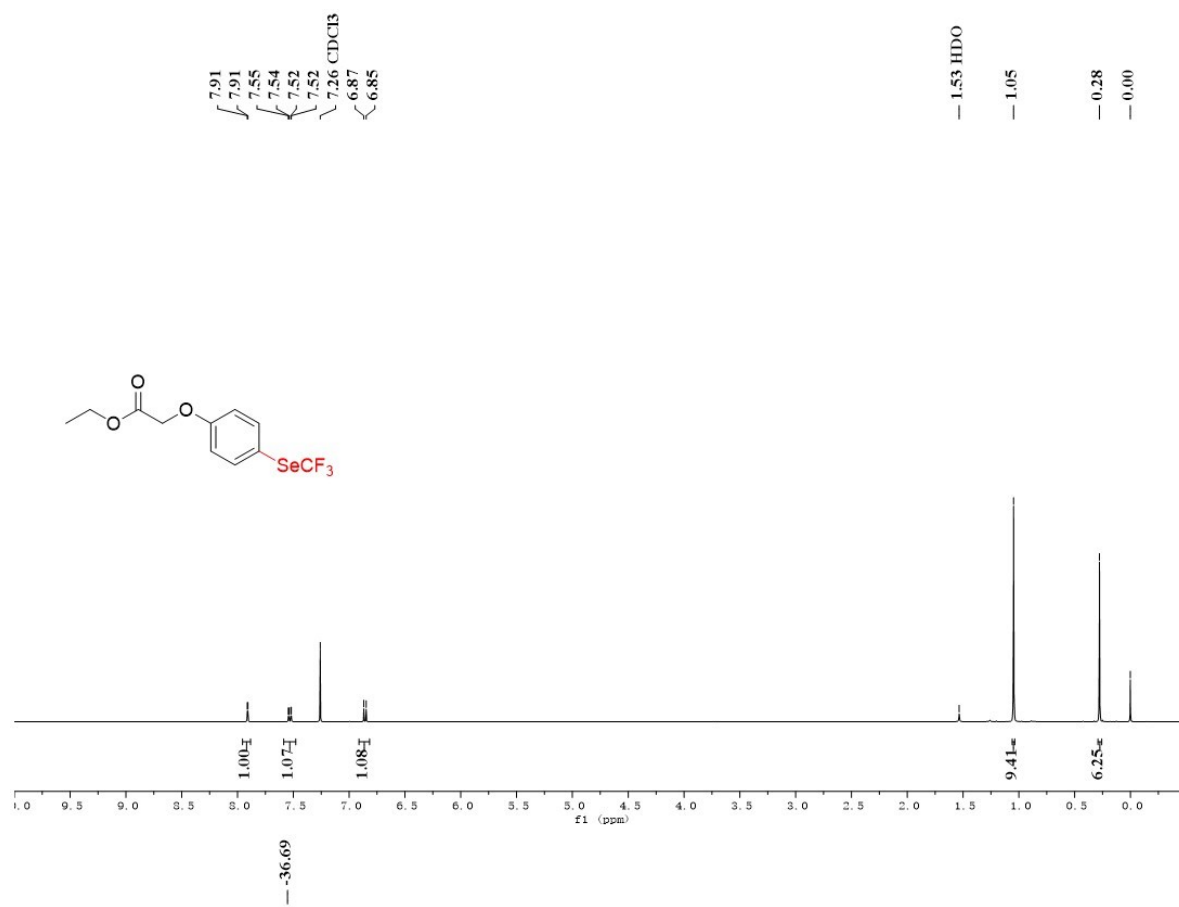


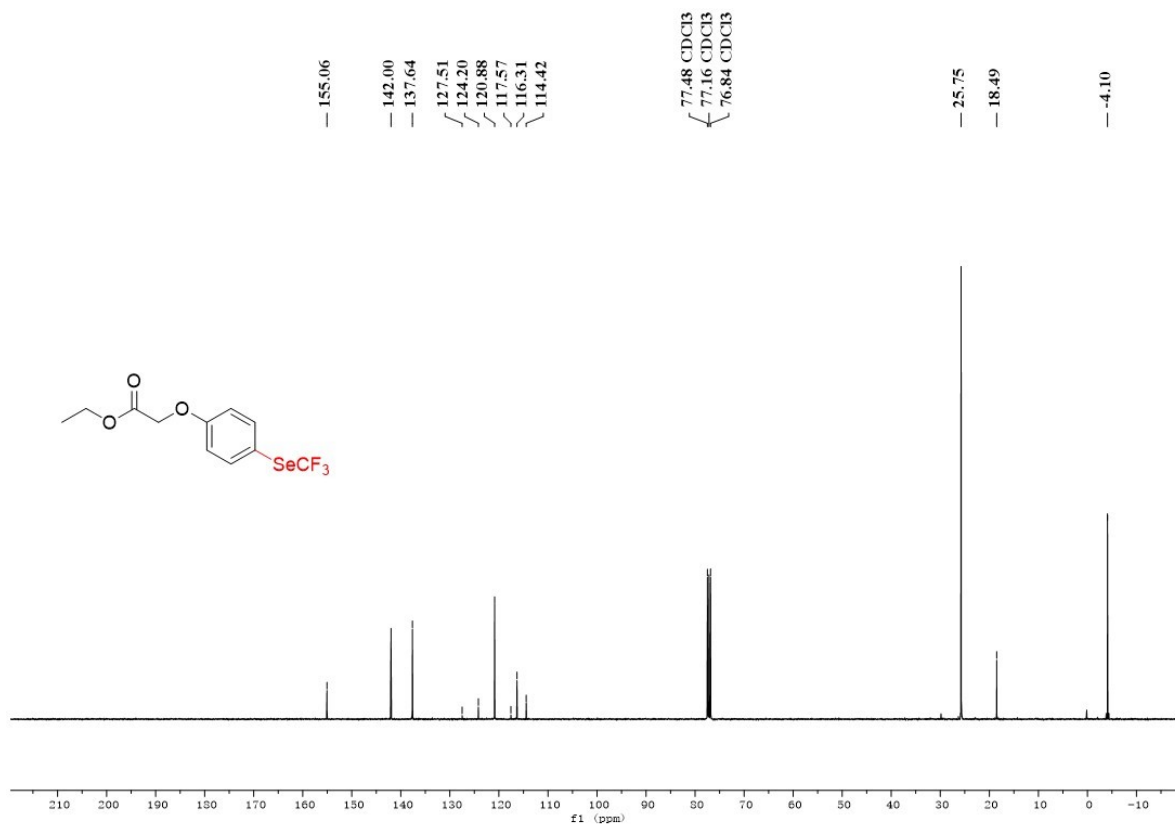
5aj (ethyl 2-(4-((trifluoromethyl)selenyl)phenoxy)acetate)



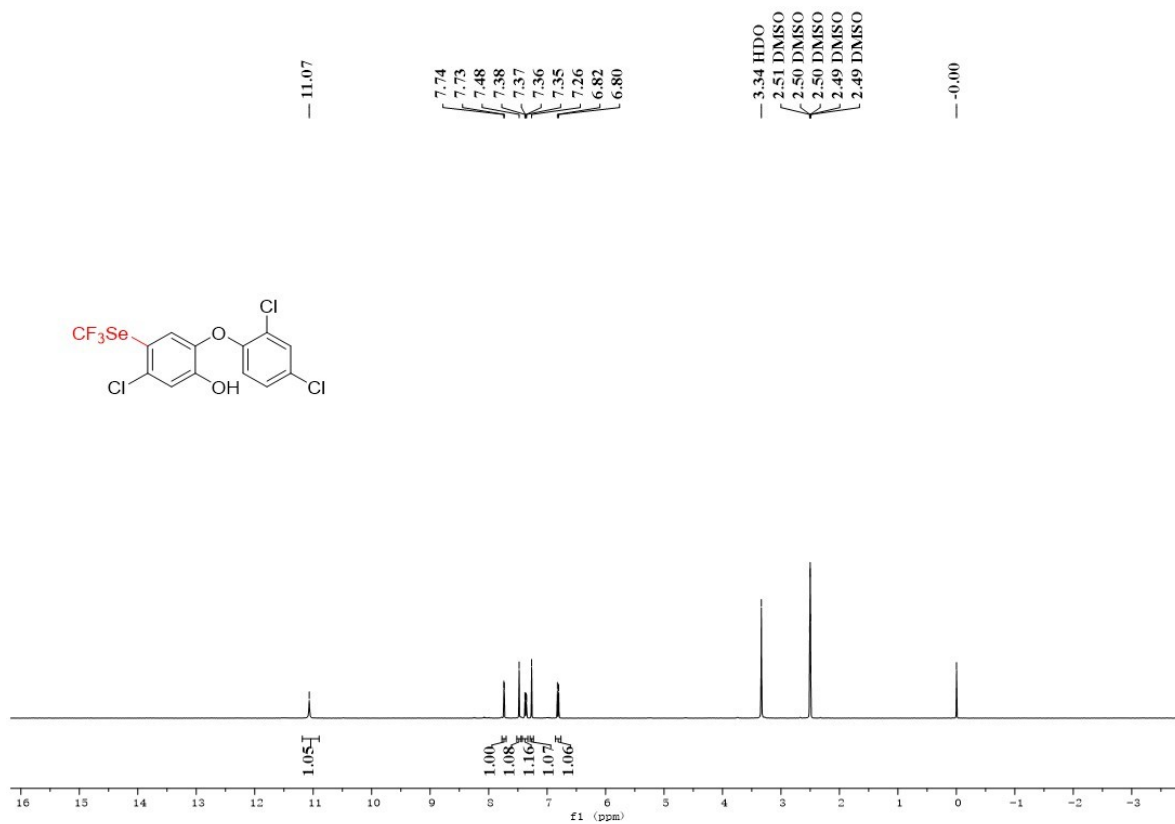


5ak ((2-bromo-4-((trifluoromethyl)selanyl)phenoxy)(tert-butyl)dimethylsilane)

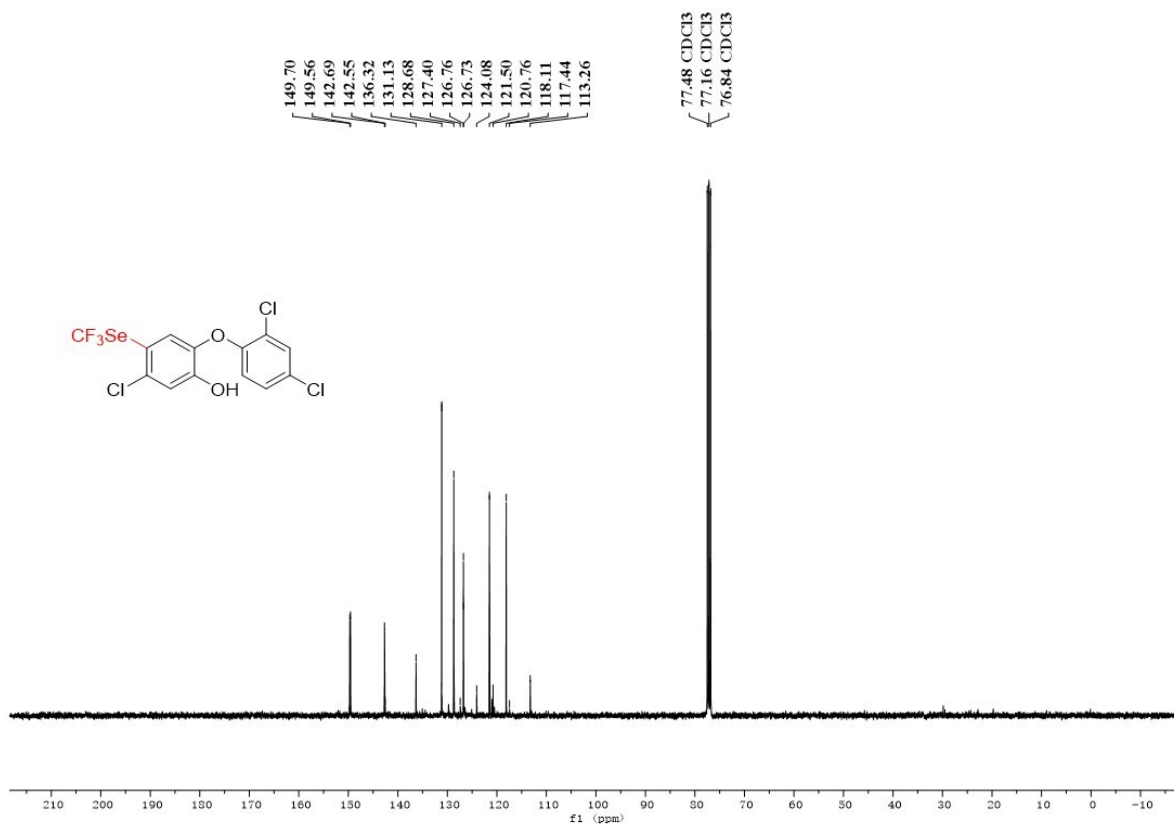
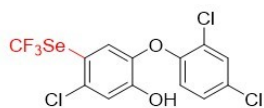
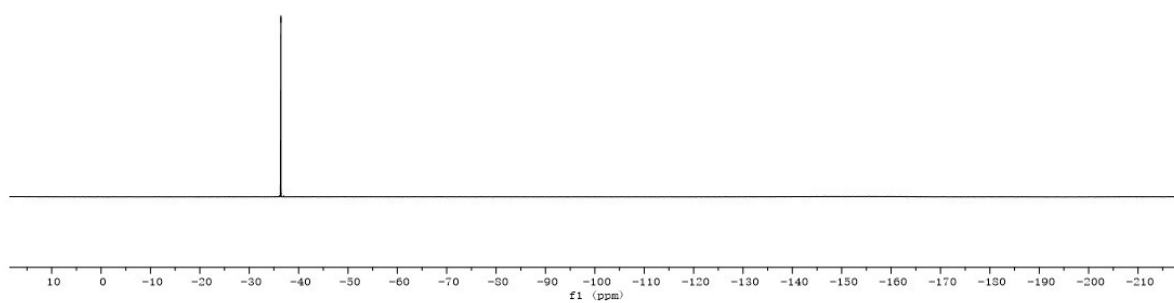
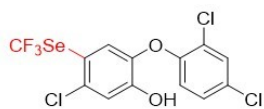




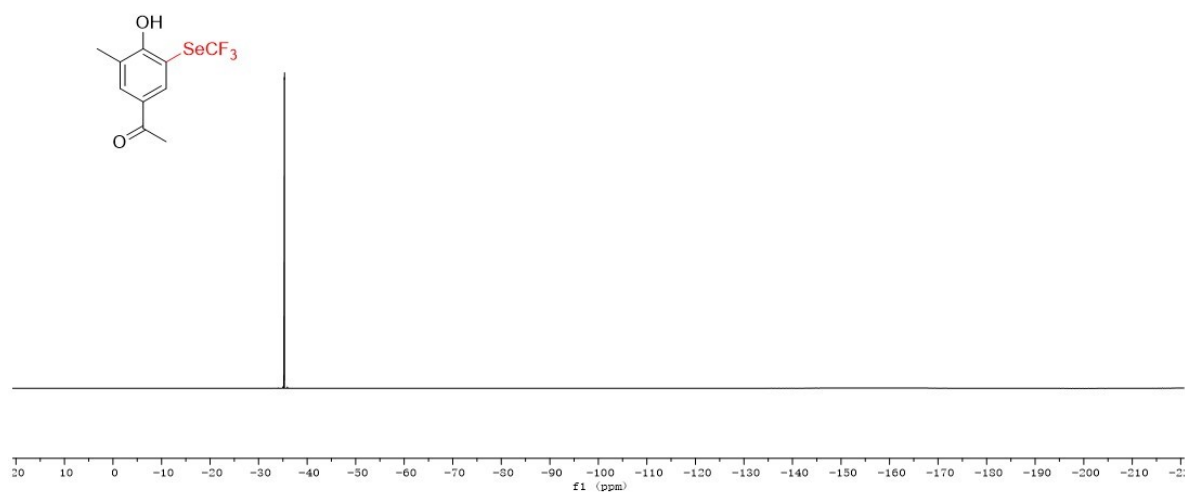
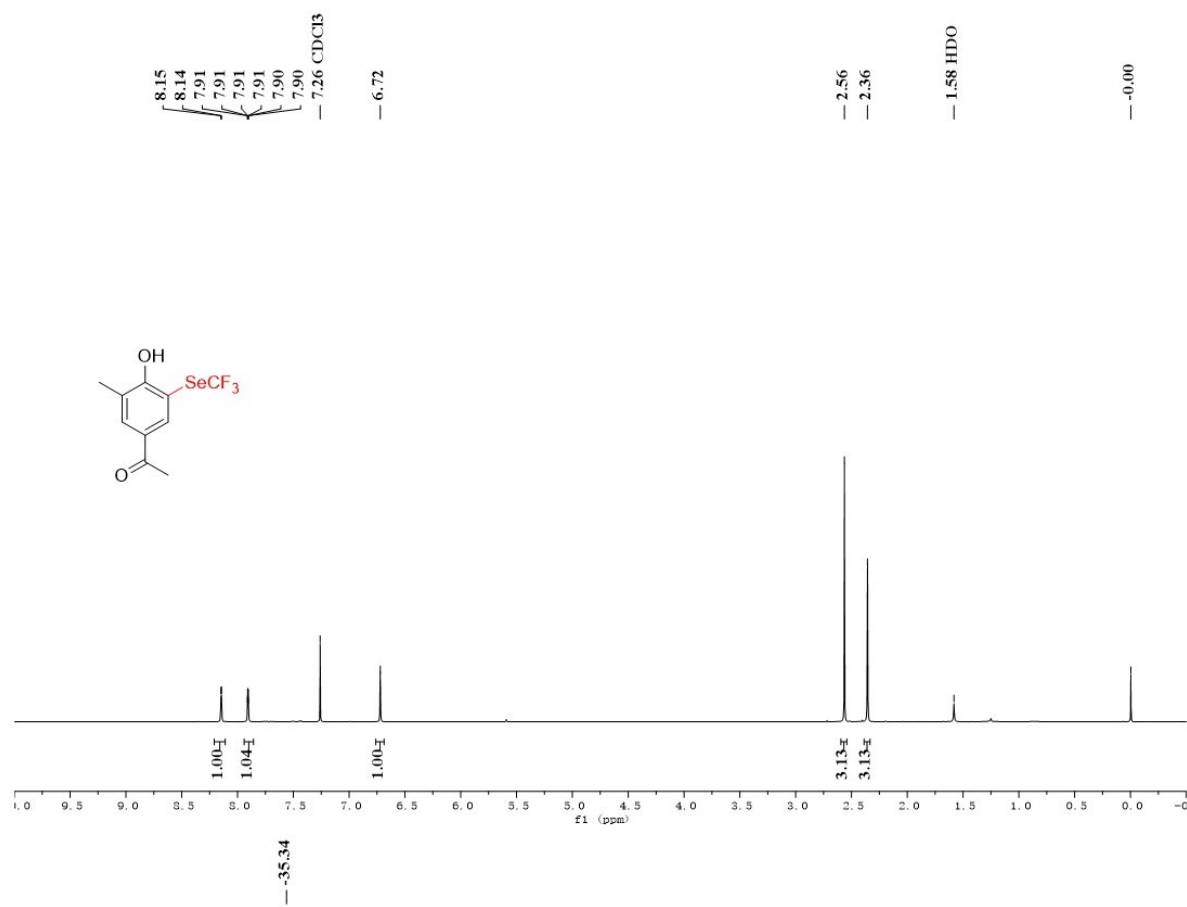
5al (5-chloro-2-(2,4-dichlorophenoxy)-4-((trifluoromethyl)selenyl)phenol)

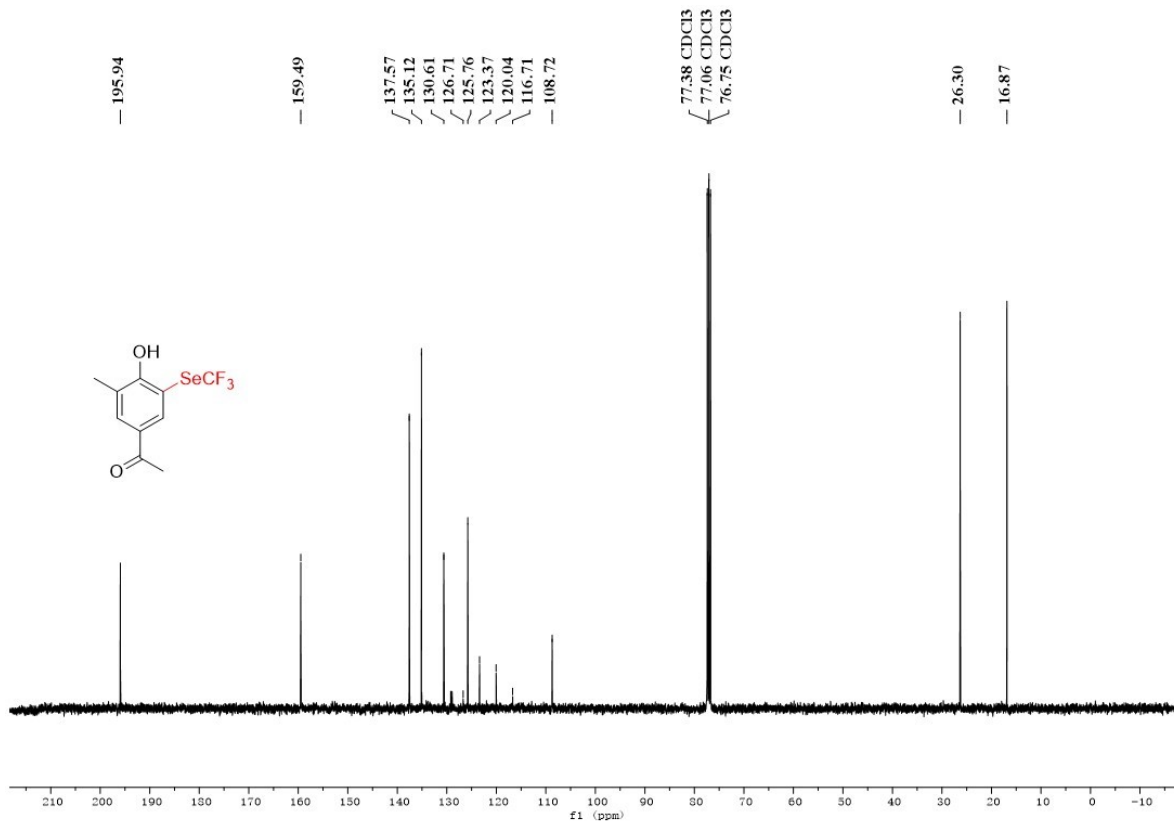


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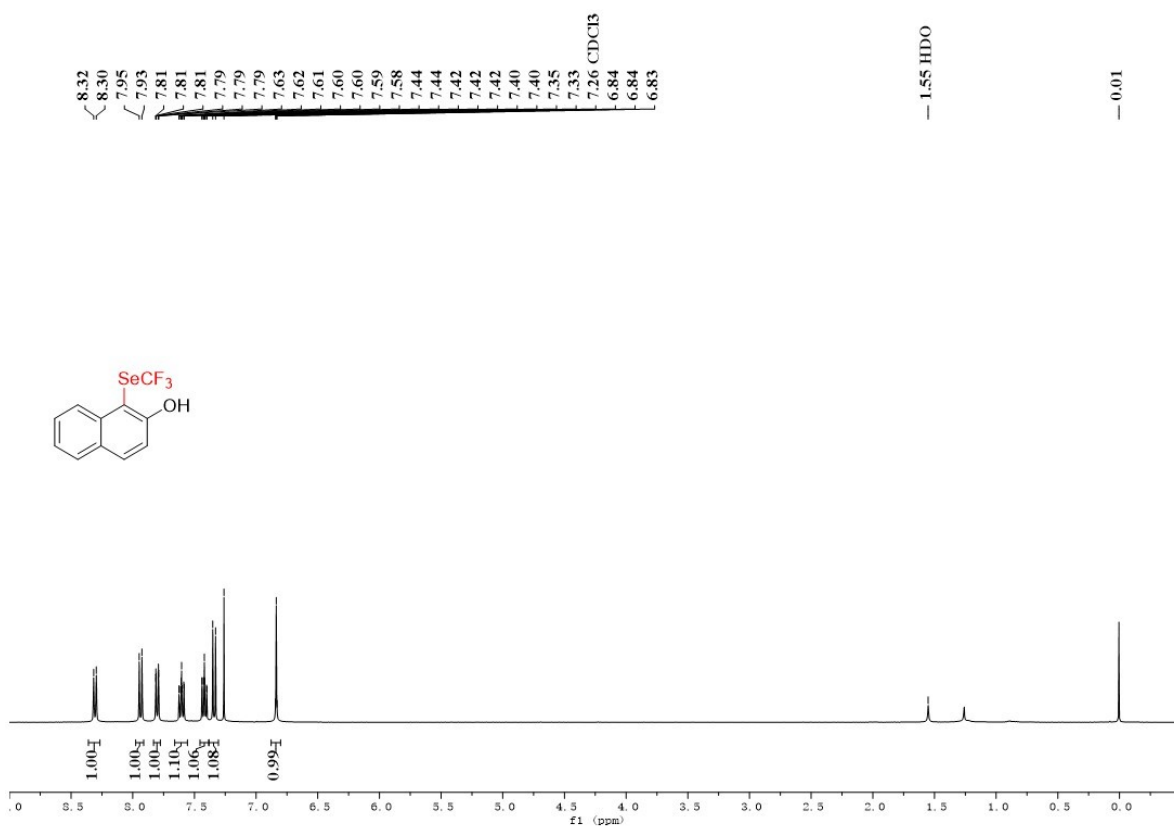


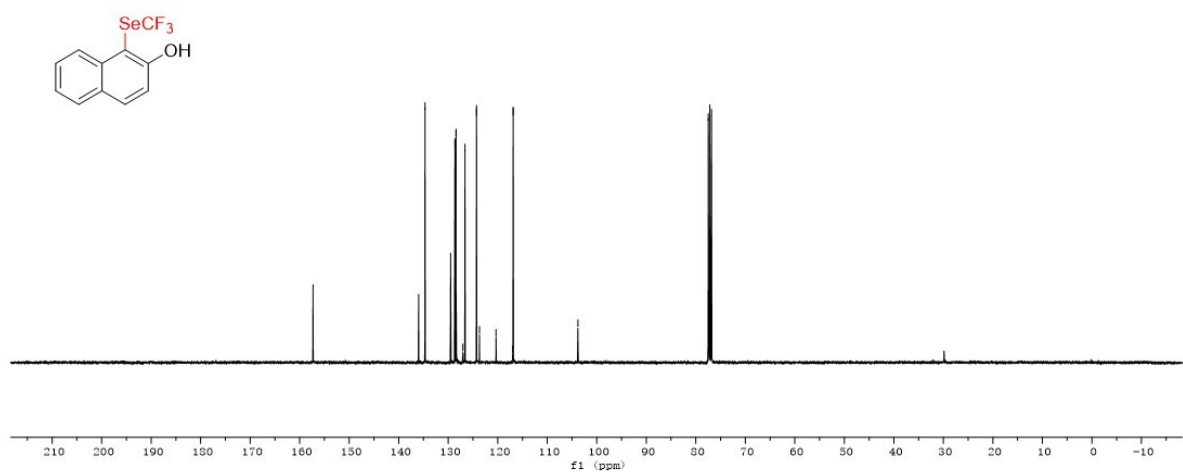
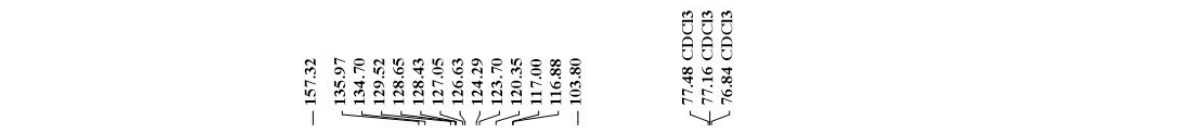
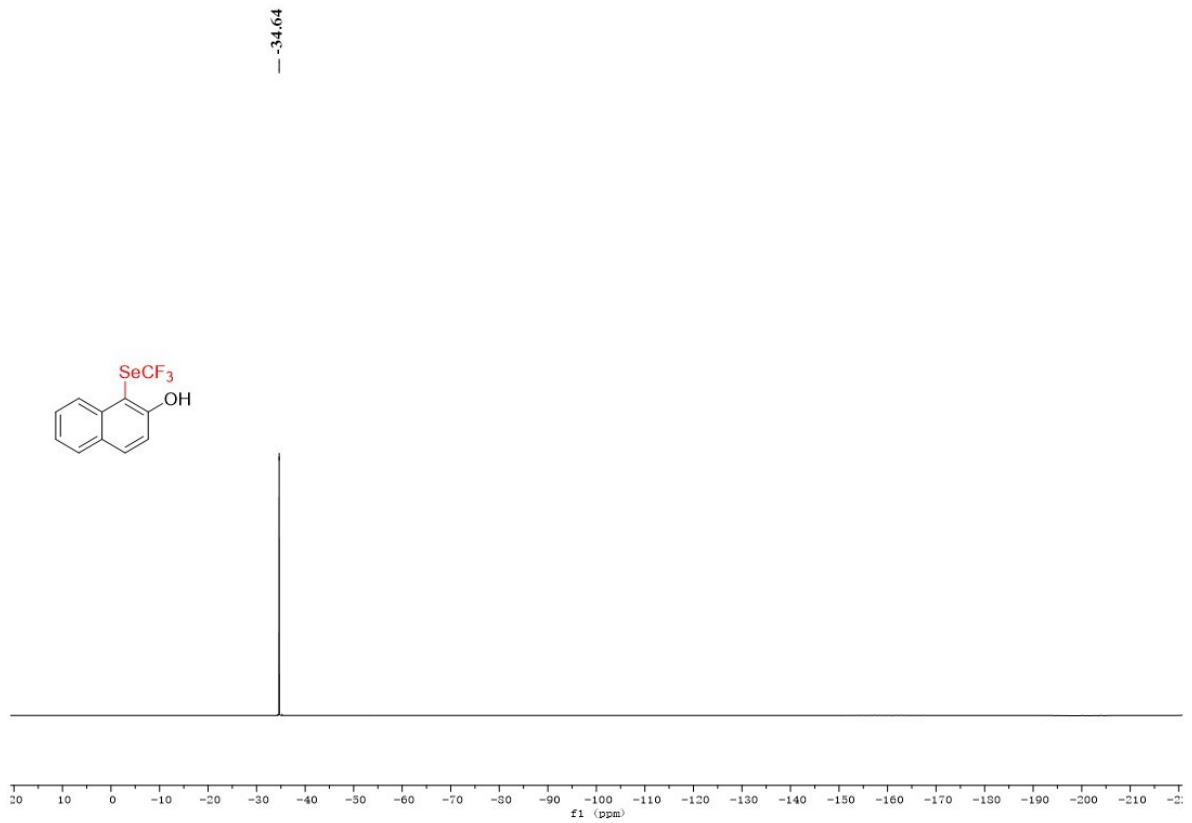
5am (1-(4-hydroxy-3-methyl-5-((trifluoromethyl)selenanyl)phenyl)ethan-1-one)



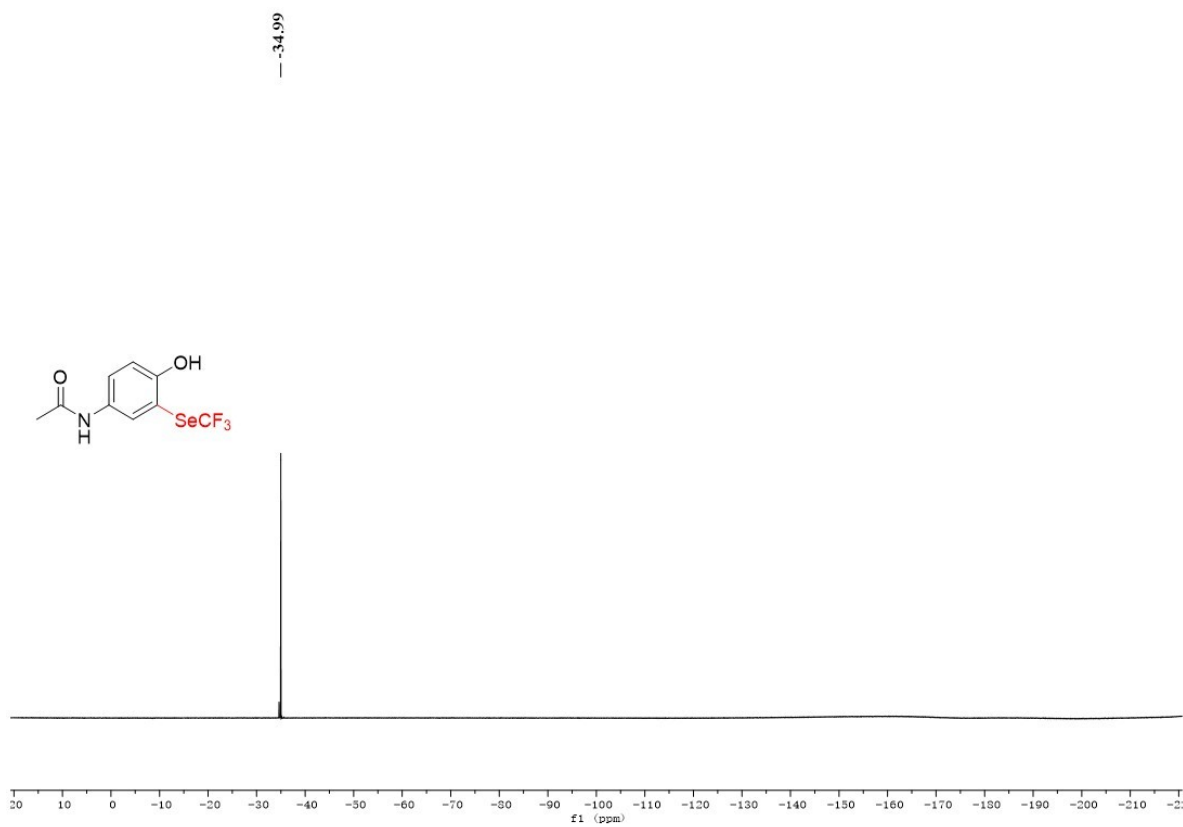
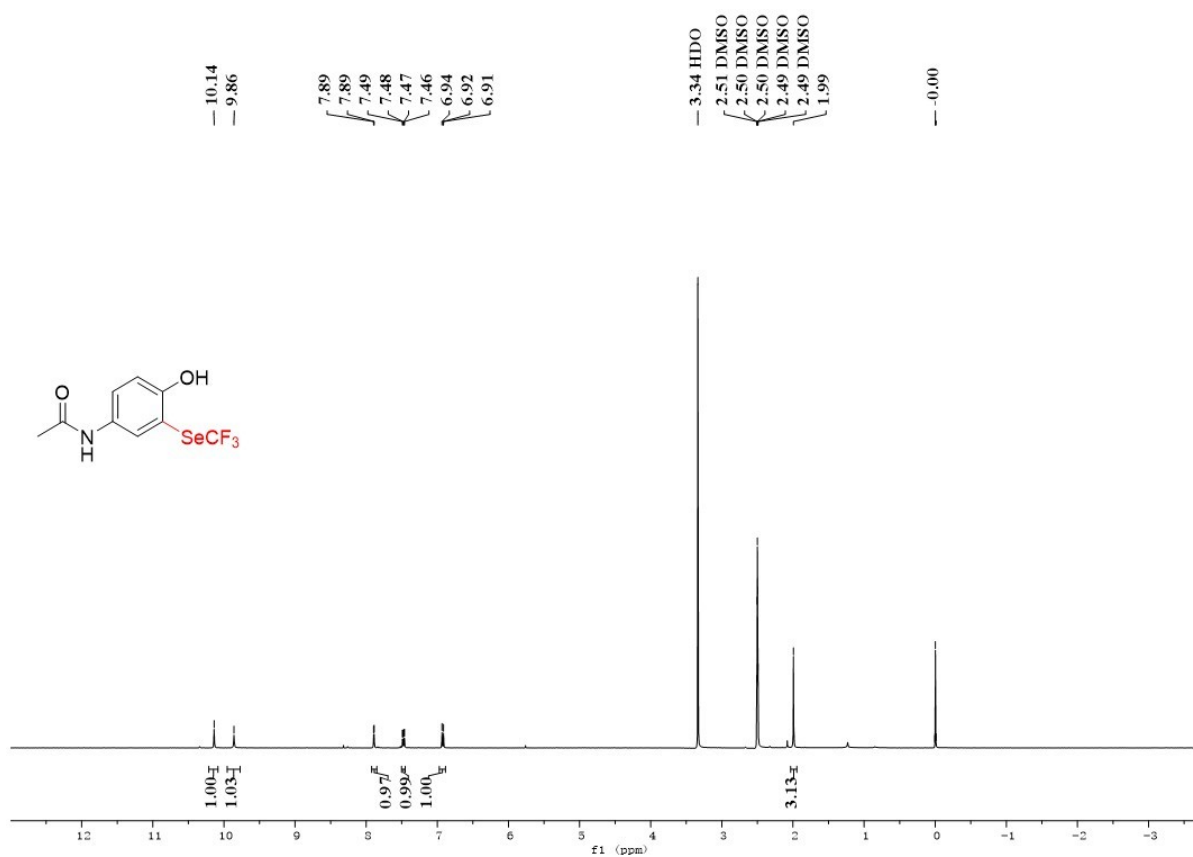


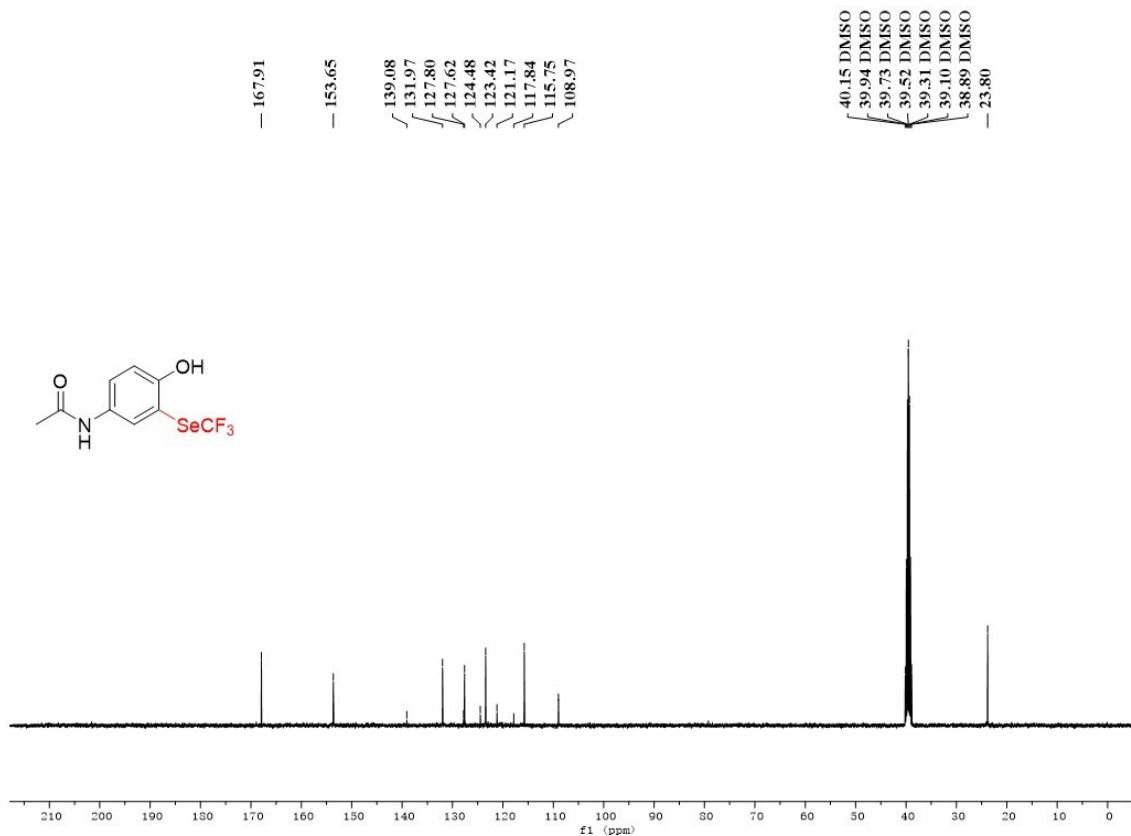
5an (1-((trifluoromethyl)selenyl)naphthalen-2-ol)



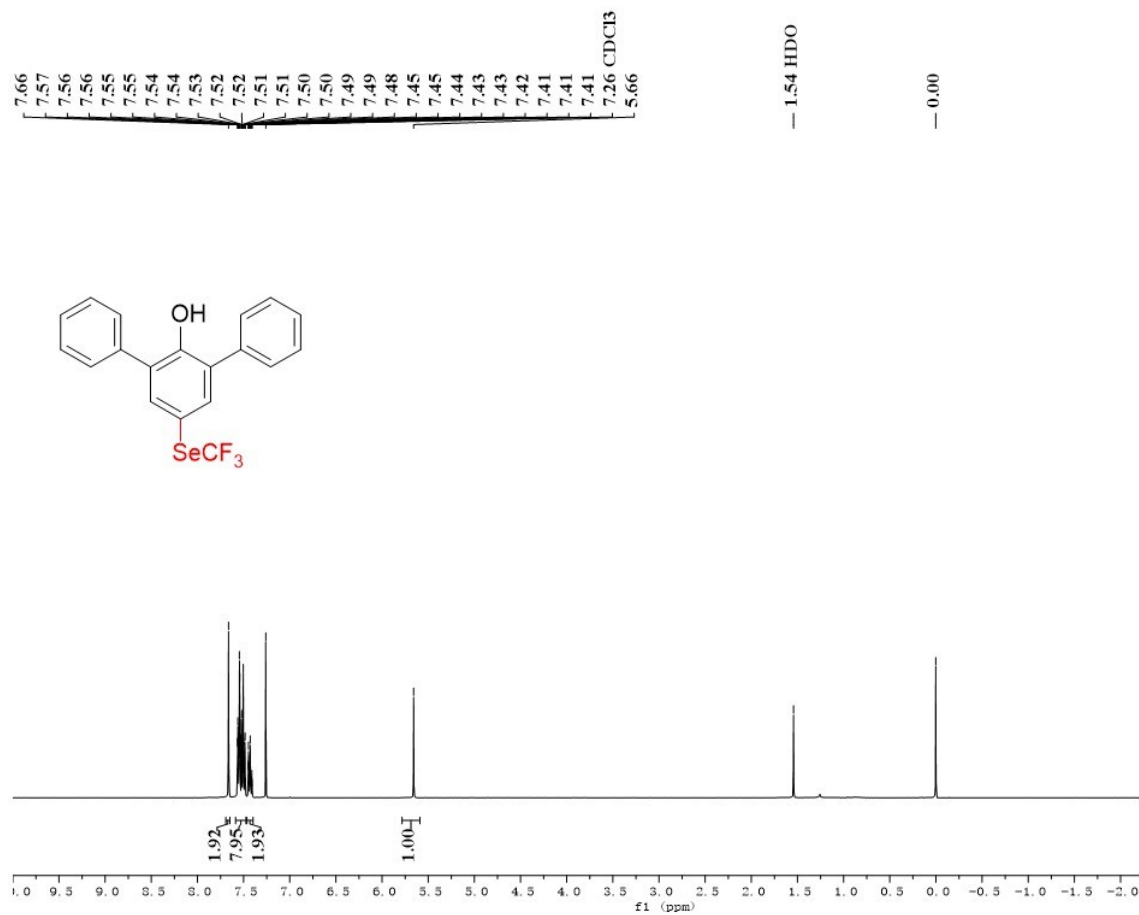


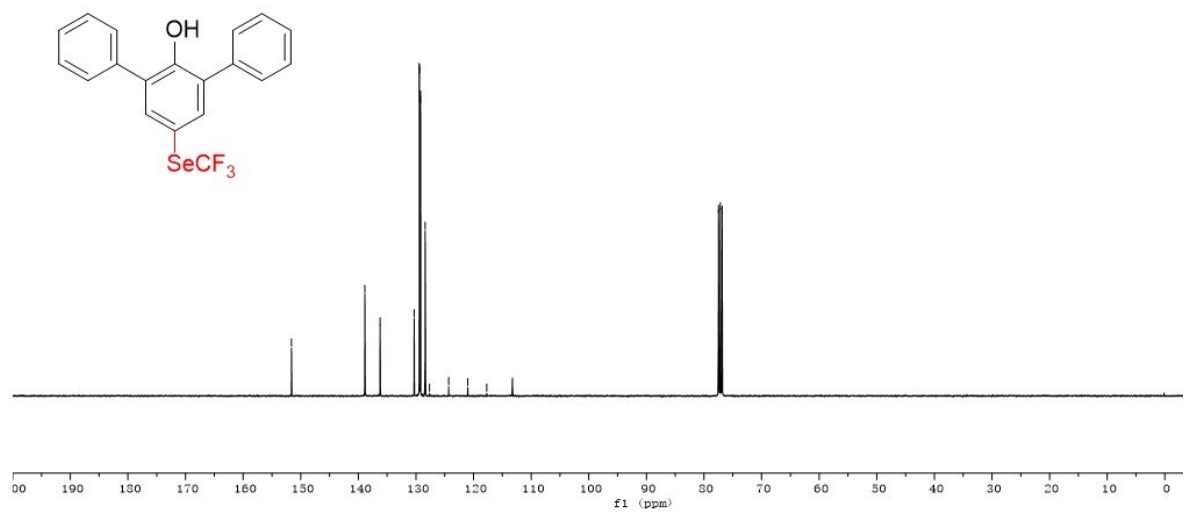
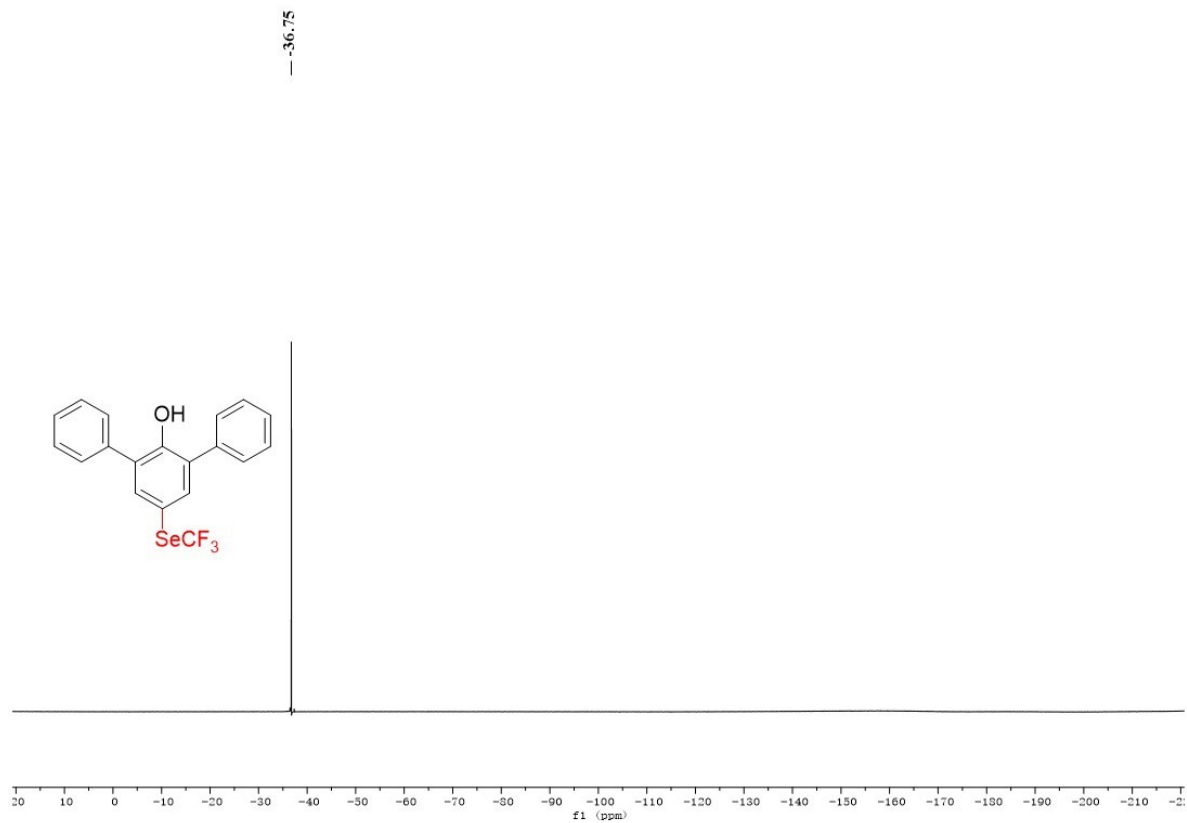
5ao (N-(4-hydroxy-3-((trifluoromethyl)selenanyl)phenyl)acetamide)



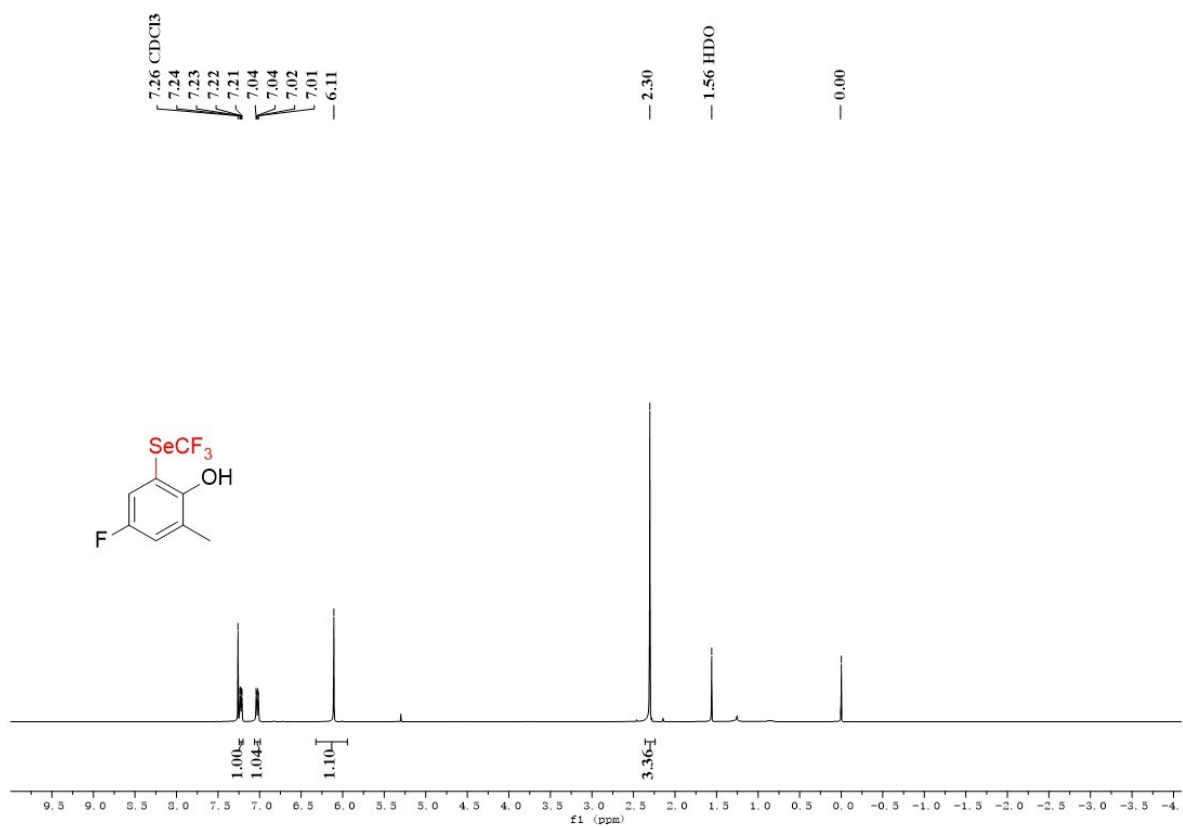


5ap (5'-((trifluoromethyl)selanyl)-[1,1':3',1''-terphenyl]-2'-ol)



