Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.
This journal is © the Partner Organisations 2024

Supporting information

Ni-catalyzed cross coupling of heteroaryl sulfone and diselenides *via* dehetroaromatization and hetroaromatization: Synthesis of heteroaryl selenides

Xin-Yu Liu,[a] Yu-Xin Dou,[a] Muhammad Hasan,[a] Daopeng Shen,[b] Weidong Rao,[c] Shusu Shen,[d] Shun-Yi Wang[a,*]

[a]Key Laboratory of Organic Synthesis of Jiangsu Province, College of Chemistry, Chemical Engineering and Materials Science & Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou, 215123, China.

[b]State Key Laboratory of Radiation Medicine and Protection, School for Radiological and Interdisciplinary Sciences (RAD-X) and Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Education Institutions, Soochow University, Suzhou, Jiangsu 215123, China

[c]Key Laboratory of Biomass-based Green Fuels and Chemicals, College of Chemical Engineering, Nanjing Forestry University, Nanjing 210037, China

[d]School of Environmental Science and Engineering, Suzhou University of Science and Technology, No.99 Xuefu Road, Huqiu District, Suzhou, 215009, PR China

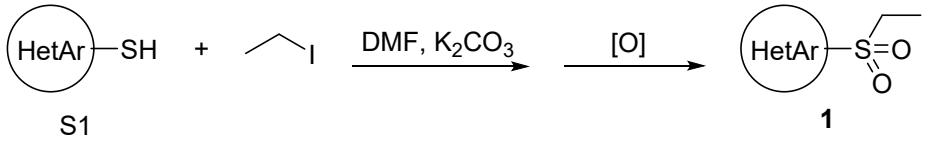
Contents

1.General Information

Unless otherwise noted, all commercially available compounds were used as provided without further purification.All the solvents for routine isolation of products and chromatography were reagent grade. Analytical thin-layer chromatography (TLC) was performed on silica gel, irradiation with UV light. For column chromatography, 300-400 mesh silica gel was used. **^{1}H-NMR** and **^{13}C-NMR** spectra were recorded on a BRUKER 400 MHz spectrometer in $CDCl_3$. Chemical shifts (δ) were reported referenced to an internal tetramethylsilane standard or the $CDCl_3$ residual peak (δ 7.26) for **^{1}H NMR**. Chemical shifts of **^{13}C NMR** are reported relative to $CDCl_3$ (δ 77.16). Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), bs (broad singlet), d (doublet), t (triplet), m (multiplet); coupling constants (J) are in Hertz (Hz). Melting points were measured on an Electrothermal digital melting point apparatus and were uncorrected. IR spectra were recorded on a BRUKER VERTEX 70 spectrophotometer and are reported in terms of frequency of absorption (cm^{-1}). HRMS spectra were obtained by using GCT Premier TOF-MS with CI source or BRUKER microTOF-Q III instrument with ESI source.

2. General procedure for synthesis of products

2.1 General procedure for synthesis of 1

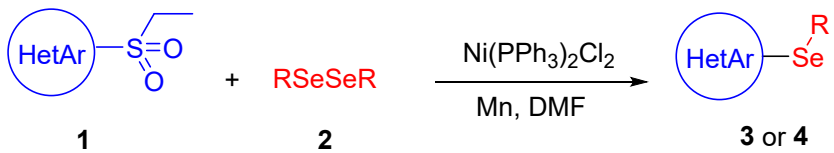


S1 **1**

According to literature reports,[1] to a 100 mL round-bottom flask was added compound S1 (5.0 mmol), ethyl iodide (7.5 mmol, 1.5 equiv), K_2CO_3 (1.0 g, 7.5 mmol, 1.5 equiv), and 30 mL DMF. The resulting solution was stirred at room temperature for 3 ~ 10 h, quenched with H_2O (50 mL), extracted with EA (50 mL × 3). The combined organic layer was washed with brine (30 mL × 3), dried over Na_2SO_4, and concentrated. The crude sulfide product was used in the next step without further purification. The sulfide was dissolved (5.0 mmol, 1 equiv) in EtOH (30 mL), $(NH_4)_6Mo_7O_{24}{\cdot}4H_2O$ (0.5 mmol, 0.1 equiv), and 30% H_2O_2(15.0 mmol) was added at 0 ºC. The resulting mixture was stirred at room temperature for 8 ~16 h. quenched with H_2O (50 mL), extracted with EA (50 mL × 3). The combined organic layer was washed with brine (30 mL × 3), dried over Na_2SO_4, and concentrated.The residue was purified by flash chromatography on a silica gel using petroleum ether and ethyl acetate (20/1~2/1, v/v) as the eluent to give substrate **1**.

2.2 General procedure for synthesis of 2[2]

2.3 General procedure for synthesis of 3 or 4



1 **2** **3** or **4**

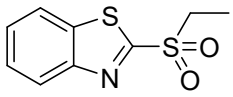
1 (0.3 mmol), **2** (0.1 mmol), $Ni(PPh_3)_2Cl_2$ (5 mmol %) and Mn(0.3 mmol, 0.0165g) were loaded in a

flask, which was subjected to evacuation/ flushing with N_2 for 3 times. DMF or MeOH (1 mL) was added to the mixture via syringe, which was stirred at rt for 12 hours. The mixture was quenched with H_2O. The aqueous layer was extracted with EtOAc. The organic layer was washed with brine, dried over Na_2SO_4, concentrated in vacuo, and purified by flash column chromatography on silica gel to give the corresponding products.

3. Reference

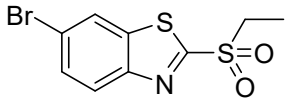
1. Cao, Y.; Wang, X.; Jiao, H.; Song,H.; Liu, X.; Wang, Q. *Green Chem*., **2022**, *24*, 4789-4793.
2. Yao, H.; LI, F.; Li, J.; Wang, S.; Ji, S. *Org. Biomol. Chem*., **2020**,*18*, 1987-1993.

4. Spectroscopic Data of Compounds



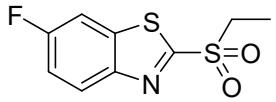
2-(ethylsulfonyl)benzo[*d*]thiazole (1a)

White solid. **Mp**:105.2-105.5 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.27 – 8.17 (m, 1H), 8.08 – 7.96 (m, 1H), 7.72 – 7.49 (m, 2H), 3.55 (q, J = 7.5 Hz, 2H), 1.45 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.3, 152.7, 136.8, 128.0, 127.6, 125.4, 122.3, 49.3, 7.2; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_9NO_2NaS_2$:249.9967, found:249.9961.



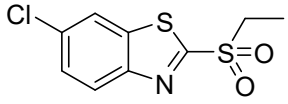
6-bromo-2-(ethylsulfonyl)benzo[*d*]thiazole (1b)

White solid. **Mp**:109.7-110.0 °C. **^{1}H NM**R (400 MHz, Chloroform-*d*) δ 8.18 (d, J = 1.9 Hz, 1H), 8.07 (d, J = 8.8 Hz, 1H), 7.75 (dd, J = 8.8, 1.9 Hz, 1H), 3.55 (q, J = 7.4 Hz, 2H), 1.45 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.9, 151.5, 138.2, 131.5, 126.5, 124.9, 122.2, 49.3, 7.1; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_8BrNO_2NaS_2$:327.9072, found:327.9054.



2-(ethylsulfonyl)-6-fluorobenzo[*d*]thiazole (1c)

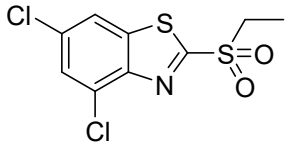
White solid. **Mp**:111.2-111.5 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.19 (dd, J = 9.1, 4.8 Hz, 1H), 7.70 (dd, J = 7.8, 2.6 Hz, 1H), 7.39 (td, J = 8.9, 2.5 Hz, 1H), 3.54 (q, J = 7.4 Hz, 2H), 1.45 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.0, 162.2 (d, J = 250 Hz), 149.4, 138.0 (d, J = 12 Hz), 126.9 (d, J = 10 Hz), 117.1 (d, J = 26 Hz), 108.3 (d, J = 27 Hz), 49.4, 7.1; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -110.12; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_8FNO_2NaS_2$:267.9873, found:267.9876.



6-chloro-2-(ethylsulfonyl)benzo[*d*]thiazole (1d)

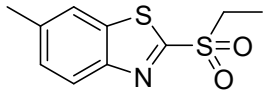
White solid. **Mp**:92.7-93.0 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.13 (d, J = 8.8 Hz, 1H), 8.01 (d, J = 2.0 Hz, 1H), 7.61 (dd, J = 8.8, 2.1 Hz, 1H), 3.55 (q, J = 7.4 Hz, 2H), 1.45 (t, J = 7.4 Hz, 3H); **^{13}C**

NMR (100 MHz, Chloroform-*d*) δ 165.9, 151.2, 137.8, 134.4, 128.8, 126.2, 121.9, 49.3, 7.1; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_{10}ClNO_2NaS_2$:283.9577, found:283.9568.



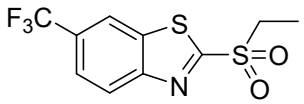
4,6-dichloro-2-(ethylsulfonyl)benzo[d]thiazole (1e)

White solid. **Mp**:122.5-122.7 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 1.9 Hz, 1H), 7.66 (d, J = 1.9 Hz, 1H), 3.61 (q, J = 7.4 Hz, 2H), 1.48 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 166.8, 148.7, 138.6, 134.4, 131.0, 128.6, 120.5, 49.1, 7.0; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_7Cl_2NO_2NaS_2$:317.9187, found:317.9182.



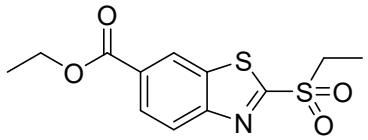
2-(ethylsulfonyl)-6-methylbenzo[*d*]thiazole (1f)

White solid. **Mp**:122.5-122.7 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (d, J = 8.5 Hz, 1H), 7.80 (dt, J = 1.7, 0.8 Hz, 1H), 7.45 (dd, J = 8.4, 1.7 Hz, 1H), 3.53 (q, J = 7.4 Hz, 2H), 2.55 (s, 3H), 1.44 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 164.0, 150.9, 138.8, 137.1, 129.5, 124.9, 121.8, 49.4, 21.8, 7.2; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{12}NO_2S_2$:242.0304, found:242.0302.



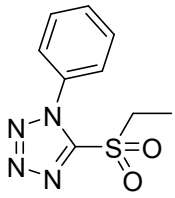
2-(ethylsulfonyl)-6-(trifluoromethyl)benzo[*d*]thiazole (1g)

Yollow solid. **Mp**:115.3-115.6 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.40 – 8.23 (m, 2H), 7.92 – 7.81 (m, 1H), 3.59 (q, J = 7.4 Hz, 2H), 1.47 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 168.7, 154.5, 136.7, 130.2 (q, J = 33 Hz), 126.1, 124.6 (q, J = 3 Hz), 123.6 (q, J = 271 Hz), 120.3 (q, J = 3 Hz), 49.3, 7.1; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -61.86; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_8F_3NO_2NaS_2$:317.9841, found:317.9836.



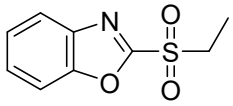
ethyl 2-(ethylsulfonyl)benzo[*d*]thiazole-6-carboxylate (1h)

White solid. **Mp**:84.2-84.5 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.75 (dd, J = 1.6, 0.7 Hz, 1H), 8.40 – 8.12 (m, 2H), 4.46 (q, J = 7.1 Hz, 2H), 3.58 (q, J = 7.5 Hz, 2H), 1.46 (q, J = 7.3 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 168.6, 165.3, 155.2, 136.6, 130.0, 128.5, 125.2, 124.6, 61.8, 49.2, 14.3, 7.1; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{12}H_{13}NO_4NaS_2$:322.0178, found:322.0170.



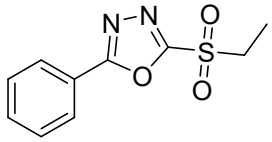
5-(ethylsulfonyl)-1-phenyl-1*H*-tetrazole (1i)

White solid. **Mp**:42.2-42.5-84.5 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.73 – 7.67 (m, 2H), 7.65 – 7.56 (m, 3H), 3.77 (q, J = 7.4 Hz, 2H), 1.55 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 168.6, 165.3, 155.2, 136.6, 130.0, 128.5, 125.2, 124.6, 61.8, 49.2, 14.3, 7.1; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_{10}N_4O_2NaS$:261.0417, found:261.0413.



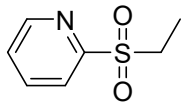
2-(ethylsulfonyl)benzo[d]oxazole (1j)

Yollow solid. **Mp**:54.5-54.7 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.95 – 7.83 (m, 1H), 7.73 – 7.63 (m, 1H), 7.60 – 7.54 (m, 1H), 7.53 – 7.47 (m, 1H), 3.59 (q, J = 7.5 Hz, 2H), 1.49 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 157.9, 150.9, 139.4, 128.6, 126.3, 122.1, 111.9, 49.4, 6.8; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_{10}NO_3S$:212.0376, found:212.0365.



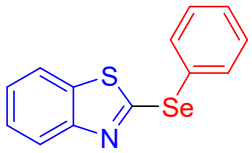
2-(ethylsulfonyl)-5-phenyl-1,3,4-oxadiazole (1k)

White solid. **Mp**:58.2-58.4 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 – 8.03 (m, 2H), 7.60 – 7.53 (m, 1H), 7.52 – 7.45 (m, 2H), 3.55 (q, J = 7.4 Hz, 2H), 1.48 (t, J = 7.4 Hz, 3H);**^{13}C NMR** (100 MHz, Chloroform-*d*) δ 166.7, 161.3, 133.3, 129.4, 127.7, 122.1, 50.1, 6.8; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{10}N_2O_3NaS$:261.0304, found:261.0301.



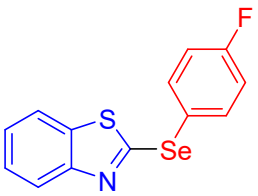
2-(ethylsulfonyl)pyridine (1m)

Colorless liquid. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.78 (ddd, J = 4.7, 1.7, 0.9 Hz, 1H), 8.11 (dt, J = 7.9, 1.1 Hz, 1H), 8.05 (td, J = 7.7, 1.7 Hz, 1H), 7.64 (ddd, J = 7.5, 4.7, 1.3 Hz, 1H), 3.44 (q, J = 7.5 Hz, 2H), 1.30 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 156.3, 150.3, 138.4, 127.6, 122.3, 46.4, 6.8; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_7H_{10}NO_2S$:172.0427, found:172.0431.



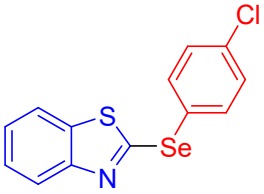
2-(phenylselanyl)benzo[*d*]thiazole (3a)

Yellow oil. yield 99% (0.0579 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.95 – 7.89 (m, 1H), 7.86 – 7.79 (m, 2H), 7.70 – 7.64 (m, 1H), 7.52 – 7.46 (m, 1H), 7.46 – 7.37 (m, 3H), 7.29 – 7.24 (m, 1H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.8, 154.6, 136.6, 136.6, 130.1, 129.9, 126.6, 126.1, 124.4, 122.0, 120.8; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 491.84; **IR (neat)**: ν = 3072, 2997, 2919, 1572, 1543, 1453, 1473, 1420, 1309, 1271, 1231 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_{10}NSSe$:291.9694, found:291.9704.



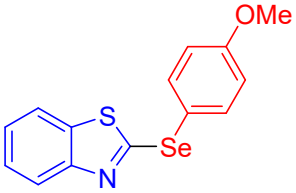
2-((4-fluorophenyl)selanyl)benzo[*d*]thiazole (3b)

Yellow oil. yield 87% (0.0536 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 – 7.88 (m, 1H), 7.84 – 7.78 (m, 2H), 7.71 – 7.66 (m, 1H), 7.42 – 7.37 (m, 1H), 7.30 – 7.25 (m, 1H), 7.16 – 7.09 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.3, 162.7, 154.6, 139.0, 136.5, 126.2, 124.5, 122.0, 121.3, 120.8, 117.3; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -109.63; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 482.65; **IR (neat)**: ν = 3088, 3059, 3029, 1733, 1581, 1481, 1454, 1396, cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_8FNNaSSe$:331.9419, found:331.9399.



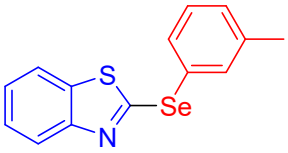
2-((4-chlorophenyl)selanyl)benzo[*d*]thiazole (3c)

Yellow oil. yield 83% (0.0539 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 – 7.83 (m, 1H), 7.70 – 7.60 (m, 3H), 7.37 – 7.29 (m, 3H), 7.24 – 7.19 (m, 1H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 161.6, 154.5, 137.8, 136.7, 136.6, 130.2, 126.2, 124.7, 124.6, 122.1, 120.9; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 482.54; **IR (neat)**: ν = **IR (neat)**: = 3069, 2958, 2924, 1556, 1472, 1453, 1421, 1386, cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_9ClNSSe$:325.9304, found:325.9306.



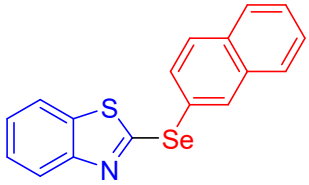
2-((4-methoxyphenyl)selanyl)benzo[*d*]thiazole (3d)

Yellow oil. yield 99% (0.0640 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.83 – 7.78 (m, 1H), 7.68 – 7.64 (m, 2H), 7.59 – 7.55 (m, 1H), 7.32 – 7.26 (m, 1H), 7.18 – 7.14 (m, 1H), 6.89 – 6.84 (m, 2H), 3.77 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.0, 161.4, 154.8, 138.8, 136.5, 125.9, 124.2, 121.8, 120.8, 116.7, 115.6, 55.4; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 481.93; **IR (neat)**: ν = 3034, 2932, 2975, 1683, 1568, 1524, 1512, 1426 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{14}H_{11}NONaSSe$:343.9619, found:343.9618.



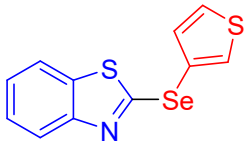
2-(*m*-tolylselanyl)benzo[*d*]thiazole (3e)

Yellow oil. yield 92% (0.0560 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.87 – 7.80 (m, 1H), 7.63 – 7.57 (m, 2H), 7.57 – 7.52 (m, 1H), 7.35 – 7.29 (m, 1H), 7.26 – 7.16 (m, 3H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 163.5, 154.6, 140.0, 137.2, 136.6, 133.6, 130.9, 129.7, 126.3, 126.0, 124.3, 121.9, 120.8, 21.3; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 491.36; **IR (neat)**: ν = 3055, 2950, 2919, 2851, 1589, 1568, 1453, 1420, 1308, 1232 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{14}H_{12}NSSe$:305.9850, found:305.9837.



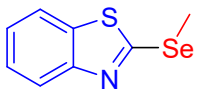
2-(naphthalen-2-ylselanyl)benzo[*d*]thiazole (3f)

White solid. yield 92% (0.0626 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:91.8-92.0 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.78 – 7.74 (m, 1H), 7.74 – 7.68 (m, 3H), 7.38 – 7.33 (m, 1H), 7.33 – 7.26 (m, 3H), 7.26 – 7.21 (m, 2H), 7.08 – 6.98 (m, 1H), 6.92 – 6.86 (m, 1H), 4.14 – 4.06 (m, 1H), 3.95 (dd, *J* = 14.4, 8.8 Hz, 1H), 3.59 (dd, *J* = 14.4, 4.4 Hz, 1H), 2.40 (s, 3H), 2.31 (dd, *J* = 14.6, 7.4 Hz, 1H), 2.26 (s, 3H), 2.15 (dd, *J* = 14.4, 4.4 Hz, 1H), 1.10 (d, *J* = 7.4 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.8, 154.6, 136.7, 136.7, 133.9, 133.6, 132.6, 129.6, 128.1, 127.9, 127.6, 126.9, 126.1, 124.4, 123.7, 122.0, 120.8; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 491.84; **IR (neat)**: ν = 2970, 2904, 2358, 1329, 2162, 2012, 1740, 1707, 1548, 1515 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{11}NNaSSe$:363.9670, found:363.9661.



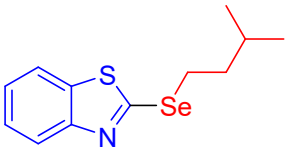
2-(thiophen-3-ylselanyl)benzo[*d*]thiazole (3g)

Yellow oil. yield 90% (0.0534 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.85 – 7.78 (m, 1H), 7.73 – 7.68 (m, 1H), 7.61 – 7.56 (m, 1H), 7.40 – 7.35 (m, 1H), 7.34 – 7.28 (m, 1H), 7.27 – 7.22 (m, 1H), 7.21 – 7.16 (m, 1H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 163.5, 154.7, 136.5, 134.1, 133.7, 127.6, 126.1, 124.3, 121.9, 120.8, 119.0; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 394.85; **IR (neat)**: ν = 3286, 3058, 2930, 2860, 1452, 1417, 1308, 1271, 1231, 1063 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{11}H_8NS_2Se$:297.9258, found:297.9260.



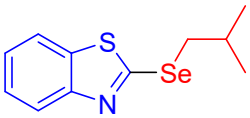
2-(methylselanyl)benzo[*d*]thiazole (3j)

White solid. yield 85% (0.0388 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:42.3-42.5 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.98 – 7.86 (m, 1H), 7.86 – 7.76 (m, 1H), 7.49 – 7.38 (m, 1H), 7.36 – 7.28 (m, 1H), 2.70 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 160.0, 154.1, 136.3, 126.0, 124.2, 121.6, 120.9, 8.0; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 291.33; **IR (neat)**: ν = 2956, 2921, 2850, 2357, 1731, 1716, 1490, 1455, 1421, 1362, 1184 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for C_8H_8NSSe:229.9537, found:227.9526.



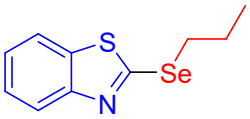
2-(isopentylselanyl)benzo[*d*]thiazole (3k)

Yellow oil. yield 90% (0.0512 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 – 7.80 (m, 1H), 7.75 – 7.63 (m, 1H), 7.38 – 7.29 (m, 1H), 7.24 – 7.18 (m, 1H), 3.32 – 3.21 (m, 2H), 1.73 – 1.67 (m, 2H), 1.67 – 1.63 (m, 1H), 0.88 (d, J = 6.3 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.4, 154.1, 136.4, 125.9, 124.2, 121.7, 120.9, 39.1, 28.5, 27.1, 22.2; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 367.85; **IR (neat)**: ν = 3060, 2953, 2926, 2867, 1454, 1421, 1384, 1365, 1307, 1260, 1232 cm^{-1}; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{12}H_{15}NNaSSe$:307.9983, found:307.9988.



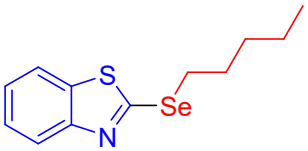
2-(isobutylselanyl)benzo[*d*]thiazole (3l)

Yellow solid. yield 80% (0.0433 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:99.7-99.9 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 – 7.77 (m, 1H), 7.76 – 7.63 (m, 1H), 7.35 – 7.30 (m, 1H), 7.25 – 7.20 (m, 1H), 3.23 (d, J = 6.7 Hz, 2H), 2.03 (dp, J = 13.3, 6.7 Hz, 1H), 1.01 (d, J = 6.7 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.6, 154.0, 136.4, 125.9, 124.2, 121.7, 120.8, 38.4, 29.3, 22.6; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 341.04; **IR (neat)**: ν = 2958, 2915, 2849, 2360, 1727, 1593,1495, 1288, 1255, 1137, 802, 754 cm^{-1}; **HRMS** (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{11}H_{14}NSSe$:272.007, found:272.006.



2-(propylselanyl)benzo[*d*]thiazole (3m)

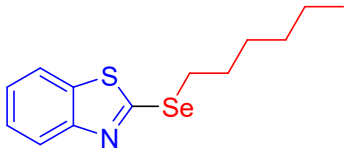
Yellow oil. yield 89% (0.0457 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.87 – 7.82 (m, 1H), 7.73 – 7.68 (m, 1H), 7.36 – 7.29 (m, 1H), 7.25 – 7.18 (m, 1H), 3.26 (t, J = 7.2 Hz, 2H), 1.85 (dt, J = 14.6, 7.3 Hz, 2H), 1.00 (t, J = 7.3 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.3, 154.1, 136.4, 125.9, 124.3, 121.7, 120.9, 31.2, 23.7, 14.4; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 361.64; **IR (neat)**: ν = 3059, 2958, 2927, 2868, 1723, 1453, 1421, 1376, 1307, 1278, 1232 cm^{-1}; **HRMS** (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{10}H_{12}NSSe$:257.9850, found:257.9844.



2-(pentylselanyl)benzo[*d*]thiazole (3n)

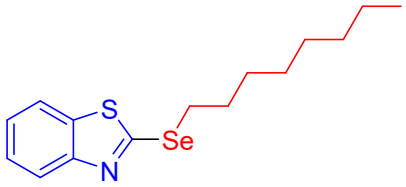
Yellow oil. yield 66% (0.0377 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 – 7.77 (m, 1H), 7.77 – 7.66 (m, 1H), 7.42 – 7.28 (m, 1H), 7.25 – 7.19 (m, 1H), 3.33 – 3.20 (m, 2H), 1.82 (p, J = 7.4 Hz, 2H), 1.43 – 1.34 (m, 2H), 1.34 – 1.27 (m, 2H), 0.84 (t, J = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.4, 154.1, 136.4, 125.9, 124.2, 121.7, 120.9, 31.9, 29.9, 29.1, 22.1, 13.9; **^{77}Se NMR** (76 MHz,

Chloroform-*d*) δ 366.07; **IR (neat)**: ν = 3059, 2954, 2924, 2853, 1702, 1453, 1421, 1307, 1270, 1232 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{12}H_{16}NSSe$:286.0163, found:286.0176.



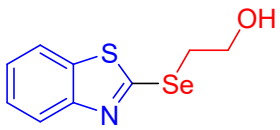
2-(hexylselanyl)benzo[*d*]thiazole (3o)

Yellow oil. yield 95% (0.0568 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 – 7.78 (m, 1H), 7.76 – 7.65 (m, 1H), 7.39 – 7.27 (m, 1H), 7.27 – 7.18 (m, 1H), 3.36 – 3.14 (m, 2H), 1.80 (p, *J* = 7.5 Hz, 2H), 1.45 – 1.35 (m, 2H), 1.24 (tt, *J* = 7.2, 3.3 Hz, 4H), 0.84 – 0.77 (m, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.4, 154.1, 136.4, 125.9, 124.2, 121.7, 120.9, 31.2, 30.2, 29.5, 29.1, 22.5, 14.0; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 365.96; **IR (neat)**: ν = 3060, 2953, 2923, 2851, 1496, 1454, 1421, 1378, 1307, 1272 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_{18}NSSe$:300.0320, found:300.0298.



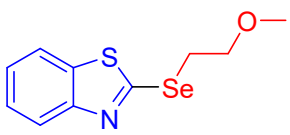
2-(octylselanyl)benzo[d]thiazole (3p)

Yellow oil. yield 78% (0.0508 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 – 7.81 (m, 1H), 7.75 – 7.66 (m, 1H), 7.37 – 7.30 (m, 1H), 7.26 – 7.19 (m, 1H), 3.34 – 3.25 (m, 2H), 1.86 – 1.77 (m, 2H), 1.41 – 1.32 (m, 2H), 1.31 – 1.18 (m, 8H), 0.86 – 0.77 (m, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.4, 154.1, 136.4, 125.9, 124.2, 121.7, 120.9, 31.8, 30.2, 29.8, 29.2, 29.1, 29.0, 22.6, 14.1; ^{77}Se NMR (76 MHz, Chloroform-*d*) δ 365.84; **IR (neat)**: ν = 3062, 2953, 2923, 2852, 1559, 1455, 1423, 1308, 1271, 1233, 963 cm^{-1}; **HRMS** (EI-TOF) m/z: M Calcd for $C_{15}H_{21}NSSe$:327.0560, found:327.0564.



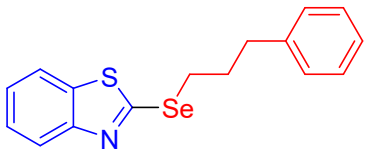
2-(benzo[*d*]thiazol-2-ylselanyl)ethan-1-ol (3q)

Yellow oil. yield 86% (0.0443 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.84 – 7.78 (m, 1H), 7.71 – 7.64 (m, 1H), 7.36 – 7.29 (m, 1H), 7.29 – 7.20 (m, 1H), 4.14 (s, 1H), 4.05 (t, *J* = 5.7 Hz, 2H), 3.42 (dd, *J* = 6.2, 5.2 Hz, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 159.4, 153.3, 136.6, 126.2, 124.7, 121.5, 121.0, 62.8, 31.9; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 354.06; **IR (neat)**: ν = 3099, 3058, 2955, 1904, 1558, 1453, 1420, 1347, 1308, 1231, 1207 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_9NONaSSe$:281.9462, found:281.9455.



