Supporting Information *for*

Copper-catalyzed synthesis of 2,2,2-trifluoroethyl selenoethers and their insecticidal activities

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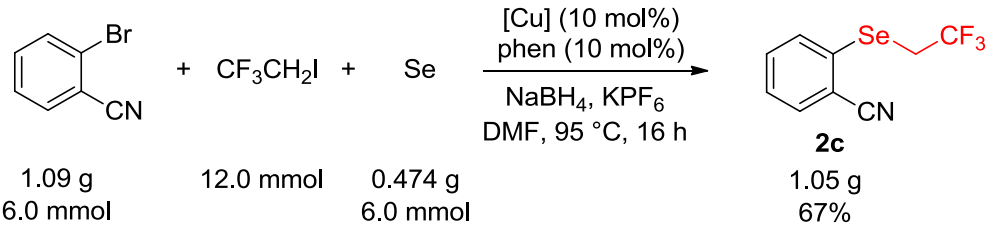
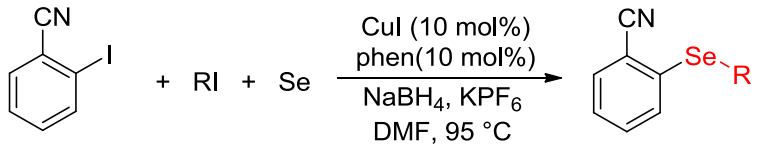
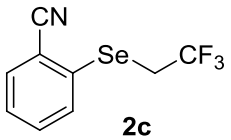
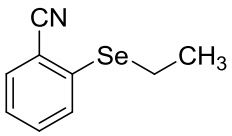
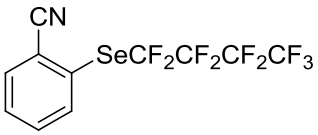
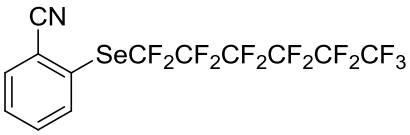
Procedure for gram scale reaction for synthesis of 2-((2,2,2-trifluoroethyl)selanyl)benzonitrile (2c)



In a drybox, CuI (0.114 g, 0.60 mmol, 10 mol%), phen (0.108 g, 0.60 mmol, 10 mol%), $NaBH_4$ (0.2269 g, 6.0 mmol, 1.0 equiv), Se (0.474 g, 6.0 mmol, 1.0 equiv), KPF_6 (2.209 g, 12.0 mmol, 2.0 equiv), ICH_2CF_3 (3.6 mL, 12.0 mmol, 2.0 equiv), 2-bromobenzonitrile (1.092 g, 6.0 mmol, 1.0 equiv), and 15 mL DMF were added to a oven-dried 100 mL test tube with Teflon screw cap. The tube was sealed and the solution was placed into a preheated 95 ℃ oil bath for 16 h. The tube was removed from the oil bath and cooled to r.t. The resulting mixture was extracted by dichloromethane (3 × 20 mL), and water (200 mL), dried over $MgSO_4$. The solvent was removed by rotary evaporation in ice bath, and the resulting product was purified by column chromatography on silica gel with pentane/dichloromethane.

The influence of RI on the reaction



Entry	RI	Product	Yield (%)[a]
1	CF_3CH_2I	 **2c**	93
2	CH_3CH_2I		0
3	$CF_3CF_2CF_2CF_2I$		Trace
4	$CF_3CF_2CF_2CF_2CF_2CF_2I$		Trace

[a] Yields were determined by ^{19}F NMR analysis of the crude reaction mixture with $PhOCF_3$ as internal standard.

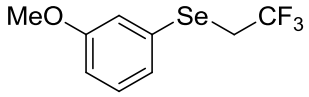
The procedure for the insecticidal assay

Each of the test compounds was first dissolved in 5 mL of mixture of acetone and methanol (1:1 by volume), and then 5 mL of water containing 0.1% Tween 80 was added to generate a 10 mL stock solution of 600 mg/L concentration.

The cabbage leaves were cut into small circular pieces (ϕ = 30 mm), and placed on the glass Petri dishes (ϕ = 60 mm) layered with filter papers that had been wet with sterilized distilled water. The cabbage leaves were prayed with the aforementioned solutions using a Airbrush sprayer (dosage 0.5 mL). After they were air dried, the third-instar insects were introduced to the cabbage leaves. They were kept in a special room for normal cultivation (temperature: 23-25 °C; RH: 40-60%, L/D: 13 h/11 h). Assessments were made after 72 h by the number of killed and size of live insects relative to that in the negative control, and evaluations were based on a percentage scale of 0-100, in which 100 was total kill and 0 was no activity. To compare their activities, the commercial products abamectin and imidacloprid was tested at the concentration of 10 mg/L under the same conditions.

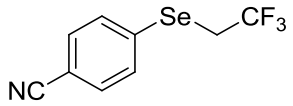
For the insecticidal activities against leucania separate, the corn leaf disks (2 mm × 5 mm) were used instead of the cabbage leaves.

Data for compounds 2 and 4



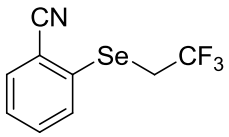
(3-Methoxyphenyl)(2,2,2-trifluoroethyl)selane (2a)

Obtained as a light yellow liquid in 97% yield (78 mg). R_f (*n*-pentane:dichloromethane 10:1) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 – 7.13 (m, 3H), 6.90 (d, *J* = 6.9 Hz, 1H), 3.84 (s, 3H), 3.40 (q, *J* = 10.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.9 (s), 130.2 (s), 129.2 (s), 126.1 (s), 125.9 (q, *J* = 274.2 Hz), 119.4 (s), 114.3 (s), 55.3 (s), 29.1 (q, *J* = 32.9 Hz). IR (ATR): ν 3012, 1587, 1476, 1416, 1288, 1259, 1226, 1110, 838, 777, 444 cm^{-1}. GC-MS m/z 270 (M^+). HRMS (EI) m/z: calcd. for $C_9H_9F_3O^{74}Se$: 263.9830; found: 263.9831.



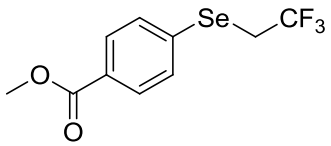
4-((2,2,2-Trifluoroethyl)selanyl)benzonitrile (2b)

Obtained as a light yellow solid in 74% yield (58 mg). M.p. 62.5-64.3 ℃ R_f (*n*-pentane: dichloromethane 1:1) = 0.69. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.6 Hz, 2H), 7.60 (d, *J* = 7.6 Hz, 2H), 3.48 (q, *J* = 9.8 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 9.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 135.3 (s), 132.9 (s), 132.6 (s), 125.5 (q, *J* = 275.8 Hz), 118.2 (s), 111.8 (s), 28.5 (q, *J* = 33.6 Hz). IR(ATR): ν 2995, 2230, 1589, 1484, 1291, 1261, 1226, 1115, 1060, 1015, 819, 649, 630, 545 cm^{-1}. GC-MS m/z 265 (M^+). HRMS (EI) m/z: calcd. for $C_9H_6F_3N^{74}Se$: 258.9677; found: 258.9683.



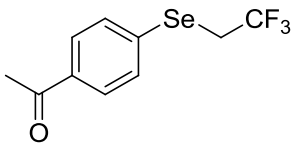
2-((2,2,2-Trifluoroethyl)selanyl)benzonitrile (2c)

Obtained as a light yellow liquid in 98% yield (77 mg). R_f (*n*-pentane:dichloromethane 4:1) = 0.36. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 3.52 (q, *J* = 10.2 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.3 (t, *J* = 10.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 135.9 (s), 134.0 (s), 133.3 (s), 131.6 (s), 129.1 (s), 125.5 (q, *J* = 274.8 Hz), 118.2 (s), 117.6 (s), 29.0 (q, *J* = 33.5 Hz). IR (ATR): ν 3027, 2964, 2240, 1568, 1417, 1269, 1217, 1116, 1061, 984, 830, 796, 663, 629, 567, 521, 439 cm^{-1}. GC-MS m/z 265 (M^+). HRMS (EI) m/z: calcd. for $C_9H_6F_3N^{74}Se$: 258.9677; found: 258.9687.



Methyl 4-((2,2,2-trifluoroethyl)selanyl)benzoate (2d)

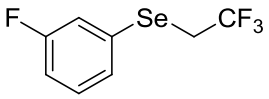
Obtained as a light yellow liquid in 68% yield (60 mg). R_f (*n*-pentane: dichloromethane 4:1) = 0.43. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 7.3 Hz, 2H), 7.64 (d, *J* = 7.3 Hz, 2H), 3.94 (s, 3H), 3.46 (q, *J* = 10.3 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.5 (s), 134.8 (s), 132.5 (s), 130.3 (s), 129.8 (s), 125.6 (q, *J* = 275.6 Hz), 52.2 (s), 28.5 (q, *J* = 33.4 Hz). IR (ATR): ν 2955, 1719, 1593, 1436, 1396, 1282, 1225, 1185, 1109, 1058, 1015, 826, 631, 475 cm^{-1}. GC-MS m/z 297 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_9F_3O_2{}^{74}Se$: 291.9779; found: 291.9782.



1-(4-((2,2,2-Trifluoroethyl)selanyl)phenyl)ethenone (2e)

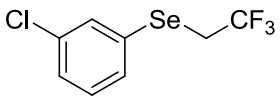
Obtained as a light yellow liquid in 73% yield (62 mg). R_f (*n*-pentane: dichloromethane 5:1)=0.35. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.2 Hz, 2H),

7.66 (d, *J* = 8.2 Hz, 2H), 3.47 (q, *J* = 10.3 Hz, 2H), 2.61 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 197.3 (s), 136.4 (s), 135.2 (s), 132.5 (s), 129.1 (s), 125.6 (q, *J* = 274.6 Hz), 28.4 (q, *J* = 33.4 Hz), 26.6 (s). IR (ATR): ν 2978, 1682, 1587, 1394, 1359, 1288, 1262, 1225, 1112, 1058, 1013, 957, 817, 631, 602, 460 cm^{-1}. GC-MS m/z 282 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_9F_3O^{74}Se$: 275.9830; found: 275.9832.



(3-Fluorophenyl)(2,2,2-trifluoroethyl)selane (2f)

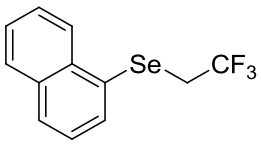
Obtained as a light yellow liquid in 83% yield (63 mg). R_f (*n*-pentane) = 0.48. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.7 Hz, 1H), 7.38 – 7.26 (m, 2H), 7.06 (t, *J* = 8.4 Hz, 1H), 3.41 (q, *J* = 10.3 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.3 Hz, 3F), -111.2 – -111.3 (m, 1F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.5 (d, *J* = 250.5 Hz), 130.7 (d, *J* = 8.1 Hz), 129.7 (d, *J* = 7.0 Hz), 129.5 (d, *J* = 3.0 Hz), 125.7 (q, *J* = 274.4 Hz), 120.8 (d, *J* = 22.4 Hz), 115.5 (d, *J* = 21.0 Hz), 29.1 (q, *J* = 33.3 Hz). IR (ATR): ν 2957, 2919, 2849, 2165, 1978, 1471, 1289, 1261, 1216, 1113, 806, 476 cm^{-1}. GC-MS m/z 257 (M^+). HRMS (EI) m/z: calcd. for $C_8H_6F_4{}^{74}Se$: 251.9630; found: 251.9637.



(3-Chlorophenyl)(2,2,2-trifluoroethyl)selane (2g)

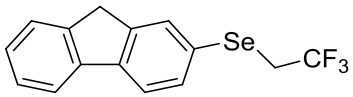
Obtained as a light yellow liquid in 77% yield (62 mg). R_f (*n*-pentane) = 0.52. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.29 – 7.21 (m, 1H), 3.40 (q, *J* = 10.1 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.1 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 134.8 (s), 133.7 (s), 132.1 (s), 130.4 (s), 129.6 (s), 128.7 (s), 125.7 (q, *J* = 274.6 Hz), 29.2 (q, *J* = 33.2 Hz). IR(ATR): ν 2955, 2926, 2872, 2854, 1457, 1378, 1291, 1263, 1116, 1060, 804, 724, 510, 435 cm^{-1}. GC-MS m/z 273 (M^+). HRMS (EI) m/z: calcd. for $C_8H_6ClF_3{}^{74}Se$:

267.9335; found: 267.9337.



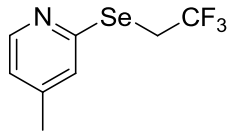
Naphthalen-1-yl(2,2,2-trifluoroethyl)selane (2h)

Obtained as a light yellow liquid in 91% yield (78 mg). R_f (*n*-pentane) = 0.71. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 7.1 Hz, 1H), 7.92 (t, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 1H), 3.41 (q, *J* = 10.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.1 (t, *J* = 10.5 H, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 135.3 (s), 134.3 (s), 134.1 (s), 130.2 (s), 128.9 (s), 127.6 (s), 127.4 (s), 127.3 (s), 126.5 (s), 125.9 (q, *J* = 274.7 Hz), 125.8 (s), 28.8 (q, *J* = 32.7 Hz). IR (ATR): ν 3054, 1589, 1501, 1411, 1377, 1287, 1257, 1220, 1104, 1053, 836, 794, 767, 695, 629 cm^{-1}. GC-MS m/z 290 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_9F_3{}^{74}Se$: 283.9881; found: 283.9890.



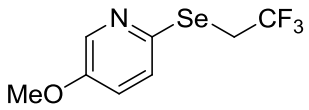
(9*H*-Fluoren-2-yl)(2,2,2-trifluoroethyl)selane (2i)

Obtained as a white solid in 99% yield (97 mg). M.p. 68.2-69.5 ℃. R_f (*n*-pentane) = 0.74. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 1H), 7.81 (d, *J* = 7.4 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.0 Hz, 1H), 7.37 (t, *J* = 7.0 Hz, 1H), 3.93 (s, 2H), 3.42 (q, *J* = 10.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.3 (t, *J* = 10.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.4 (s), 143.3 (s), 142.3 (s), 140.8 (s), 133.2 (s), 131.3 (s), 127.4 (s), 127.0 (s), 126.1 (s), 126.0 (q, *J* = 275.6 Hz), 125.1 (s), 120.6 (s), 120.2 (s), 36.8 (s), 29.6 (q, *J* = 32.6 Hz). IR (ATR): ν 2922, 1449, 1405, 1286, 1259, 1221, 1104, 1053, 963, 823, 763, 629, 572, 518 cm^{-1}. GC-MS m/z 328 (M^+). HRMS (EI) m/z: calcd. for $C_{15}H_{11}F_3{}^{74}Se$: 322.0038; found: 322.0042.



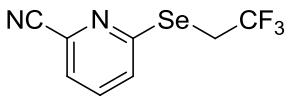
4-Methyl-2-((2,2,2-trifluoroethyl)selanyl)pyridine (**2j**)

Obtained as a light yellow liquid in 81% yield (61 mg). R_f (*n*-pentane: dichloromethane 5:1) = 0.34. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, *J* = 4.8 Hz, 1H), 7.21 (s, 1H), 6.93 (d, *J* = 4.7 Hz, 1H), 3.95 (q, *J* = 10.6 Hz, 2H), 2.32 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 151.1 (s), 149.6 (s), 147.9 (s), 126.1 (q, *J* = 274.1 Hz), 125.7 (s), 122.6 (s), 25.1 (q, *J* = 33.5 Hz), 20.7 (s). IR(ATR): ν 2923, 2850, 2169, 2050, 1984, 1591, 1541, 1465, 1010, 1373, 1291, 1262, 1216, 1113, 1087, 849, 817, 701, 631, 519, 428 cm^{-1}. GC-MS m/z 254 (M^+). HRMS (EI) m/z: calcd. for $C_8H_8F_3N^{74}Se$: 248.9834; found: 248.9837.



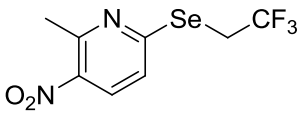
5-Methoxy-2-((2,2,2-trifluoroethyl)selanyl)pyridine (2k)

Obtained as a light yellow liquid in 84% yield (67 mg). R_f (*n*-pentane: dichloromethane 20:3) = 0.34. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, *J* = 2.9 Hz, 1H), 7.33 (d, *J* = 8.6 Hz, 1H), 7.12 (dd, *J* = 8.6, 3.0 Hz, 1H), 3.86 (s, 3H), 3.84 (q, *J* = 10.6 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.6 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.8 (s), 140.8 (s), 137.5 (s), 126.1 (q, *J* = 274.1 Hz), 126.0 (s), 122.5 (s), 55.7 (s), 26.0 (q, *J* = 33.4 Hz). IR (ATR): ν 2956, 1564, 1464, 1377, 1268, 1222, 1112, 1060, 1028, 823, 631 cm^{-1}. GC-MS m/z 270 (M^+). HRMS (EI) m/z: calcd. for $C_8H_8F_3NO^{74}Se$: 264.9783; found: 264.9787.



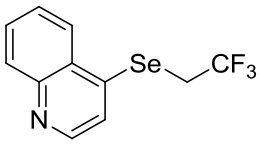
2-Ethynyl-6-((2,2,2-trifluoroethyl)selanyl)pyridine (2l)

Obtained as a light yellow liquid in 75% yield (59 mg). R_f (*n*-pentane: dichloromethane 4:1) = 0.44. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (t, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.52 (d, *J* = 7.4 Hz, 1H), 3.96 (q, *J* = 10.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.5 (s), 136.9 (s), 134.0 (s), 128.4 (s), 125.9 (s), 125.6 (q, *J* = 274.3 Hz), 116.7 (s), 25.5 (q, *J* = 34.0 Hz). IR (ATR): ν 2995, 2227, 1463, 1412, 1291, 1261, 1225, 1114, 1061, 631, 555, 461 cm^{-1}. GC-MS m/z 266 (M^+). HRMS (EI) m/z: calcd. for $C_8H_5F_3N_2{}^{74}Se$: 259.9630; found: 259.9637.



2-Methyl-3-nitro-6-((2,2,2-trifluoroethyl)selanyl)pyridine (2m)

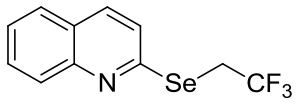
Obtained as a light yellow liquid in 79% yield (70 mg). R_f (*n*-pentane: dichloromethane 5:1) = 0.39. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J* = 8.5 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 1H), 4.03 (q, *J* = 10.4 Hz, 2H), 2.91 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.4 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.5 (s), 154.6 (s), 143.6 (s), 132.6 (s), 125.6 (q, *J* = 274.3 Hz), 122.5 (s), 25.7 (q, *J* = 34.0 Hz), 24.4 (s). IR(ATR): ν 2919, 1584, 1560, 1514, 1425, 1359, 1338, 1289, 1262, 1114, 1068, 982, 903, 893, 823, 752, 631, 522 cm^{-1}. GC-MS m/z 299 (M^+). HRMS (EI) m/z: calcd. for $C_8H_7F_3N_2O_2{}^{74}Se$: 293.9684; found: 293.9677.



4-((2,2,2-Trifluoroethyl)selanyl)quinolone (2n)

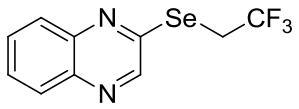
Obtained as a white solid in 41% yield (36 mg). M.p. 98.9-100.0 ℃. R_f (*n*-pentane: dichloromethane 4:1) = 0.40. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96 (d, *J* = 4.2 Hz, 1H), 8.18 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.61 – 7.39 (m, 2H), 3.66 (q, *J* = 10.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.4 (t, *J* =

10.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.7 (s), 146.5 (s), 136.6 (s), 132.0 (s), 128.7 (s), 128.5 (s), 127.0 (s), 126.5 (s), 126.2 (q, *J* = 274.7 Hz), 121.9 (s), 25.1 (q, *J* = 32.9 Hz). IR (ATR): ν 2957, 1490, 1289, 1261, 1226, 1111, 1053, 820, 786 cm^{-1}. GC-MS m/z 291 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3N^{74}Se$: 284.9834; found: 284.9828.



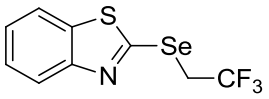
2-((2,2,2-Trifluoroethyl)selanyl)quinolone (2o)

Obtained as a light yellow liquid in 51% yield (44 mg). R_f (*n*-pentane: dichloromethane 20:3) = 0.67. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J* = 8.5 Hz, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 1H), 4.18 (q, *J* = 10.7 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.1 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.0 (s), 148.7 (s), 136.0 (s), 130.0 (s), 128.3 (s), 127.8 (s), 126.8 (s), 126.1 (s), 126.0 (q, *J* = 274.2 Hz), 122.6 (s), 25.1 (q, *J* = 33.6 Hz). IR (ATR): ν 2931, 1588, 1556, 1497, 1418, 1288, 1264, 1222, 1113, 1077, 813, 778, 630, 576, 474, 420 cm^{-1}. GC-MS m/z 291 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3N^{74}Se$: 284.9834; found: 284.9836.



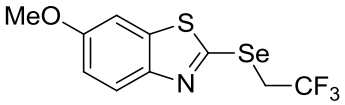
2-((2,2,2-Trifluoroethyl)selanyl)quinoxaline (2p)

Obtained as a light yellow liquid in 44% yield (38 mg). R_f (*n*-pentane: dichloromethane 5:1) = 0.42. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (s, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.86 – 7.64 (m, 2H), 4.11 (q, *J* = 10.4 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.2 (t, *J* = 10.4 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.4 (s), 145.5 (s), 143.5 (s), 141.0 (s), 130.6 (s), 129.4 (s), 129.1 (s), 128.1 (s), 125.7 (q, *J* = 274.2 Hz), 24.8 (q, *J* = 34.1 Hz). IR(ATR): ν 2943, 1544, 1488, 1403, 1307, 1271, 1241, 1127, 1084, 961, 908, 845, 759, 639, 596, 534 cm^{-1}. GC-MS m/z 292 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_7F_3N_2{}^{74}Se$: 285.9786; found: 285.9784.



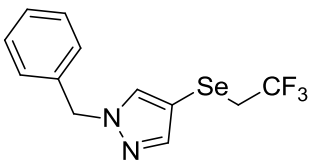
2-((2,2,2-Trifluoroethyl)selanyl)benzo[*d*]thiazole (2q)

Obtained as a light yellow liquid in 55% yield (48 mg). R_f (*n*-pentane: dichloromethane 5:1) = 0.46. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 4.08 (q, *J* = 10.1 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.3 (t, *J* = 10.1 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.3 (s), 153.3 (s), 136.8 (s), 126.3 (s), 125.4 (q, *J* = 274.7 Hz), 124.9 (s), 122.1 (s), 121.2 (s), 27.8 (q, *J* = 34.3 Hz). IR(ATR): ν 2959, 1560, 1457, 1290, 1260, 1224, 1113, 1061, 969, 839, 754, 726, 703, 669, 630, 521, 427 cm^{-1}. GC-MS m/z 296 (M^+). HRMS (EI) m/z: calcd. for $C_9H_6F_3NS^{74}Se$: 290.9398; found: 290.9392.



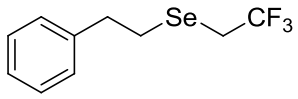
6-Methoxy-2-((2,2,2-trifluoroethyl)selanyl)benzo[d]thiazole (2r)

Obtained as a light yellow solid in 47% yield (46 mg). M.p. 59.5-60.2 ℃ R_f (*n*-pentane: dichloromethane 4:1) =0.42. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.9 Hz, 1H), 7.30 (s, 1H), 7.08 (d, *J* = 8.9 Hz, 1H), 3.99 (q, *J* = 10.4 Hz, 2H), 3.89 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.4 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.6 (s), 151.4 (s), 147.9 (s), 138.3 (s), 125.3 (q, *J* = 274.4 Hz), 122.6 (s), 115.4 (s), 103.9 (s), 55.8 (s), 28.1 (q, *J* = 34.3 Hz). IR (ATR): ν 2997, 2254, 1602, 1475, 1292, 1262, 1221, 1120, 1062, 974, 830 cm^{-1}. GC-MS m/z 327 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_8F_3NOS^{74}Se$: 320.9503; found: 320.9502.



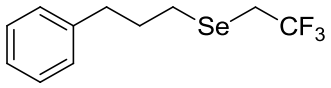
1-Benzyl-4-((2,2,2-trifluoroethyl)selanyl)-1*H*-pyrazole (2s)

Obtained as a light yellow liquid in 21% yield (20 mg). R_f (*n*-pentane: dichloromethane 1:1) = 0.45. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (s, 1H), 7.54 (s, 1H), 7.43 – 7.33 (m, 3H), 7.25 (d, *J* = 6.6 Hz, 2H), 5.33 (s, 2H), 3.11 (q, *J* = 10.4 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.7 (t, *J* = 10.4 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1 (s), 135.7 (s), 135.2 (s), 129.0 (s), 128.4 (s), 127.9 (s), 125.8 (q, *J* = 274.0 Hz), 100.7 (s), 56.4 (s), 30.3 (q, *J* = 32.1 Hz). IR(ATR): ν 2925, 1289, 1261, 1222, 1108, 1060, 903, 724, 649, 628 cm^{-1}. GC-MS m/z 319 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{11}F_3N_2{}^{74}Se$: 314.0099; found: 314.0110.



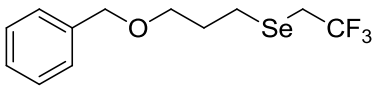
Phenethyl(2,2,2-trifluoroethyl)selane (4a)

Obtained as a light yellow liquid in 82% yield (65 mg). R_f (*n*-pentane) = 0.58. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (t, *J* = 7.3 Hz, 2H), 7.32 – 7.20 (m, 3H), 3.09 (q, *J* = 10.2 Hz, 2H), 3.02 – 2.90 (m, 4H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.4 (t, *J* = 10.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.4 (s), 128.6 (s), 128.4 (s), 126.7 (s), 126.3 (q, *J* = 274.2 Hz), 36.7 (s), 26.8 (s), 24.0 (q, *J* = 33.1 Hz). IR(ATR): ν 3011, 1496, 1454, 1411, 1291, 1260, 1108, 1055, 837, 727, 699, 649, 542, 488 cm^{-1}. GC-MS m/z 268 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_{11}F_3{}^{74}Se$: 262.0038; found: 262.0033.



(3-Phenylpropyl)(2,2,2-trifluoroethyl)selane (4b)

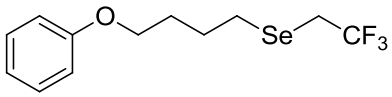
Obtained as a light yellow liquid in 84% yield (71 mg). R_f (*n*-pentane) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (t, *J* = 7.1 Hz, 2H), 7.29 – 7.19 (m, 3H), 3.08 (q, *J* = 10.5 Hz, 2H), 2.78 (dd, *J* = 13.4, 6.5 Hz, 4H), 2.05 (p, *J* = 7.1 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 141.0 (s), 128.5 (s), 128.4 (s), 126.3 (q, *J* = 274.2 Hz), 126.1 (s), 35.6 (s), 31.5 (s), 25.3 (s), 23.9 (q, *J* = 33.0 Hz). IR (ATR): ν 2973, 2247, 2179, 2001, 1291, 1262, 1110, 1060, 904, 649, 419 cm^{-1}. GC-MS m/z 282 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_{13}F_3{}^{74}Se$: 276.0194; found: 276.0201.



(3-(Benzyloxy)propyl)(2,2,2-trifluoroethyl)selane (4c)

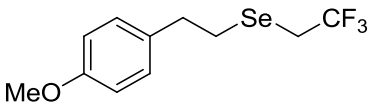
Obtained as a light yellow liquid in 72% yield (66 mg). R_f (*n*-pentane: dichloromethane 20:3) = 0.34. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 – 7.29 (m, 5H), 4.55 (s, 2H), 3.59 (t, *J* = 5.6 Hz, 2H), 3.08 (q, *J* = 10.3 Hz, 2H), 2.88 (t, *J* = 6.6 Hz,

2H), 2.22 – 1.88 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 138.3 (s), 128.4 (s), 127.7 (s), 126.3 (q, *J* = 275.1 Hz), 73.1 (s), 69.1 (s), 30.2 (s), 24.1 (q, *J* = 33.0 Hz), 22.8 (s). IR(ATR): ν 2858, 1495, 1454, 1411, 1363, 1291, 1260, 1226, 1101, 1055, 1028, 836, 732, 697, 649, 630, 518, 460 cm^{-1}. GC-MS m/z 311 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{15}F_3O^{74}Se$: 306.0300; found: 306.0293.



(4-Phenoxybutyl)(2,2,2-trifluoroethyl)selane (4d)

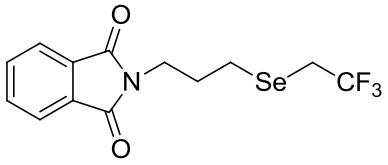
Obtained as a light yellow liquid in 77% yield (72 mg). R_f (*n*-pentane: dichloromethane 20:3) = 0.61. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (t, *J* = 7.6 Hz, 2H), 6.99 (t, *J* = 7.3 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 2H), 4.02 (t, *J* = 4.8 Hz, 2H), 3.10 (q, *J* = 10.6 Hz, 2H), 2.85 (t, *J* = 6.4 Hz, 2H), 1.99 – 1.87 (m, 4H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9 (s), 129.5 (s), 126.0 (q, *J* = 276.3 Hz), 120.7 (s), 114.5 (s), 67.0 (s), 34.3 (q, *J* = 32.7 Hz), 33.0 (s), 28.2 (s), 25.8 (s). IR (ATR): ν 2938, 1597, 1496, 1291, 1244, 1110, 1059, 649, 511 cm^{-1}. GC-MS m/z 312 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{15}F_3O^{74}Se$: 306.0300; found: 306.0308.



(4-Methoxyphenethyl)(2,2,2-trifluoroethyl)selane (4e)

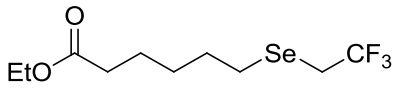
Obtained as a light yellow liquid in 72% yield (64 mg). R_f (*n*-pentane:dichloromethane 4:1)=0.53. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15 (d, *J* = 7.1 Hz, 2H), 6.88 (d, *J* = 7.1 Hz, 2H), 3.83 (s, 3H), 3.05 (q, *J* = 10.6 Hz, 2H), 3.02 – 2.90 (m, 4H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.4 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.4 (s), 132.4 (s), 129.4 (s), 126.3 (q, *J* = 274.5 Hz), 114.0 (s), 55.3 (s), 35.7 (s), 27.3 (s), 24.0 (q, *J* = 33.0 Hz). IR (ATR): ν 2956, 2926, 2872, 1513,

1464, 1378, 1292, 1264, 1111, 1056, 816, 741, 518, 419 cm^{-1}. GC-MS m/z 297 (M^+). HRMS (EI) m/z: calcd. for$C_{11}H_{13}F_3O^{74}Se$: 292.0143; found: 292.0146.