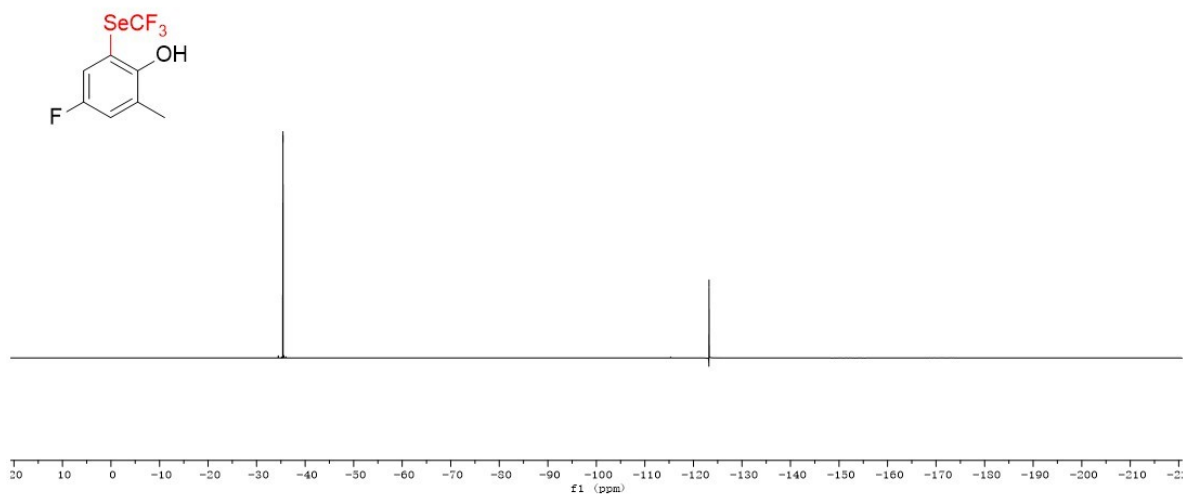


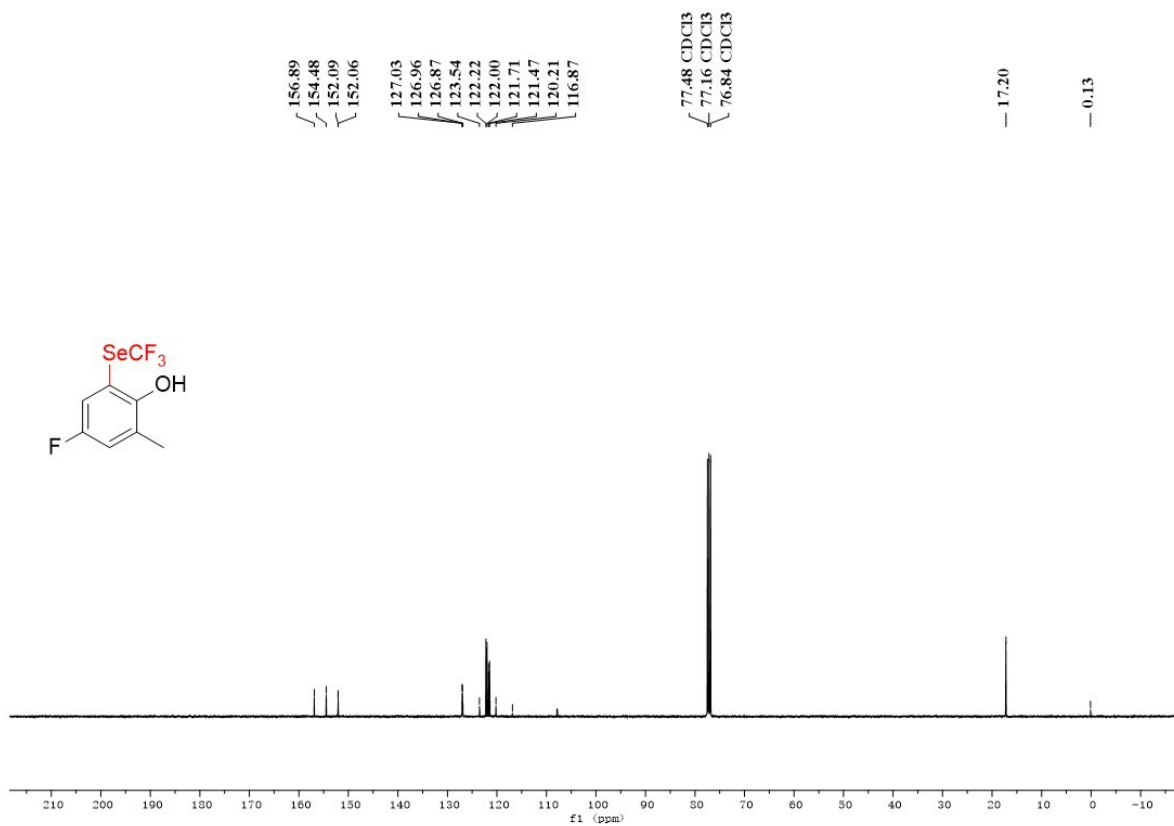
5aq (4-fluoro-2-methyl-6-((trifluoromethyl)selenanyl)phenol)



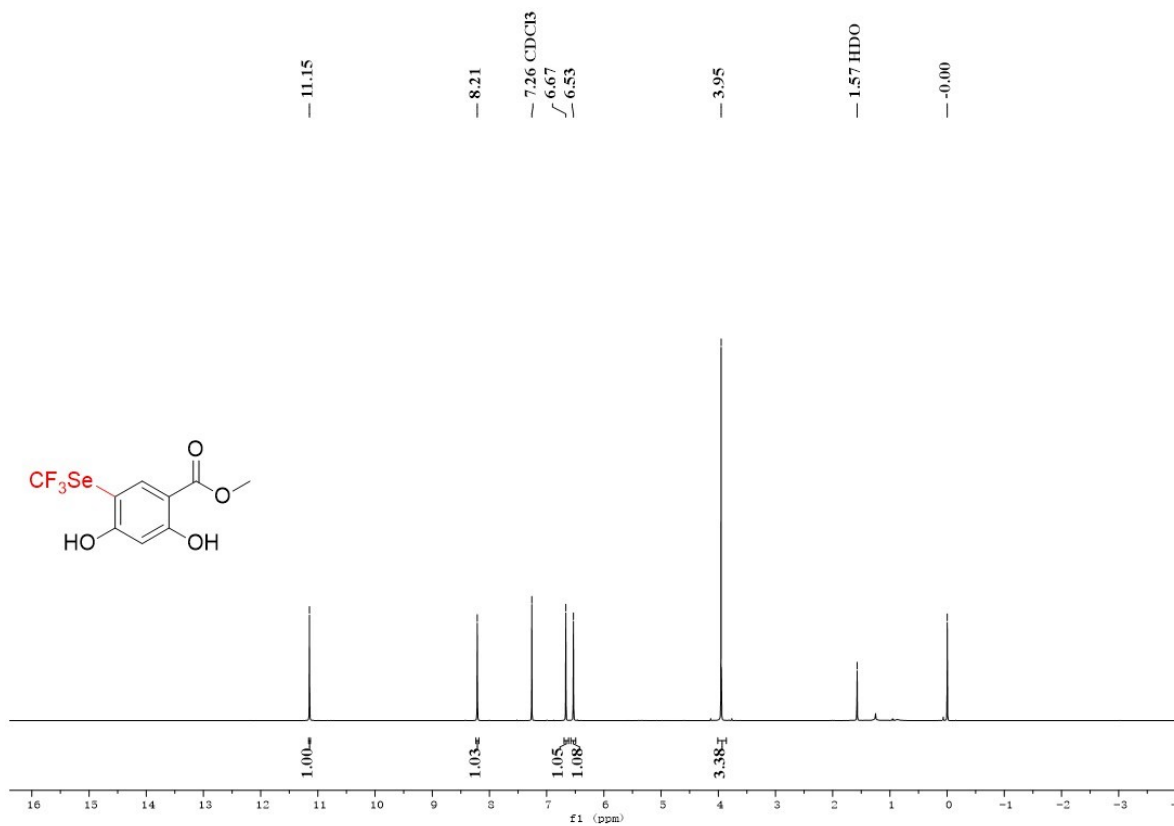
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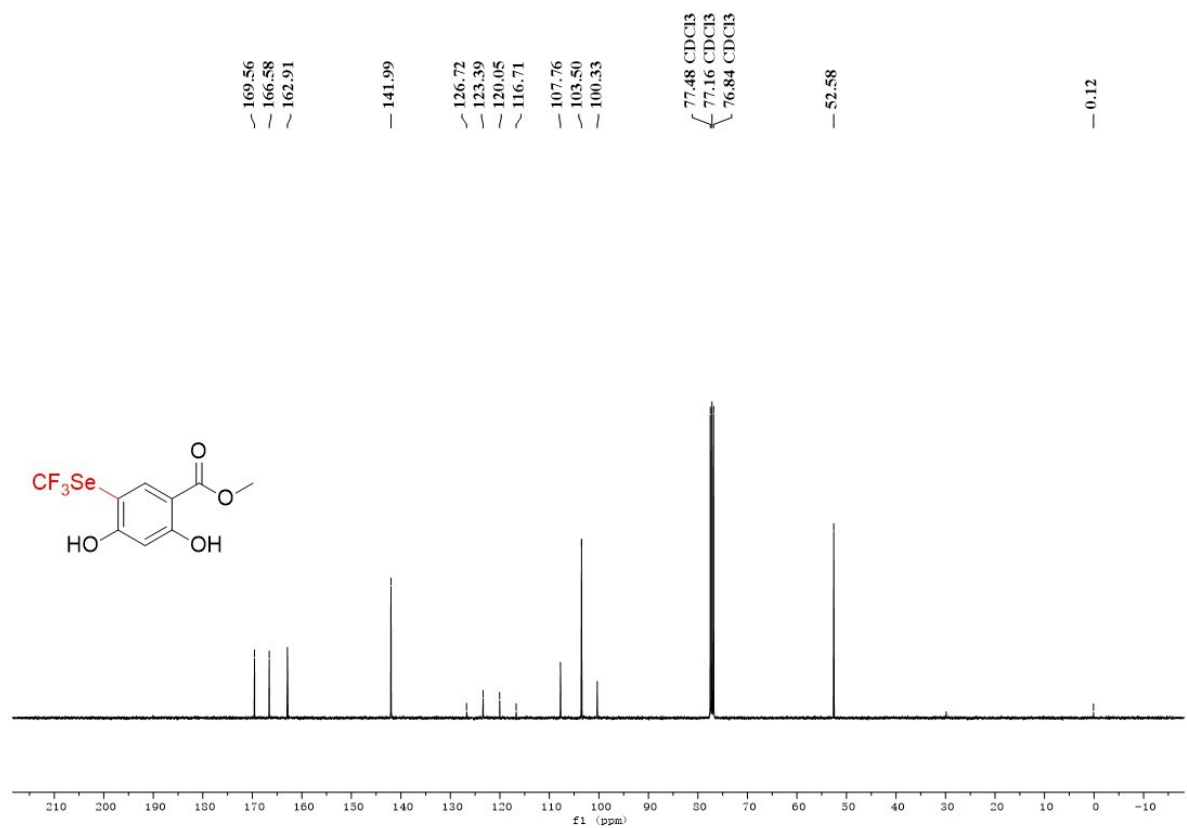
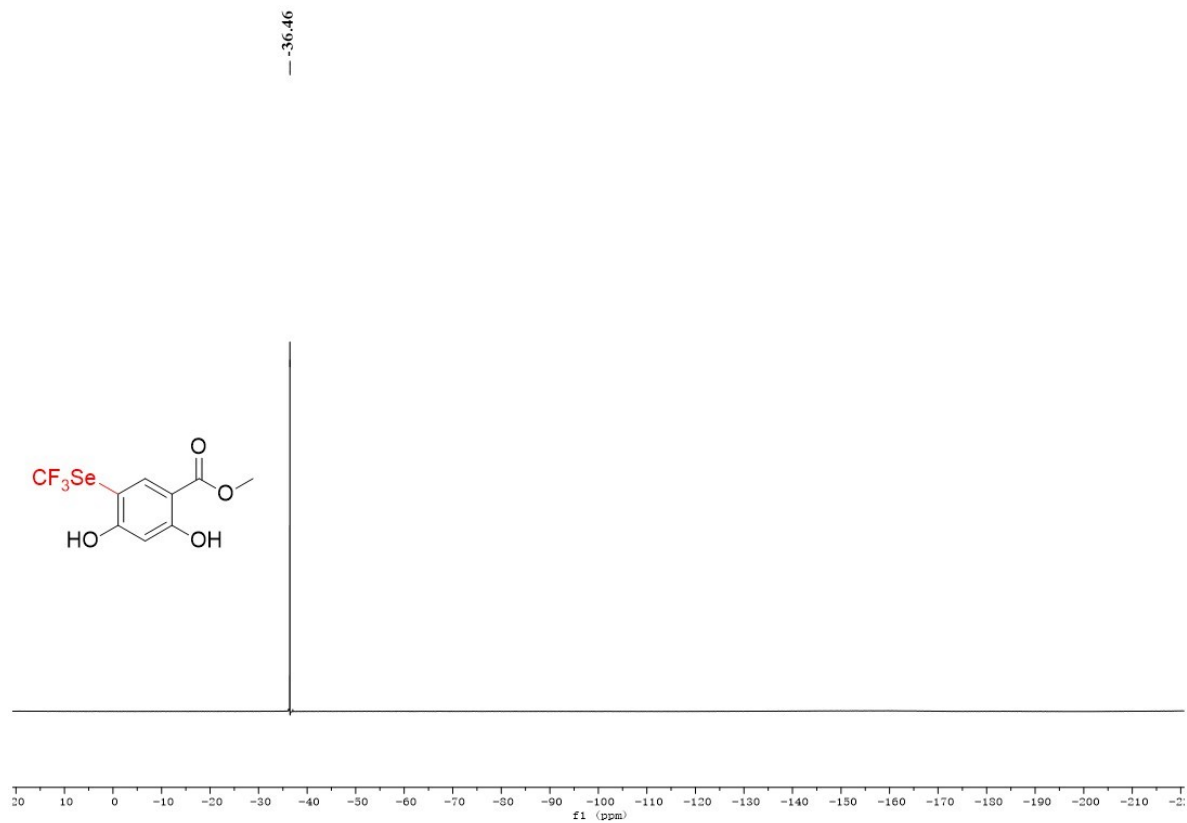
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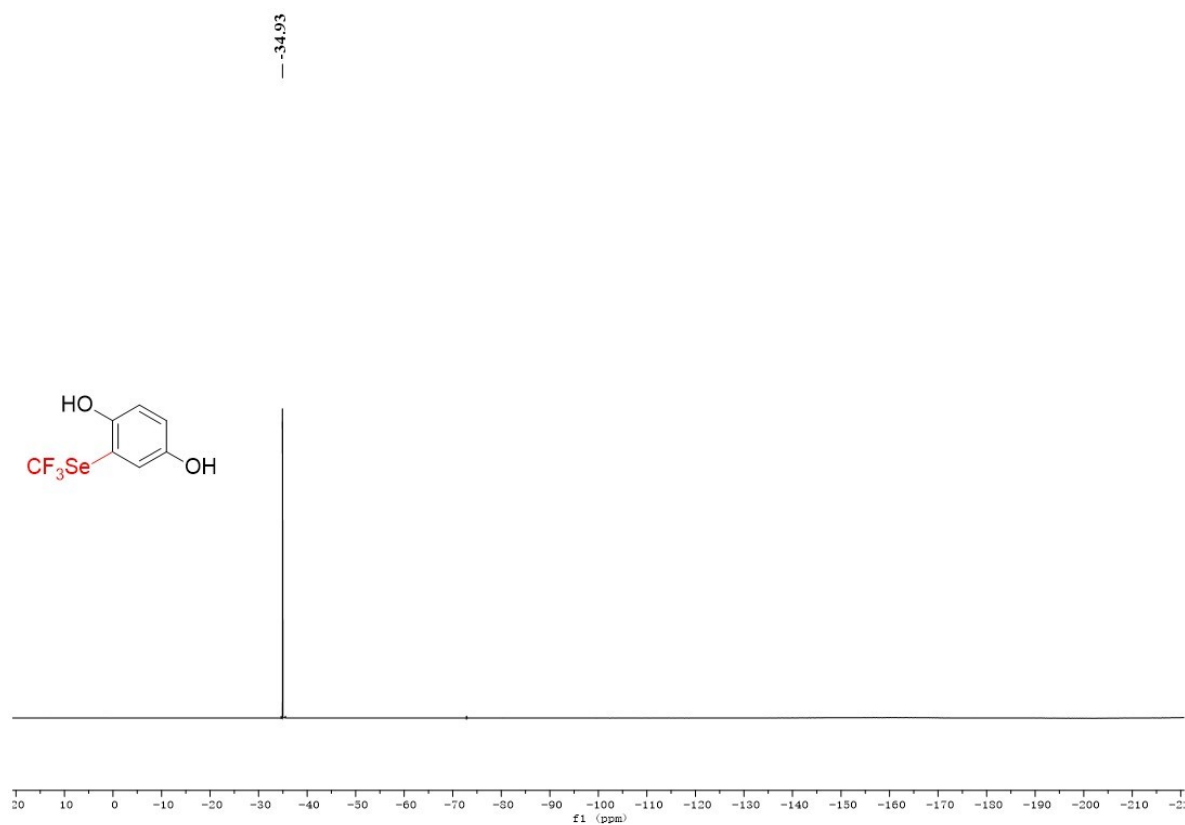
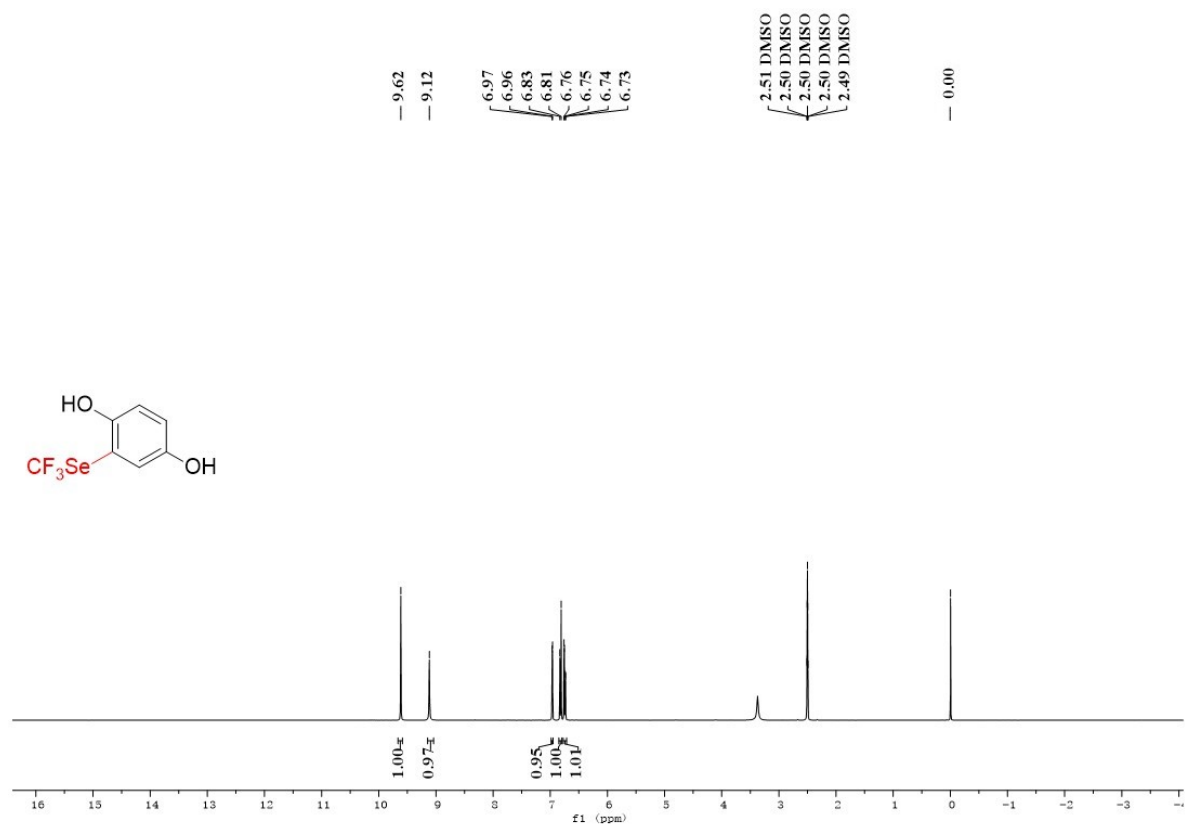


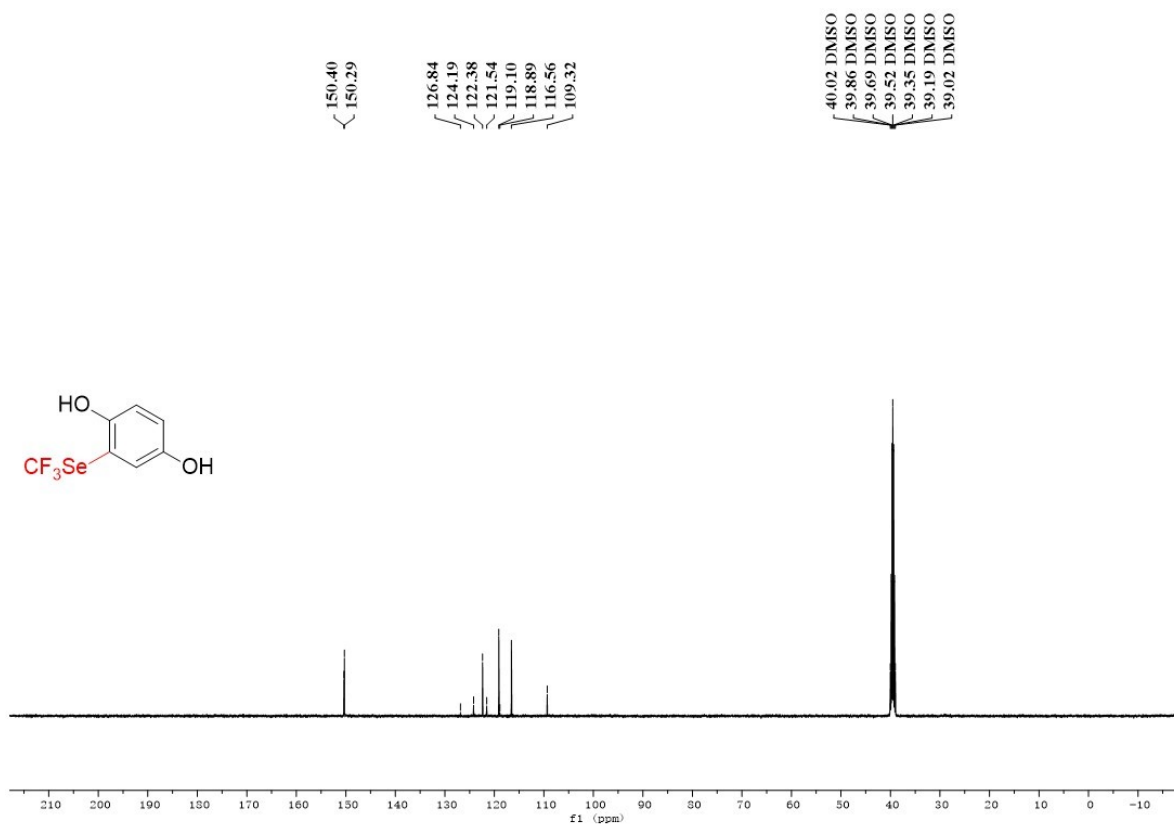
5ar (methyl 2,4-dihydroxy-5-((trifluoromethyl)selanyl)benzoate)



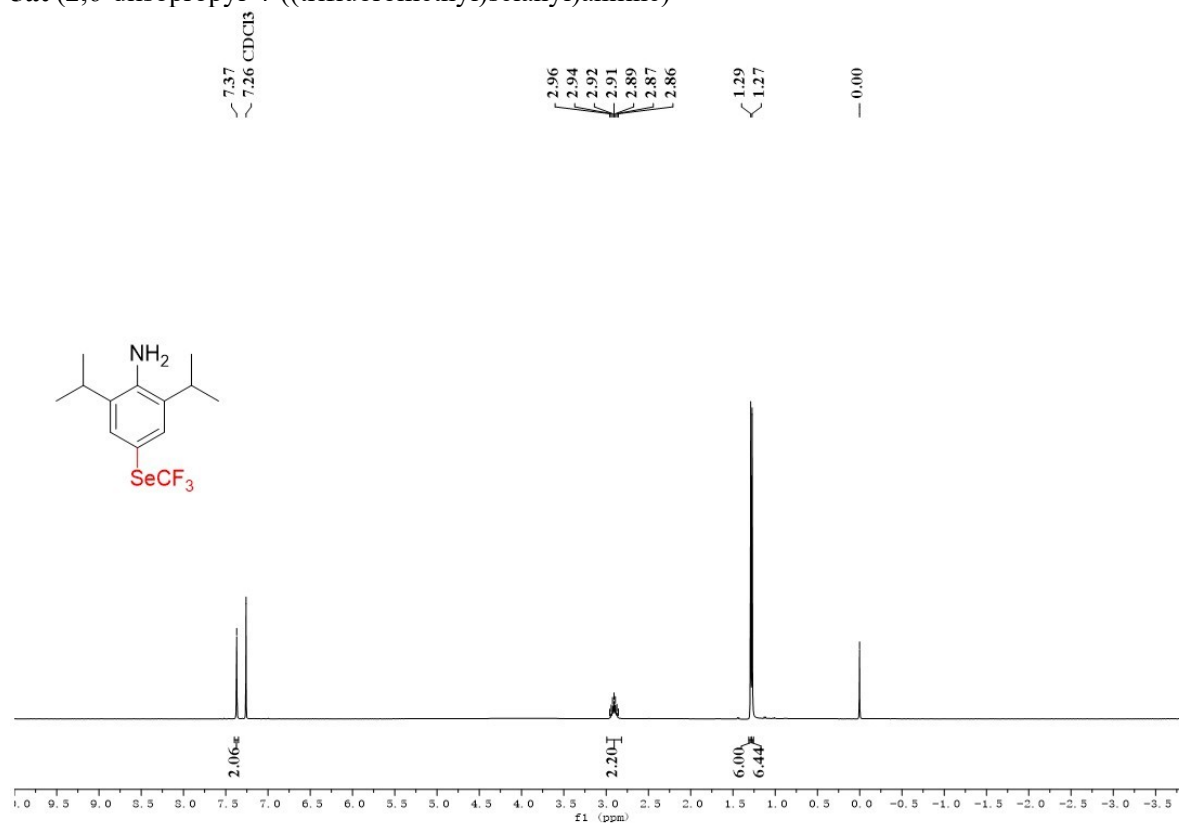


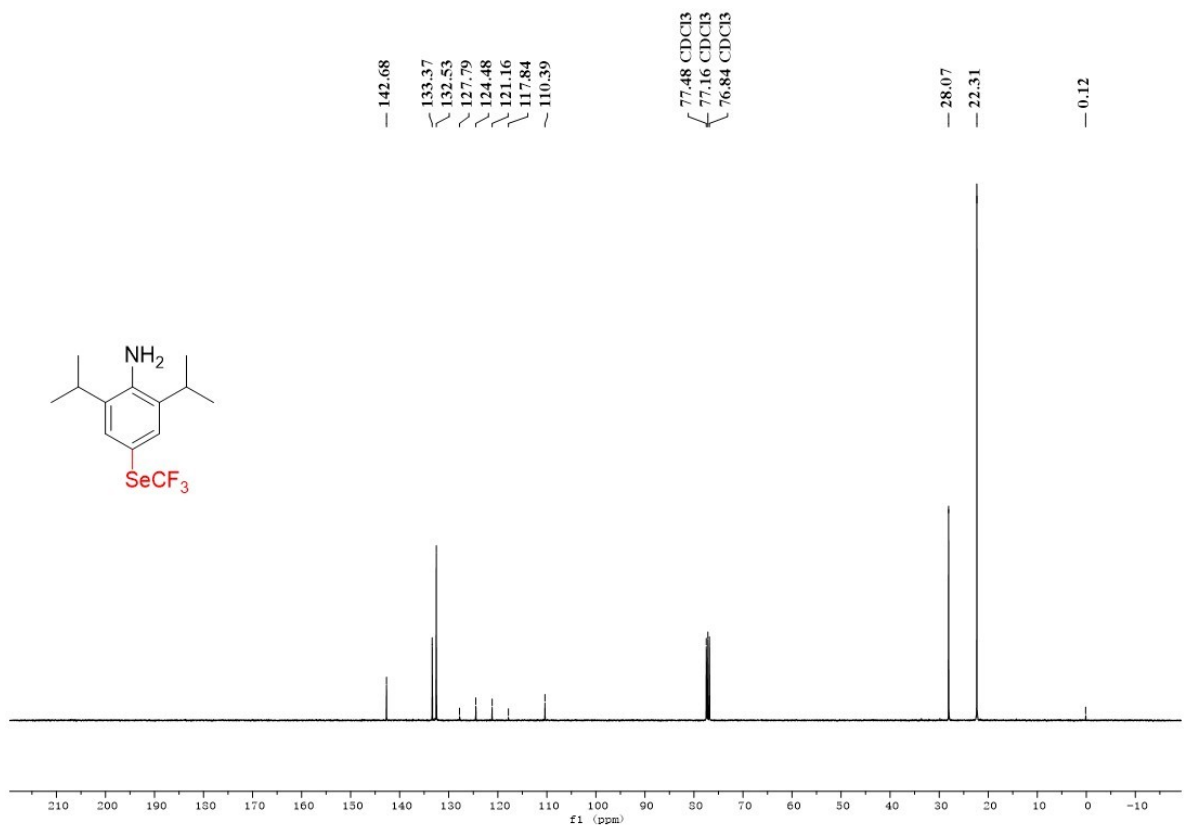
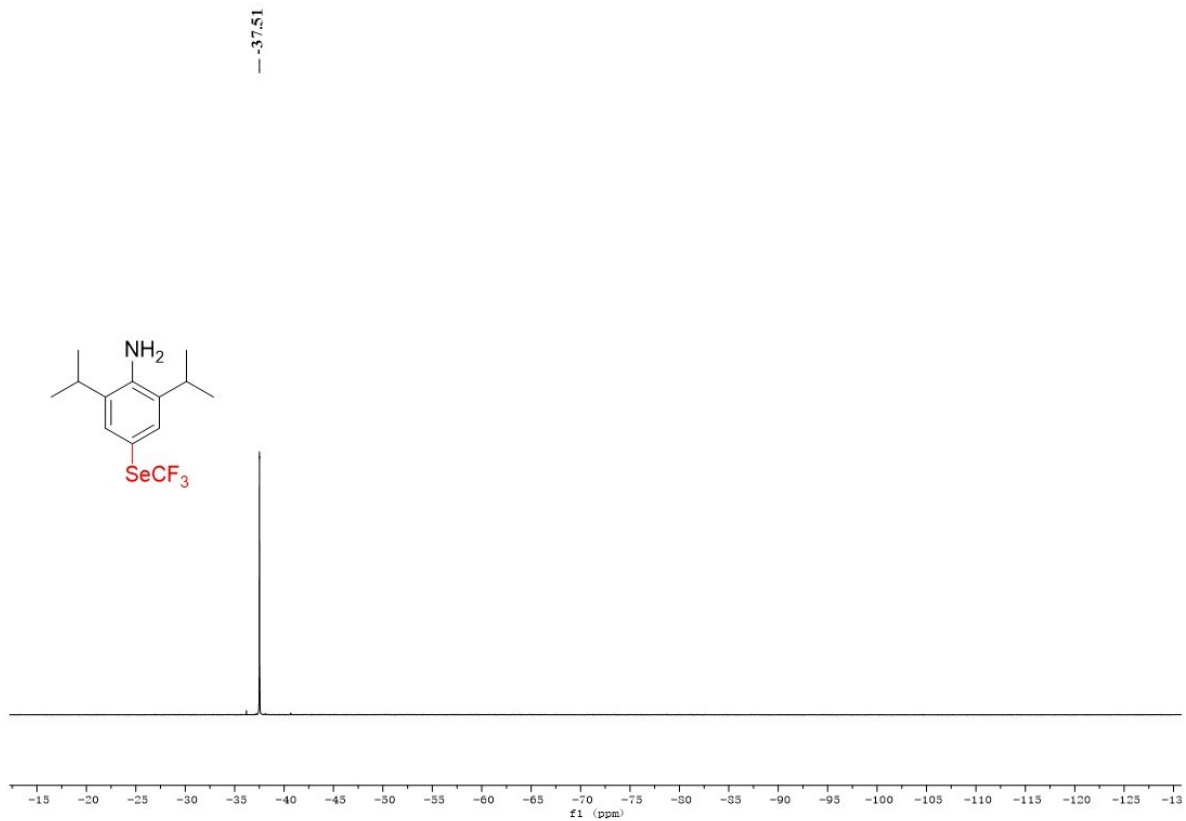
5as (2-((trifluoromethyl)selanyl)benzene-1,4-diol)



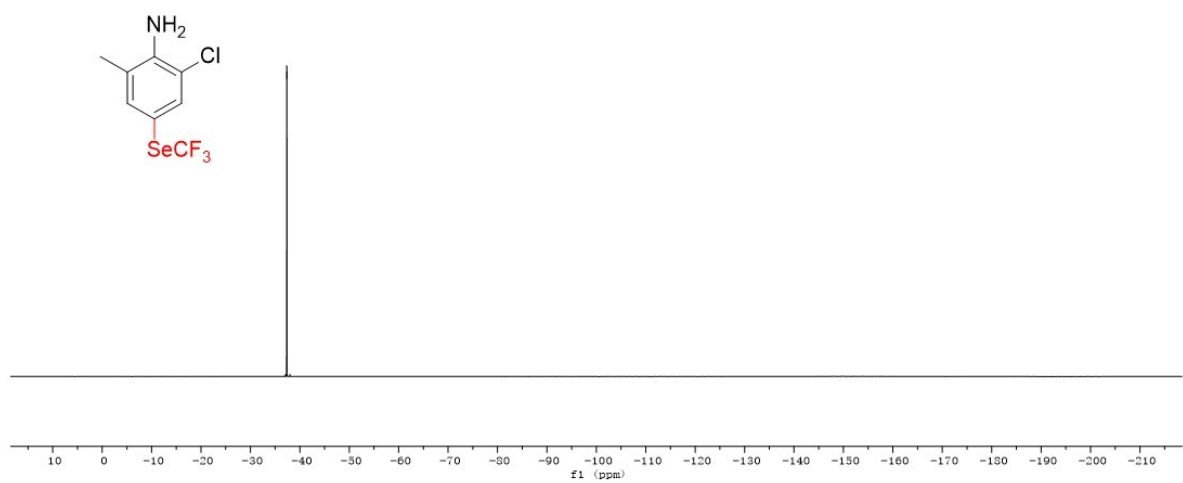
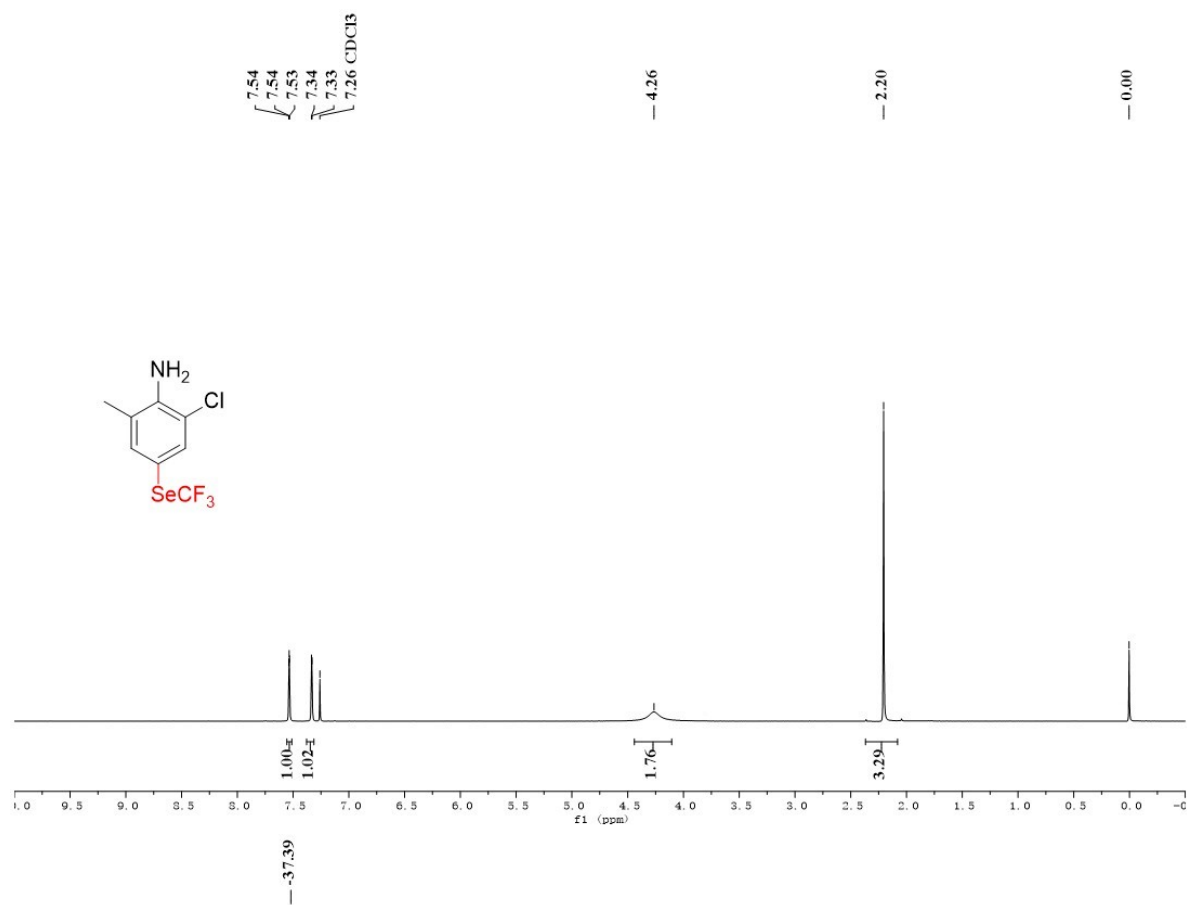


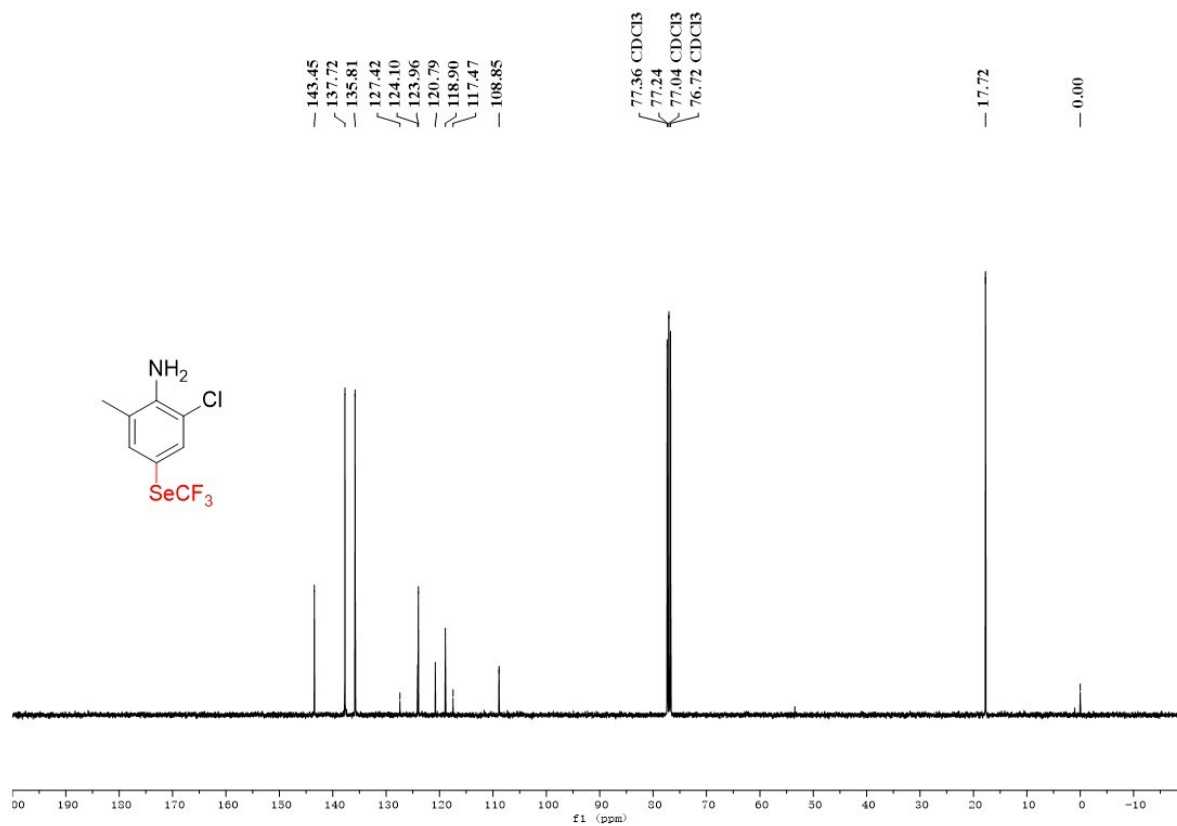
5at (2,6-diisopropyl-4-((trifluoromethyl)selenyl)aniline)



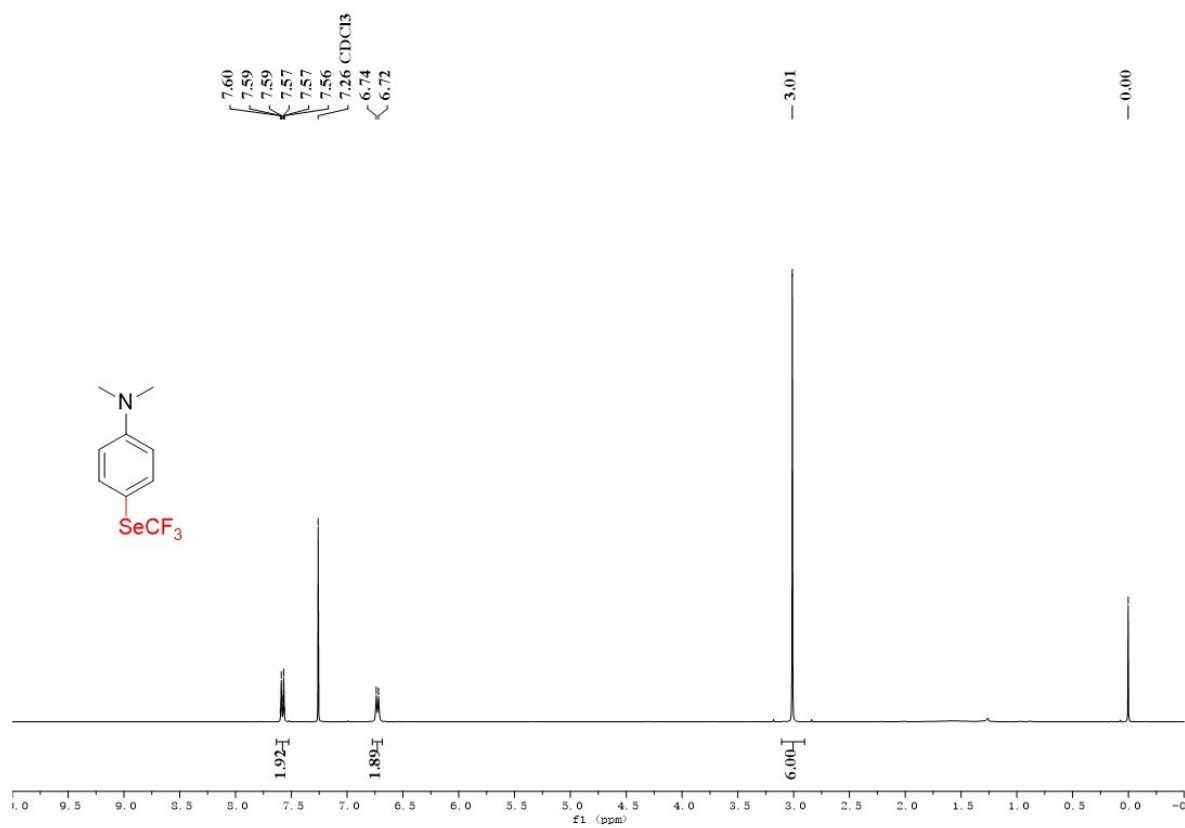


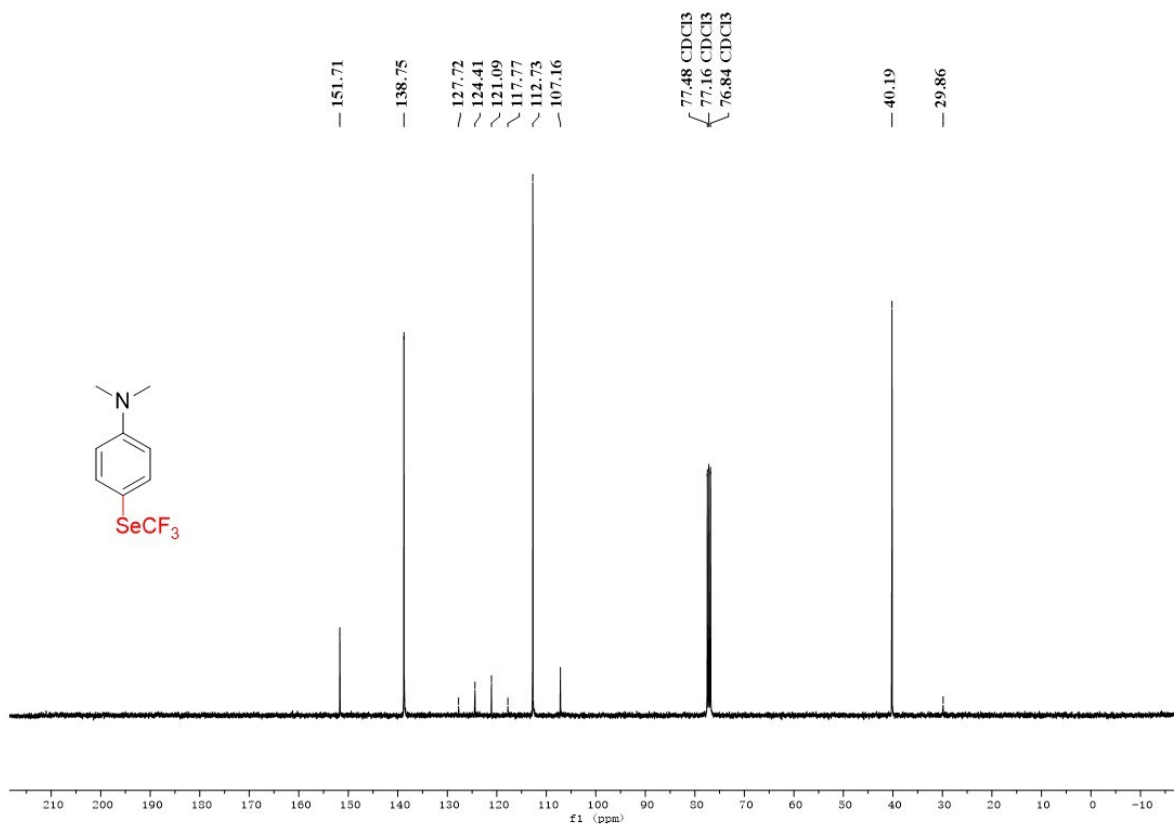
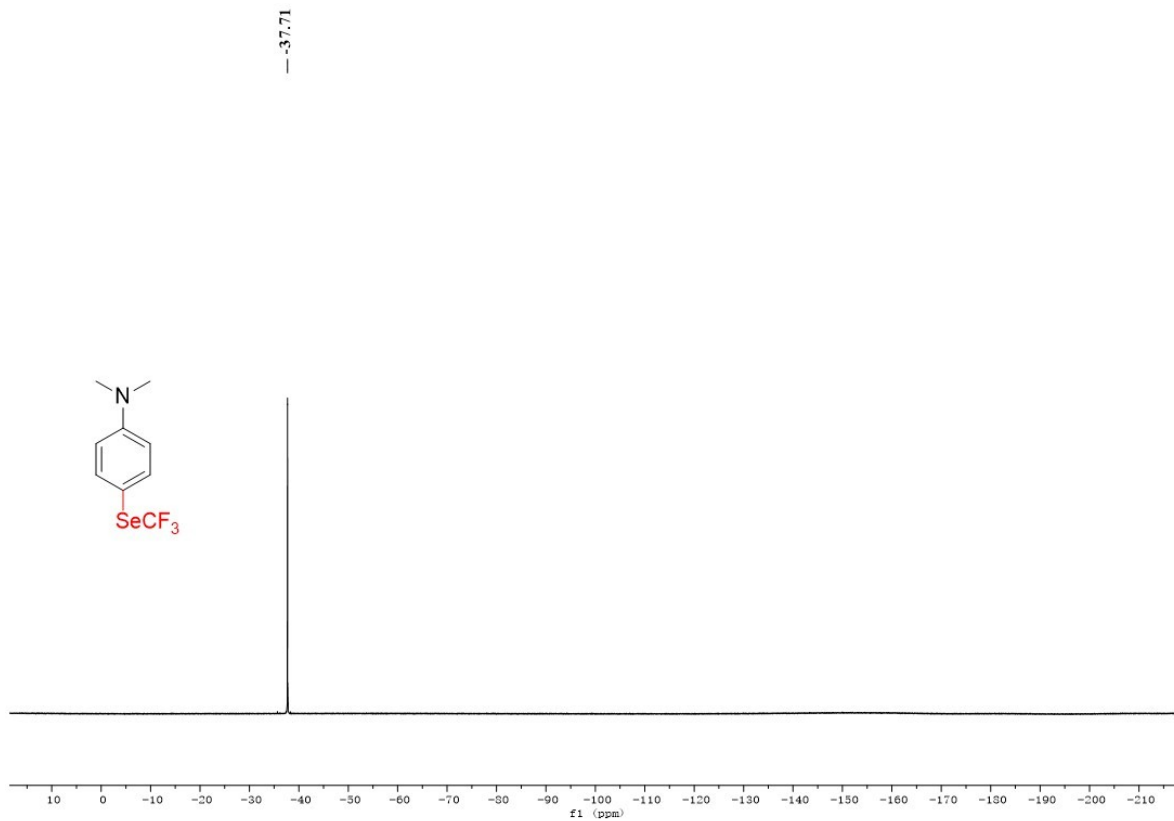
5au (2-chloro-6-methyl-4-((trifluoromethyl)selanyl)aniline)