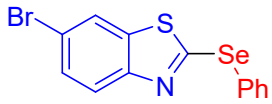
2-((2-methoxyethyl)selanyl)benzo[*d*]thiazole (3r)

Yellow oil. yield 86% (0.0468 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 – 7.81 (m, 1H), 7.81 – 7.68 (m, 1H), 7.39 – 7.31 (m, 1H), 7.29 – 7.21 (m, 1H), 3.77 (t, *J* = 6.4 Hz, 2H), 3.50 (t, *J* = 6.4 Hz, 2H), 3.34 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 158.6, 153.9, 136.5, 125.9, 124.3, 121.7, 120.9, 71.6, 58.8, 27.9; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 344.22; **IR (neat)**: ν = 3058, 2981, 2923, 2821, 1558, 1453, 1421, 1376, 1308, 1270, 1232 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{10}H_{12}NOSSe$:273.9799, found:273.9793.



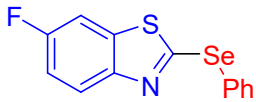
2-((3-phenylpropyl)selanyl)benzo[*d*]thiazole (3s)

Yellow oil. yield 99% (0.0666 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.85 – 7.81 (m, 1H), 7.70 – 7.66 (m, 1H), 7.34 – 7.27 (m, 1H), 7.21 – 7.15 (m, 3H), 7.13 – 7.08 (m, 3H), 3.25 (t, *J* = 7.3 Hz, 2H), 2.70 (dd, *J* = 8.3, 6.7 Hz, 2H), 2.17 – 2.10 (m, 2H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 158.9, 154.1, 140.9, 136.5, 128.6, 128.5, 126.1, 126.0, 124.3, 121.8, 120.9, 35.7, 31.8, 28.4; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 363.85; **IR (neat)**: ν = 3326, 3055, 2913, 1667, 1595, 1577, 1467, 1446, 1411, 1304, 1270 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{16}NSSe$:334.0163, found:334.0145.



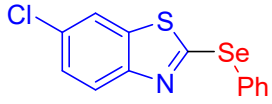
6-bromo-2-(phenylselanyl)benzo[*d*]thiazole (4a)

White solid. yield 86% (0.0632 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:57.2-57.4 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.76 – 7.69 (m, 2H), 7.69 – 7.61 (m, 2H), 7.43 – 7.31 (m, 4H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 163.9, 153.5, 138.1, 136.7, 130.4, 130.1, 129.5, 126.1, 123.3, 122.9, 118.0; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 497.96; **IR (neat)**: ν = 3054, 2959, 2920, 2849, 1595, 1557, 1542, 1440, 1416, 1390, 1250 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_9BrNSSe$:369.8799, found:369.8807.



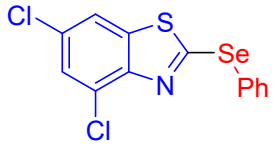
6-fluoro-2-(phenylselanyl)benzo[*d*]thiazole (4b)

Yellow solid. yield 99% (0.0625 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:40.1-40.3 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.85 – 7.69 (m, 3H), 7.45 – 7.39 (m, 1H), 7.39 – 7.32 (m, 2H), 7.31 – 7.24 (m, 1H), 7.10 – 7.00 (m, 1H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.1, 160.0 (d, *J* = 245 Hz), 151.3, 137.5 (d, *J* = 11 Hz), 136.6, 130.2, 130.0, 126.4, 122.8 (d, *J* = 10 Hz), 114.5 (d, *J* = 25 Hz), 107.2 (d, *J* = 26 Hz); **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -116.83; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 494.67; **IR (neat)**: ν = 2959, 2920, 2855, 2356, 2227, 2170, 1694, 1561, 1465, 1435 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_8NFNaSSe$:331.9419, found:331.9414.



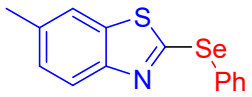
6-chloro-2-(phenylselanyl)benzo[*d*]thiazole (4c)

Yellow solid. yield 99% (0.0712 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:78.7-79.0 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.76 – 7.67 (m, 3H), 7.54 – 7.50 (m, 1H), 7.45 – 7.38 (m, 1H), 7.38 – 7.31 (m, 2H), 7.27 – 7.22 (m, 1H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 163.7, 153.2, 137.7, 136.7, 130.4, 130.3, 130.1, 126.8, 126.2, 122.6, 120.5; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 497.51; **IR (neat)**: ν = 3058, 2954, 2851, 1730, 1574, 1573, 1473, 1454, 1427, 1393, 1299, 1254 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_9ClNSSe$:325.9304, found:325.9302.



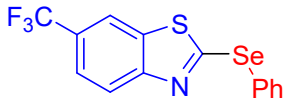
4,6-dichloro-2-(phenylselanyl)benzo[*d*]thiazole (4d)

White solid. yield 87% (0.0624 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:106.7-106.9 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.77 – 7.71 (m, 2H), 7.48 – 7.42 (m, 1H), 7.40 – 7.35 (m, 3H), 7.31 – 7.28 (m, 1H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 166.4, 150.5, 138.4, 137.0, 130.7, 130.2, 130.1, 126.7, 126.7, 125.9, 118.9; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 512.78; **IR (neat)**: ν = 3063, 2961, 2838, 2366, 1717, 1571, 1541, 1439, 1420, 1370, 1258 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{13}H_8Cl_2NSSe$:359.8914, found:359.8907.



6-methyl-2-(phenylselanyl)benzo[*d*]thiazole (4e)

Yellow oil. yield 84% (0.0511 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.77 – 7.67 (m, 3H), 7.42 – 7.28 (m, 4H), 7.14 – 7.07 (m, 1H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 160.9, 152.7, 136.9, 136.4, 134.6, 129.9, 129.9, 127.6, 126.8, 121.5, 120.6, 21.5; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 486.36; **IR (neat)**: ν = 2961, 2912, 2863, 1715, 1470, 1433, 1259, 1090, 1019 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{14}H_{12}NSSe$:305.9850, found:305.9837.

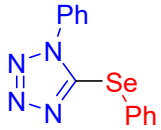


2-(phenylselanyl)-6-(trifluoromethyl)benzo[*d*]thiazole (4f)

Yellow oil. yield 99% (0.0707 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 – 7.81 (m, 2H), 7.78 – 7.70 (m, 2H), 7.57 – 7.49 (m, 1H), 7.49 – 7.41 (m, 1H), 7.41 – 7.31 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 167.7, 156.6, 136.9 (q, J = 3.6 Hz), 136.6, 130.6, 130.2, 126.3 (q, J = 33 Hz), 125.88, 124.1 (q, J = 273 Hz), 123.1 (q, J = 3.6 Hz), 122.1, 118.3 (q, J = 4 Hz); **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 506.91; **IR (neat)**: ν = 3058, 2961, 2921, 2850, 1607, 1470, 1437, 1405, 1313, 1268, 1161 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{14}H_9F_3SSe$:359.9568, found:359.9575.

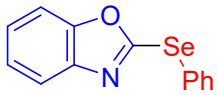
ethyl 2-(phenylselanyl)benzo[d]thiazole-6-carboxylate (4g)

White solid. yield 20% (0.0141 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:76.2-76.4 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.31 – 8.28 (m, 1H), 8.02 – 7.97 (m, 1H), 7.84 – 7.78 (m, 1H), 7.78 – 7.72 (m, 2H), 7.48 – 7.41 (m, 1H), 7.40 – 7.35 (m, 2H), 4.29 (q, J = 7.2 Hz, 2H), 1.30 (t, J = 7.1 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 168.1, 166.1, 157.4, 136.9, 136.3, 130.5, 130.1, 127.4, 126.3, 125.9, 122.8, 121.4, 61.2, 14.3; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 507.06; **IR (neat)**: ν = 2959, 2918, 2850, 1702, 1594, 1538, 1363, 1285, 1261, 1110 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{13}NO_2SNaSe$:385.9724, found:385.9707.



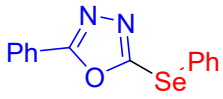
1-phenyl-5-(phenylselanyl)-1*H*-tetrazole (4h)

Yellow oil. yield 56% (0.0334 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.63 – 7.57 (m, 2H), 7.57 – 7.51 (m, 3H), 7.50 – 7.45 (m, 2H), 7.42 – 7.36 (m, 1H), 7.35 – 7.29 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 147.0, 135.2, 134.0, 130.5, 129.8, 129.8, 129.7, 124.7, 124.2; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 331.47; **IR (neat)**: ν = 3066, 2921, 2851, 1592, 1573, 1495, 1461, 1437, 1406, 1379, 1272, 1229, 1087, 1072 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_{10}N_4NaSe$:324.9963, found:324.9953.



2-(phenylselanyl)benzo[d]oxazole (4i)

Yellow oil. yield 90% (0.0490 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.72 – 7.67 (m, 2H), 7.56 – 7.51 (m, 1H), 7.37 – 7.29 (m, 4H), 7.21 – 7.12 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 158.0, 152.6, 142.3, 135.6, 129.8, 129.6, 124.6, 124.3, 124.3, 119.1, 110.1; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 404.28; **IR (neat)**: ν = 3057, 1577, 1488, 1447, 1327, 1232, 1204, 1115, 1080 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_9NONaSe$:297.9742, found:297.9741.

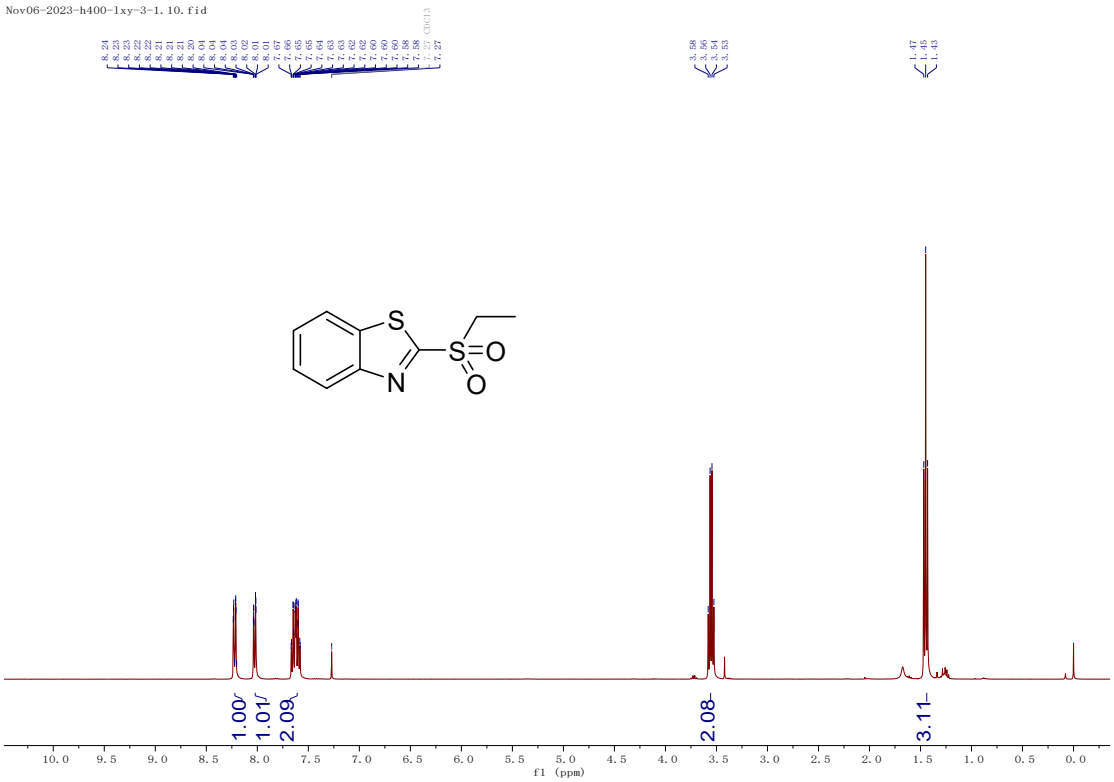


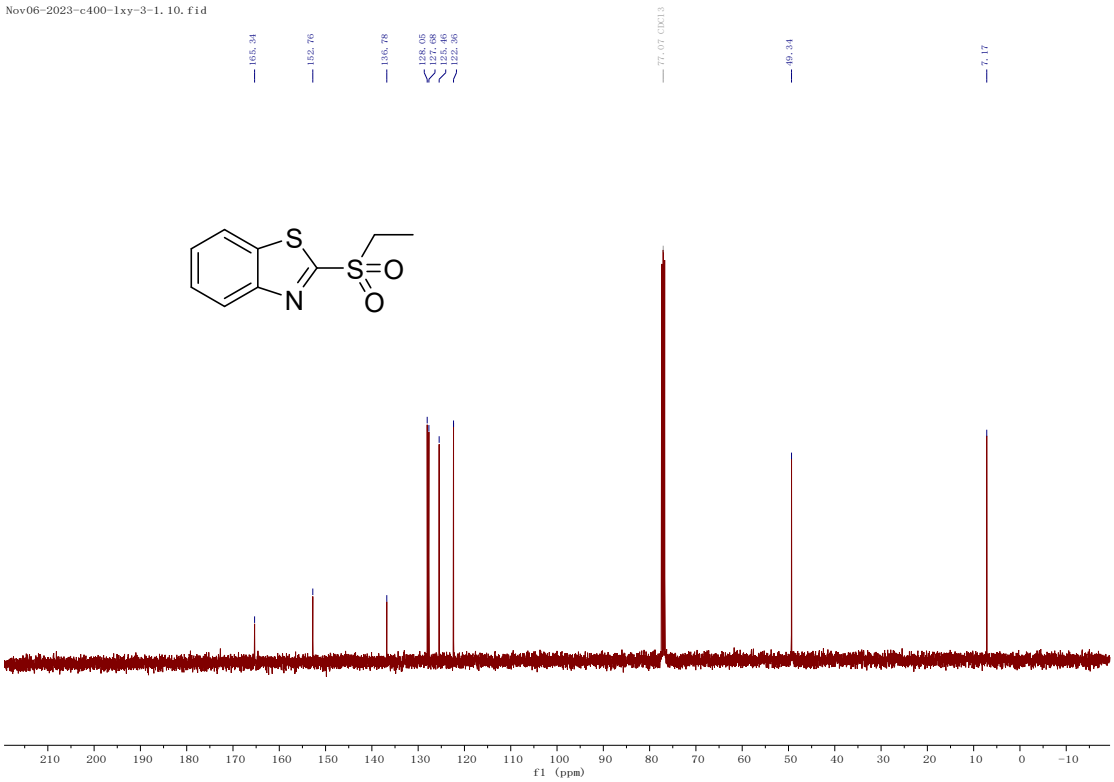
2-phenyl-5-(phenylselanyl)-1,3,4-oxadiazole (4j)

White solid. yield 95% (0.0570 g, 0.2 mmol scale) , and purified by flash column chromatography on silica gel (PE /EA = 50/1); **Mp**:46.7-46.9 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 – 7.82 (m, 2H), 7.71 – 7.64 (m, 2H), 7.45 – 7.27 (m, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 167.7, 156.2, 135.1, 131.8, 129.9, 129.7, 129.0, 126.8, 124.2, 123.5; **^{77}Se NMR** (76 MHz, Chloroform-*d*) δ 366.88; **IR (neat)**: ν = 2960, 2918, 2849, 1551, 1460, 1438, 1155, 1064, 1021, 982 cm^{-1}; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{14}H_{11}N_2OSe$:303.0031, found:303.0030.

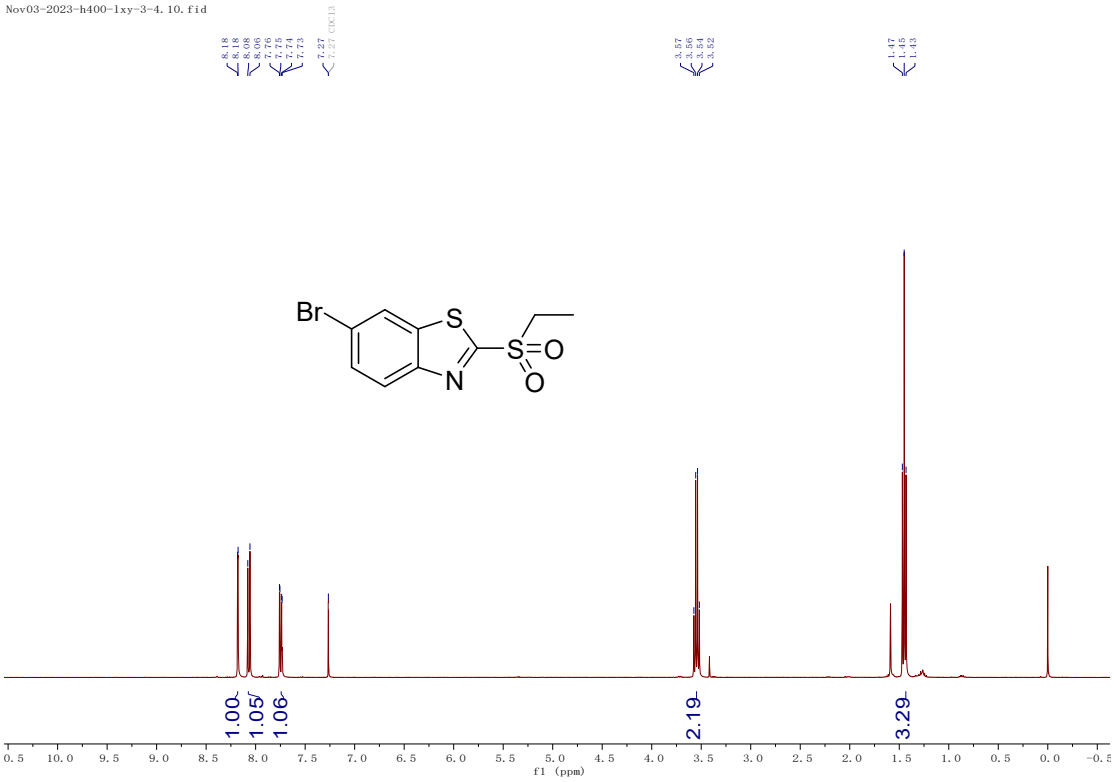
5. Copies of 1H , 13C NMR, 19F NMR,77Se NMR Spectra for Compounds

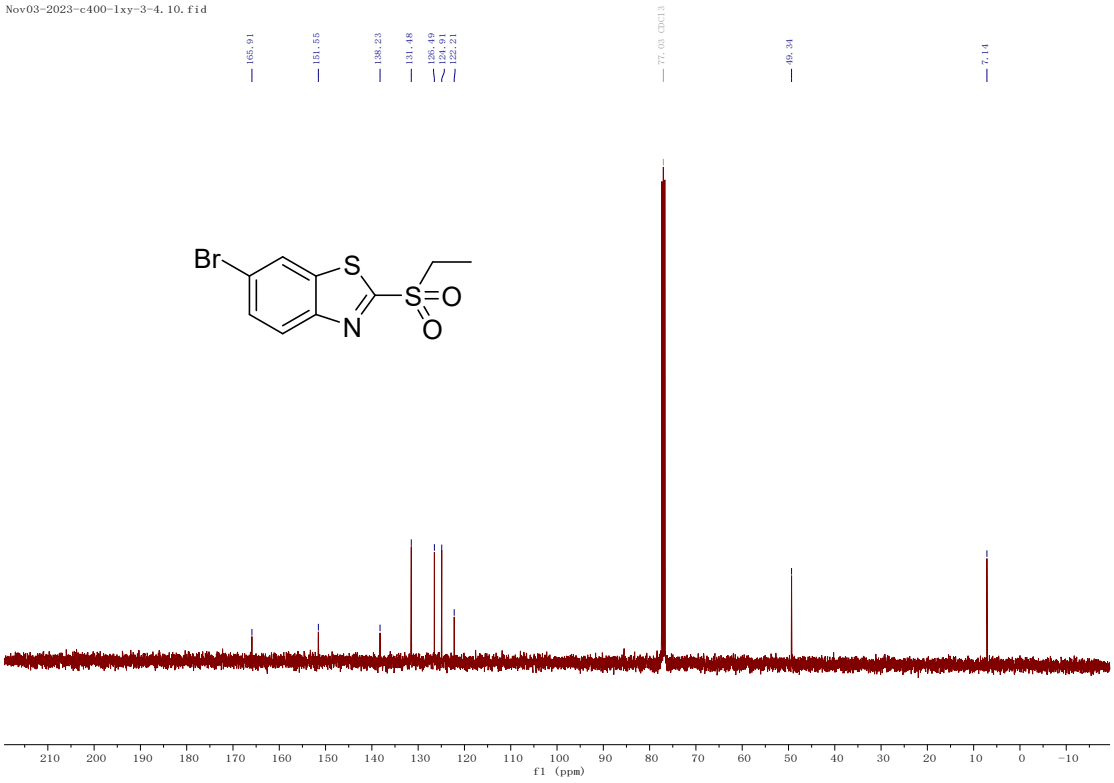
2-(ethylsulfonyl)benzo[*d*]thiazole (1a)



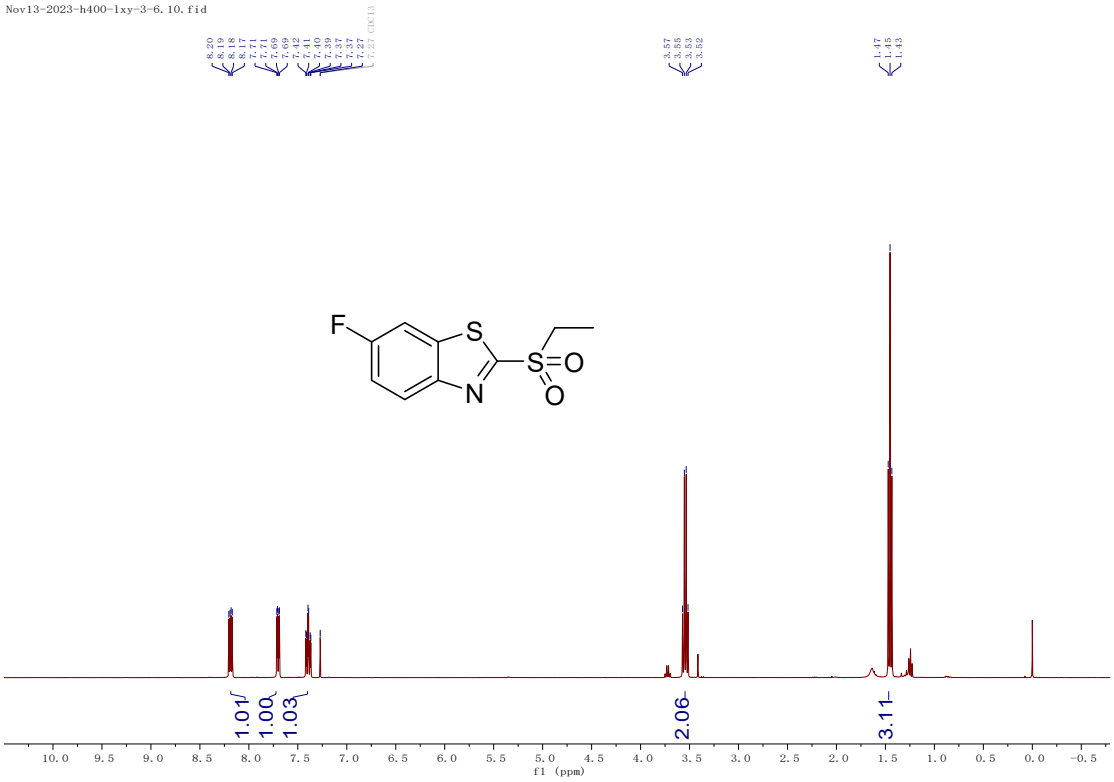


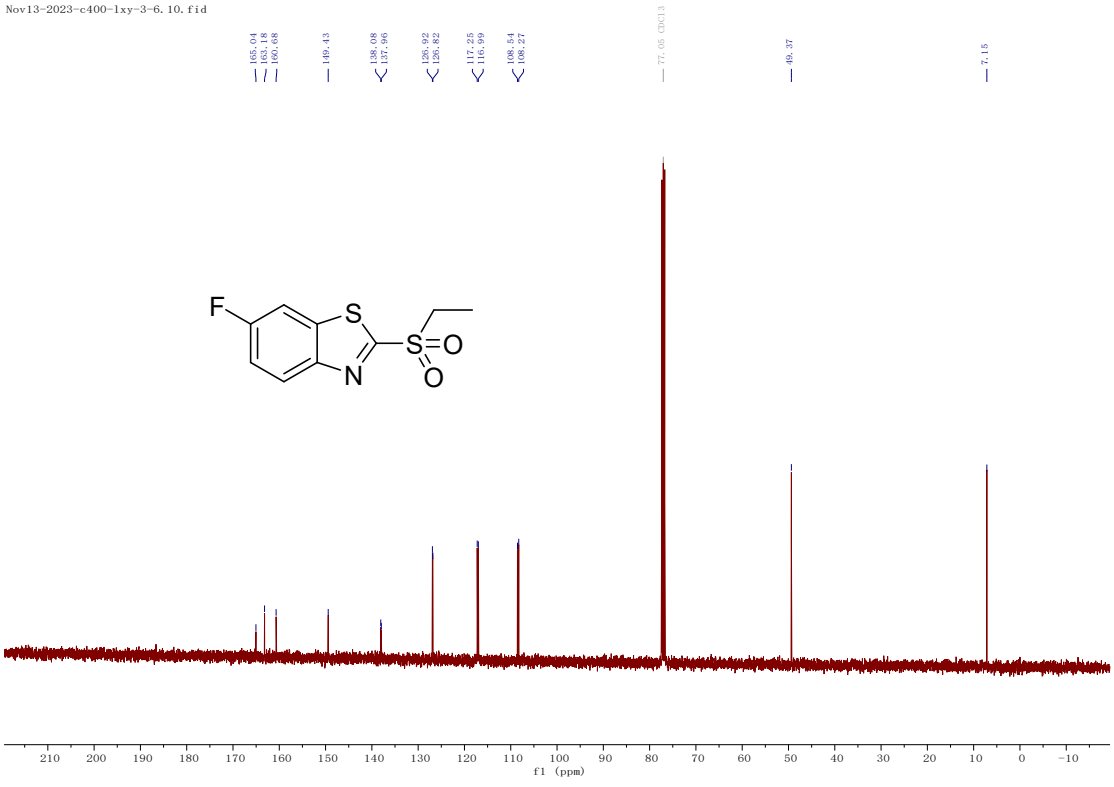
6-bromo-2-(ethylsulfonyl)benzo[*d*]thiazole (1b)