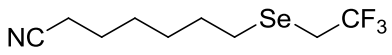
2-(3-((2,2,2-Trifluoroethyl)selanyl)propyl)isoindoline-1,3-dione (4f)

Obtained as a light yellow liquid in 61% yield (64 mg). R_f (*n*-pentane: dichloromethane 2:1) = 0.36. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 – 7.80 (m, 2H), 7.80 – 7.70 (m, 2H), 3.83 (t, *J* = 6.7 Hz, 2H), 3.11 (q, *J* = 10.6 Hz, 2H), 2.77 (t, *J* = 7.2 Hz, 2H), 2.09 (p, *J* = 7.0 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.4 (s), 134.1 (s), 132.0 (s), 126.2 (q, *J* = 274.4 Hz), 123.3 (s), 37.5 (s), 28.8 (s), 24.0 (q, *J* = 33.1 Hz), 22.5 (s). IR(ATR): ν 2943, 1772, 1706, 1614, 1436, 1395, 1361, 1290, 1260, 1224, 1103, 1054, 1001, 879, 835, 794, 715, 629, 527 cm^{-1}. GC-MS m/z 351 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_{12}F_3NO_2{}^{74}Se$: 345.0045; found: 345.0040.



Ethyl 6-((2,2,2-trifluoroethyl)selanyl)hexanoate (4g)

Obtained as a light yellow liquid in 66% yield (60 mg). R_f (*n*-pentane: dichloromethane 5:2) = 0.42. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.15 (q, *J* = 6.6 Hz, 2H), 3.06 (q, *J* = 10.3 Hz, 2H), 2.75 (t, *J* = 6.9 Hz, 2H), 2.32 (t, *J* = 6.9 Hz, 2H), 1.83 – 1.62 (m, 4H), 1.54 – 1.39 (m, 2H), 1.28 (t, *J* = 6.7 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 173.5 (s), 126.3 (q, *J* = 274.2 Hz), 60.3 (s), 34.1 (s), 29.6 (s), 29.1 (s), 25.7 (s), 24.4 (s), 23.9 (q, *J* = 33.1 Hz), 14.2 (s). IR(ATR): ν 2937, 1727, 1412, 1374, 1291, 1260, 1226, 1193, 1108, 1057, 649, 630 cm^{-1}. GC-MS m/z 306 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_{17}F_3O_2{}^{74}Se$: 300.0405; found: 300.0404.



7-((2,2,2-Trifluoroethyl)selanyl)heptanenitrile (4h)

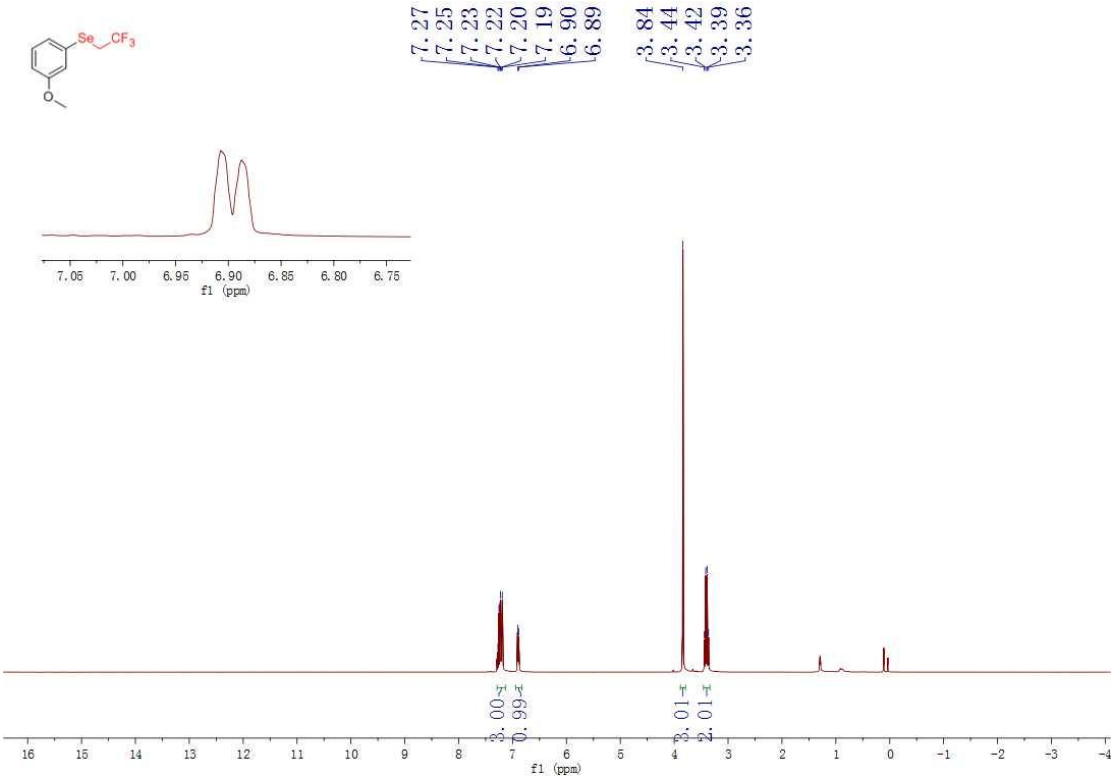
Obtained as a light yellow liquid in 58% yield (47 mg). R_f (*n*-pentane: dichloromethane 1:1) = 0.59. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.07 (q, *J* = 10.2 Hz, 2H), 2.76 (t, *J* = 6.8 Hz, 2H), 2.37 (t, *J* = 6.6 Hz, 2H), 1.82 – 1.59 (m, 4H), 1.57 – 1.41 (m, 4H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -64.5 (t, *J* = 10.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$): δ 126.3 (q, *J* = 274.2 Hz), 119.6 (s), 29.6 (s), 28.7 (s), 28.1 (s), 25.7 (s), 25.2 (s), 23.9 (q, *J* = 33.0 Hz), 17.1 (s). IR(ATR): ν 2937, 2253, 1411, 1291, 1260, 1227, 1108, 1057, 904, 649, 630 cm^{-1}. GC-MS m/z 272 (M^+). HRMS (EI) m/z: calcd. for $C_9H_{14}F_3N^{74}Se$: 267.0303; found: 267.0305.

References

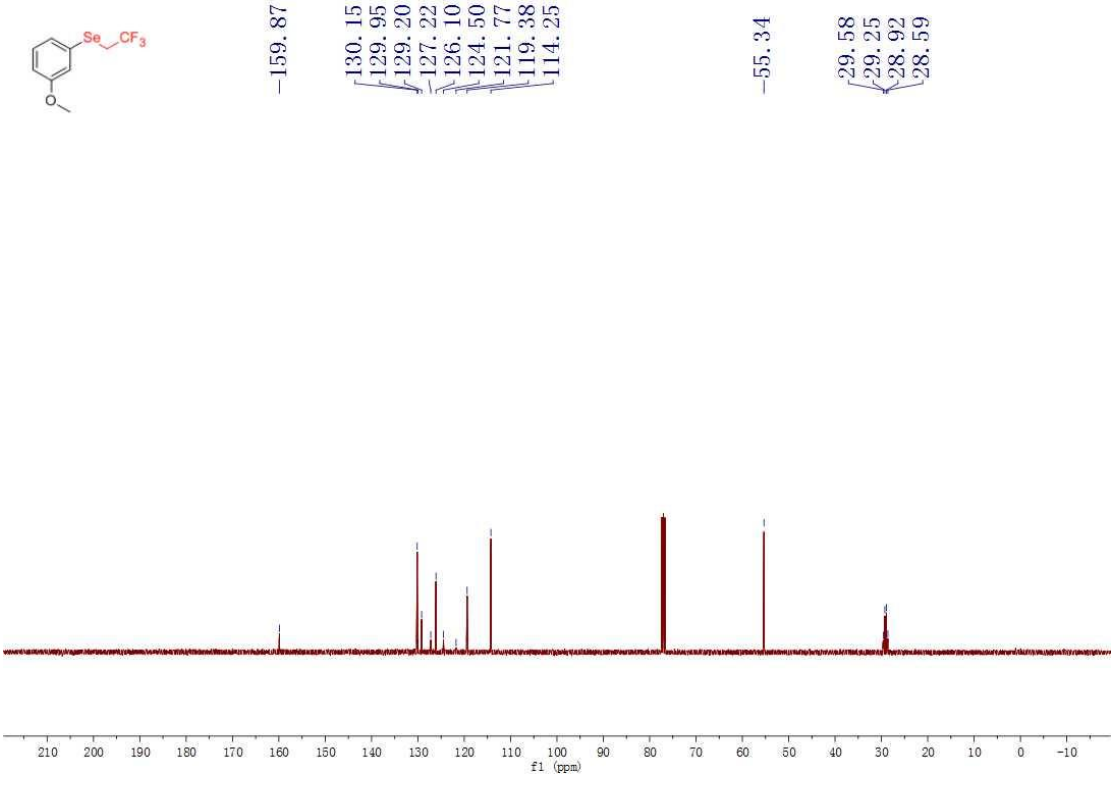
1. SHELXTL version 5.03; Bruker Analytical X-ray Systems, Madison, WI, 1997.

Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra

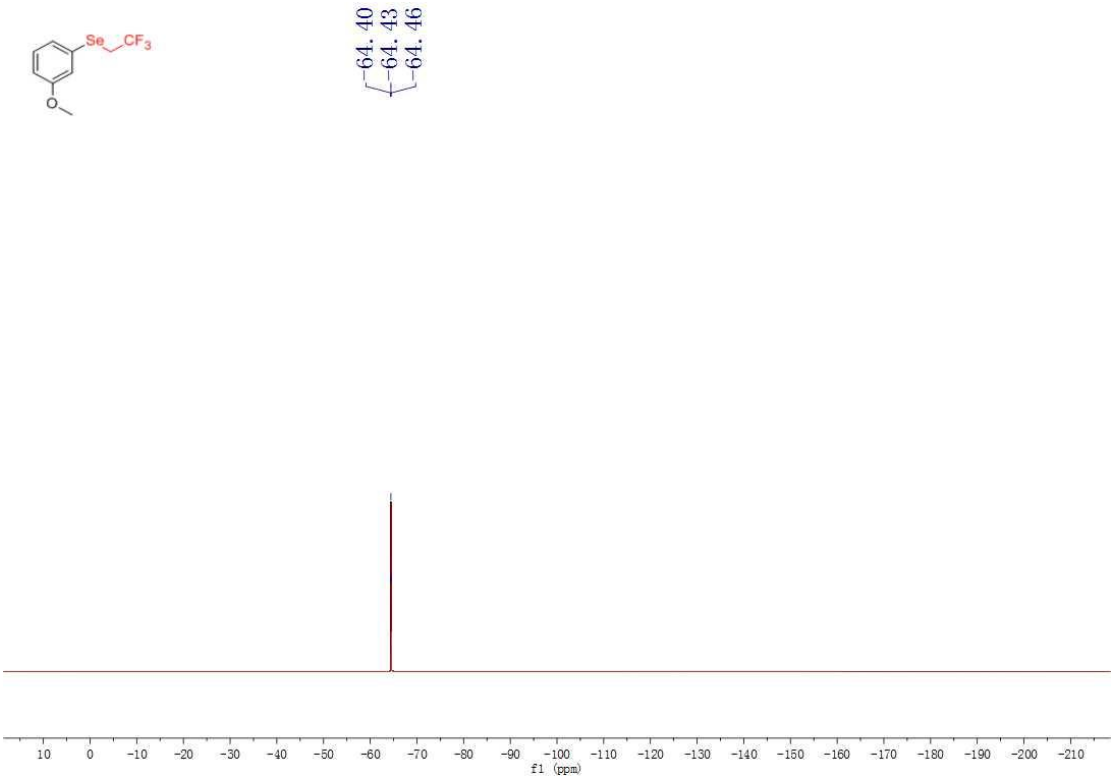
^{1}H NMR spectrum of **2a** in $CDCl_3$



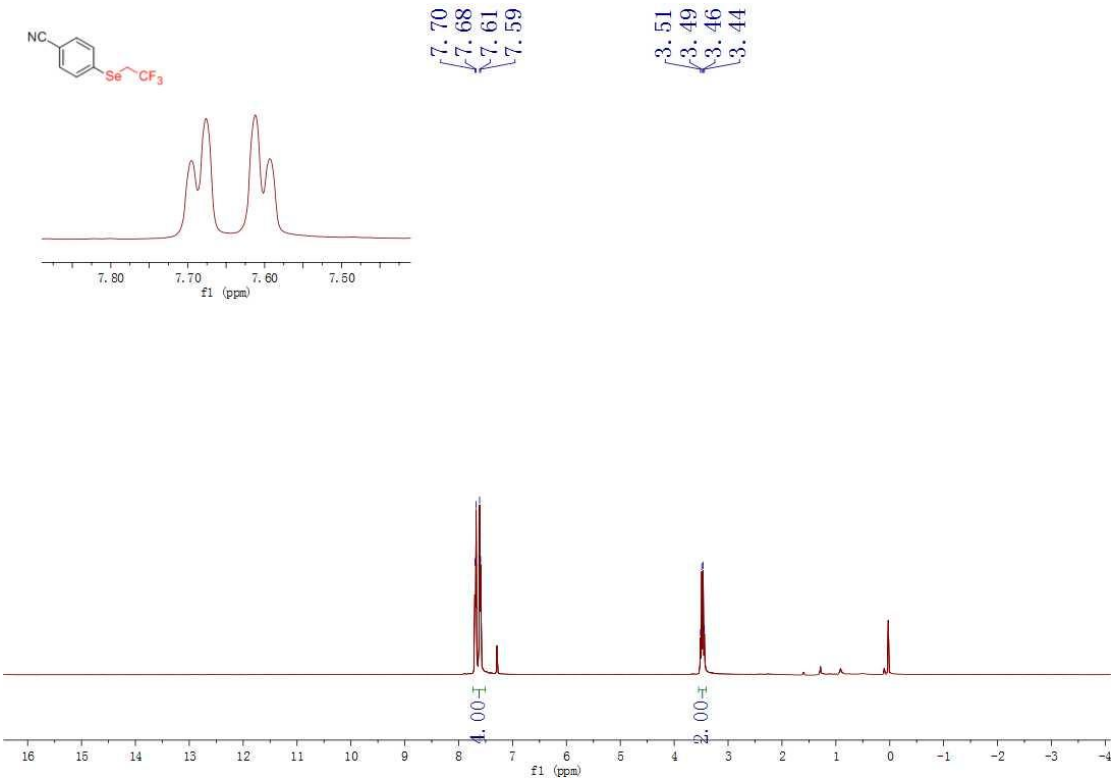
^{13}C NMR spectrum of **2a** in $CDCl_3$



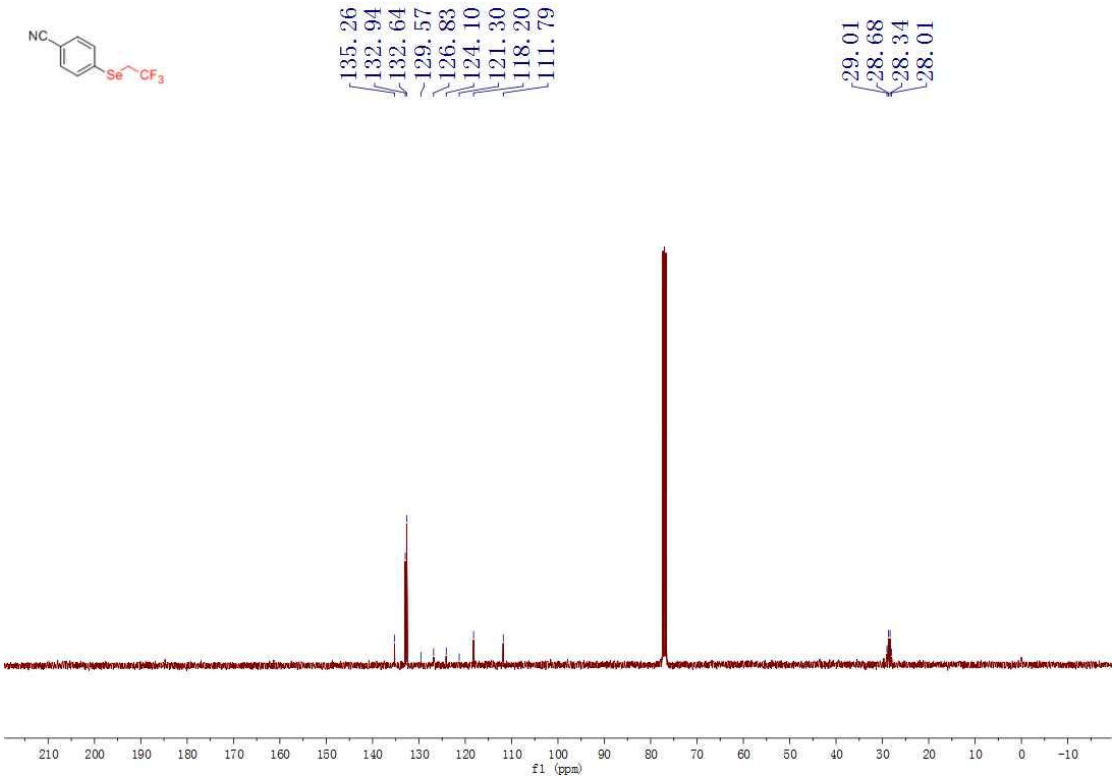
^{19}F NMR spectrum of **2a** in $CDCl_3$



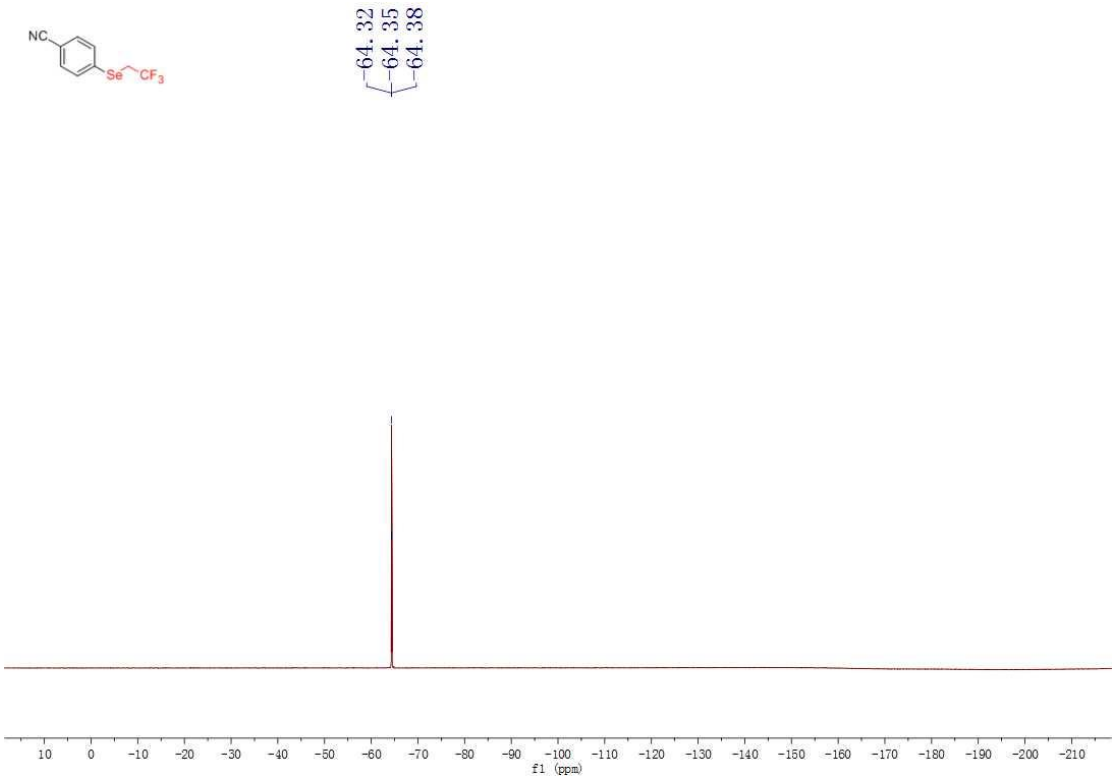
^{1}H NMR spectrum of **2b** in $CDCl_3$



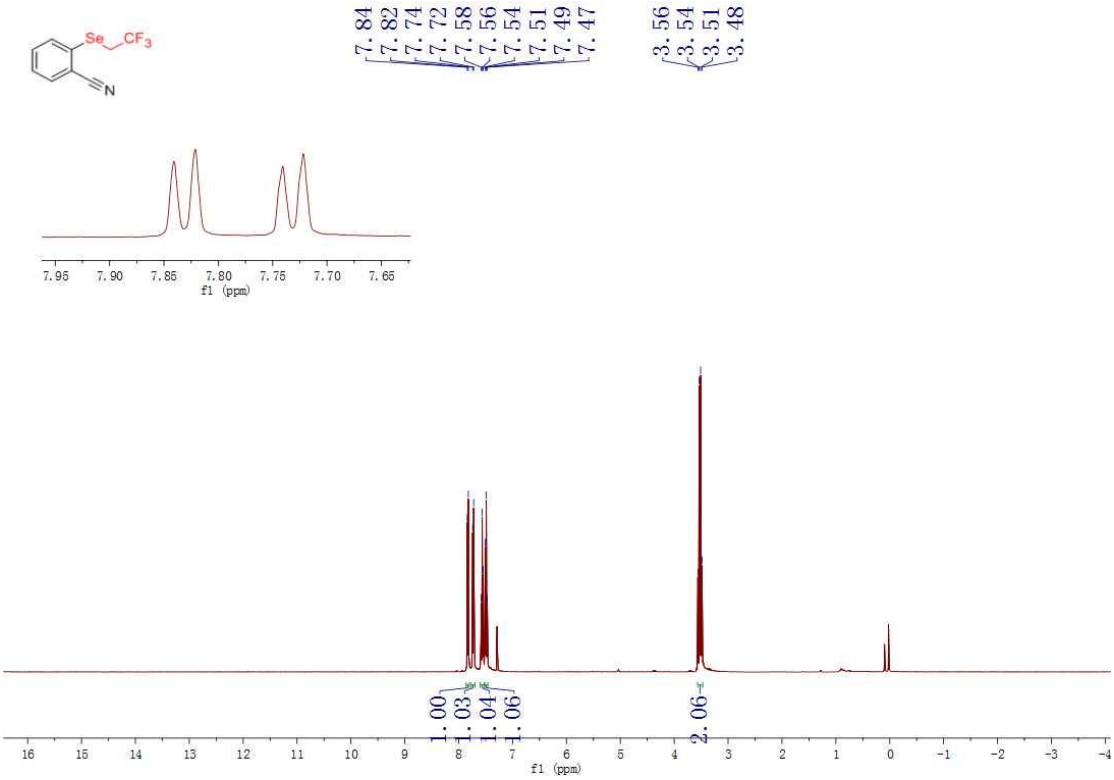
^{13}C NMR spectrum of **2b** in $CDCl_3$



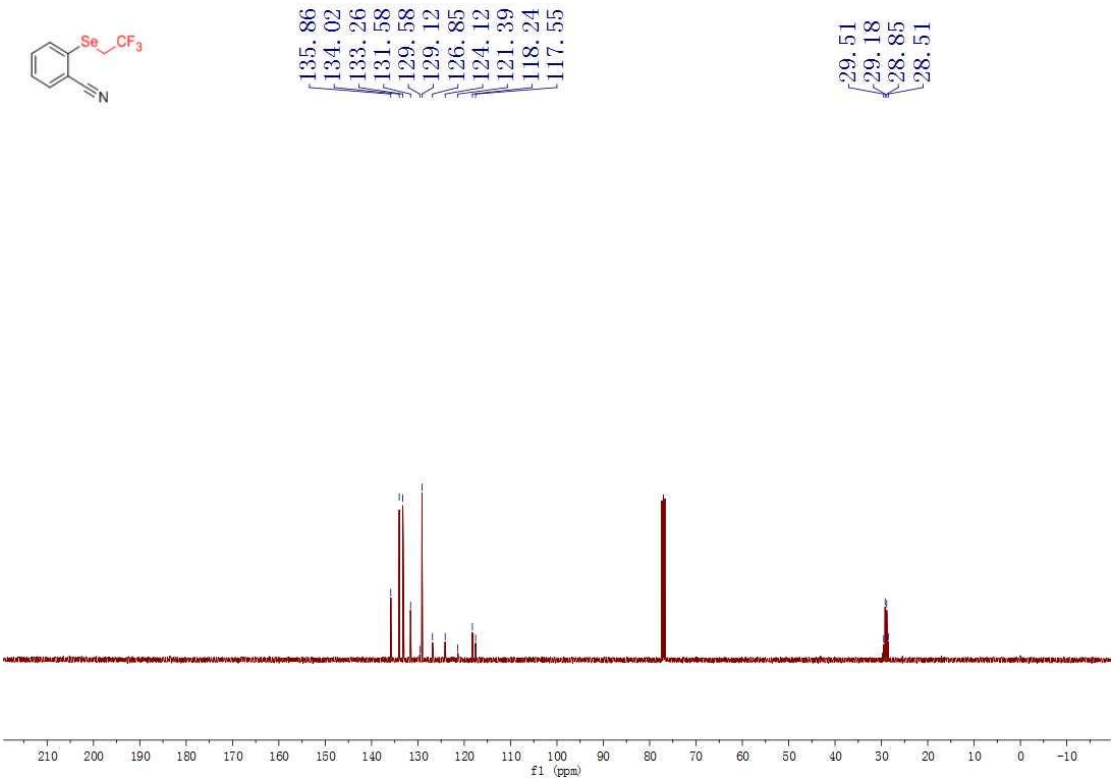
^{19}F NMR spectrum of **2b** in $CDCl_3$



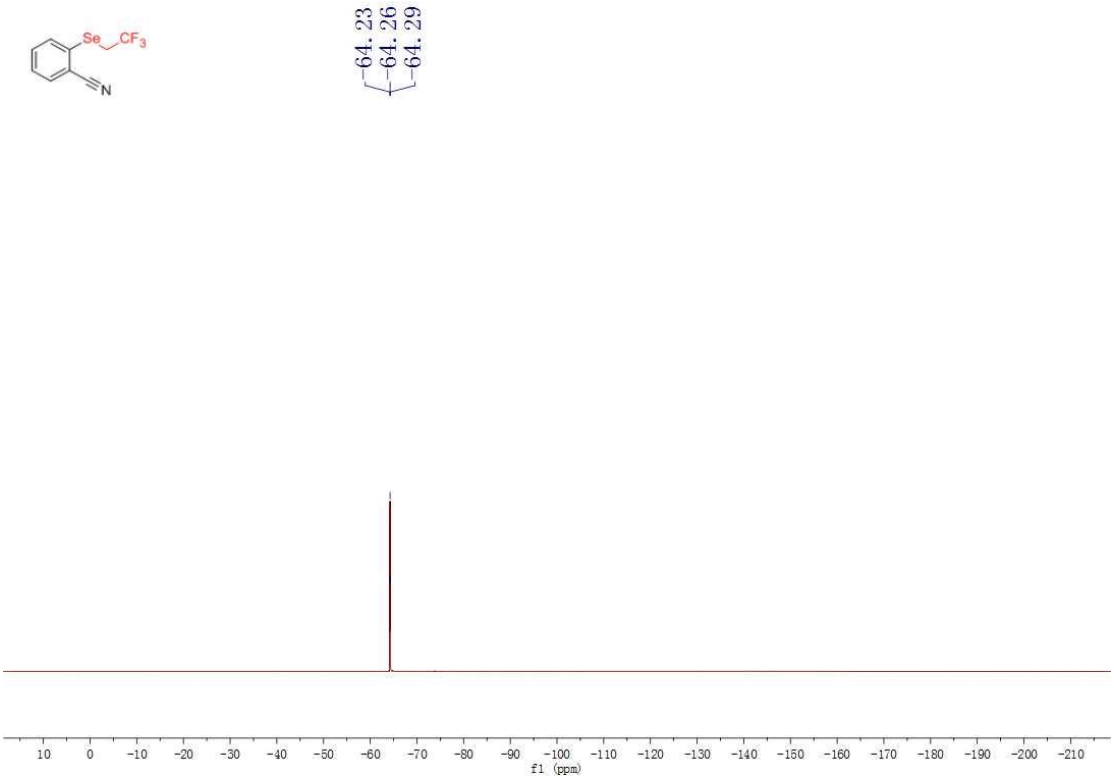
^{1}H NMR spectrum of **2c** in $CDCl_3$



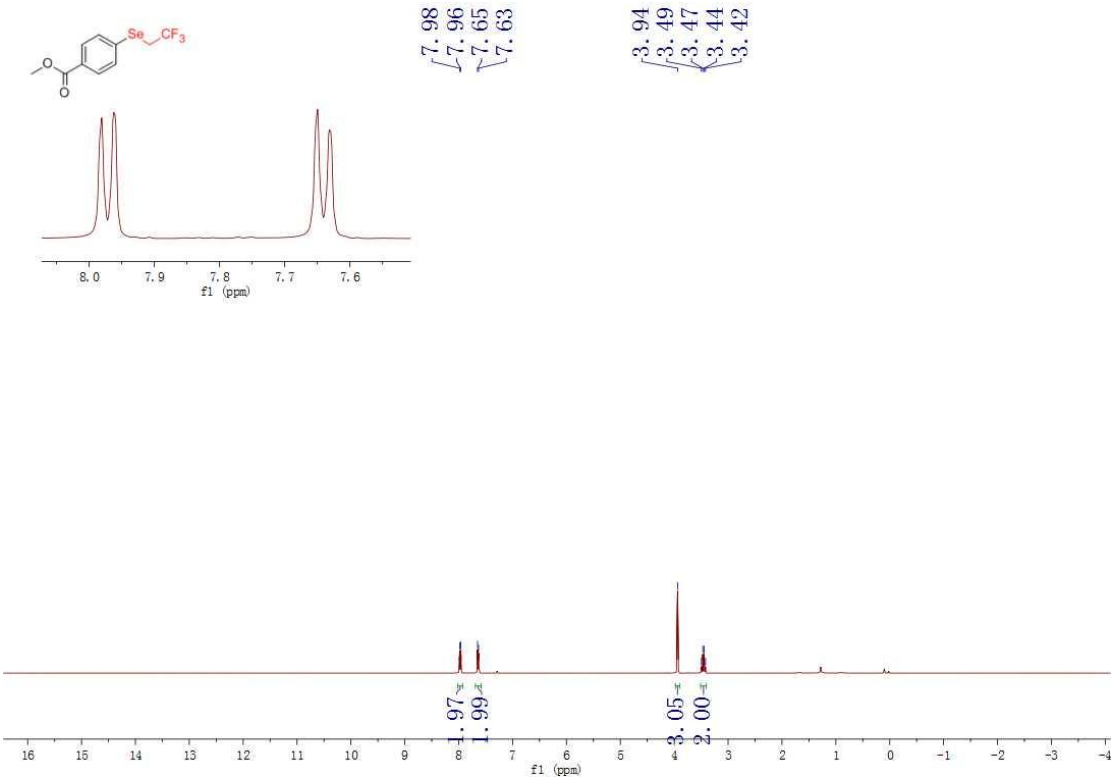
^{13}C NMR spectrum of **2c** in $CDCl_3$