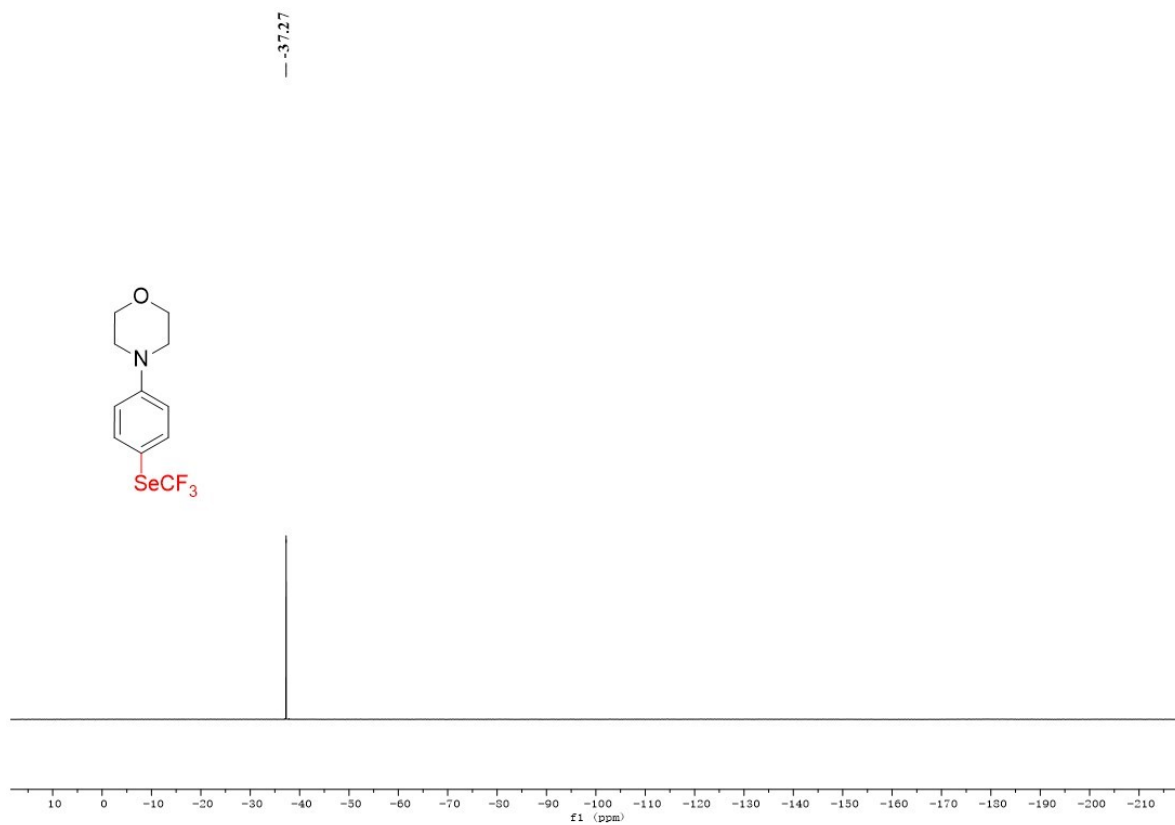
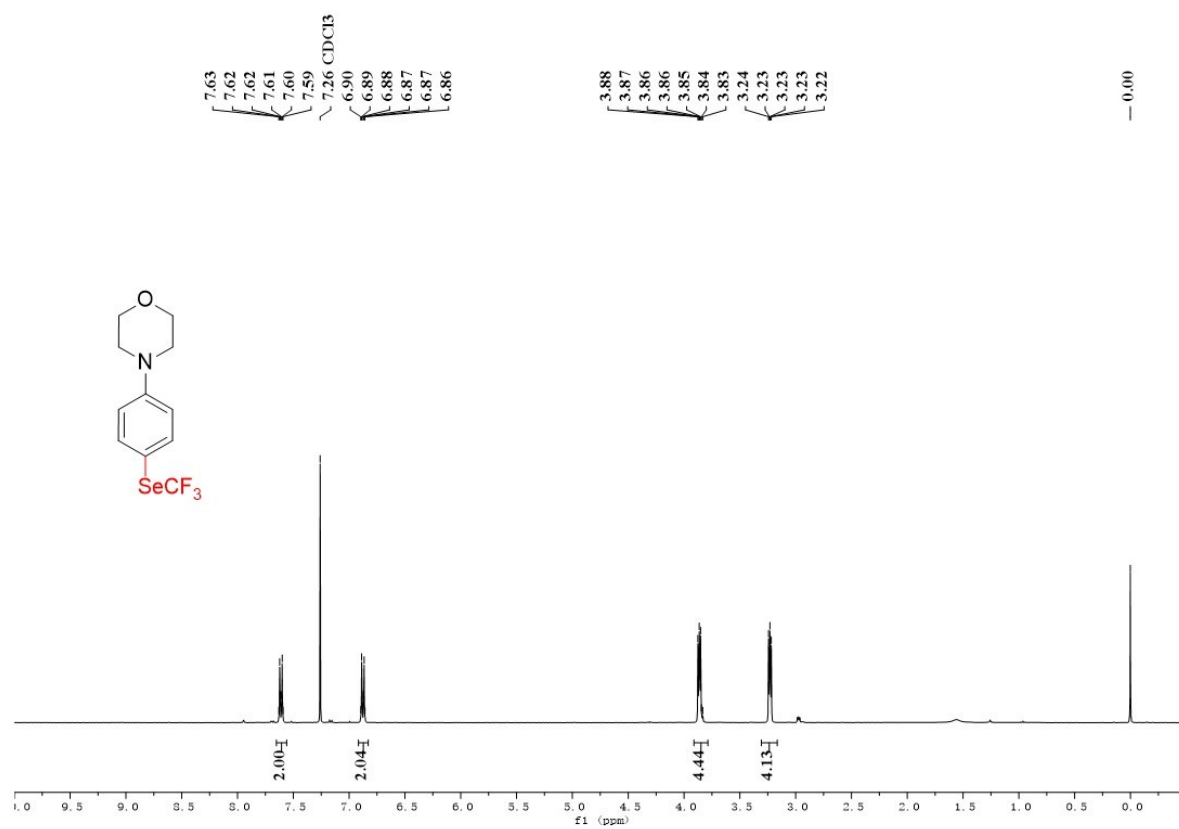


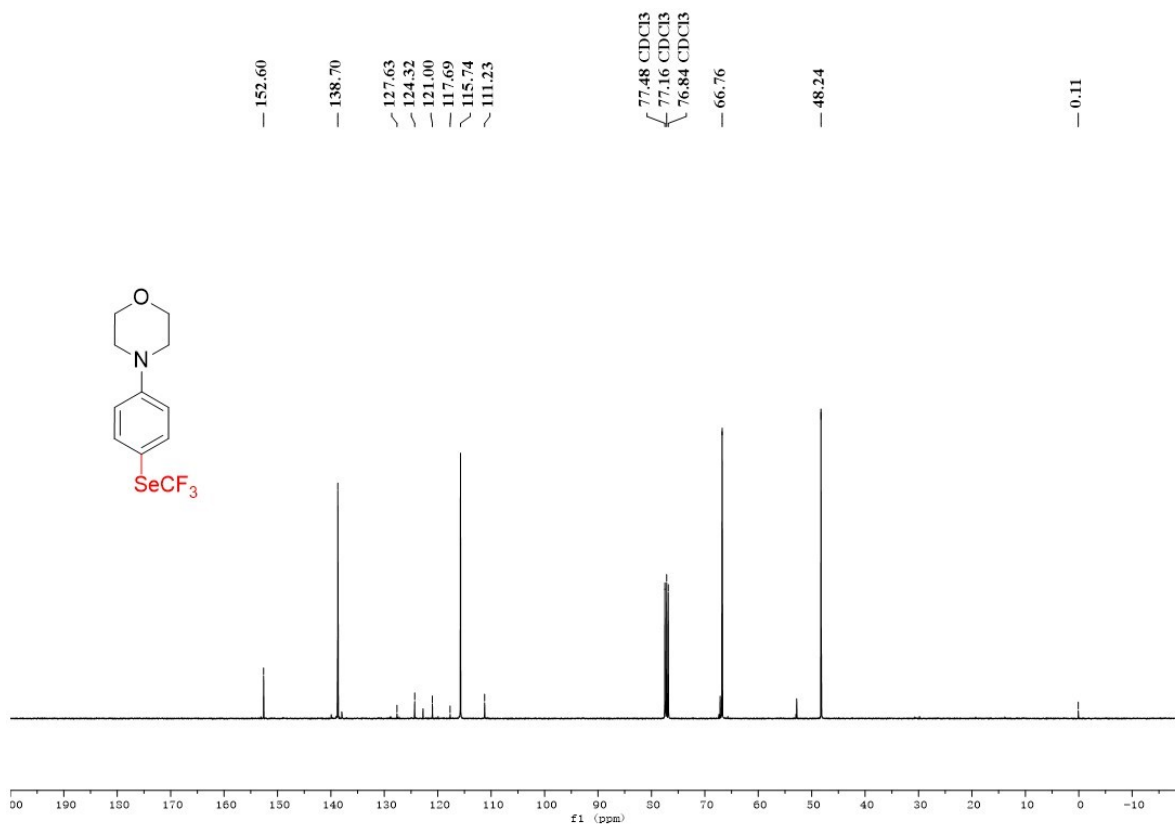
5av (N,N-dimethyl-4-((trifluoromethyl)selanyl)aniline)



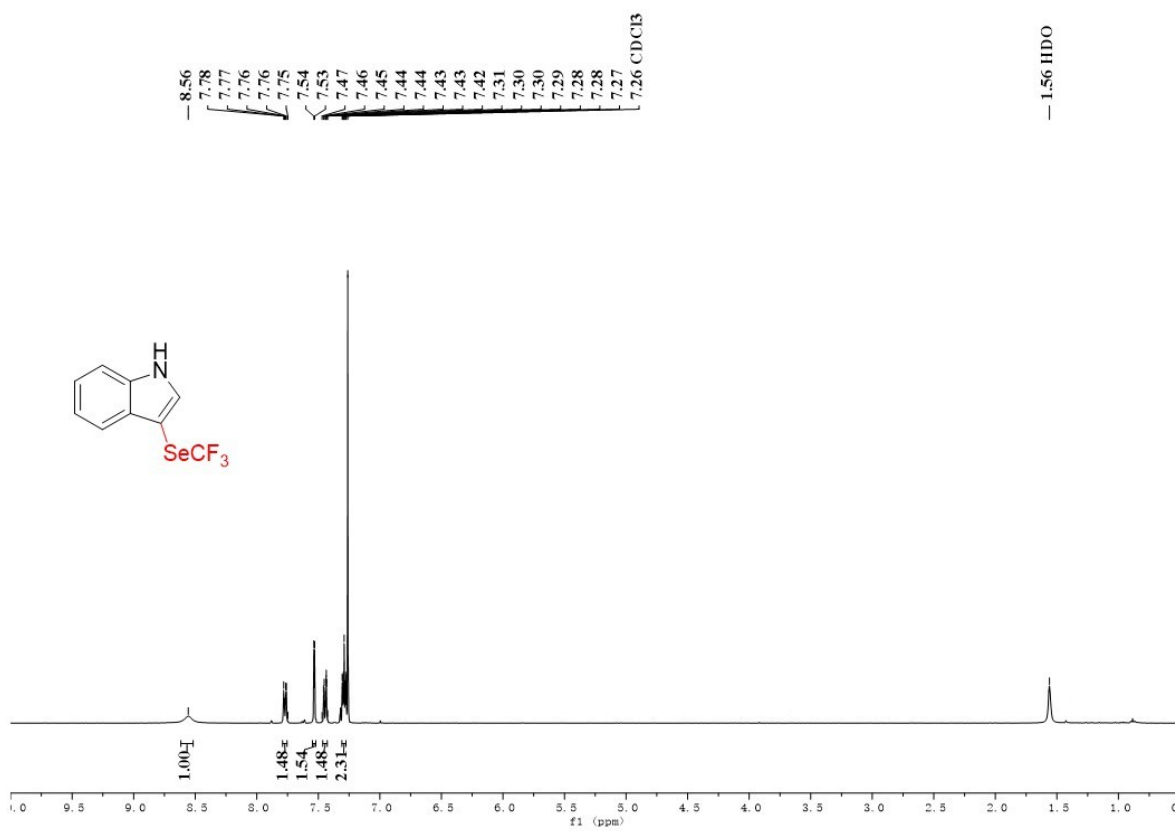


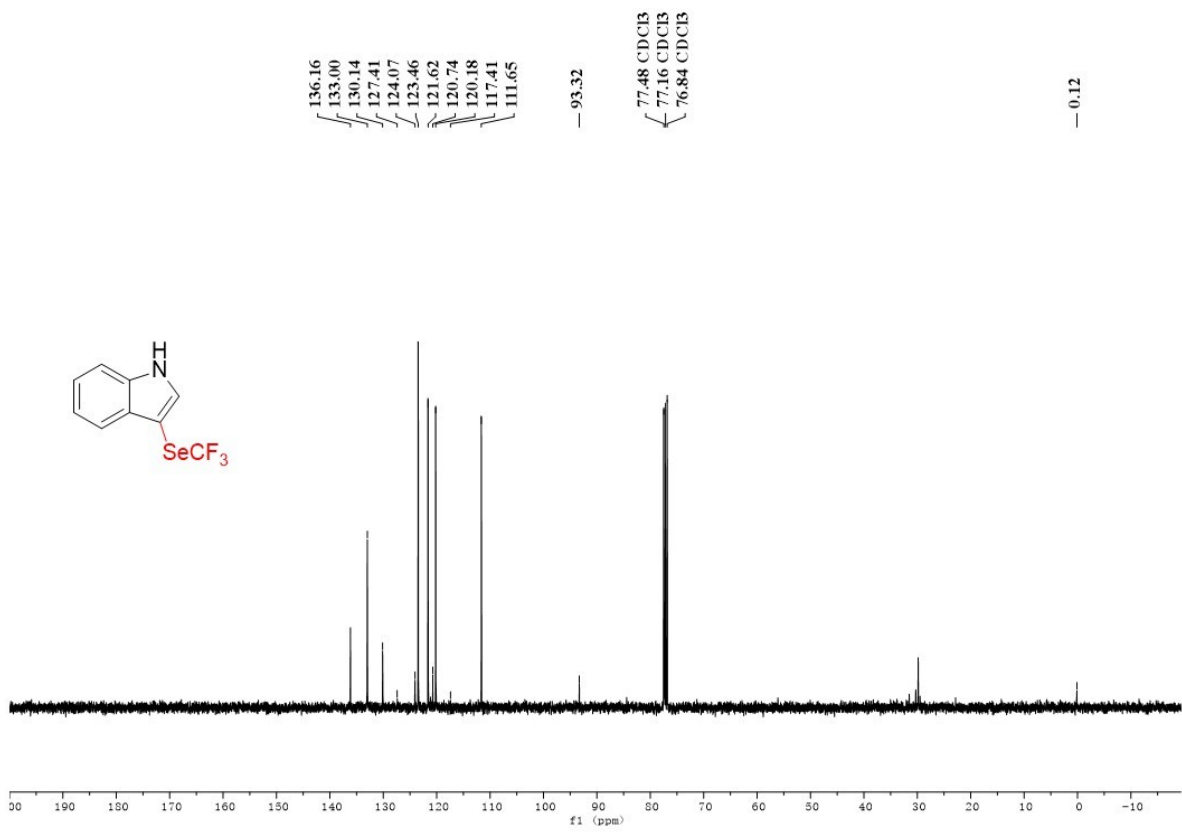
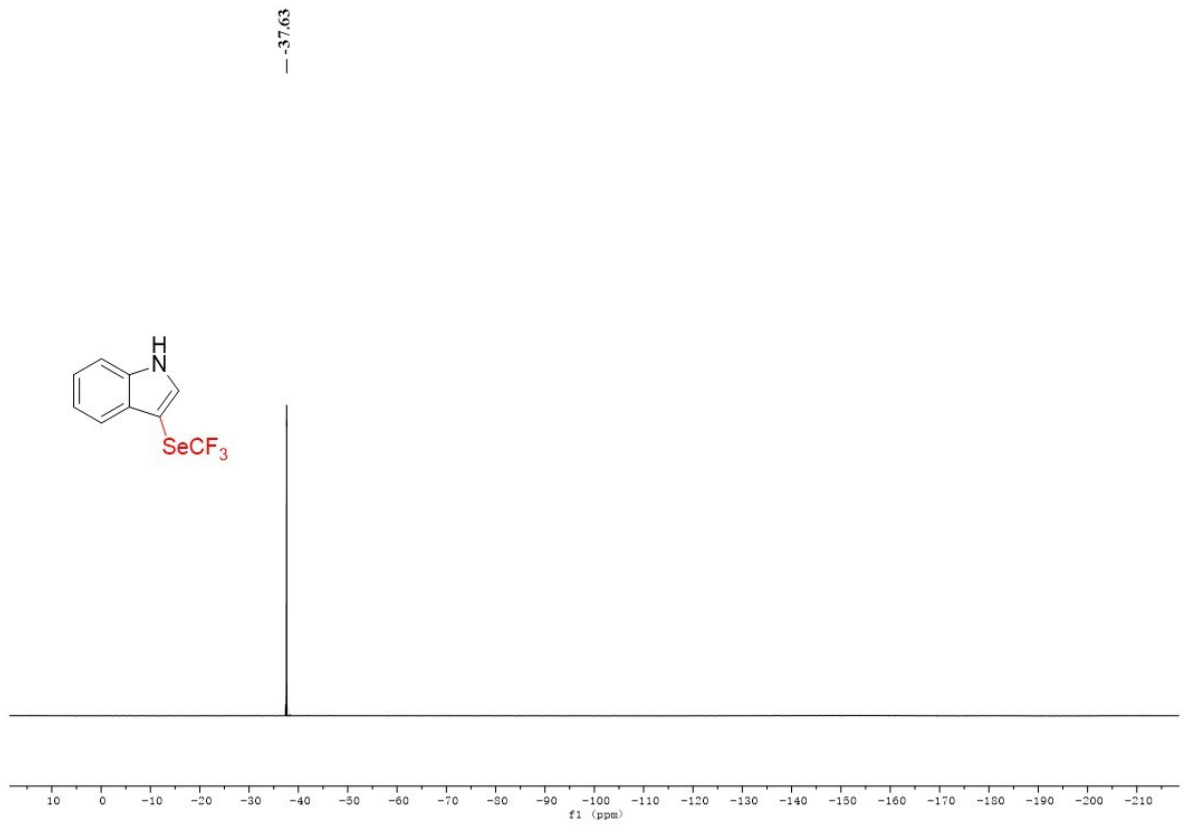
5aw (4-(4-((trifluoromethyl)selenanyl)phenyl)morpholine)



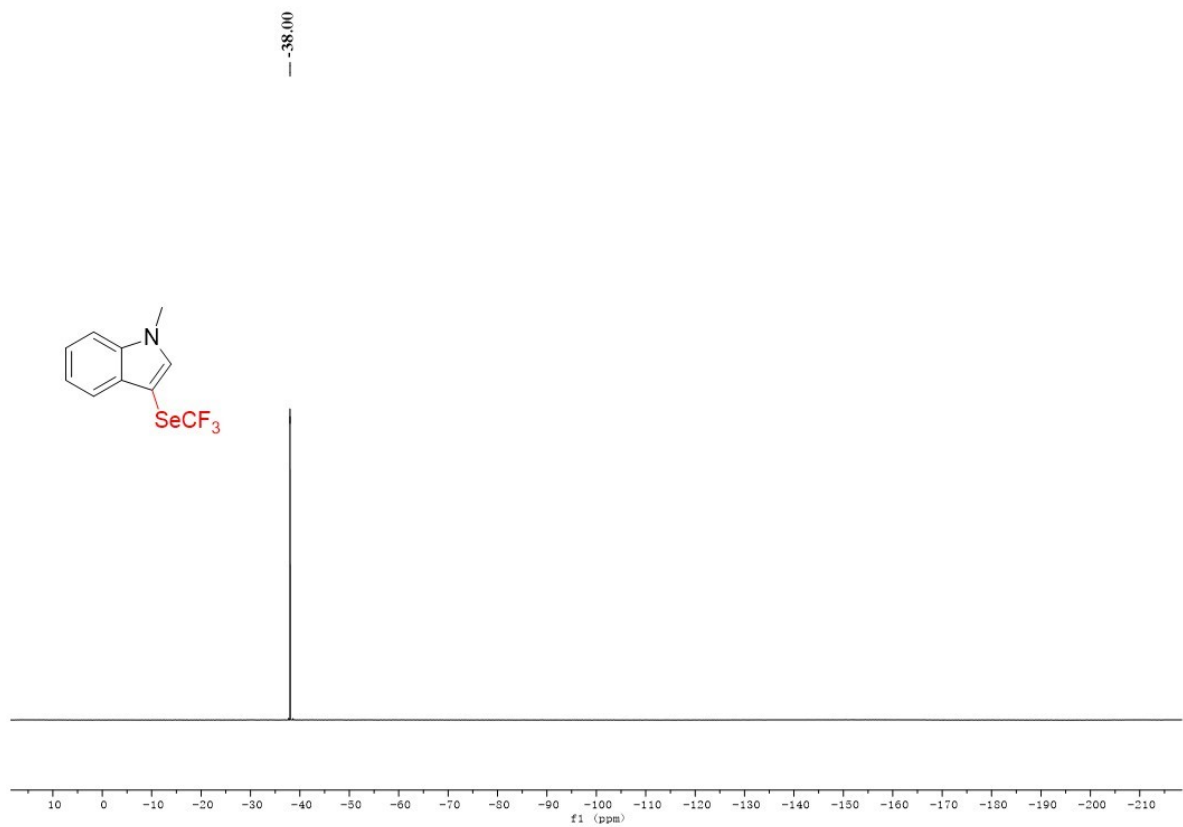
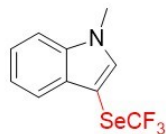
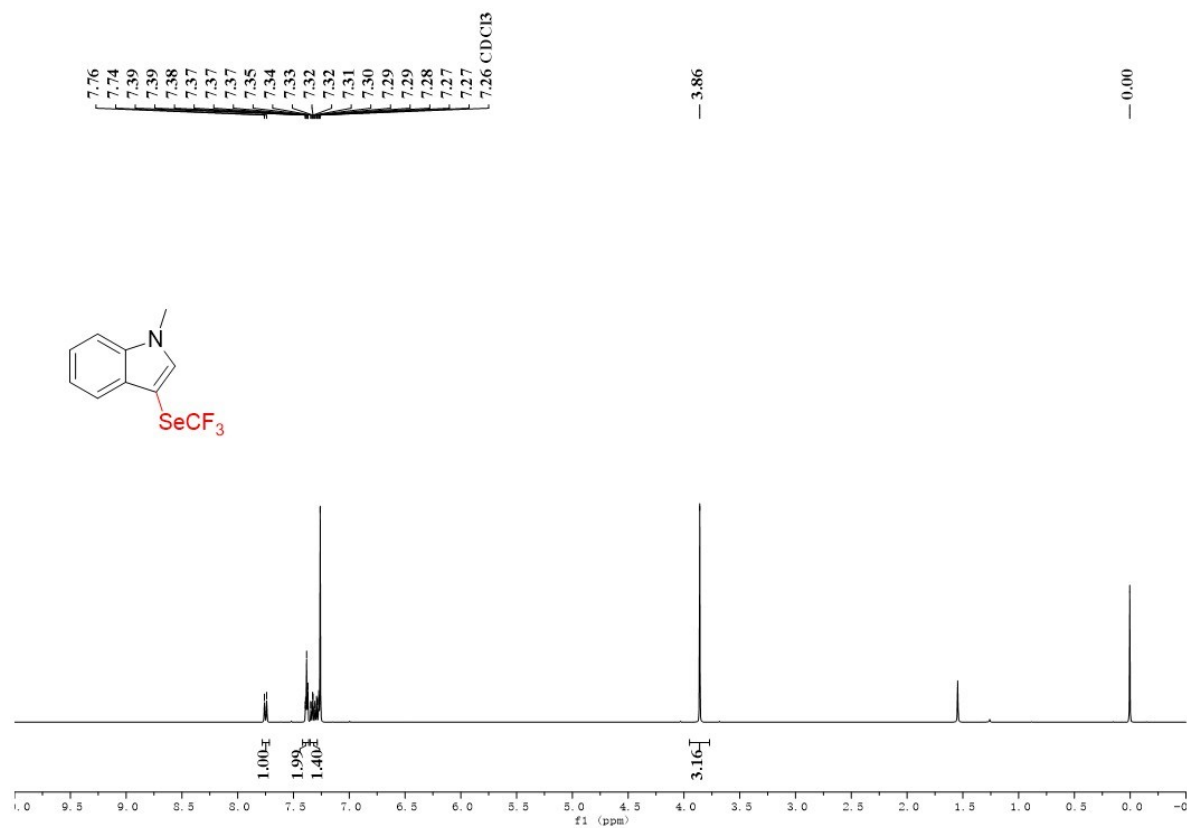


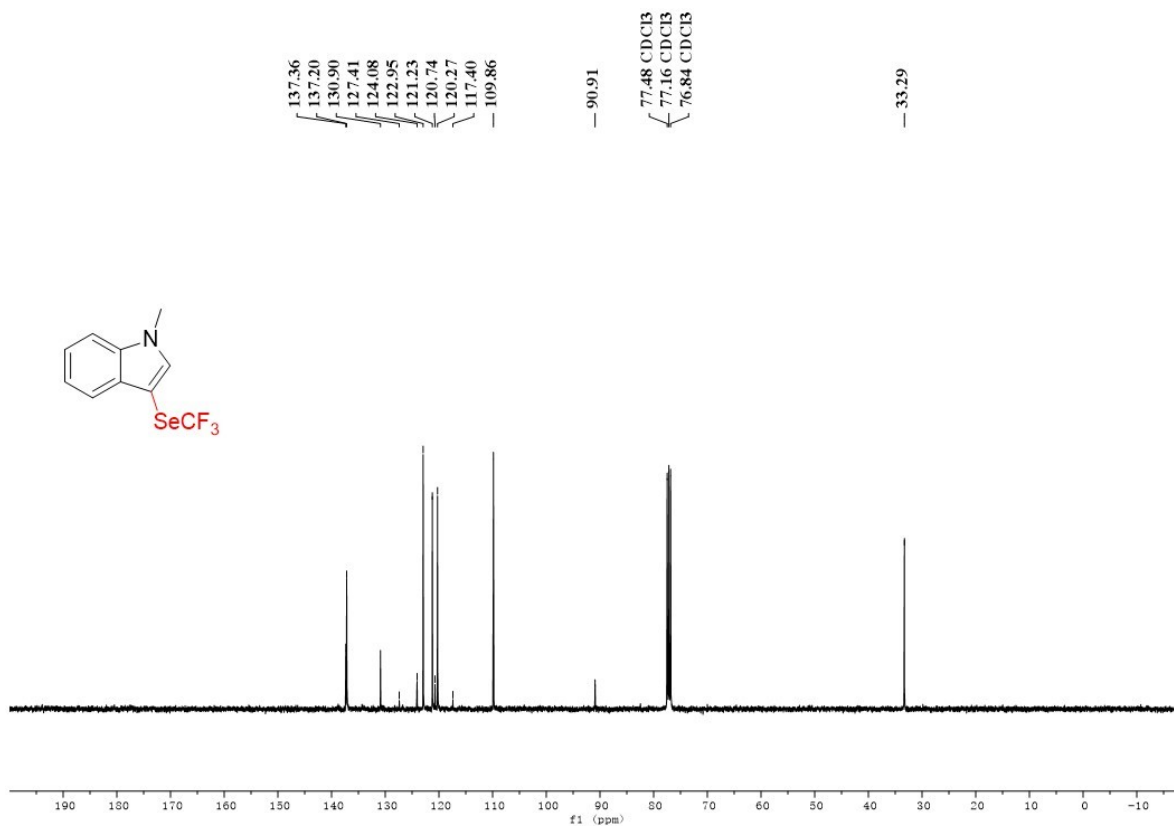
5axa (3-((trifluoromethyl)selenanyl)-1H-indole)



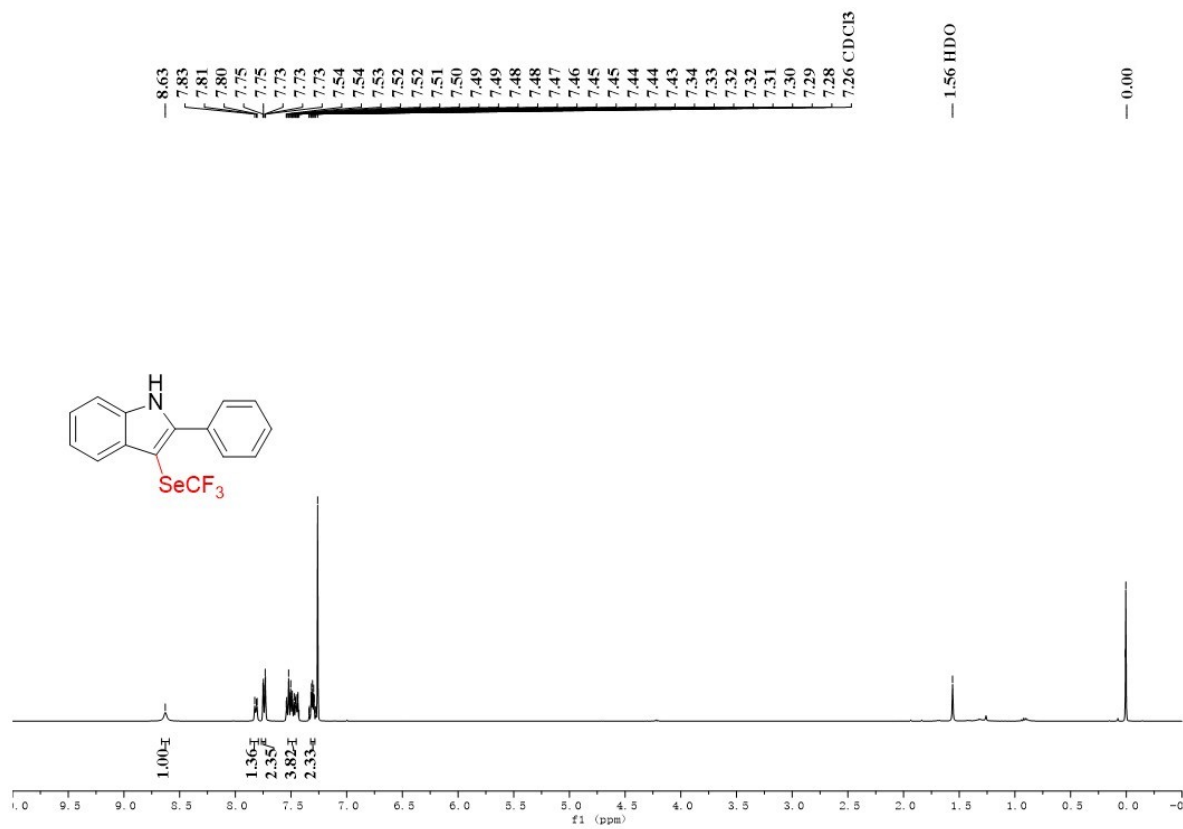


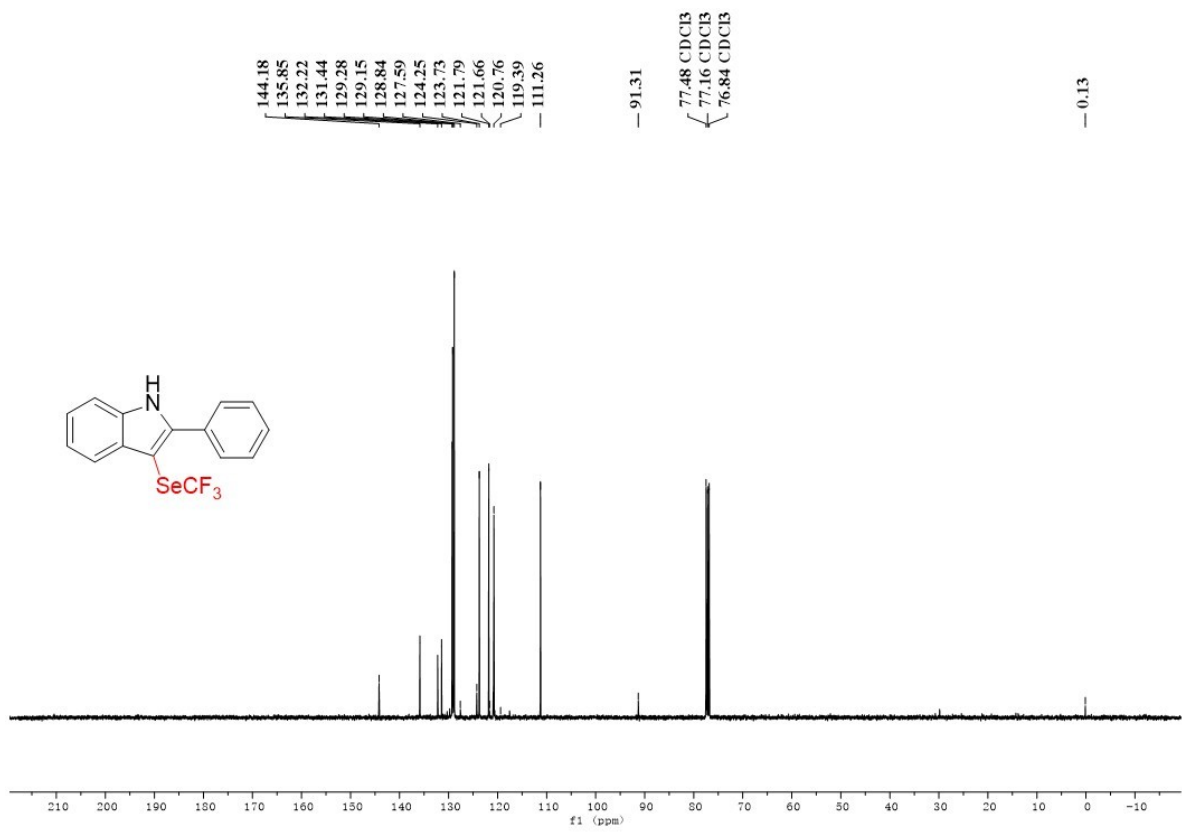
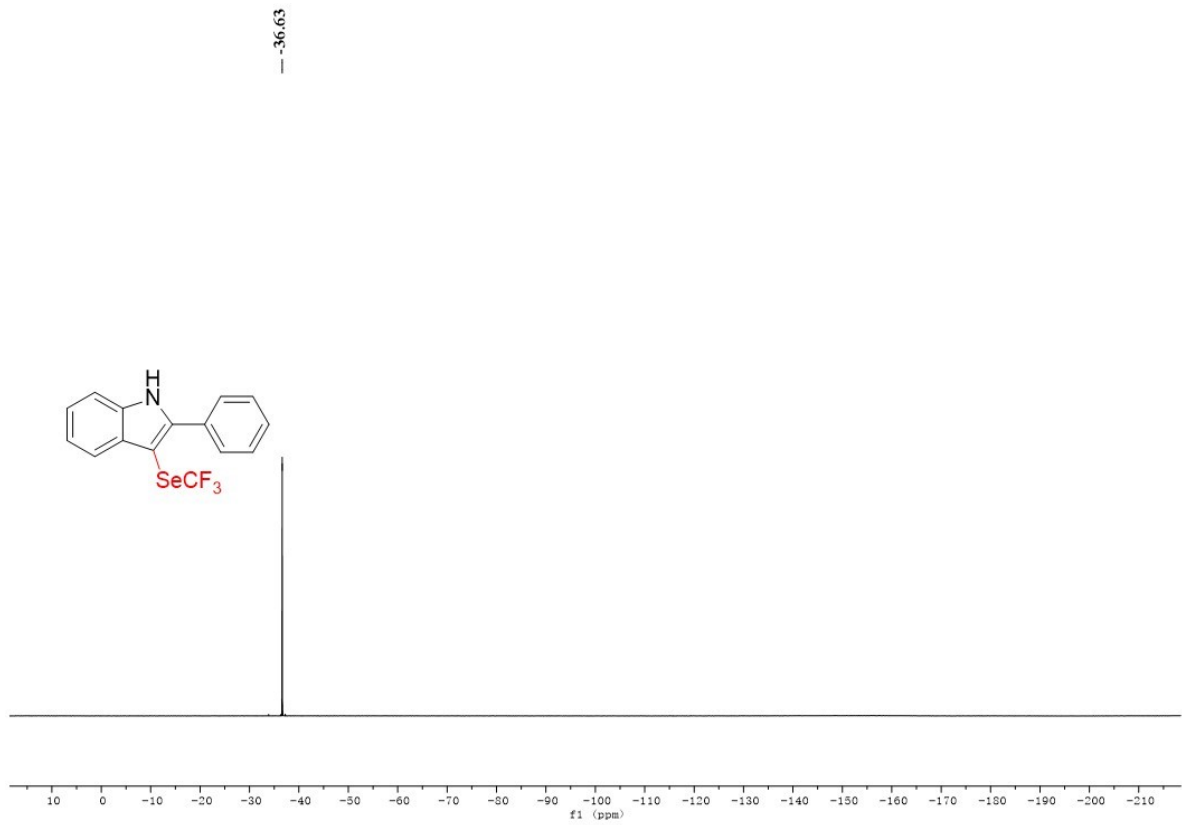
5axb (3-((trifluoromethyl)selanyl)-1H-indole)



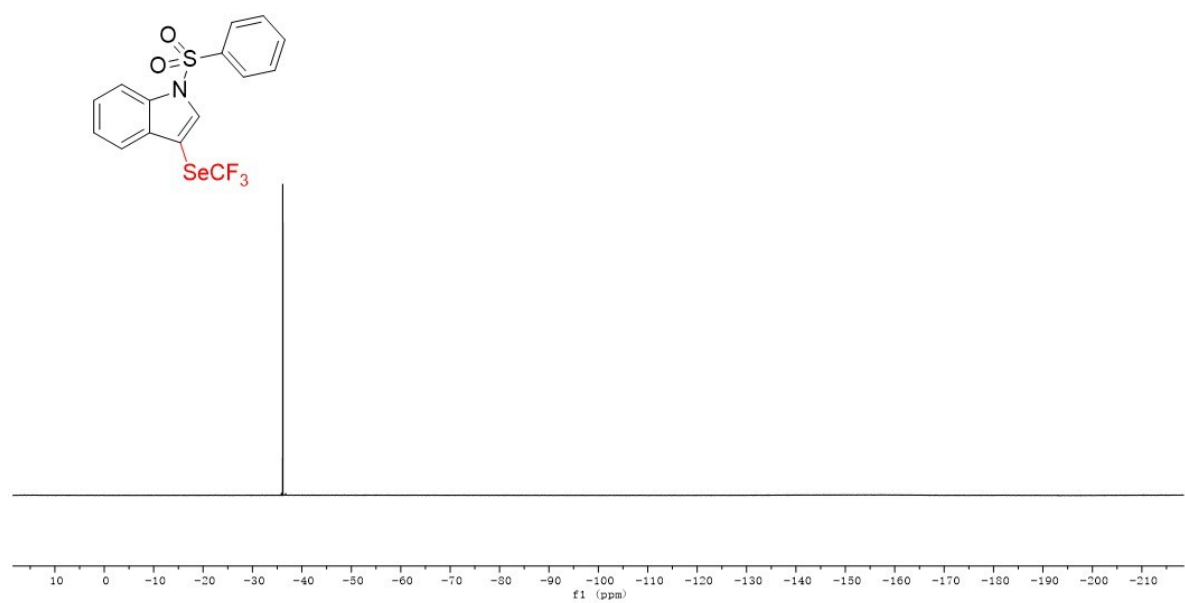
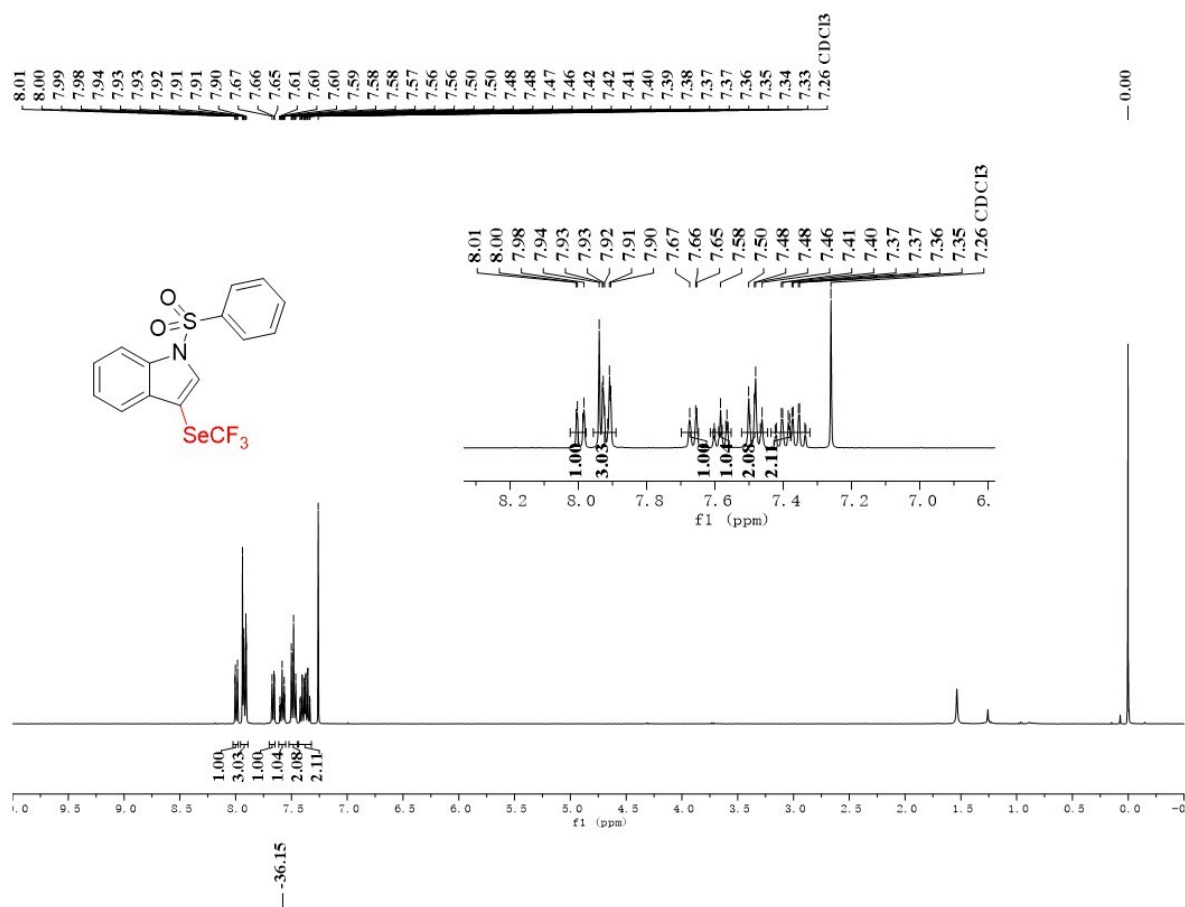


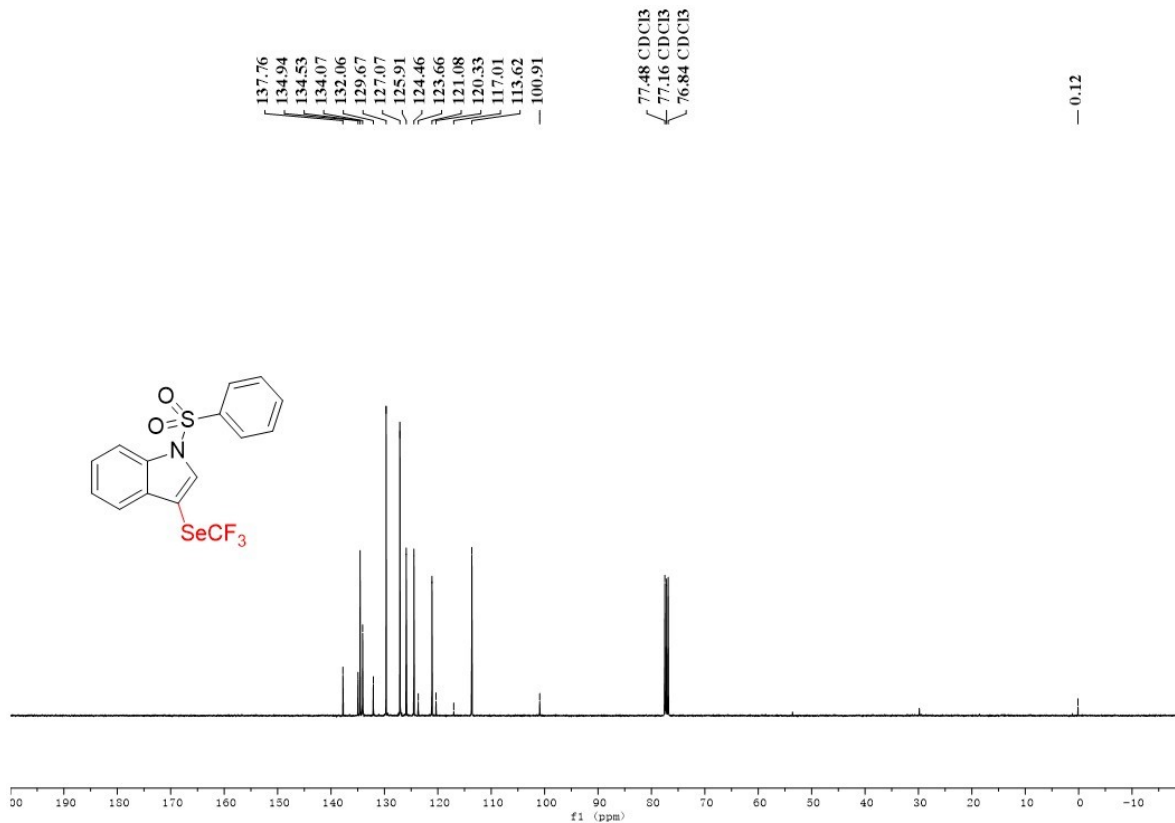
5axc (2-phenyl-3-((trifluoromethyl)selenyl)-1H-indole)



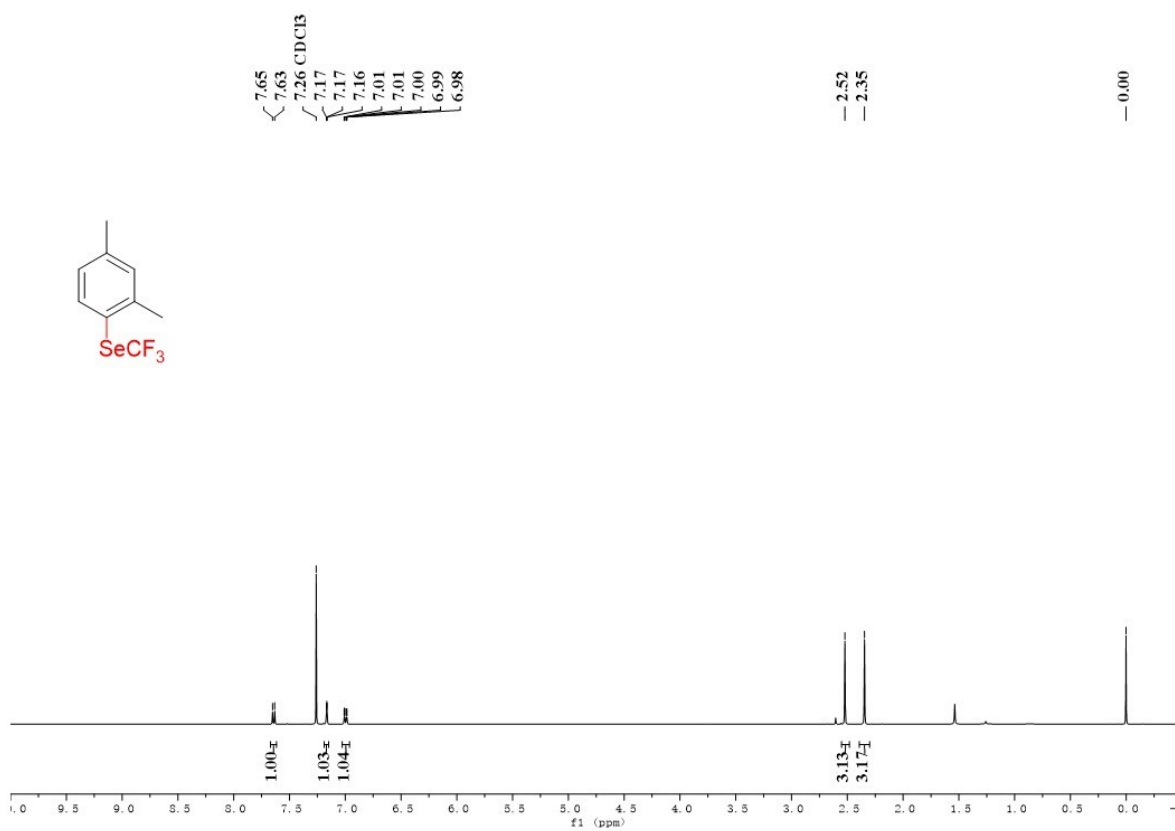


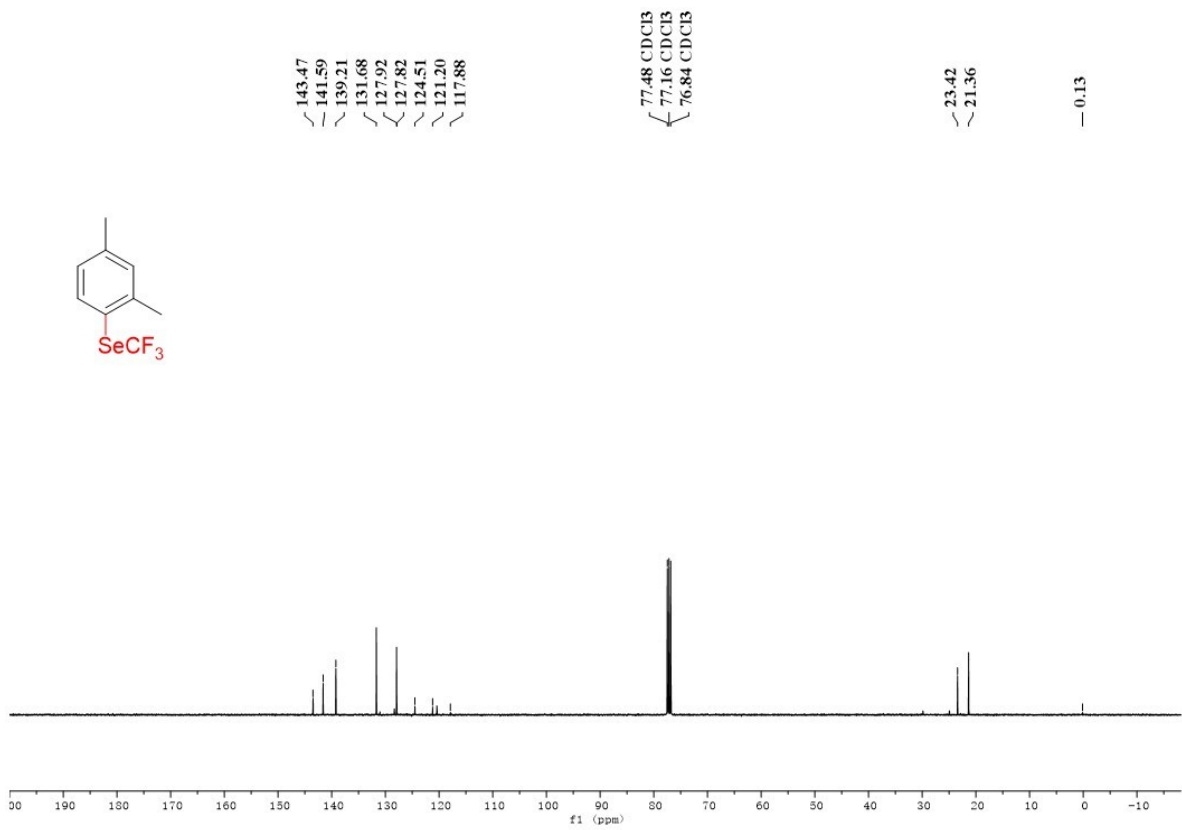
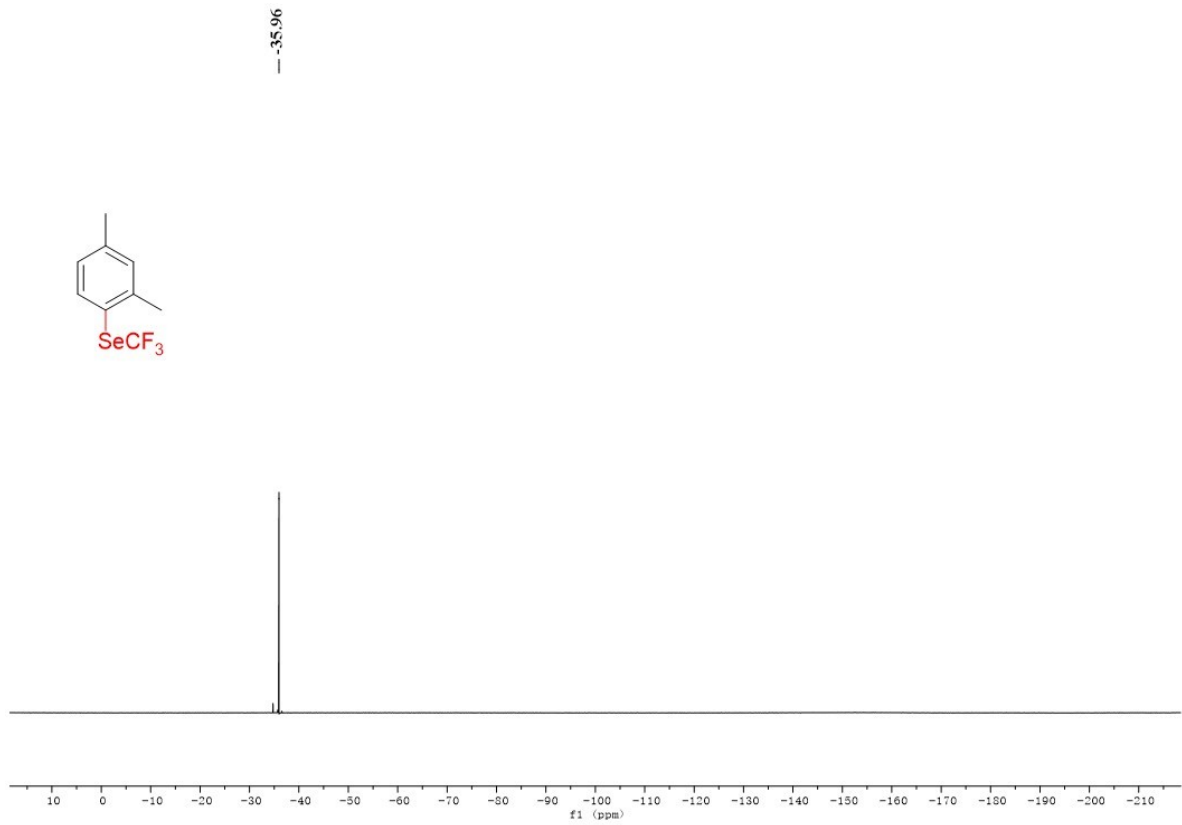
5axd (1-(phenylsulfonyl)-3-((trifluoromethyl)selenyl)-1H-indole)