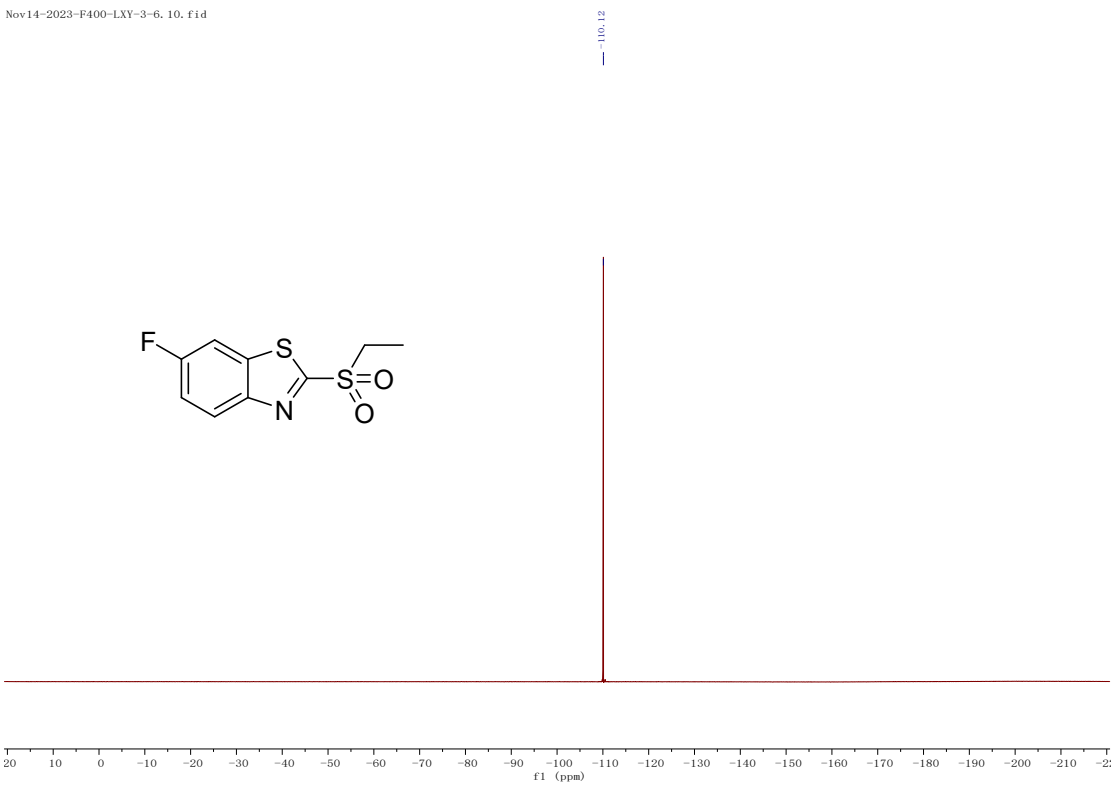




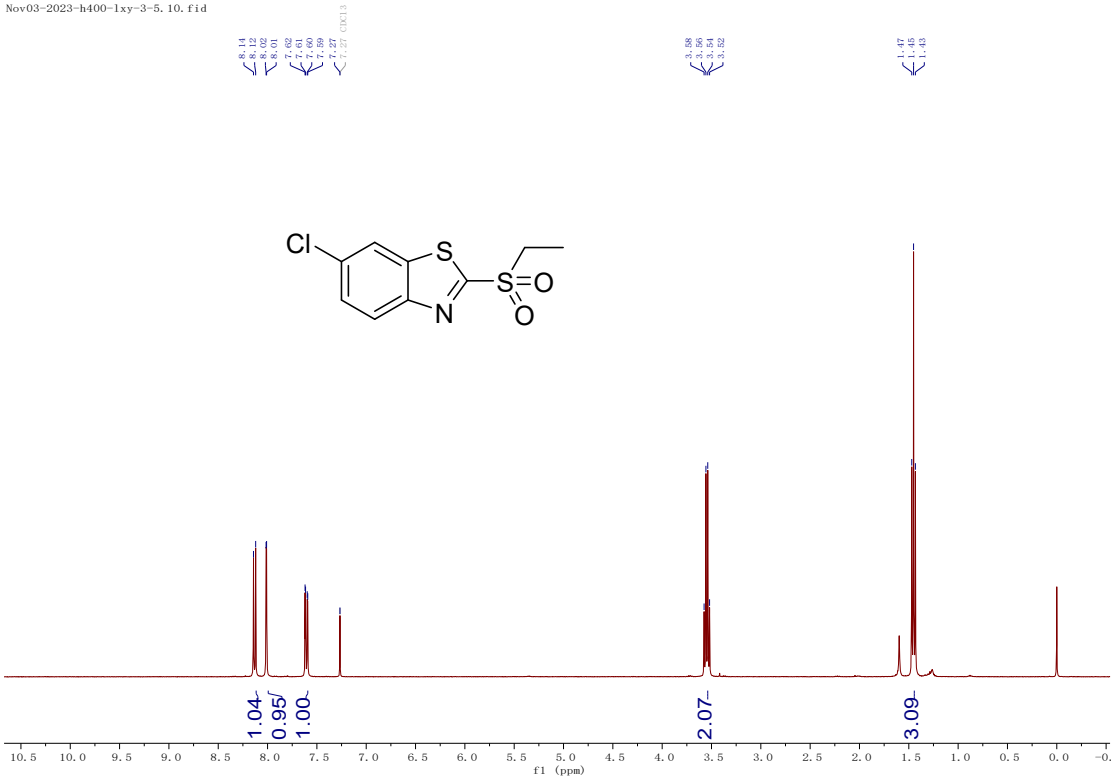
2-(ethylsulfonyl)-6-fluorobenzo[*d*]thiazole (1c)

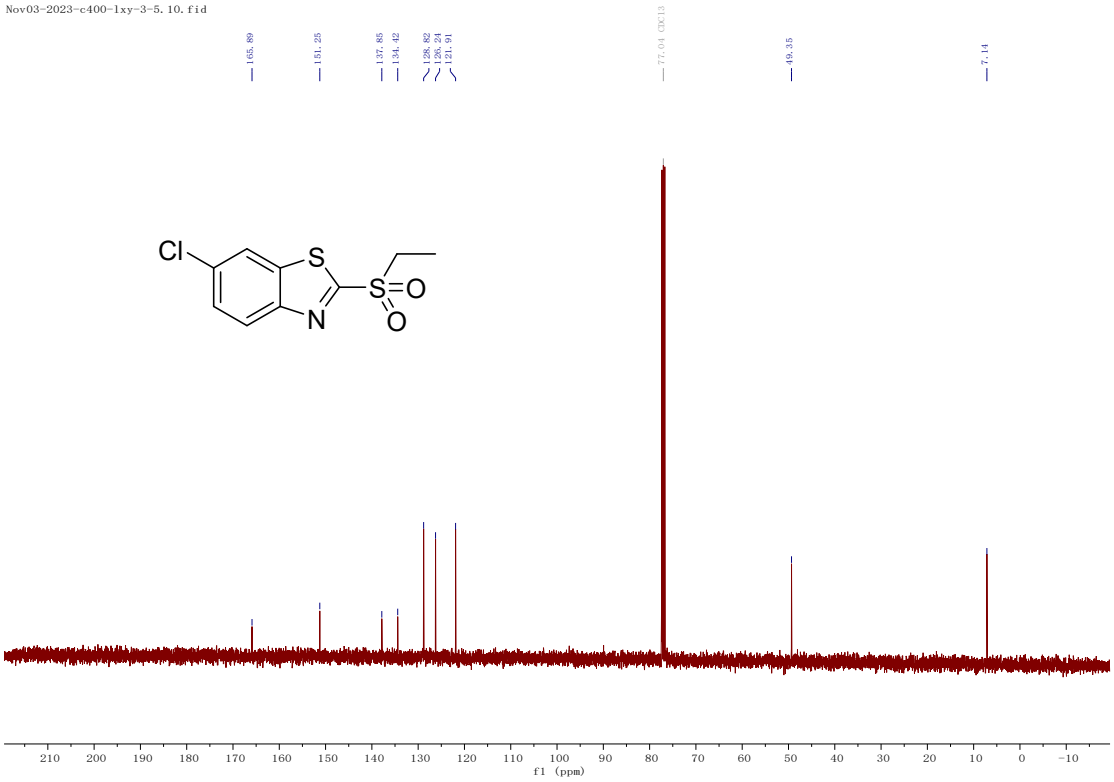

Nov13-2023-h400-lxy-3-6.10.fid
8.20
8.19
8.18
8.17
7.71
7.71
7.69
7.69
7.42
7.41
7.40
7.39
7.37
7.37
7.27
7.27 CDCl3
3.57
3.55
3.53
3.52
1.47
1.45
1.43
F
S
S
O
O
N
1.01
1.00
1.03
2.06
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Nov13-2023-c400-lxy-3-6.10.fid
165.04
163.18
160.68
149.43
138.08
137.96
126.92
126.82
117.25
116.99
108.54
108.27
77.05 CDCl3
49.37
7.15
F
S
S
O
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

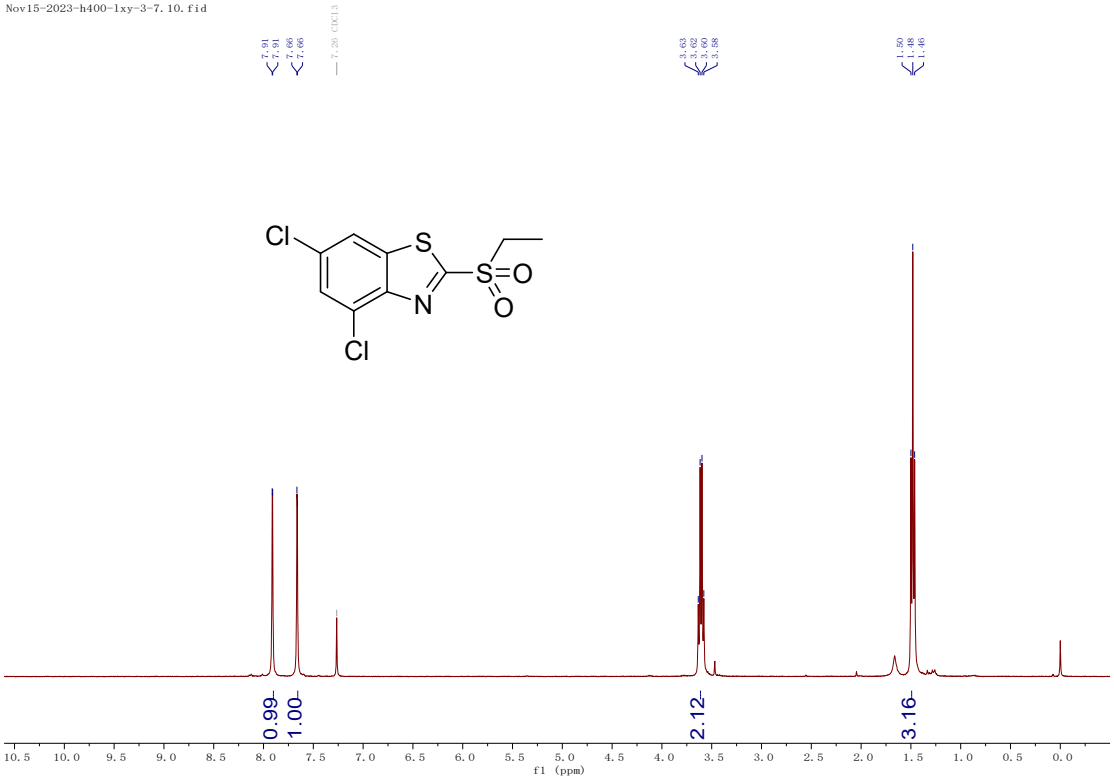


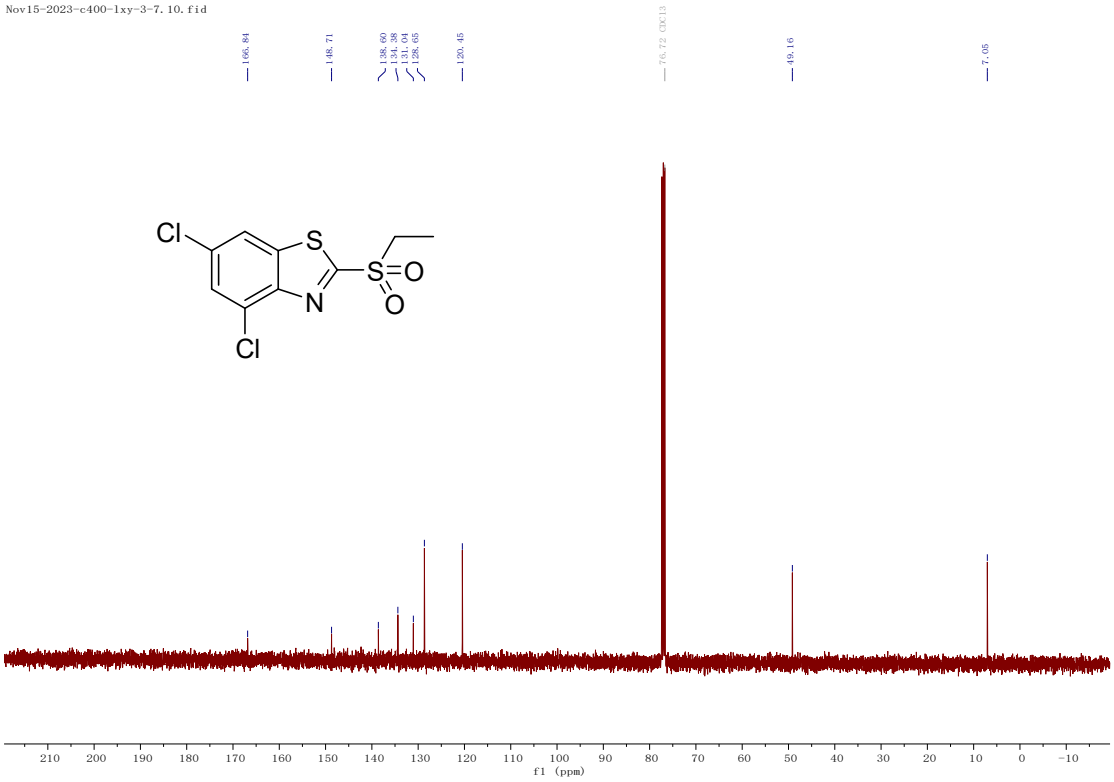
6-chloro-2-(ethylsulfonyl)benzo[*d*]thiazole (1d)



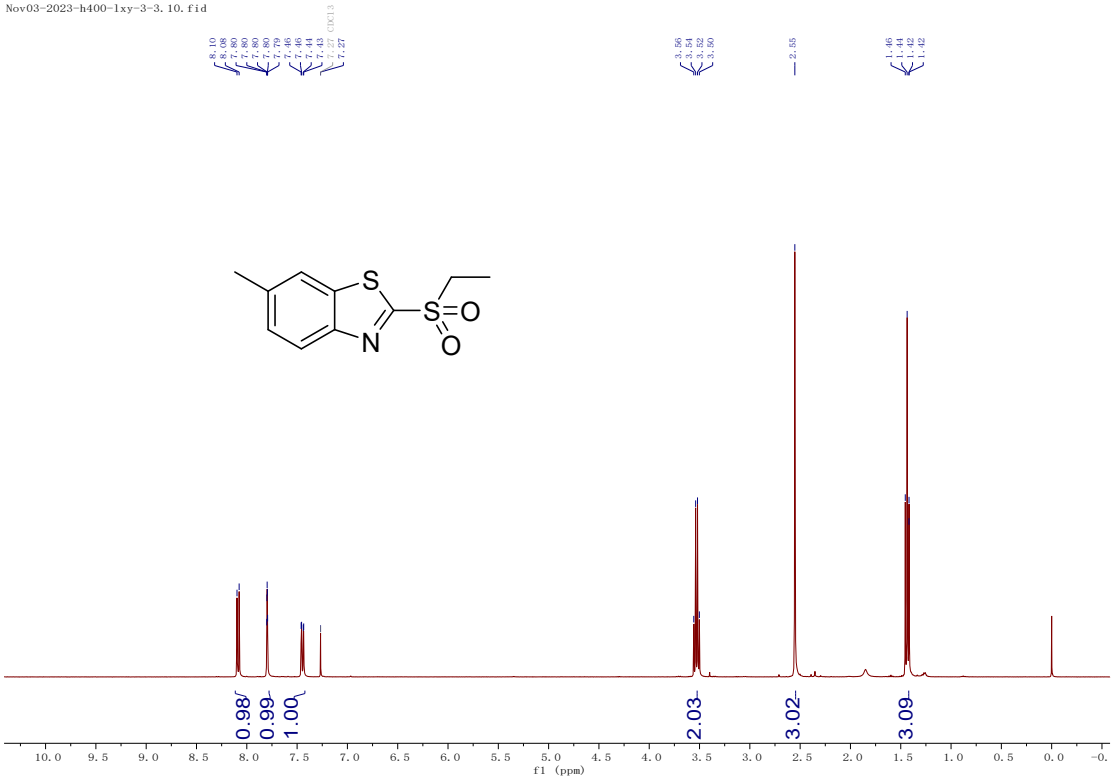


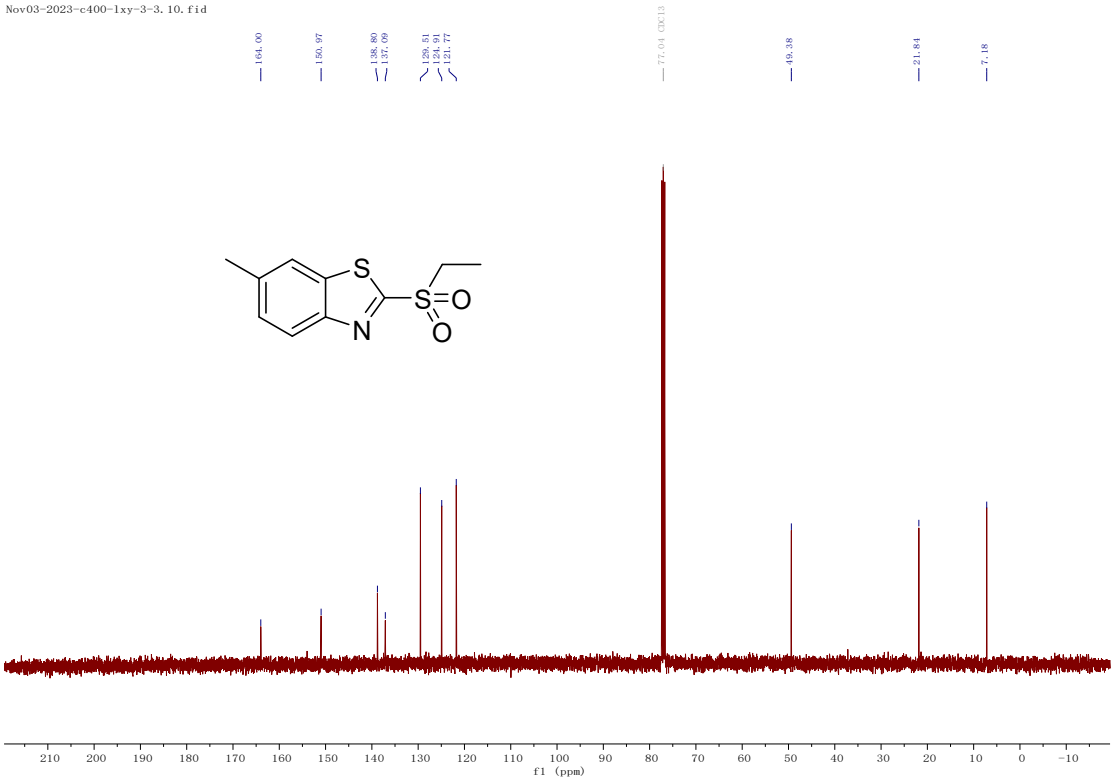
4,6-dichloro-2-(ethylsulfonyl)benzo[d]thiazole (1e)



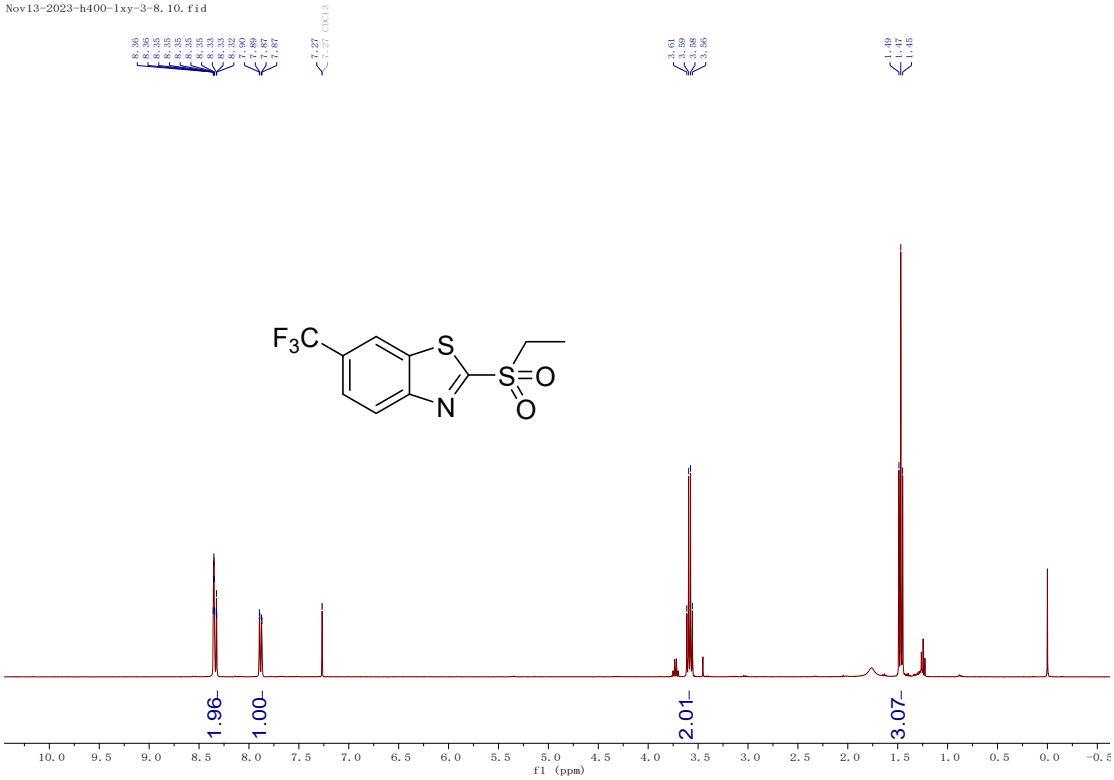


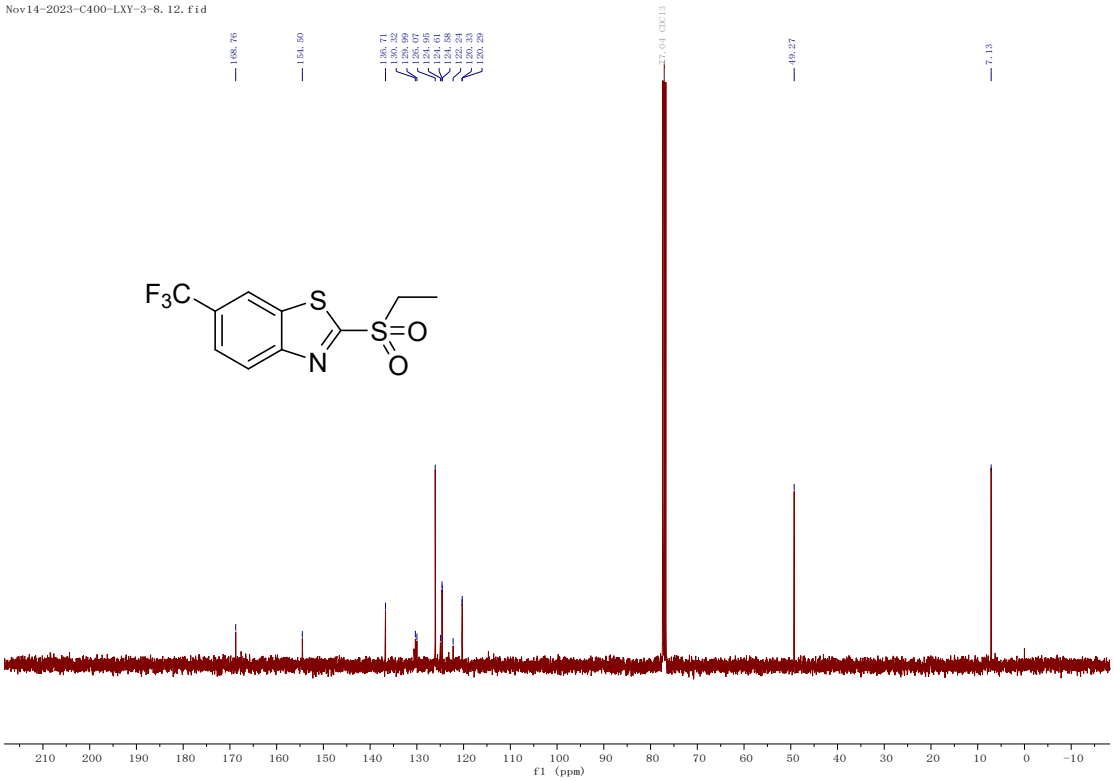
2-(ethylsulfonyl)-6-methylbenzo[*d*]thiazole (1f)

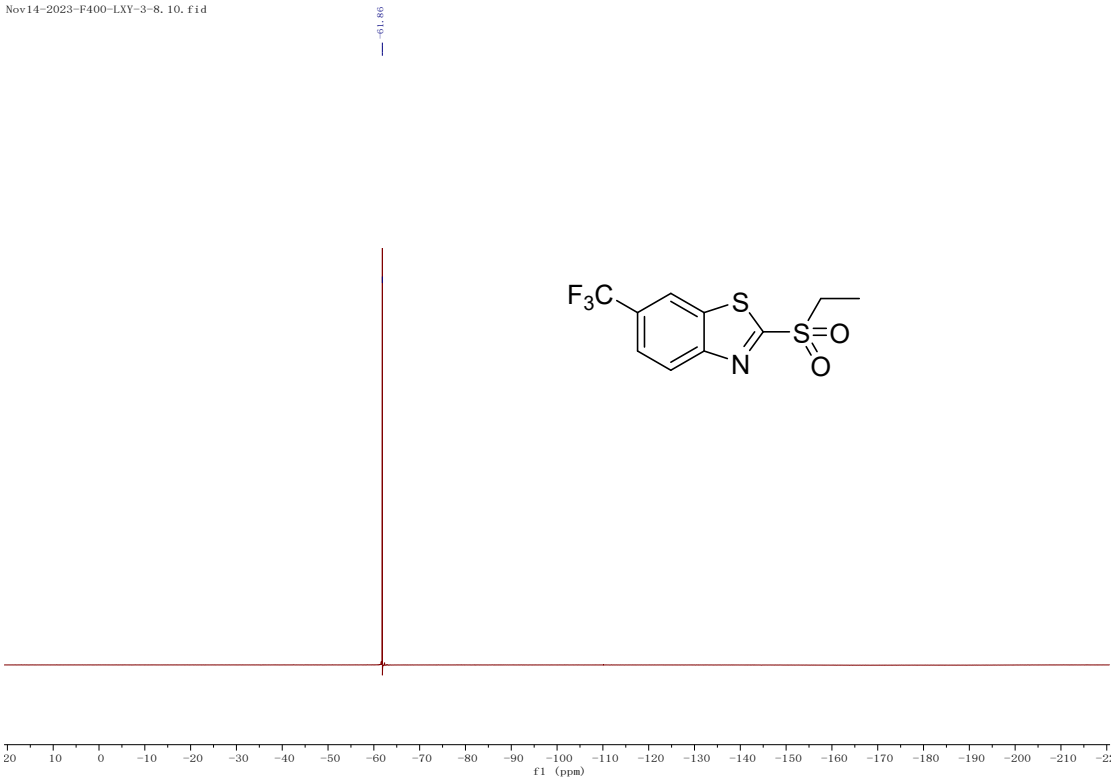




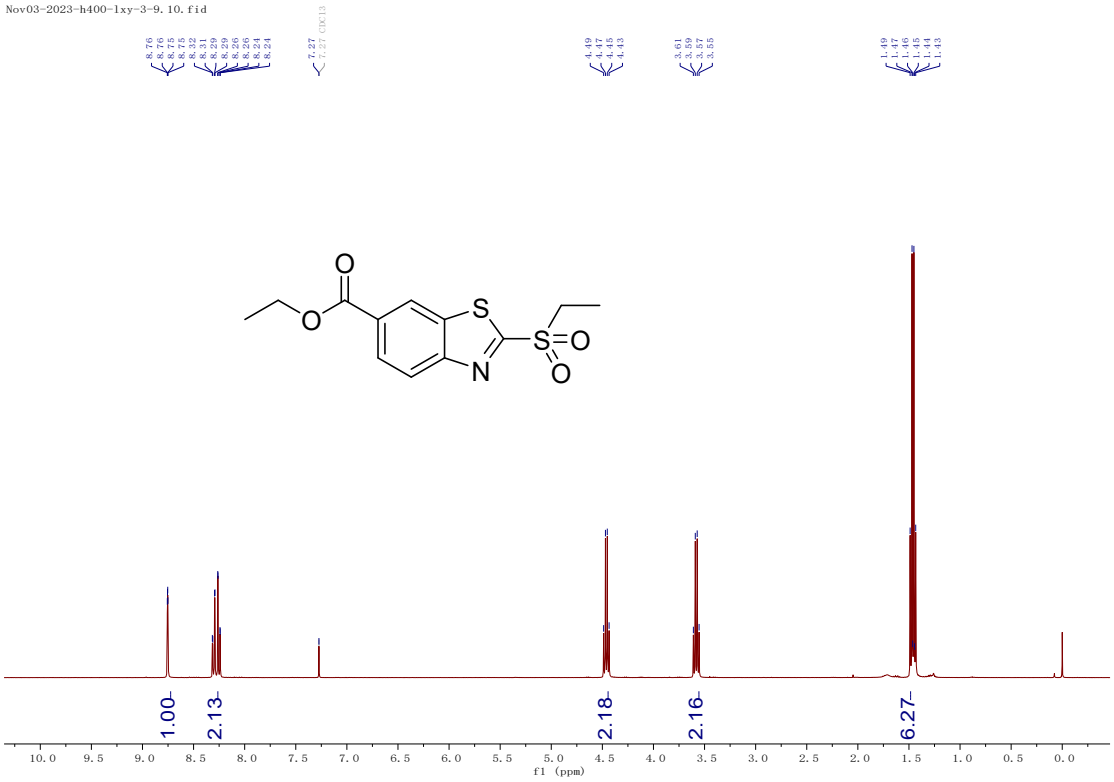
2-(ethylsulfonyl)-6-(trifluoromethyl)benzo[*d*]thiazole (1g)