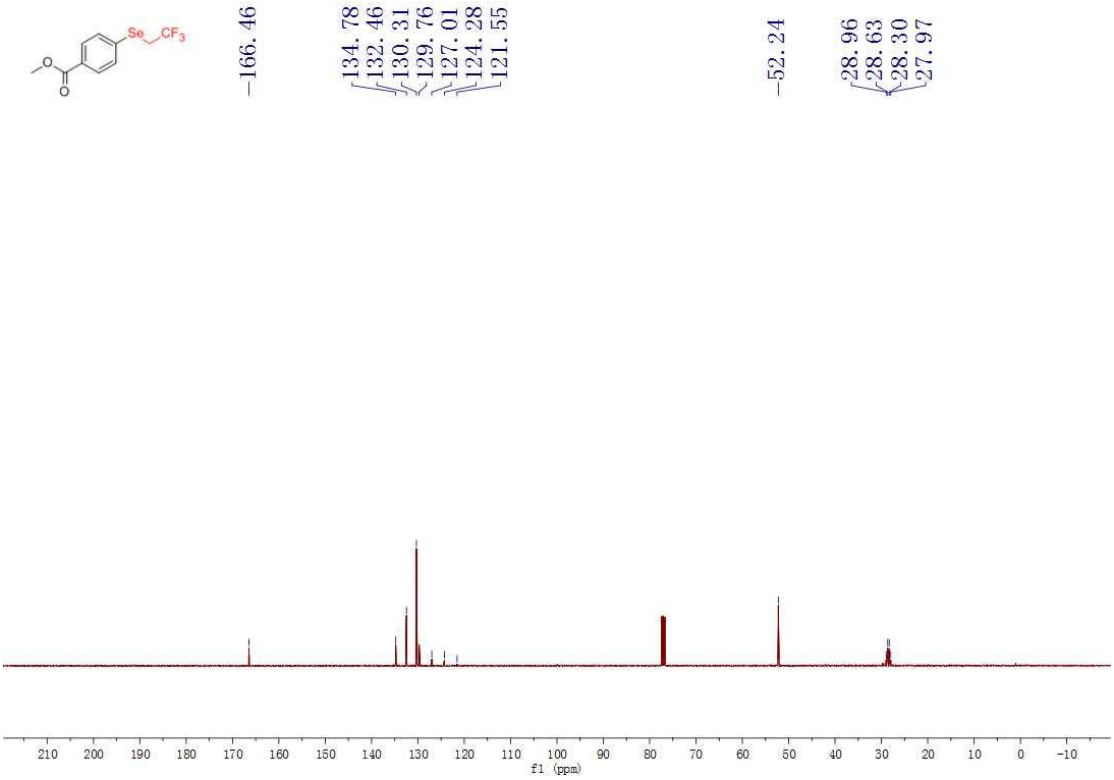
^{19}F NMR spectrum of **2c** in $CDCl_3$



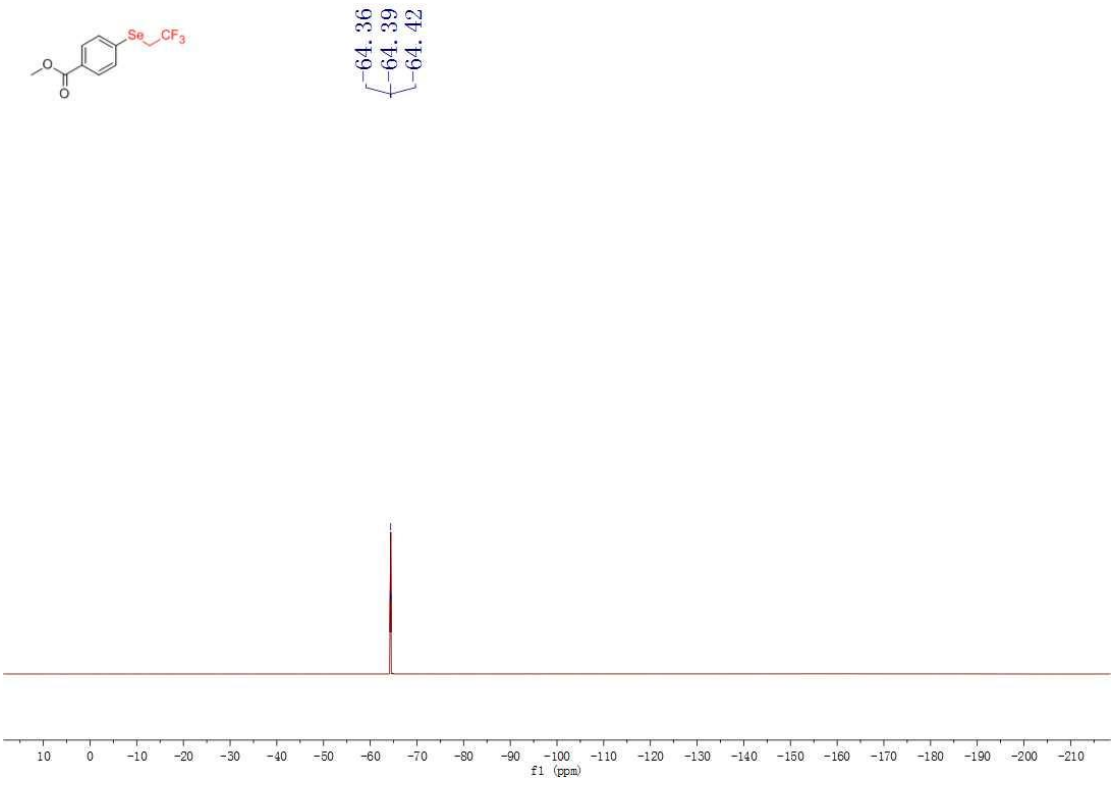
^{1}H NMR spectrum of **2d** in $CDCl_3$



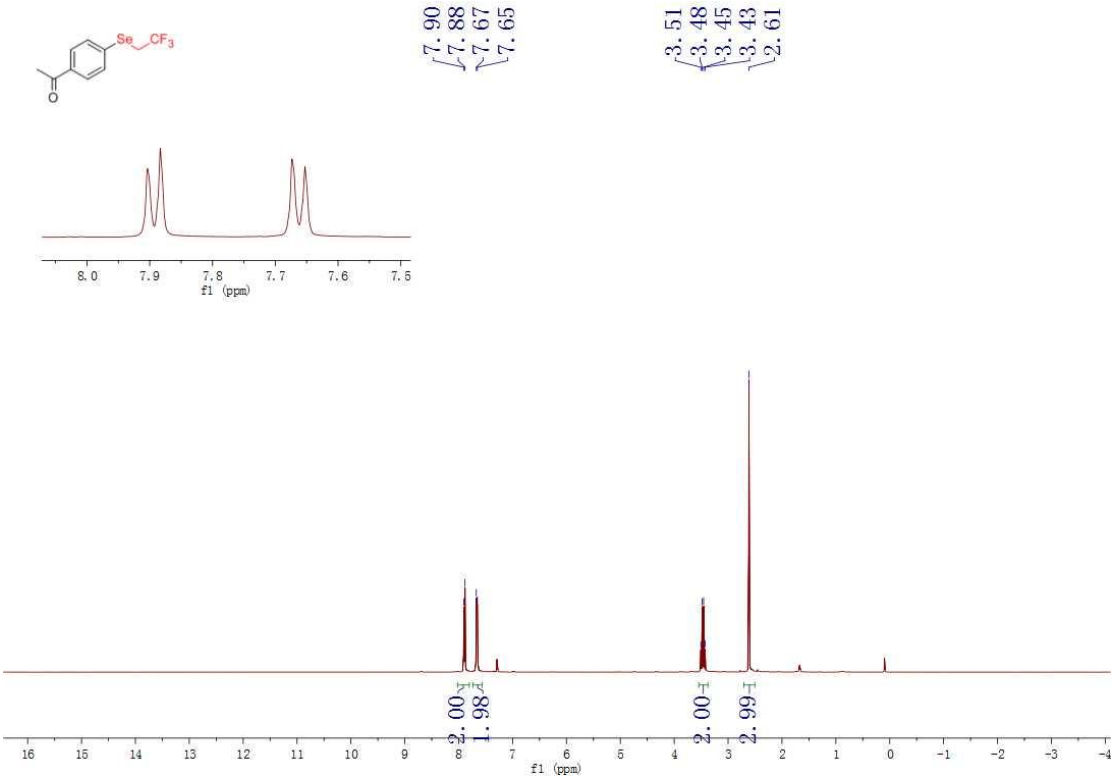
^{13}C NMR spectrum of **2d** in $CDCl_3$



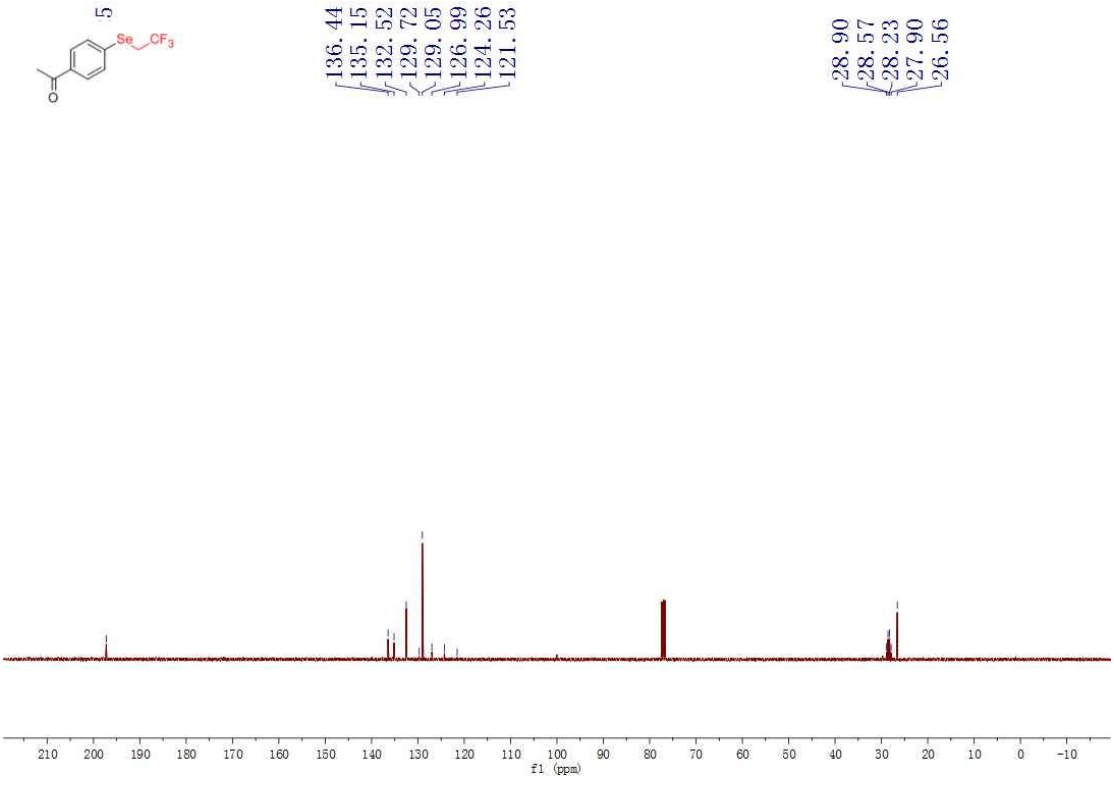
^{19}F NMR spectrum of **2d** in $CDCl_3$



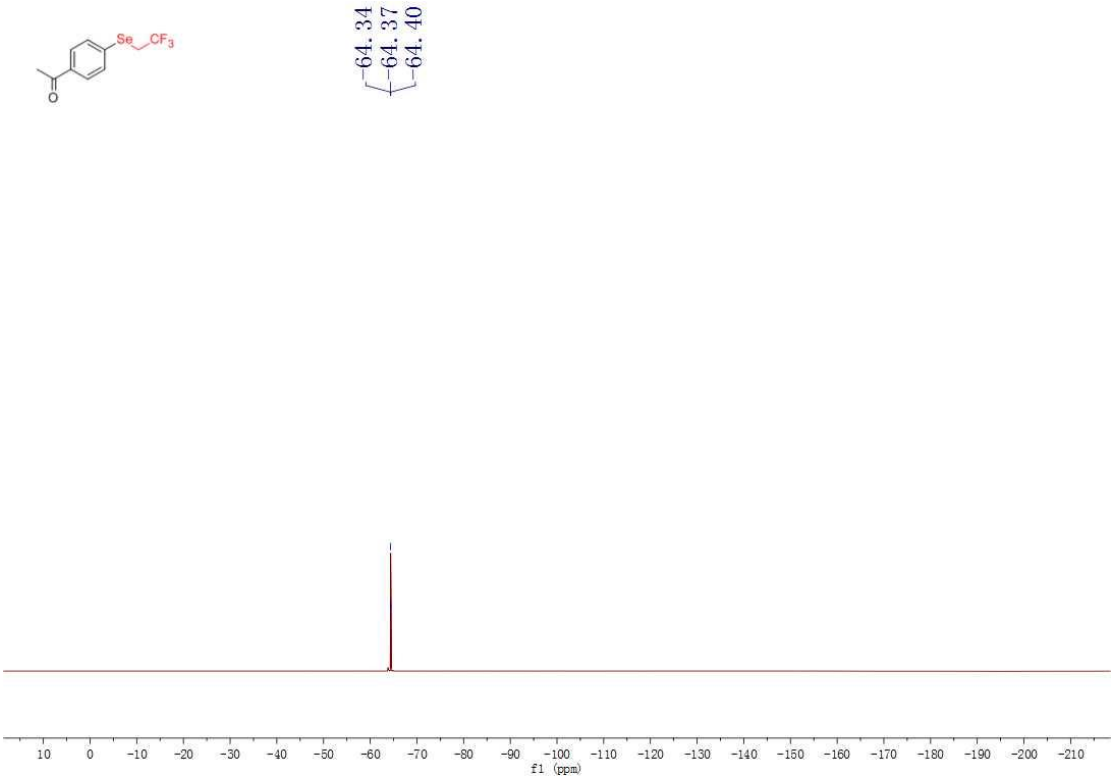
^{1}H NMR spectrum of **2e** in $CDCl_3$



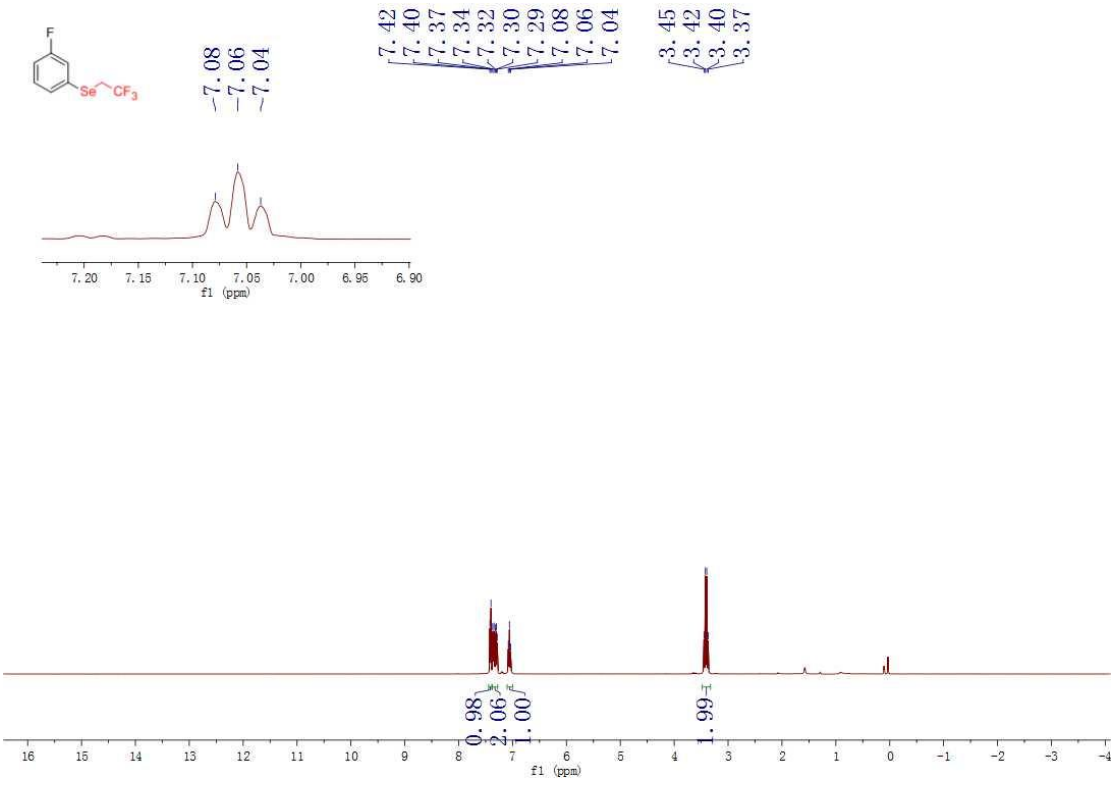
^{13}C NMR spectrum of **2e** in $CDCl_3$



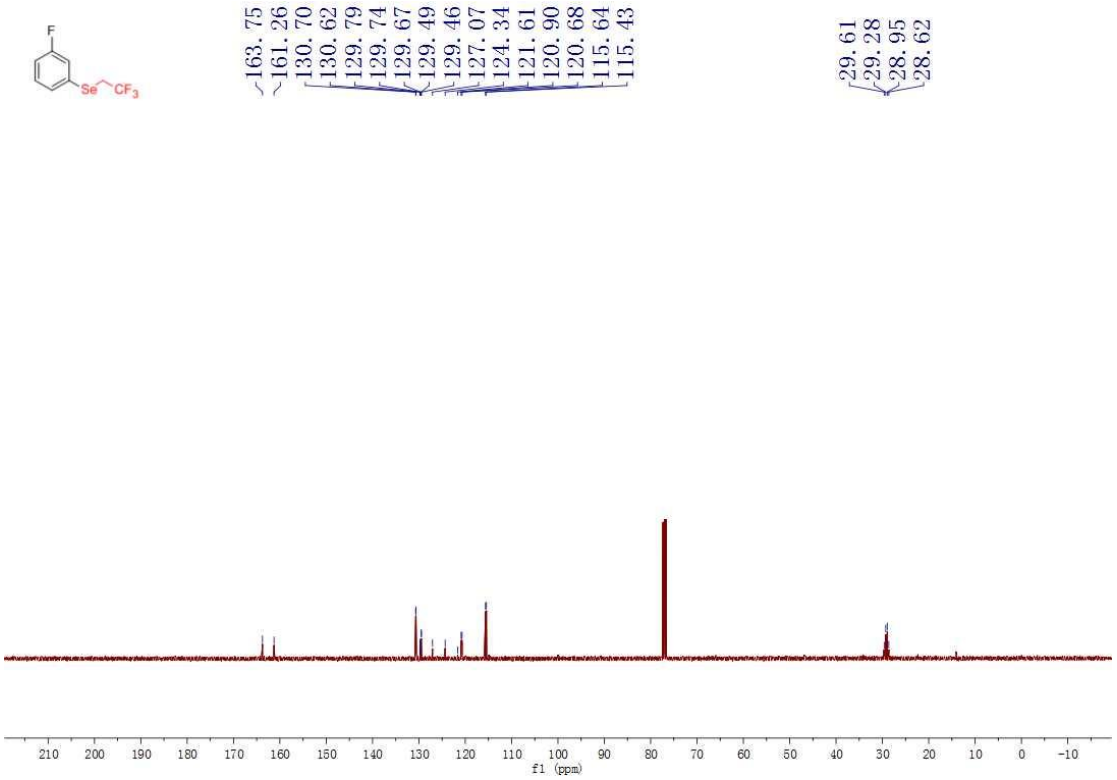
^{19}F NMR spectrum of **2e** in $CDCl_3$



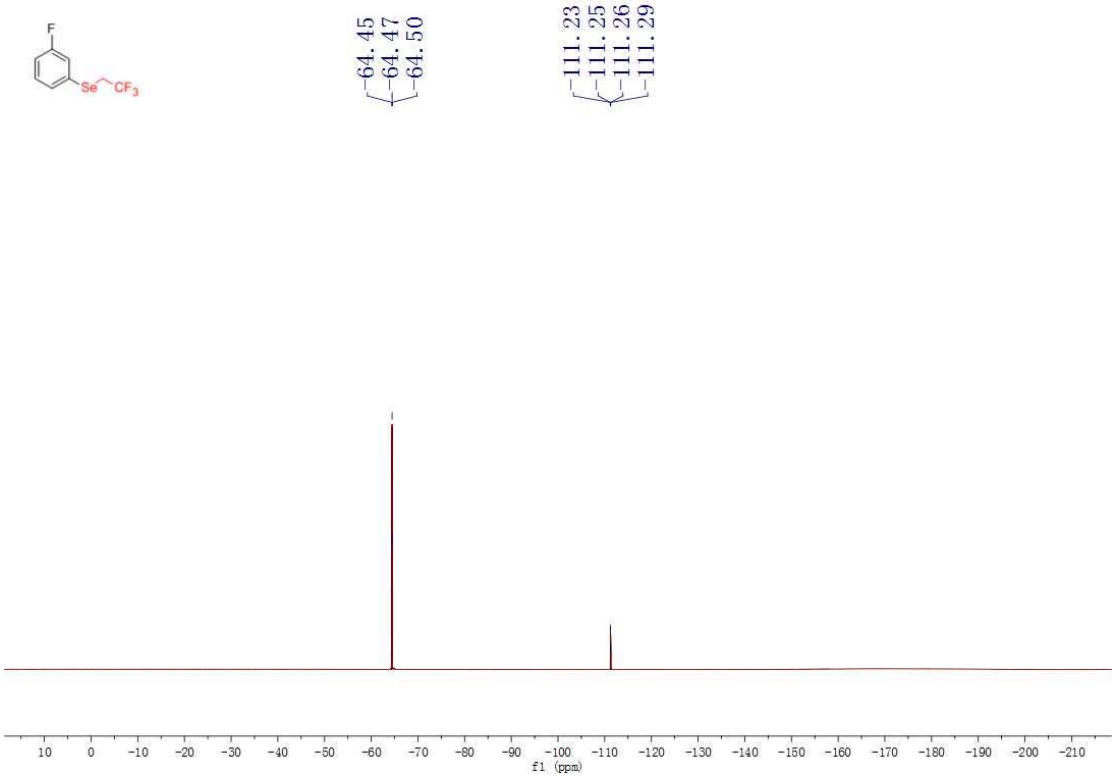
^{1}H NMR spectrum of **2f** in $CDCl_3$



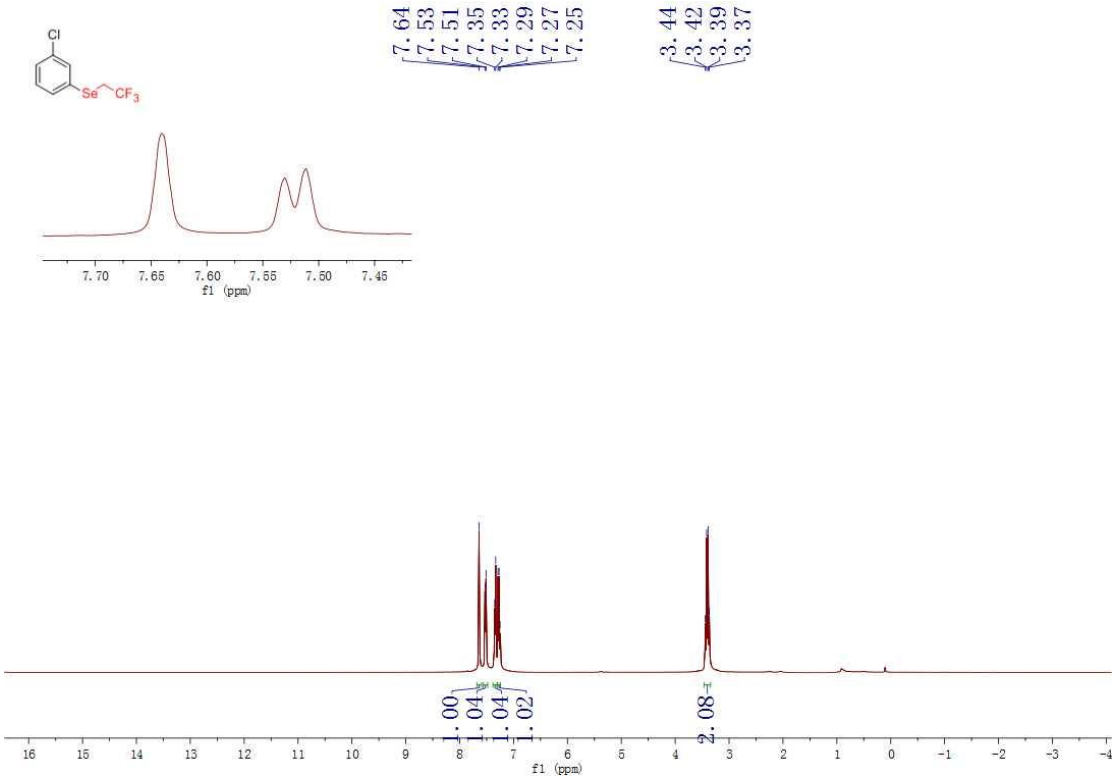
^{13}C NMR spectrum of **2f** in $CDCl_3$



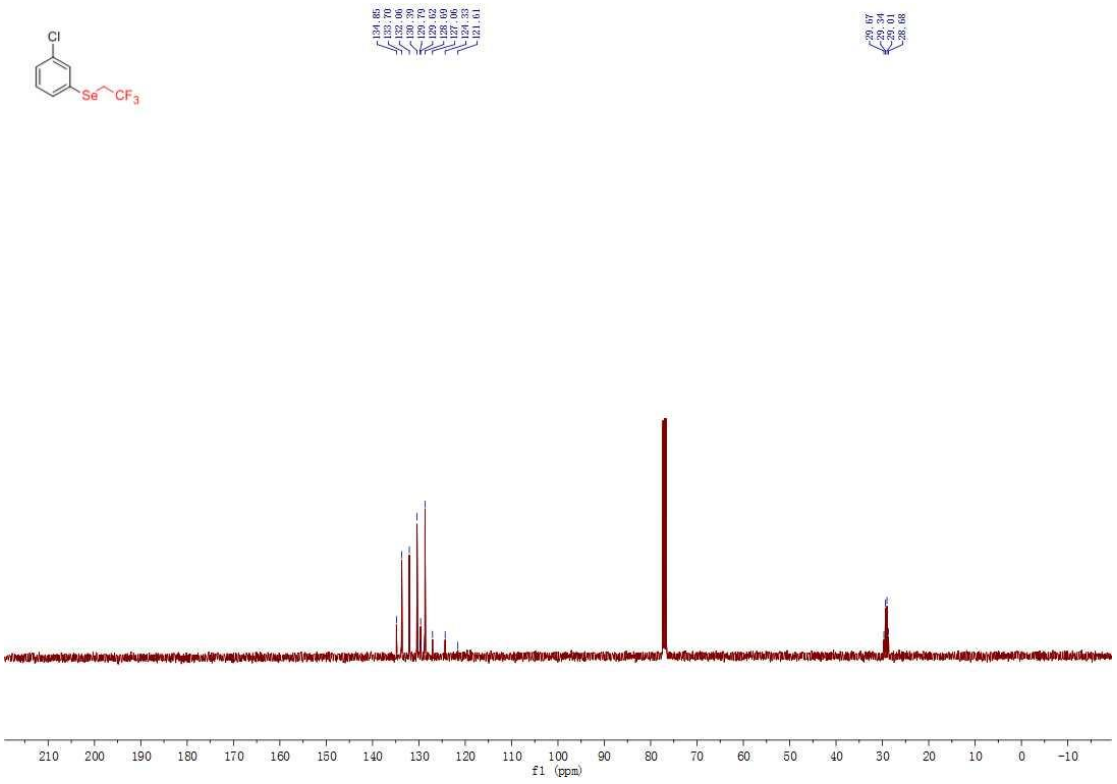
^{19}F NMR spectrum of **2f** in $CDCl_3$



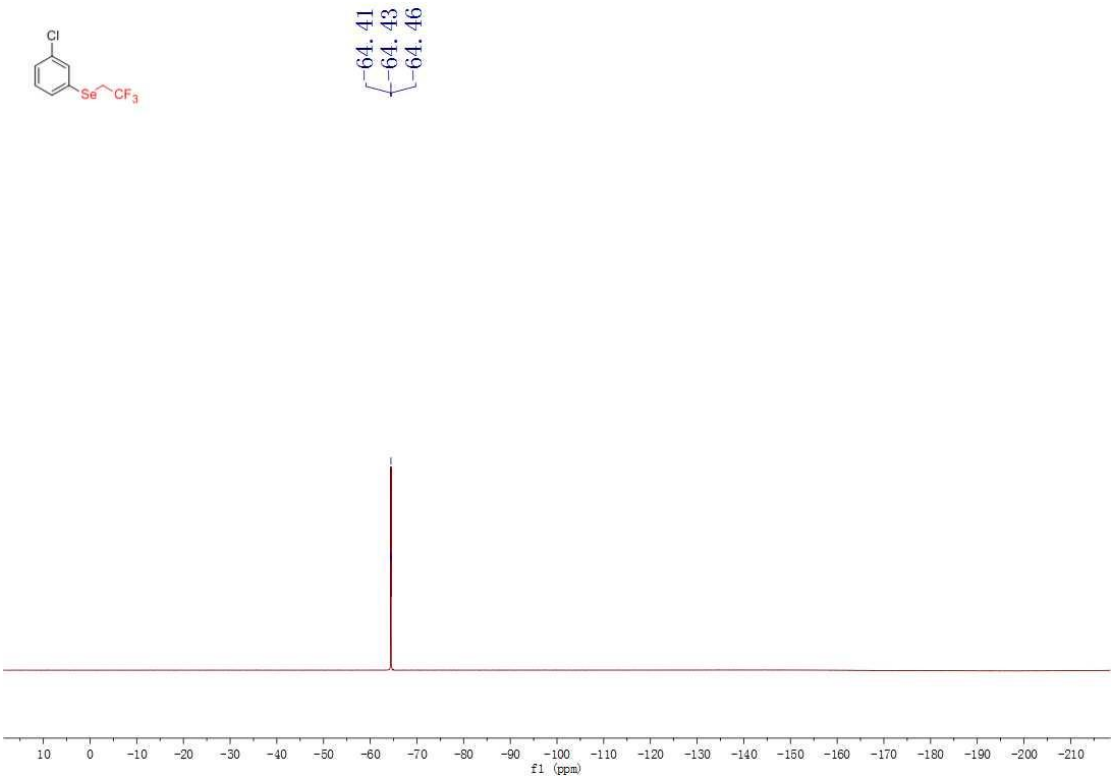
^{1}H NMR spectrum of **2g** in $CDCl_3$