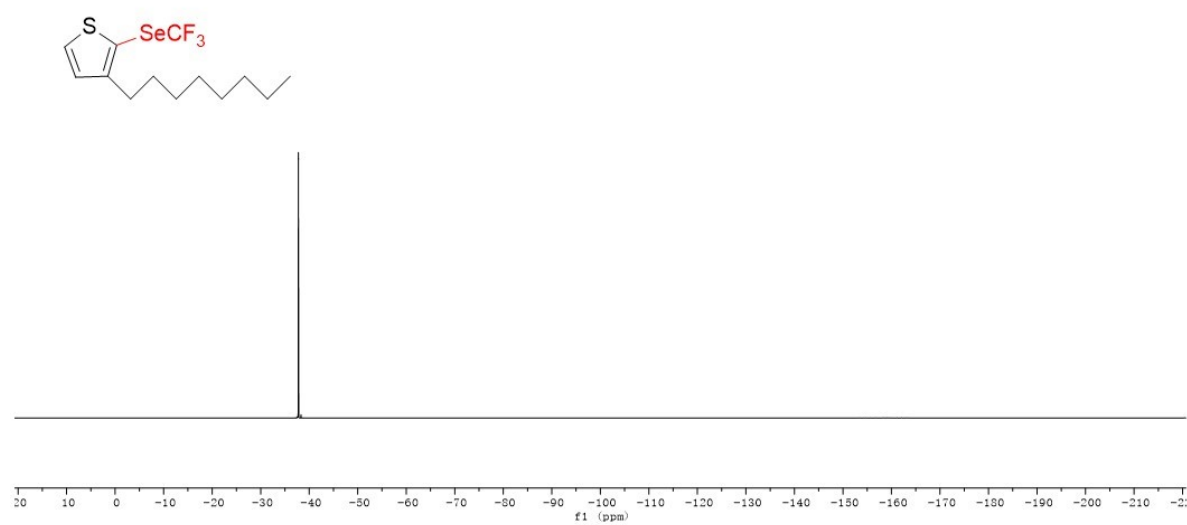
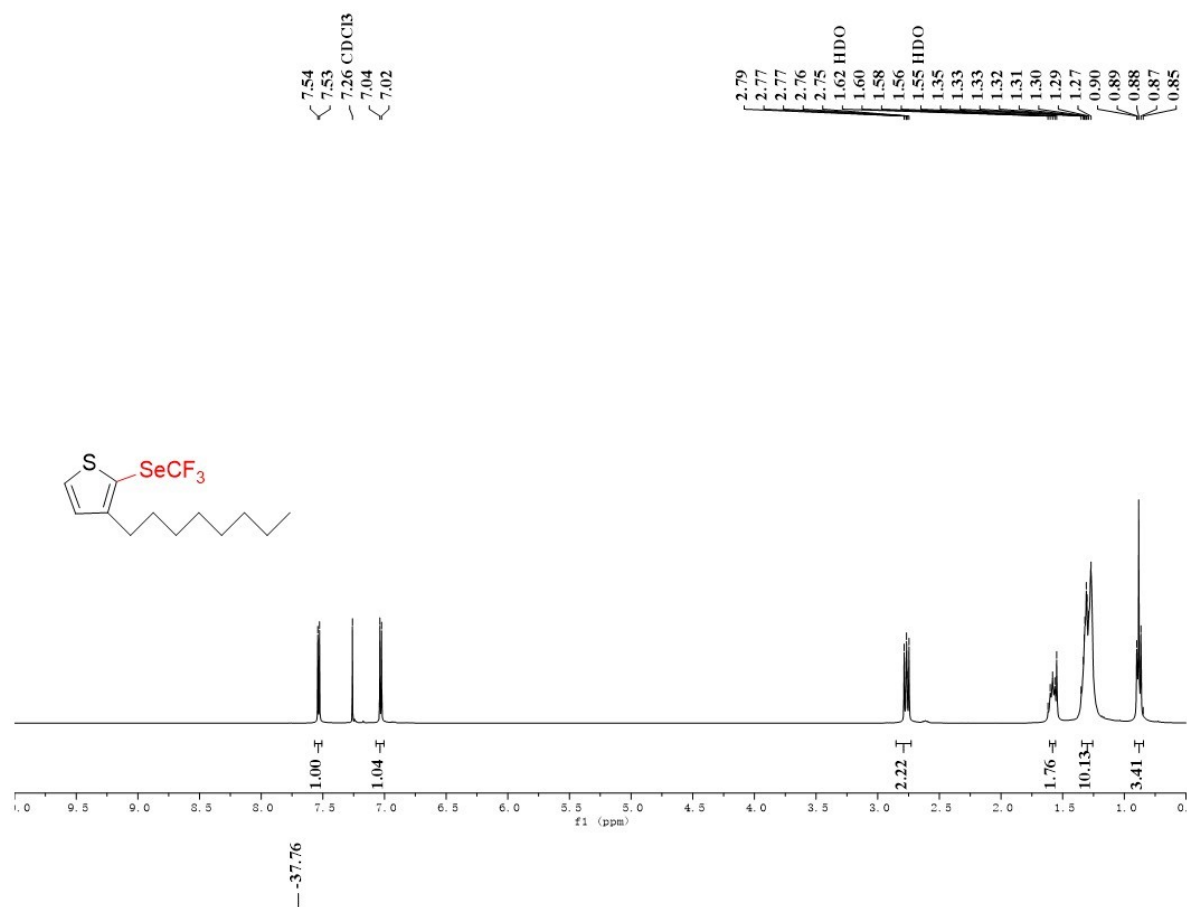


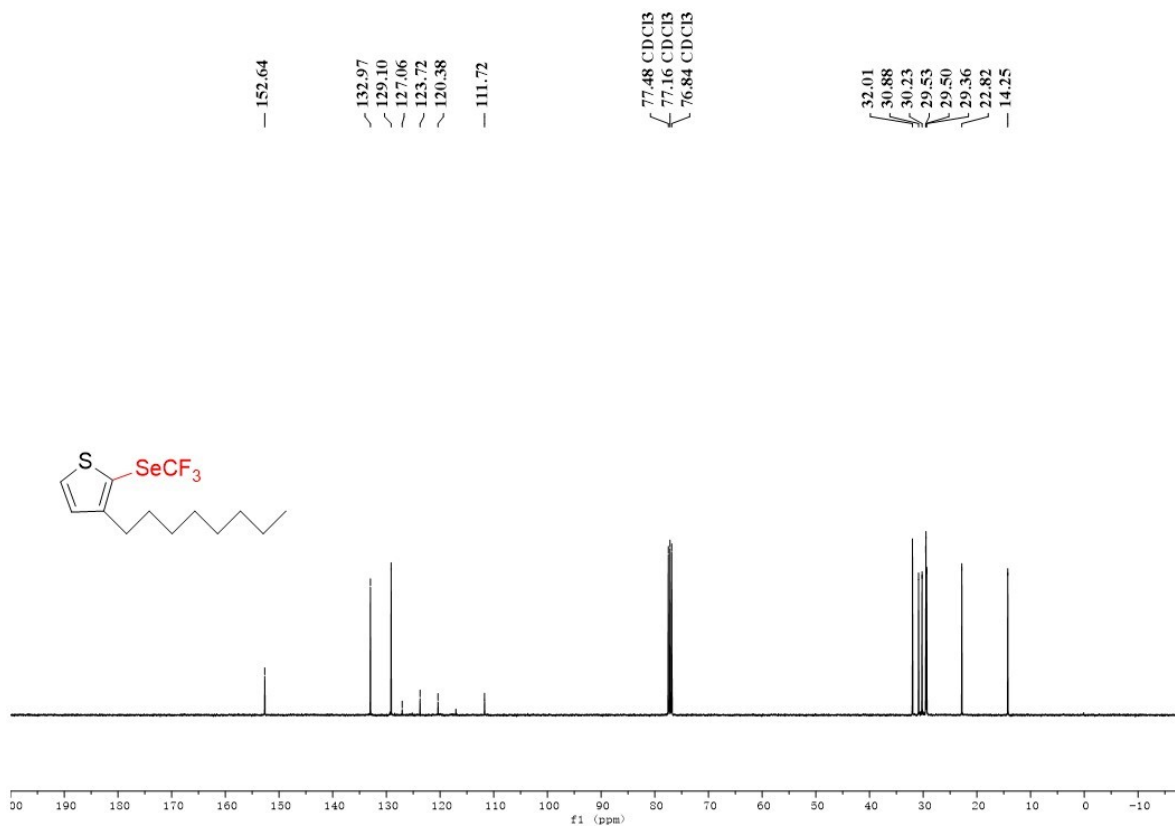
5ay ((2,4-dimethylphenyl)(trifluoromethyl)selane)



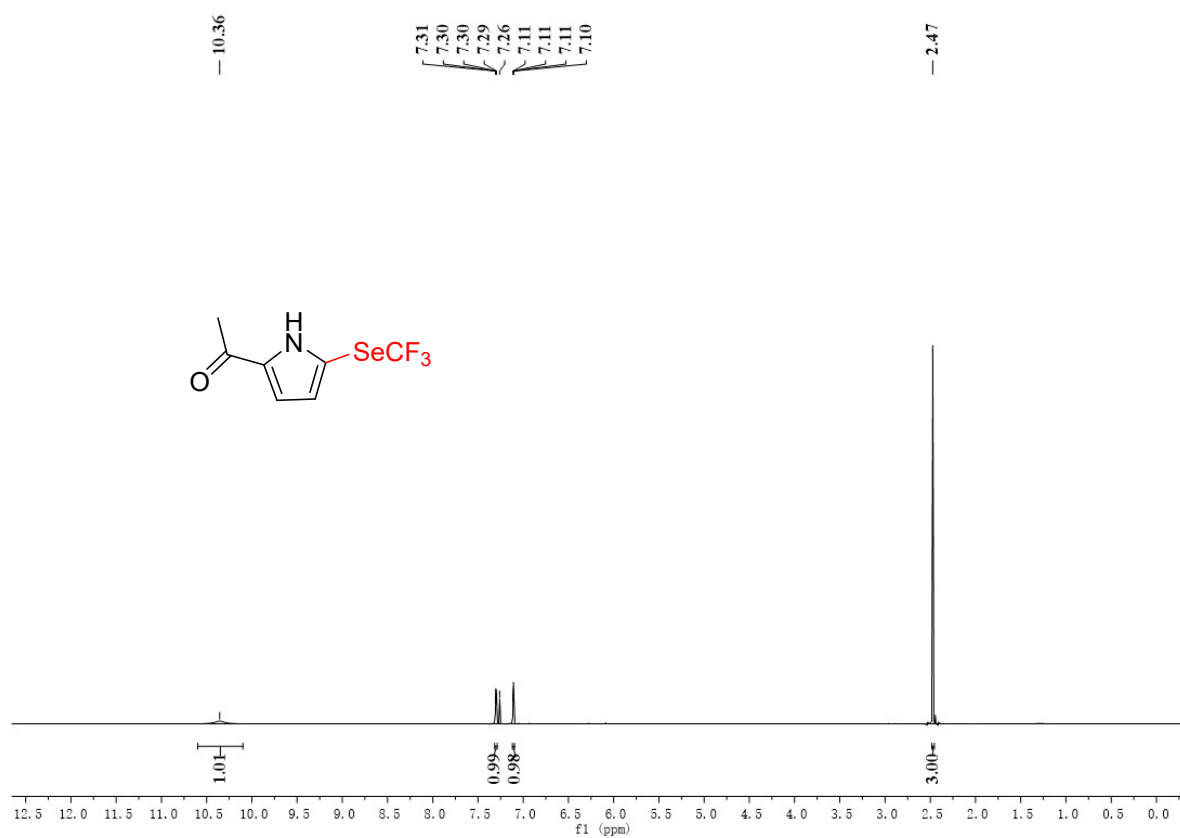


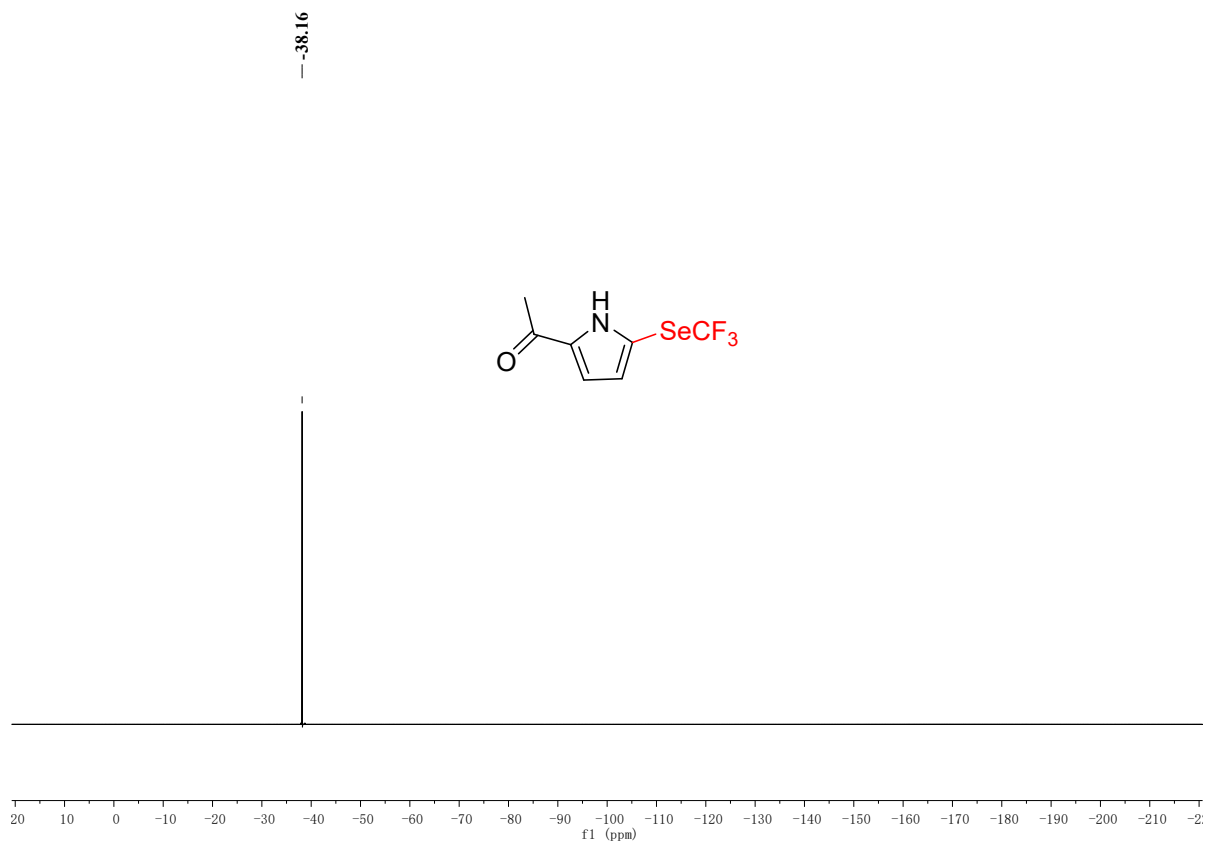
5aza (3-octyl-2-((trifluoromethyl)selanyl)thiophene)





5azb 1-(5-((trifluoromethyl)selanyl)-1H-pyrrol-2-yl)ethan-1-one





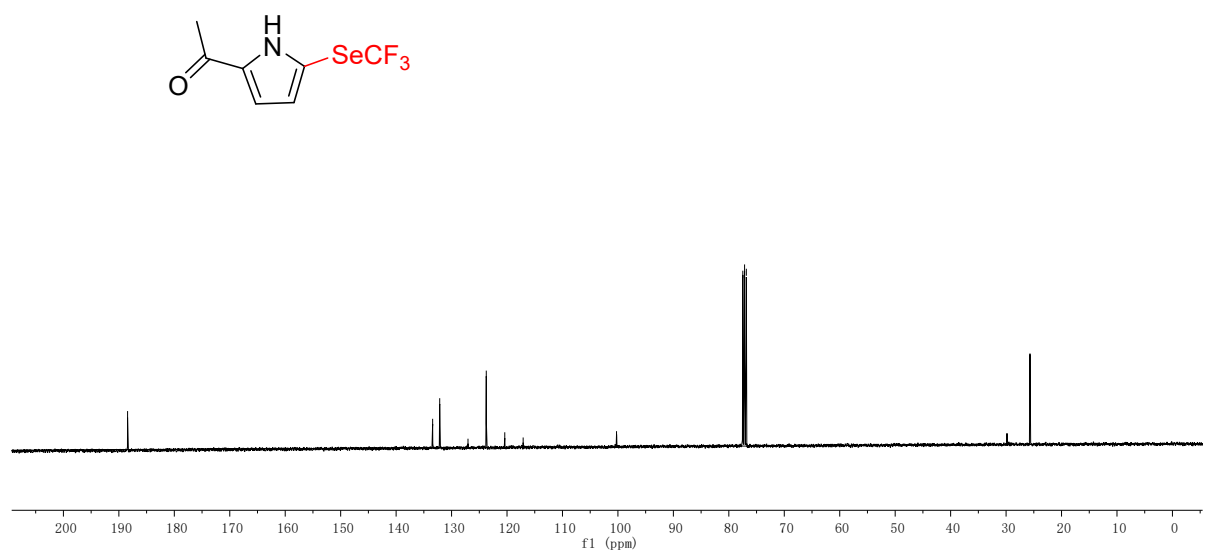
188.43

133.41
132.14
127.04
123.74
120.41
117.09

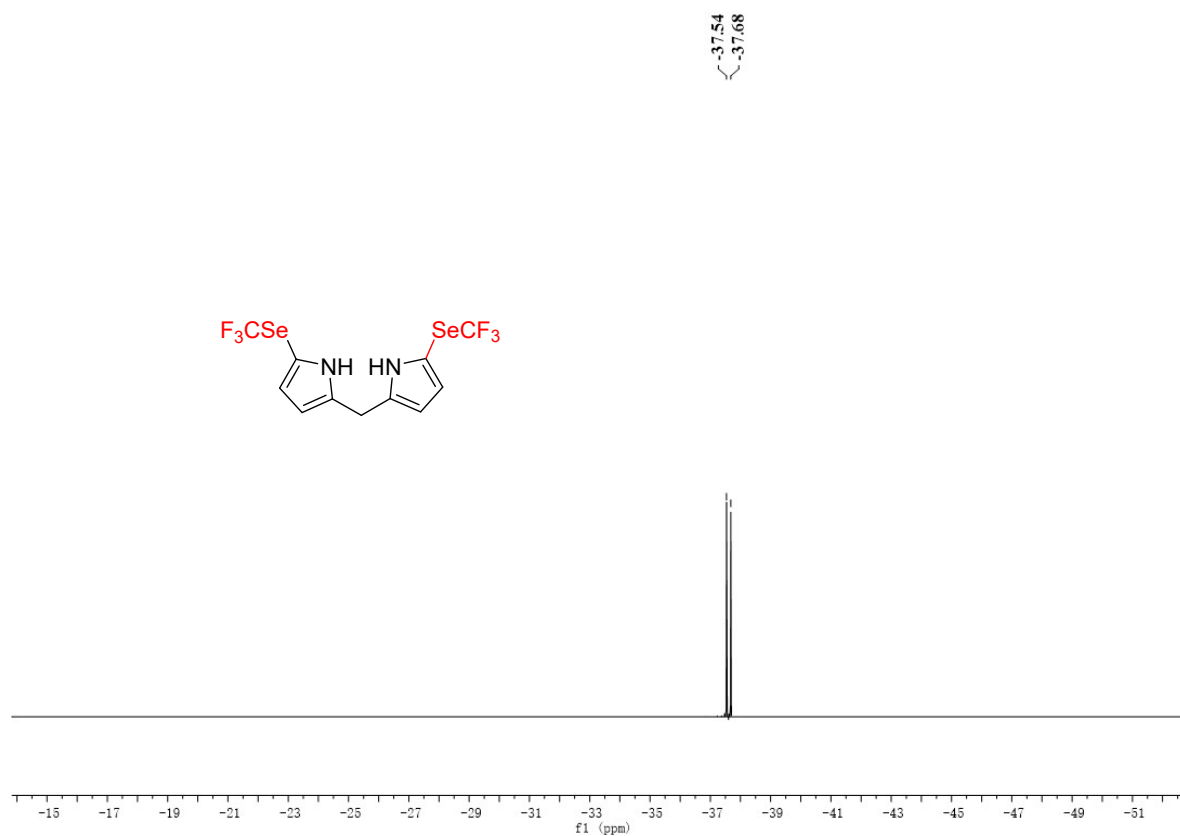
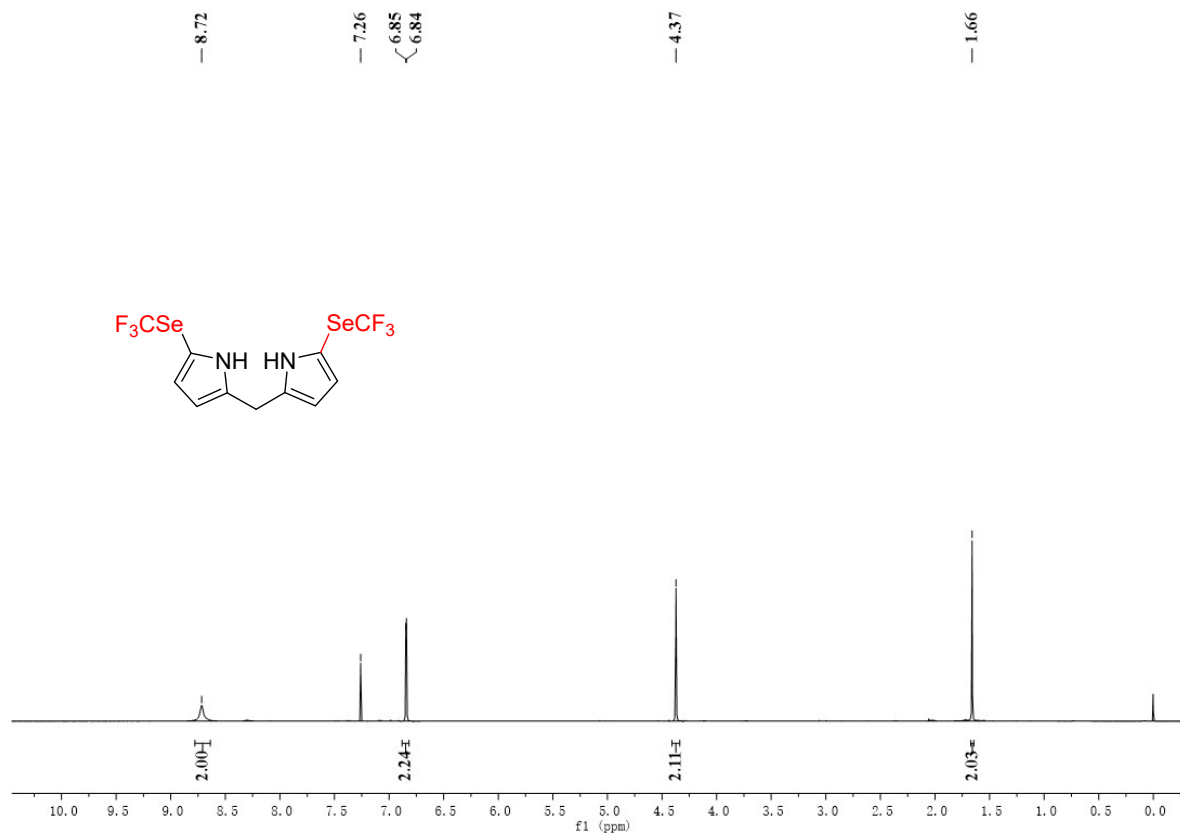
100.25

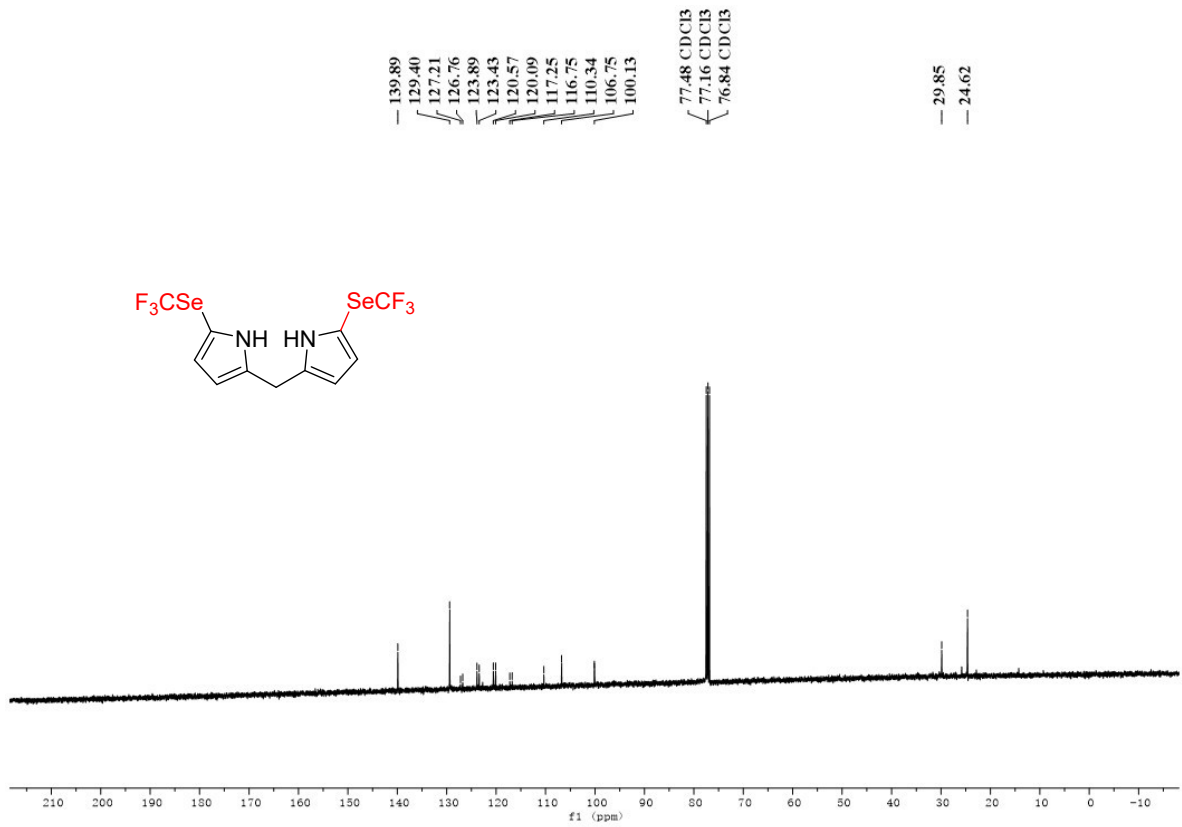
77.48
77.36
77.16
76.84

25.69

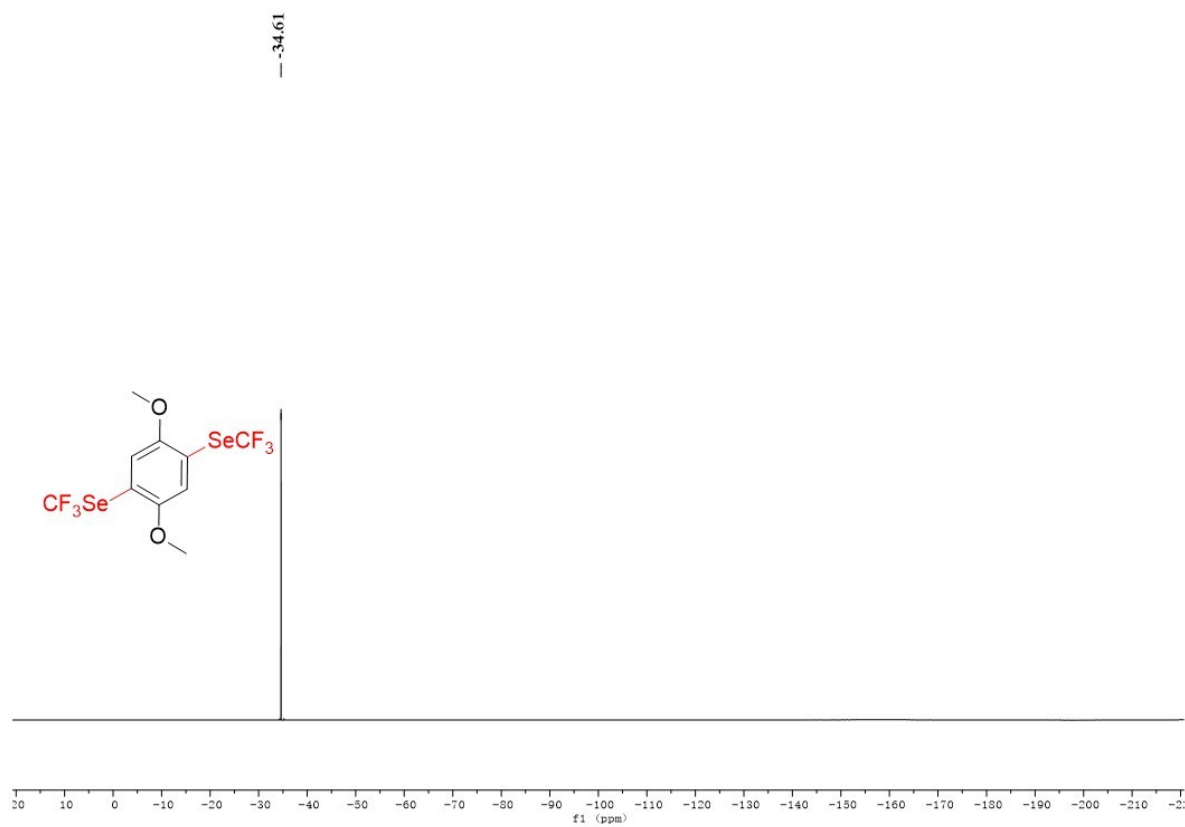
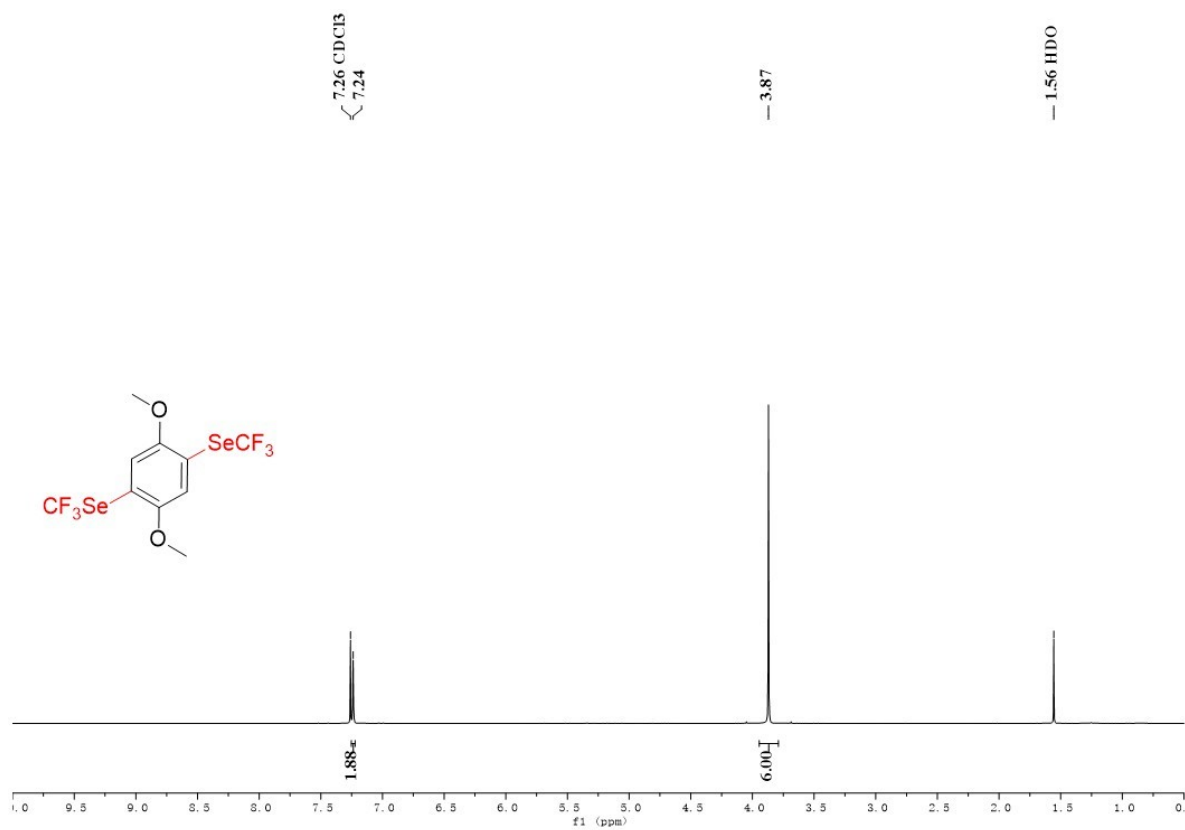


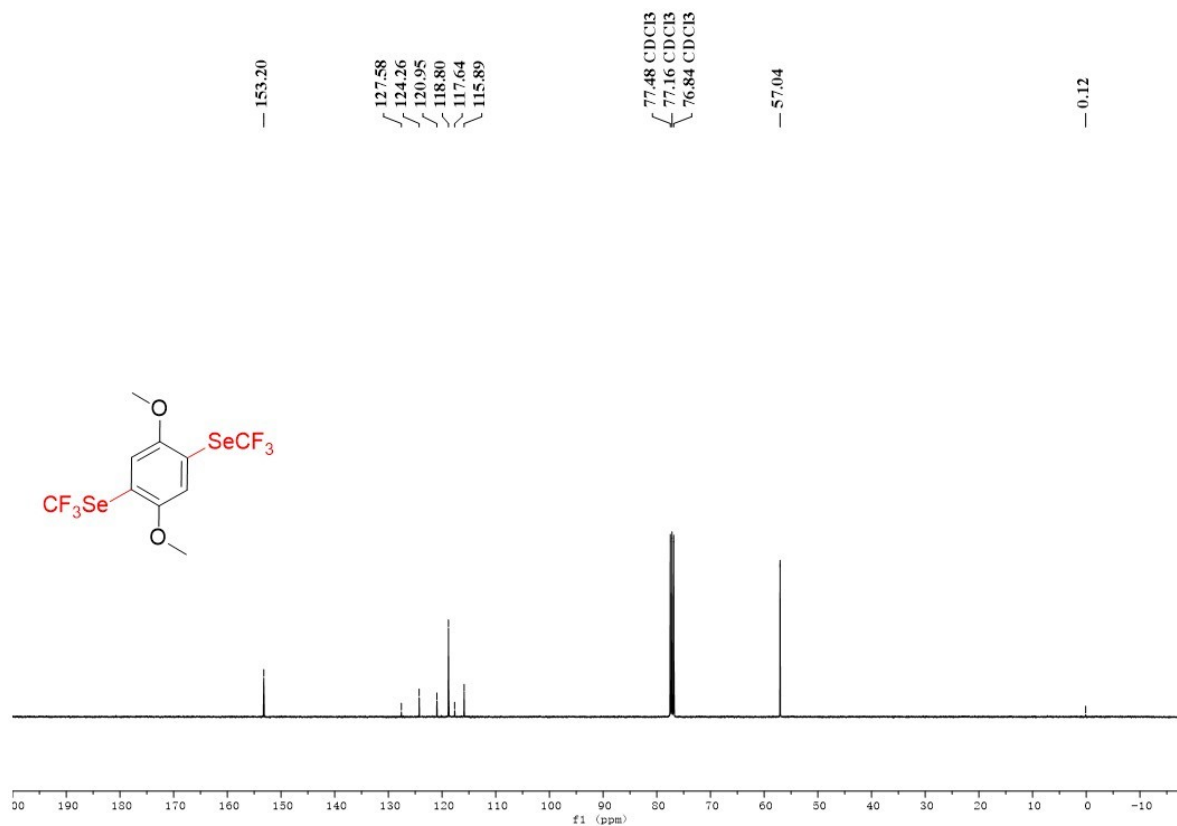
5azc bis(5-((trifluoromethyl)selanyl)-1H-pyrrol-2-yl)methane



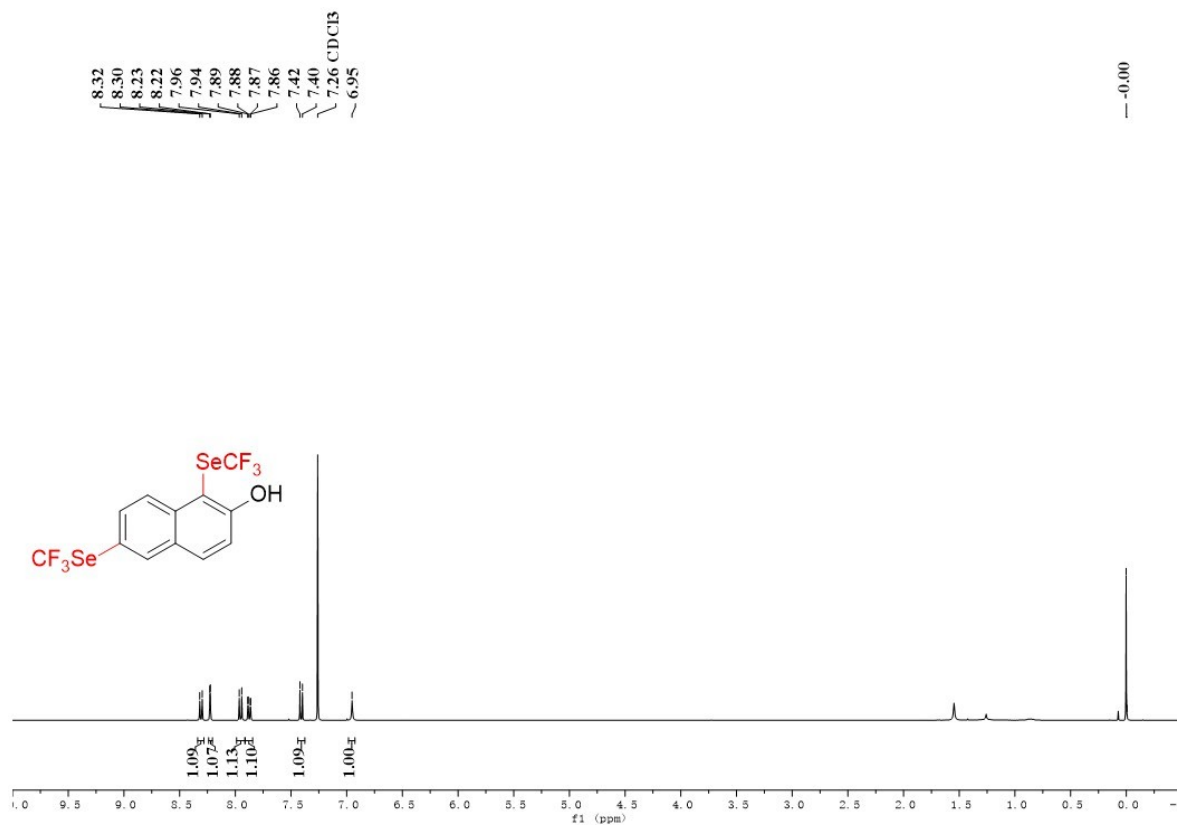


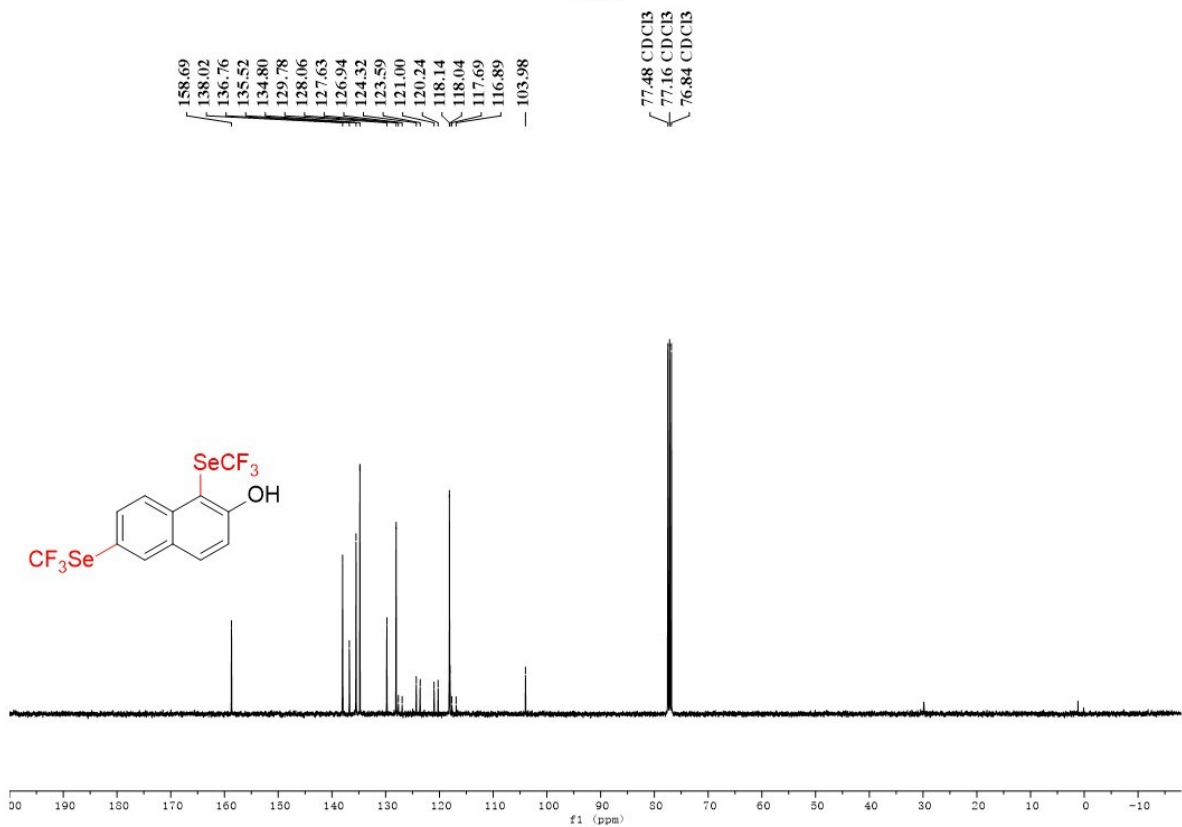
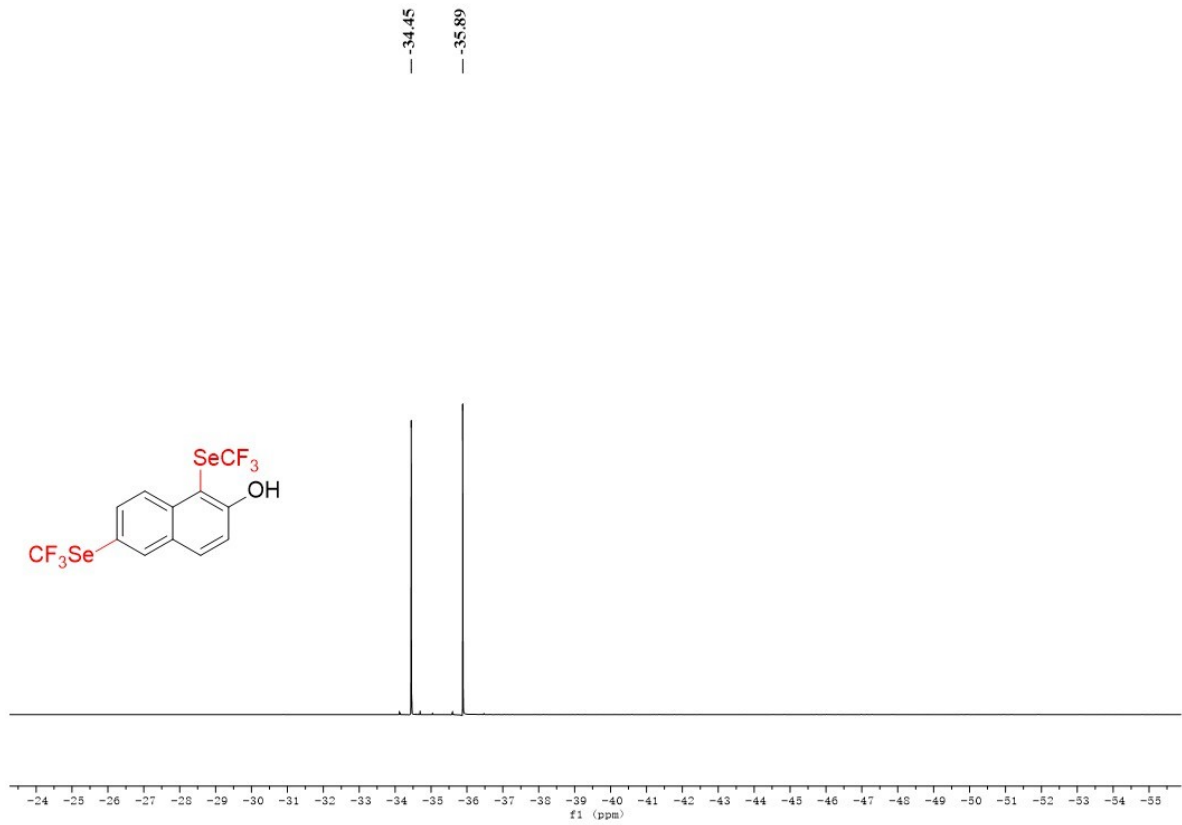
5ba ((2,5-dimethoxy-1,4-phenylene)bis((trifluoromethyl)selane))



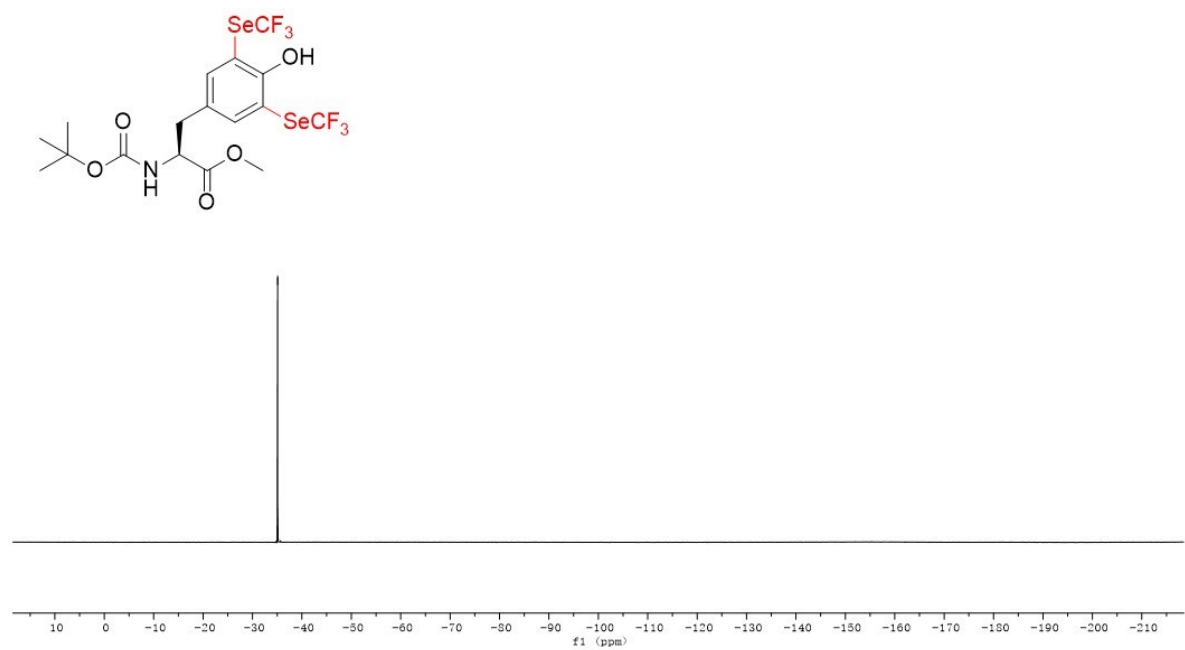
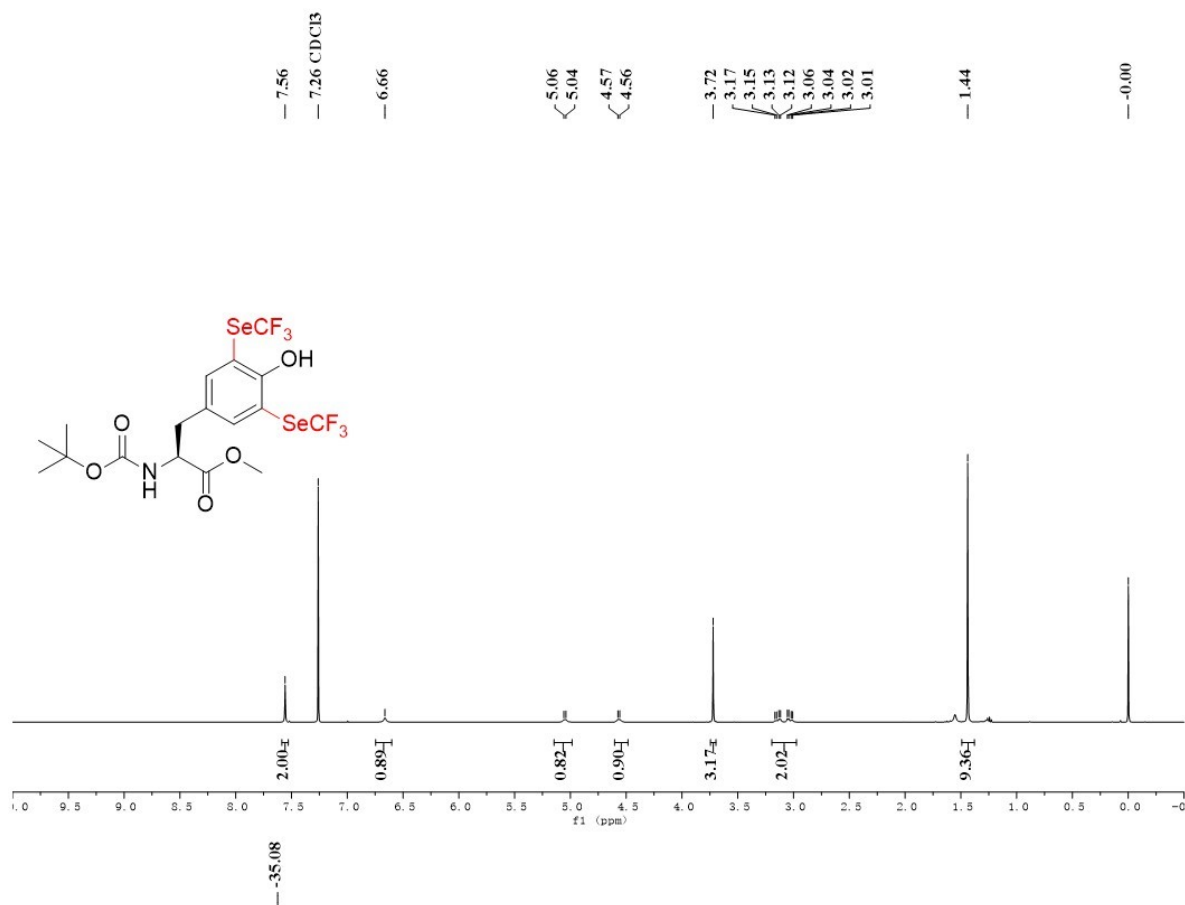