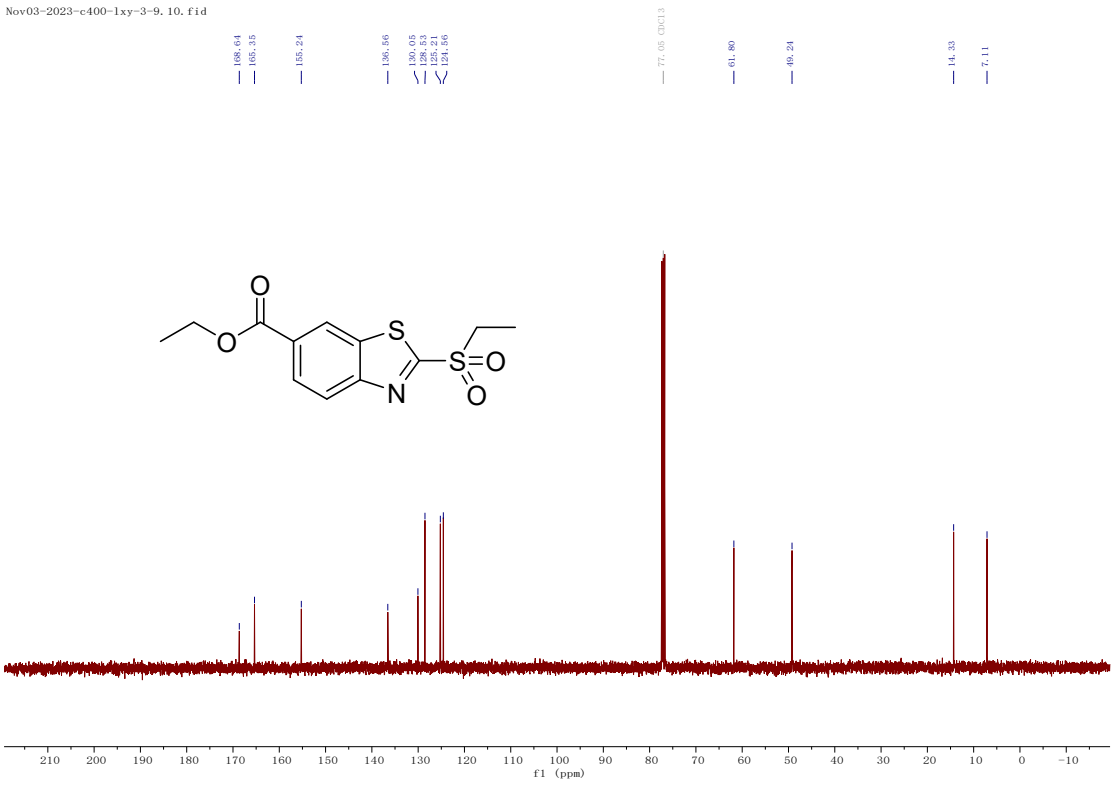




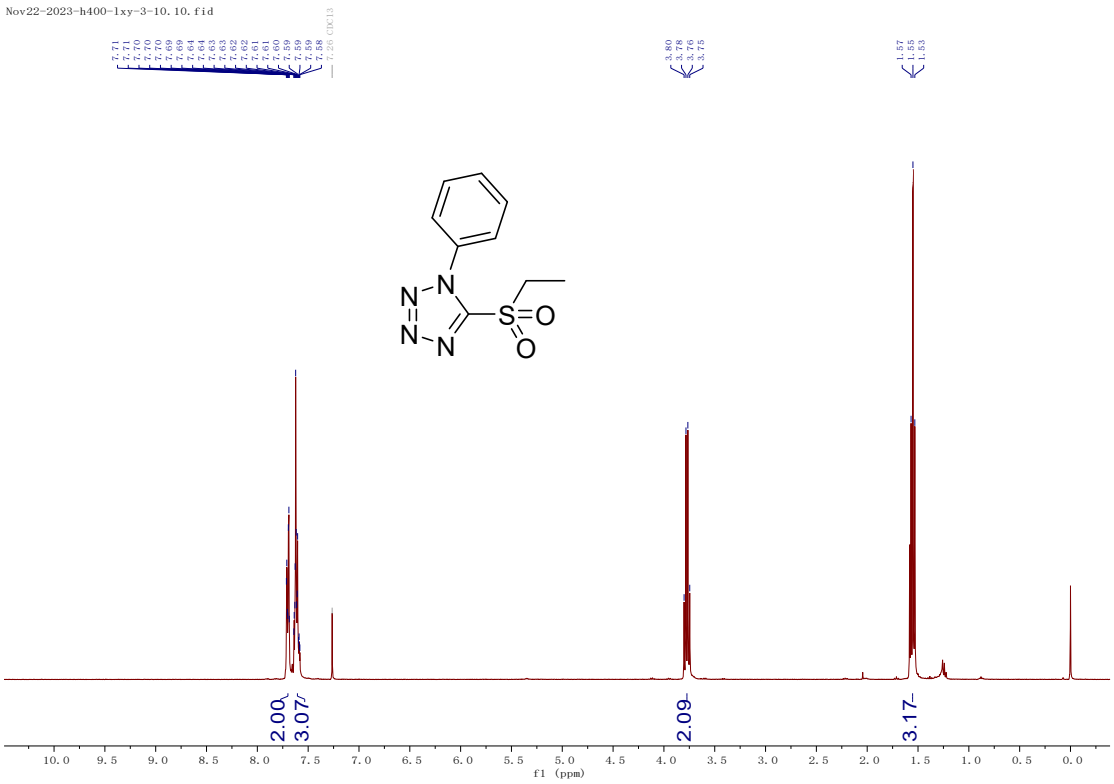


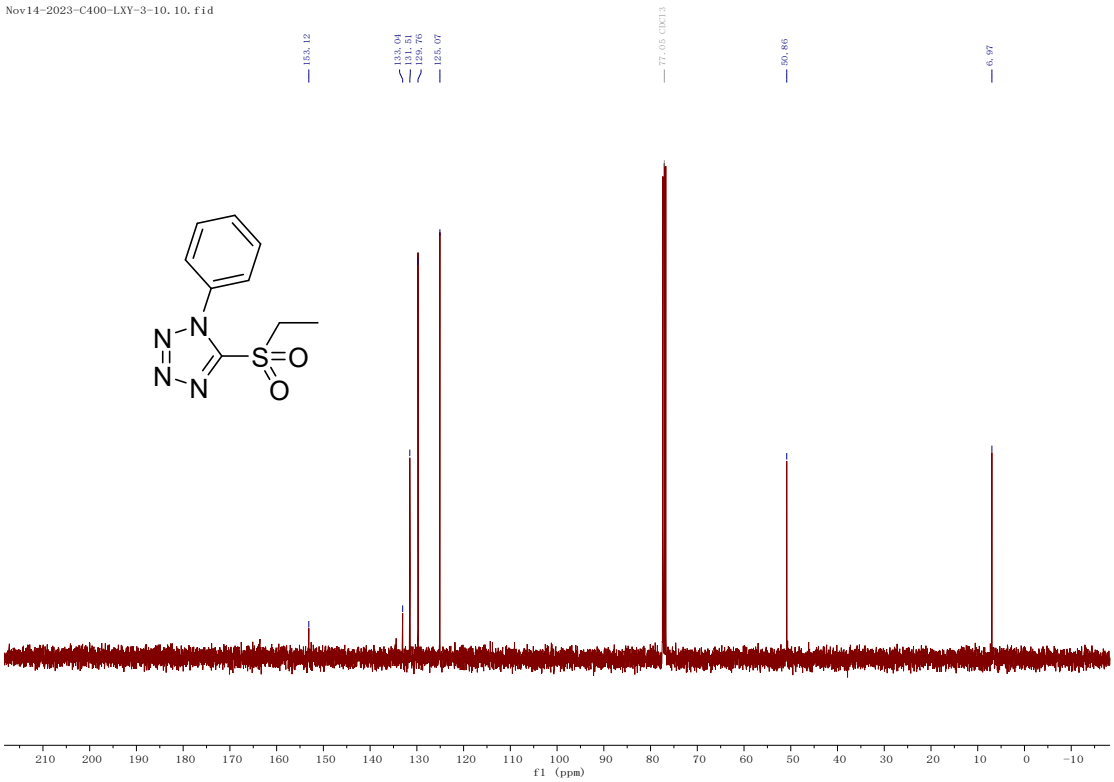
ethyl 2-(ethylsulfonyl)benzo[*d*]thiazole-6-carboxylate (1h)



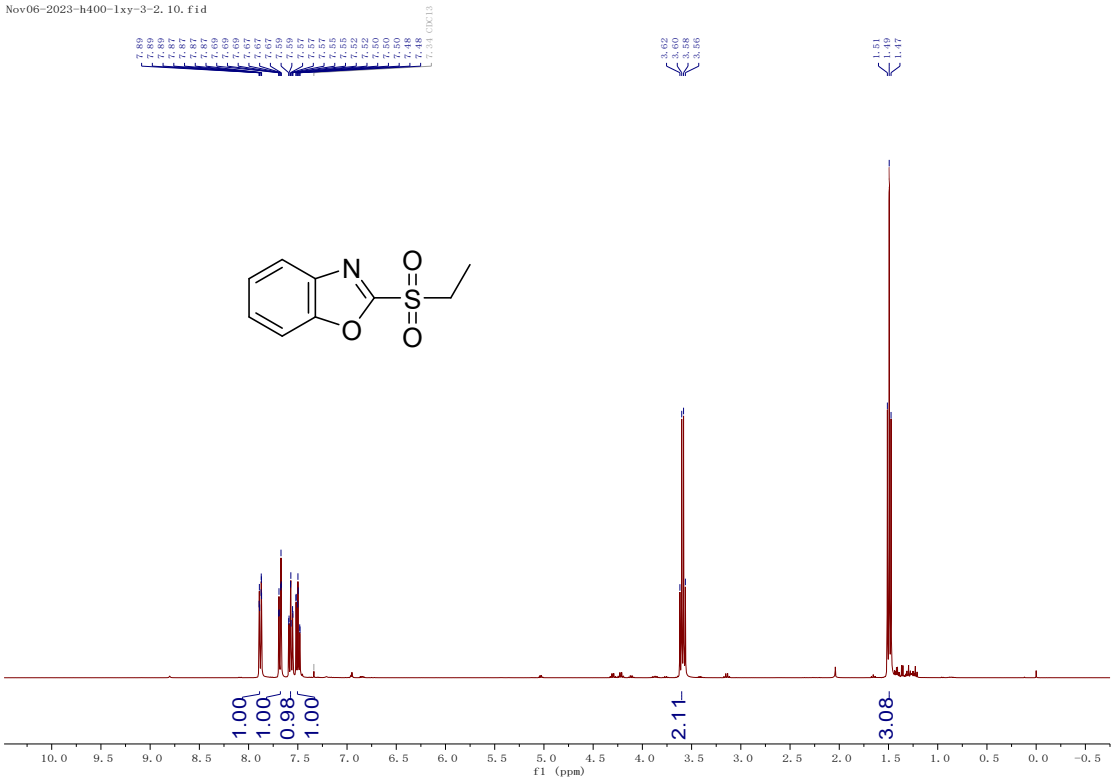


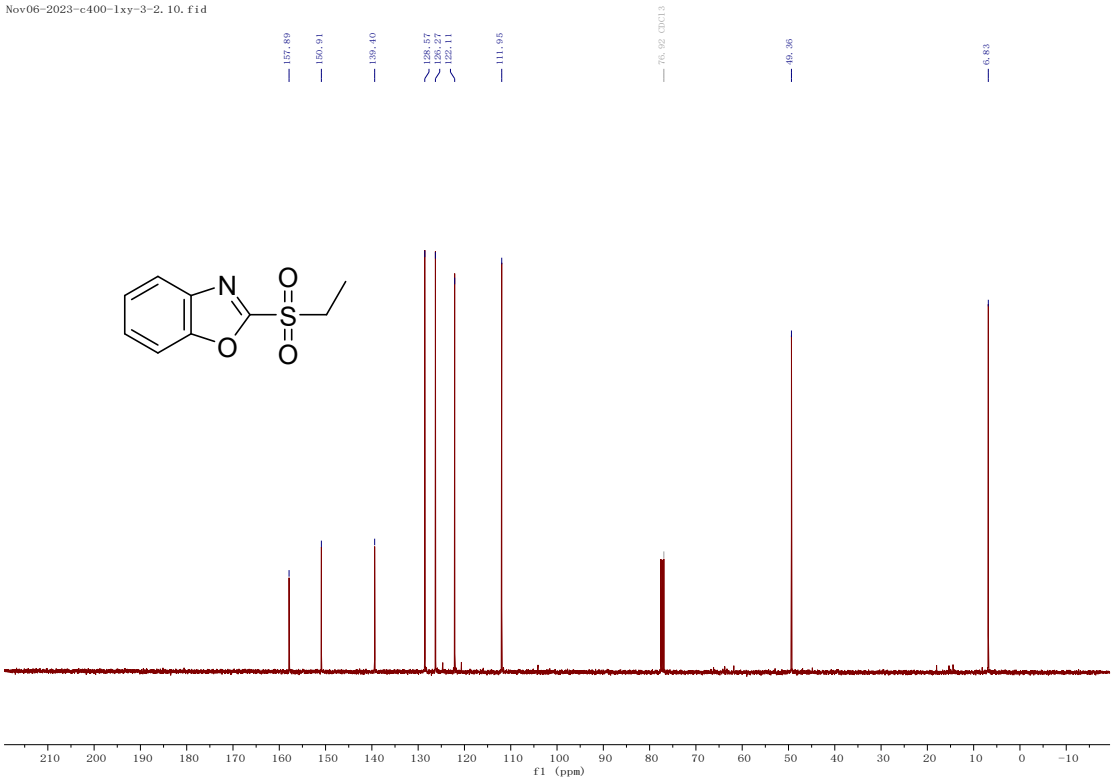
5-(ethylsulfonyl)-1-phenyl-1*H*-tetrazole (1i)



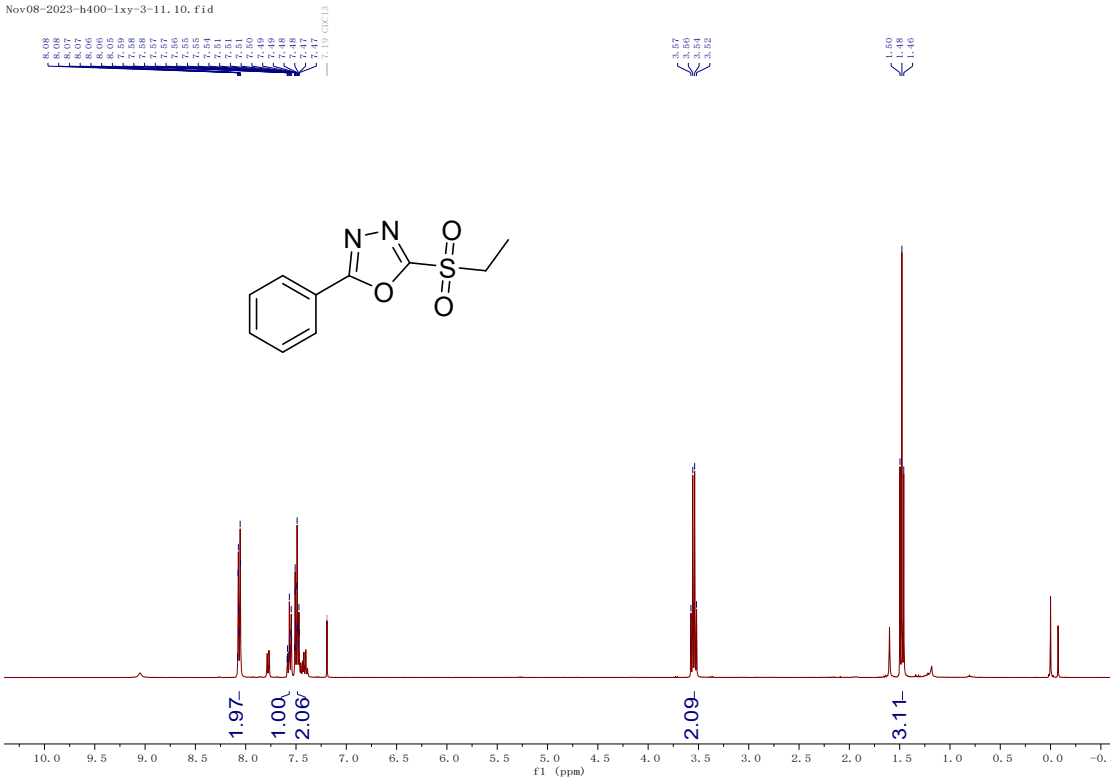


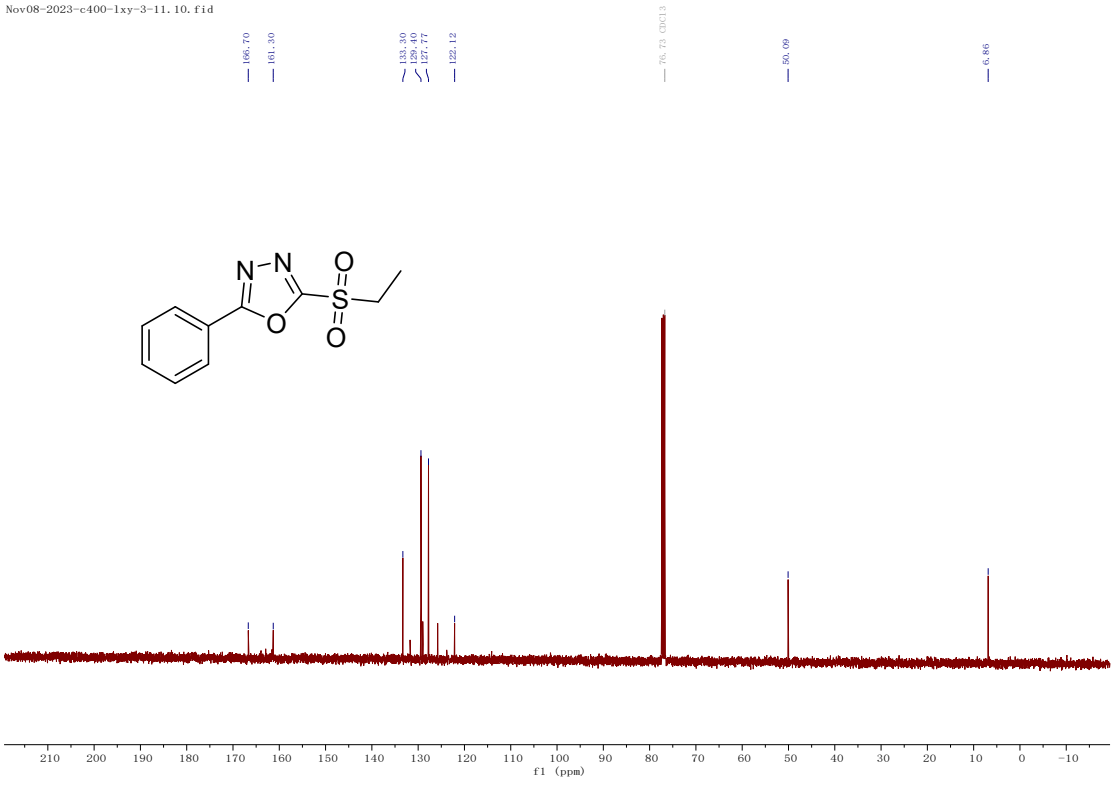
2-(ethylsulfonyl)benzo[d]oxazole (1j)



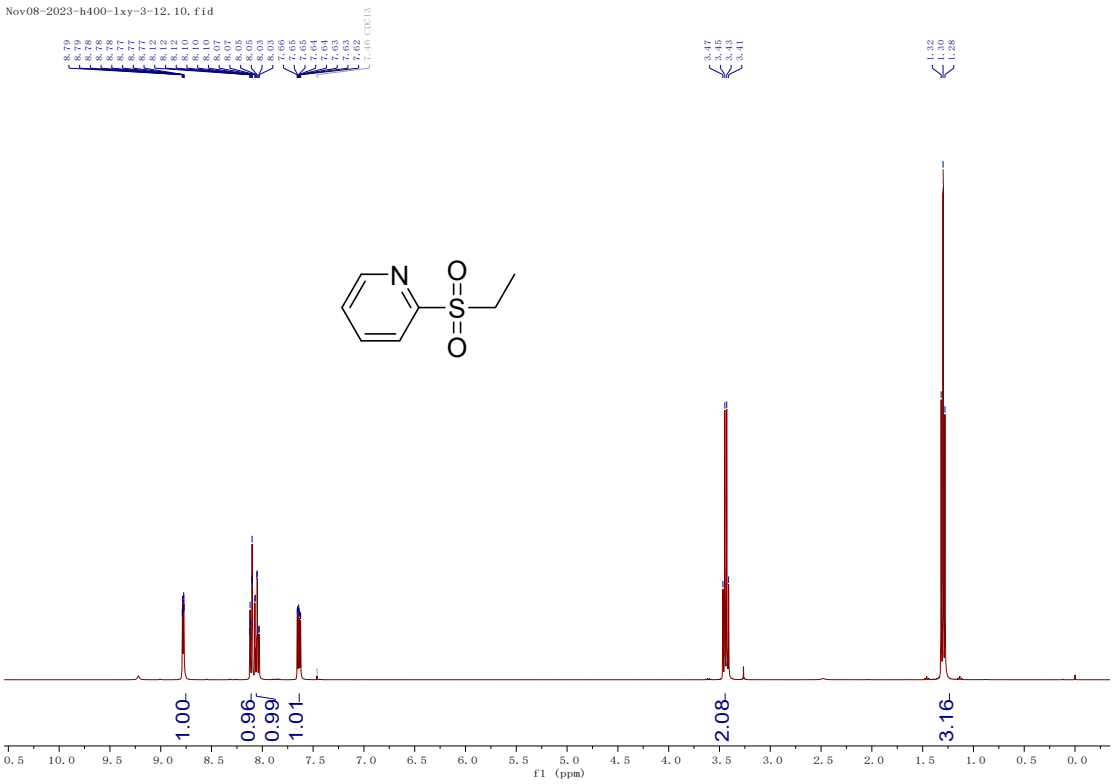


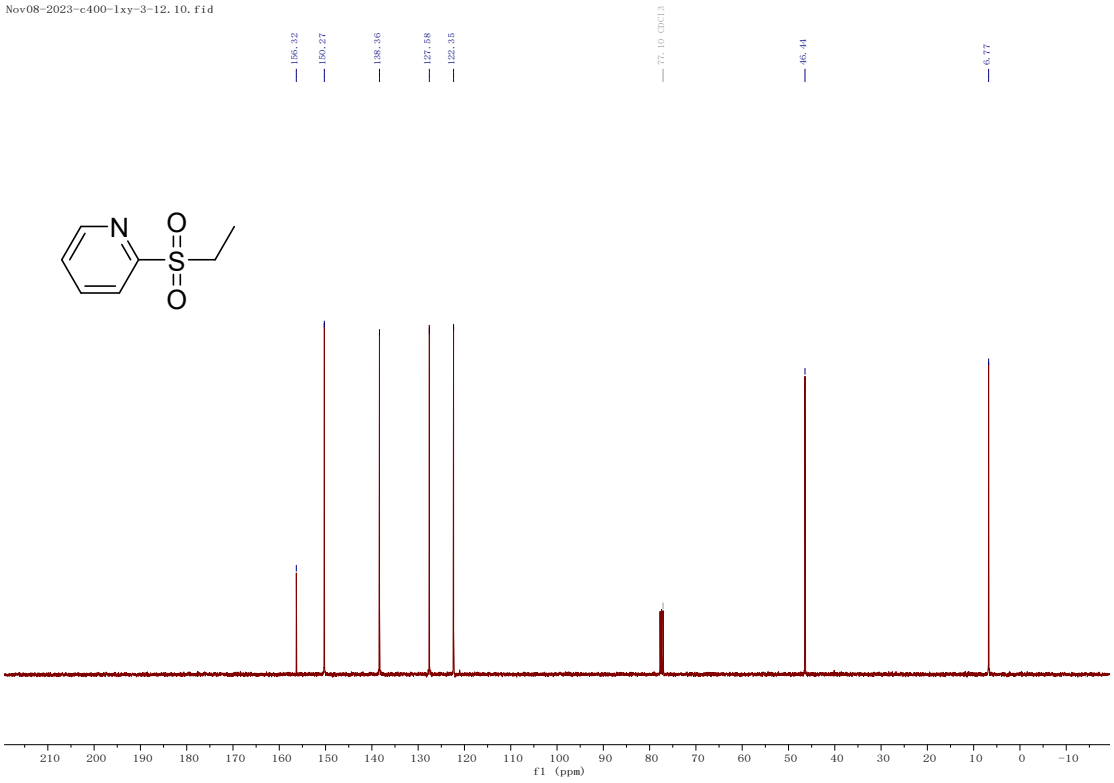
2-(ethylsulfonyl)-5-phenyl-1,3,4-oxadiazole (1k)





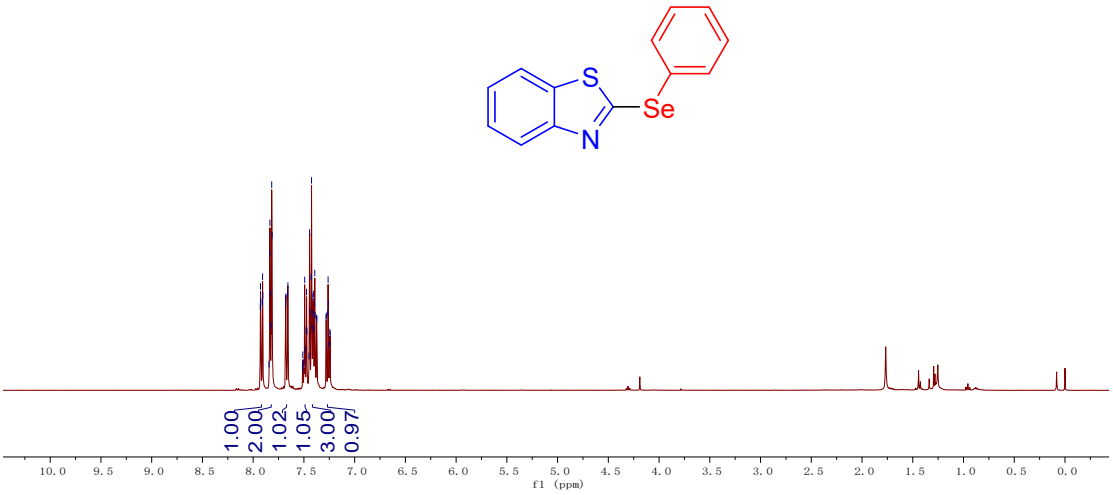
2-(ethylsulfonyl)pyridine (1m)