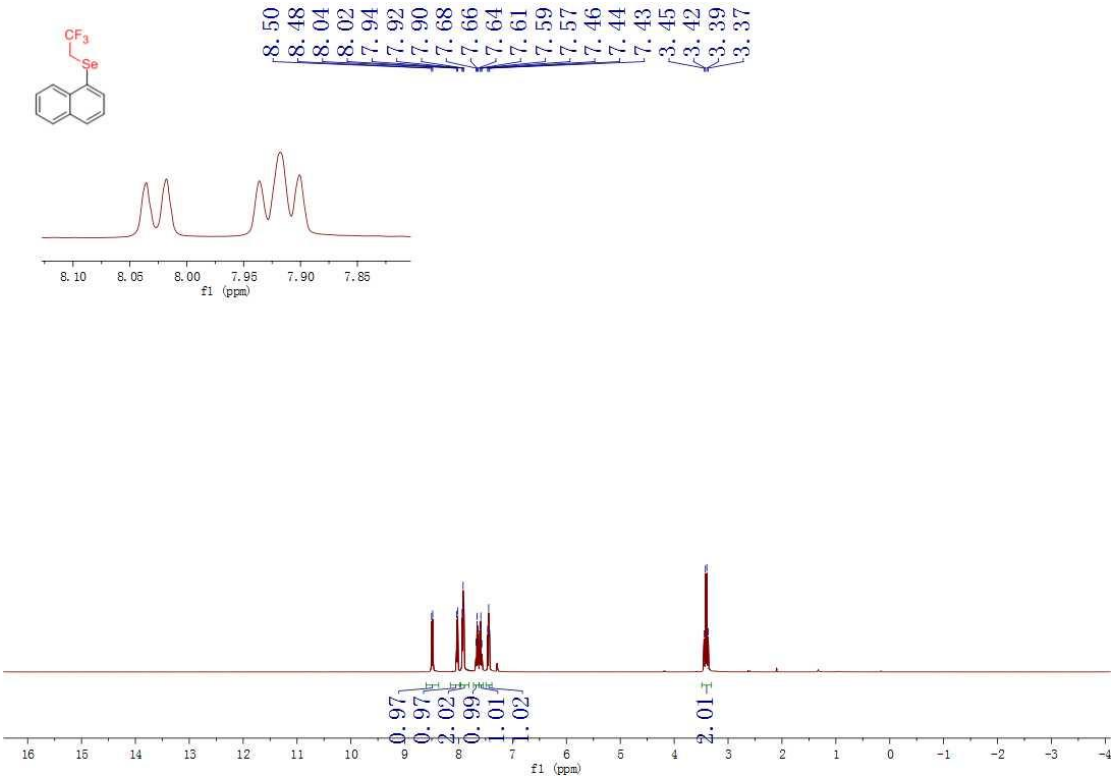
^{13}C NMR spectrum of **2g** in $CDCl_3$



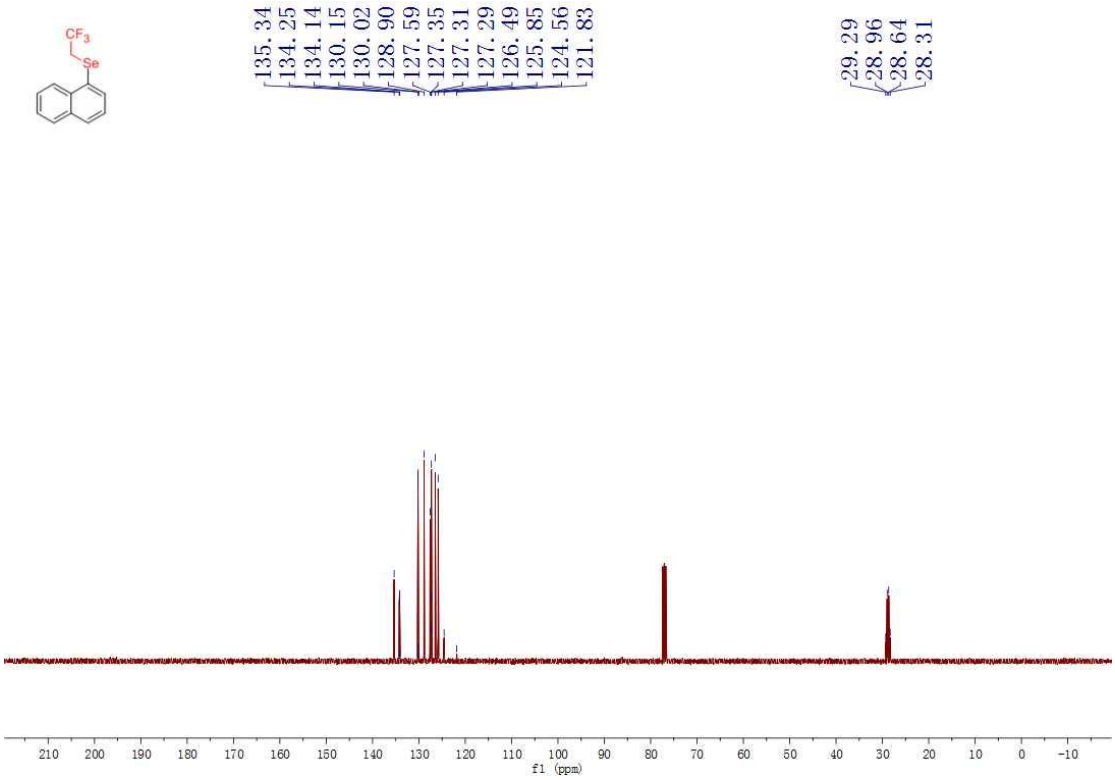
^{19}F NMR spectrum of **2g** in $CDCl_3$



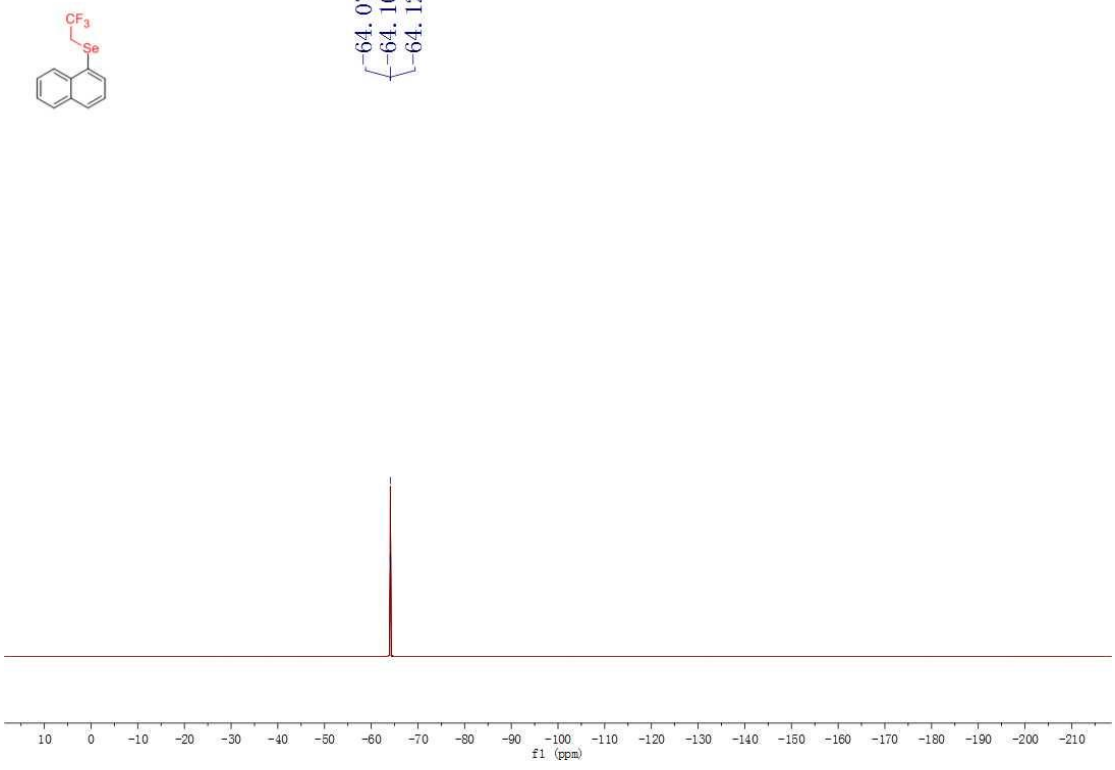
^{1}H NMR spectrum of **2h** in $CDCl_3$



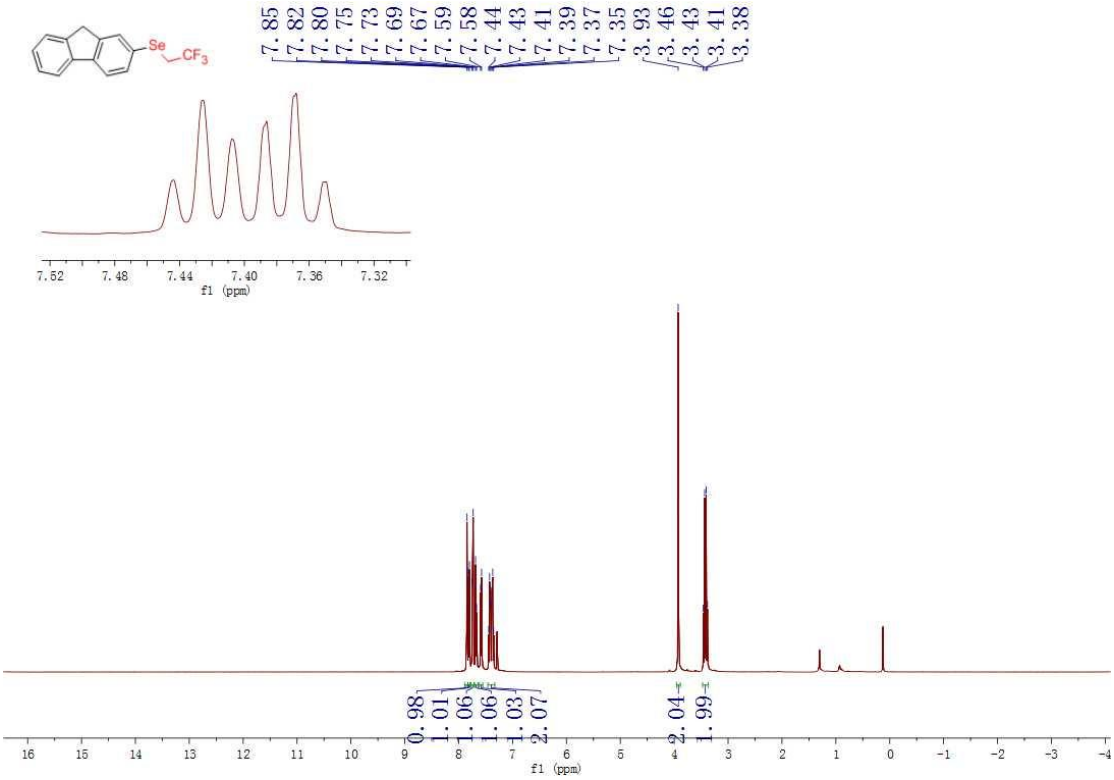
^{13}C NMR spectrum of **2h** in $CDCl_3$



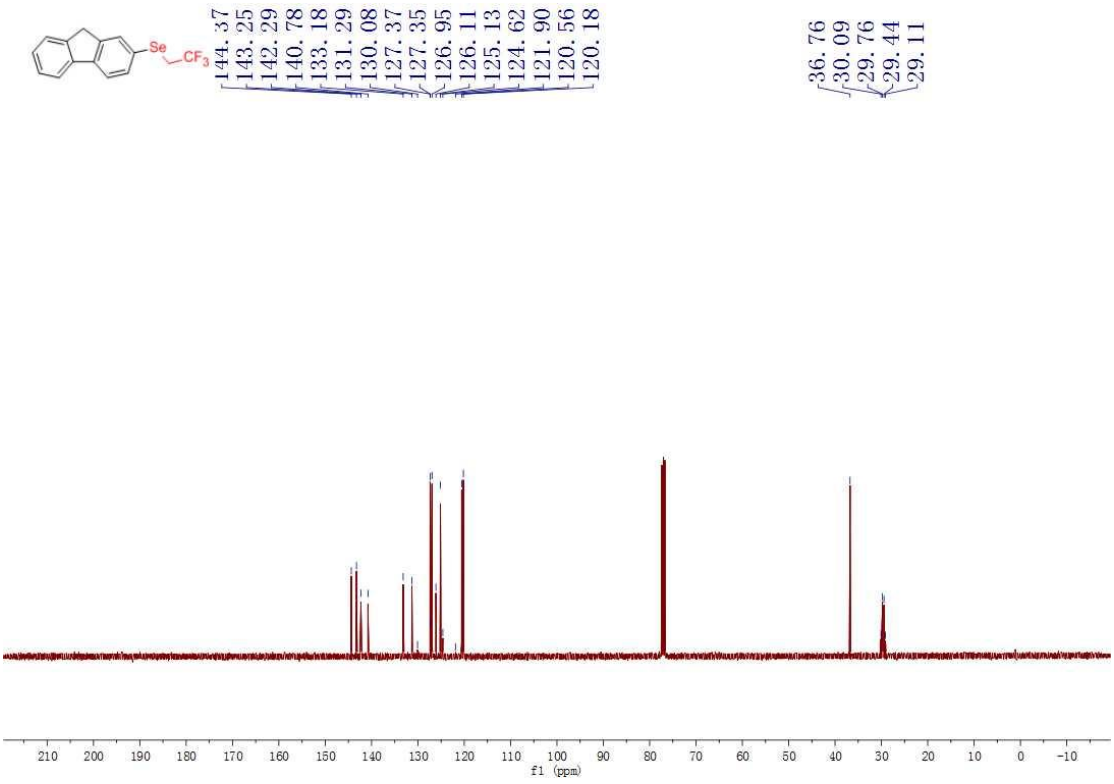
^{19}F NMR spectrum of **2h** in $CDCl_3$



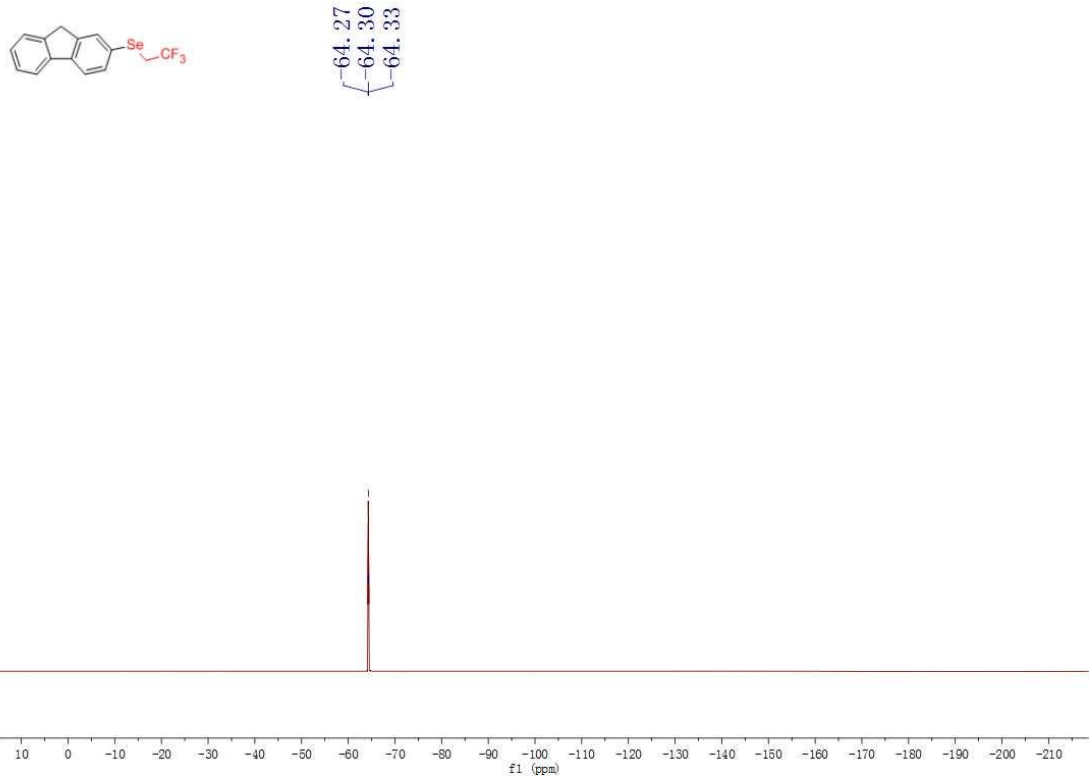
^{1}H NMR spectrum of **2i** in $CDCl_3$



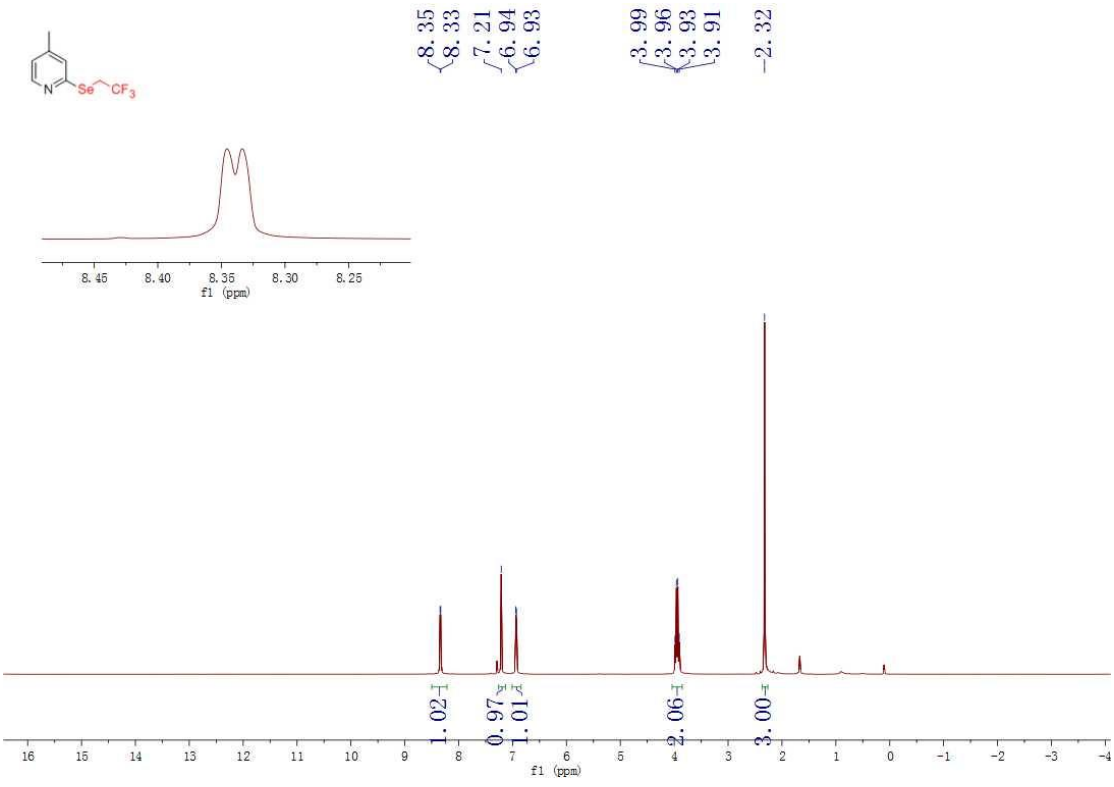
^{13}C NMR spectrum of **2i** in $CDCl_3$



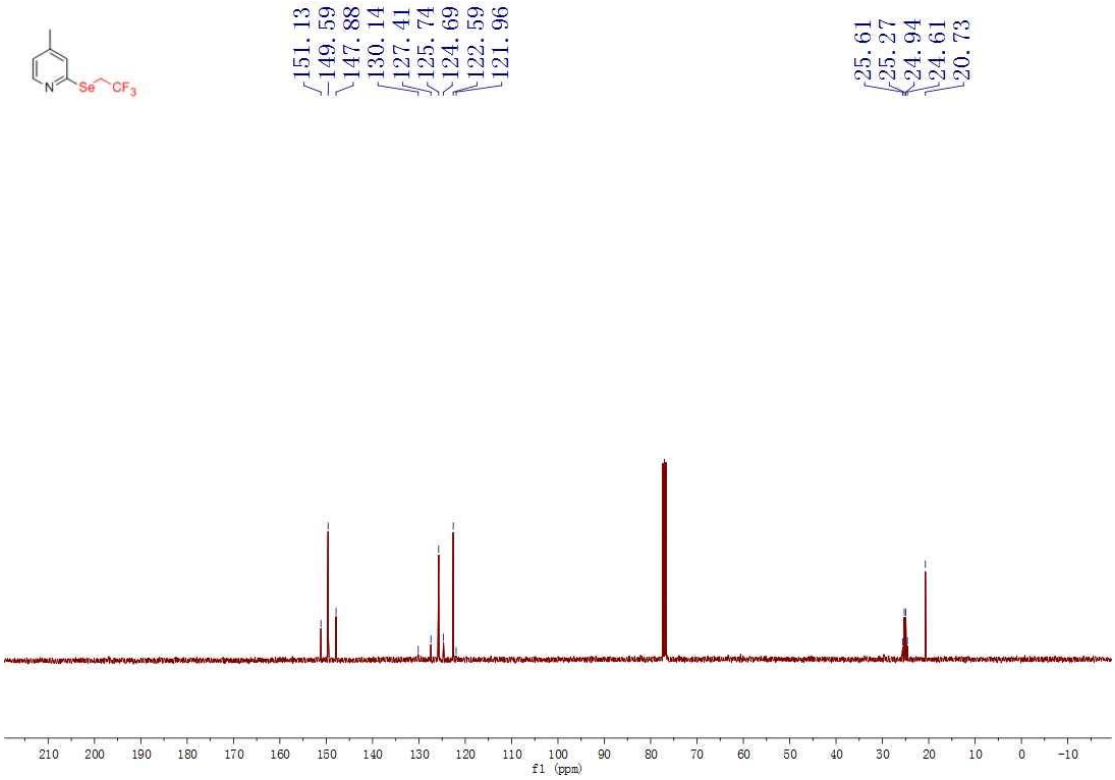
^{19}F NMR spectrum of **2i** in $CDCl_3$



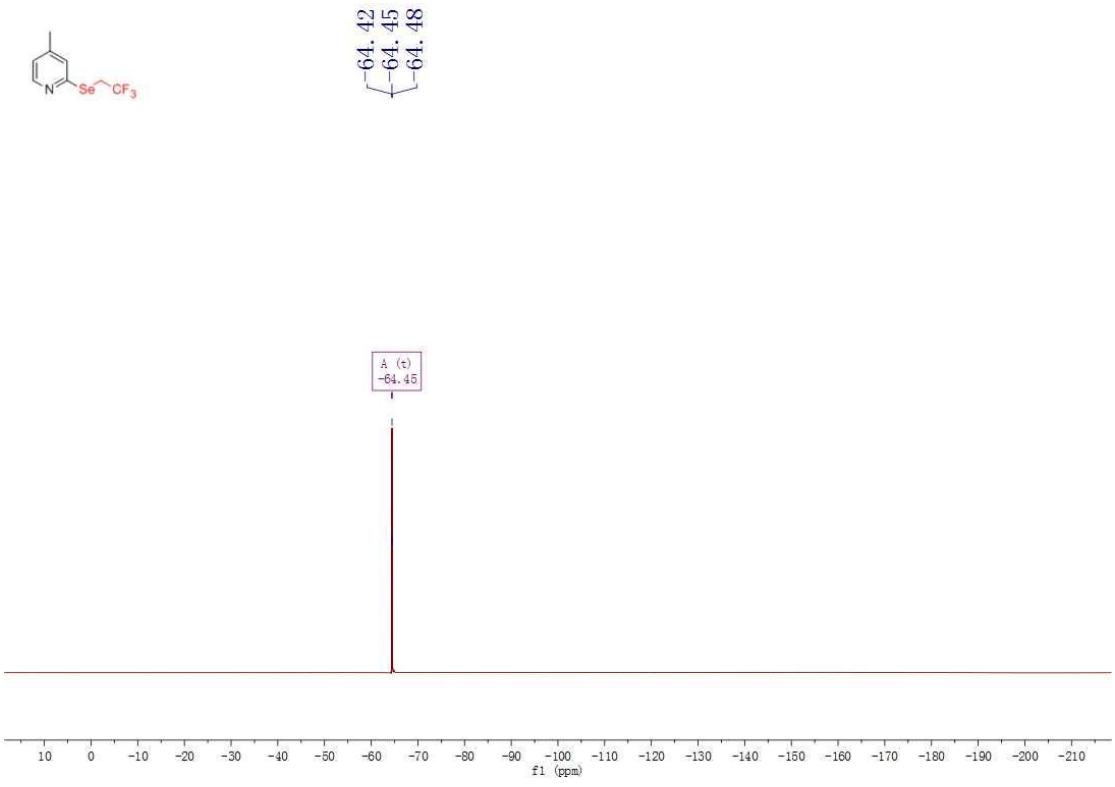
^{1}H NMR spectrum of **2j** in $CDCl_3$



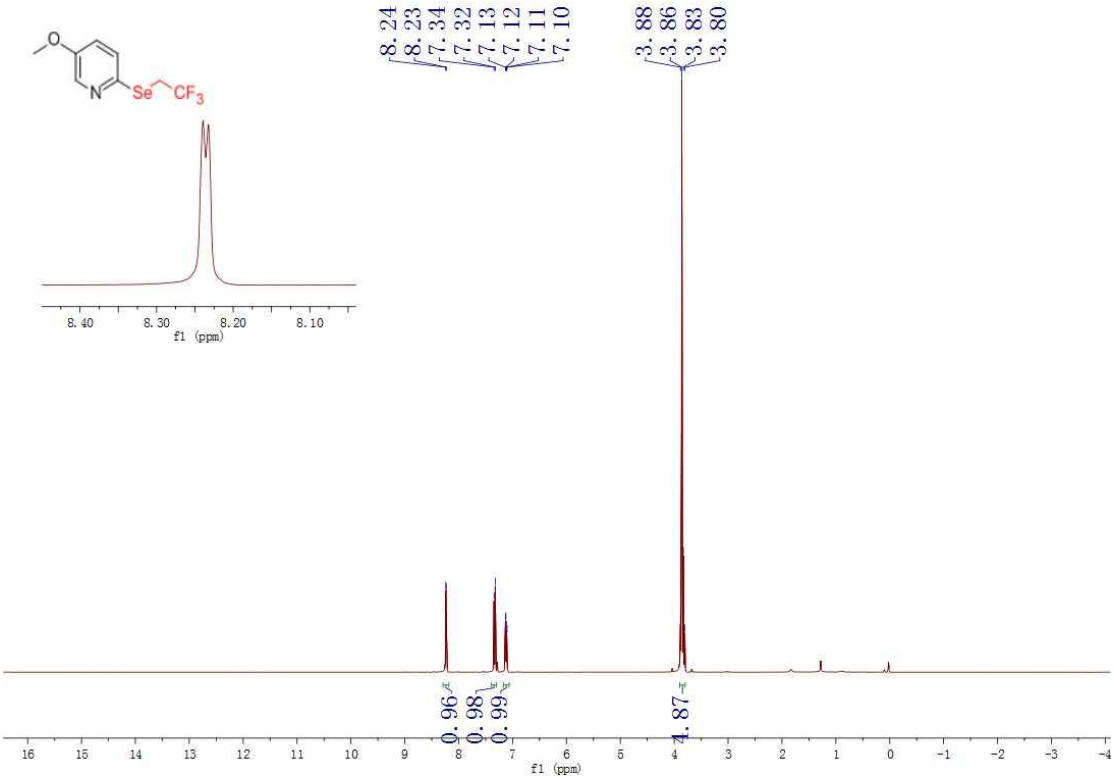
^{13}C NMR spectrum of **2j** in $CDCl_3$



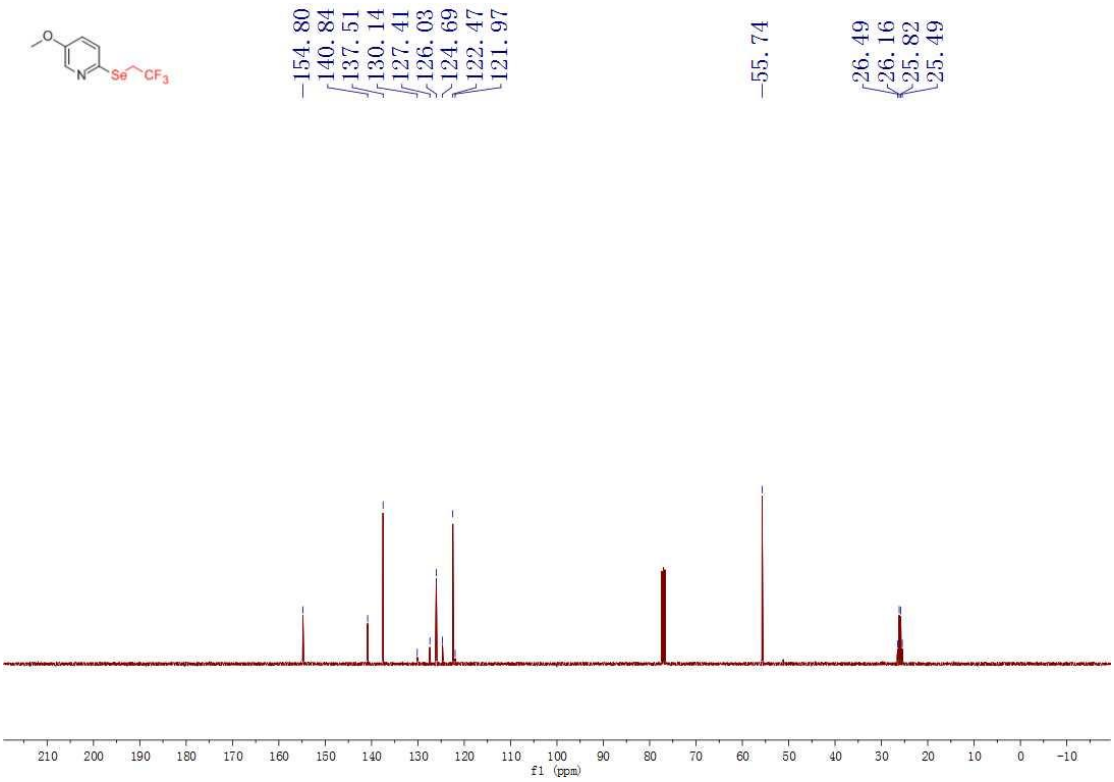
^{19}F NMR spectrum of **2j** in $CDCl_3$