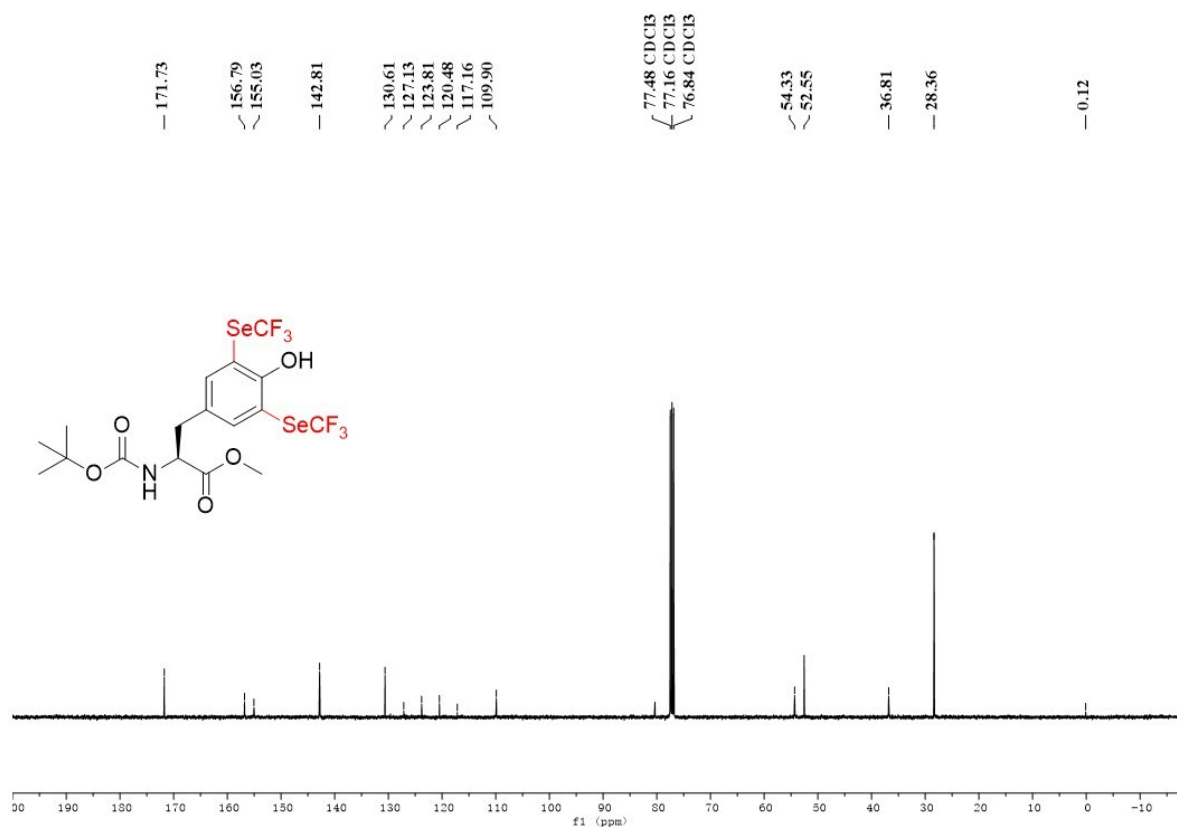
5bb (1,6-bis((trifluoromethyl)selenyl)naphthalen-2-ol)



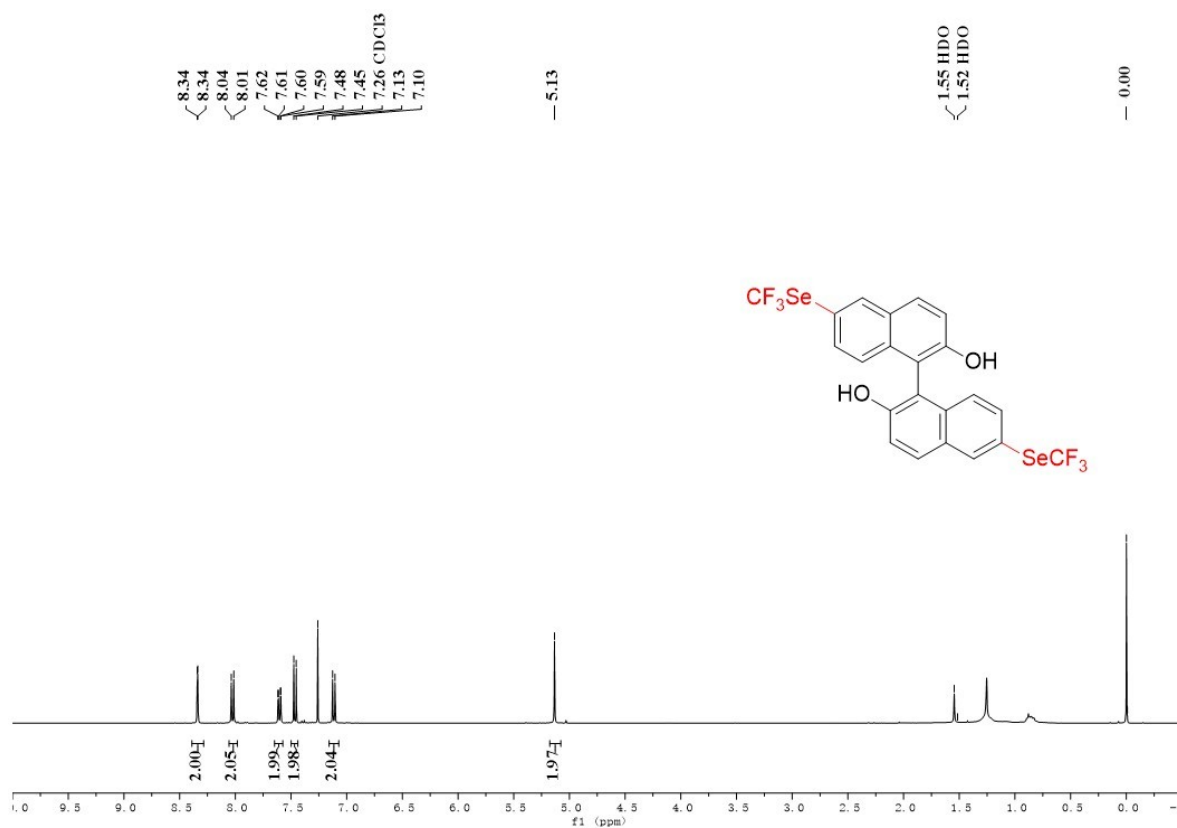


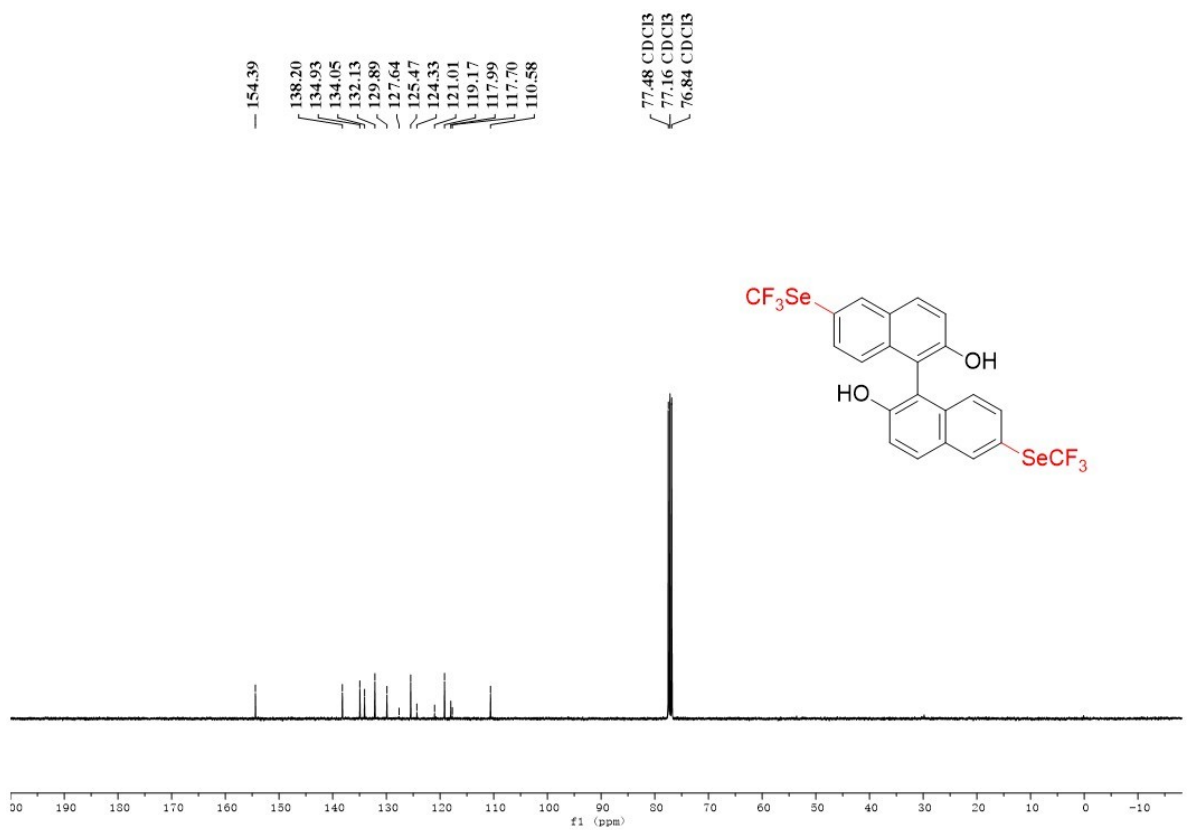
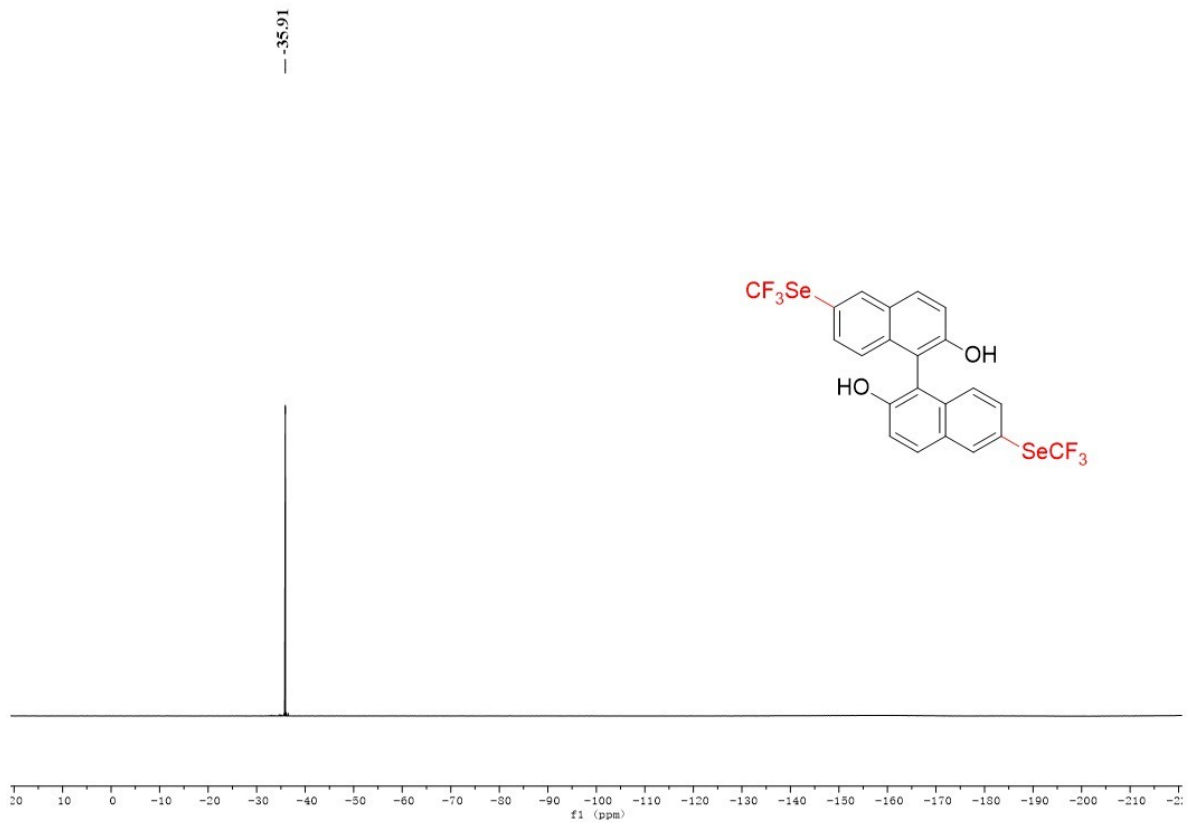
5bc (methyl (S)-2-((tert-butoxycarbonyl)amino)-3-(4-hydroxy-3,5-bis((trifluoromethyl)selenanyl)phenyl)propanoate)



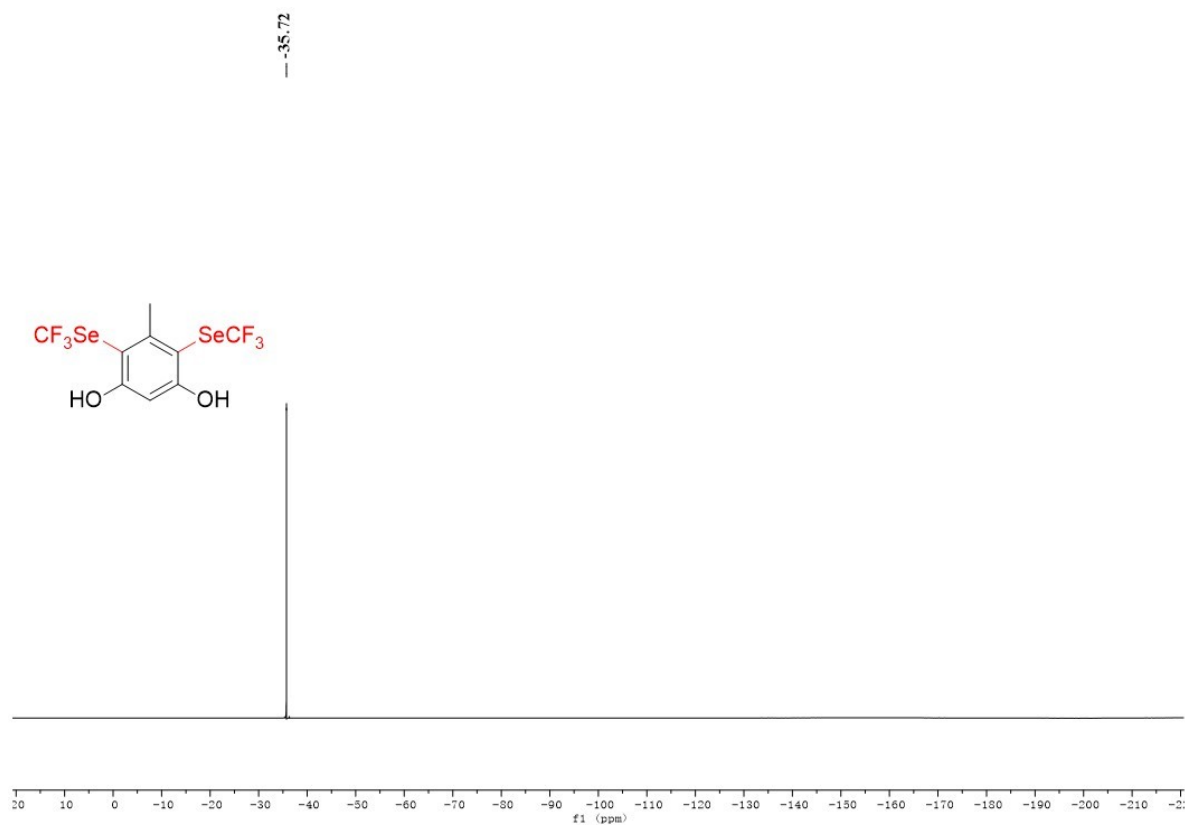
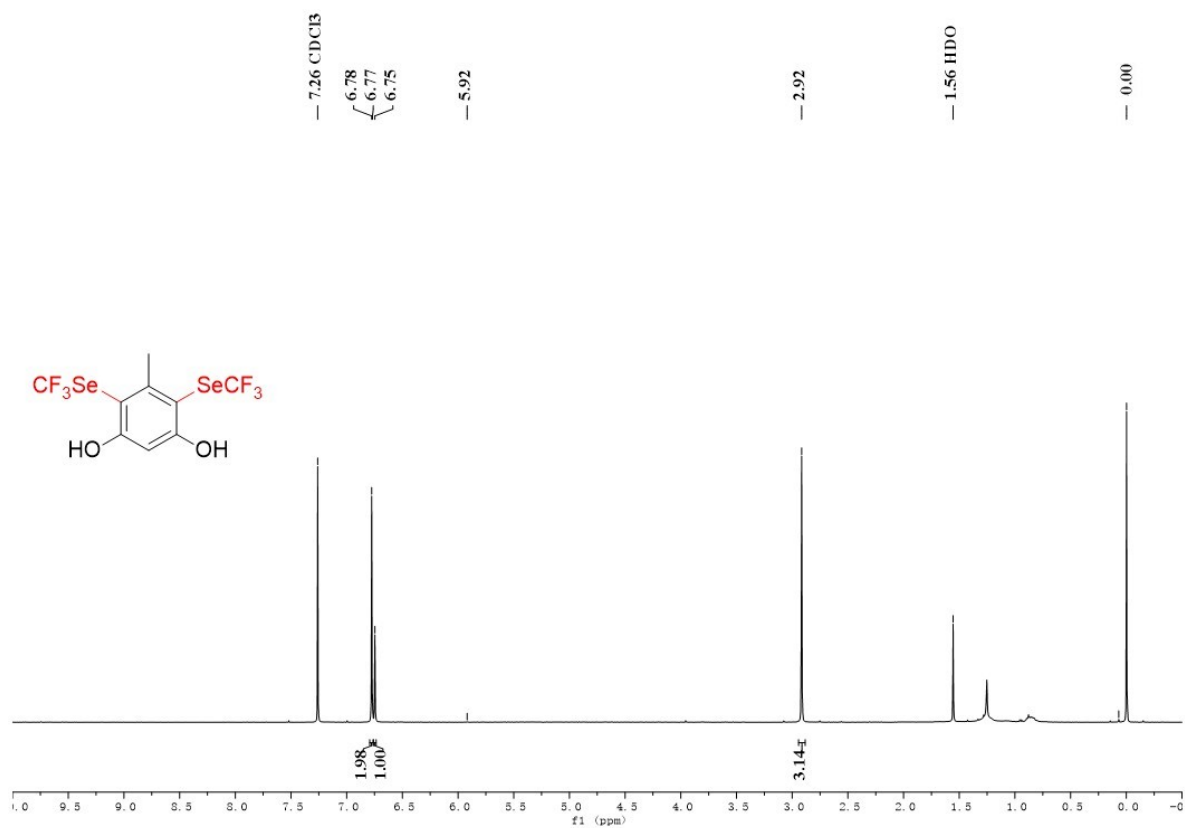


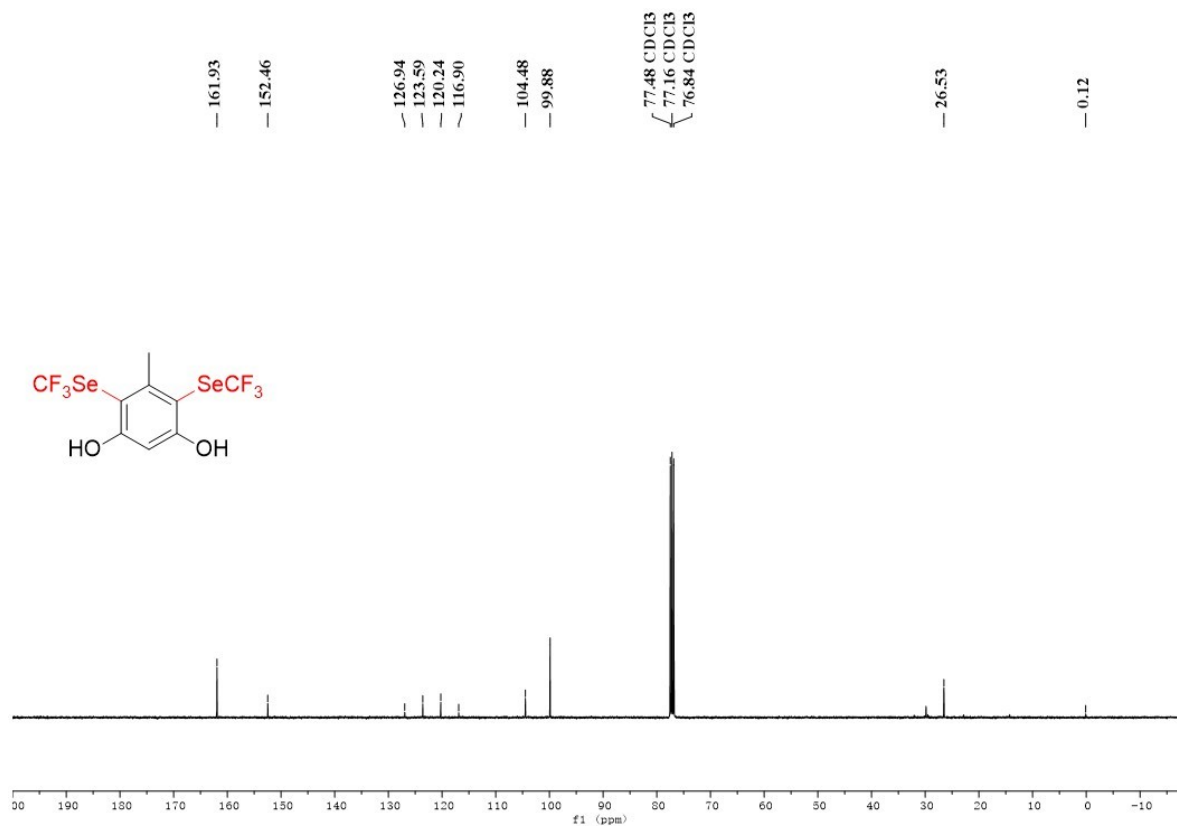
5bd (6,6'-bis((trifluoromethyl)selenanyl)-[1,1'-binaphthalene]-2,2'-diol)



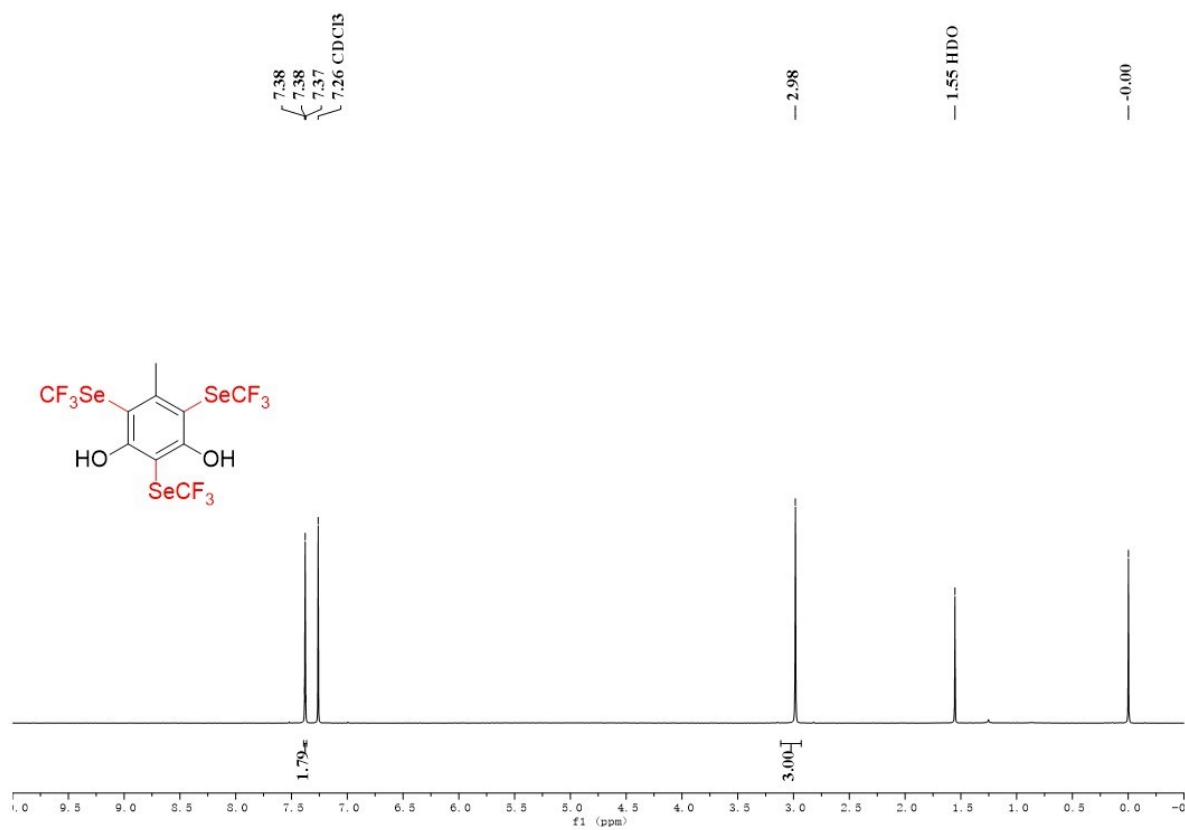


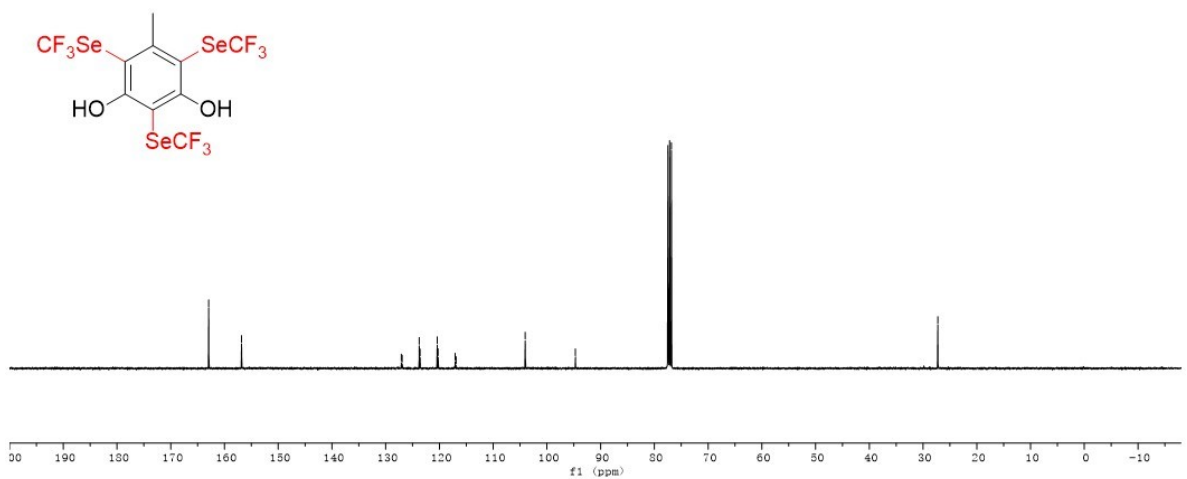
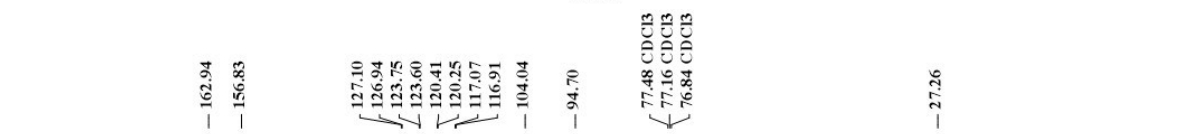
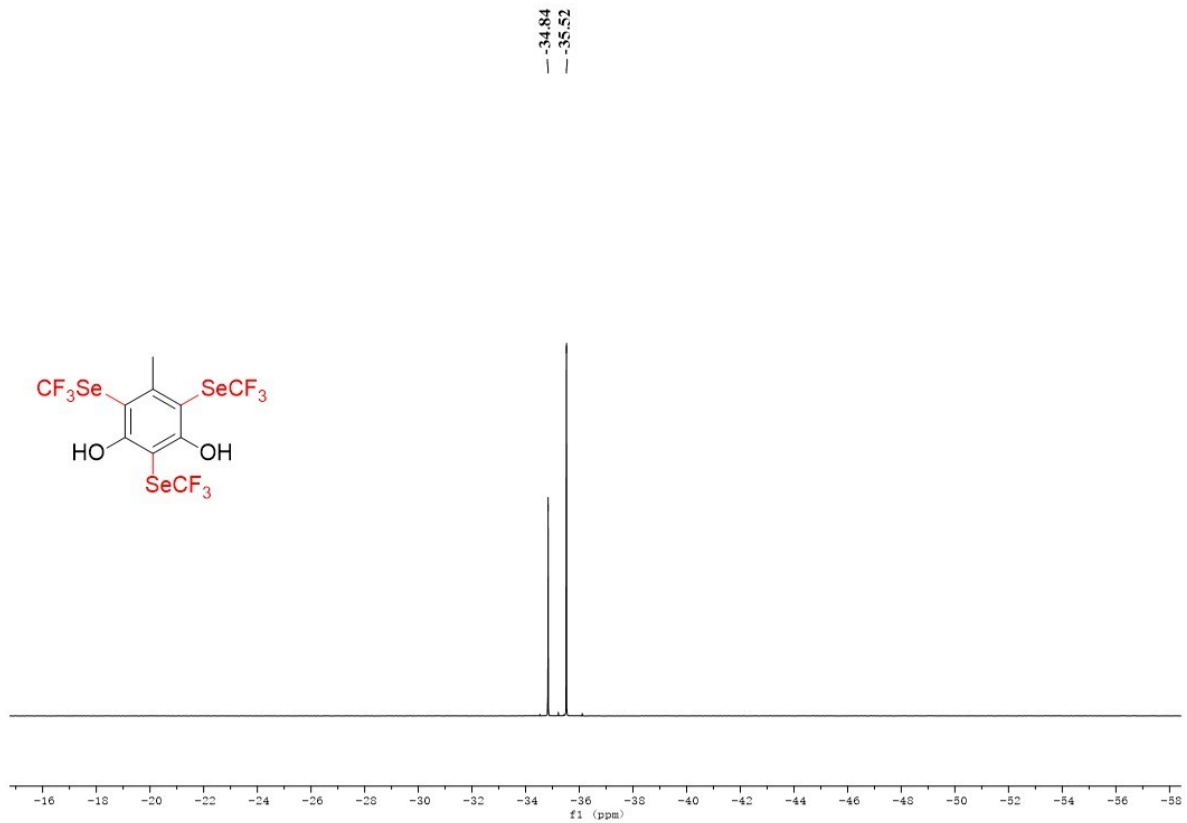
5be (5-methyl-4,6-bis((trifluoromethyl)selanyl)benzene-1,3-diol)



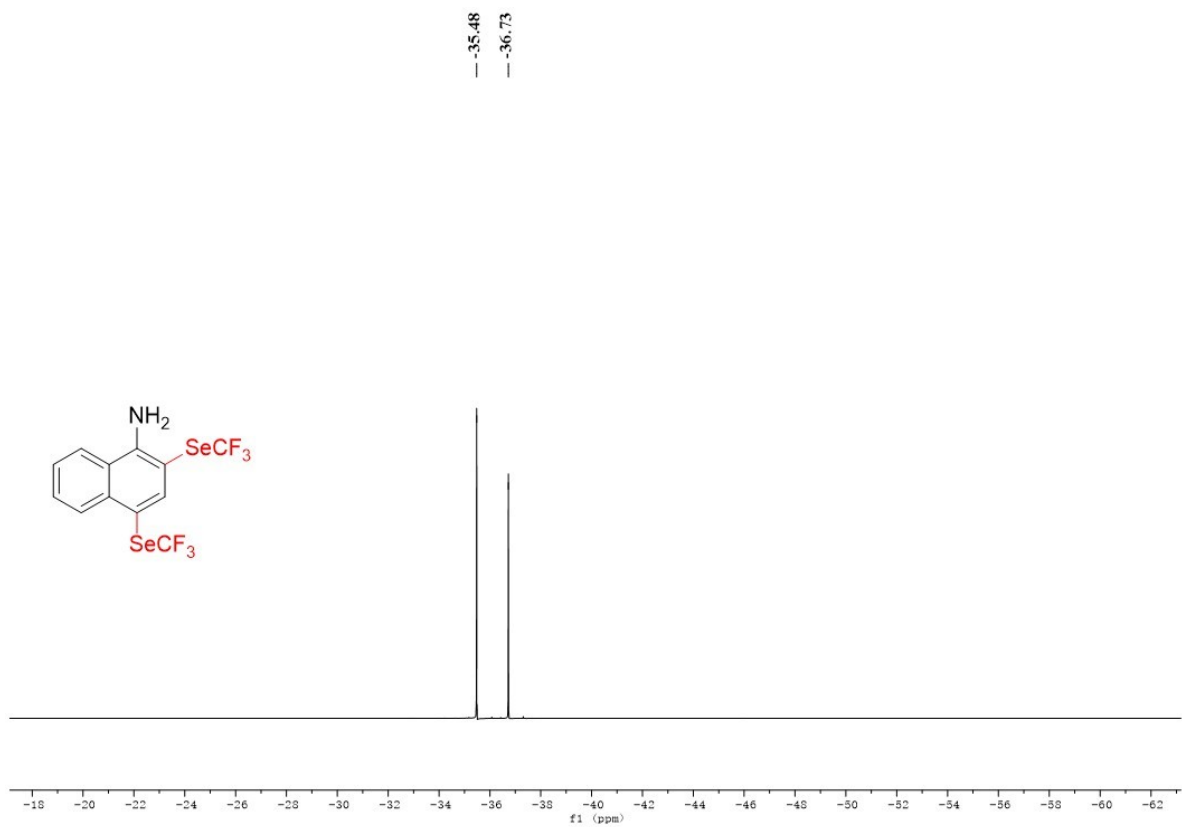
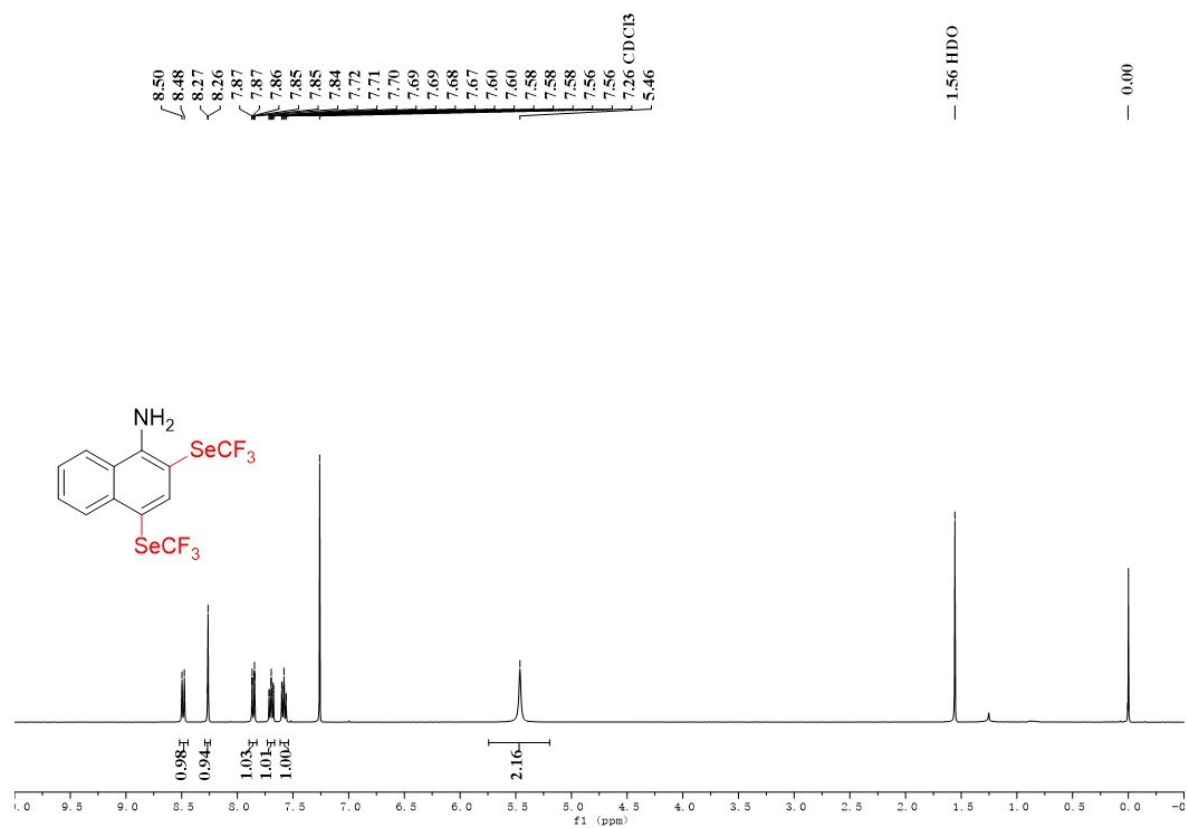


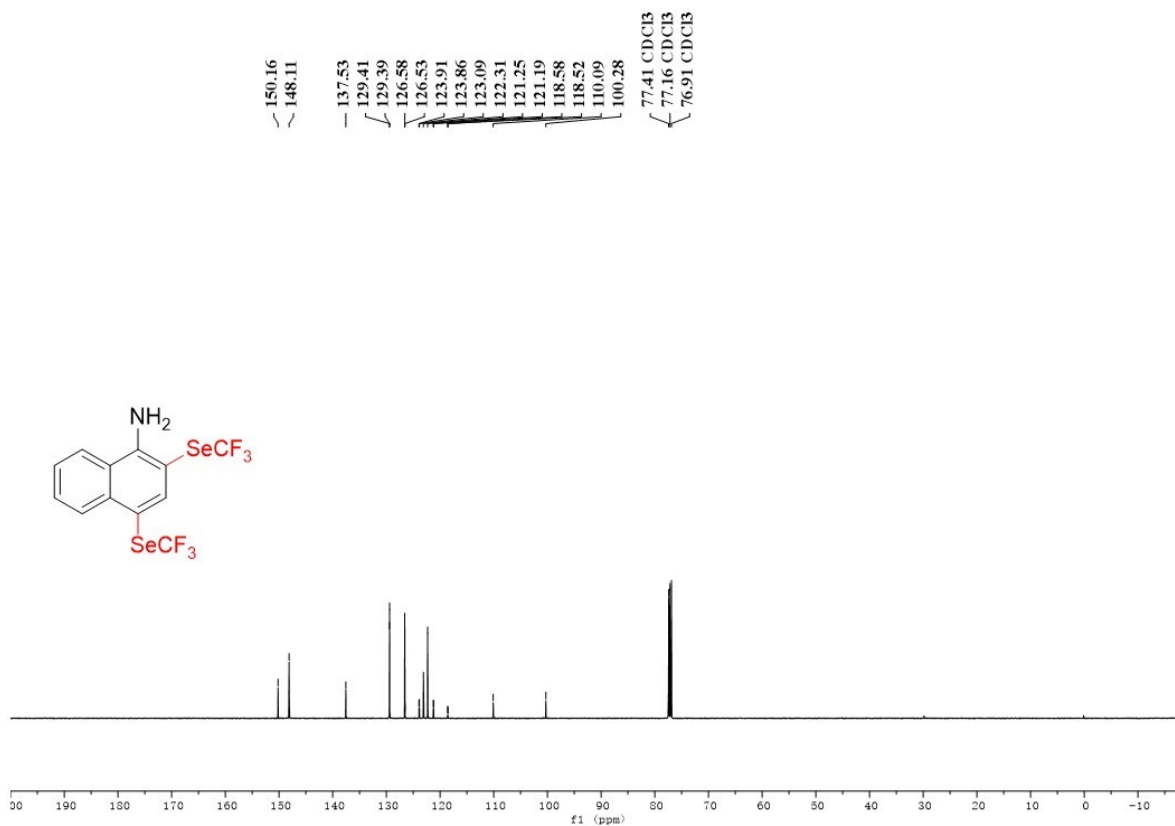
5bf (5-methyl-2,4,6-tris((trifluoromethyl)selenanyl)benzene-1,3-diol)



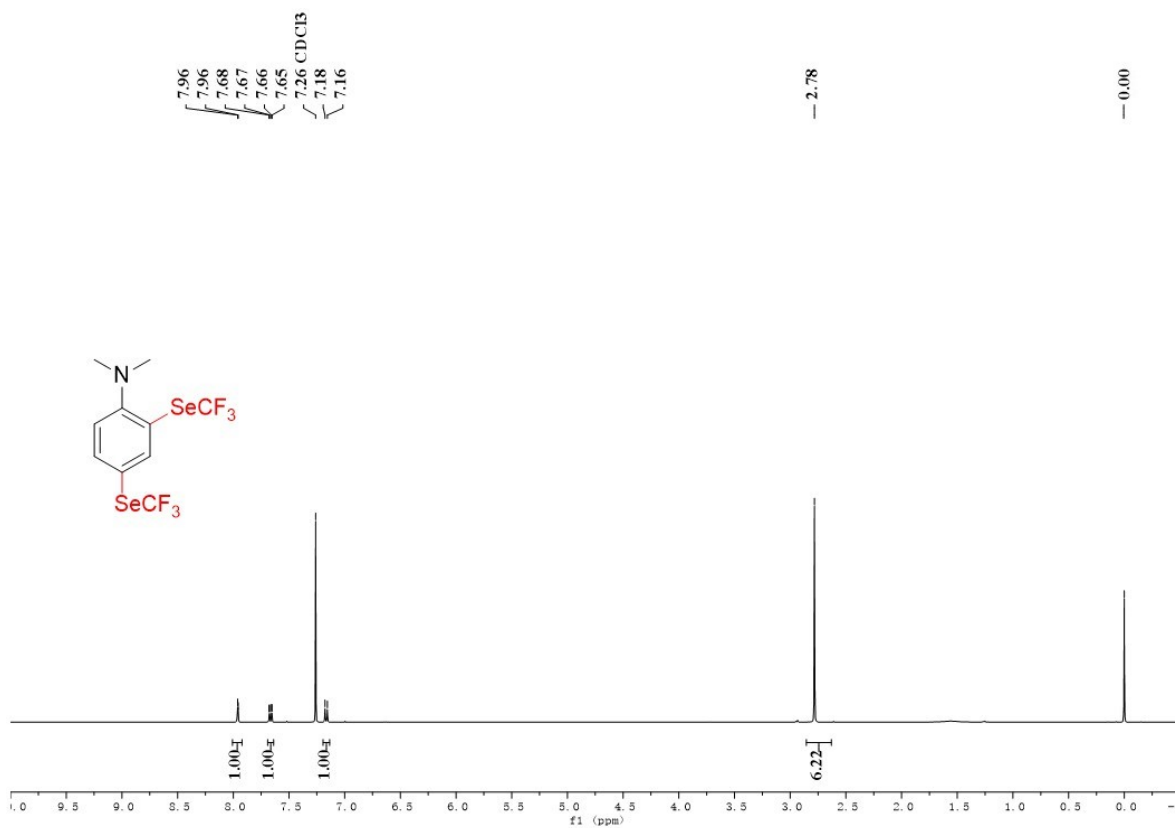


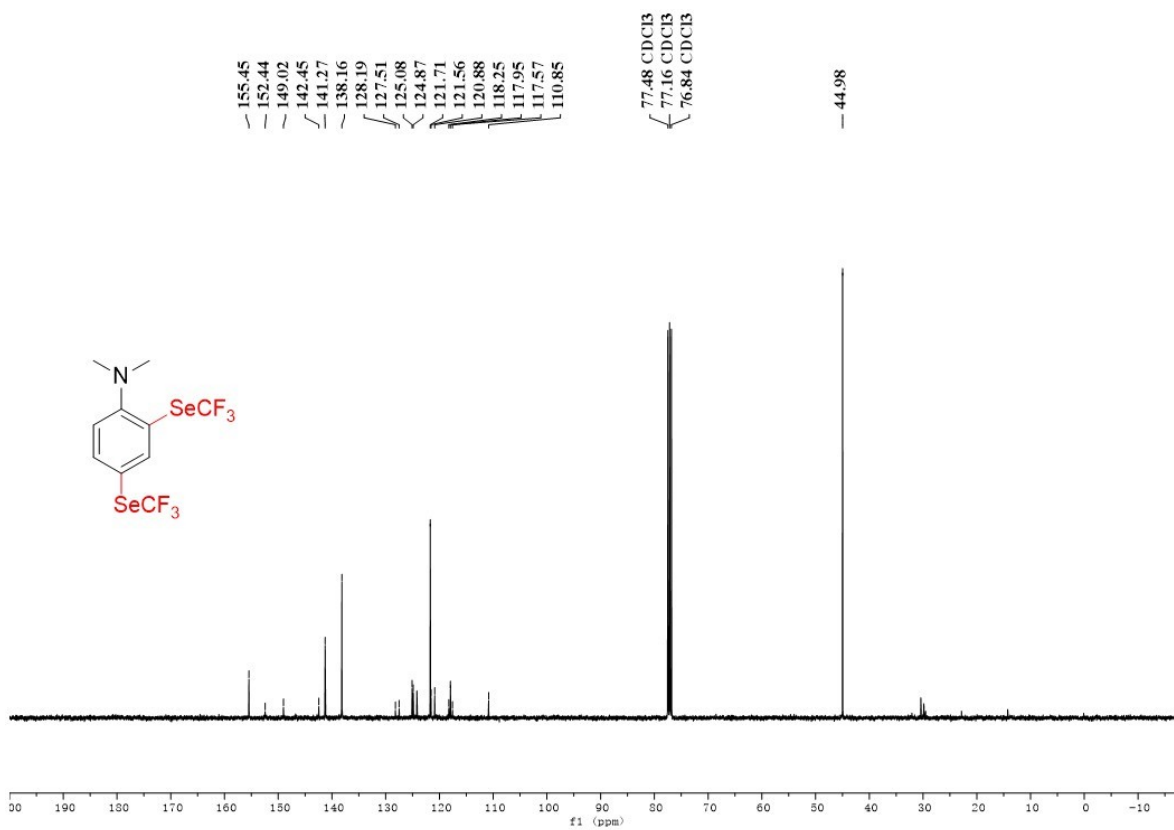
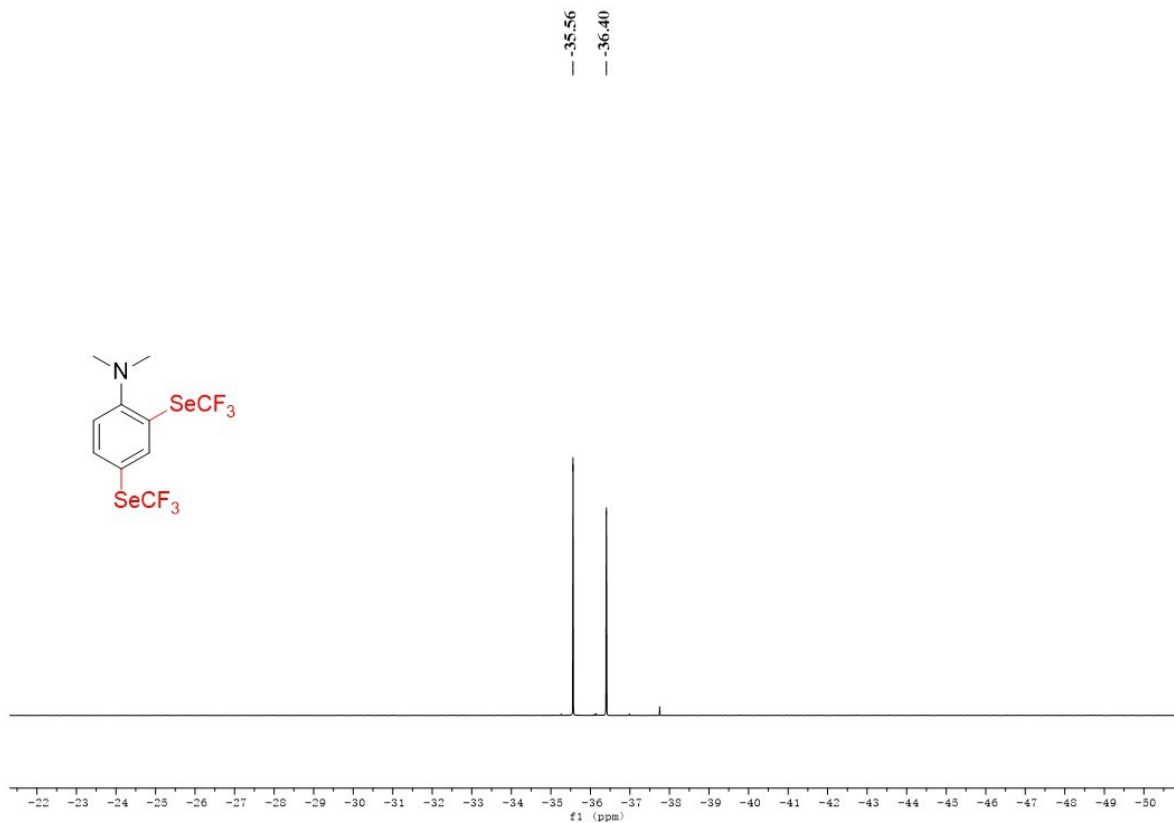
5bg (2,4-bis((trifluoromethyl)selanyl)naphthalen-1-amine)