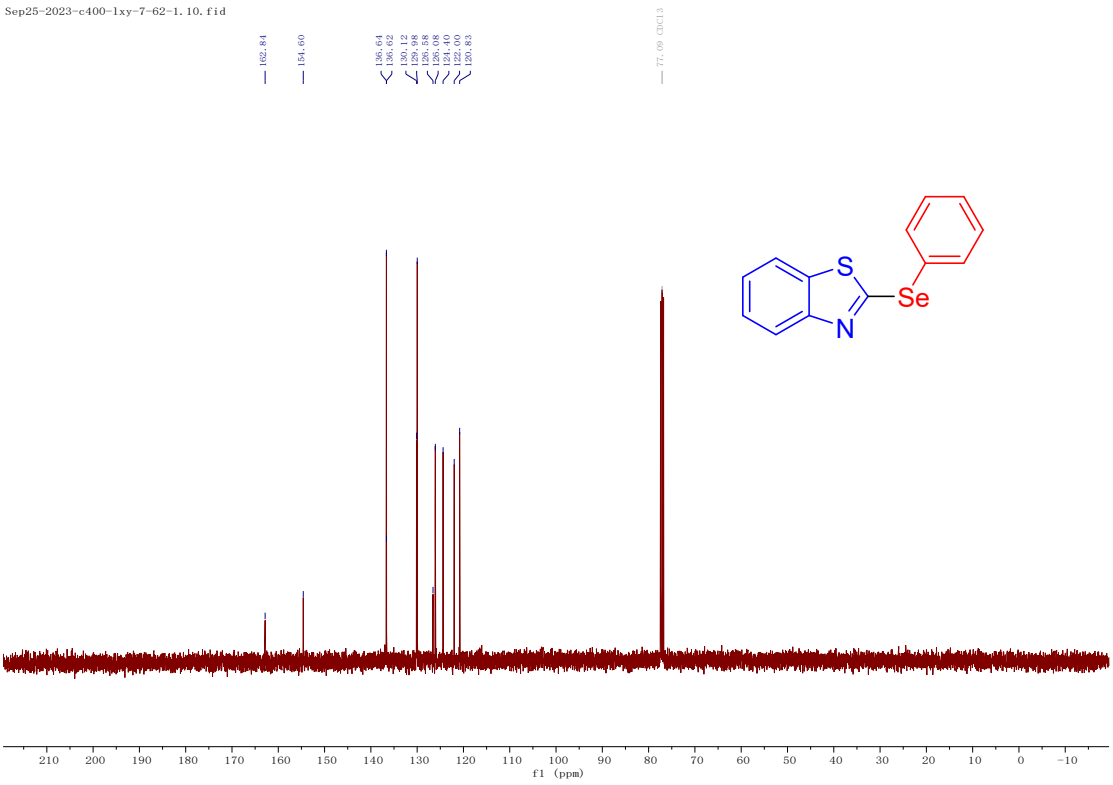


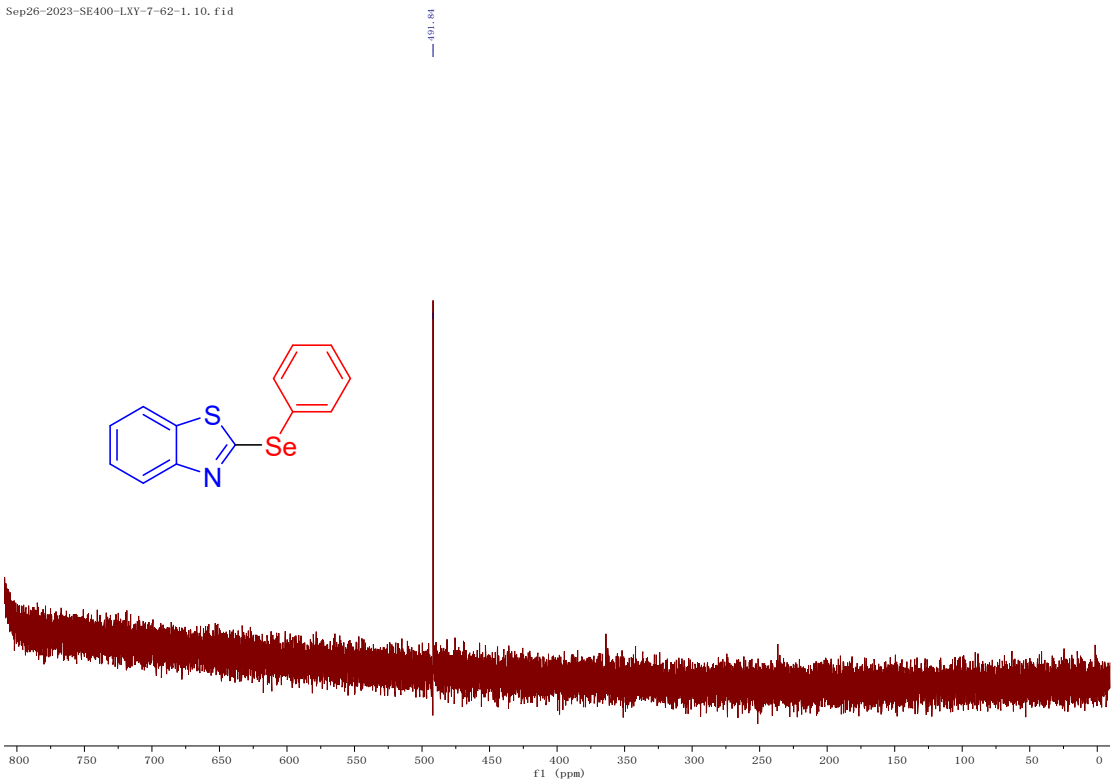
2-(phenylselanyl)benzo[*d*]thiazole (3a)

Sep25-2023-h400-1xy-7-62-1.10.fid

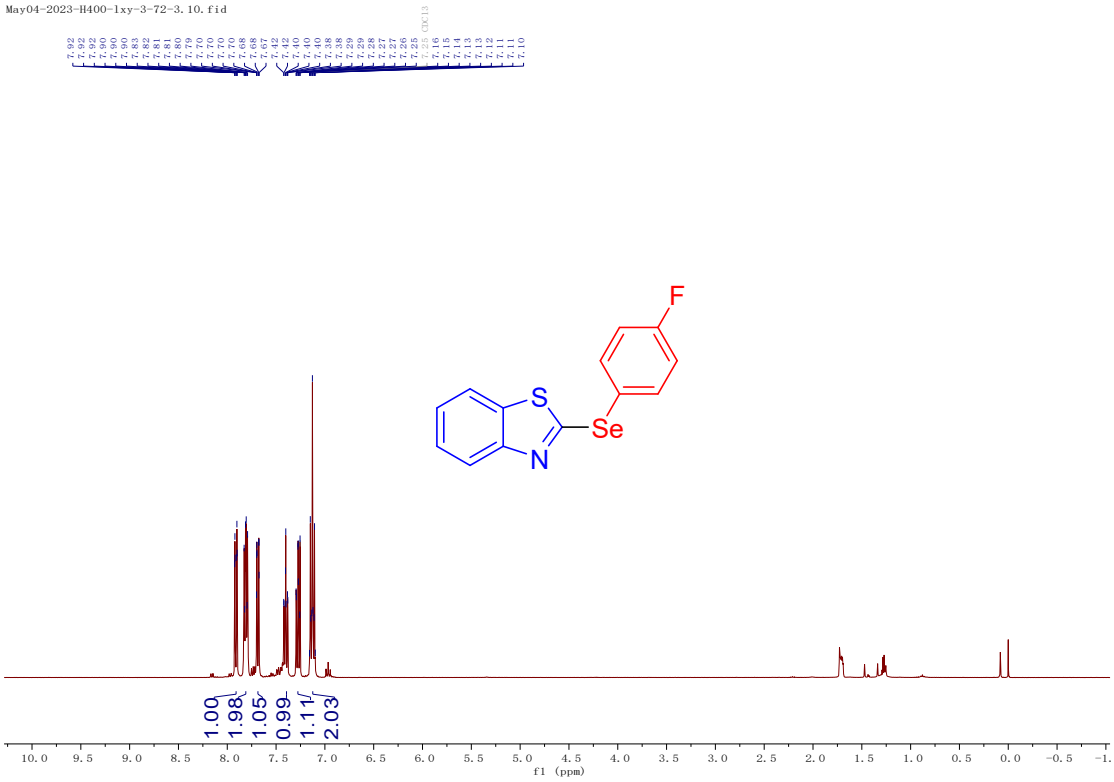


Sep25-2023-c400-1xy-7-62-1.10.fid

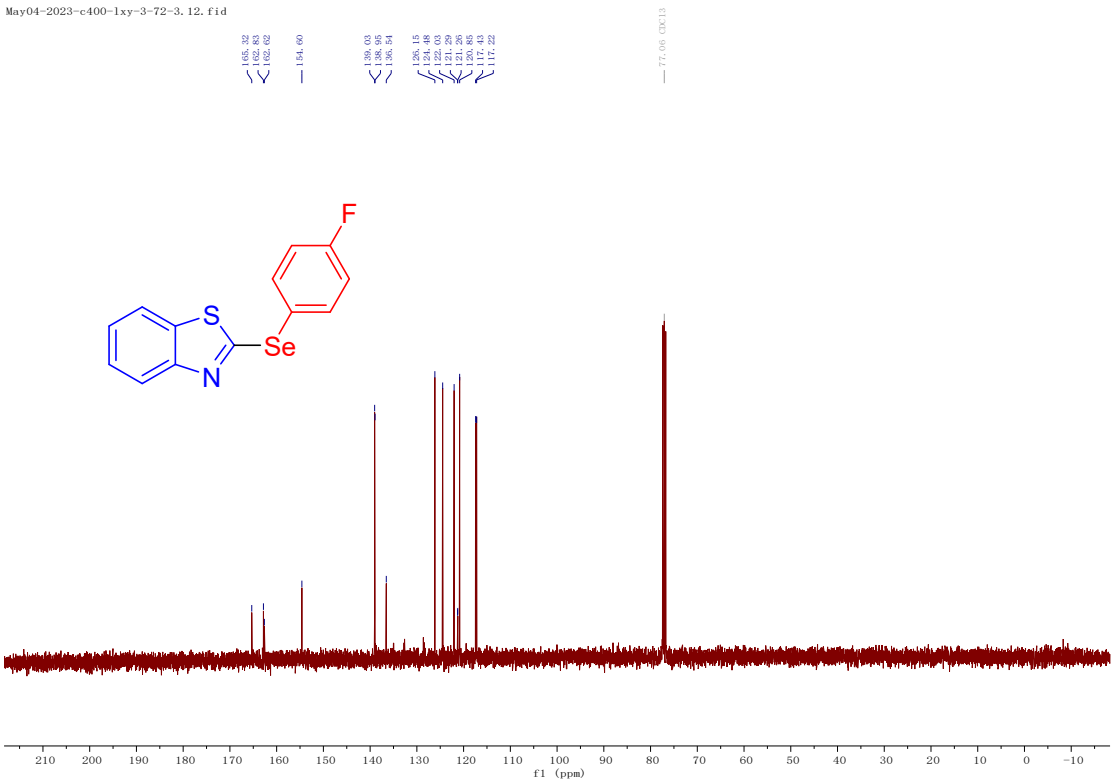




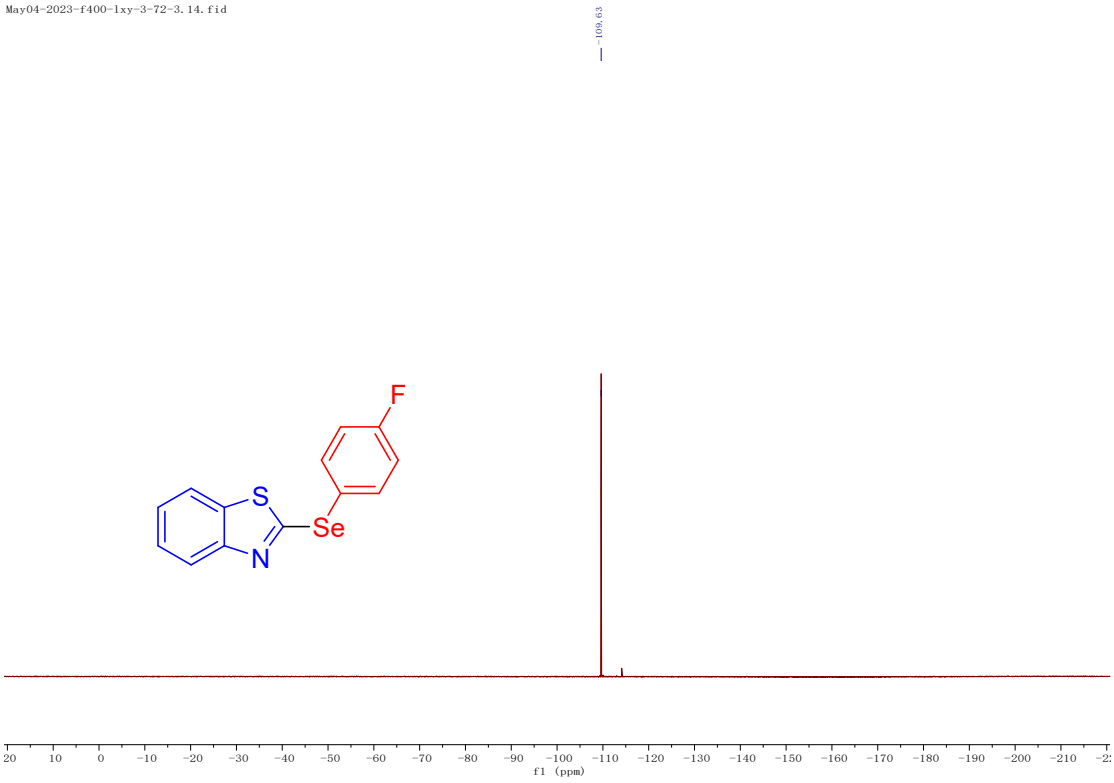
2-((4-fluorophenyl)selanyl)benzo[*d*]thiazole (3b)

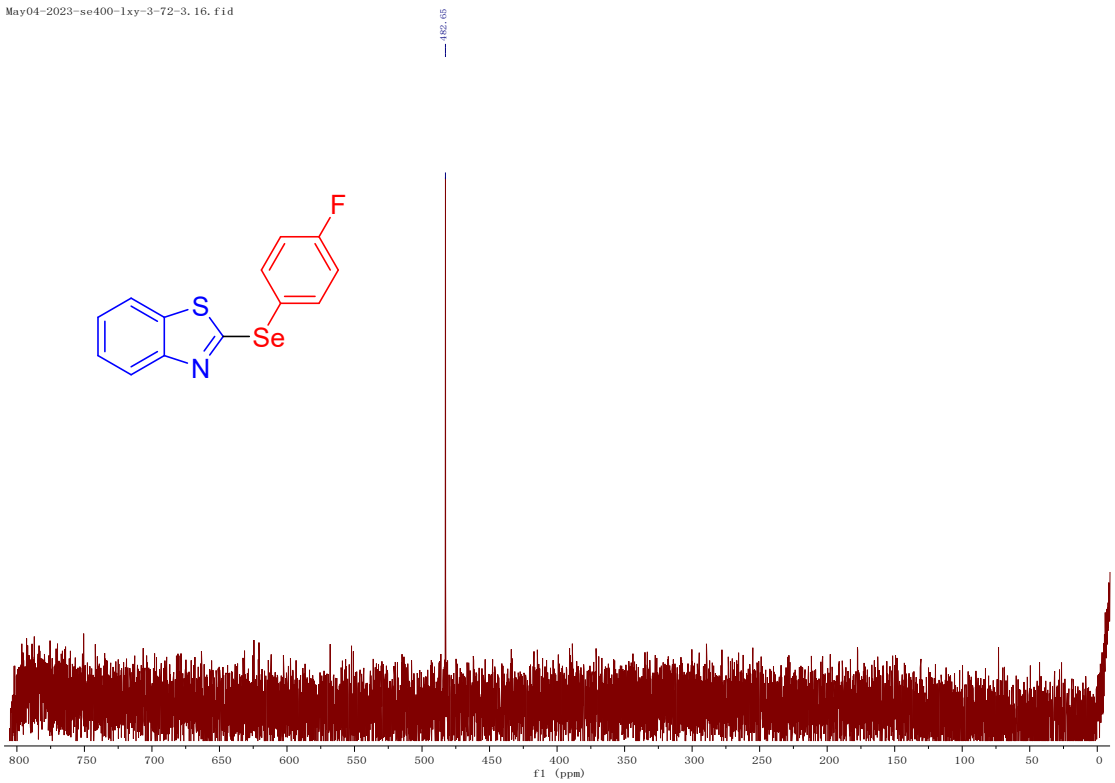


May04-2023-c400-lxy-3-72-3.12.fid

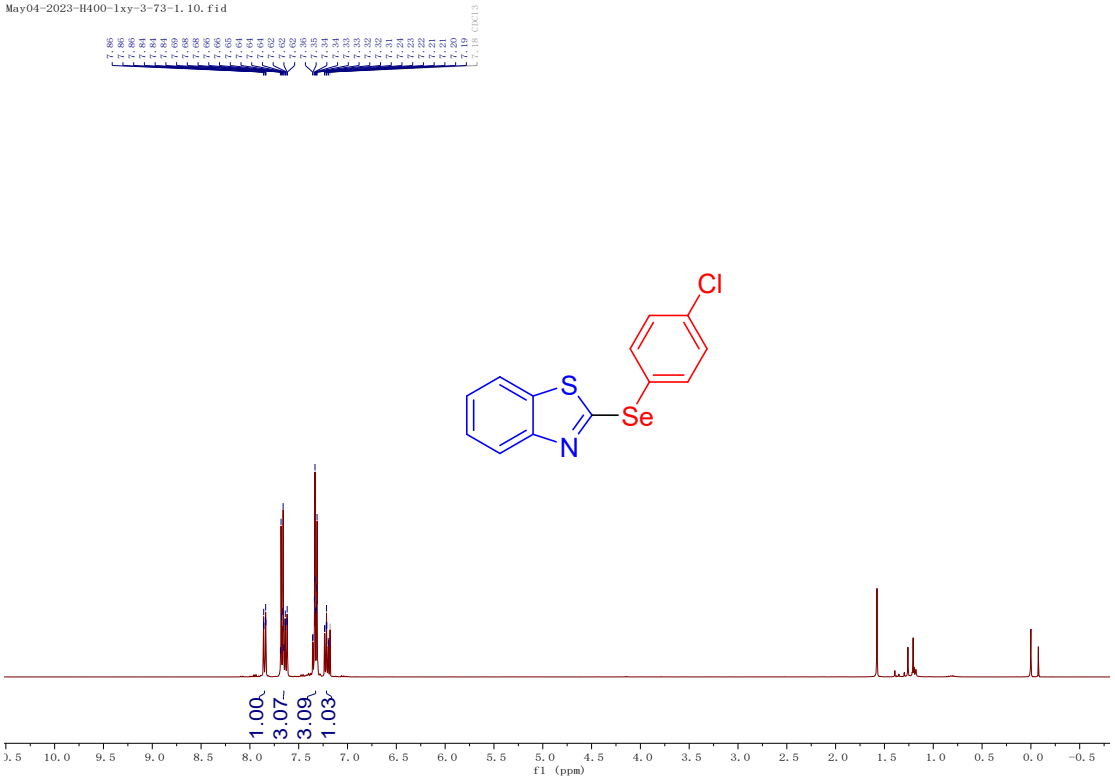


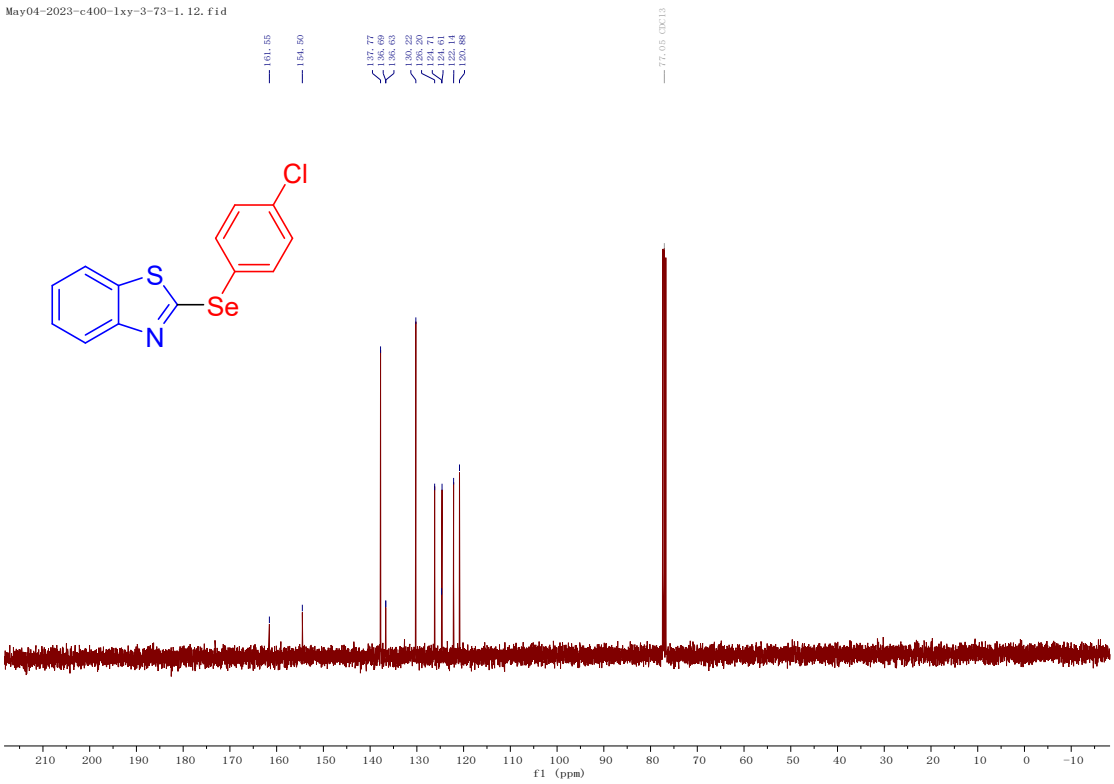
May04-2023-f400-lxy-3-72-3.14.fid

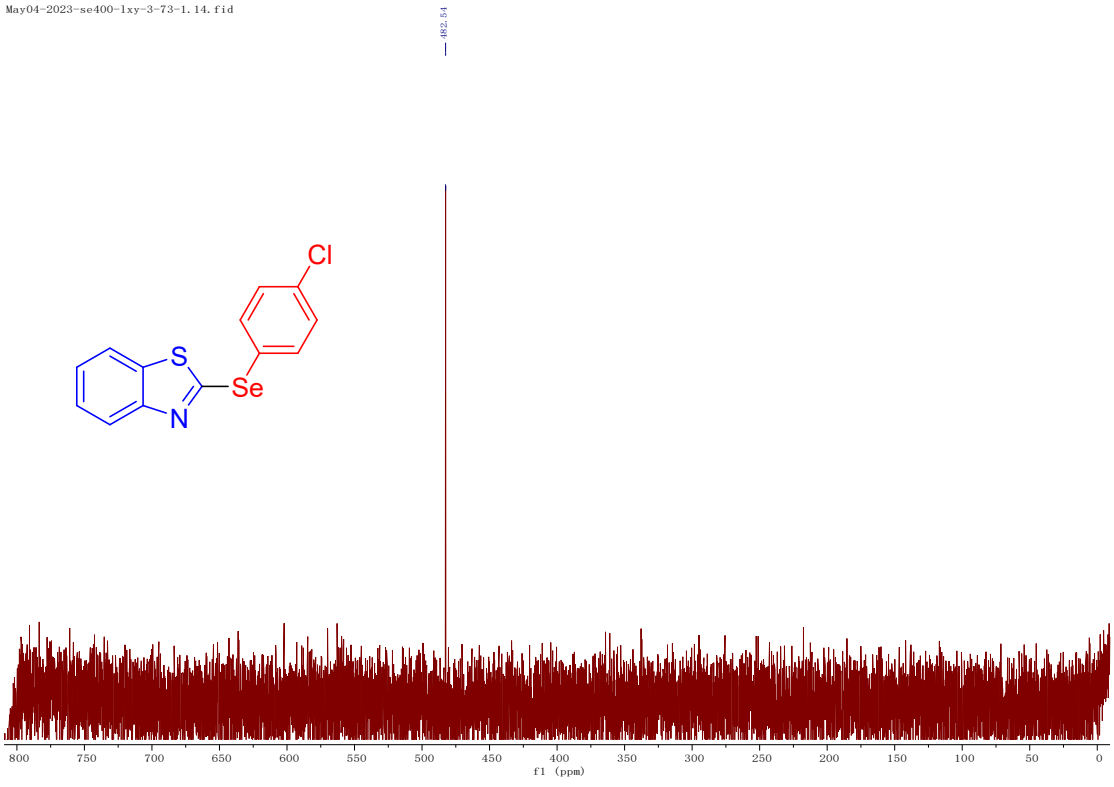




2-((4-chlorophenyl)selanyl)benzo[*d*]thiazole (3c)

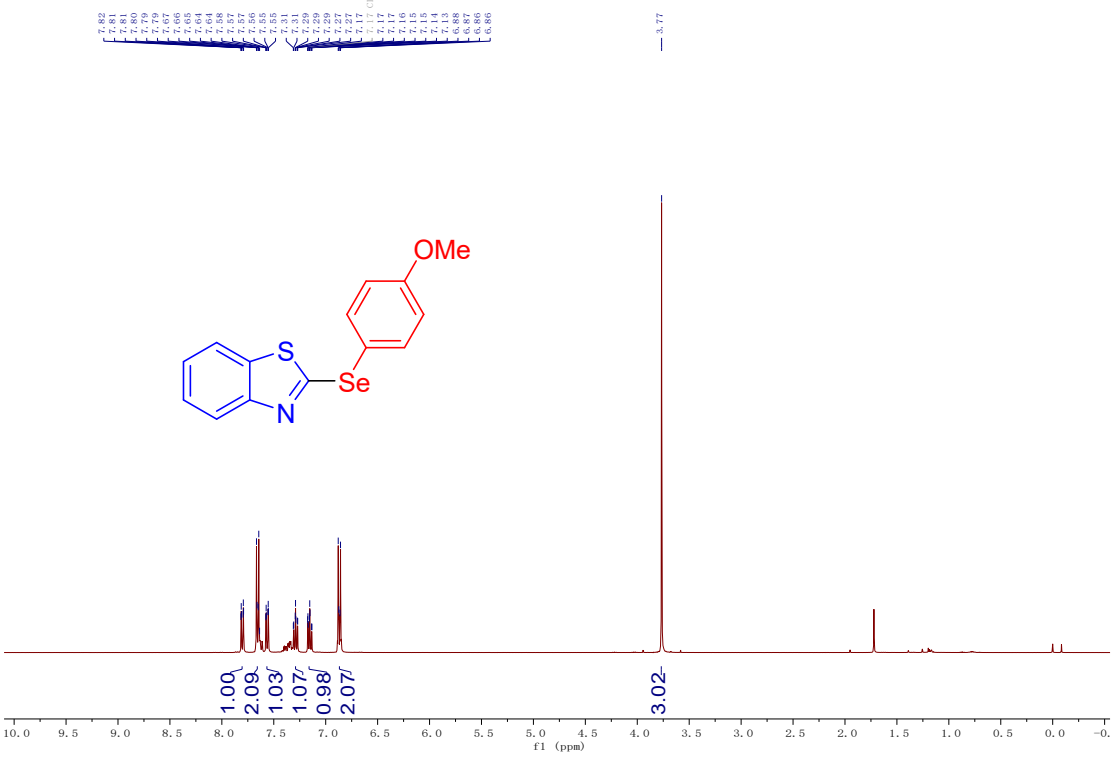




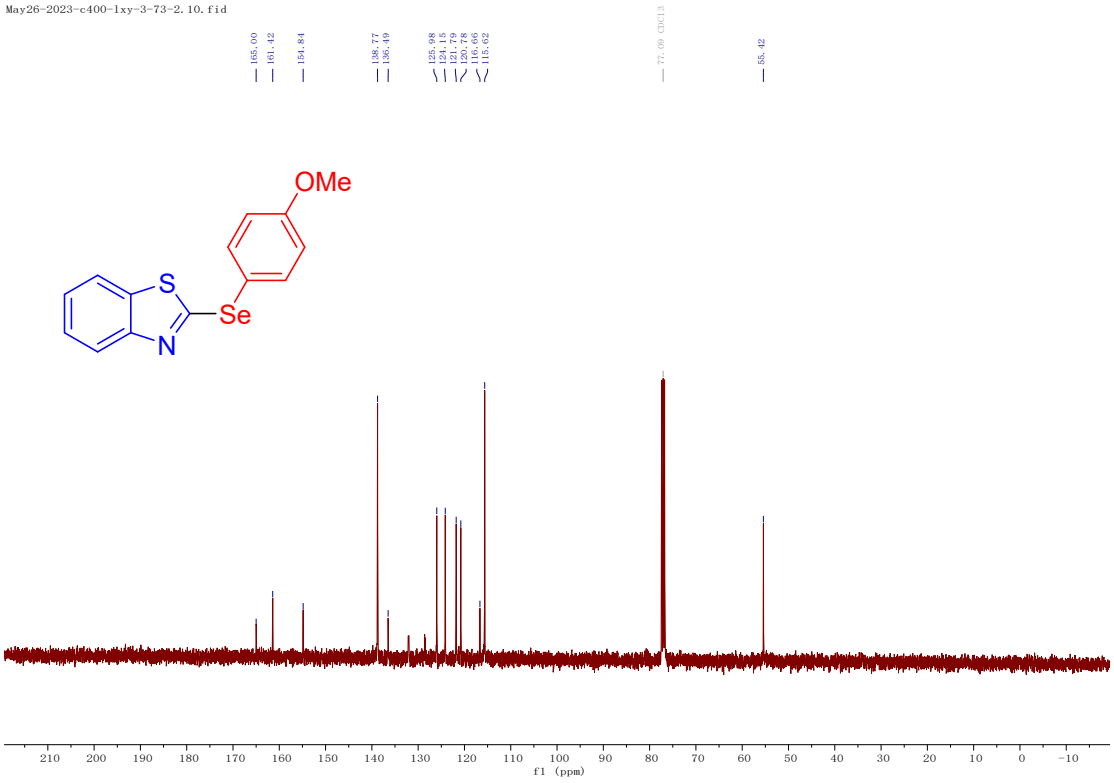


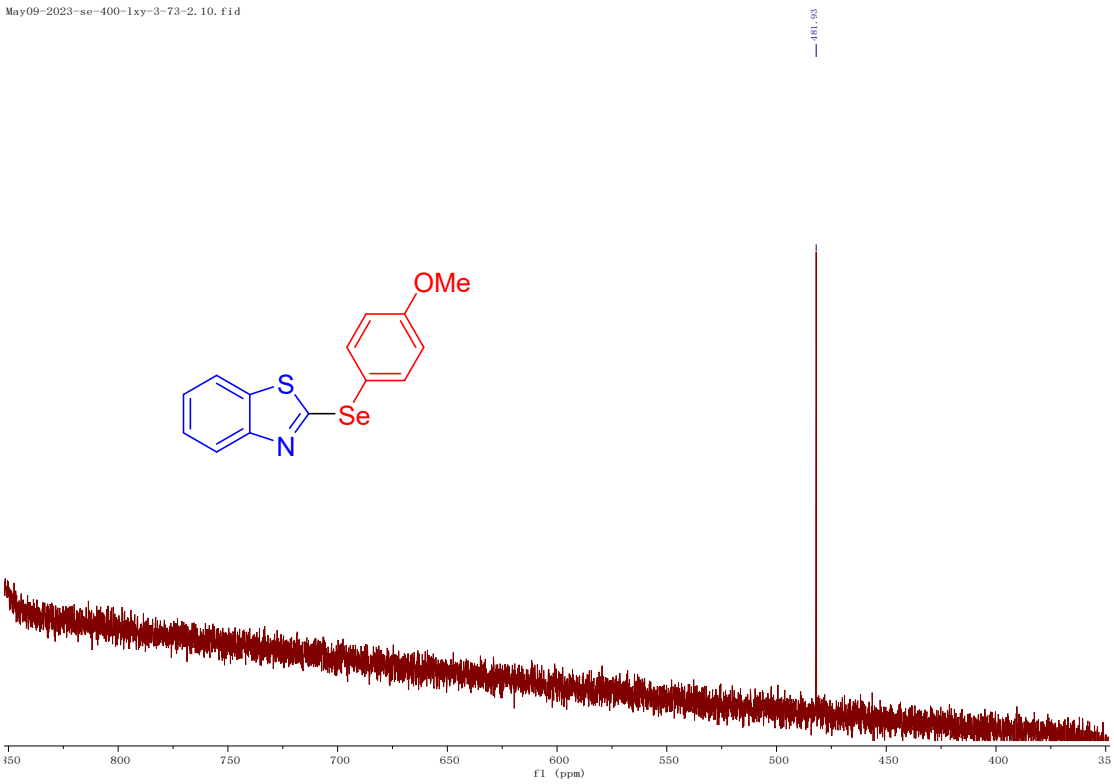
2-((4-methoxyphenyl)selanyl)benzo[*d*]thiazole (3d)