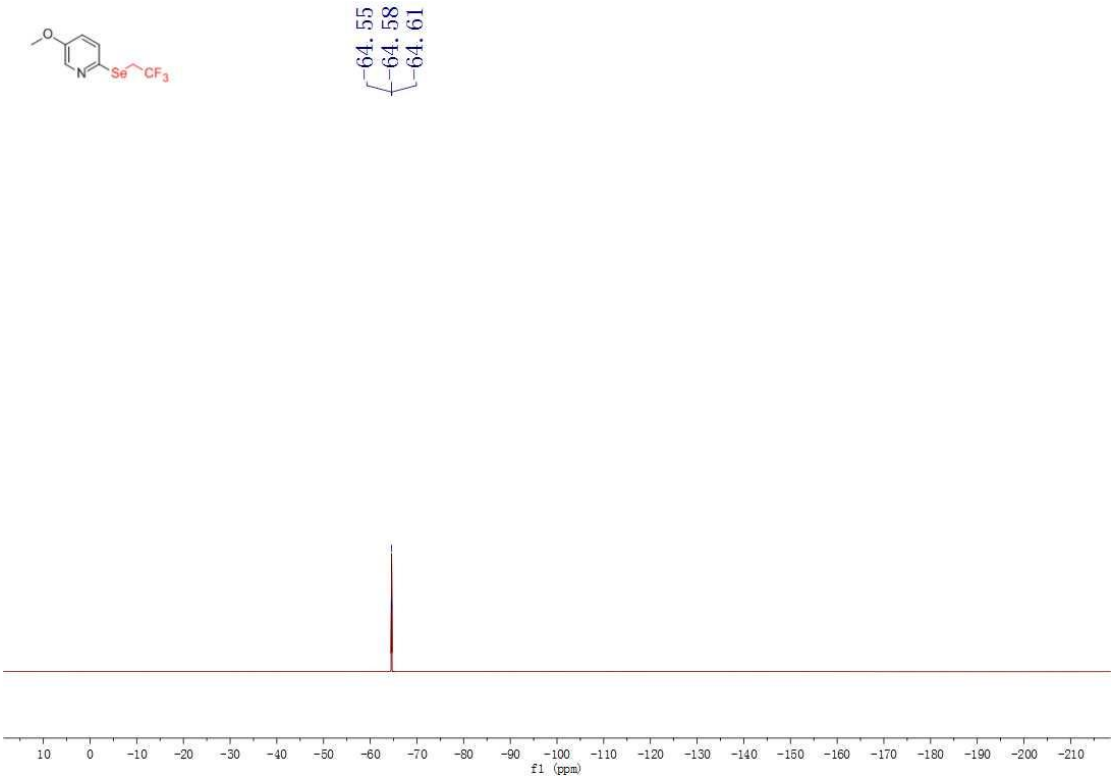
^{1}H NMR spectrum of **2k** in $CDCl_3$



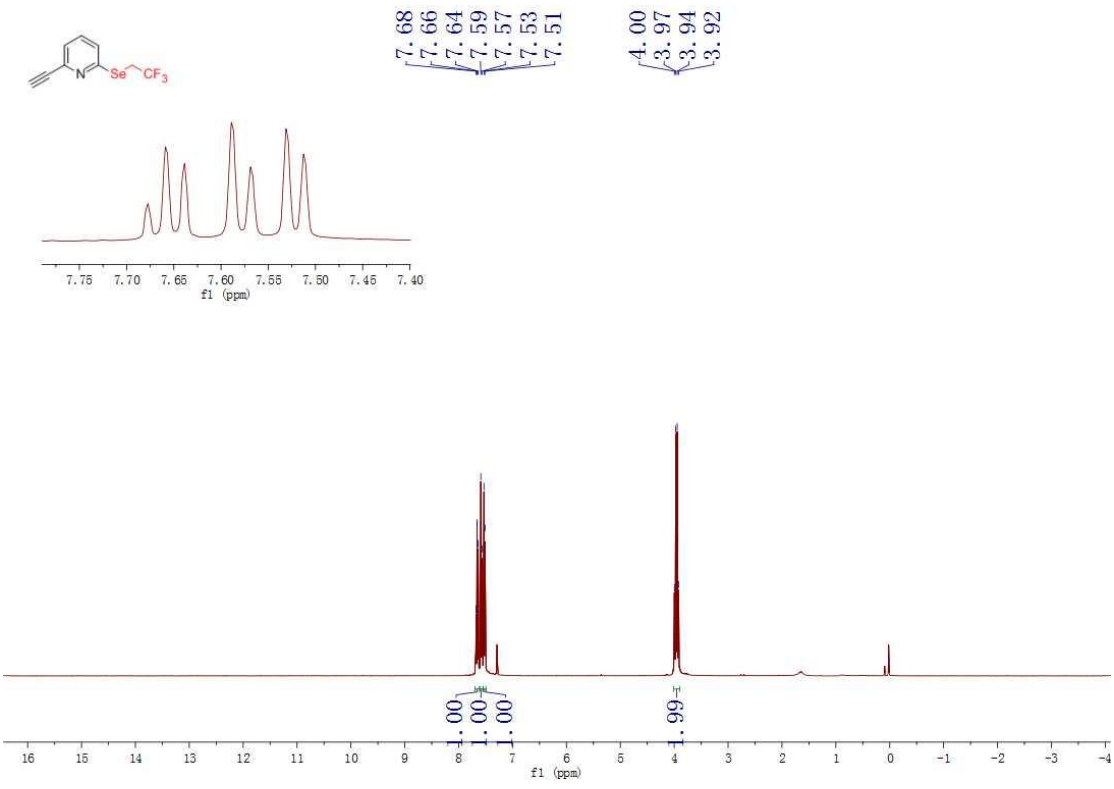
^{13}C NMR spectrum of **2k** in $CDCl_3$



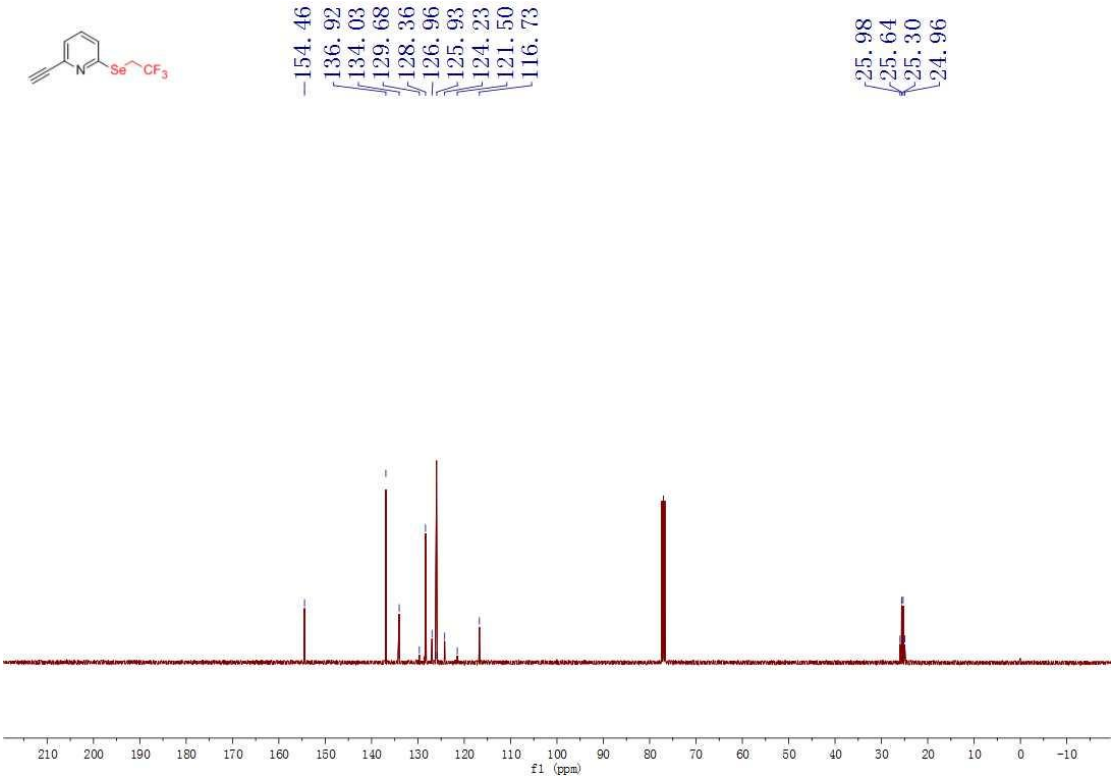
^{19}F NMR spectrum of **2k** in $CDCl_3$



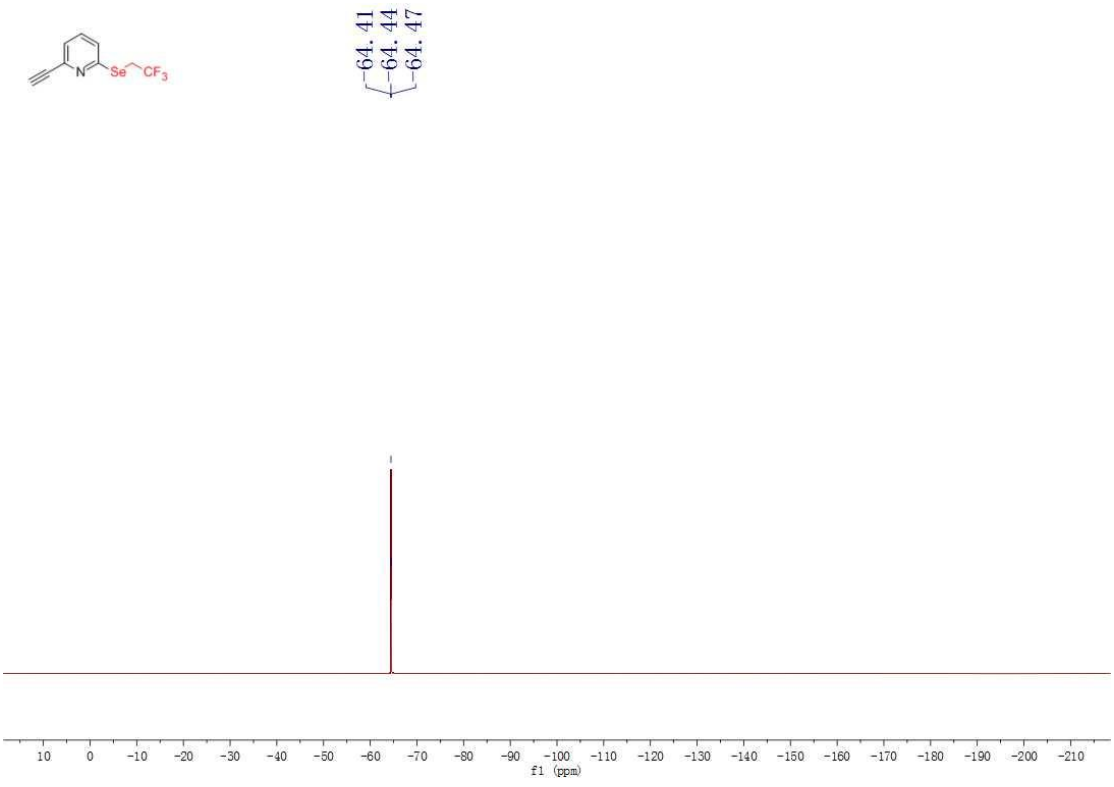
^{1}H NMR spectrum of **2l** in $CDCl_3$



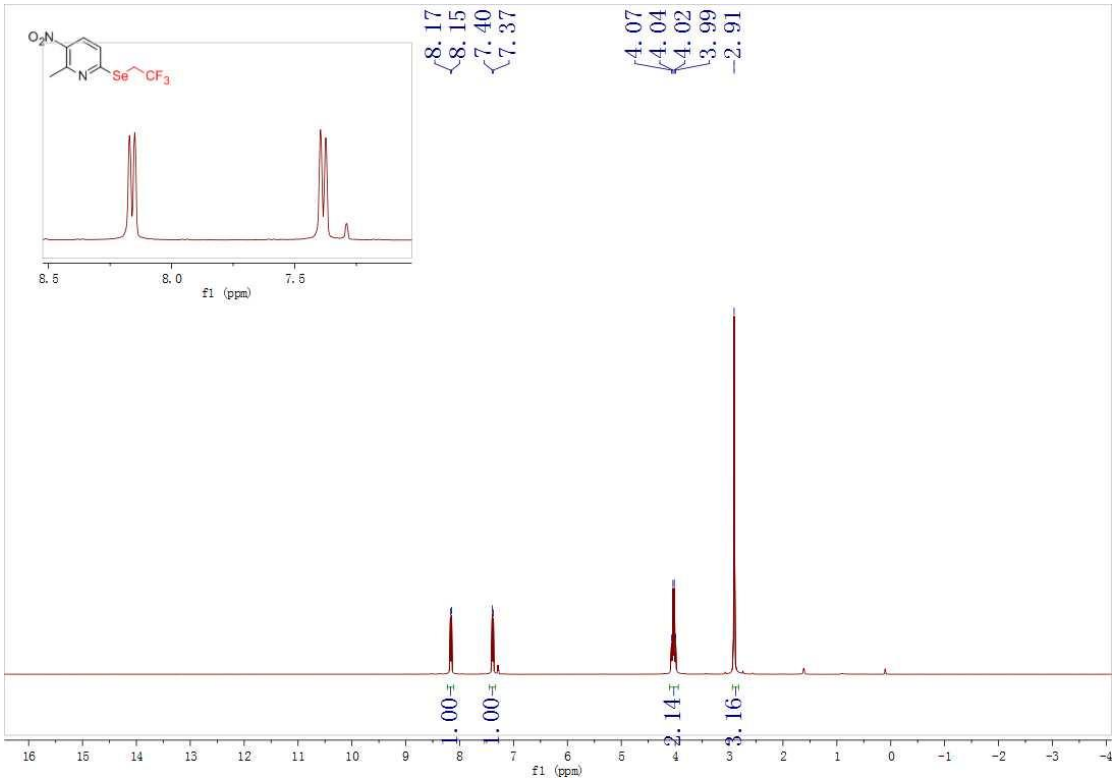
^{13}C NMR spectrum of **2l** in $CDCl_3$



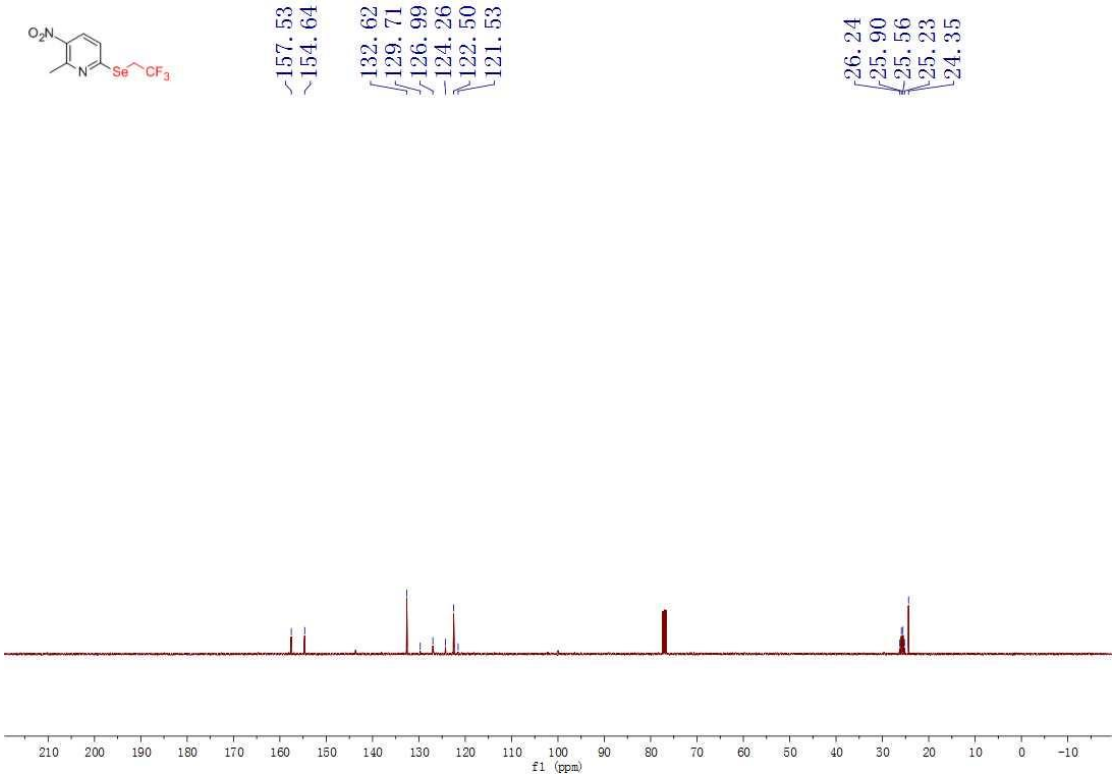
^{19}F NMR spectrum of **2l** in $CDCl_3$



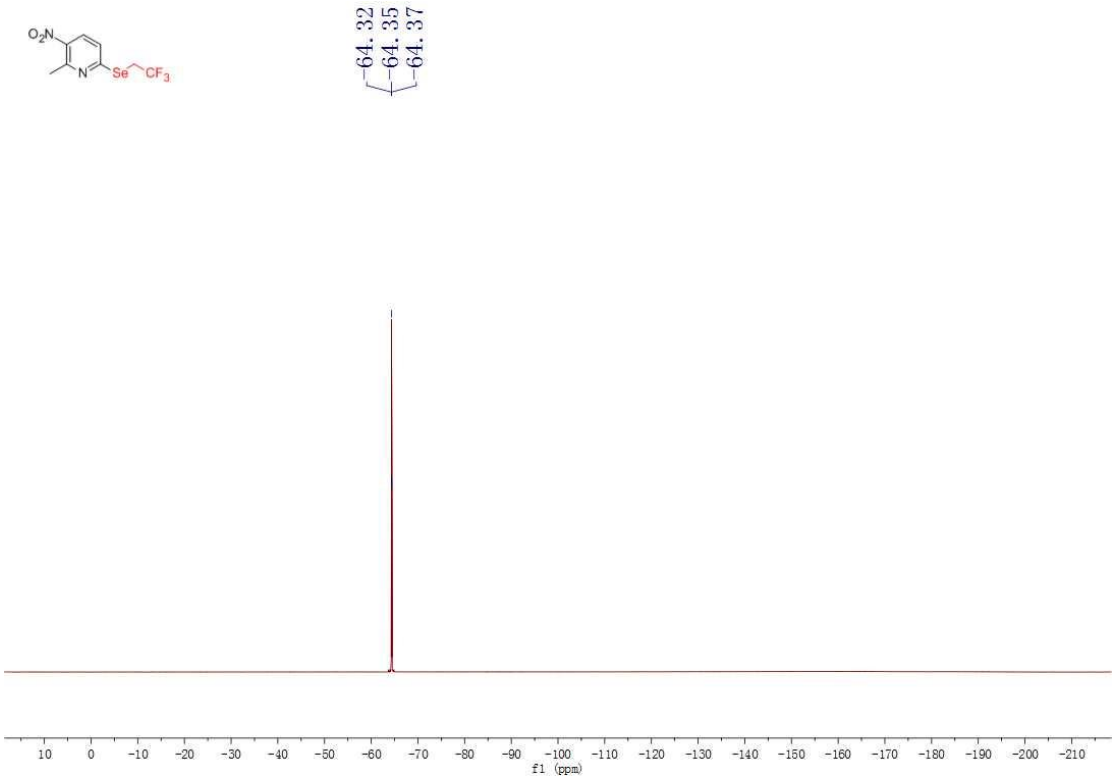
^{1}H NMR spectrum of **2m** in $CDCl_3$



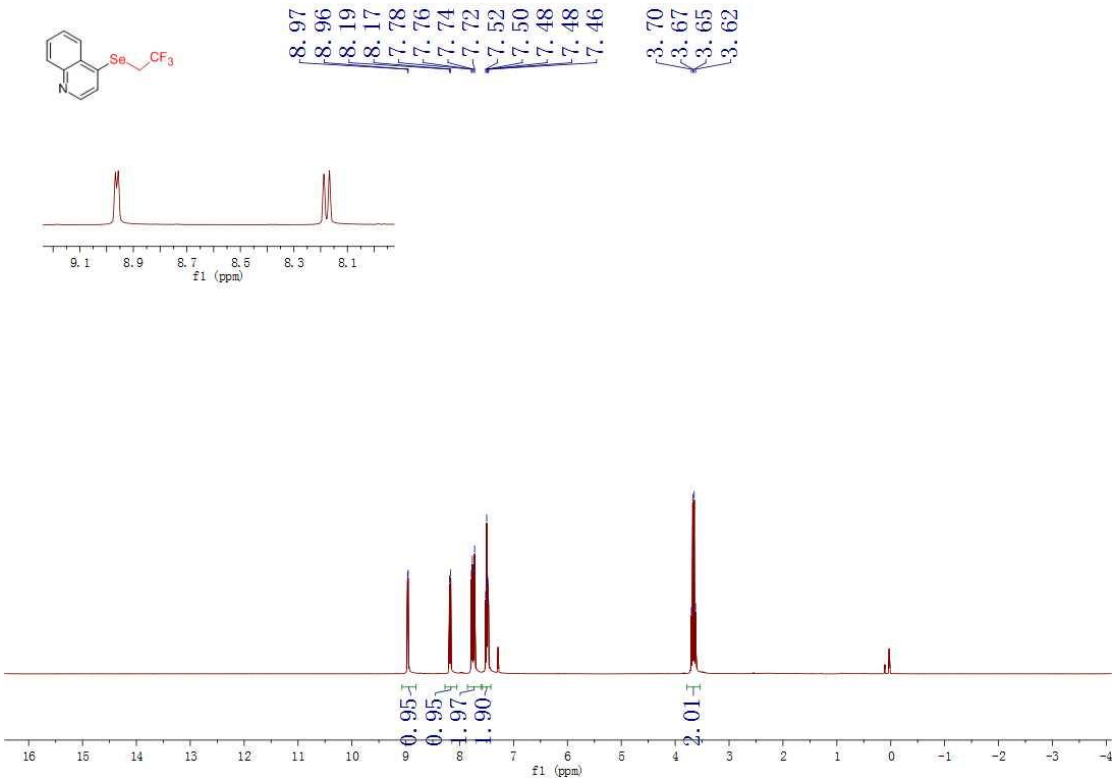
^{13}C NMR spectrum of **2m** in $CDCl_3$



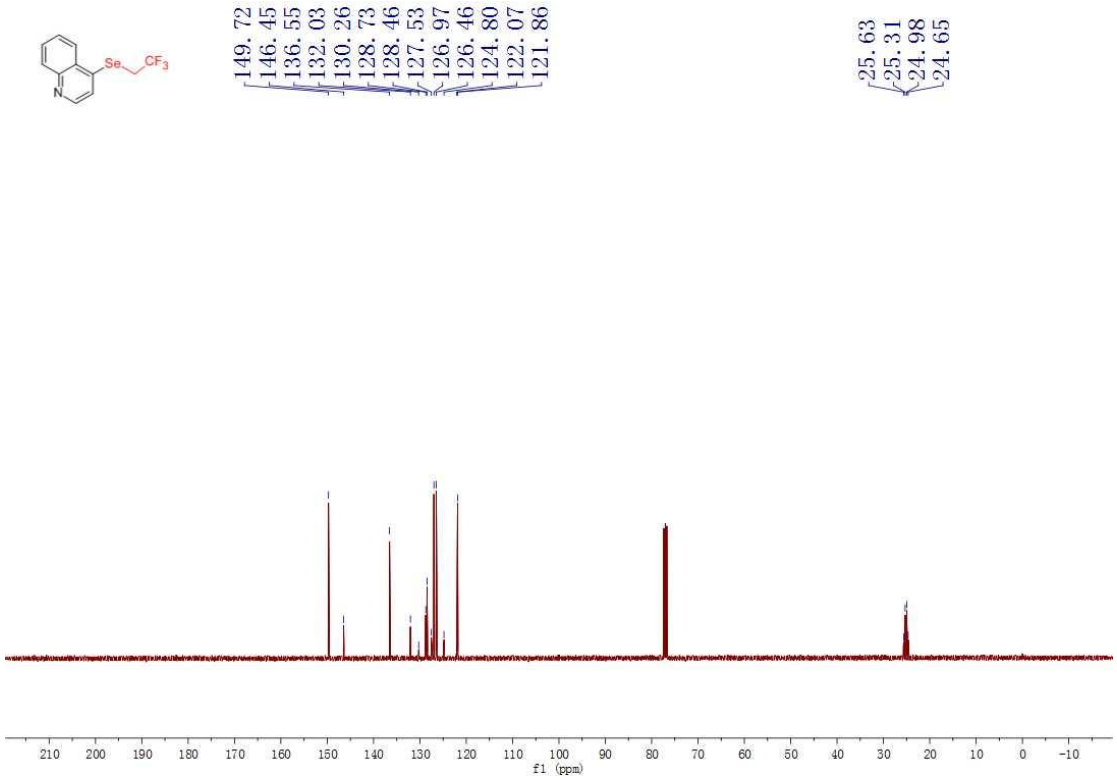
^{19}F NMR spectrum of **2m** in $CDCl_3$



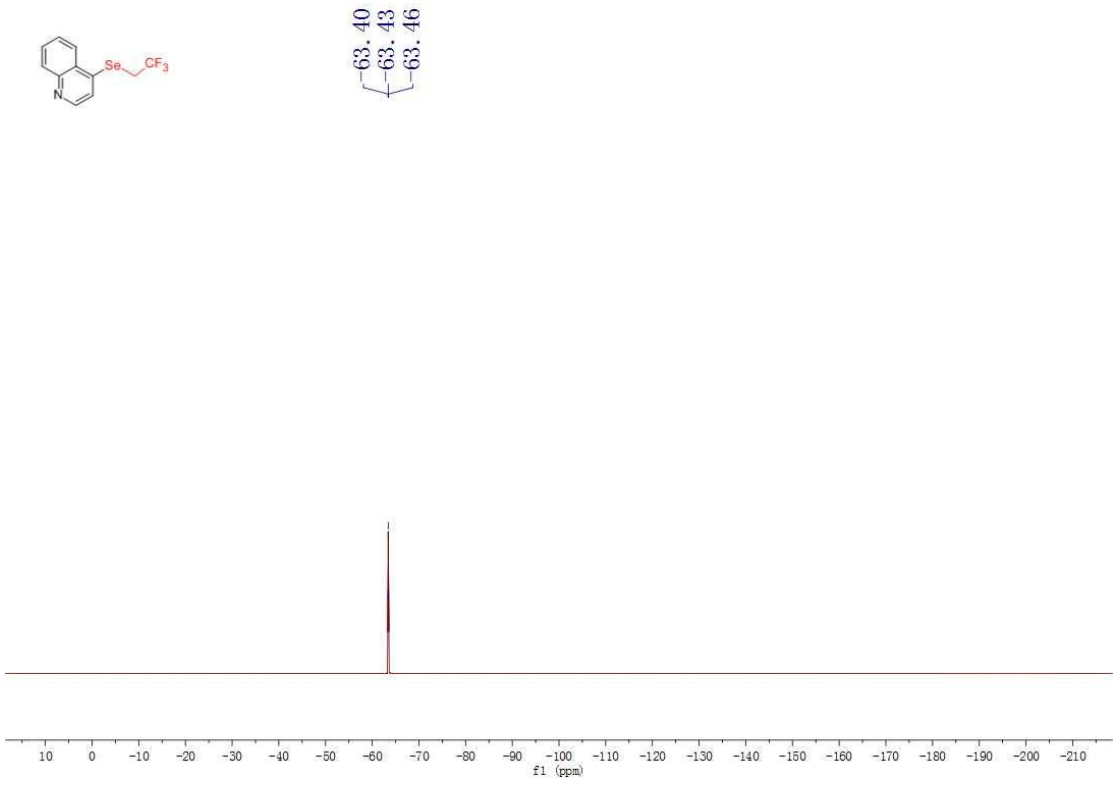
^{1}H NMR spectrum of **2n** in $CDCl_3$



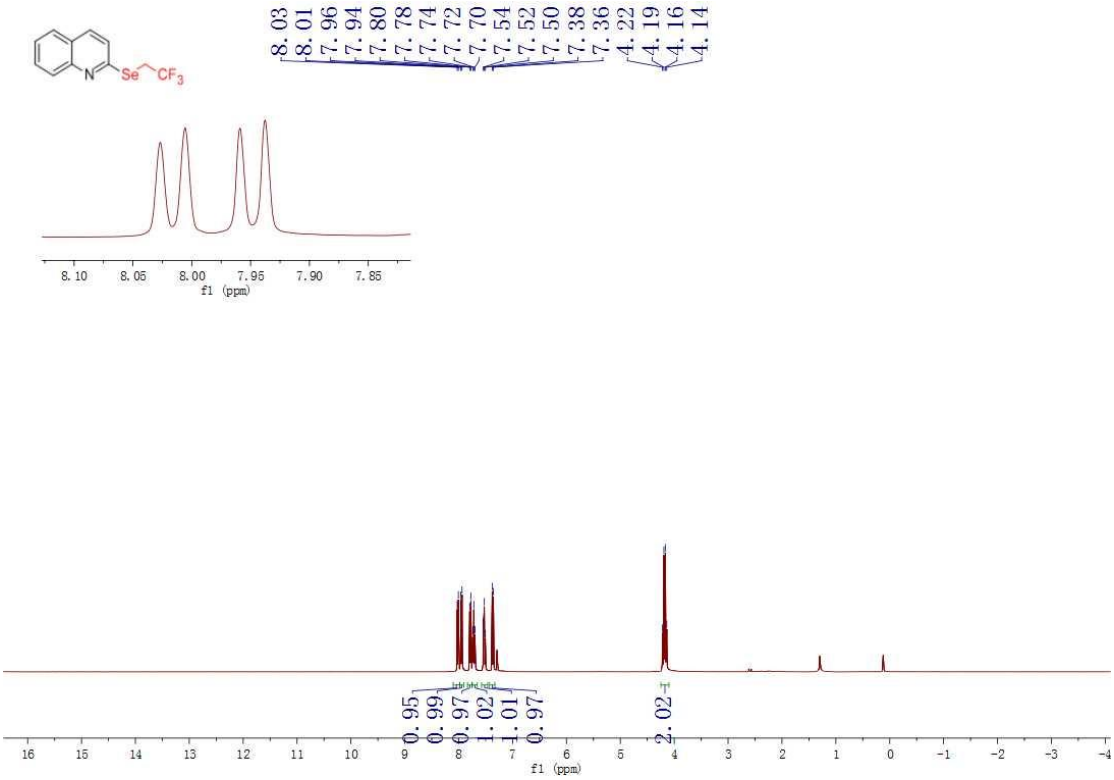
^{13}C NMR spectrum of **2n** in $CDCl_3$



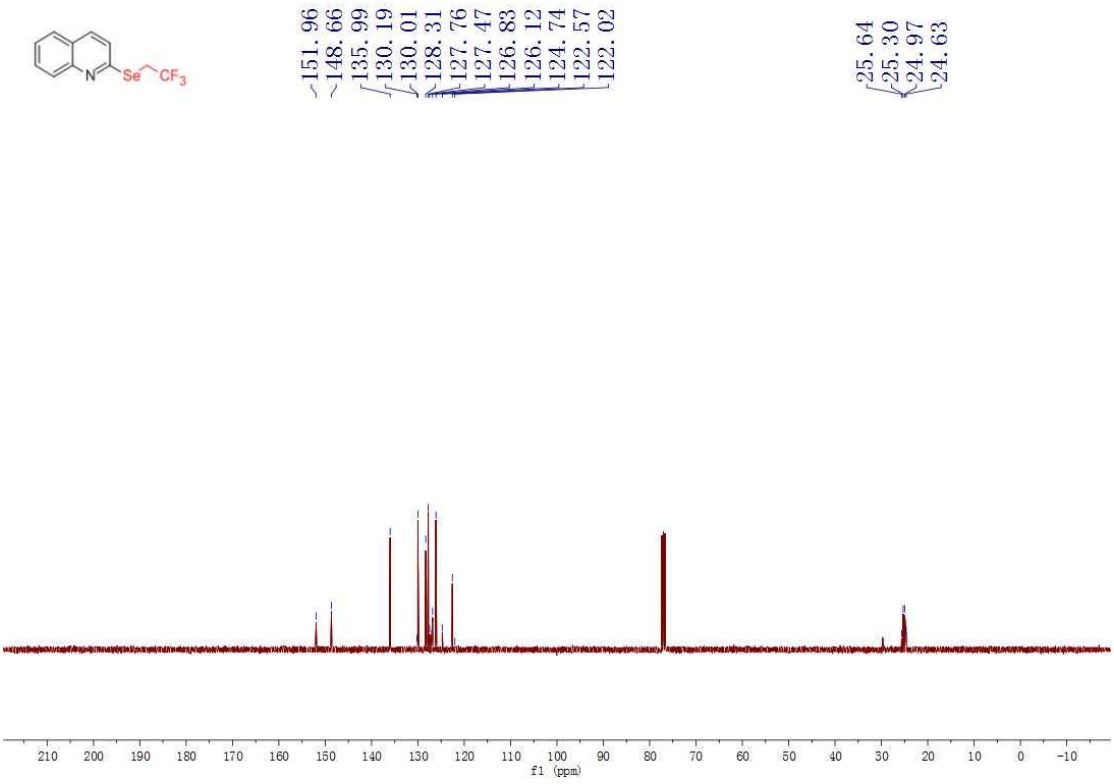
^{19}F NMR spectrum of **2n** in $CDCl_3$