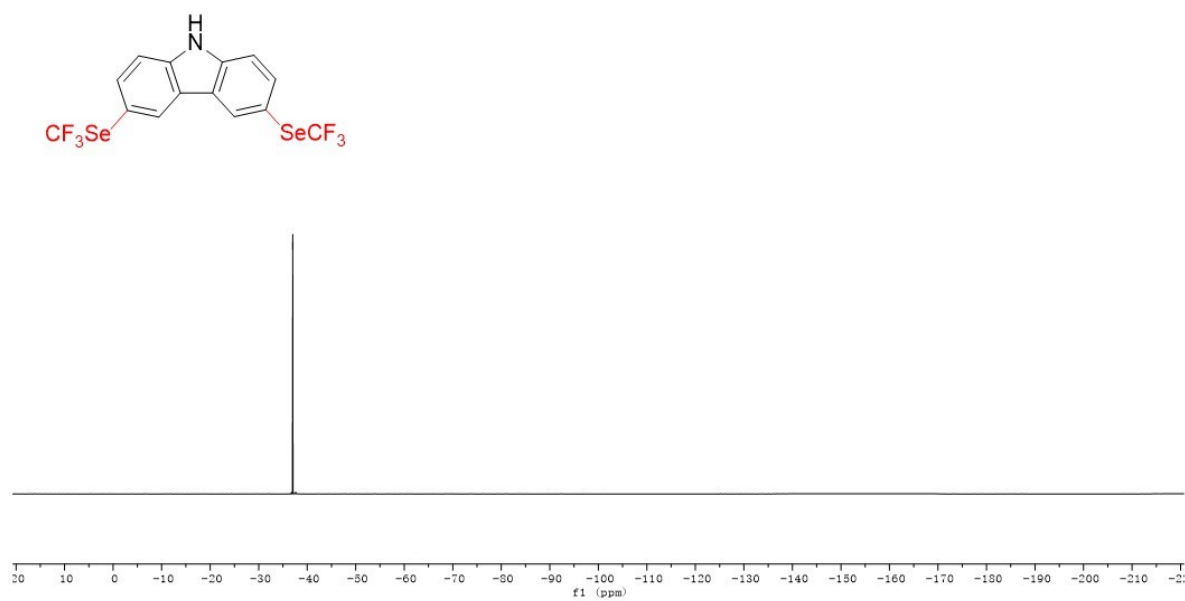
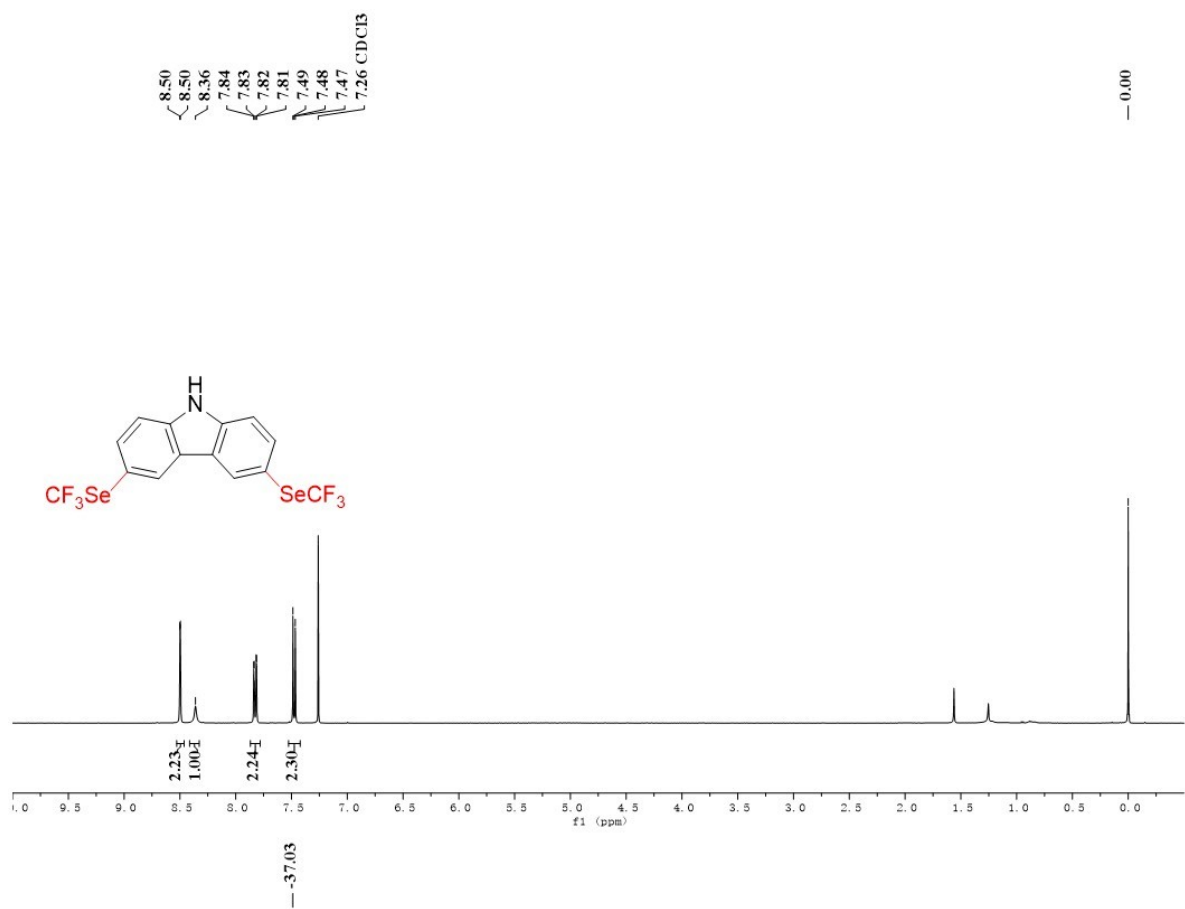


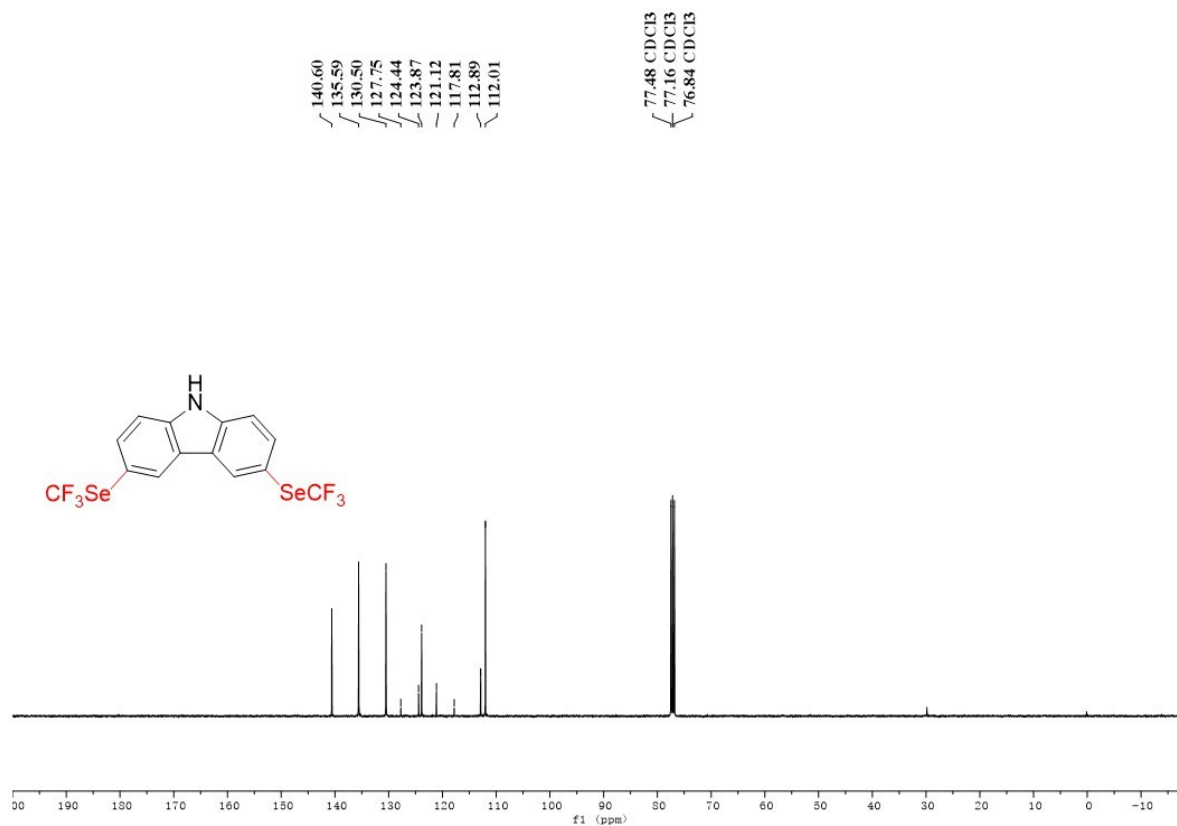
5bh (N,N-dimethyl-2,4-bis((trifluoromethyl)selenyl)aniline)



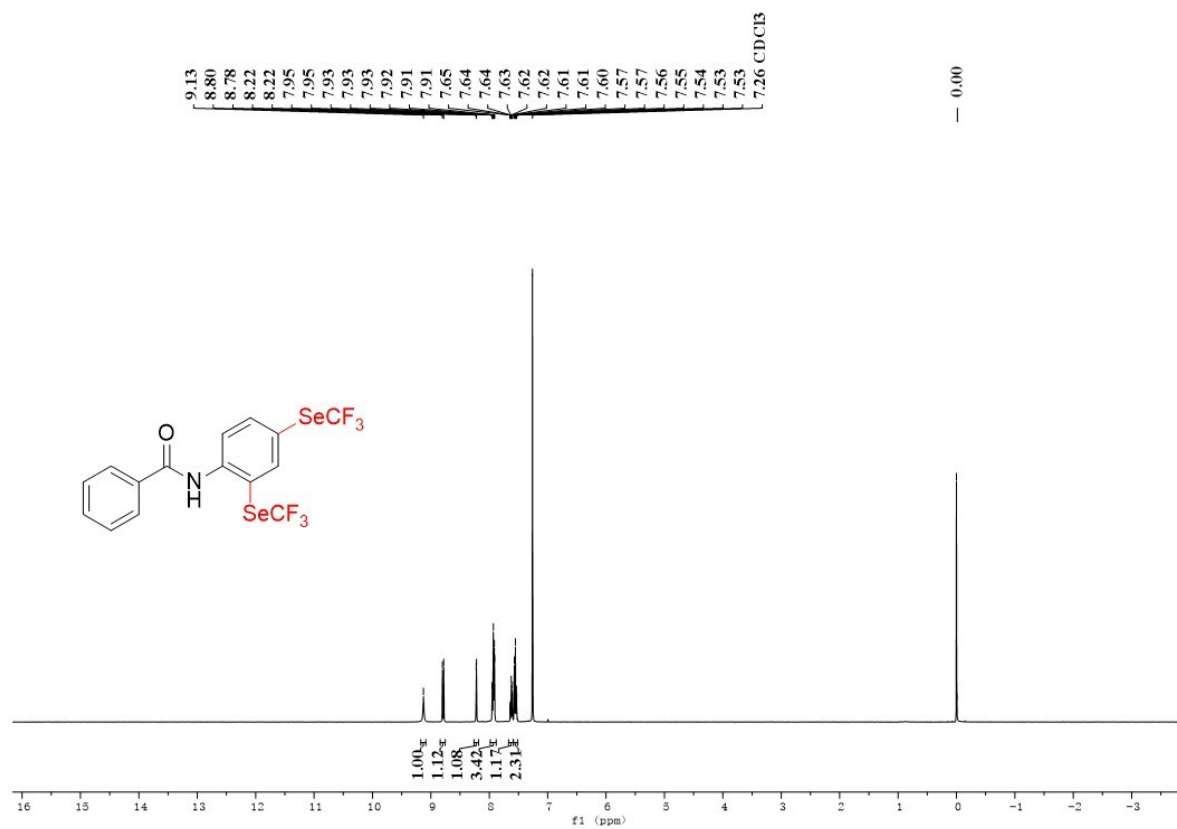


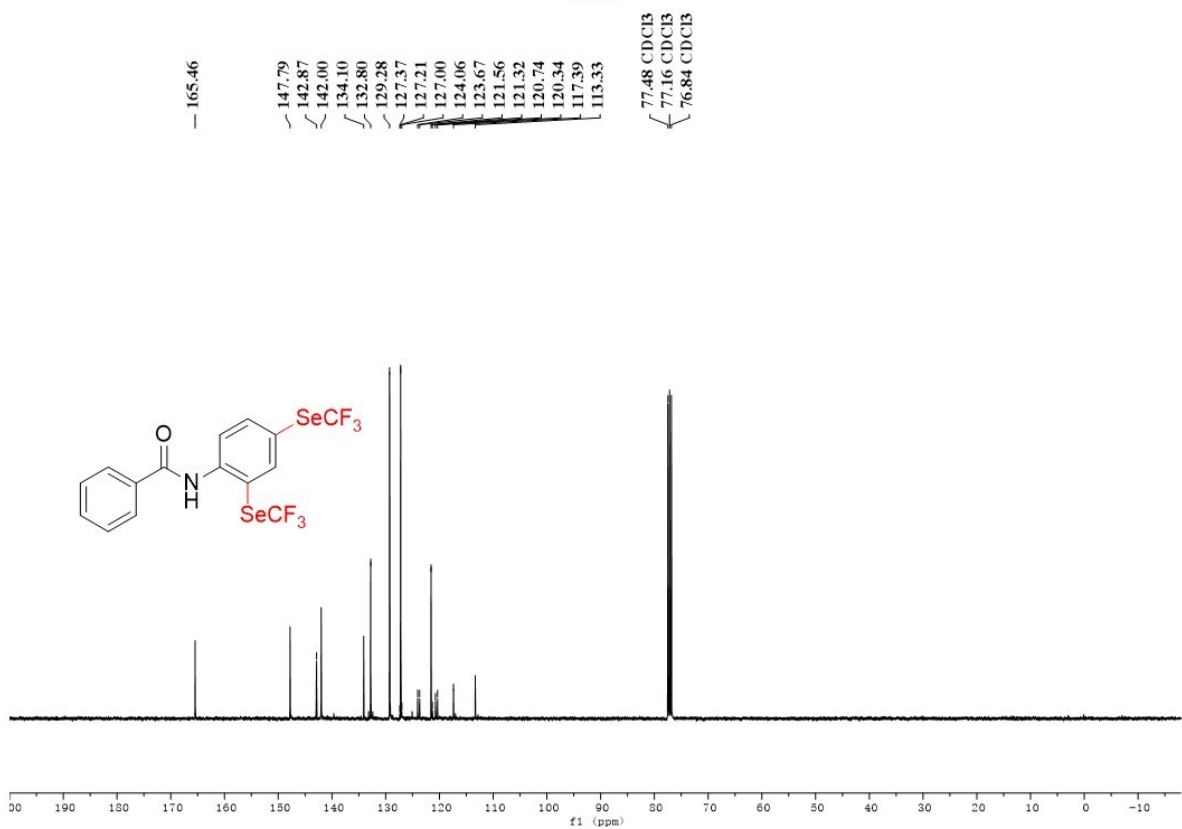
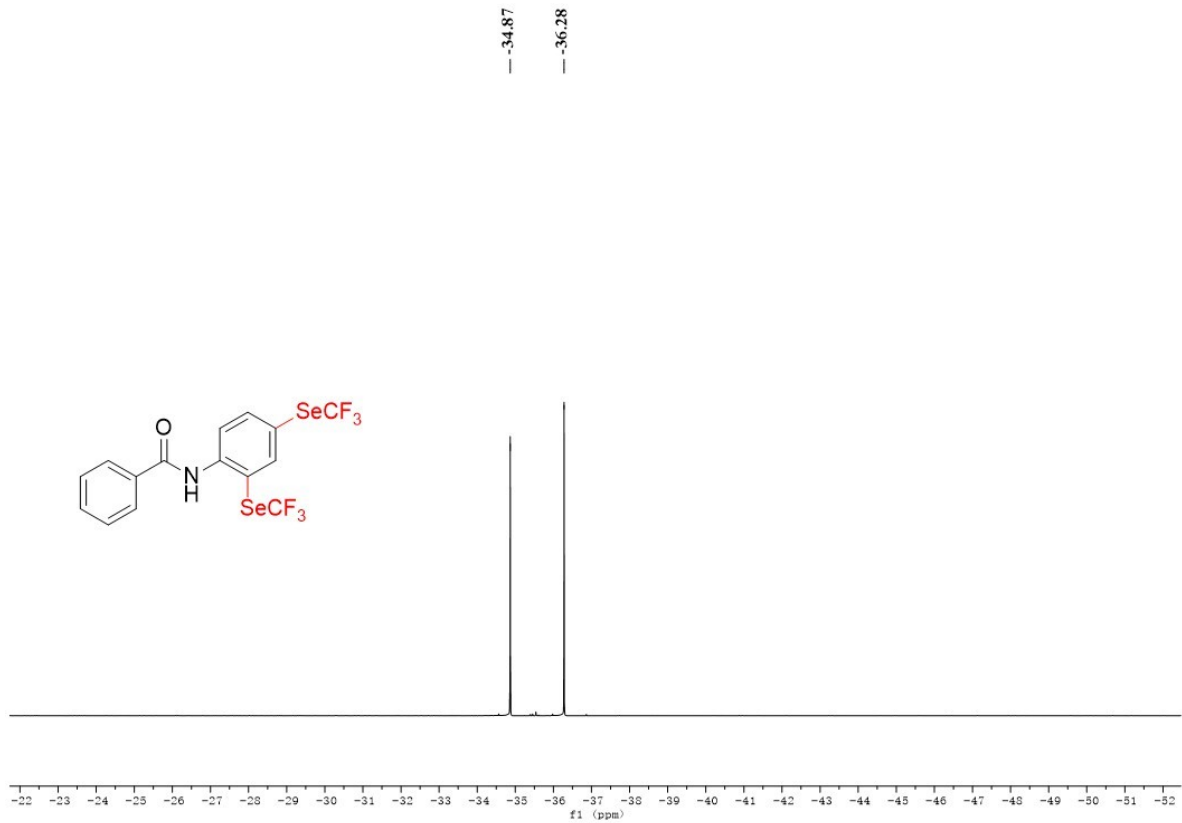
5bi (3,6-bis((trifluoromethyl)selanyl)-9H-carbazole)



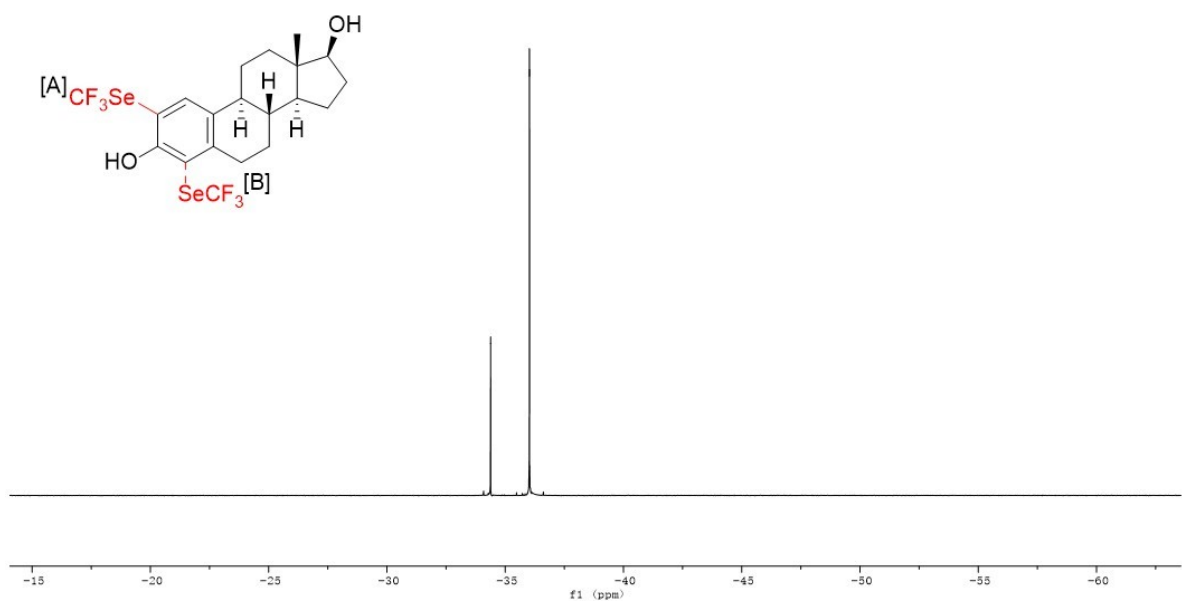
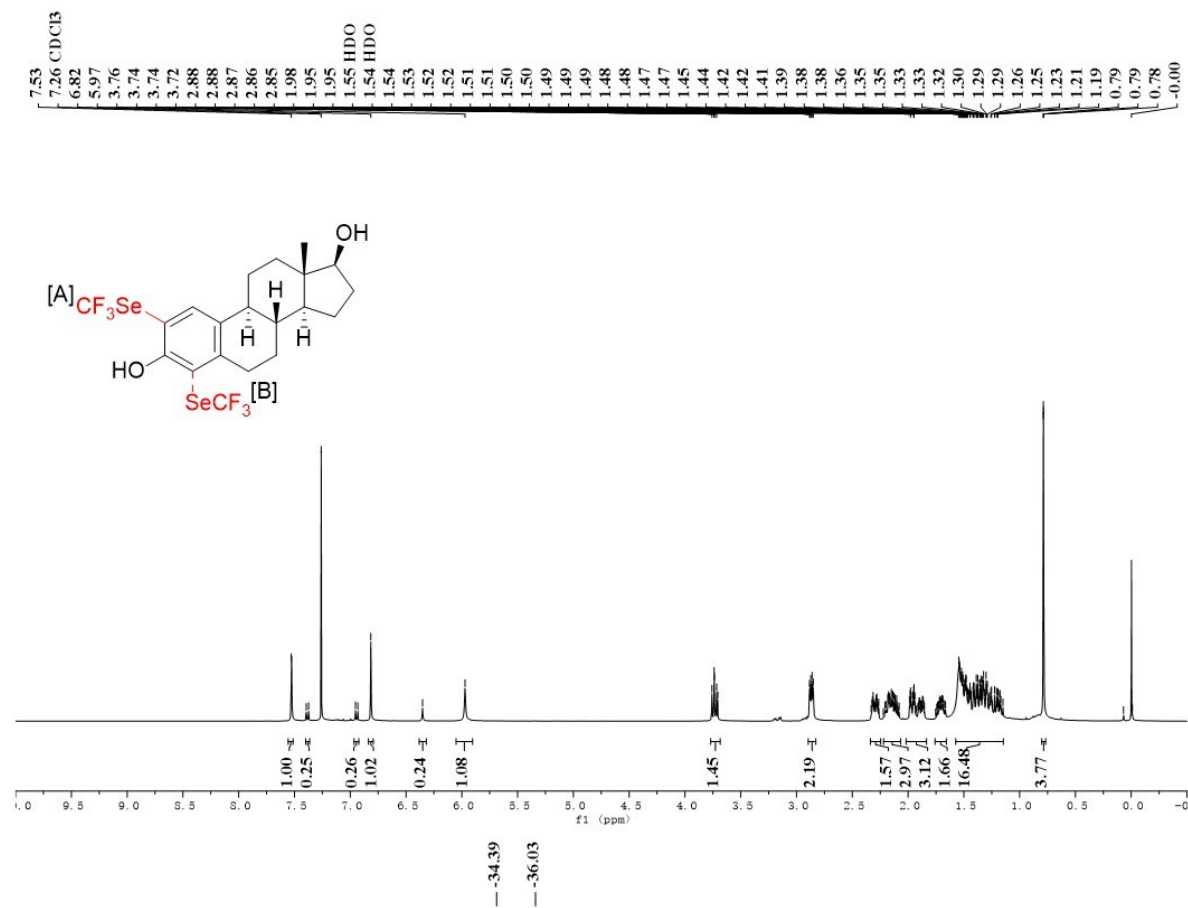


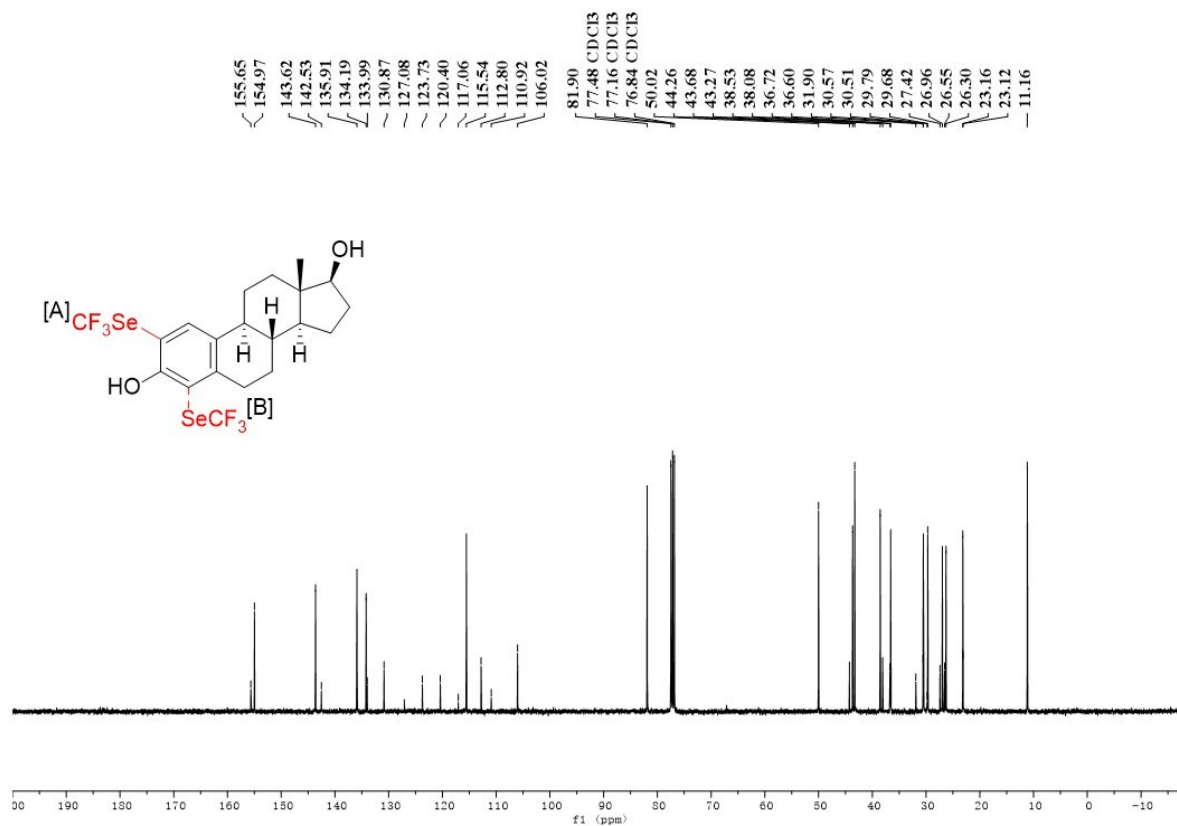
5bj (N-(2,4-bis((trifluoromethyl)selanyl)phenyl)benzamide)



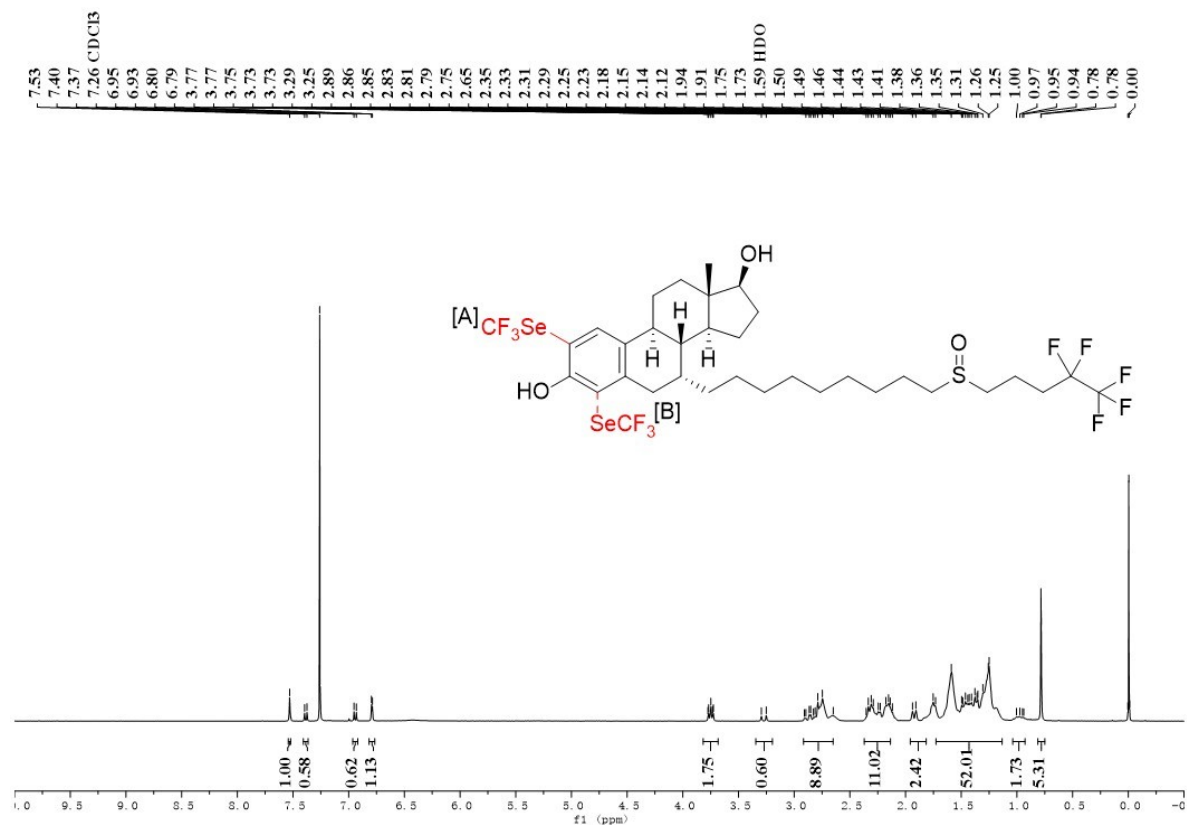


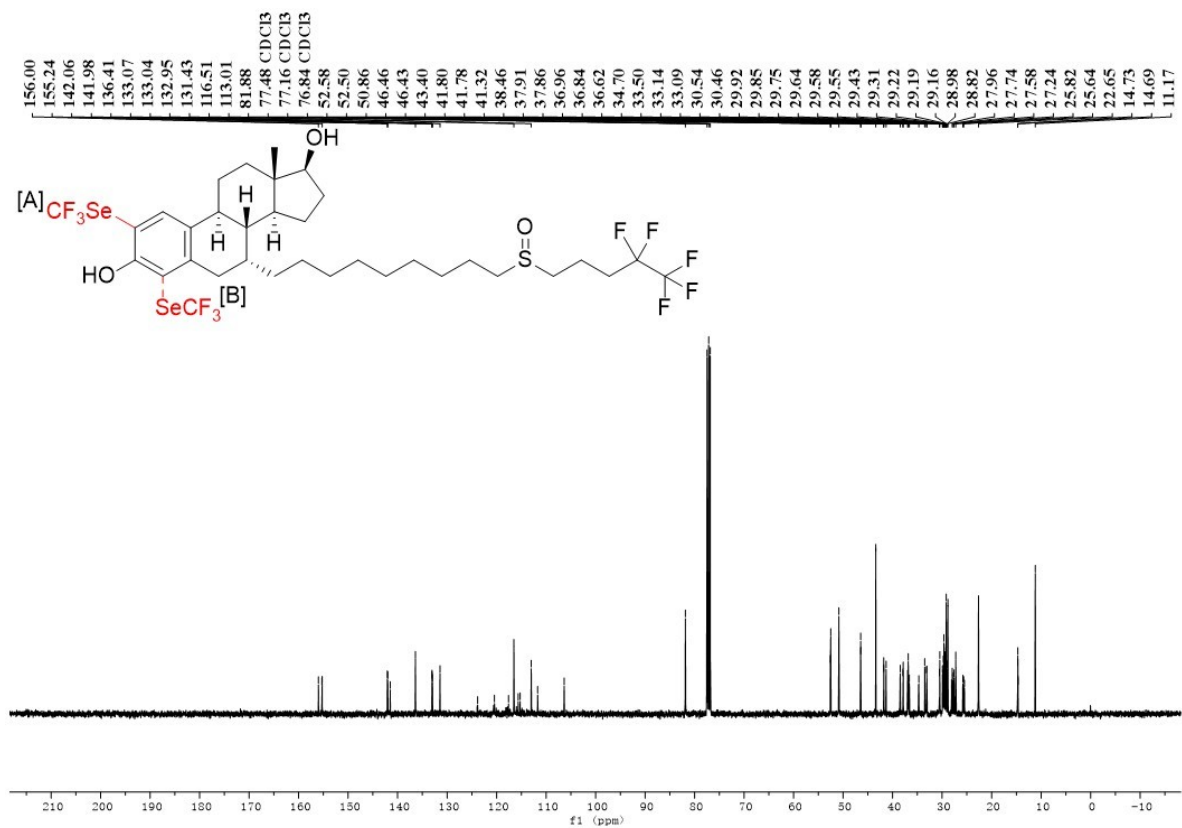
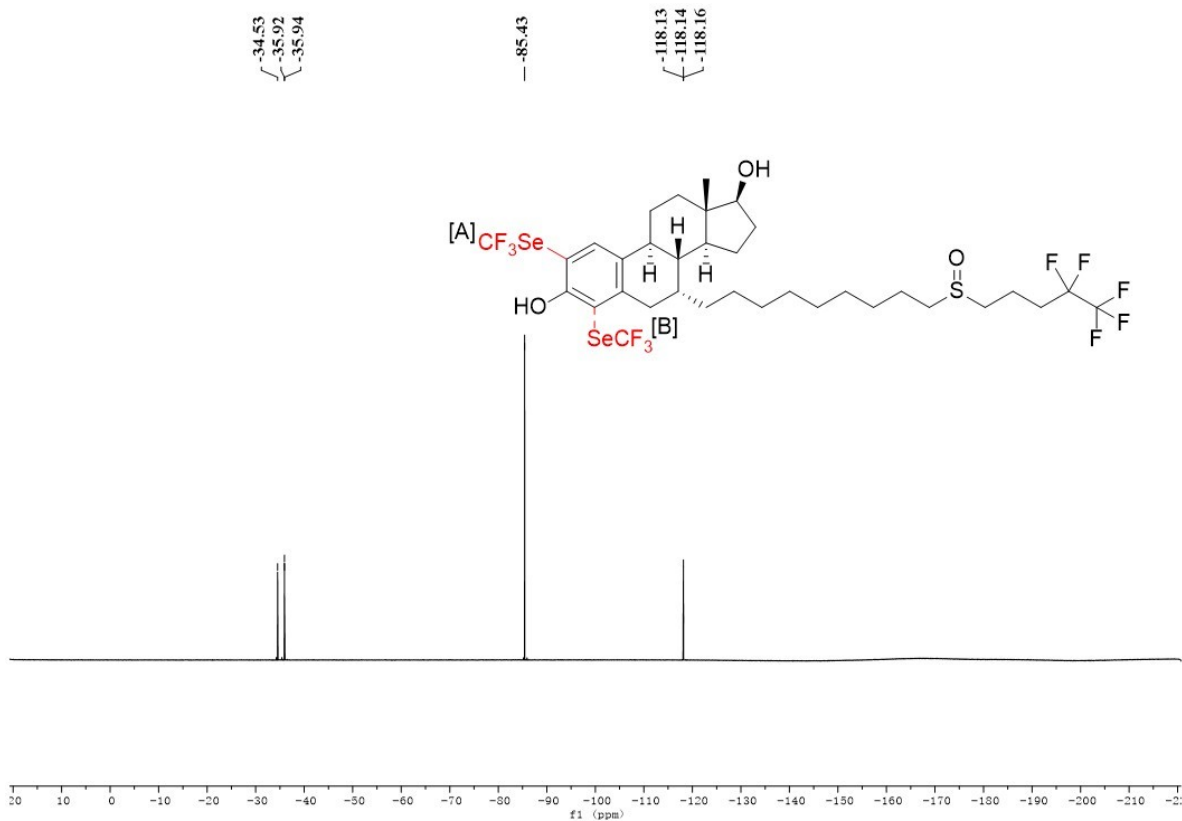
5ca ([A]: (8R,9S,13S,14S,17S)-13-methyl-2-((trifluoromethyl)selenanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol; [B]: (8R,9S,13S,14S,17S)-13-methyl-4-((trifluoromethyl)selenanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol)



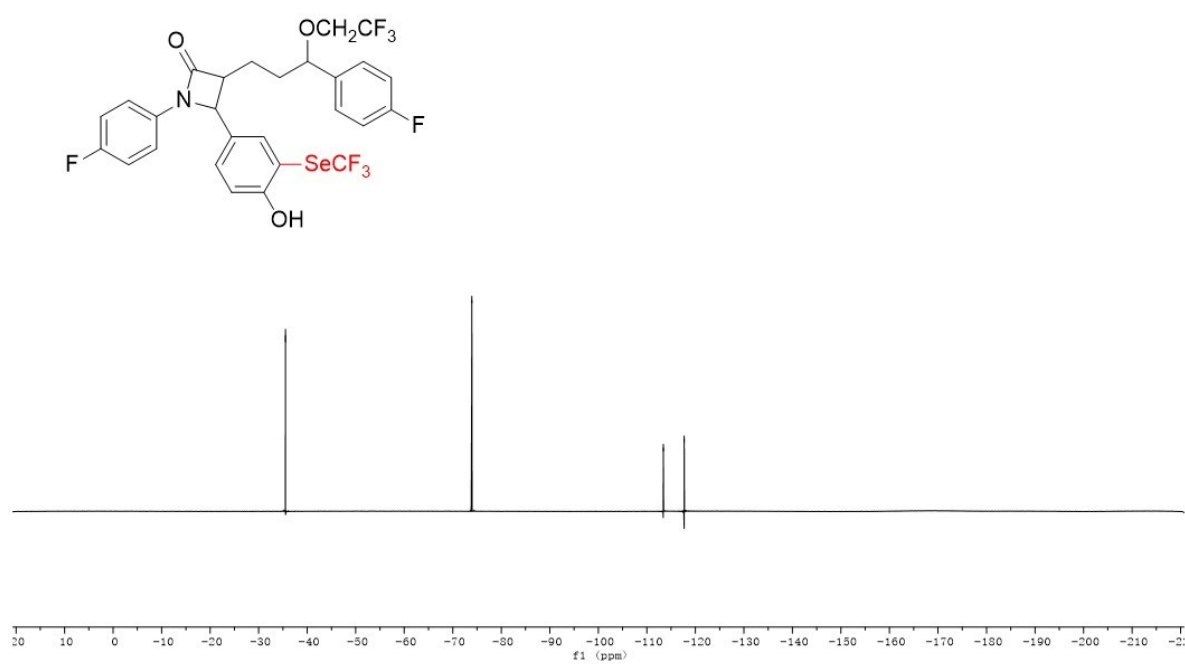
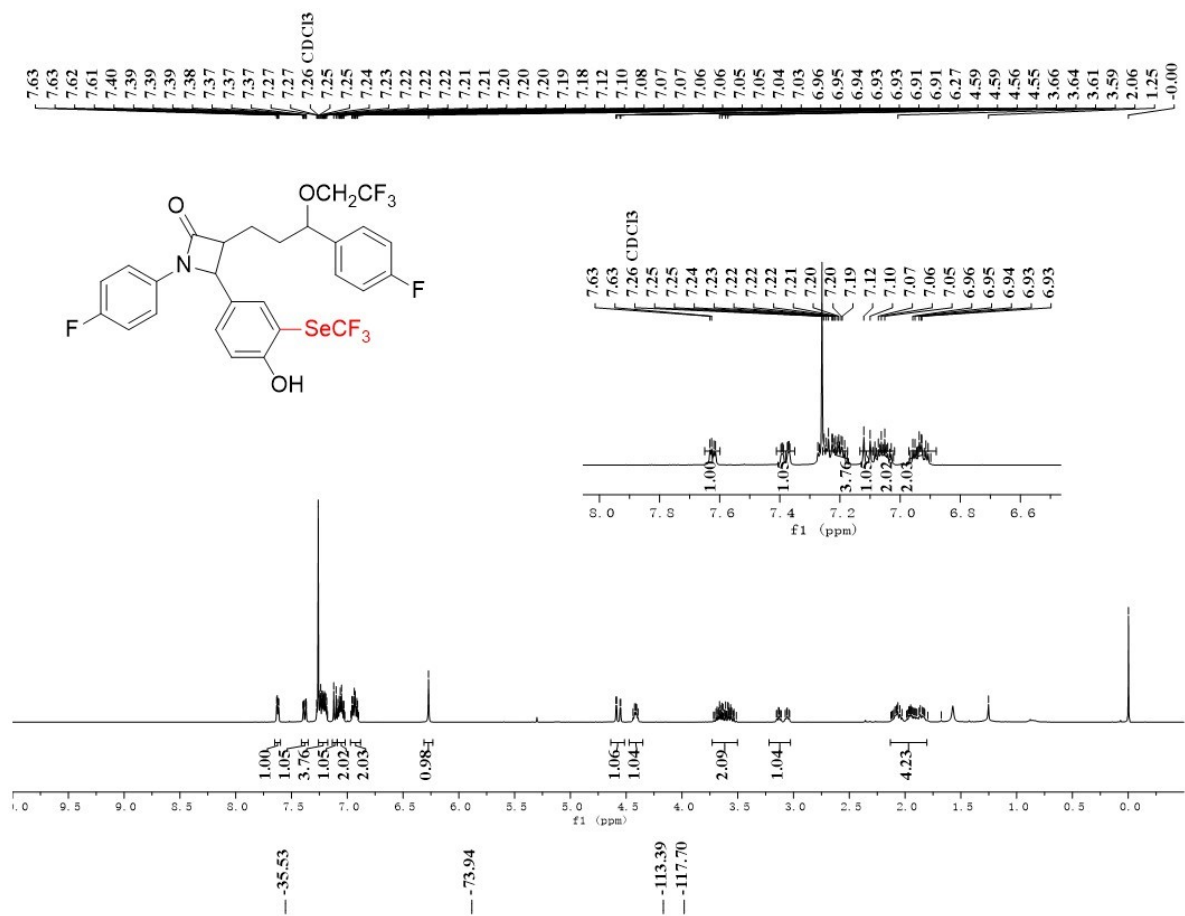


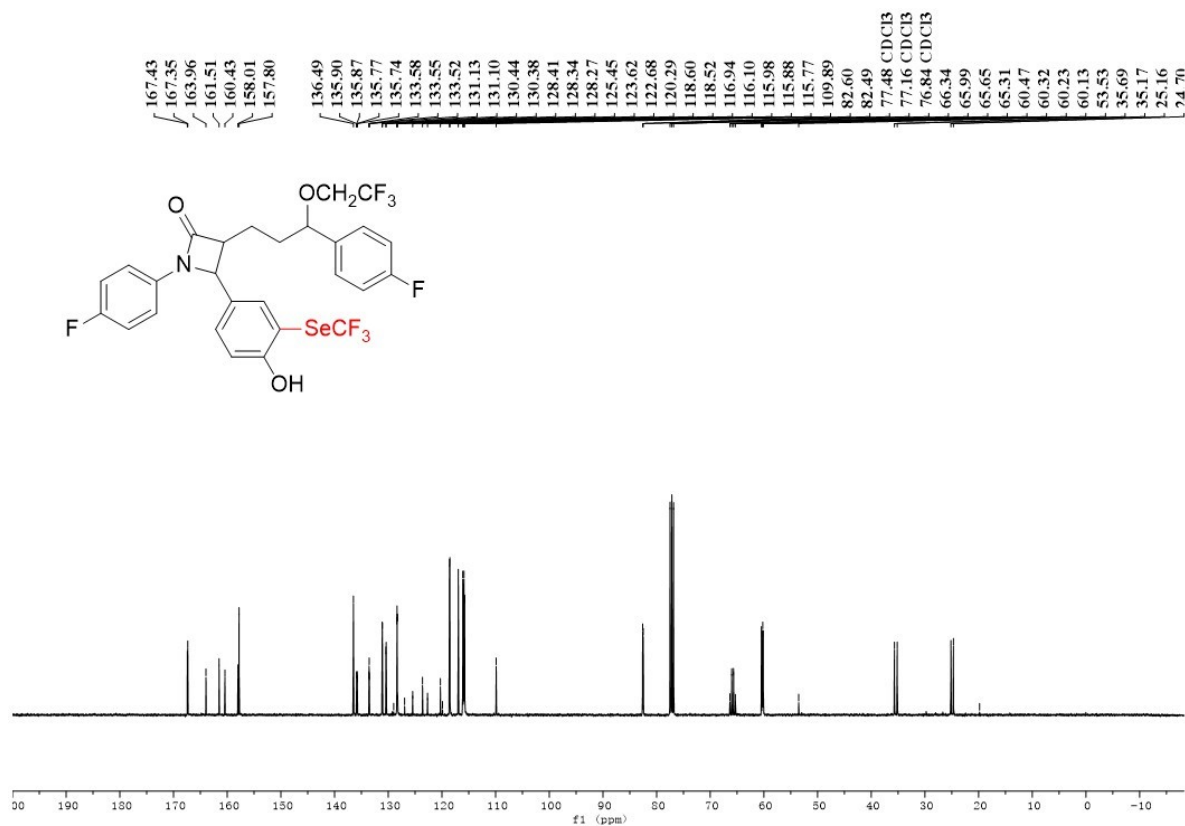
5cb ([A]: (7R,8R,9S,13S,14S,17S)-13-methyl-7-(9-((4,4,5,5,5-pentafluoropentyl)sulfinyl)nonyl)-2-((trifluoromethyl)selanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol; [B]: (7R,8R,9S,13S,14S,17S)-13-methyl-7-(9-((4,4,5,5,5-pentafluoropentyl)sulfinyl)nonyl)-4-((trifluoromethyl)selanyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol)



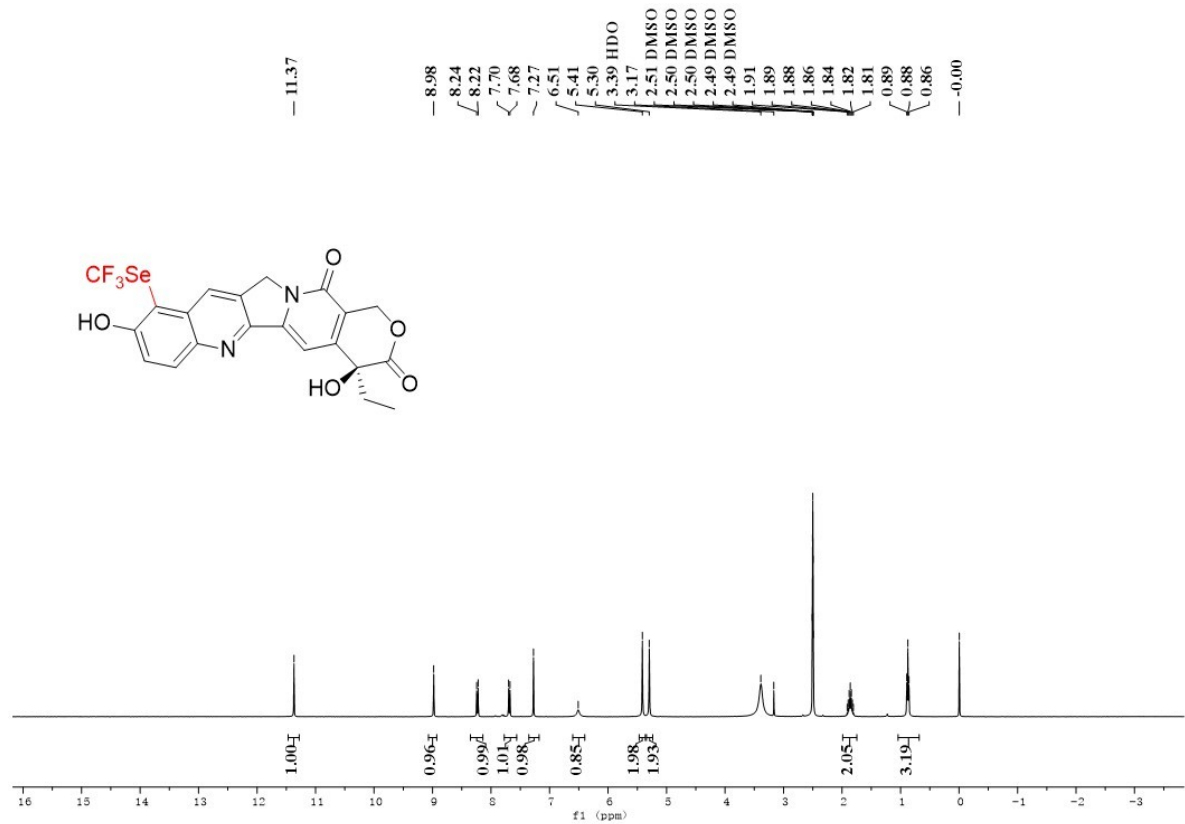


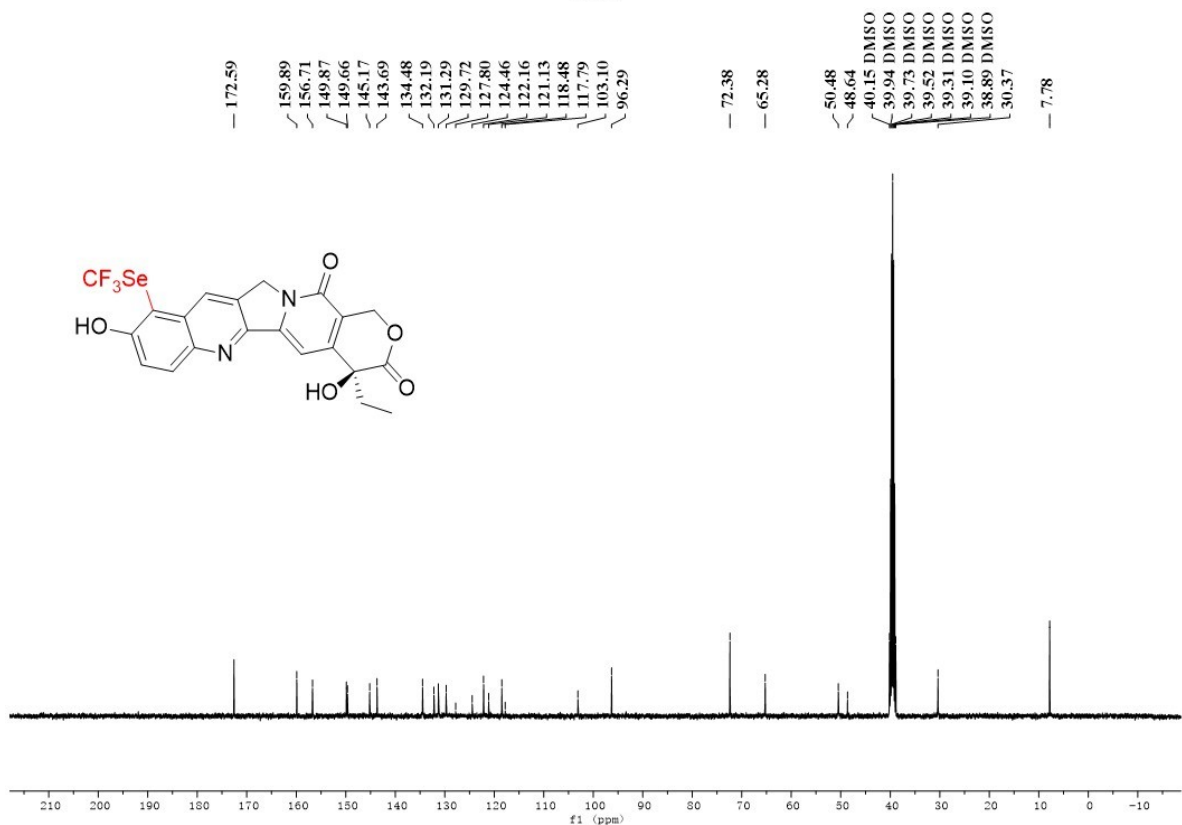
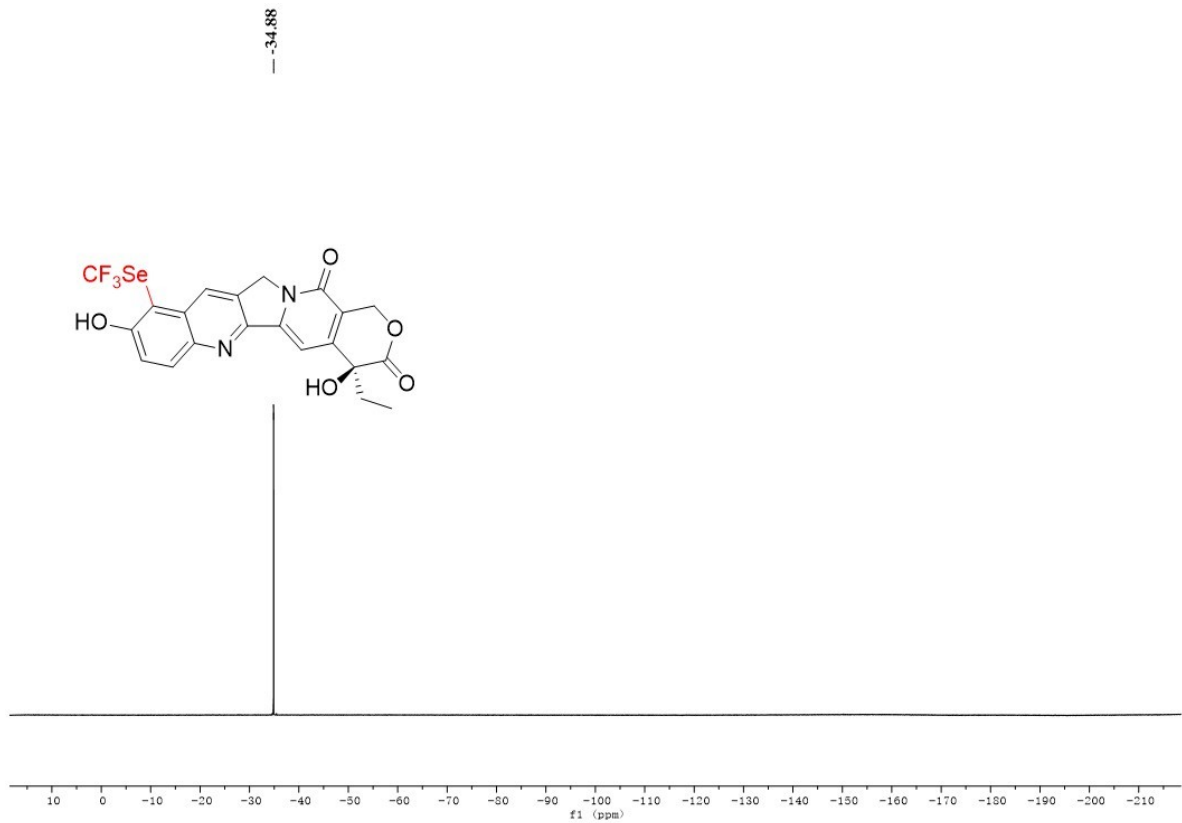
5cc (1-(4-fluorophenyl)-3-(3-(4-fluorophenyl)-3-(2,2,2-trifluoroethoxy)propyl)-4-(4-hydroxy-3-((trifluoromethyl)selenanyl)phenyl)azetid-2-one)