May03-2023-h400-lxy-3-73-2.10.fid

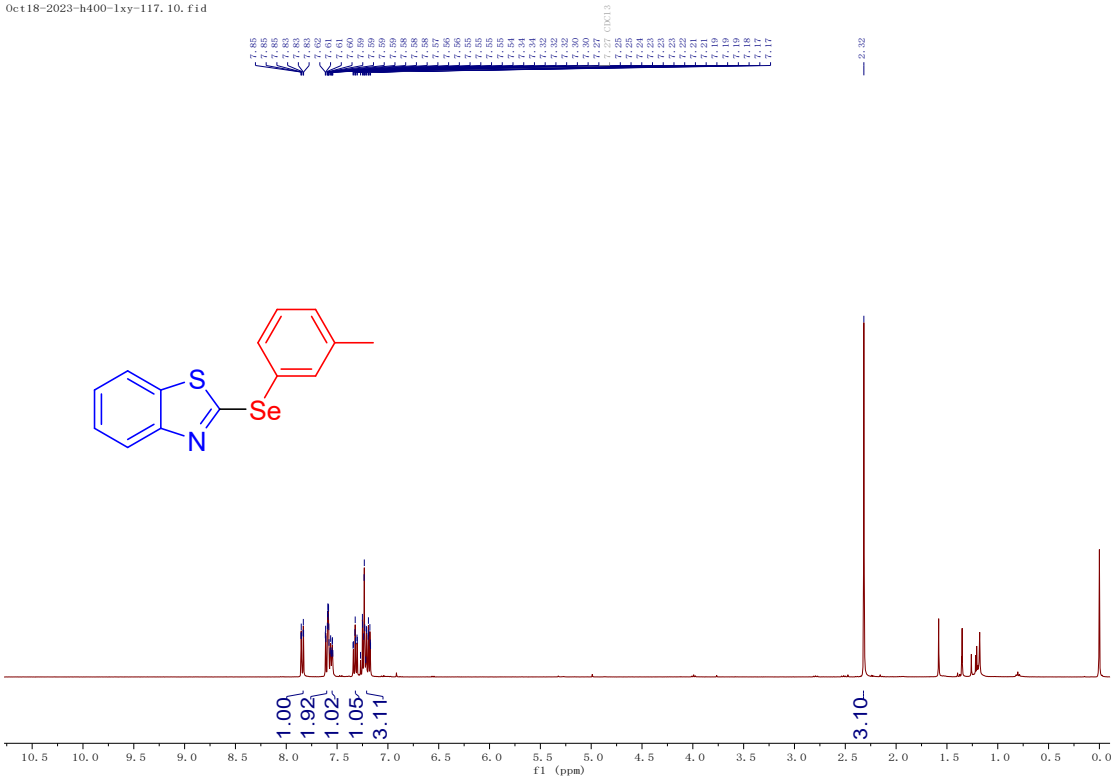


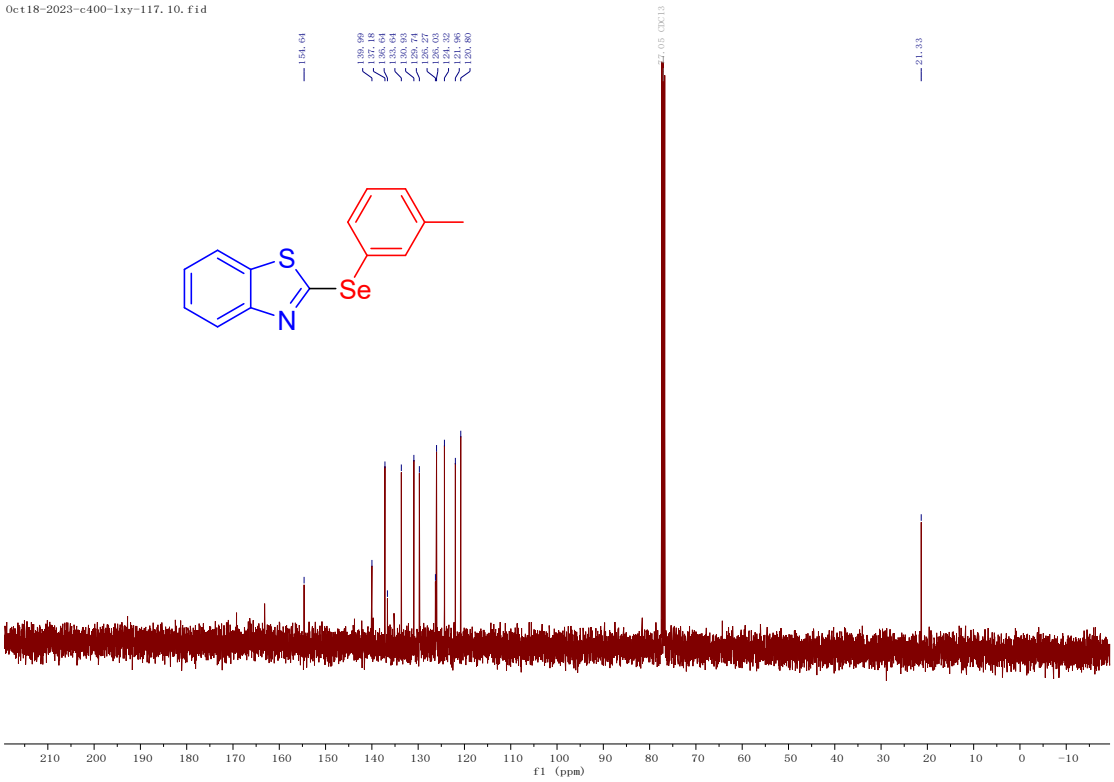
May26-2023-c400-lxy-3-73-2.10.fid

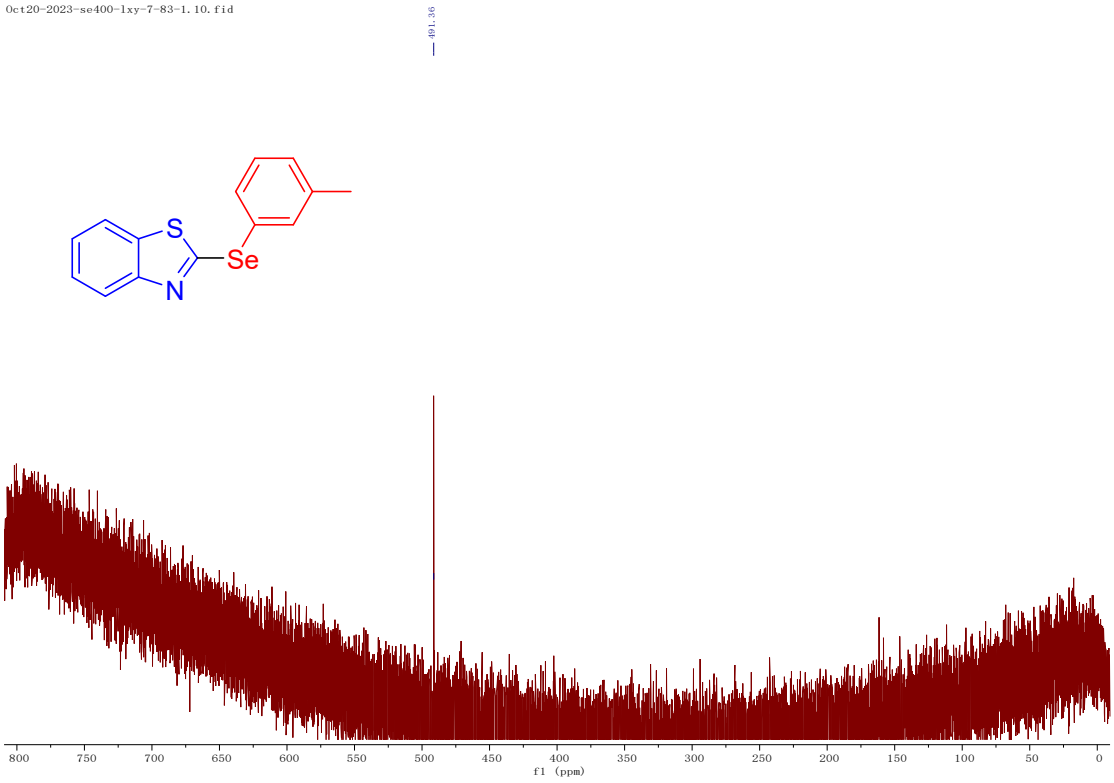




2-(*m*-tolylselanyl)benzo[*d*]thiazole (3e)

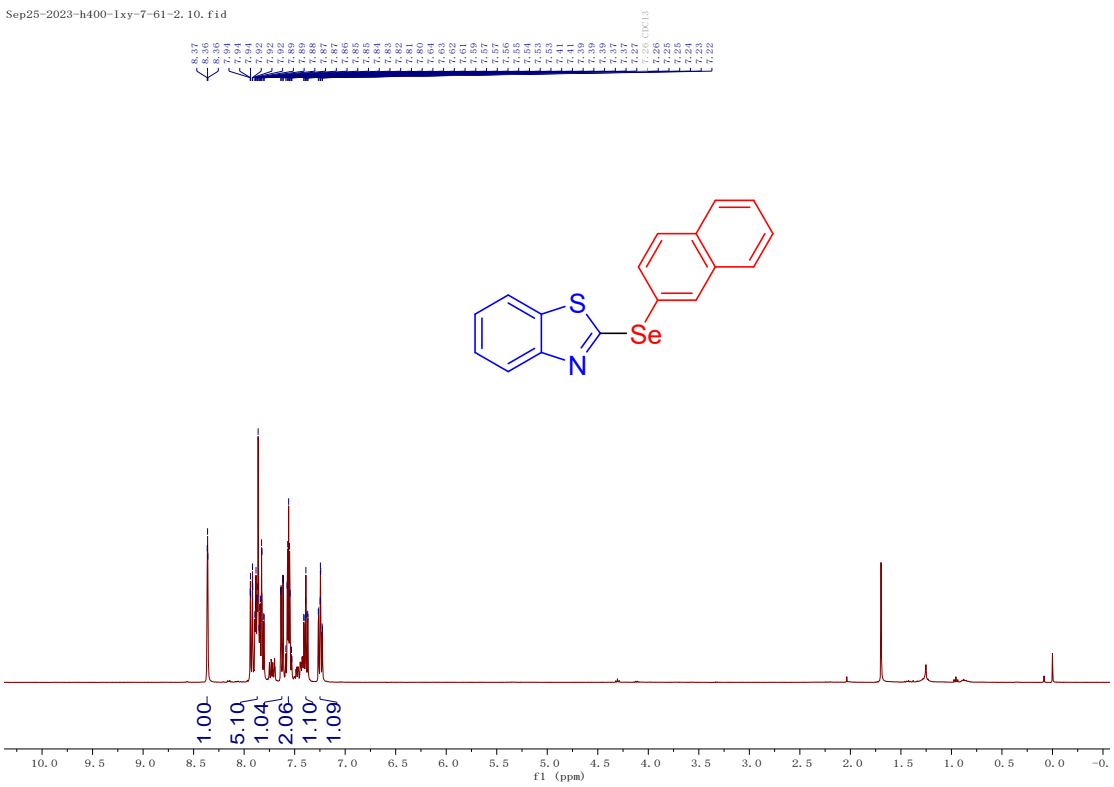




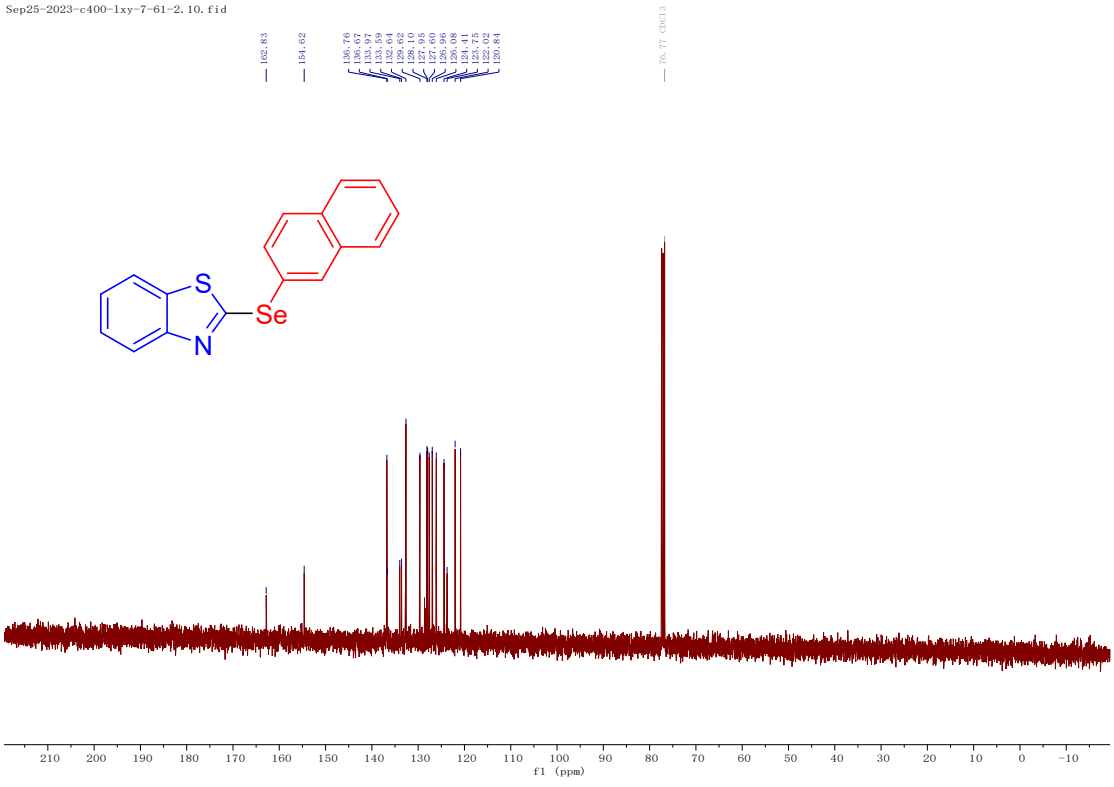


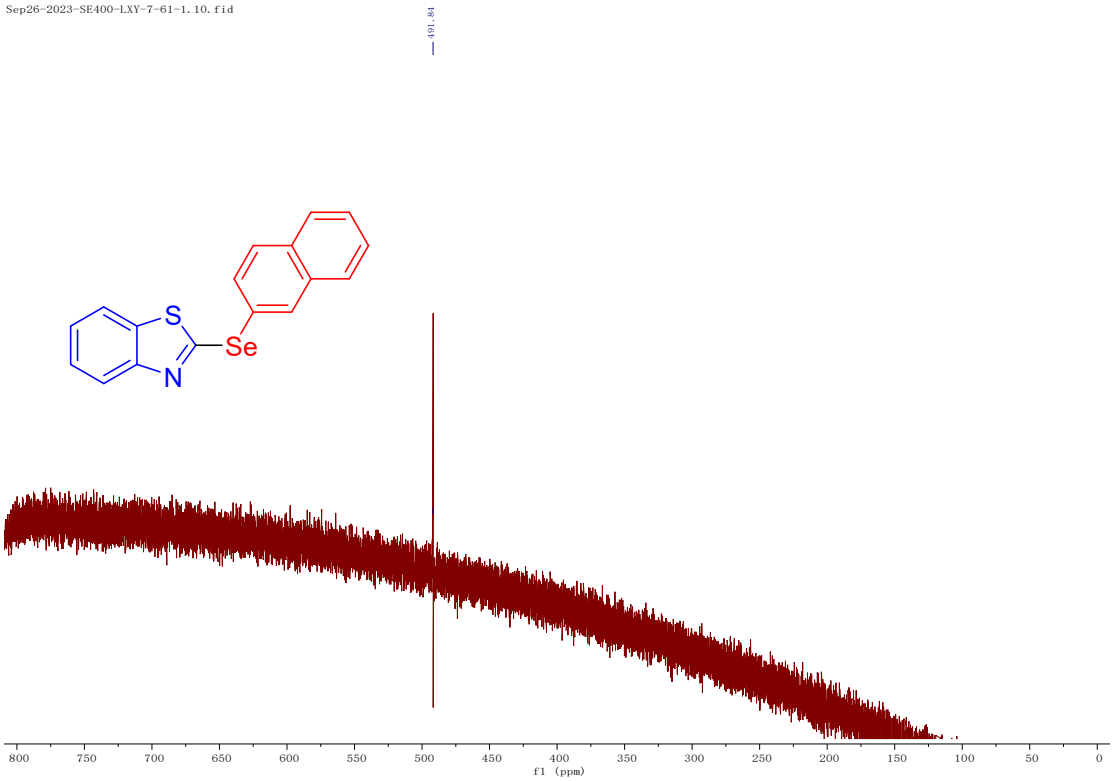
2-(naphthalen-2-ylselanyl)benzo[*d*]thiazole (3f)

Sep25-2023-h400-lxy-7-61-2.10.fid

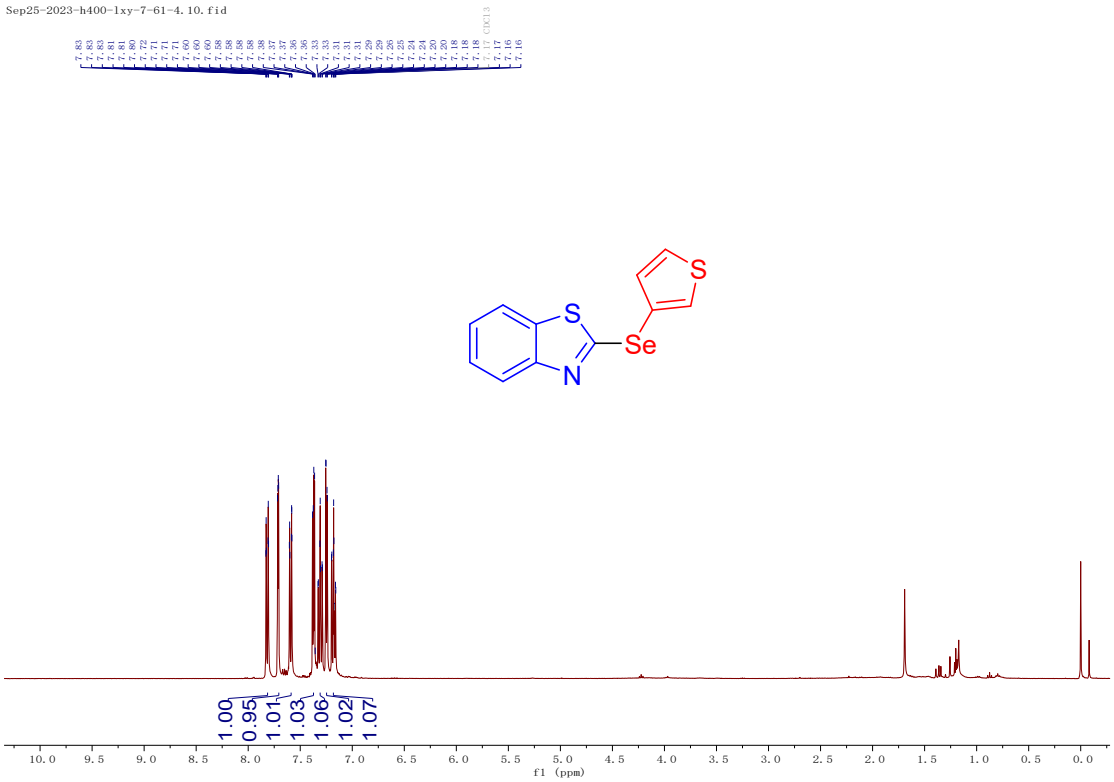


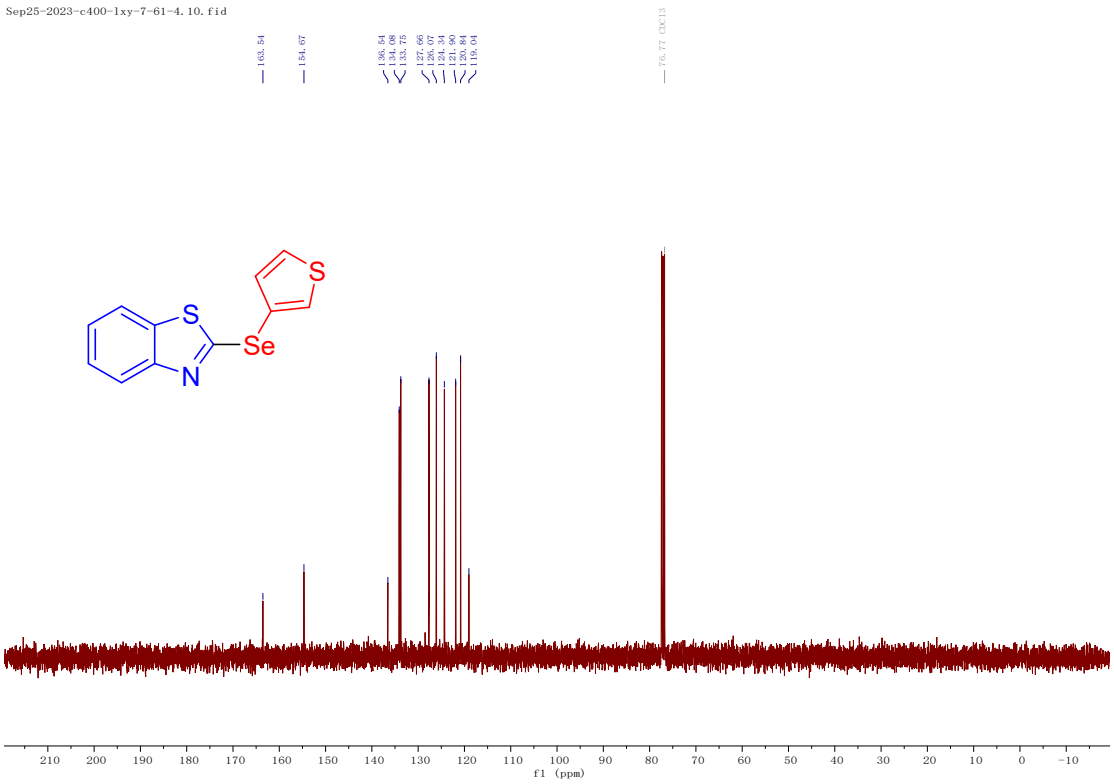
Sep25-2023-c400-lxy-7-61-2.10.fid

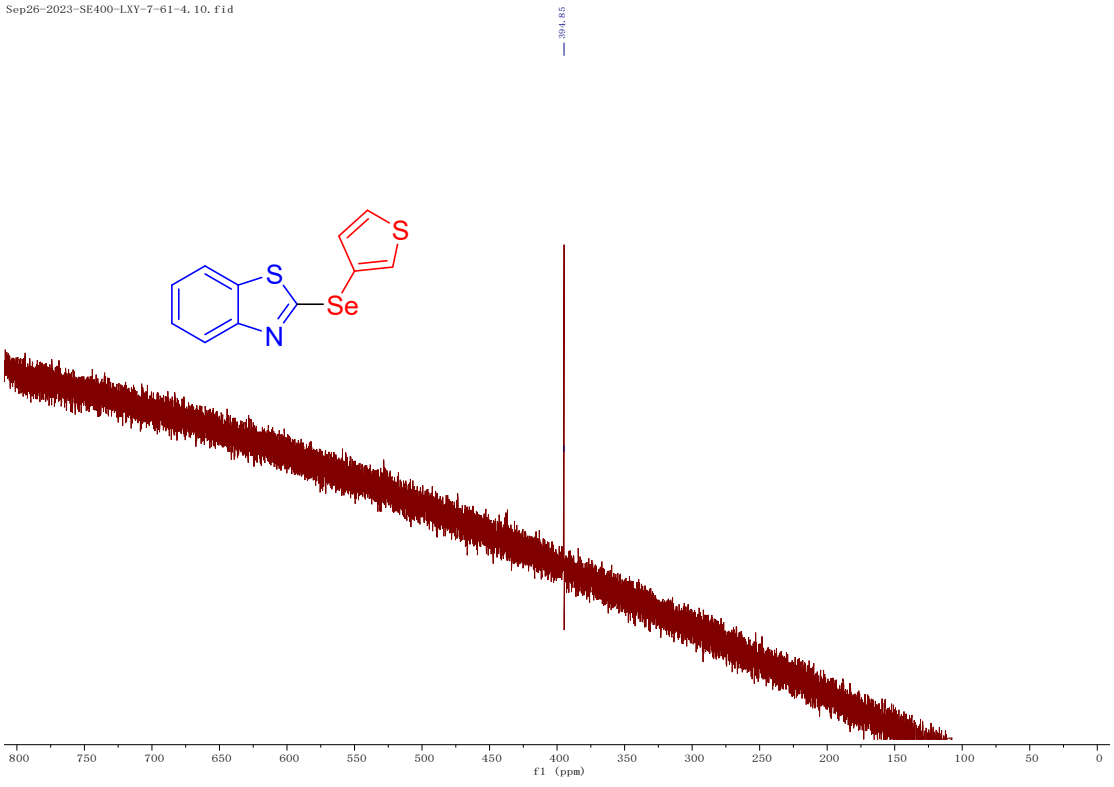




2-(thiophen-3-ylselanyl)benzo[*d*]thiazole (3g)