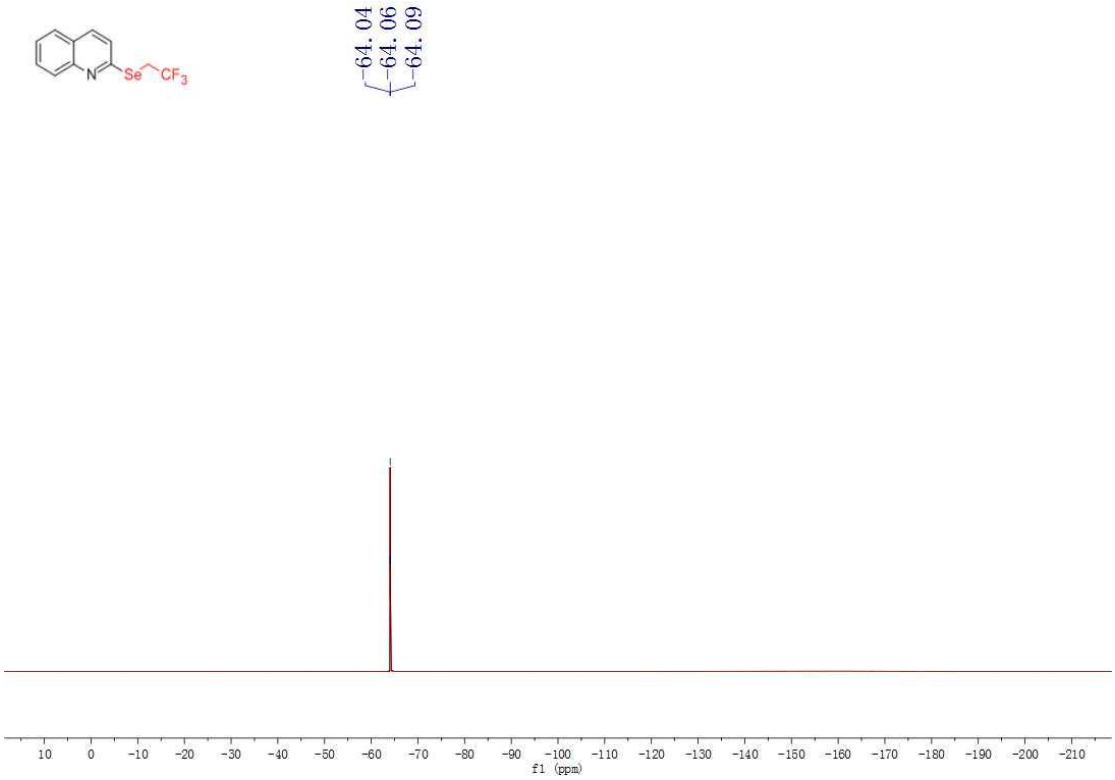
^{1}H NMR spectrum of **2o** in $CDCl_3$



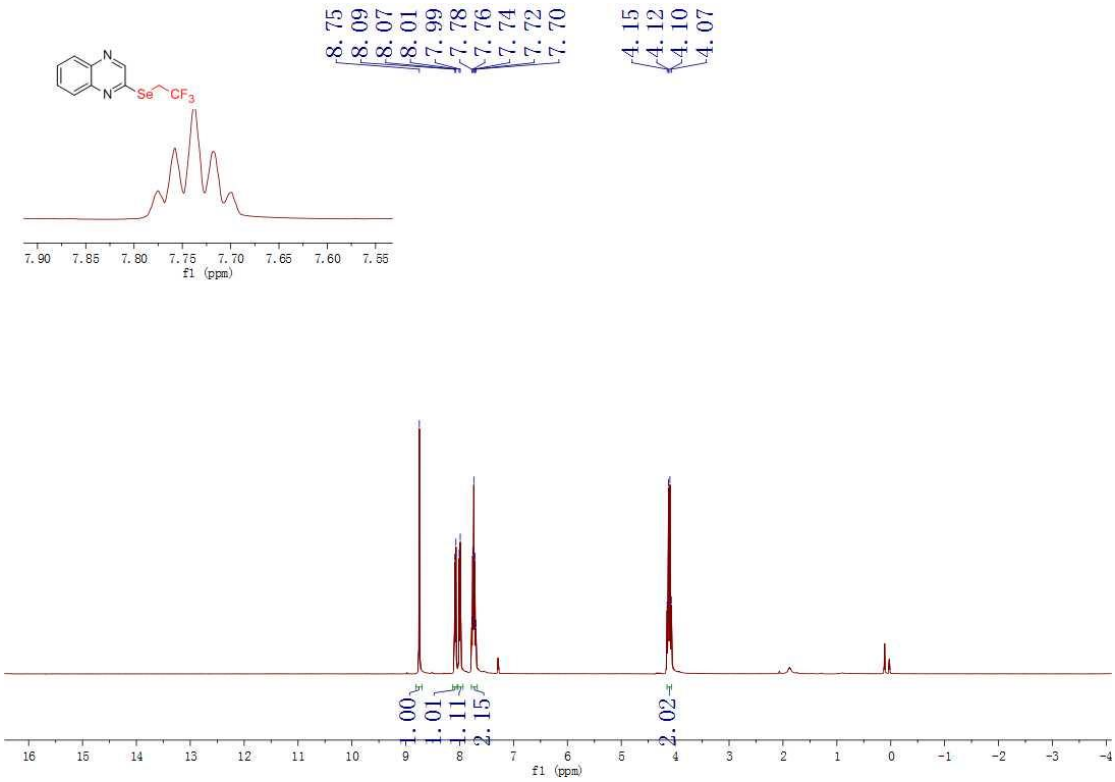
^{13}C NMR spectrum of **2o** in $CDCl_3$



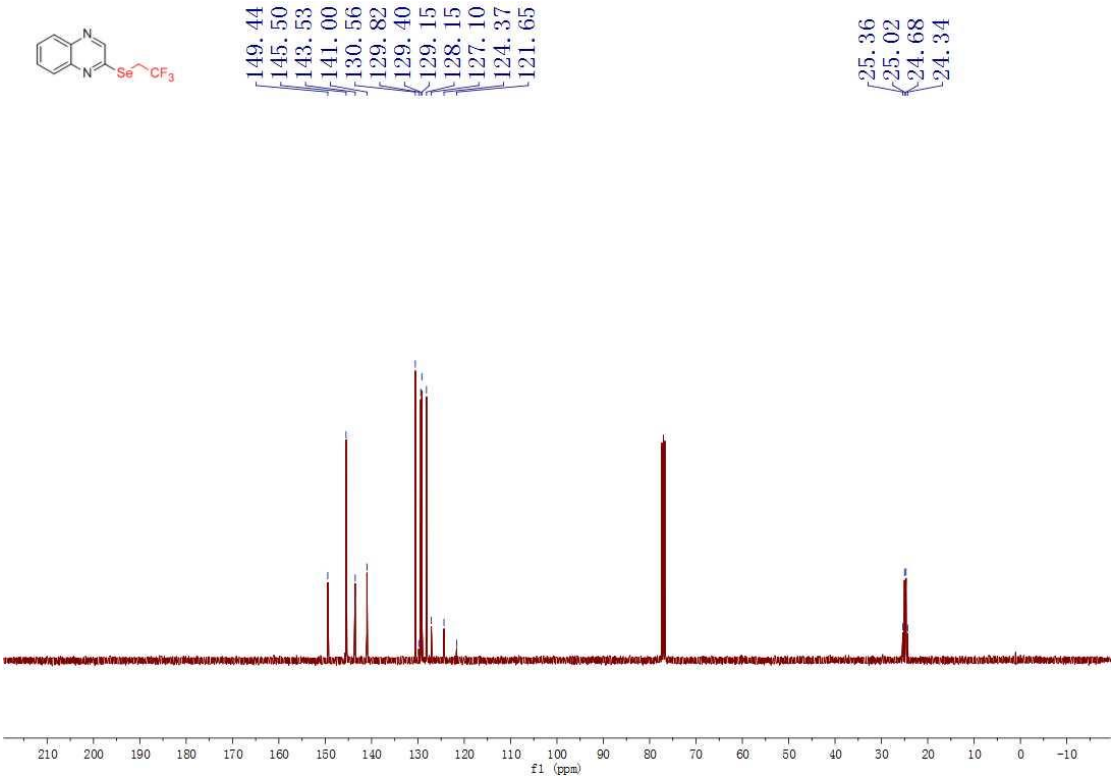
^{19}F NMR spectrum of **2o** in $CDCl_3$



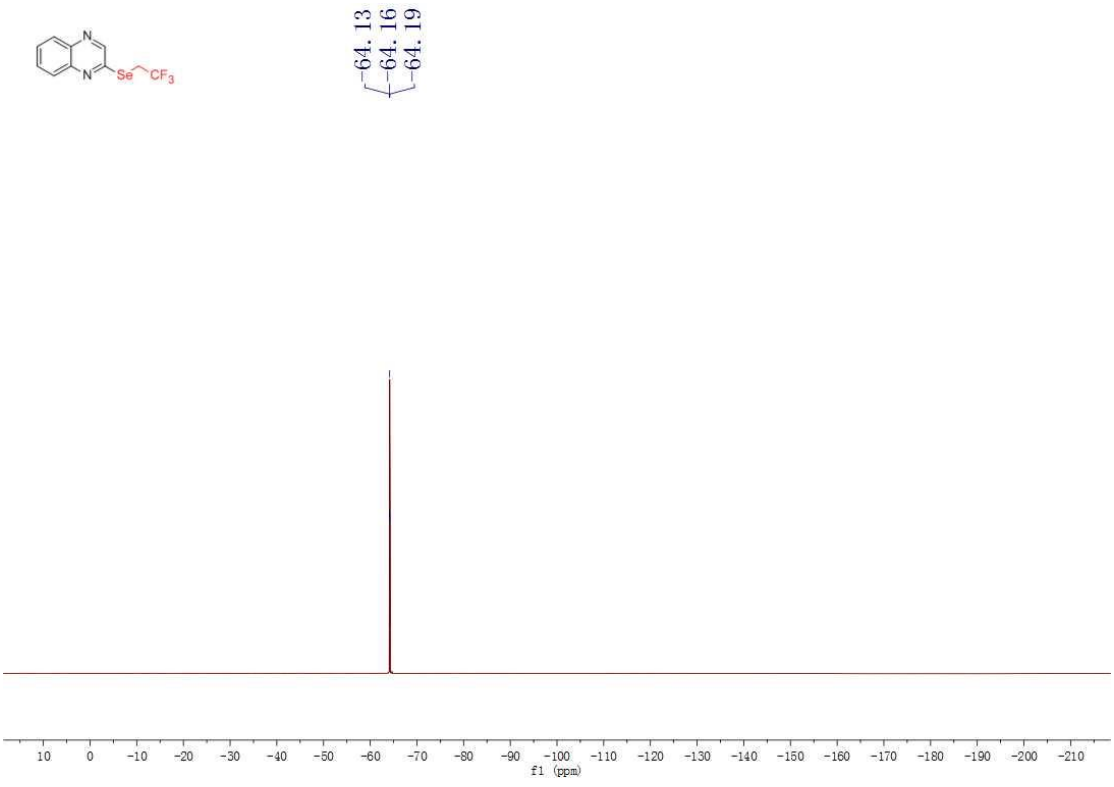
^{1}H NMR spectrum of **2p** in $CDCl_3$



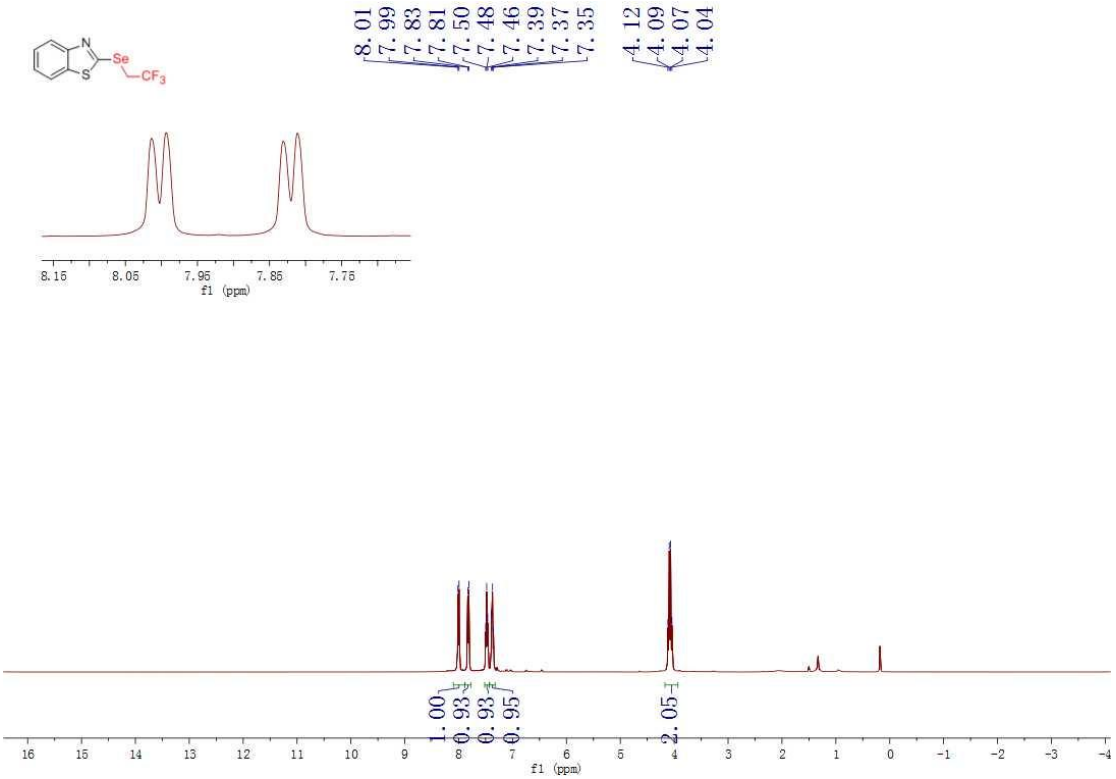
^{13}C NMR spectrum of **2p** in $CDCl_3$



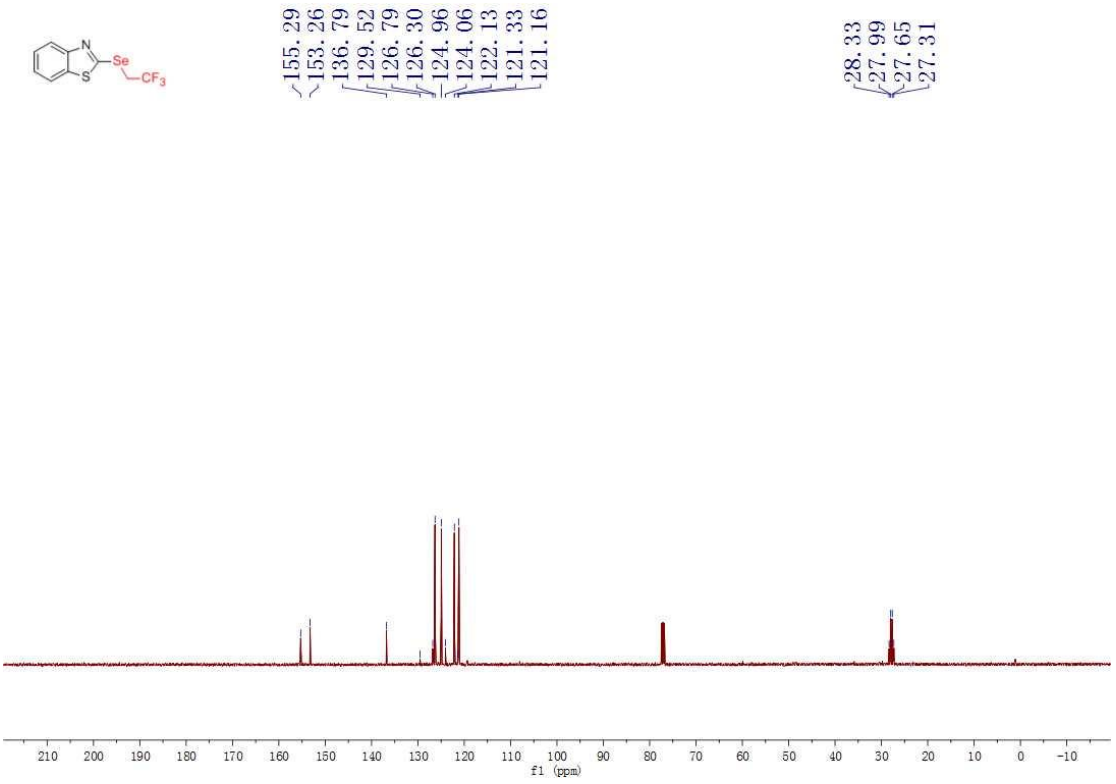
^{19}F NMR spectrum of **2p** in $CDCl_3$



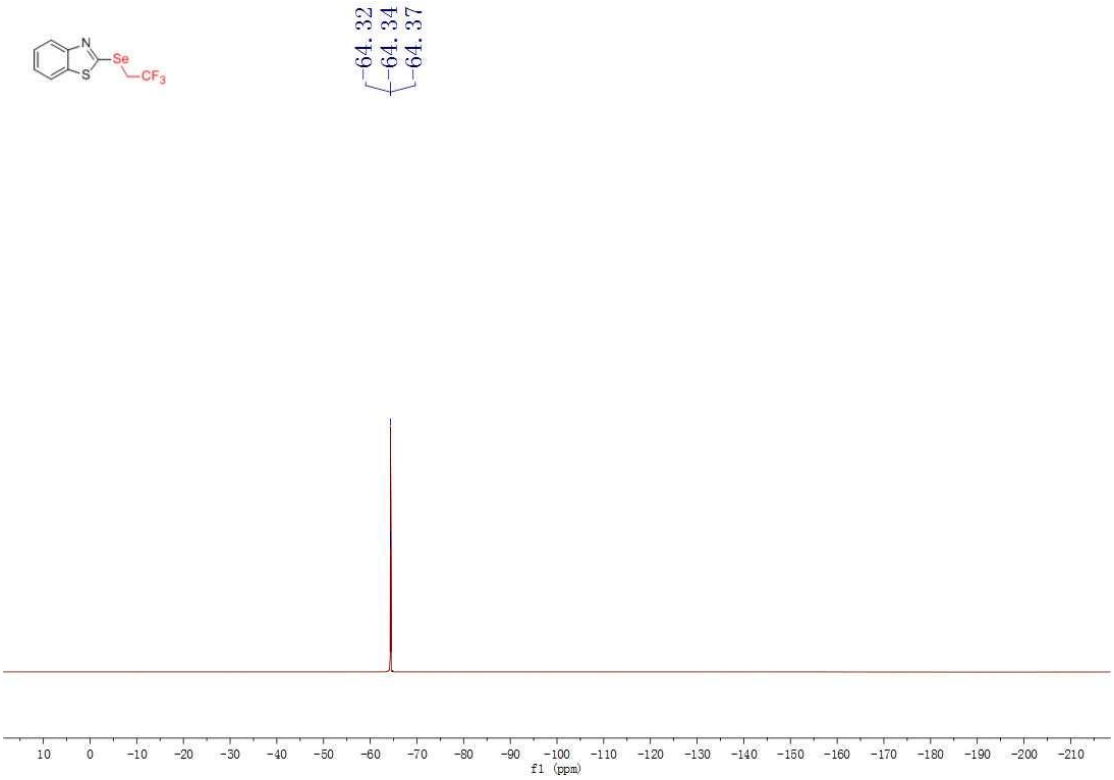
^{1}H NMR spectrum of **2q** in $CDCl_3$



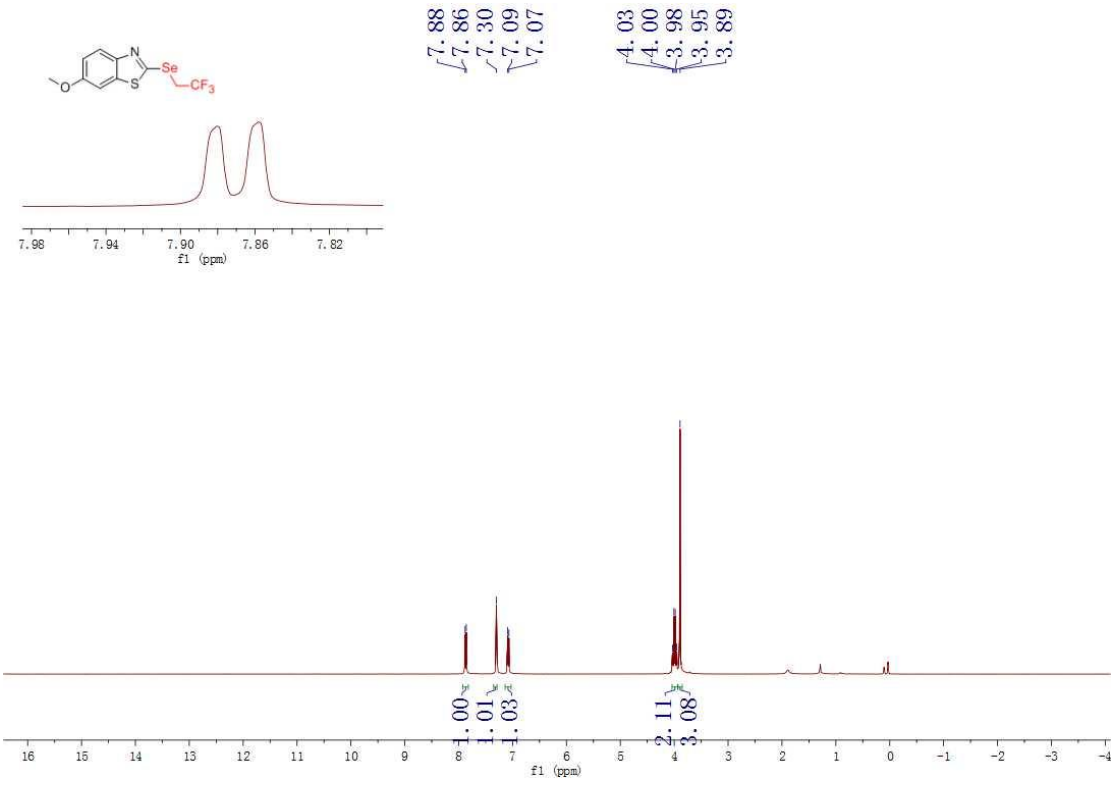
^{13}C NMR spectrum of **2q** in $CDCl_3$



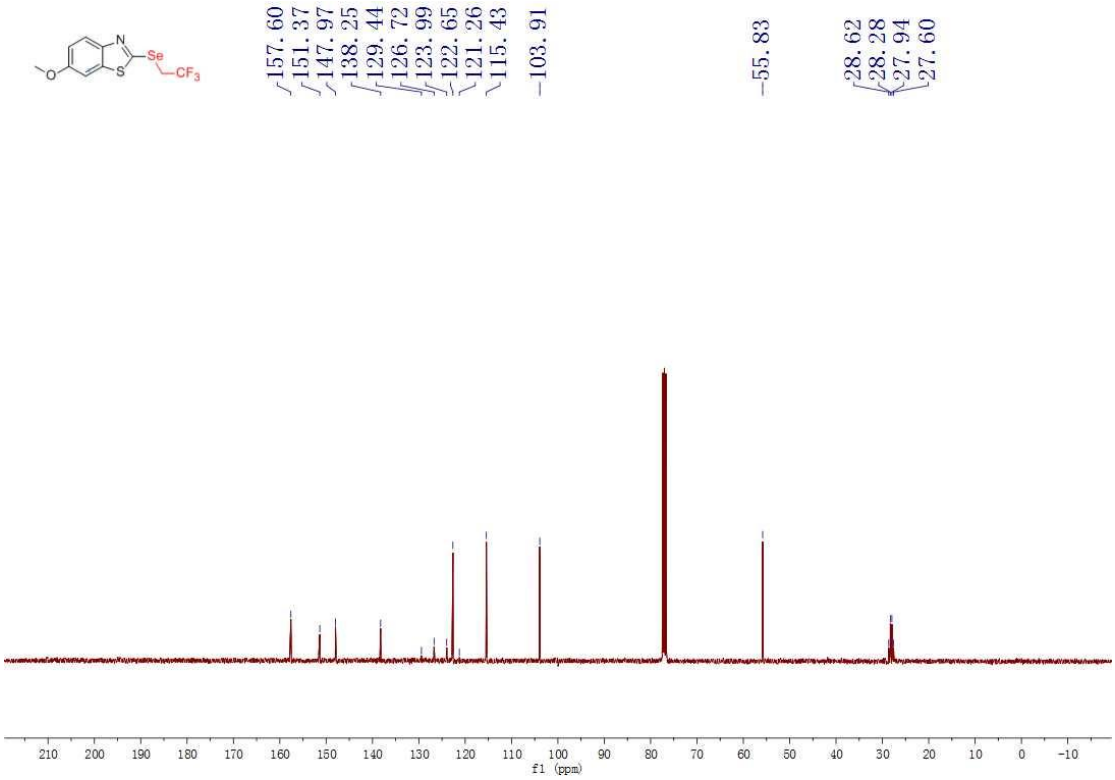
^{19}F NMR spectrum of **2q** in $CDCl_3$



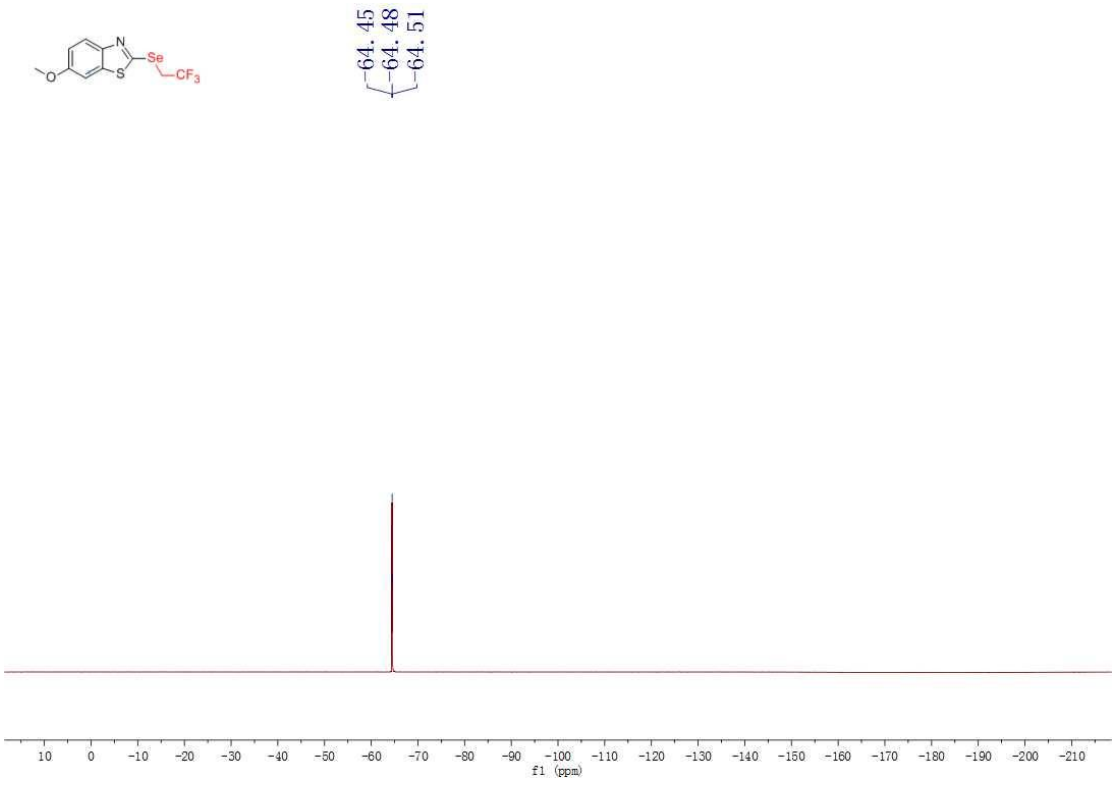
^{1}H NMR spectrum of **2r** in $CDCl_3$



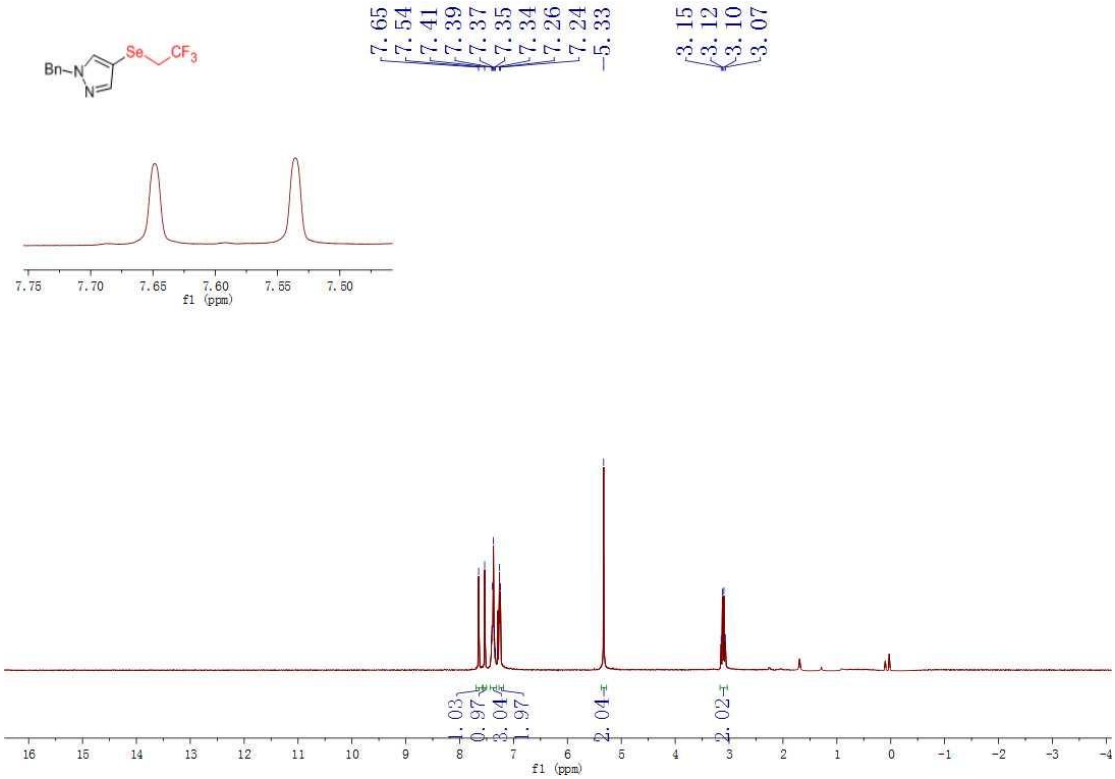
^{13}C NMR spectrum of **2r** in $CDCl_3$