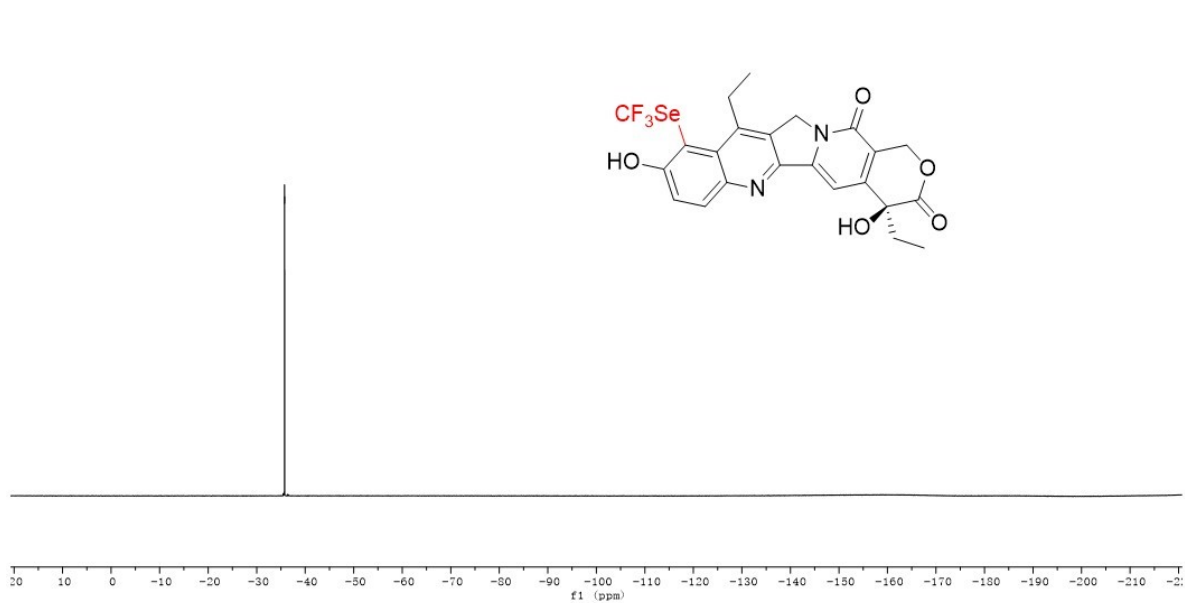
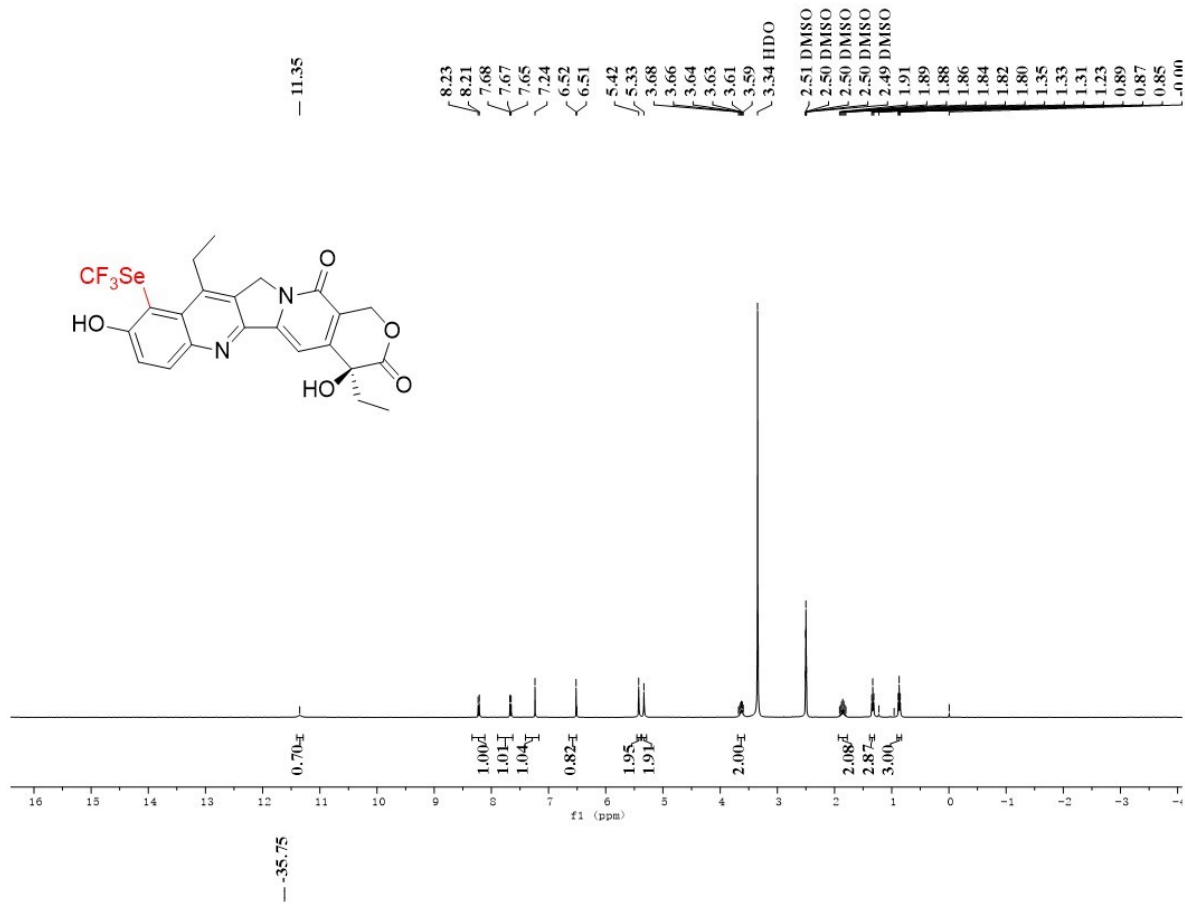


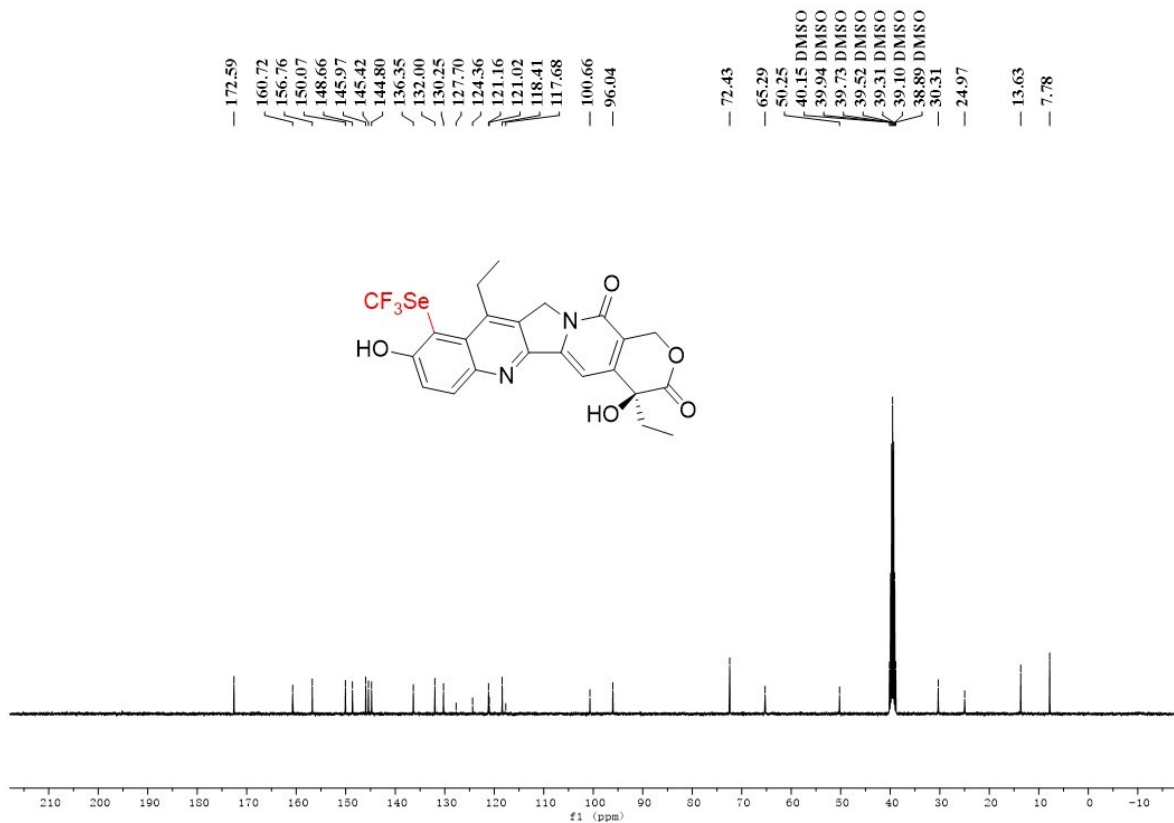
5cd ((S)-4-ethyl-4,9-dihydroxy-10-((trifluoromethyl)selanyl)-1,12-dihydro-14H-pyrano[3',4':6,7]indolizino[1,2-b]quinoline-3,14(4H)-dione)



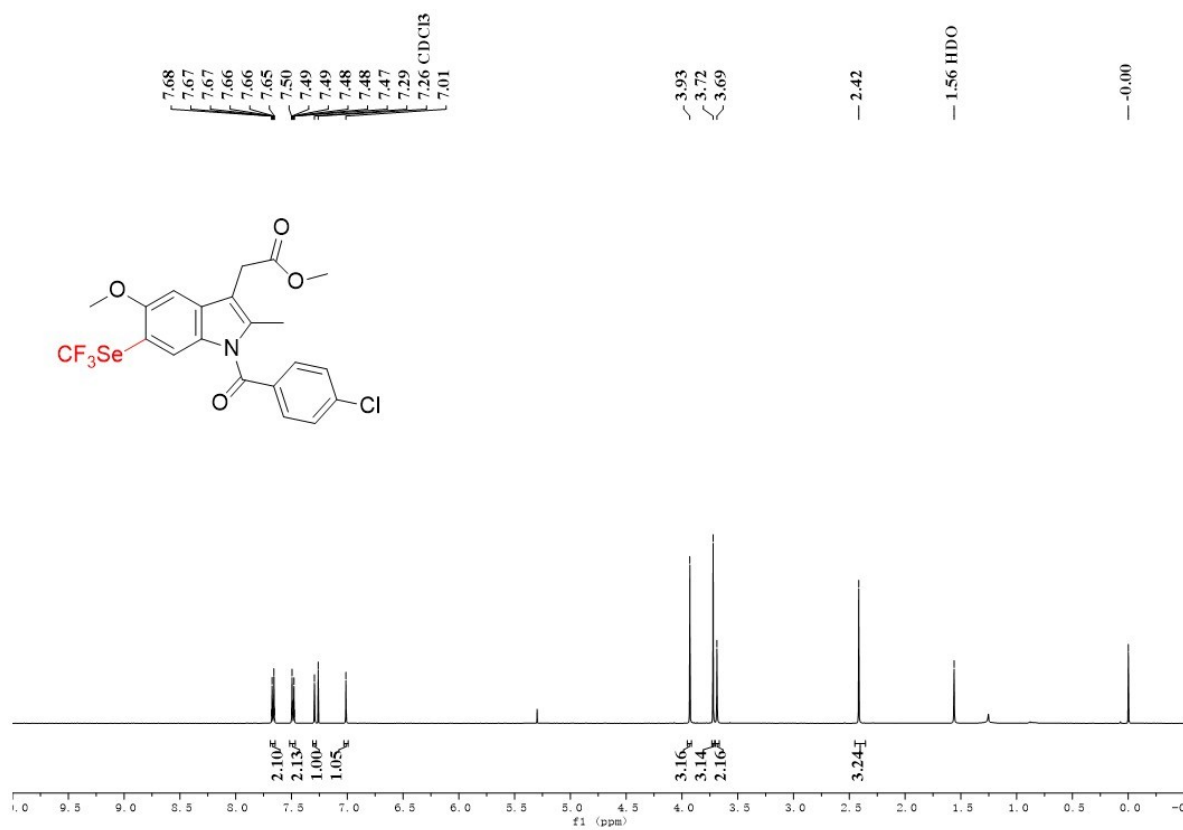


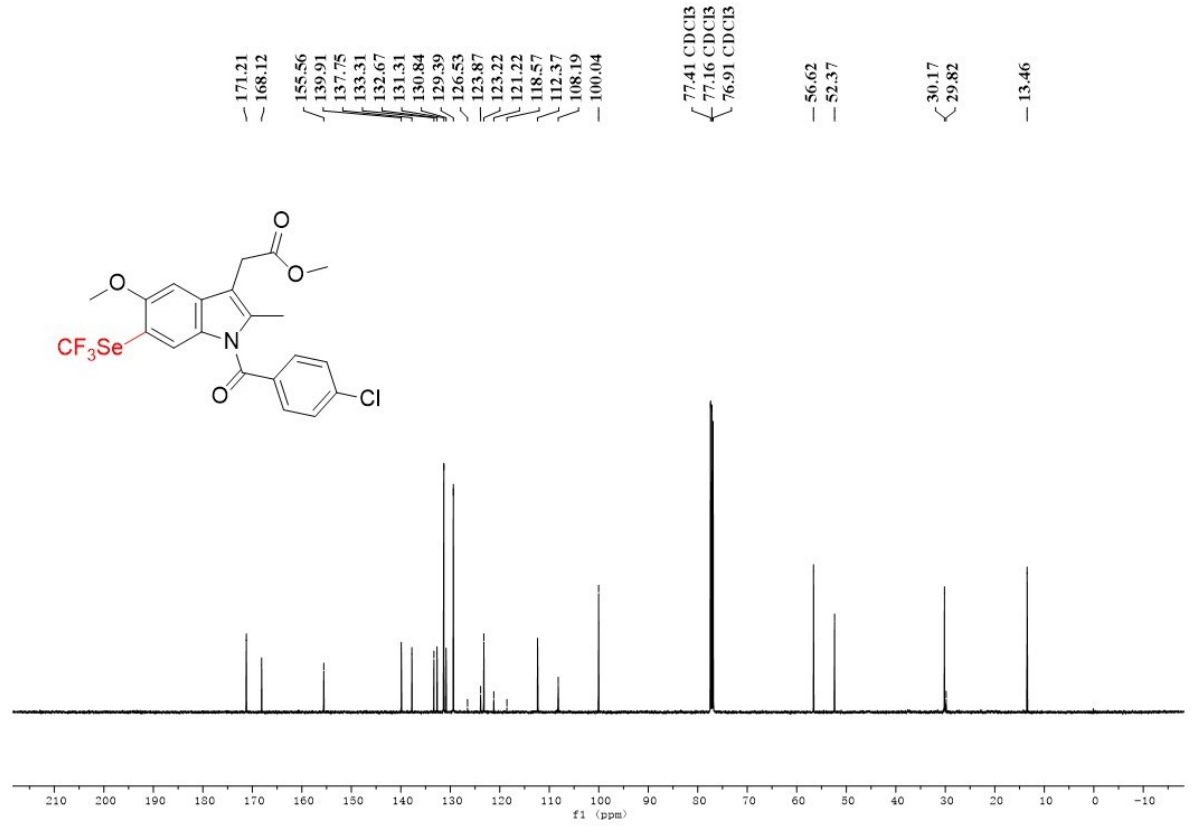
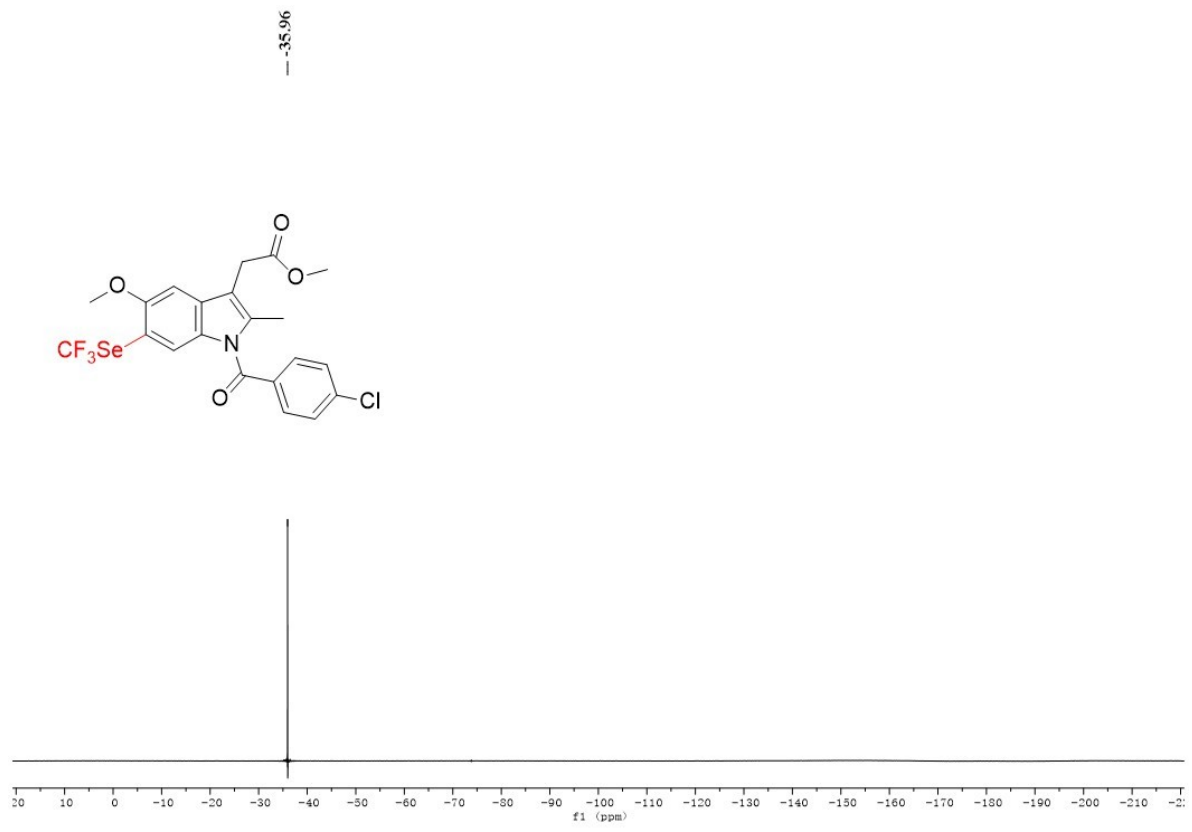
5ce ((S)-4,11-diethyl-4,9-dihydroxy-10-((trifluoromethyl)selanyl)-1,12-dihydro-14H-pyrano[3',4':6,7]indolizino[1,2-b]quinoline-3,14(4H)-dione)



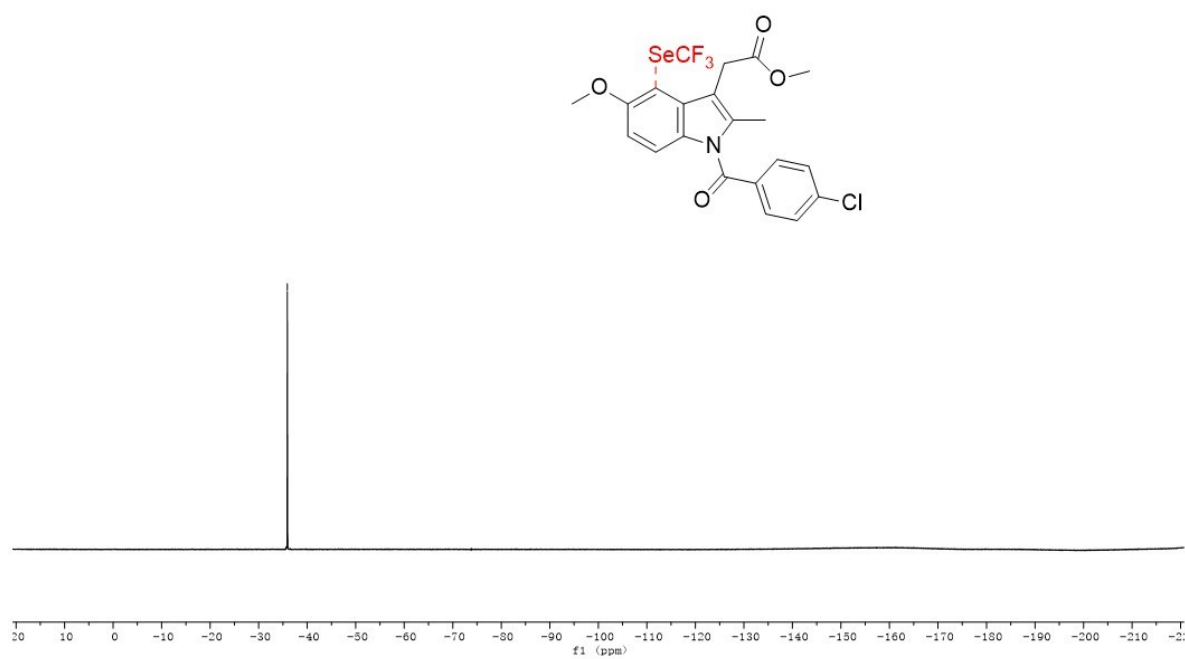
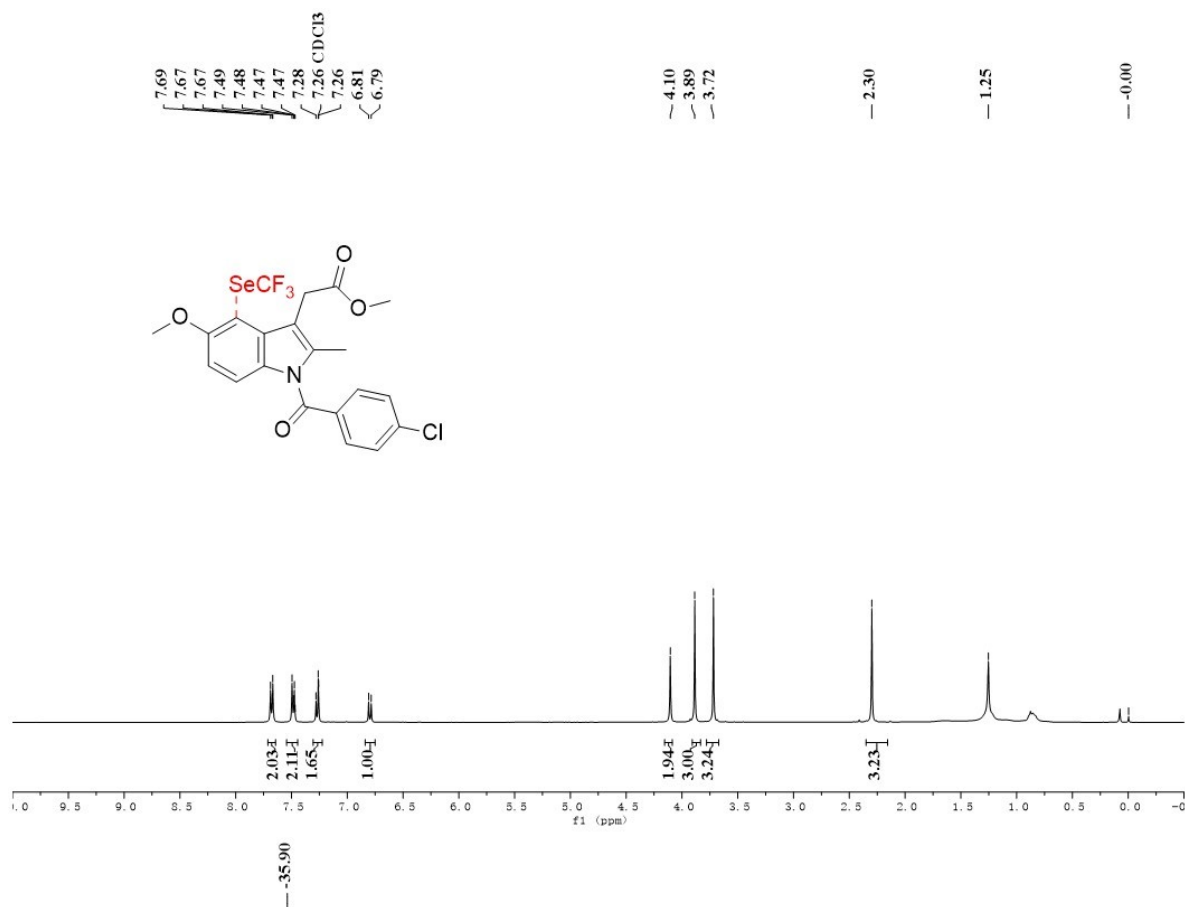


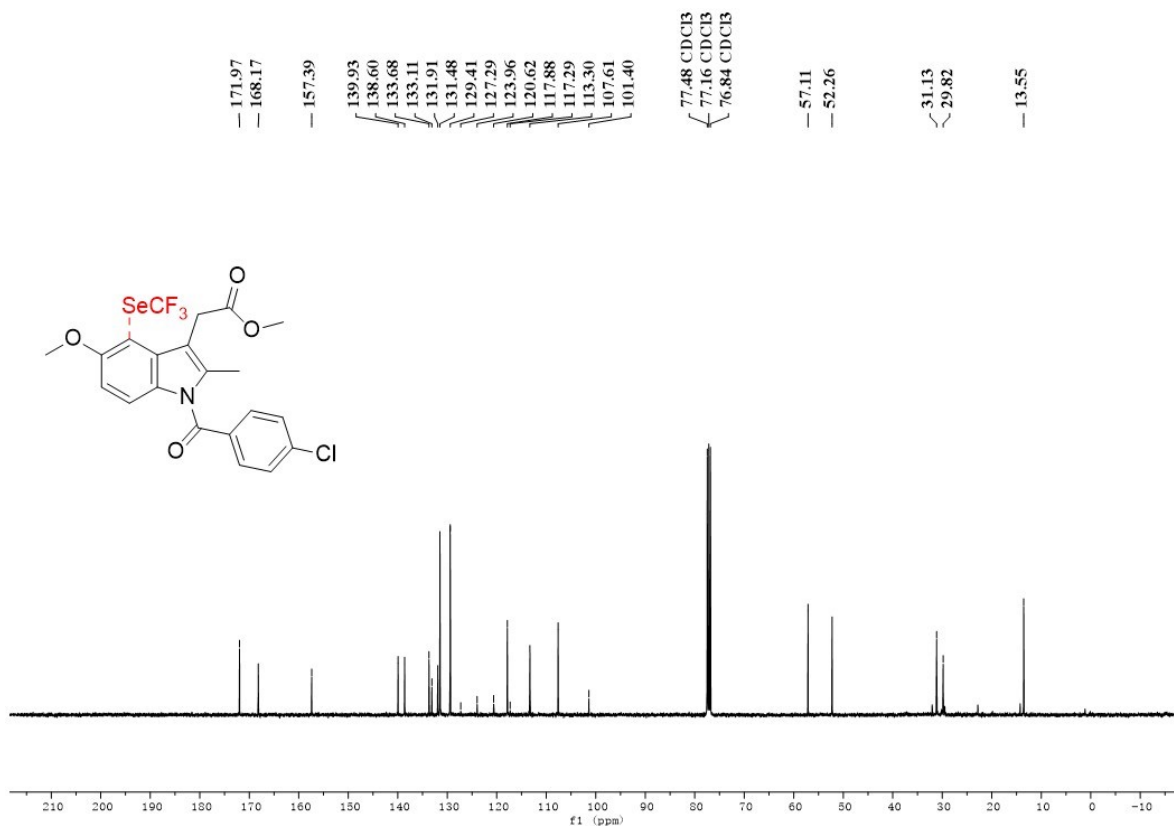
5cf, [A] : [B] = 3 : 2, A (methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-6-((trifluoromethyl)selenyl)-1H-indol-3-yl)acetate)



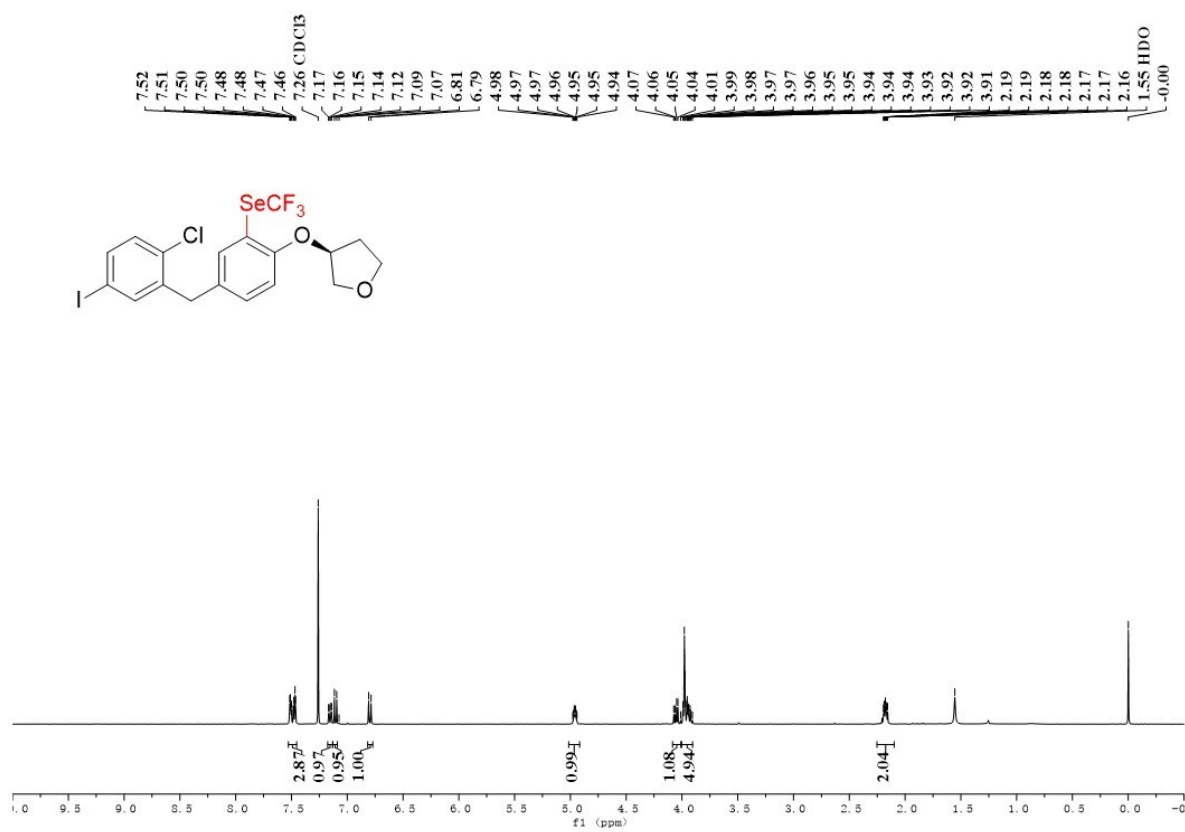


5cf, B (methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-4-((trifluoromethyl)selenanyl)-1H-indol-3-yl)acetate)

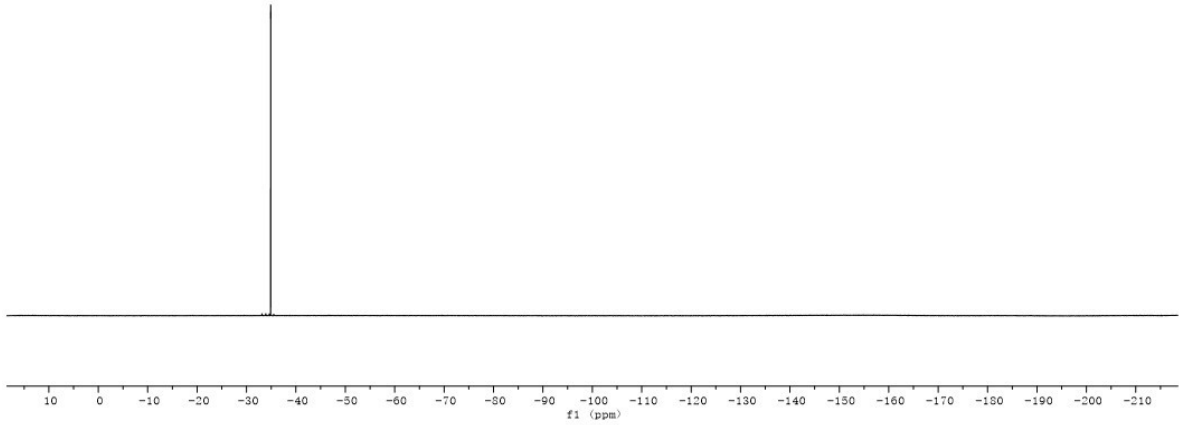
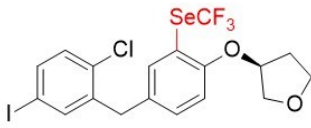




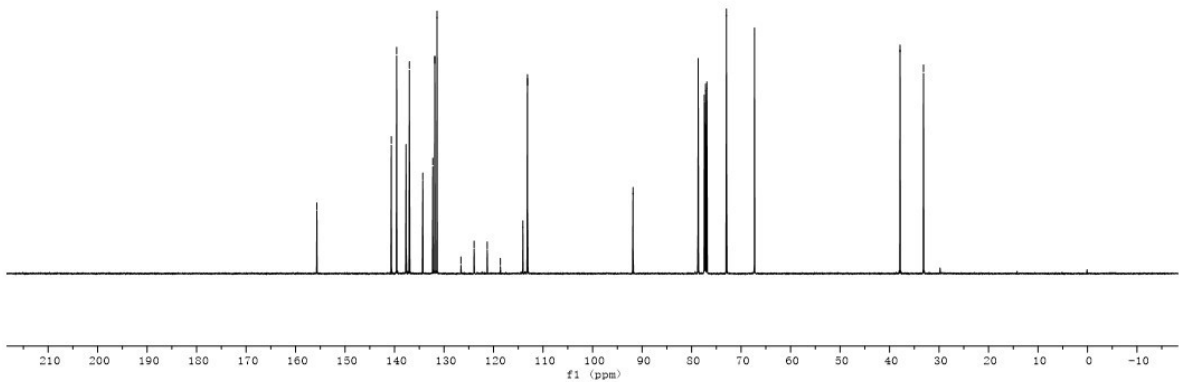
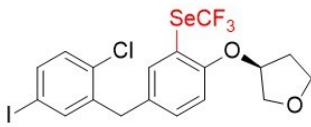
5cg ((S)-3-(4-(2-chloro-5-iodobenzyl)-2-((trifluoromethyl)selanyl)phenoxy) tetrahydrofuran)



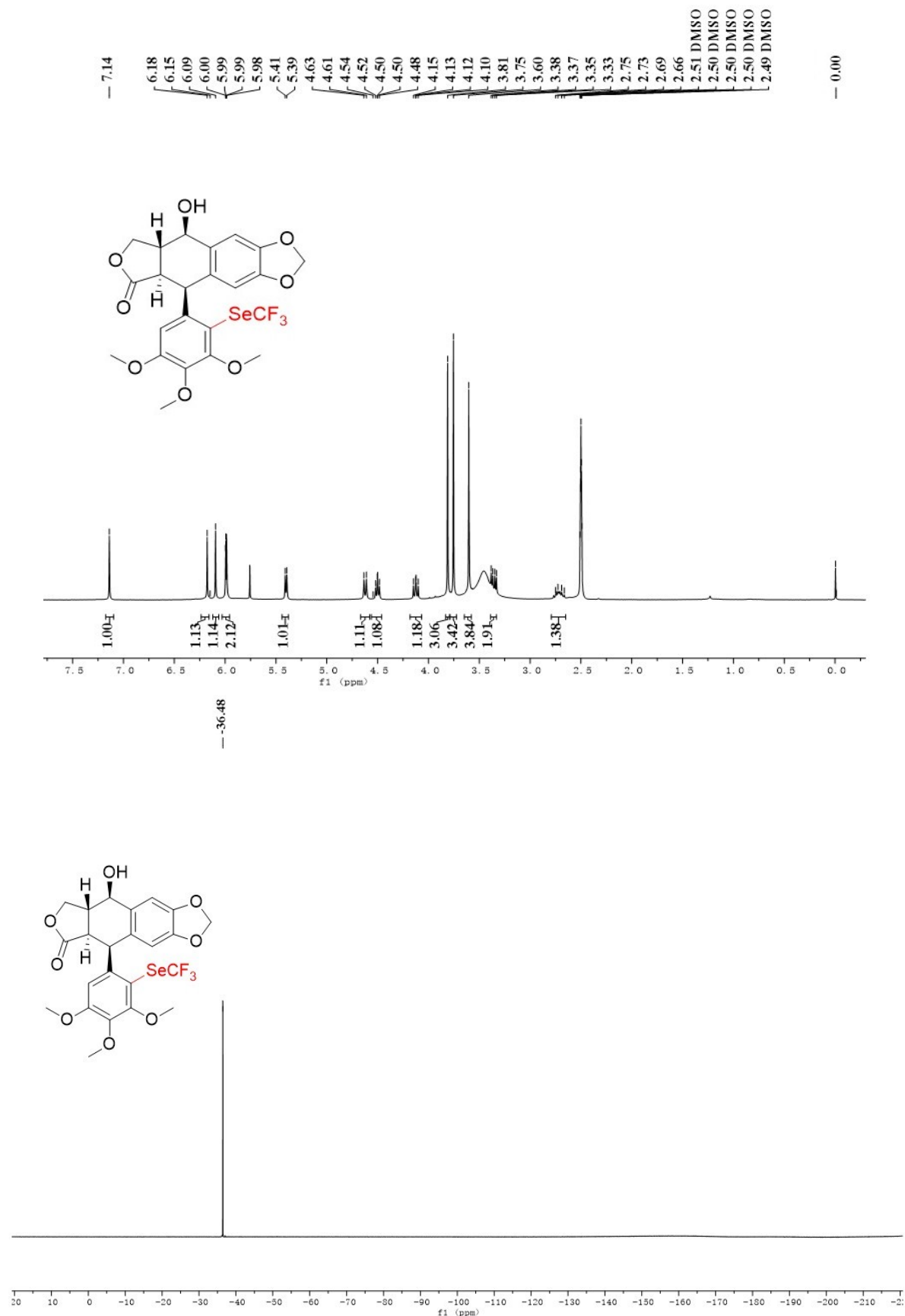
-34.91

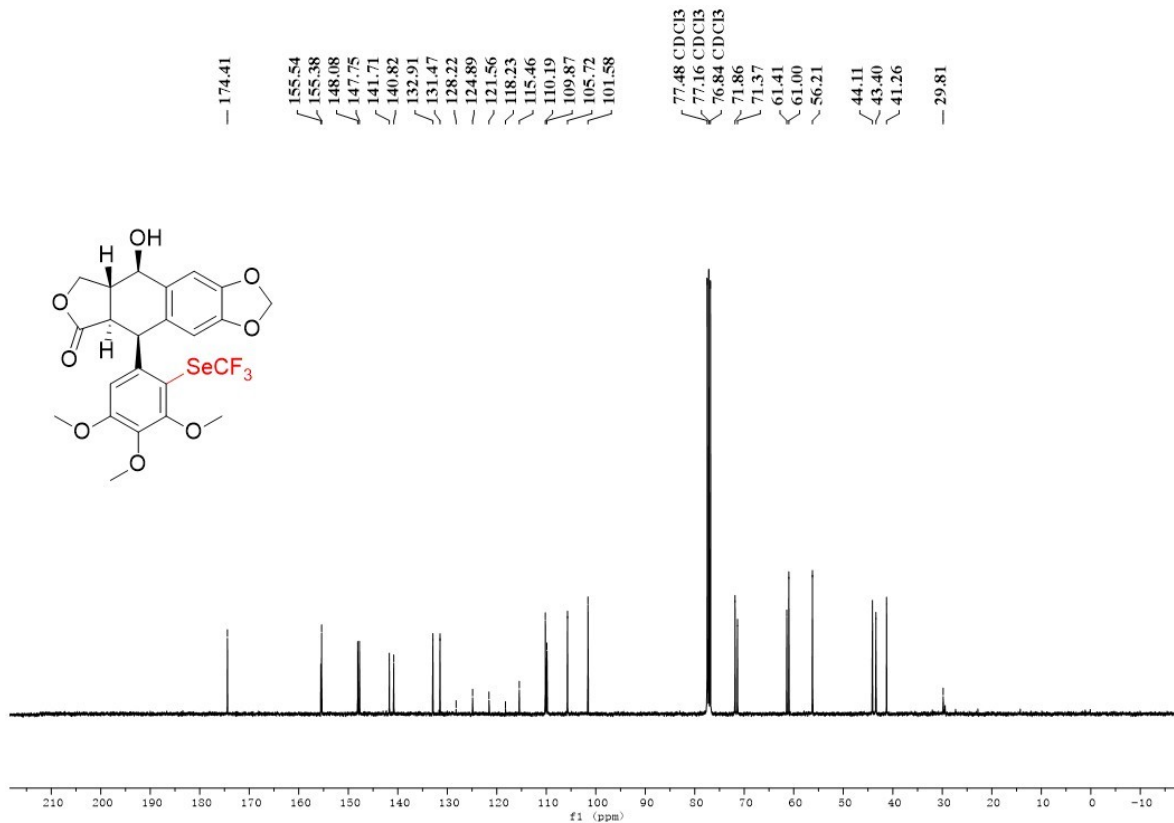


155.71
140.66
139.58
137.68
137.01
134.30
132.28
131.87
131.42
126.59
123.94
121.29
118.64
114.07
113.15
- 91.84
78.68
77.41 CDCl₃
77.16 CDCl₃
76.91 CDCl₃
72.95
67.28
- 37.87
- 33.14

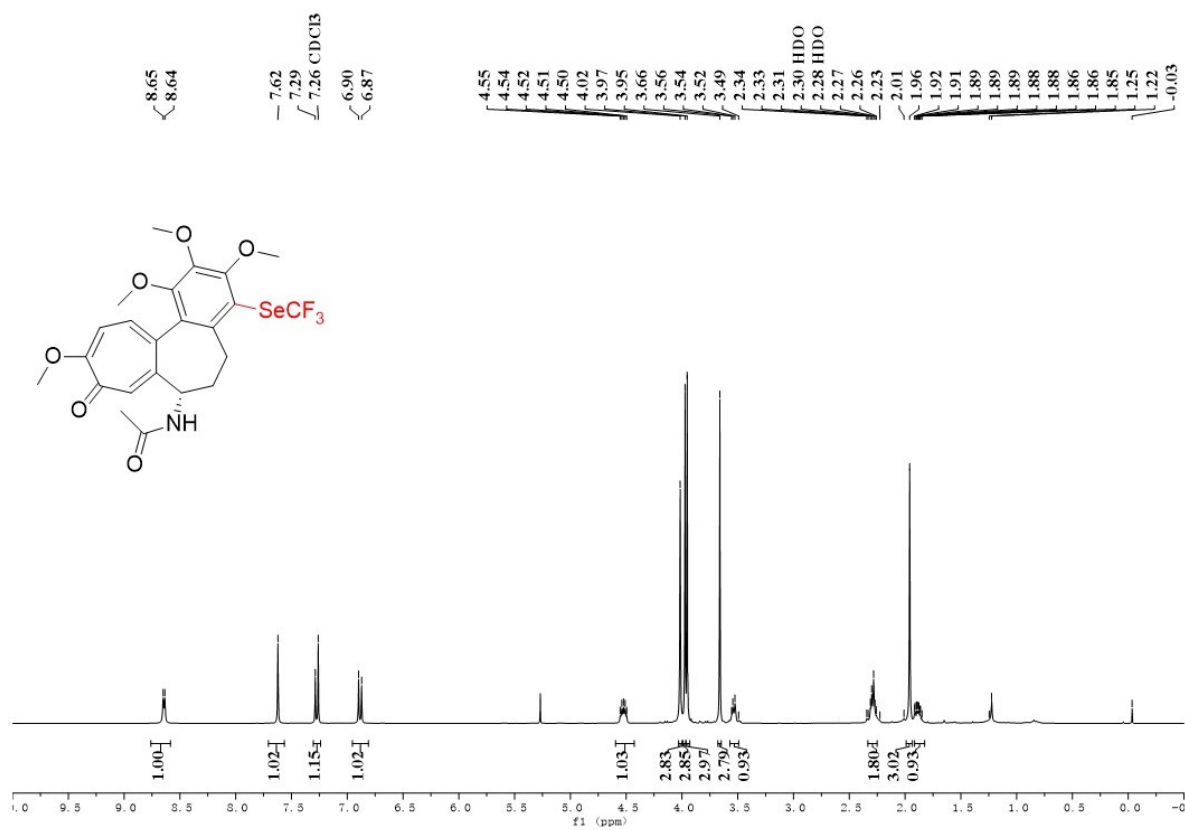


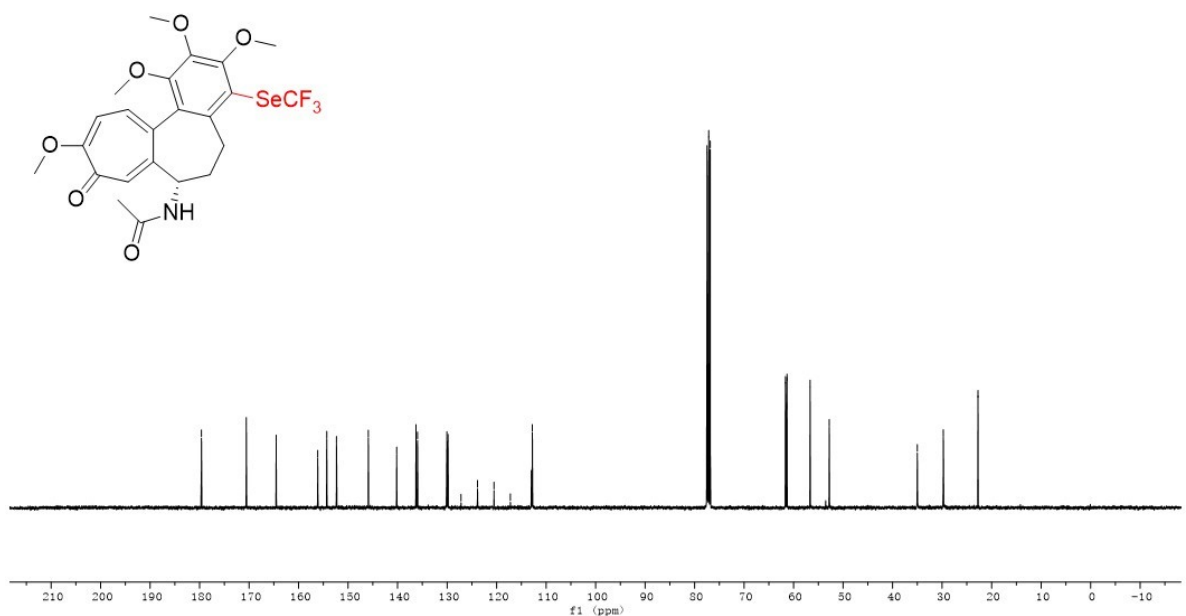
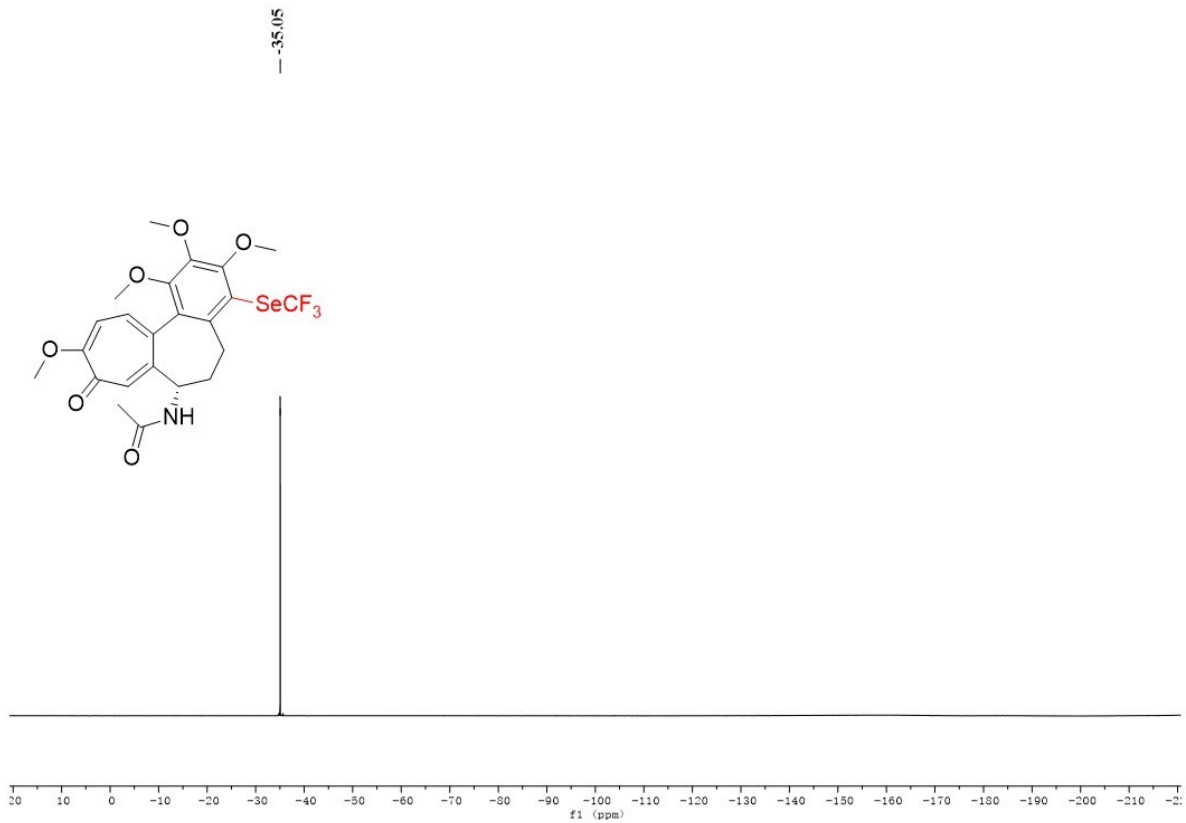
5ch ((5S,5aR,8aR,9R)-9-hydroxy-5-(3,4,5-trimethoxy-2-((trifluoromethyl)selenyl)phenyl)-5,8,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one)