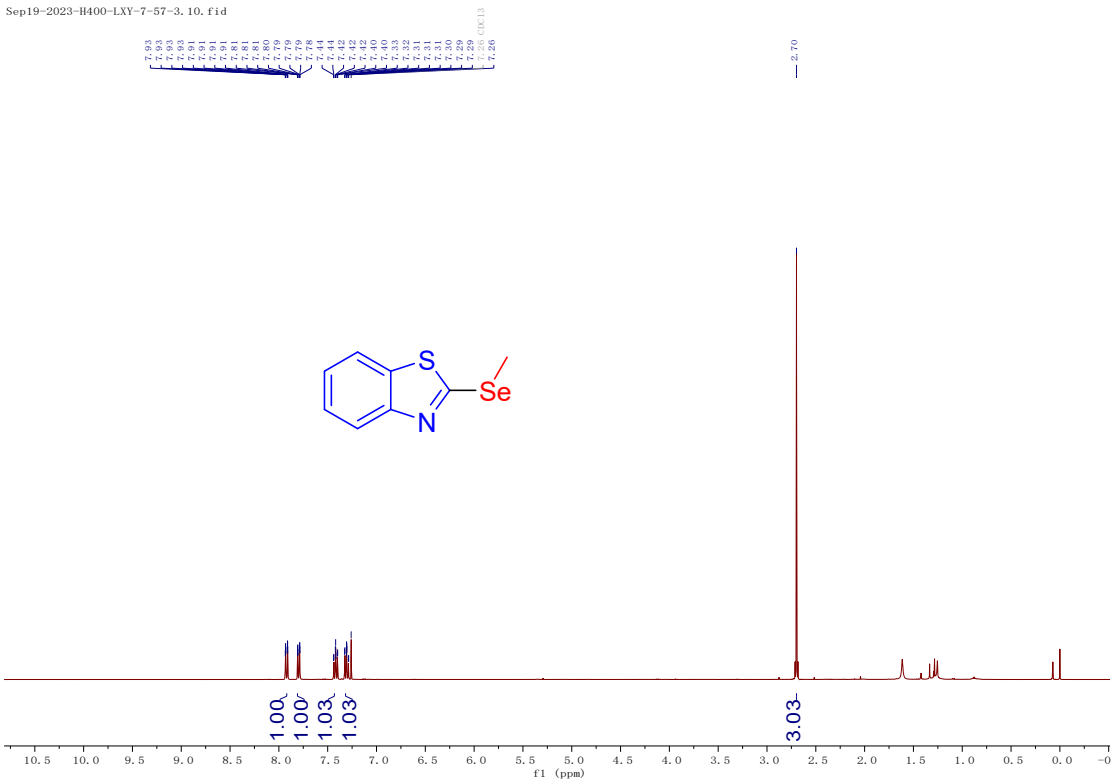




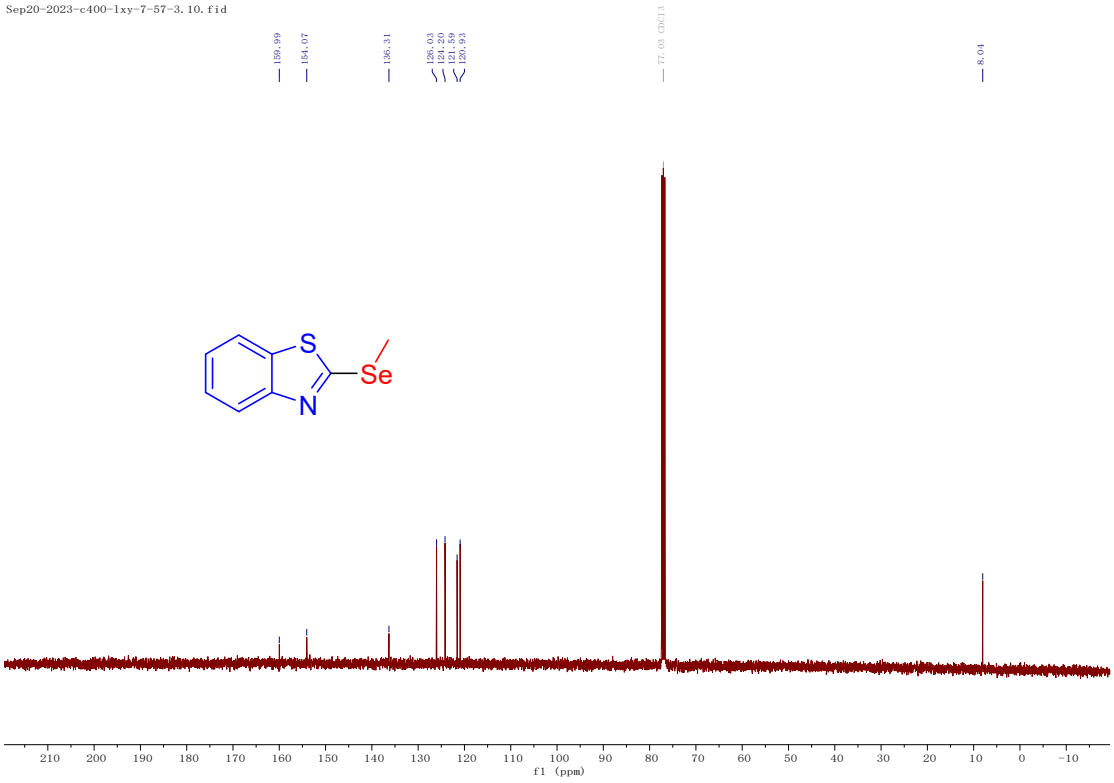


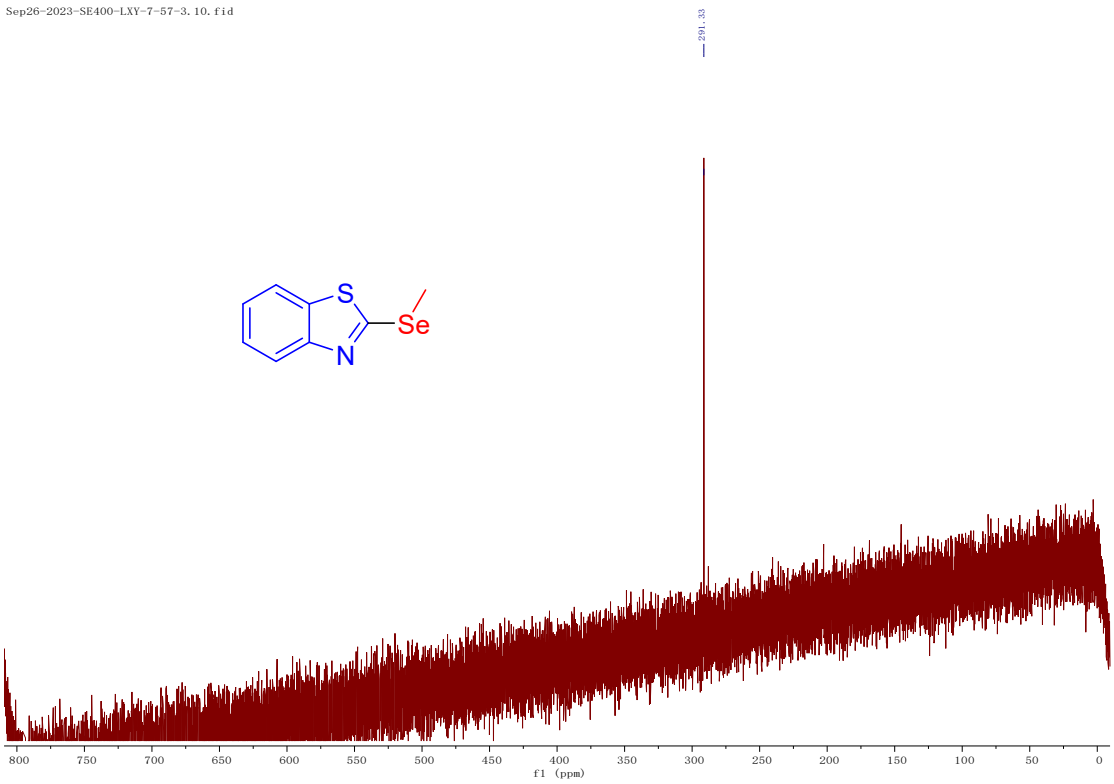
2-(methylselanyl)benzo[*d*]thiazole (3j)

Sep19-2023-H400-LXY-7-57-3.10.fid

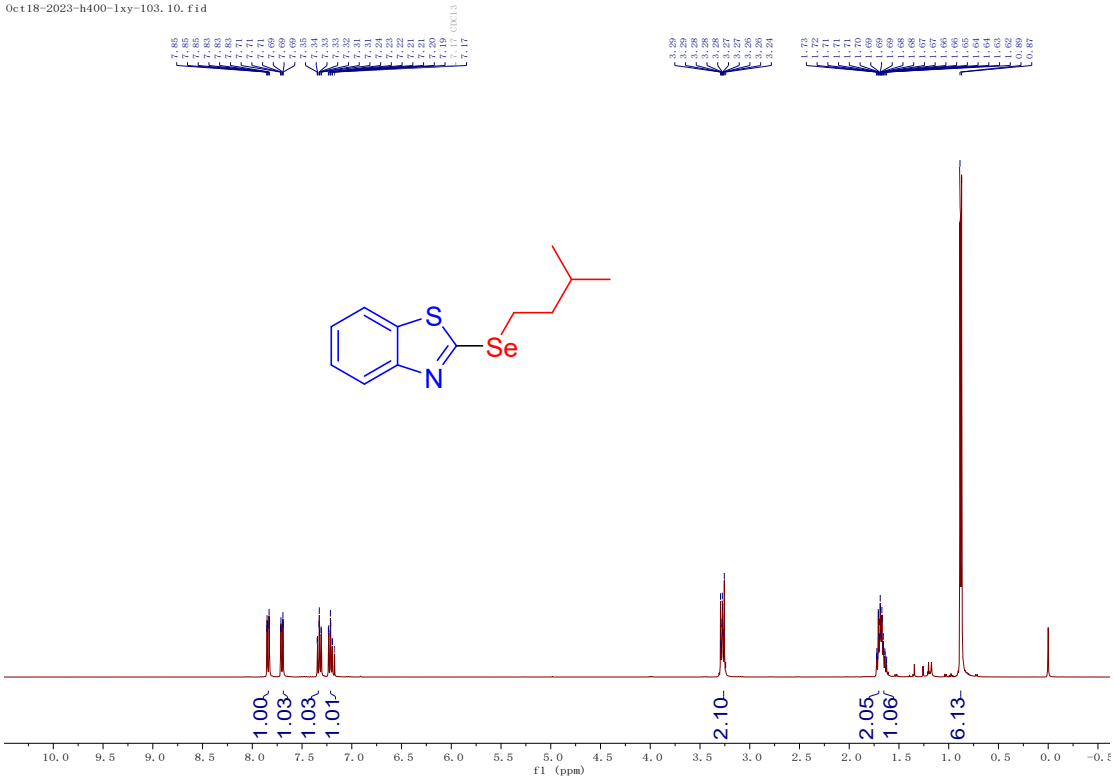


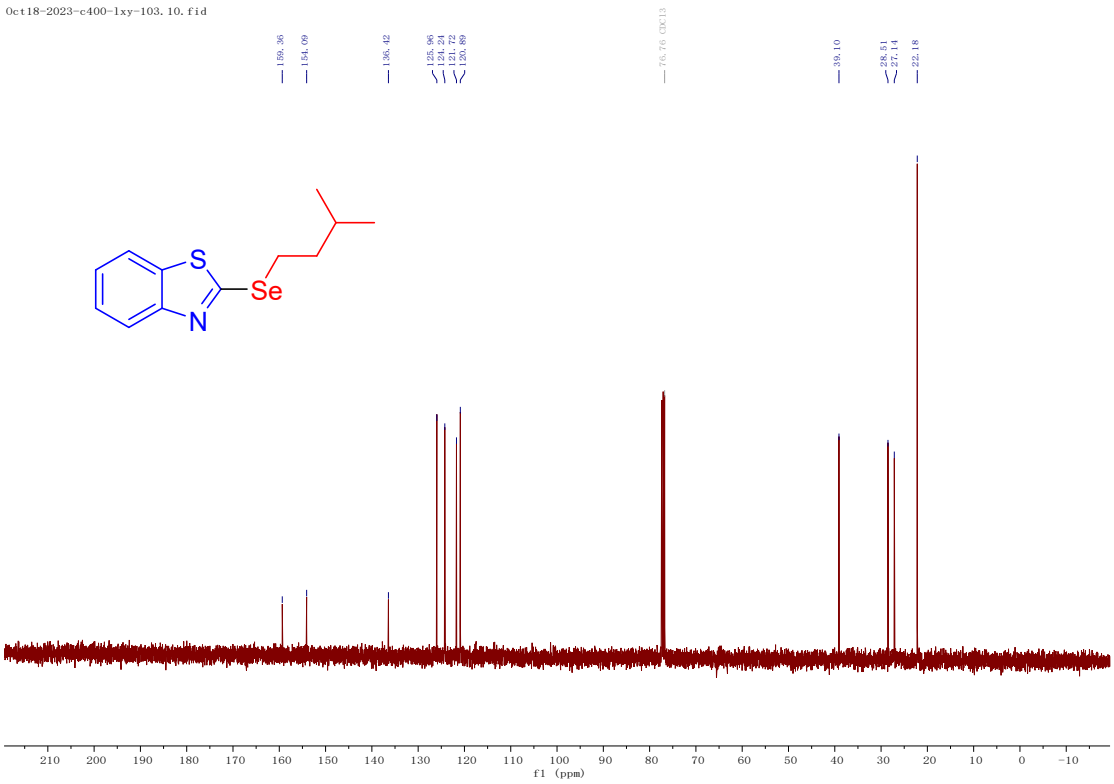
Sep20-2023-c400-lxy-7-57-3.10.fid

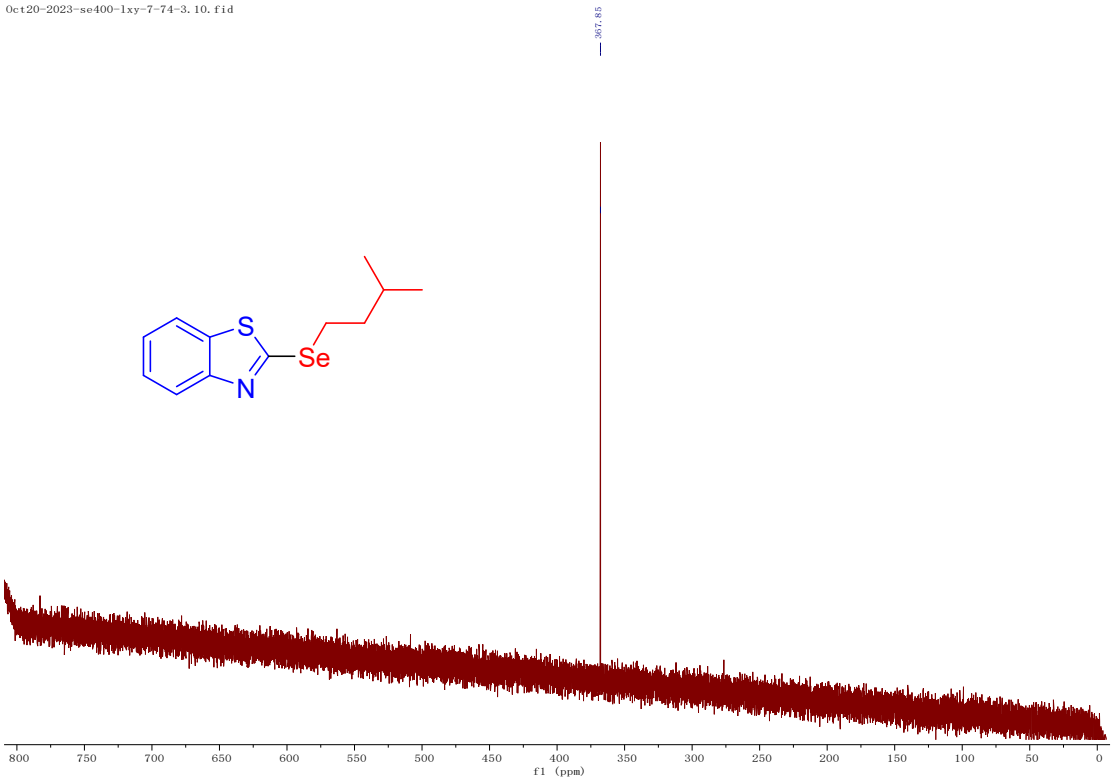




2-(isopentylselanyl)benzo[*d*]thiazole (3k)

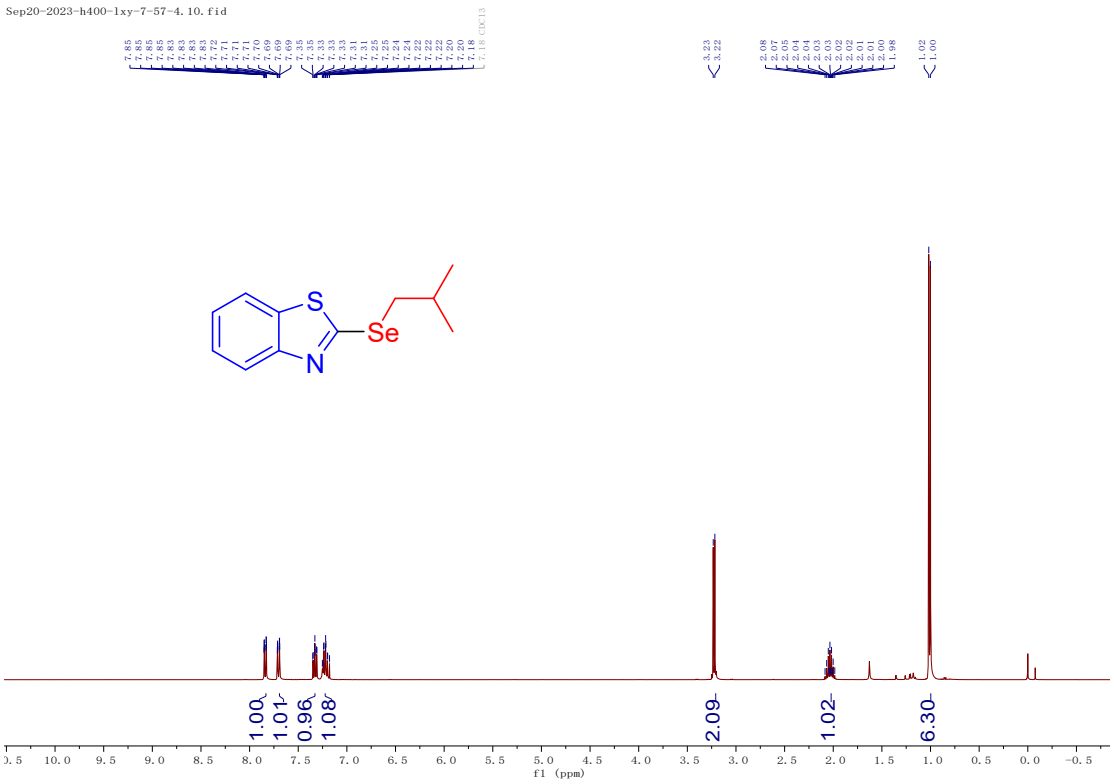




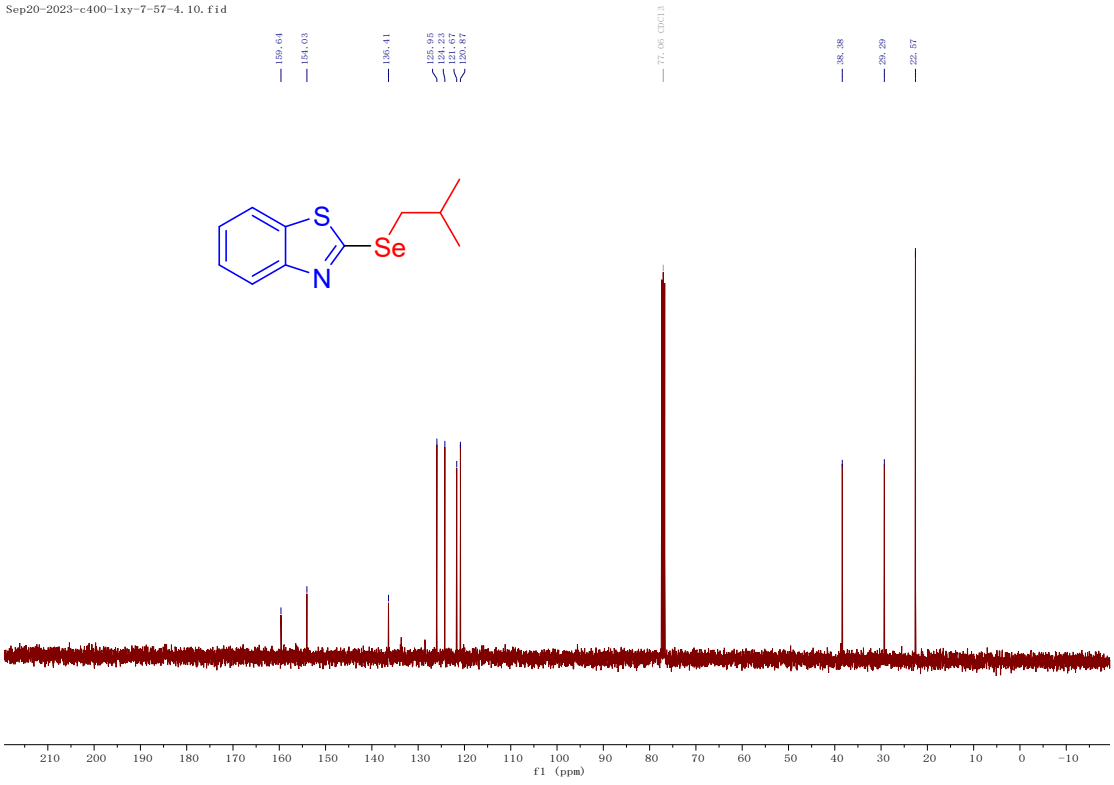


2-(isobutylselanyl)benzo[*d*]thiazole (3l)

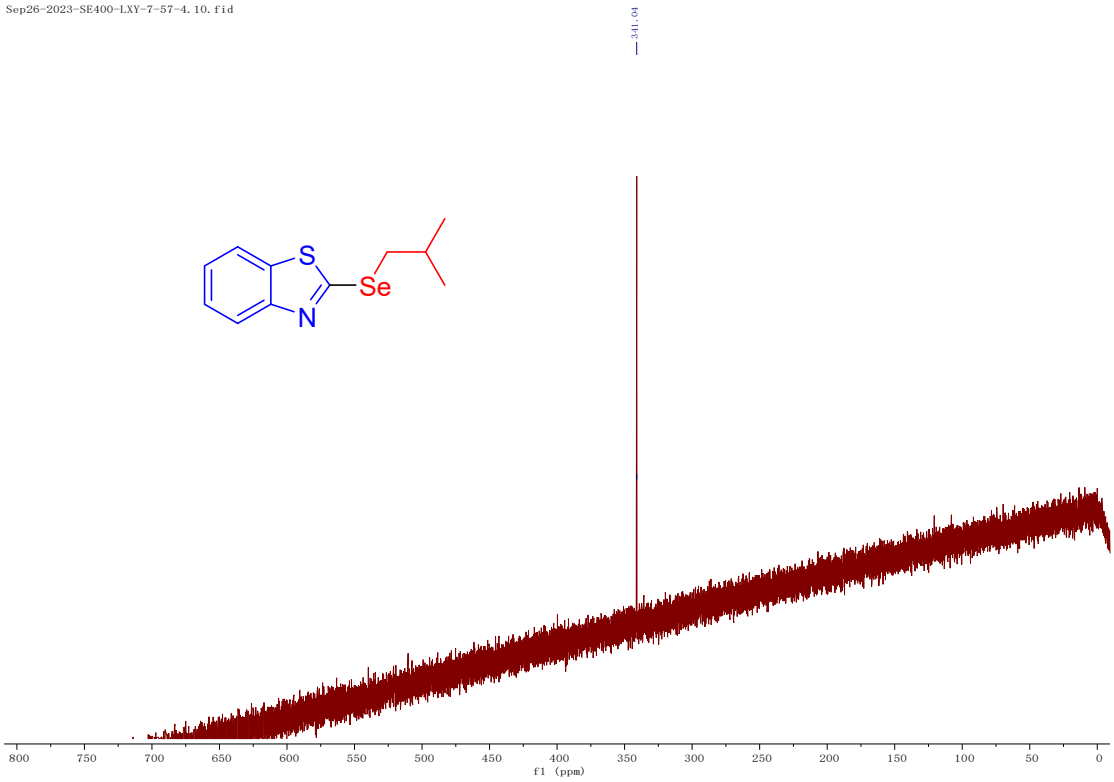
Sep20-2023-h400-1xy-7-57-4.10.fid



Sep20-2023-c400-1xy-7-57-4.10.fid

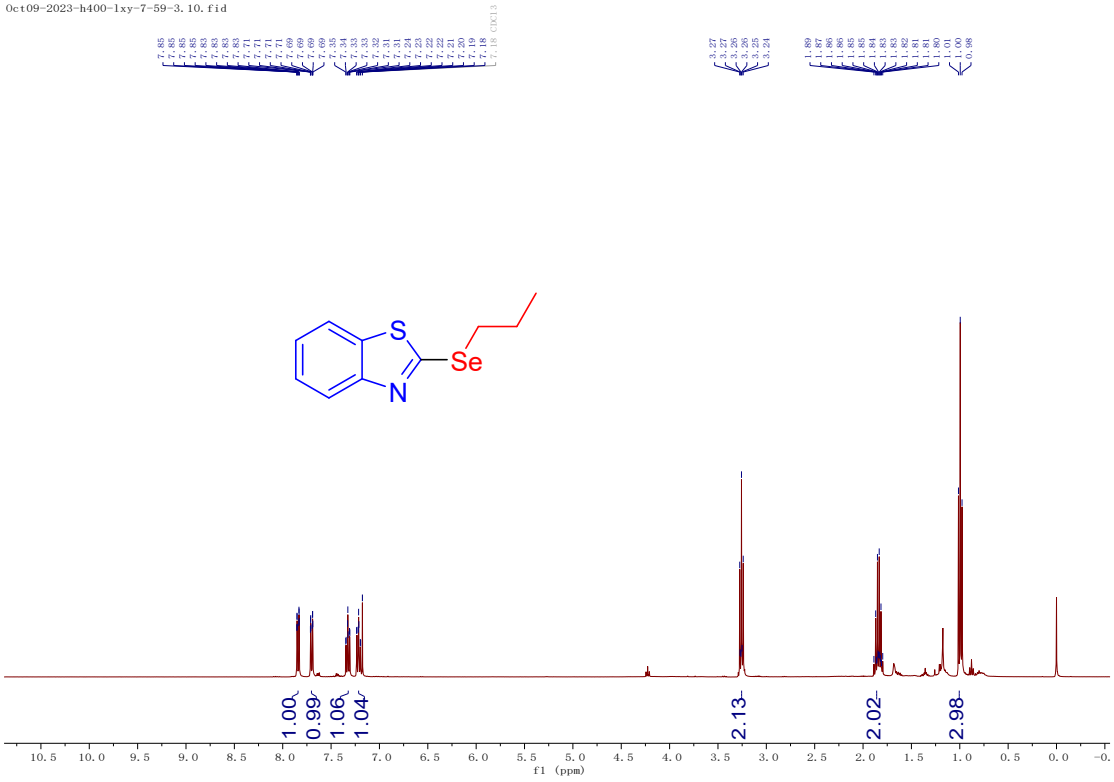


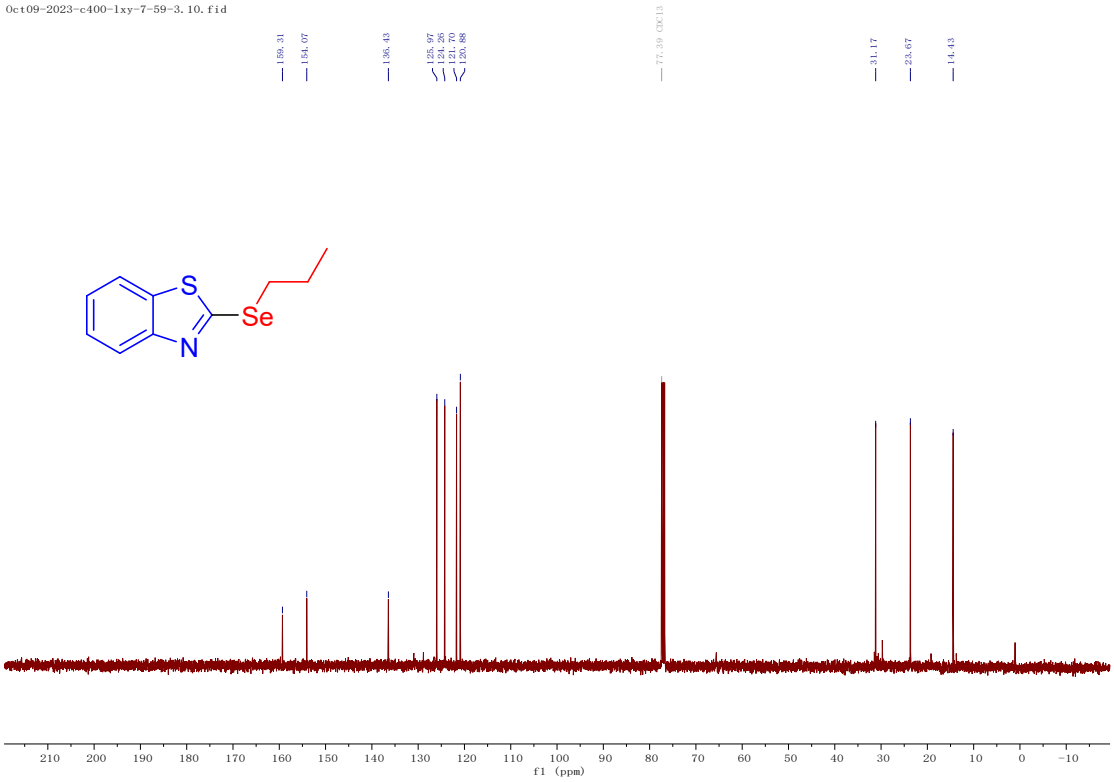
Sep26-2023-SE400-LXY-7-57-4.10.fid

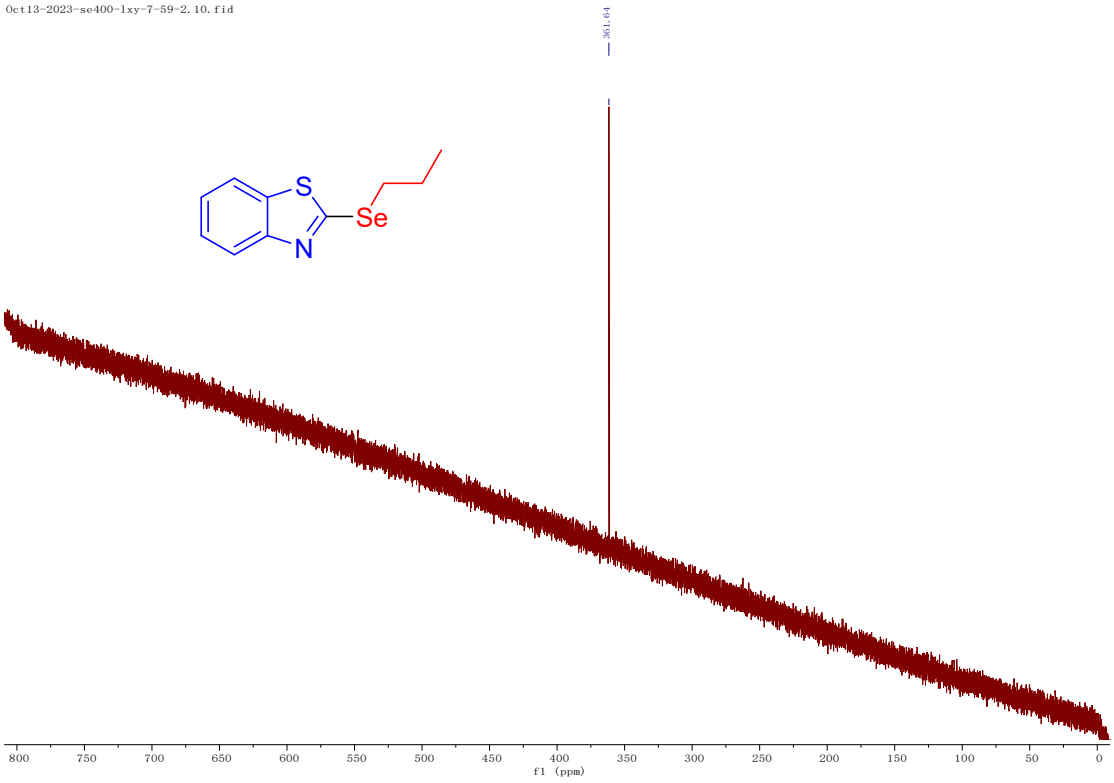


2-(propylselanyl)benzo[*d*]thiazole (3m)