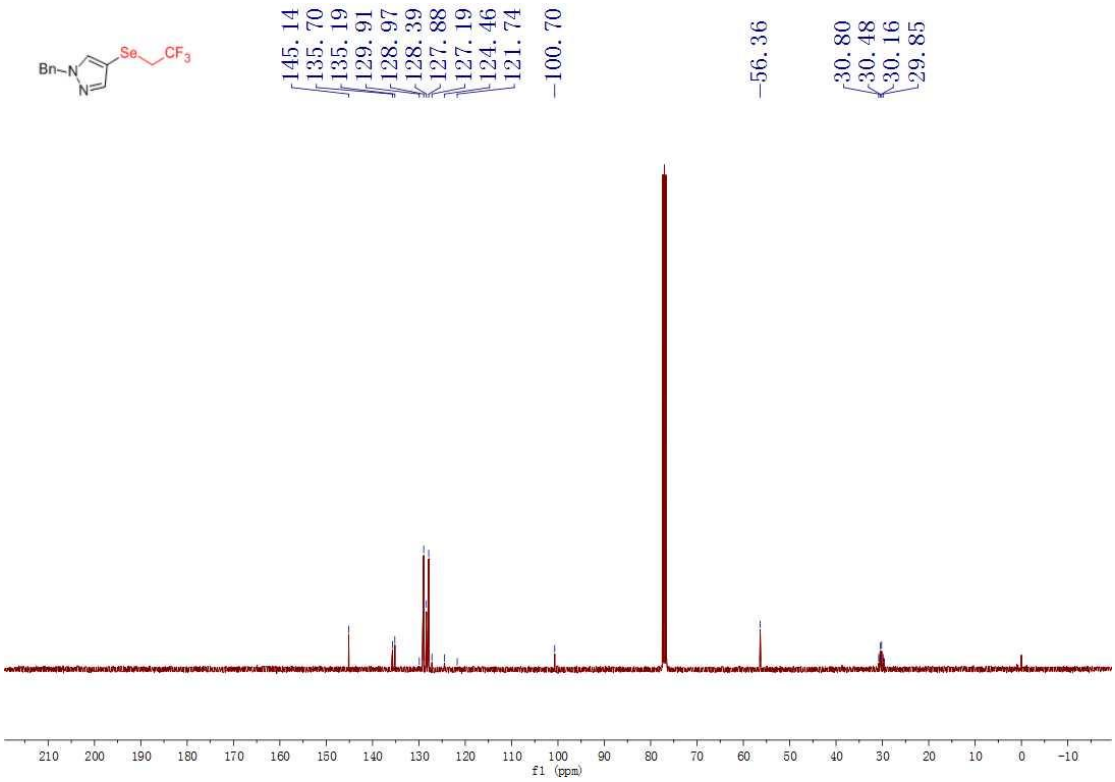
^{19}F NMR spectrum of **2r** in $CDCl_3$



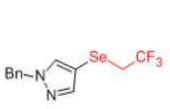
^{1}H NMR spectrum of **2s** in $CDCl_3$

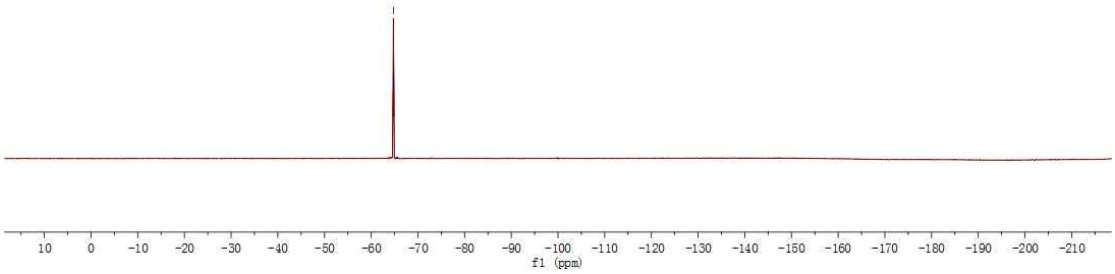


^{13}C NMR spectrum of **2s** in $CDCl_3$

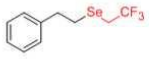


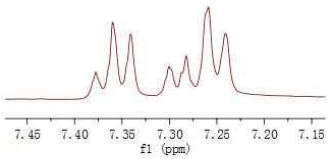
^{19}F NMR spectrum of **2s** in $CDCl_3$

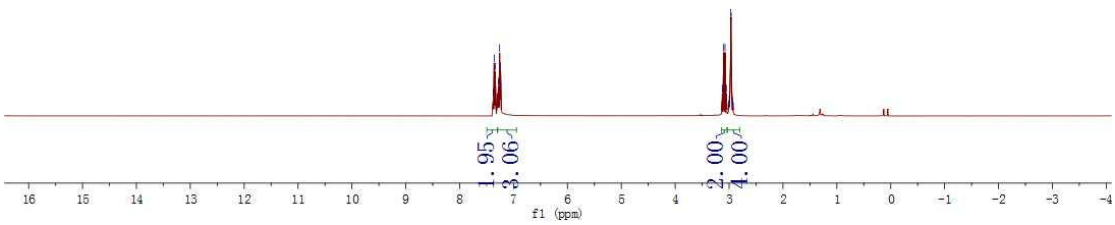




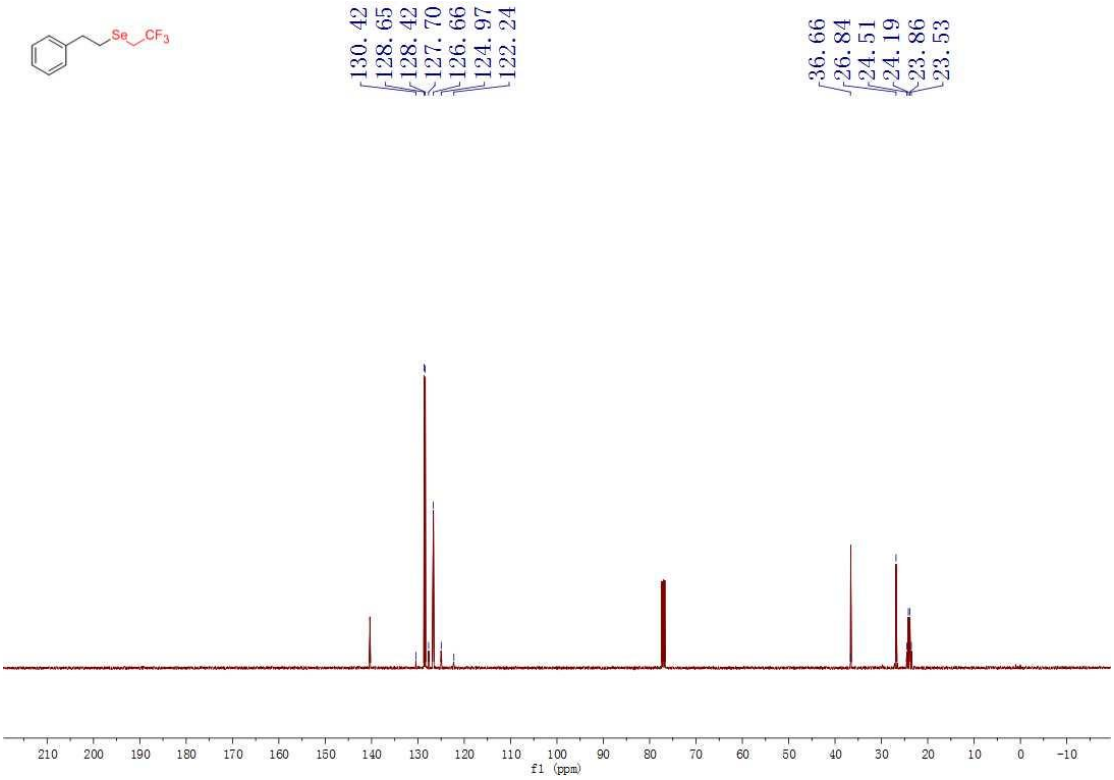
^{1}H NMR spectrum of **4a** in $CDCl_3$



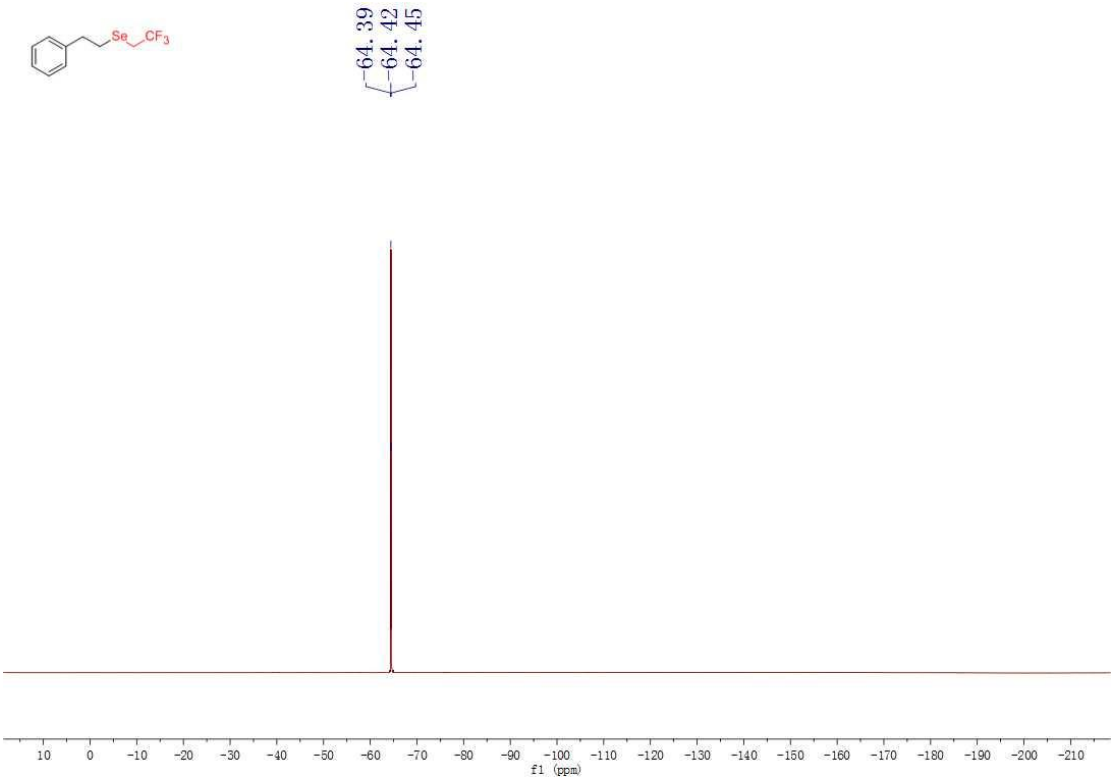




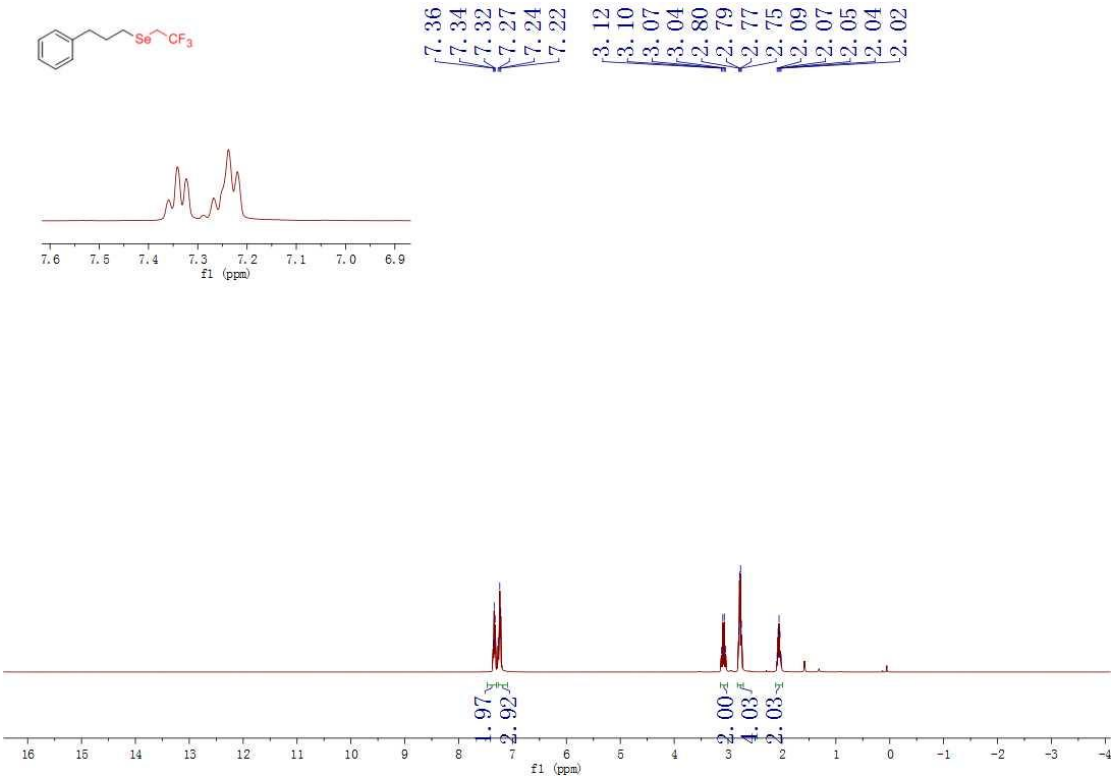
^{13}C NMR spectrum of **4a** in $CDCl_3$



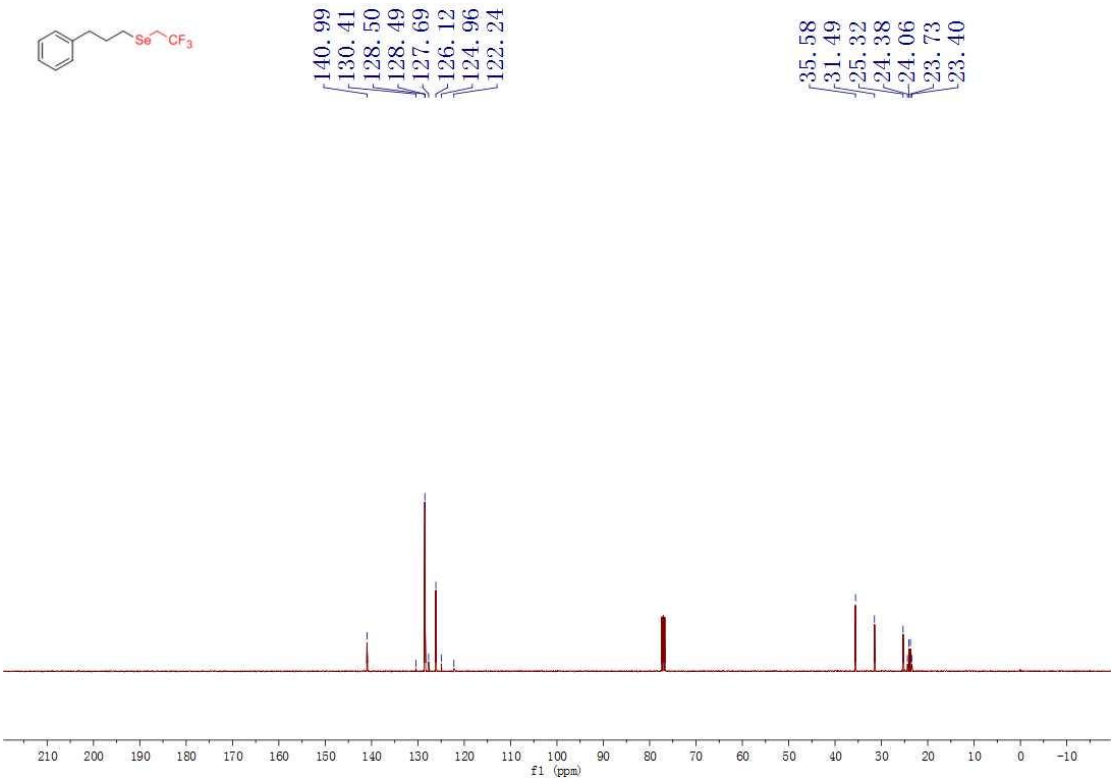
^{19}F NMR spectrum of **4a** in $CDCl_3$



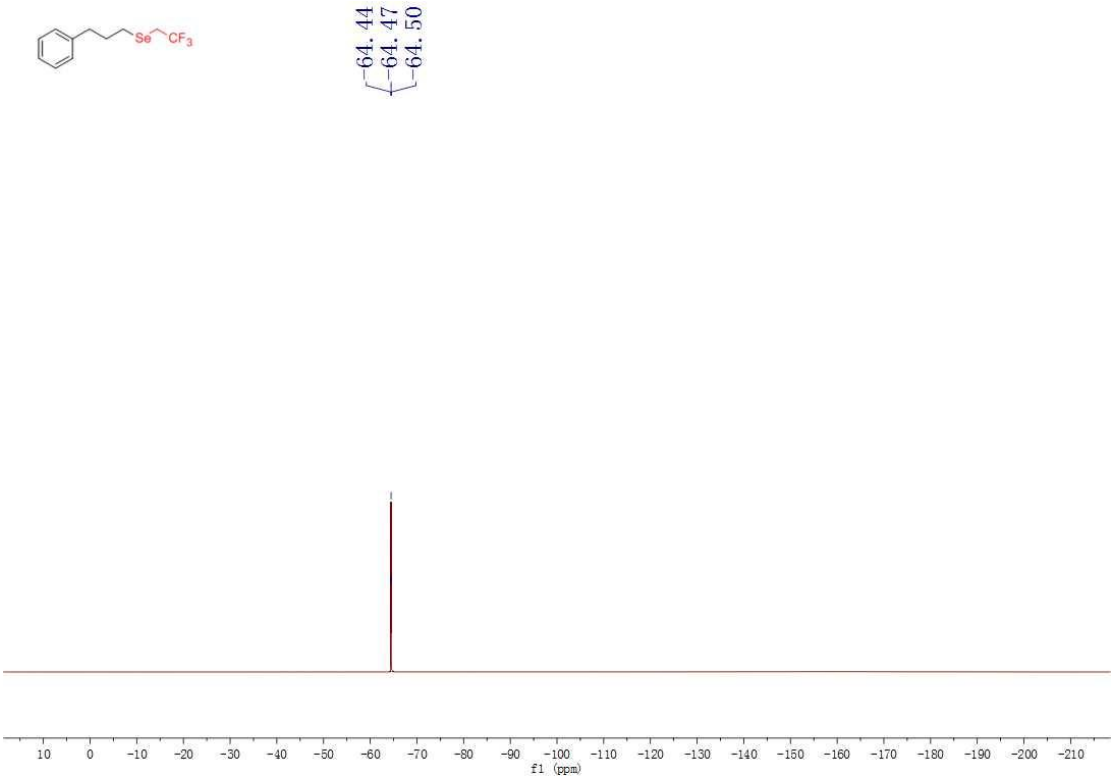
^{1}H NMR spectrum of **4b** in $CDCl_3$



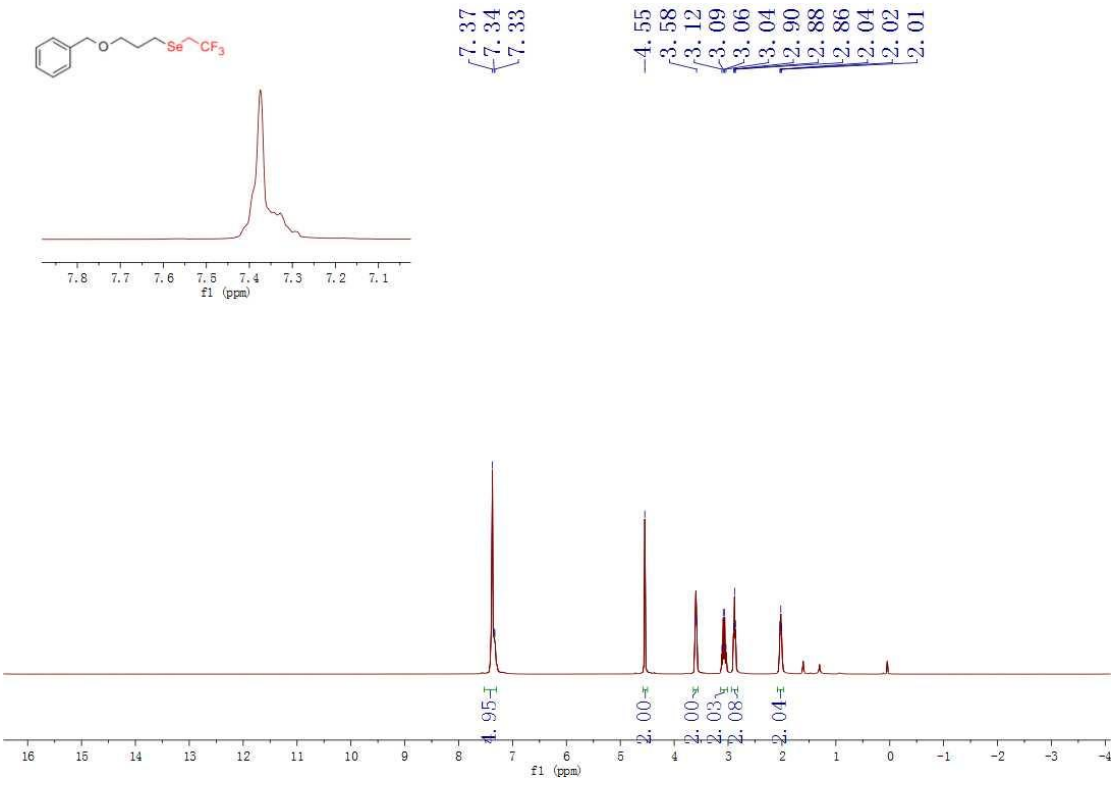
^{13}C NMR spectrum of **4b** in $CDCl_3$



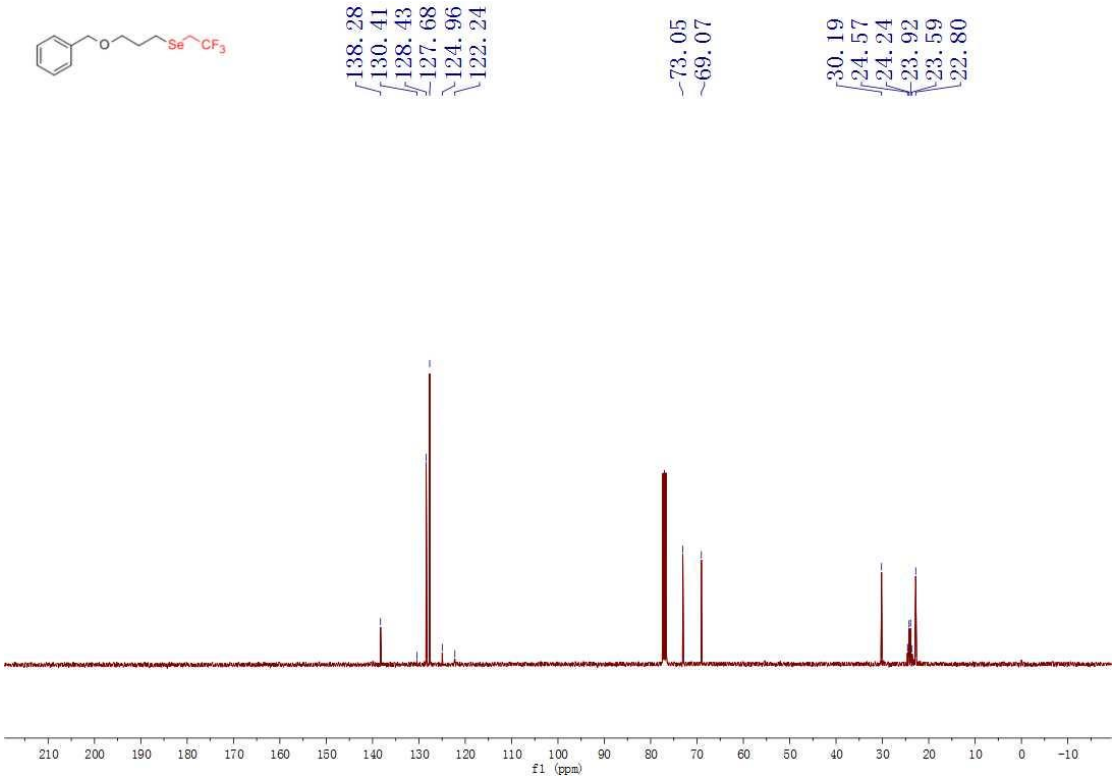
^{19}F NMR spectrum of **4b** in $CDCl_3$



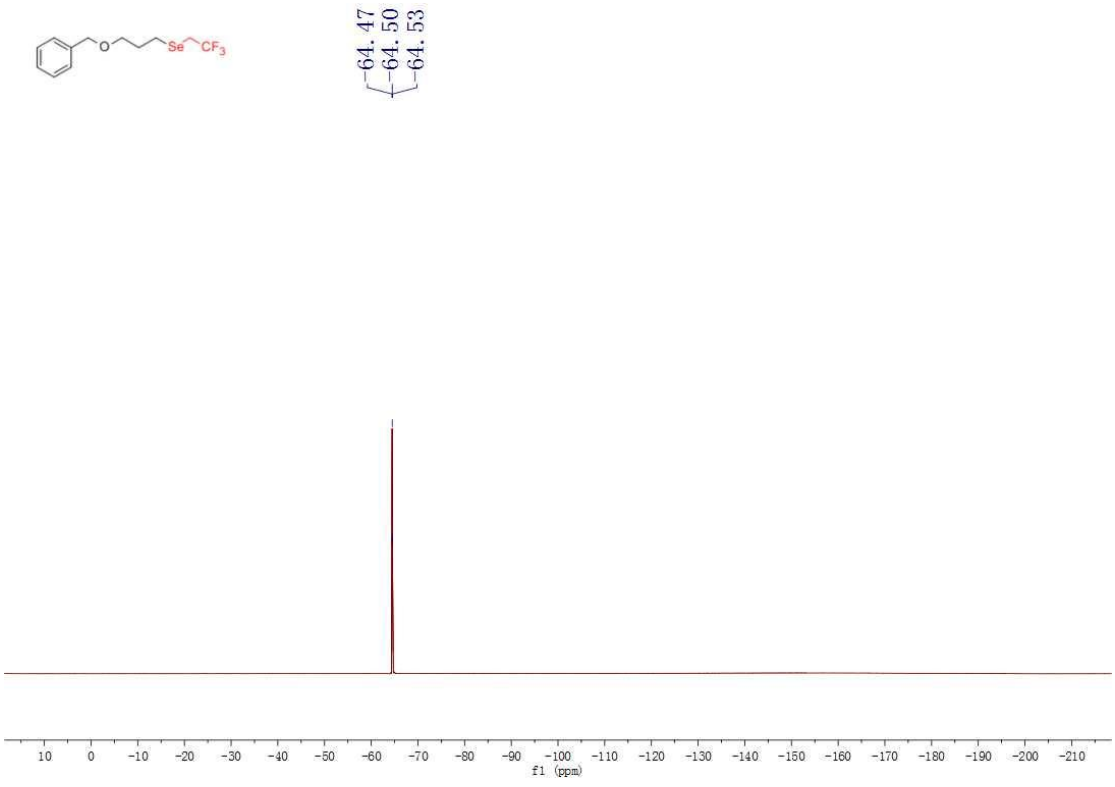
^{1}H NMR spectrum of **4c** in $CDCl_3$



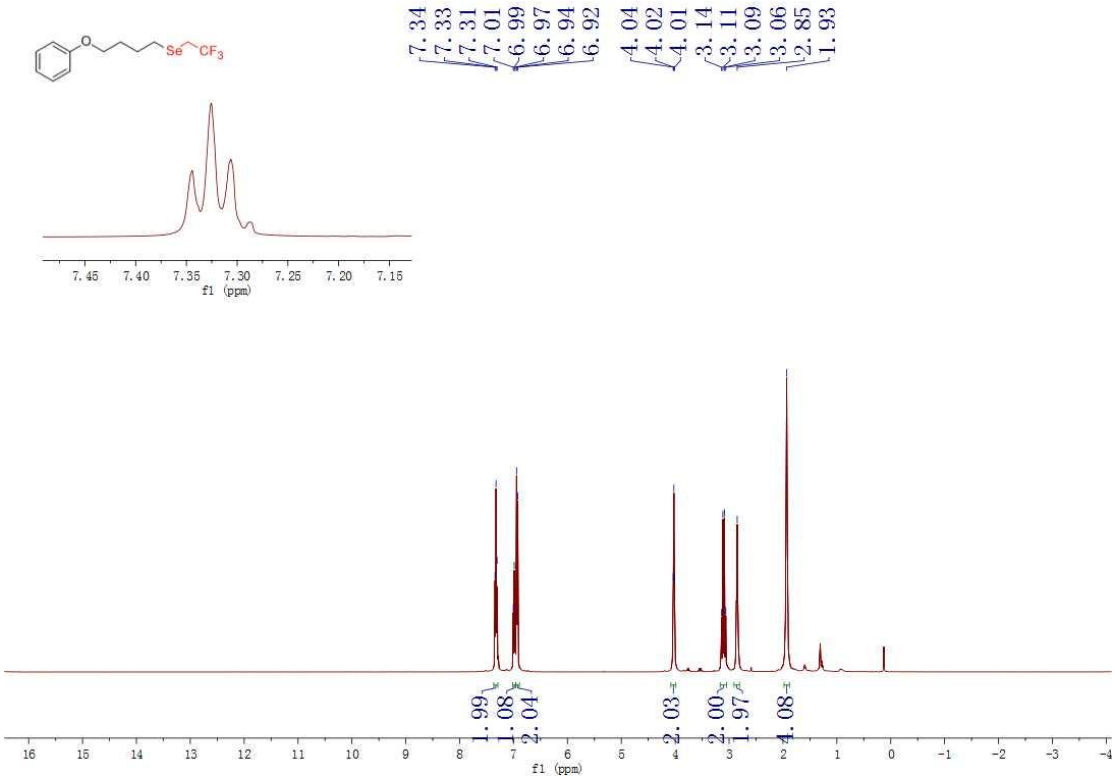
^{13}C NMR spectrum of **4c** in $CDCl_3$