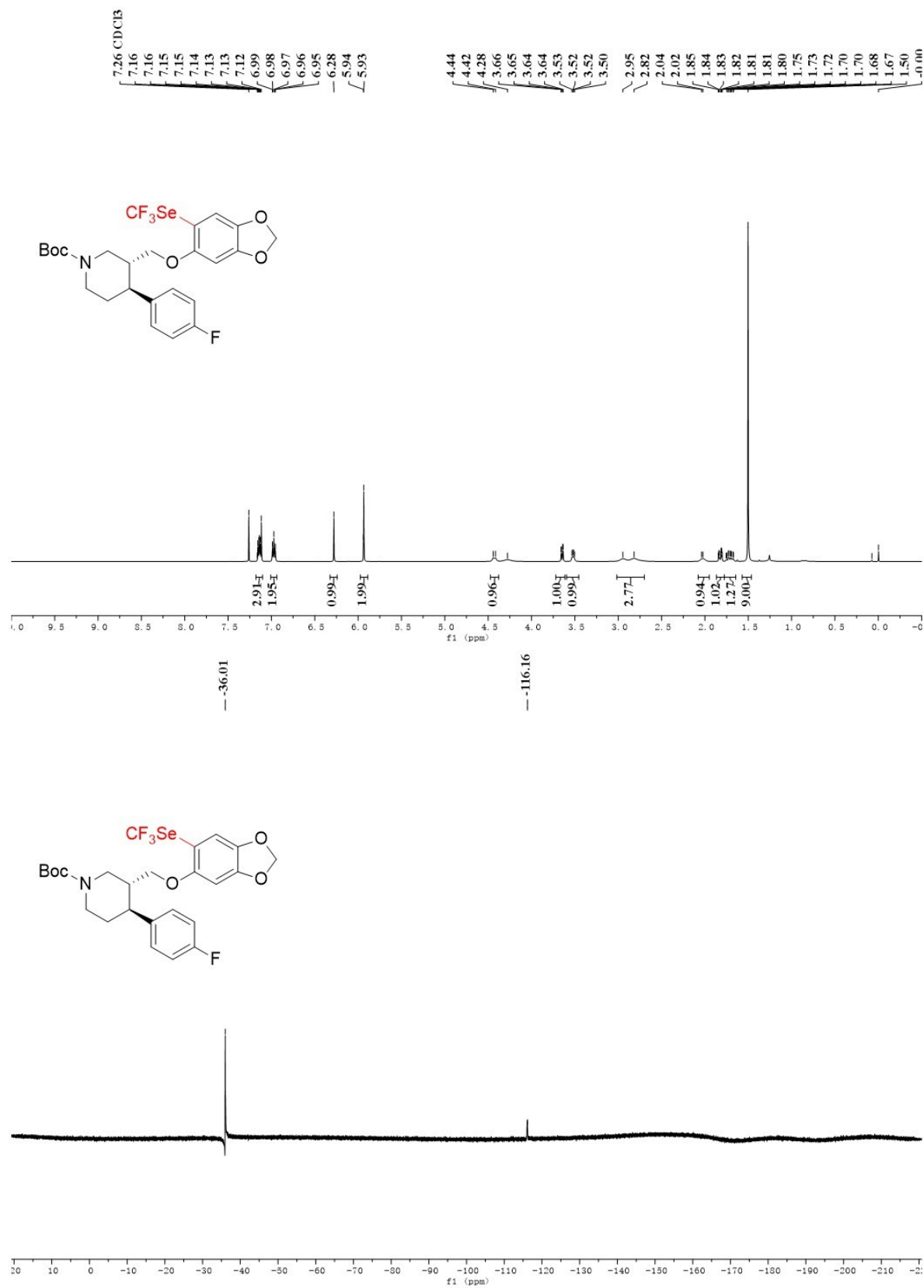


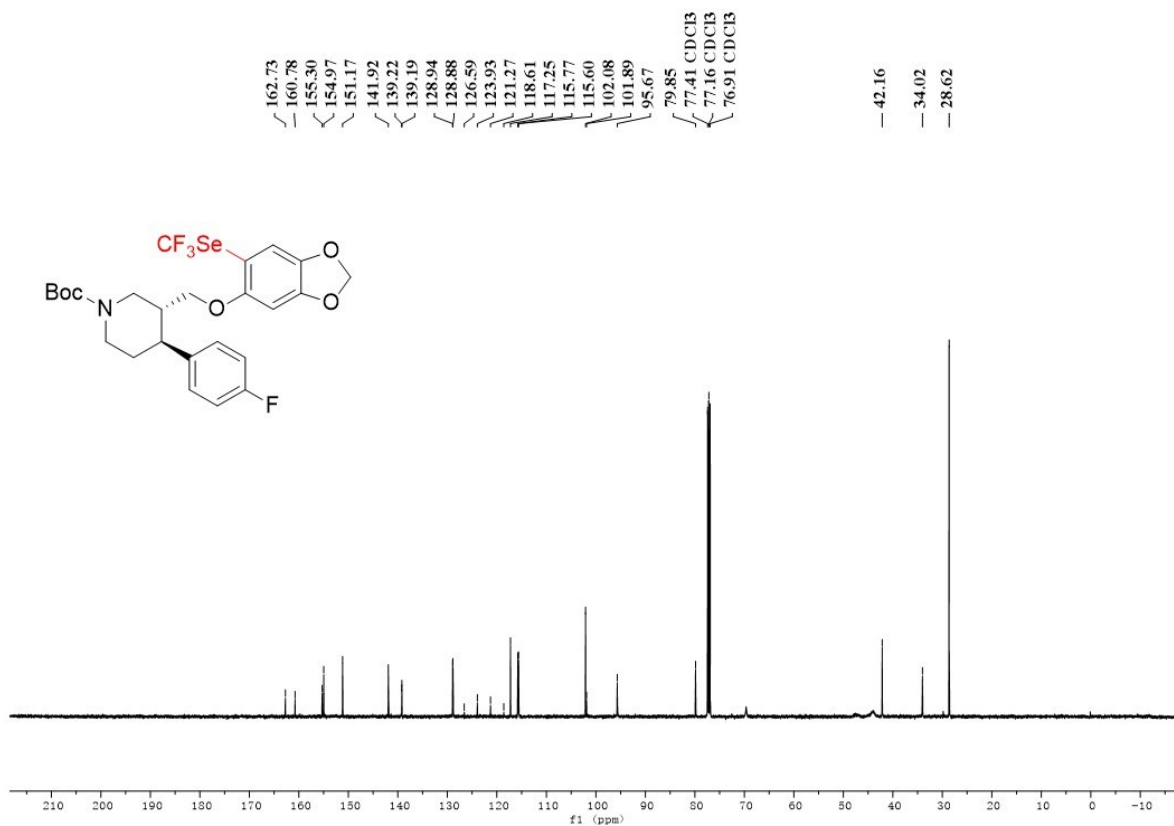
5ci ((S)-N-(1,2,3,10-tetramethoxy-9-oxo-4-((trifluoromethyl)selenanyl)-5,6,7,9-tetrahydrobenzo[a]heptalen-7-yl)acetamide)



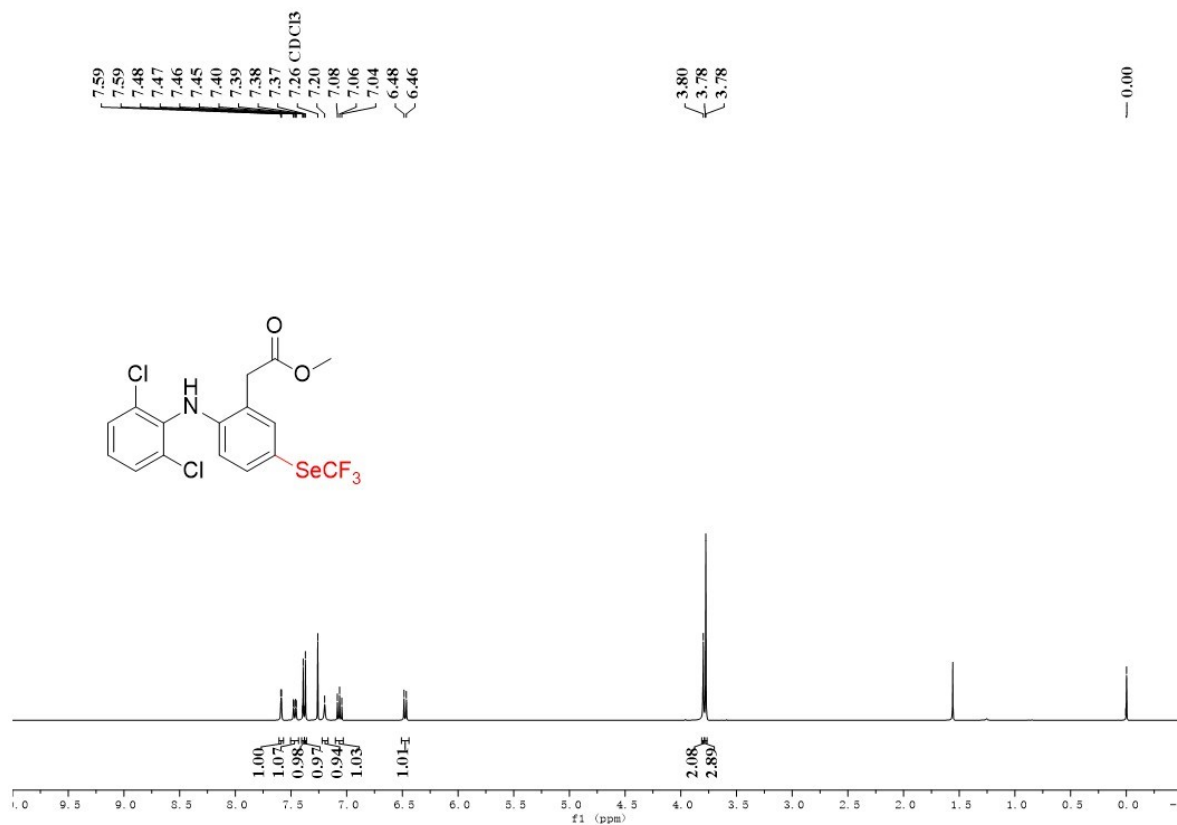


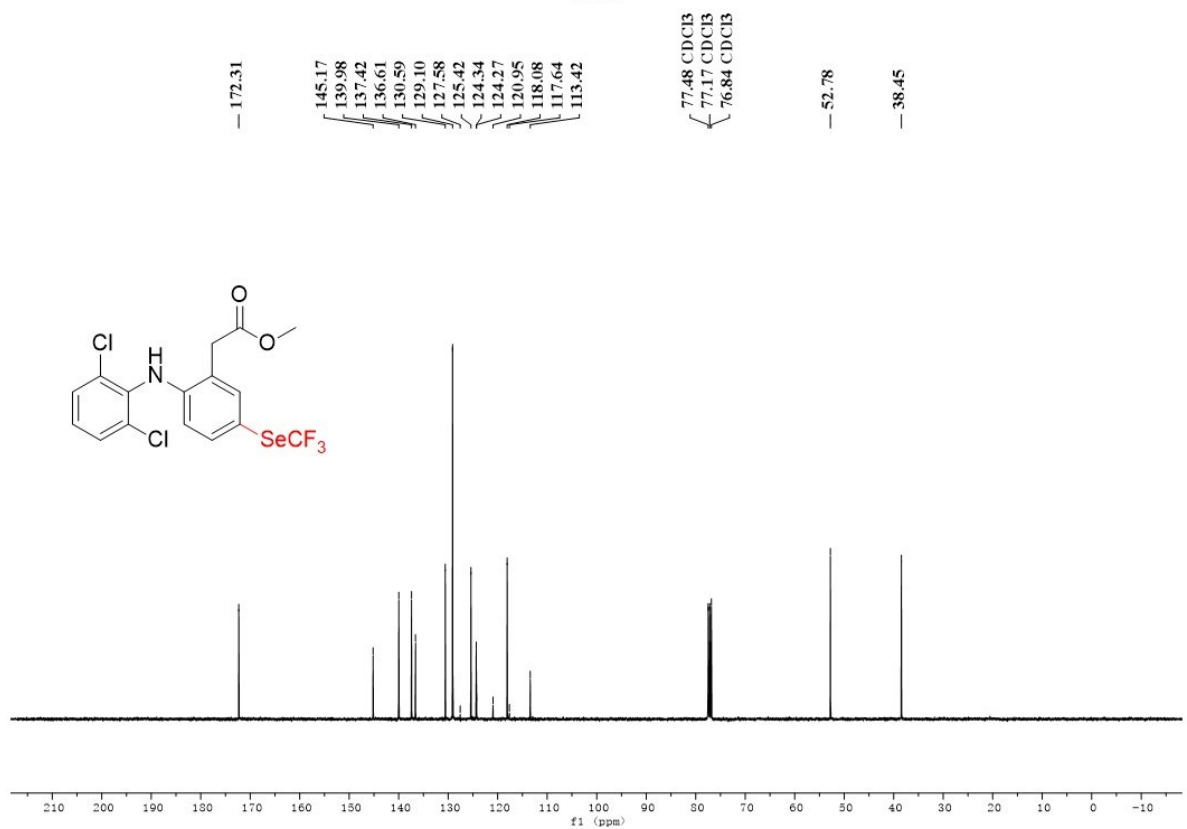
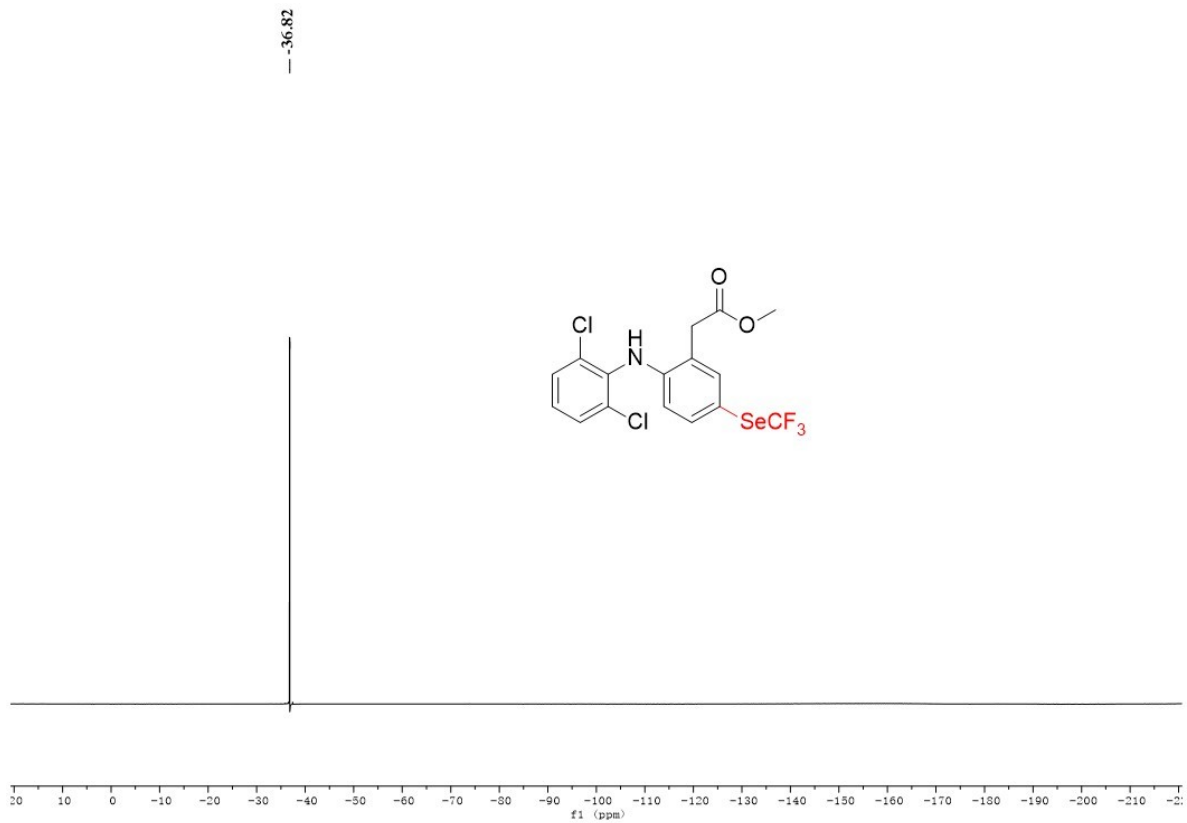
5cj (tert-butyl (3R,4S)-4-(4-fluorophenyl)-3-(((6-((trifluoromethyl)selenanyl)benzo[d][1,3]dioxol-5-yl)oxy)methyl)piperidine-1-carboxylate)



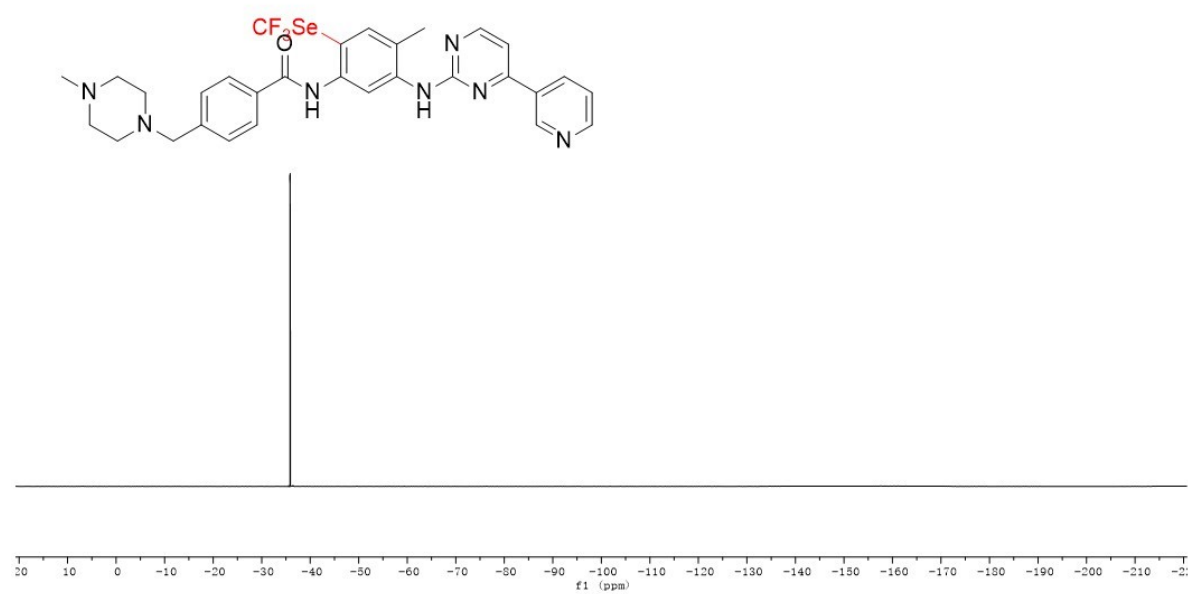
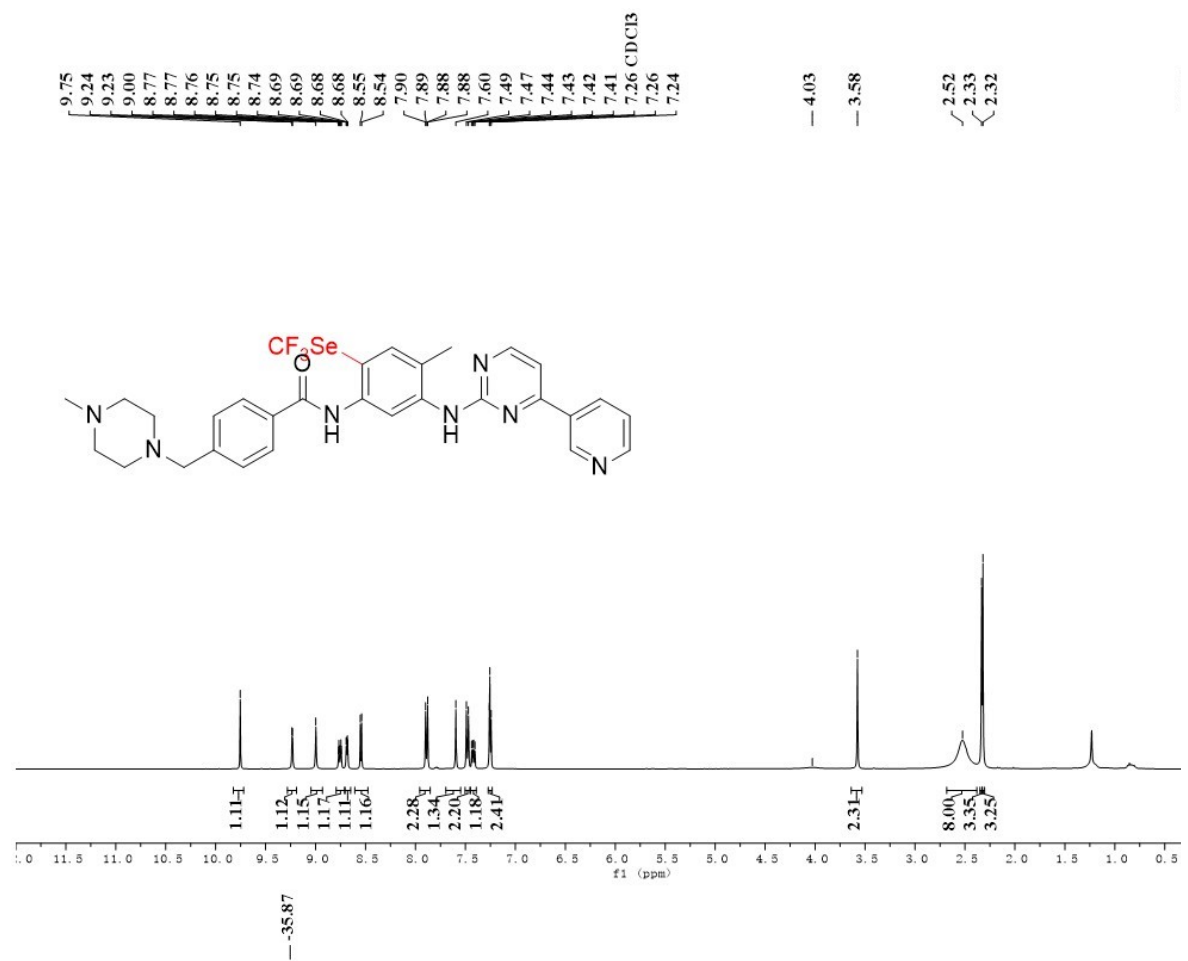


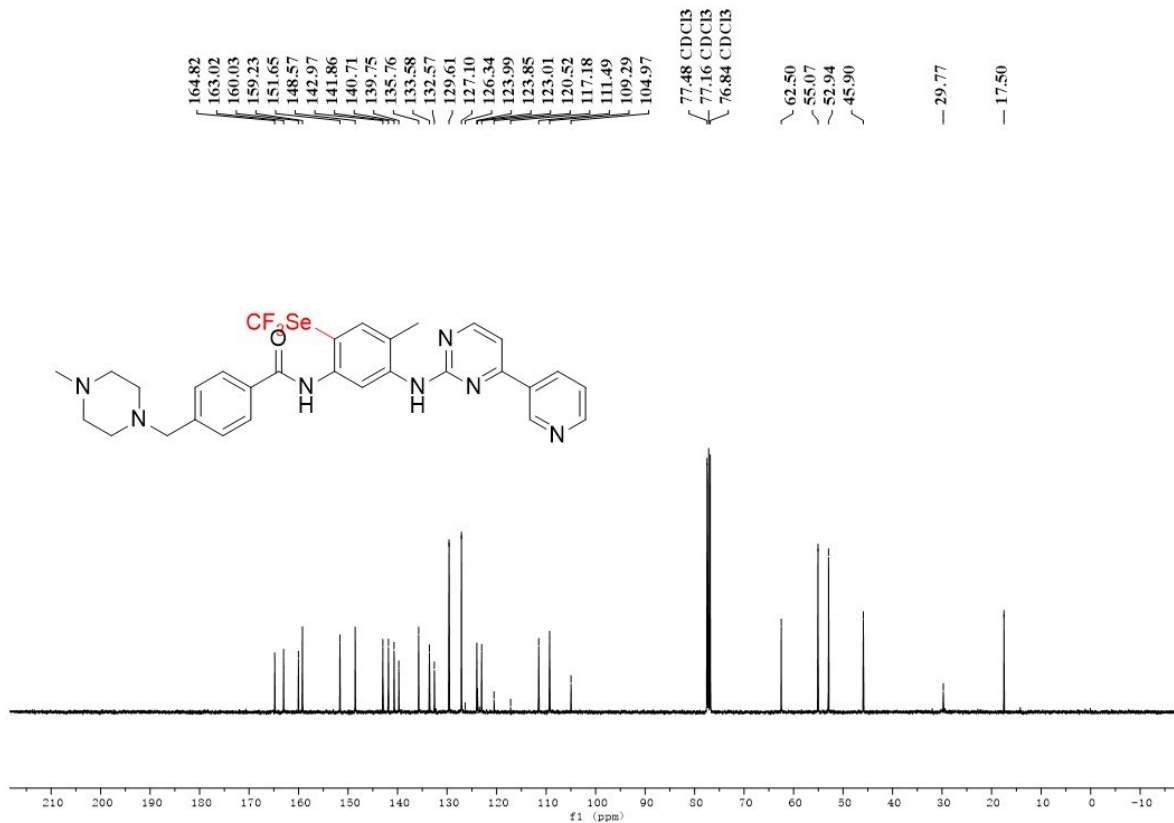
5ck (methyl 2-(2-((2,6-dichlorophenyl)amino)-5-((trifluoromethyl)selanyl)phenyl)acetate)



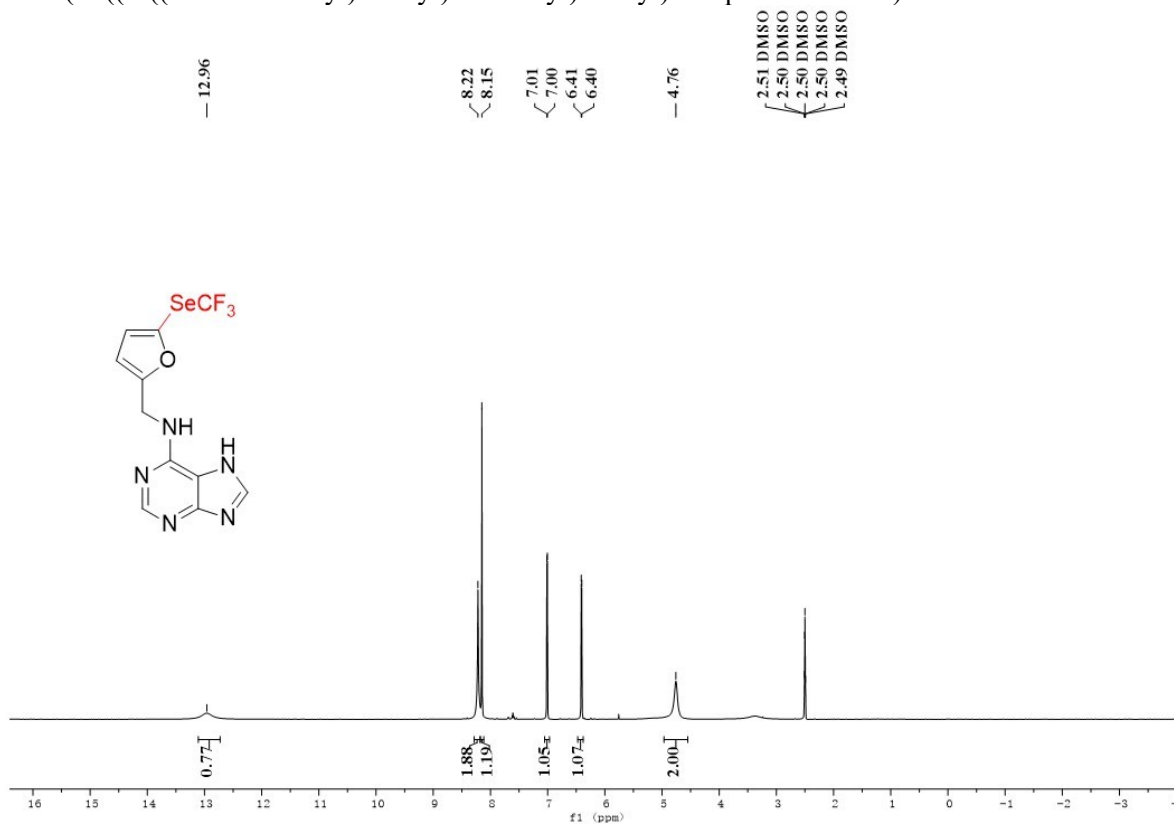


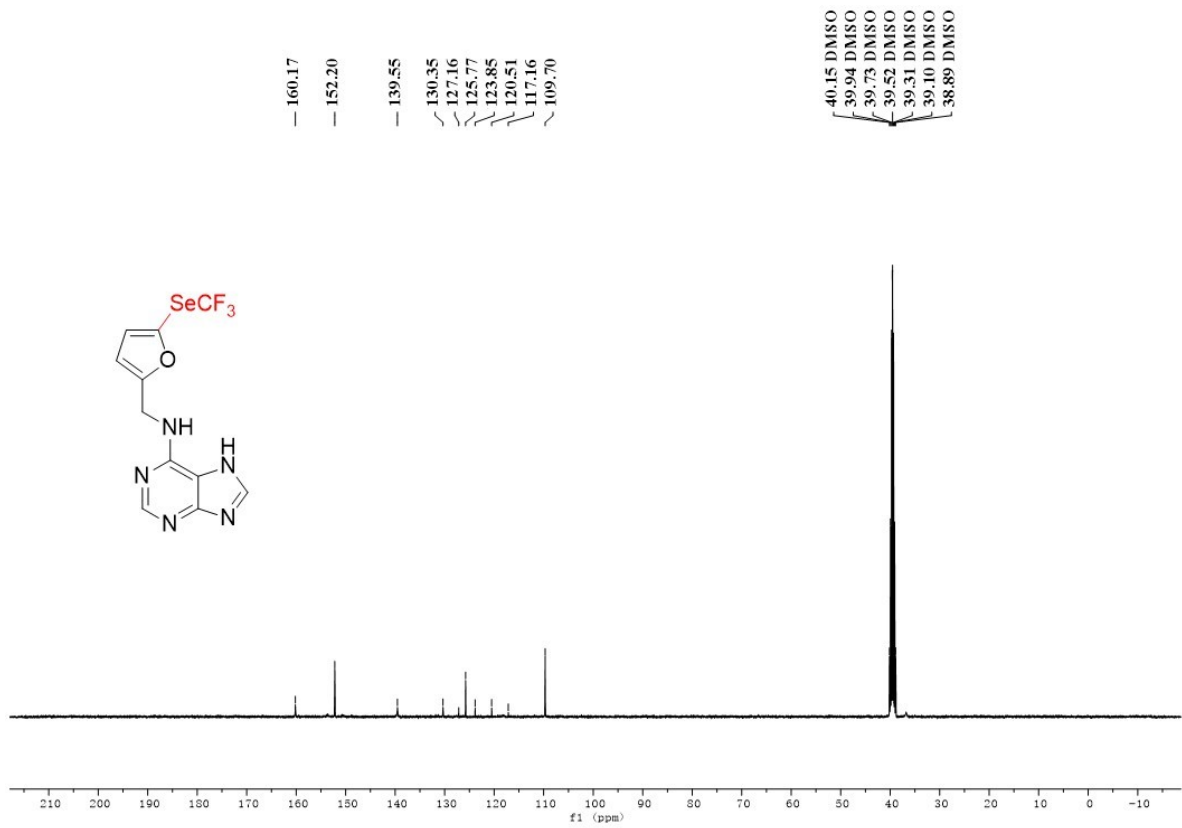
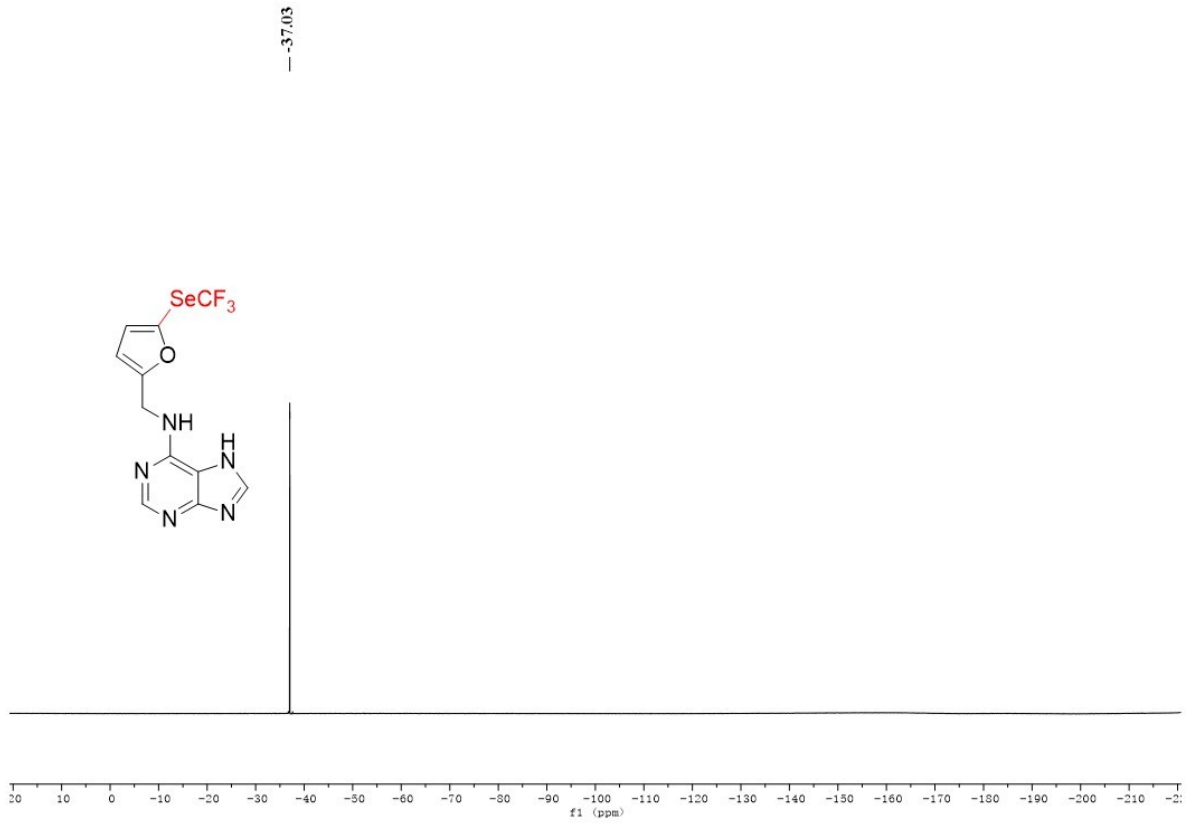
5cl (N-(4-methyl-5-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)-2-((trifluoromethyl)selenyl)phenyl)-4-((4-methylpiperazin-1-yl)methyl)benzamide)



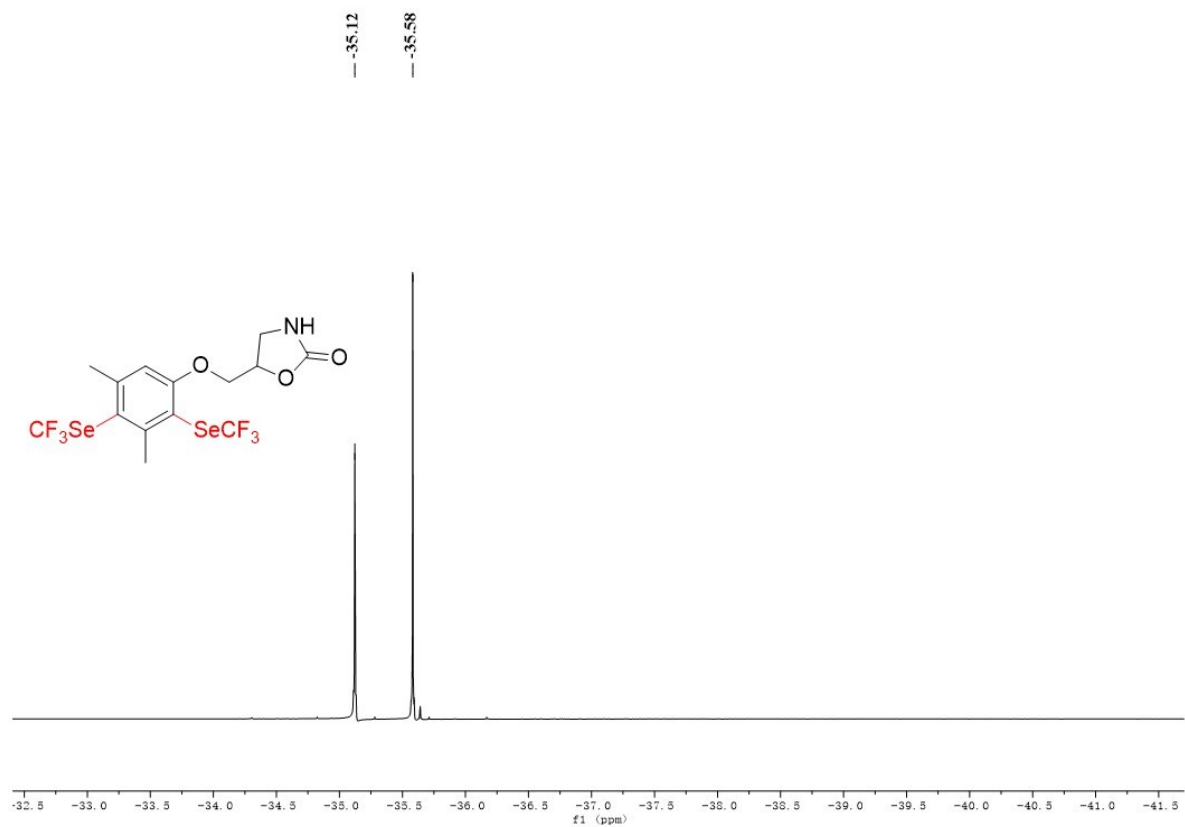
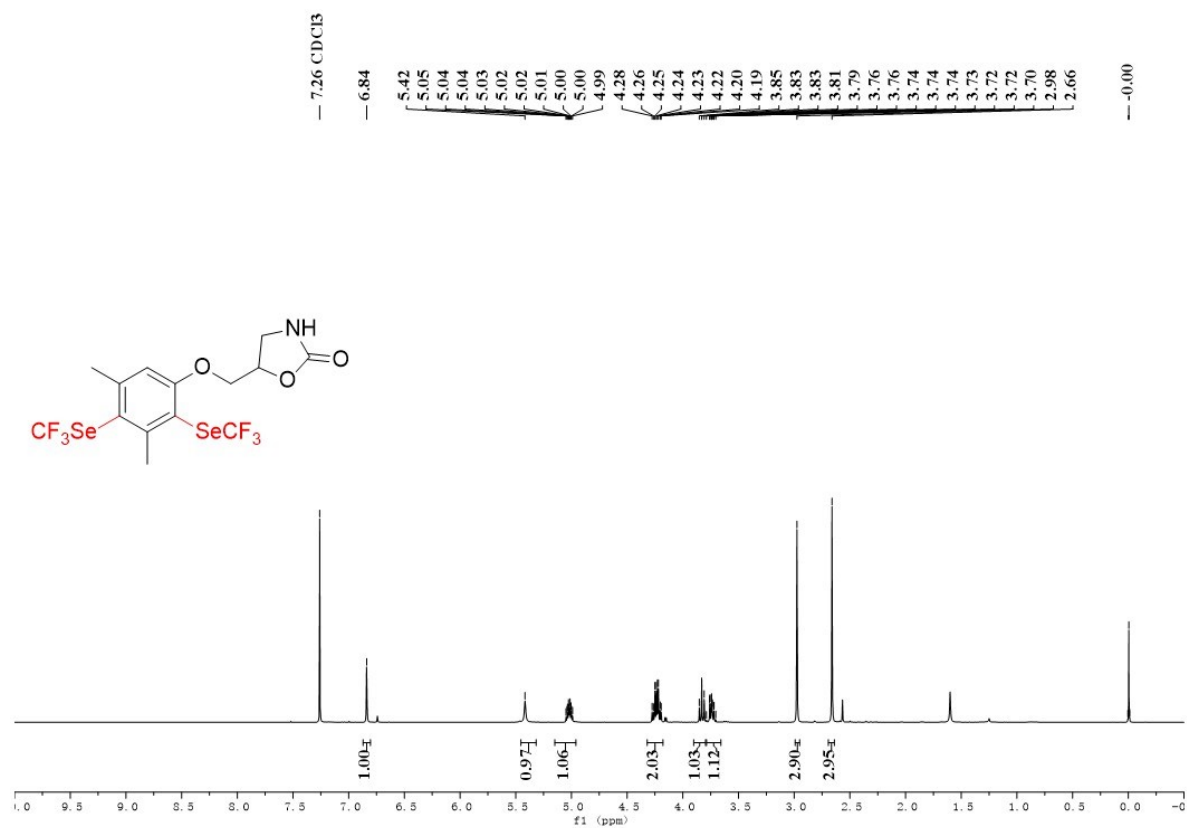


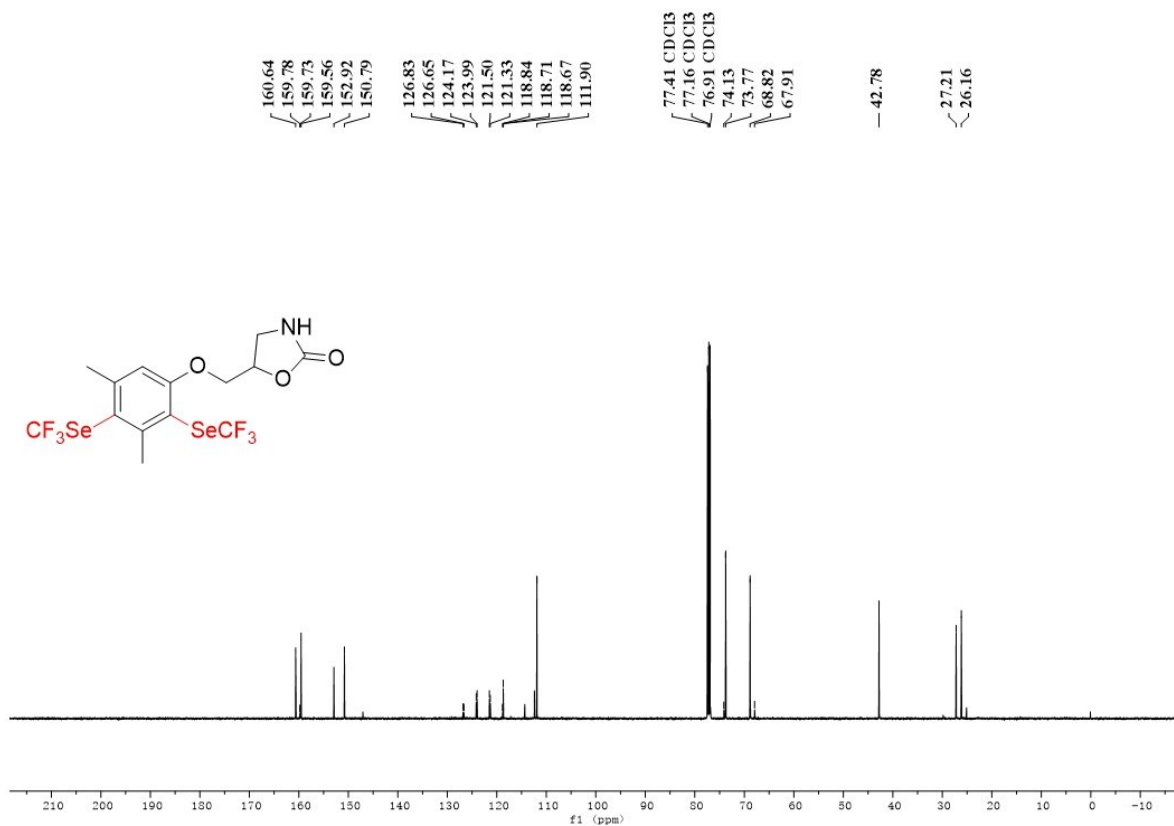
5cm (N-((5-((trifluoromethyl)selenanyl)furan-2-yl)methyl)-7H-purin-6-amine)



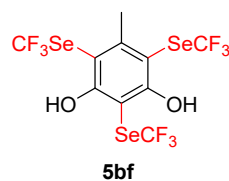
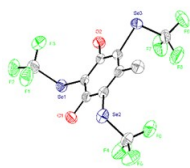


5cn (5-((3,5-dimethyl-2,4-bis((trifluoromethyl)selenyl)phenoxy)methyl)oxazolidin-2-one)

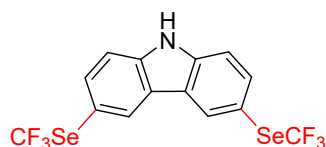
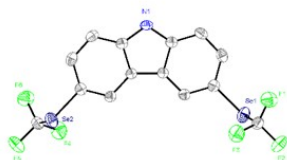




10) X-Ray Crystal data for complexes

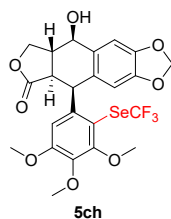
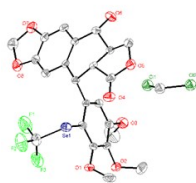


Identification code	5bf
CCDC deposition number	2363156
Empirical formula	C ₁₀ H ₅ F ₉ O ₂ Se ₃
Formula weight	565.02
Temperature/K	296(2)
Crystal system	monoclinic
Space group	P ₂₁ /m
a/Å	5.5035(7)
b/Å	14.3112(18)
c/Å	10.2822(14)
α/°	90
β/°	95.415(2)
γ/°	90
Volume/Å ³	806.23(18)
Z	2
ρ _{calc} /cm ³	2.327
μ/mm ⁻¹	6.940
F(000)	528.0
Crystal size/mm ³	0.24 × 0.23 × 0.21
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.892 to 49.994
Index ranges	-6 ≤ h ≤ 6, -13 ≤ k ≤ 17, -12 ≤ l ≤ 12
Reflections collected	4078
Independent reflections	1479 [R _{int} = 0.0394, R _{sigma} = 0.0526]
Data/restraints/parameters	1479/0/120
Goodness-of-fit on F ²	0.989
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0429, wR ₂ = 0.1179
Final R indexes [all data]	R ₁ = 0.0623, wR ₂ = 0.1268
Largest diff. peak/hole / e Å ⁻³	0.70/-0.50

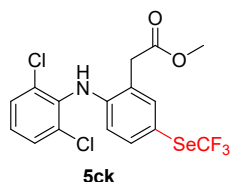
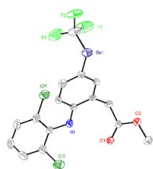


5bi

Identification code	5bi
CCDC deposition number	2363182
Empirical formula	C ₁₄ H ₇ F ₆ NSe ₂
Formula weight	461.13
Temperature/K	296(2)
Crystal system	monoclinic
Space group	C ₂ /c
a/Å	13.120(3)
b/Å	15.873(4)
c/Å	7.9225(17)
α/°	90
β/°	113.703(3)
γ/°	90
Volume/Å ³	1510.7(6)
Z	4
ρ _{calc} /cm ³	2.027
μ/mm ⁻¹	4.955
F(000)	880.0
Crystal size/mm ³	0.24 × 0.22 × 0.2
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.784 to 49.998
Index ranges	-15 ≤ h ≤ 14, -18 ≤ k ≤ 18, -9 ≤ l ≤ 9
Reflections collected	3795
Independent reflections	1335 [R _{int} = 0.0200, R _{sigma} = 0.0225]
Goodness-of-fit on F ²	1.054
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0258, wR ₂ = 0.0699
Final R indexes [all data]	R ₁ = 0.0326, wR ₂ = 0.0727
Largest diff. peak/hole / e Å ⁻³	0.35/-0.41



Identification code	5ch
CCDC deposition number	2363183
Empirical formula	C ₂₄ H ₂₃ C ₁₂ F ₃ O ₈ Se
Formula weight	646.28
Temperature/K	296(2)
Crystal system	orthorhombic
Space group	P ₂ /12121
a/Å	11.7699(17)
b/Å	13.869(2)
c/Å	16.099(2)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	2627.9(7)
Z	4
ρ _{calc} /cm ³	1.633
μ/mm ⁻¹	1.700
F(000)	1304.0
Crystal size/mm ³	0.24 × 0.21 × 0.19
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.852 to 49.998
Index ranges	-13 ≤ h ≤ 13, -15 ≤ k ≤ 16, -13 ≤ l ≤ 19
Reflections collected	13444
Independent reflections	4601 [R _{int} = 0.0418, R _{sigma} = 0.0734]
Data/restraints/parameters	4601/0/347
Goodness-of-fit on F ²	0.905
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0405, wR ₂ = 0.0921
Final R indexes [all data]	R ₁ = 0.0613, wR ₂ = 0.0998
Largest diff. peak/hole / e Å ⁻³	0.46/-0.42
Flack parameter	-0.001(7)



Identification code	5ck
CCDC deposition number	2363185
Empirical formula	C ₁₆ H ₁₂ Cl ₂ F ₃ NO ₂ Se
Formula weight	457.13
Temperature/K	296(2)
Crystal system	monoclinic
Space group	C ₂ /c
a/Å	24.132(11)
b/Å	11.467(4)
c/Å	16.411(7)
α/°	90
β/°	125.672(12)
γ/°	90
Volume/Å ³	3689(3)
Z	8
ρ _{calc} /cm ³	1.646
μ/mm ⁻¹	2.363
F (000)	1808.0
Crystal size/mm ³	0.23 × 0.22 × 0.18
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.284 to 49.99
Index ranges	-28 ≤ h ≤ 22, -13 ≤ k ≤ 13, -17 ≤ l ≤ 19
Reflections collected	9015
Independent reflections	3232 [R _{int} = 0.0933, R _{sigma} = 0.0964]
Data/restraints/parameters	3232/0/228
Goodness-of-fit on F ₂	0.957
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0581, wR ₂ = 0.1463
Final R indexes [all data]	R ₁ = 0.0978, wR ₂ = 0.1623
Largest diff. peak/hole / e Å ⁻³	0.55/-1.17