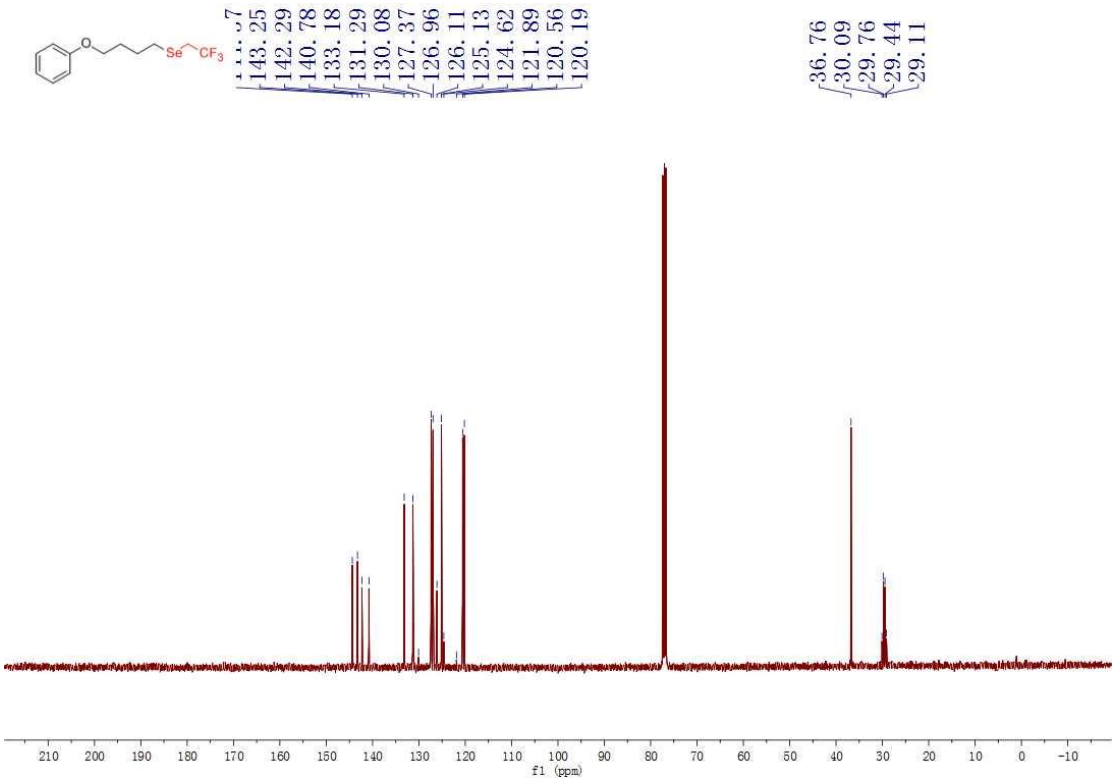
^{19}F NMR spectrum of **4c** in $CDCl_3$



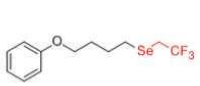
^{1}H NMR spectrum of **4d** in $CDCl_3$

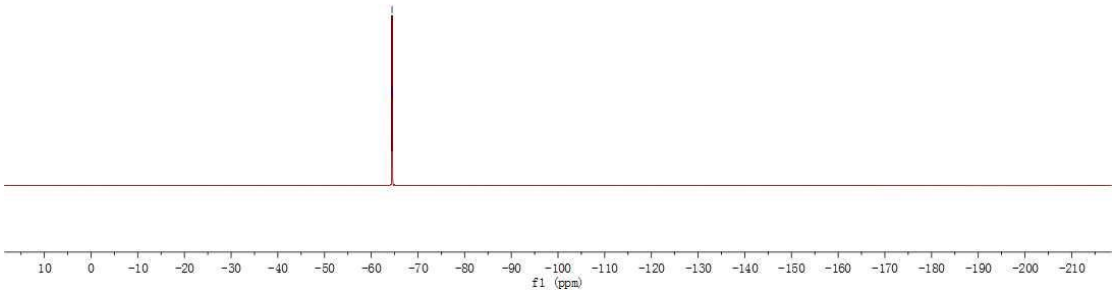


^{13}C NMR spectrum of **4d** in $CDCl_3$

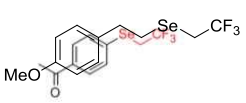


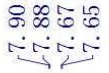
^{19}F NMR spectrum of **4d** in $CDCl_3$

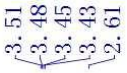


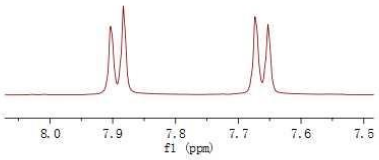


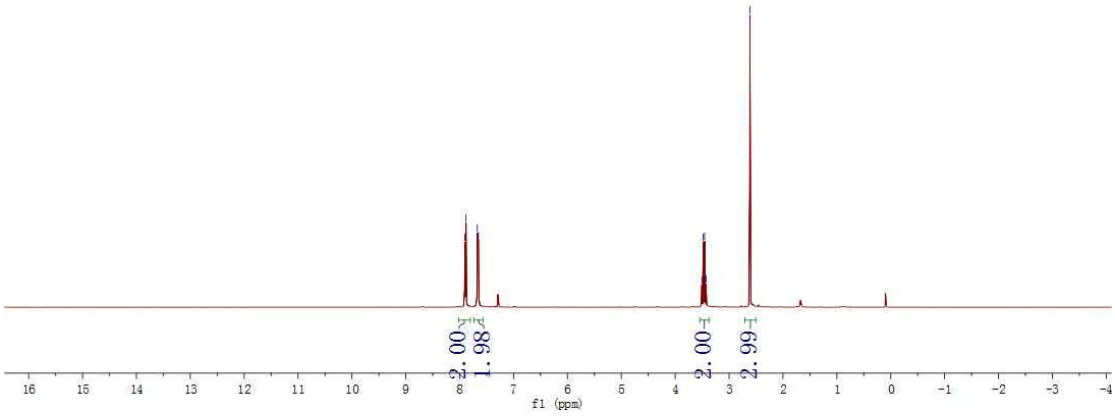
^{1}H NMR spectrum of **4e** in $CDCl_3$



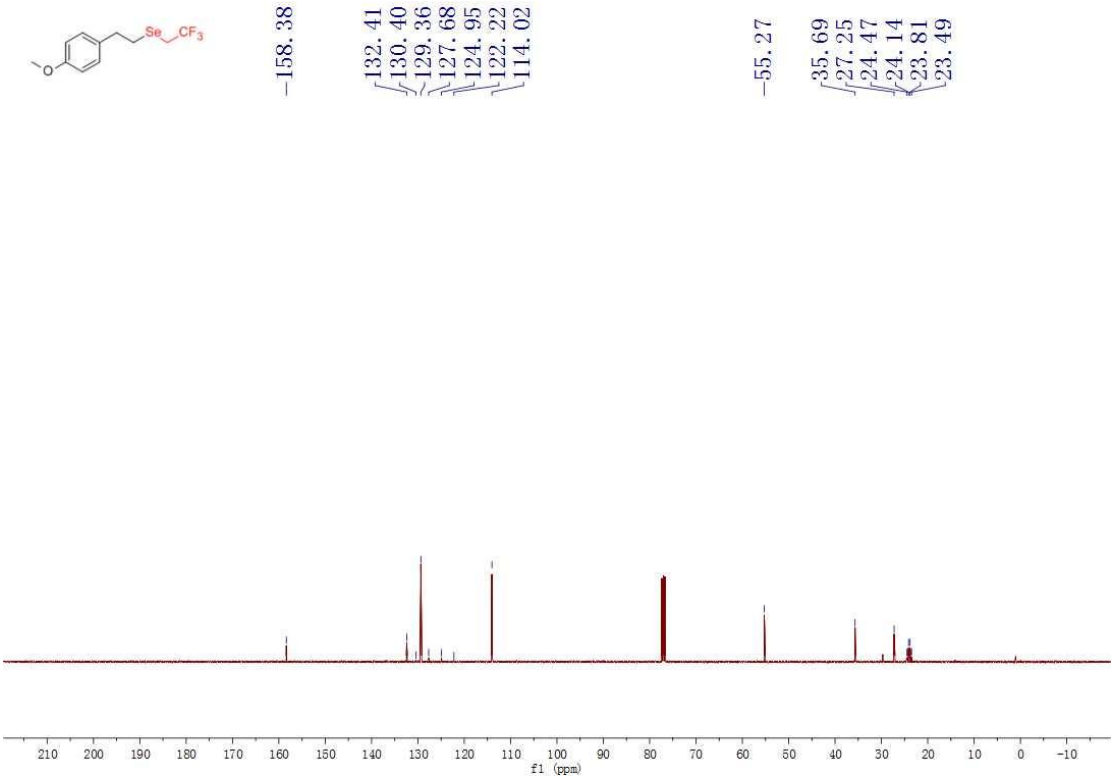




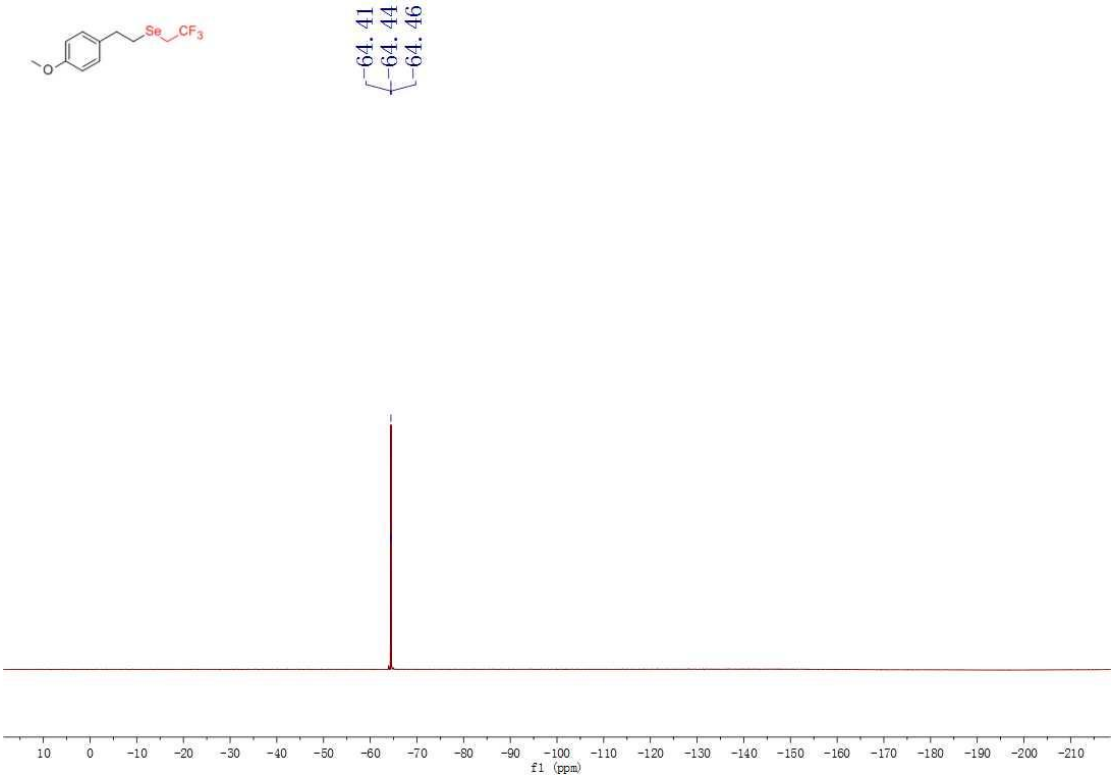




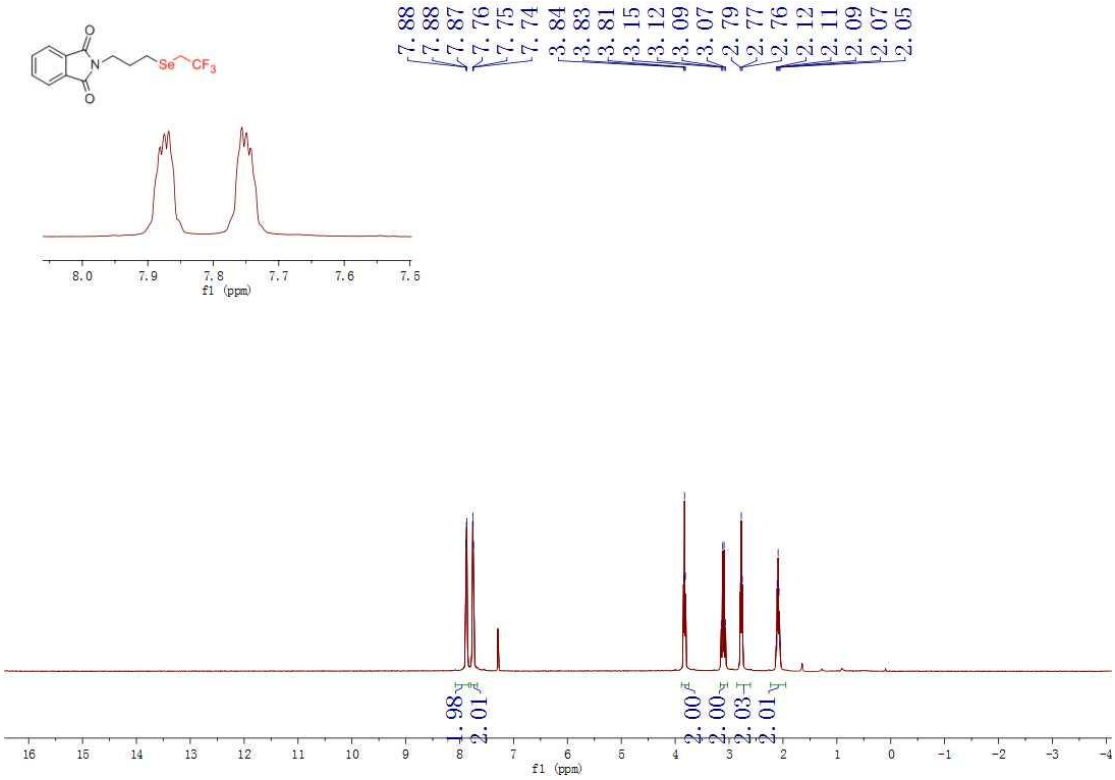
^{13}C NMR spectrum of **4e** in $CDCl_3$



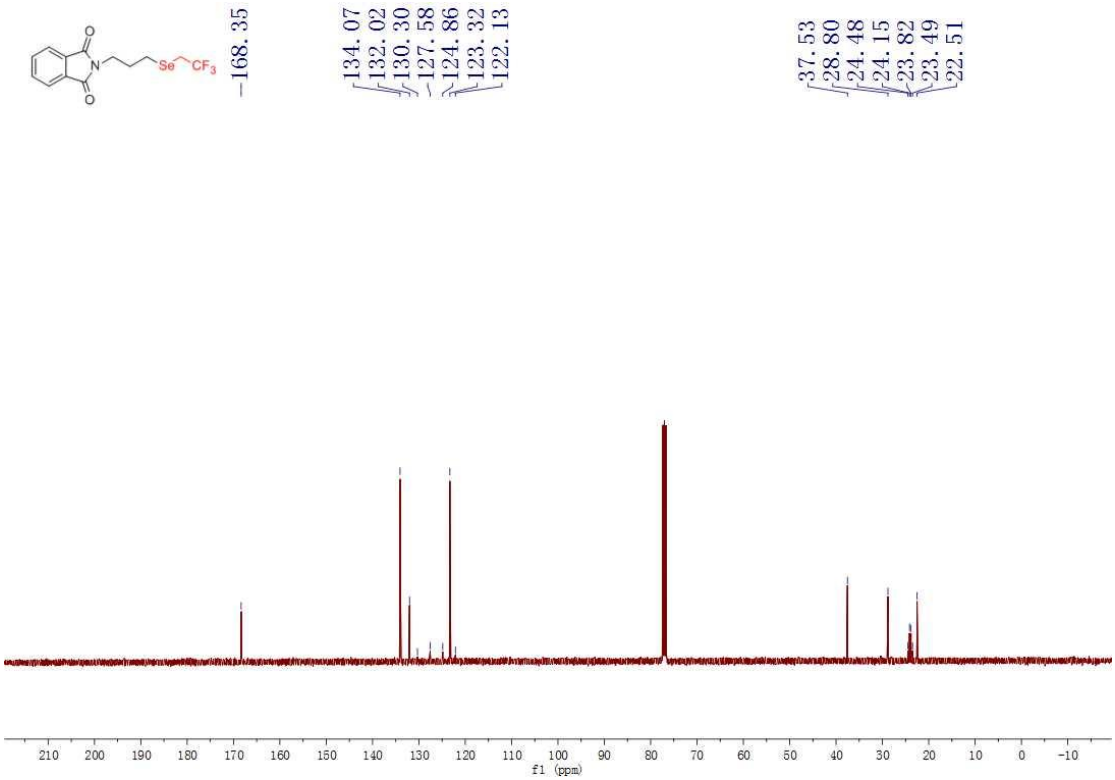
^{19}F NMR spectrum of **4e** in $CDCl_3$



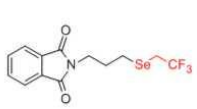
^{1}H NMR spectrum of **4f** in $CDCl_3$

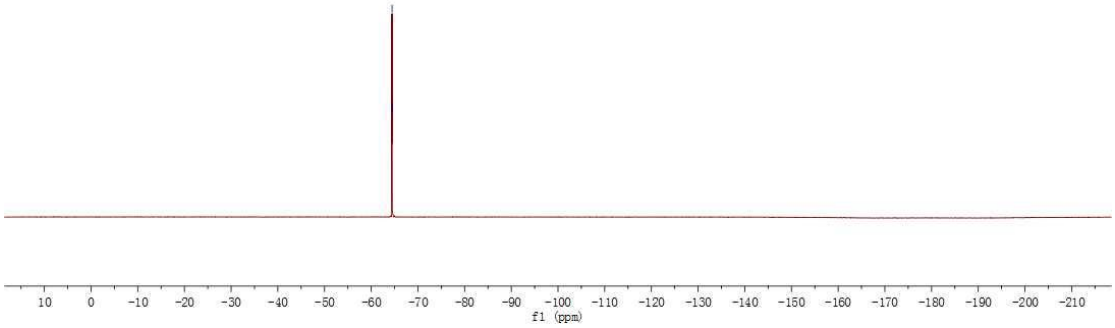


^{13}C NMR spectrum of **4f** in $CDCl_3$

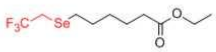


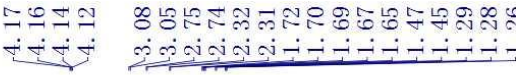
^{19}F NMR spectrum of **4f** in $CDCl_3$

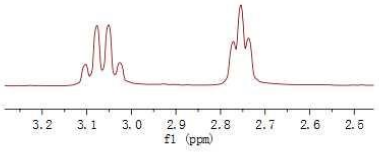


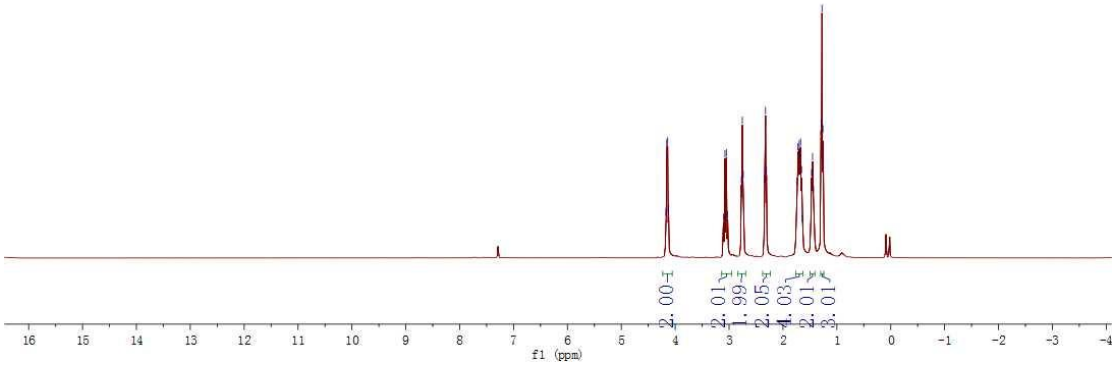


^{1}H NMR spectrum of **4g** in $CDCl_3$

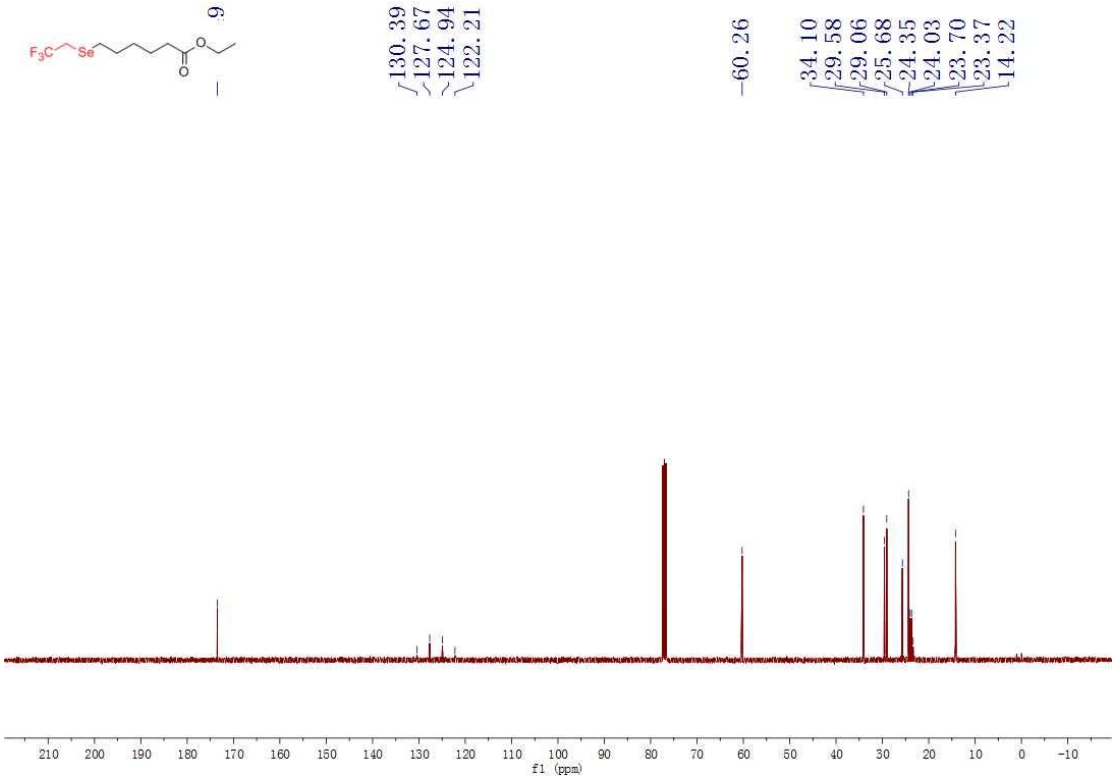




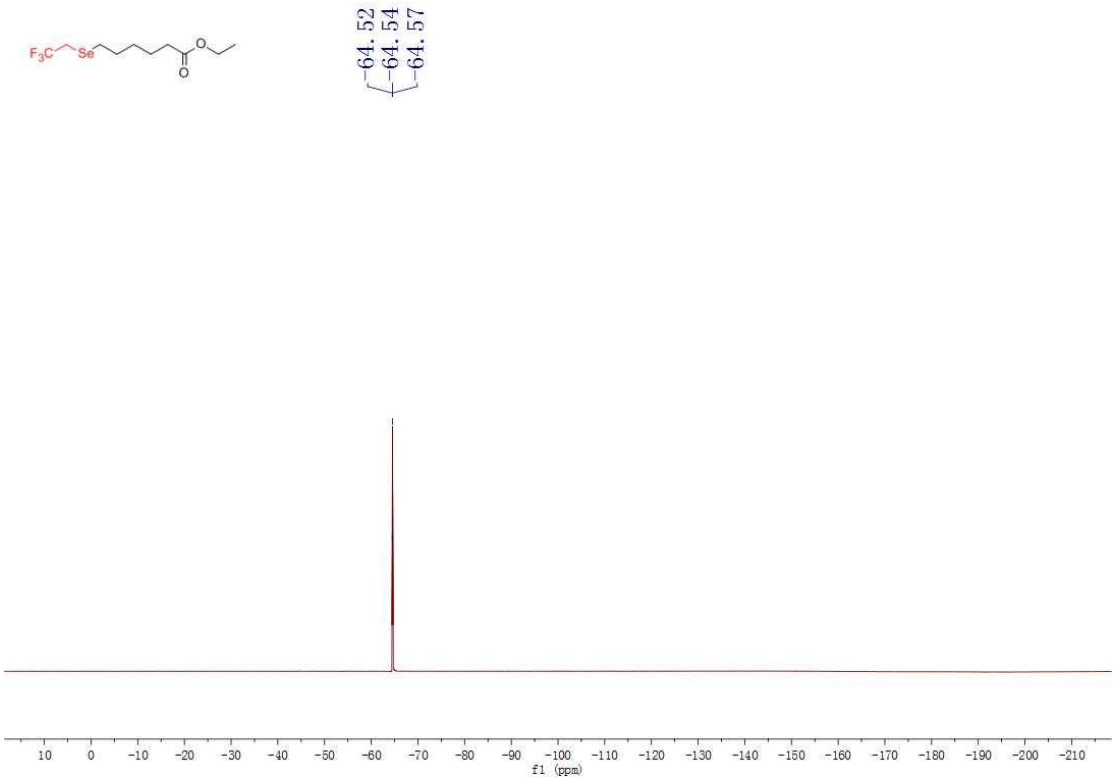




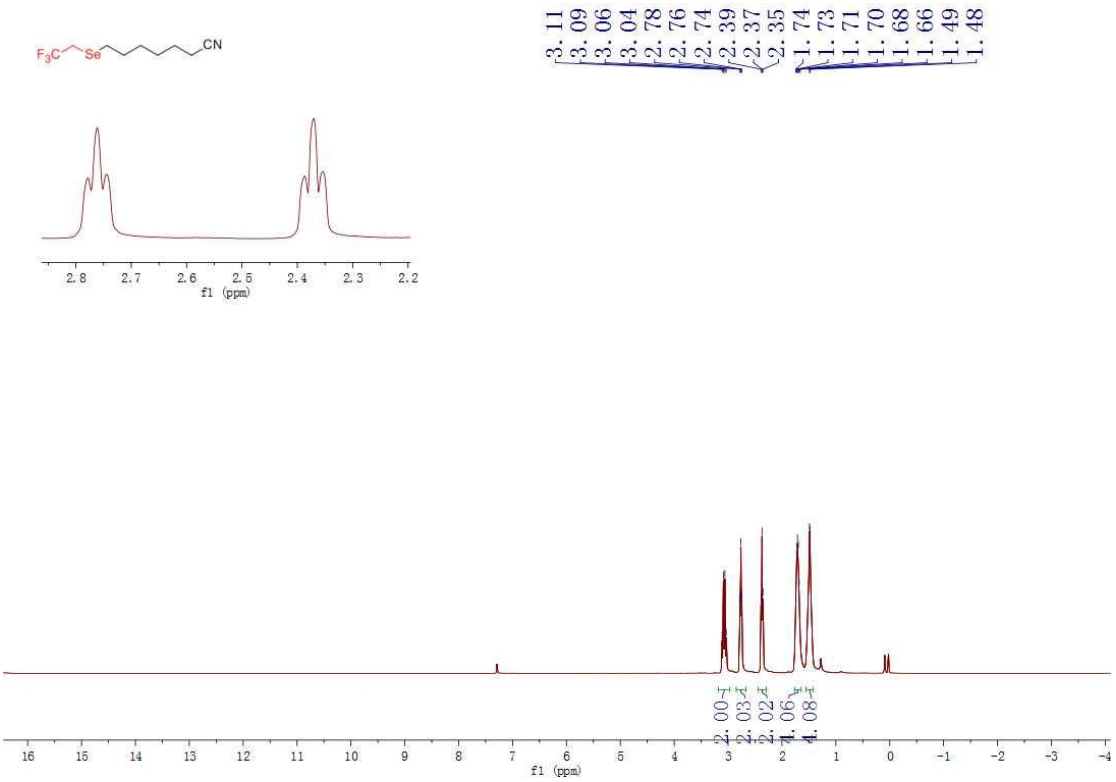
^{13}C NMR spectrum of **4g** in $CDCl_3$



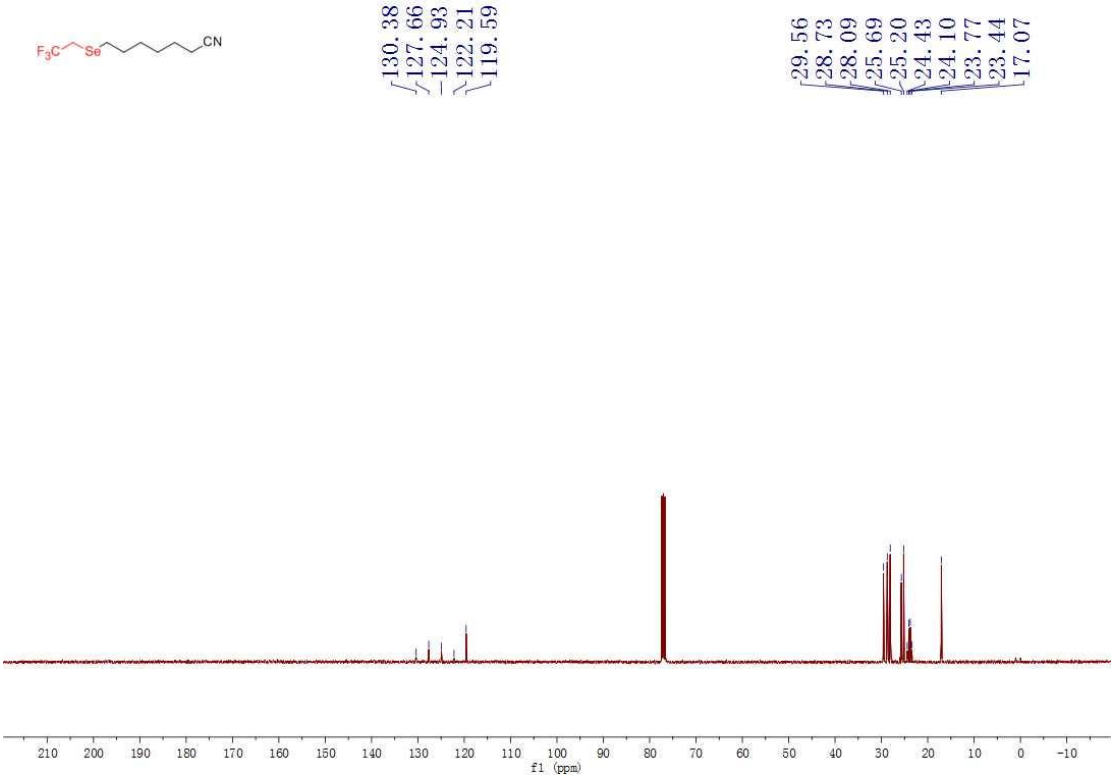
^{19}F NMR spectrum of **4g** in $CDCl_3$



^{1}H NMR spectrum of **4h** in $CDCl_3$



^{13}C NMR spectrum of **4h** in $CDCl_3$



^{19}F NMR spectrum of **4h** in $CDCl_3$