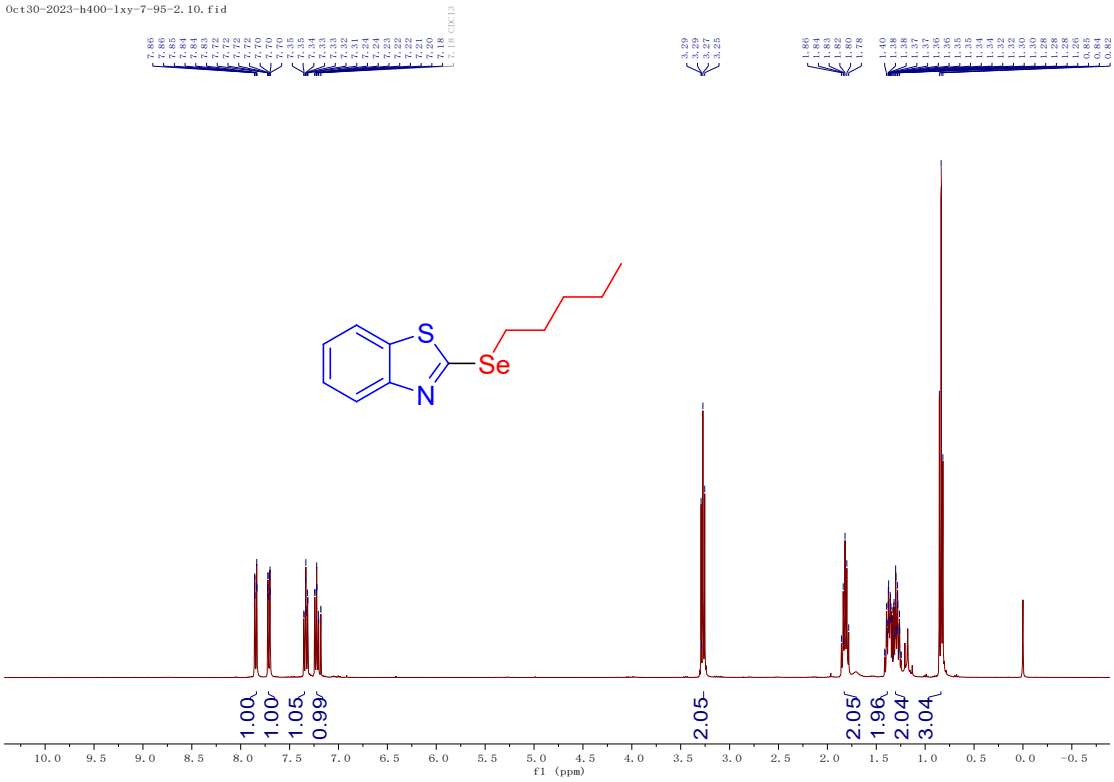
Oct09-2023-h400-lxy-7-59-3.10.fid

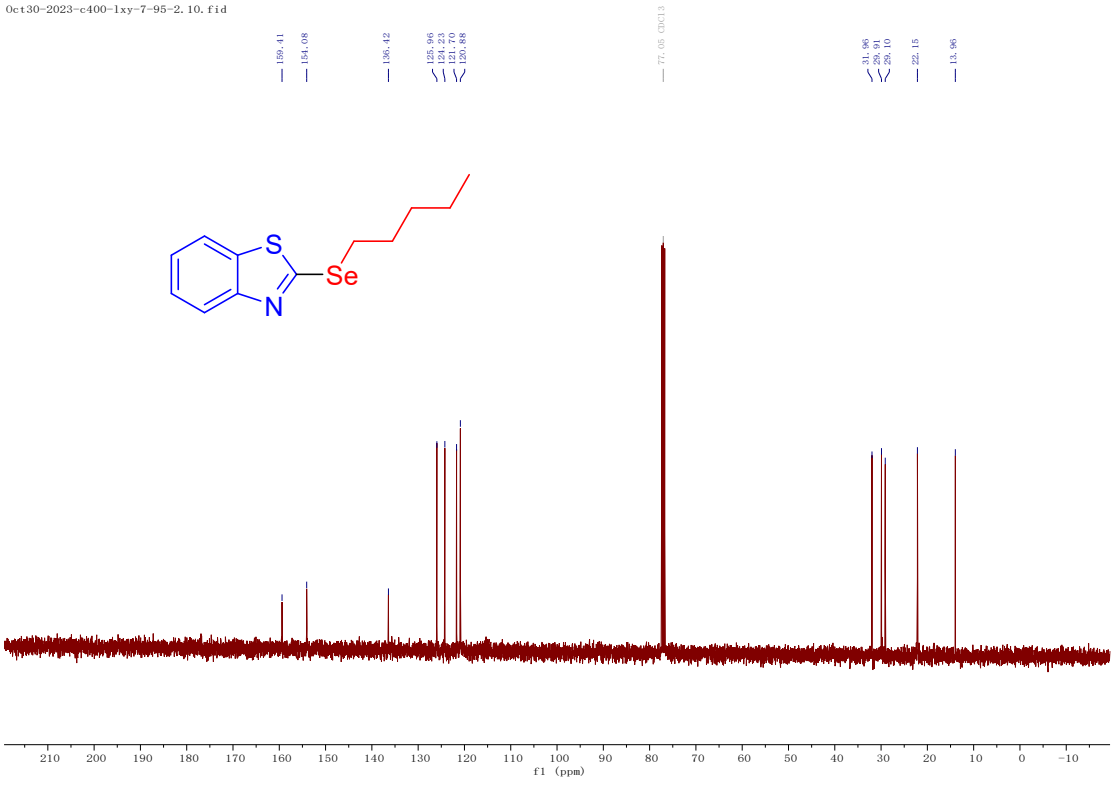


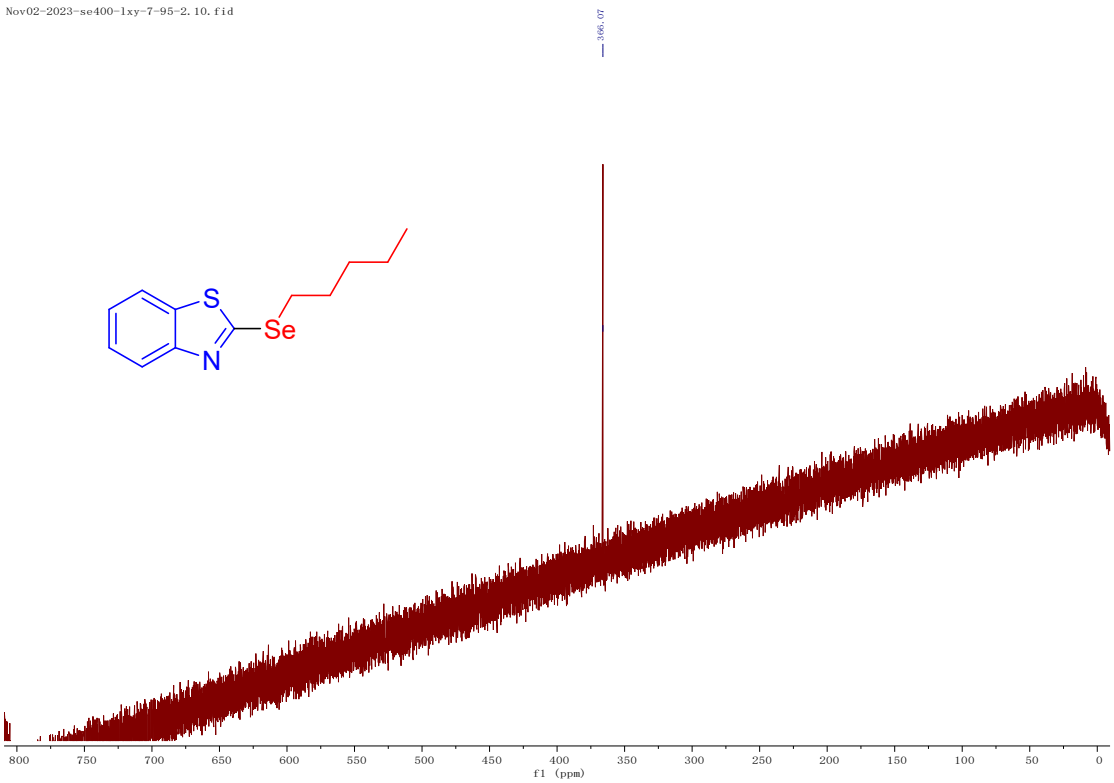




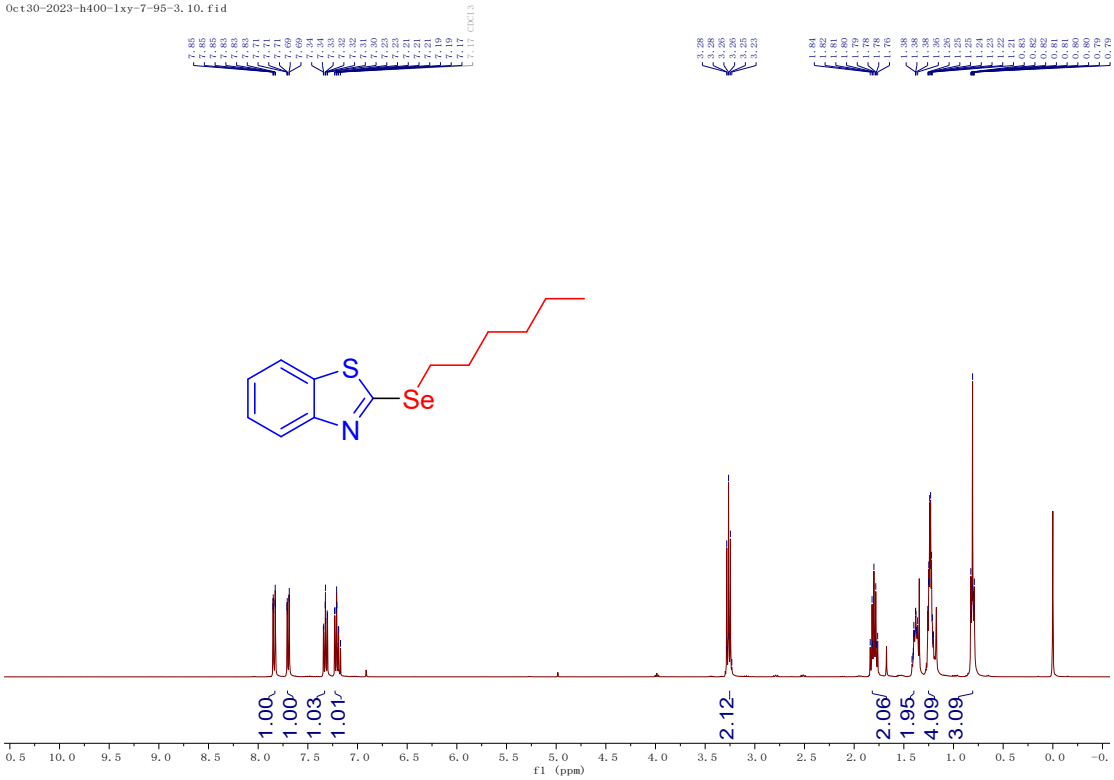
2-(pentylselanyl)benzo[*d*]thiazole (3n)

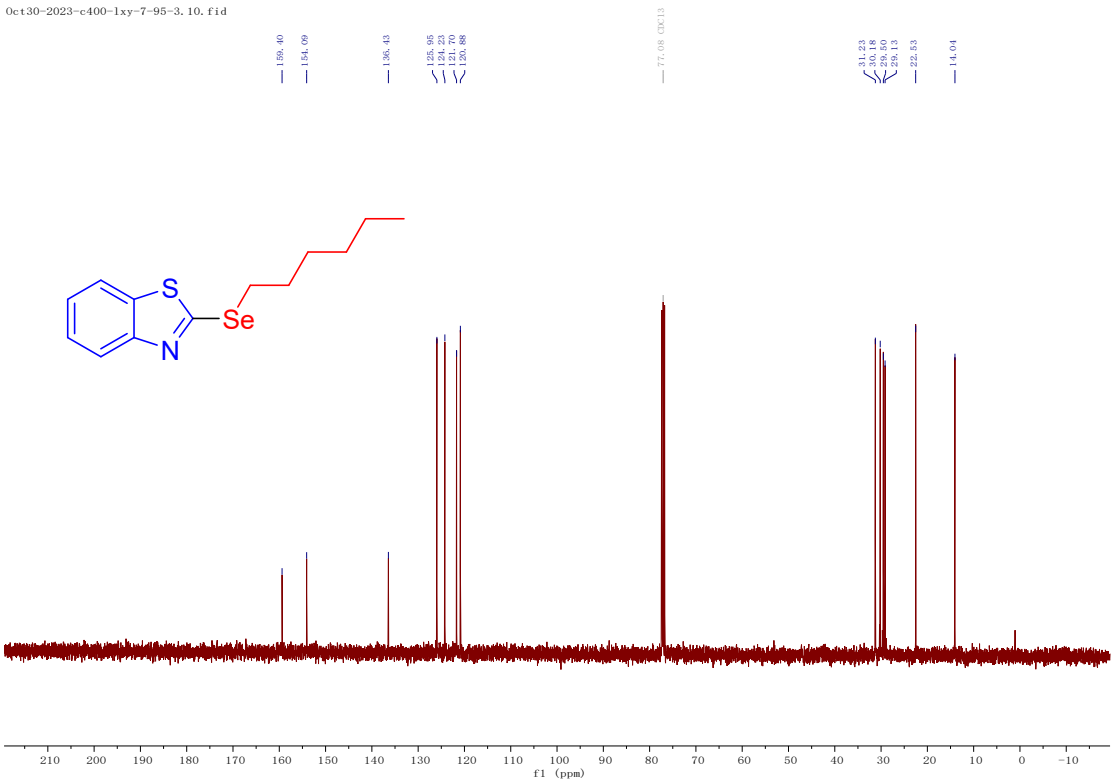

0ct30-2023-h400-lxy-7-95-2.10.fid
S
Se
N
1.00
1.00
1.05
0.99
2.05
2.05
1.96
2.04
3.04
f1 (ppm)

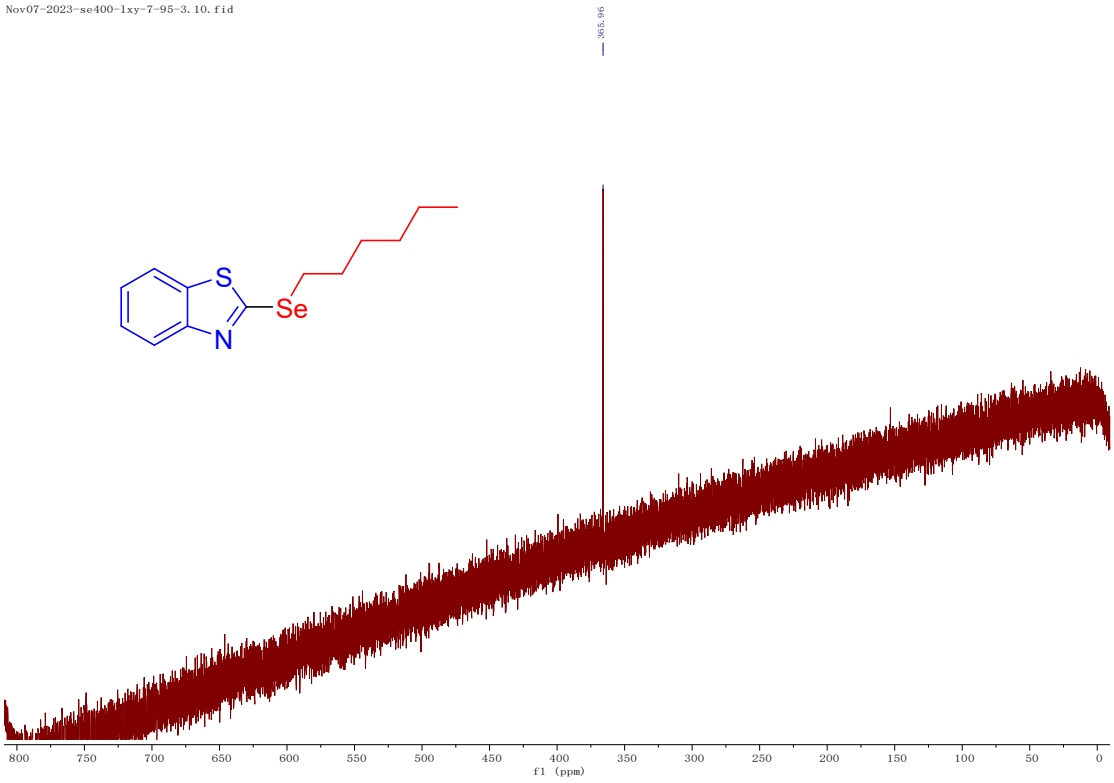

0ct30-2023-c400-lxy-7-95-2.10.fid
159.41
154.08
136.42
125.96
124.23
121.70
120.88
77.05 CDCl3
31.96
29.91
29.10
22.15
13.96
S
Se
N
f1 (ppm)



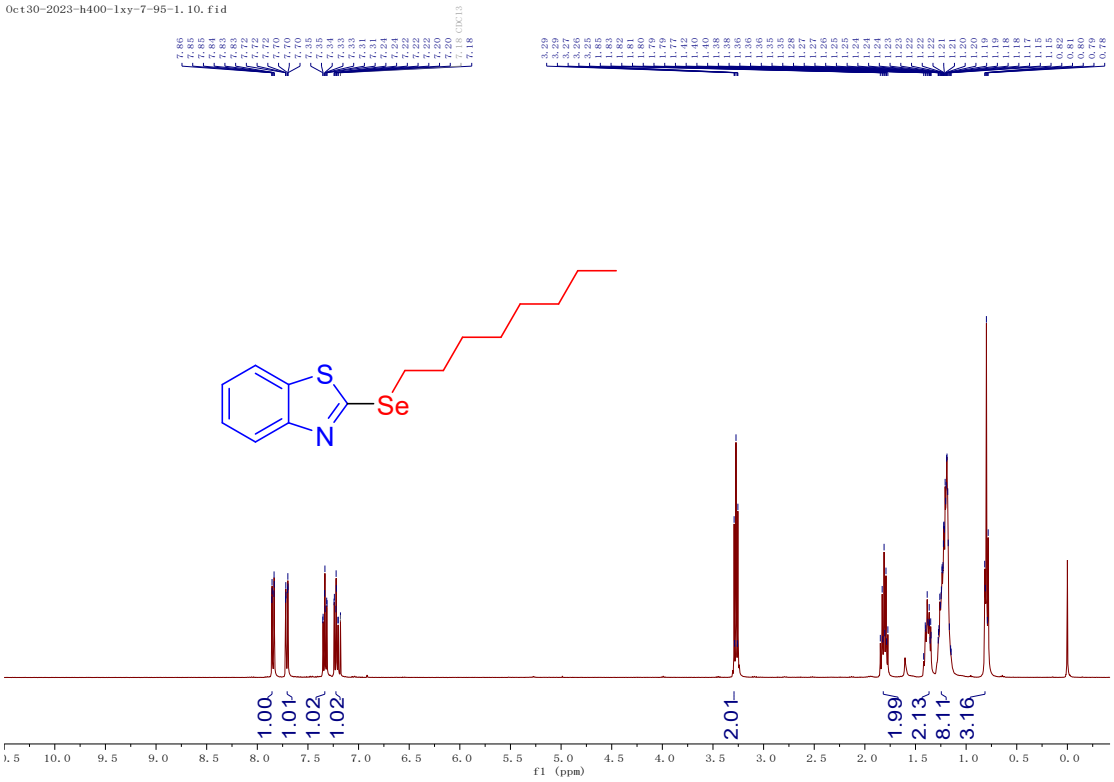
2-(hexylselanyl)benzo[*d*]thiazole (3o)

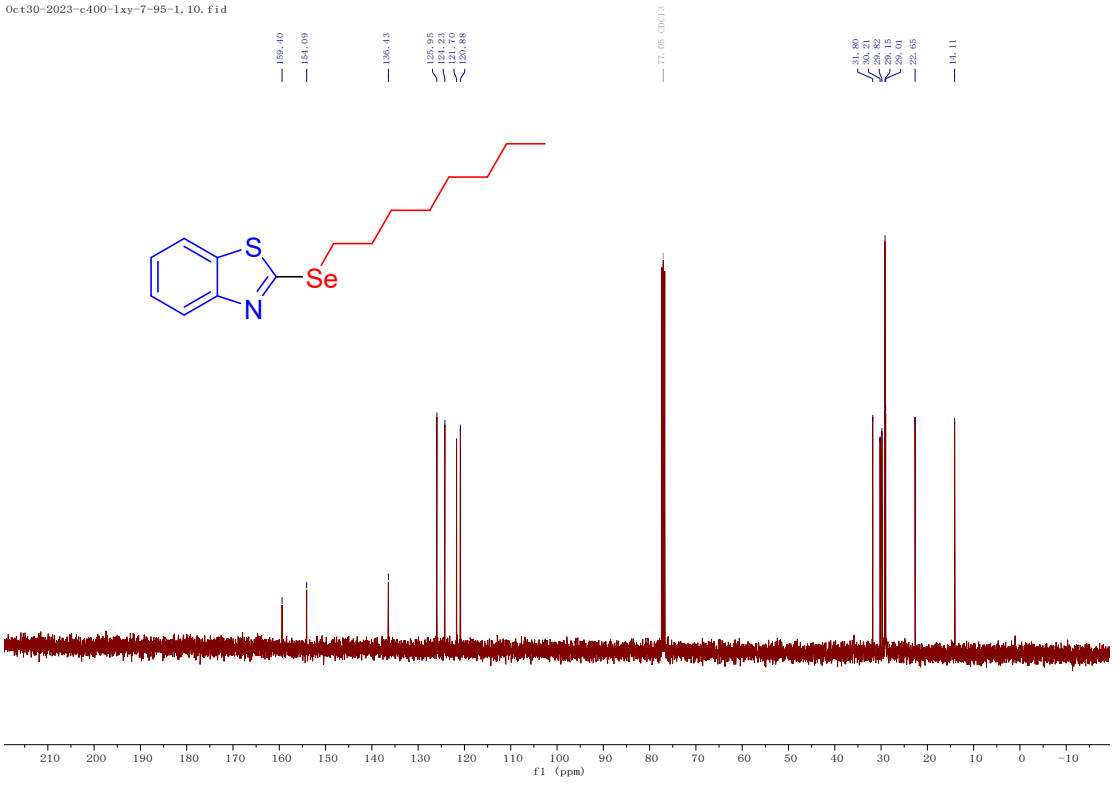


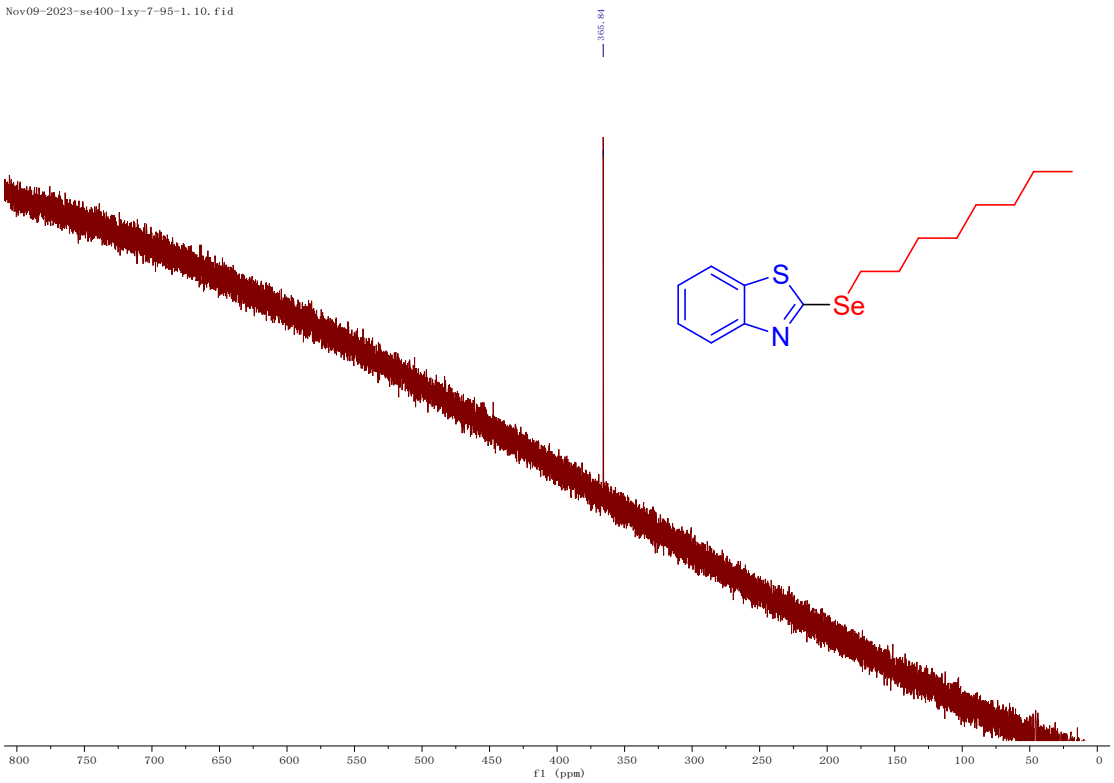




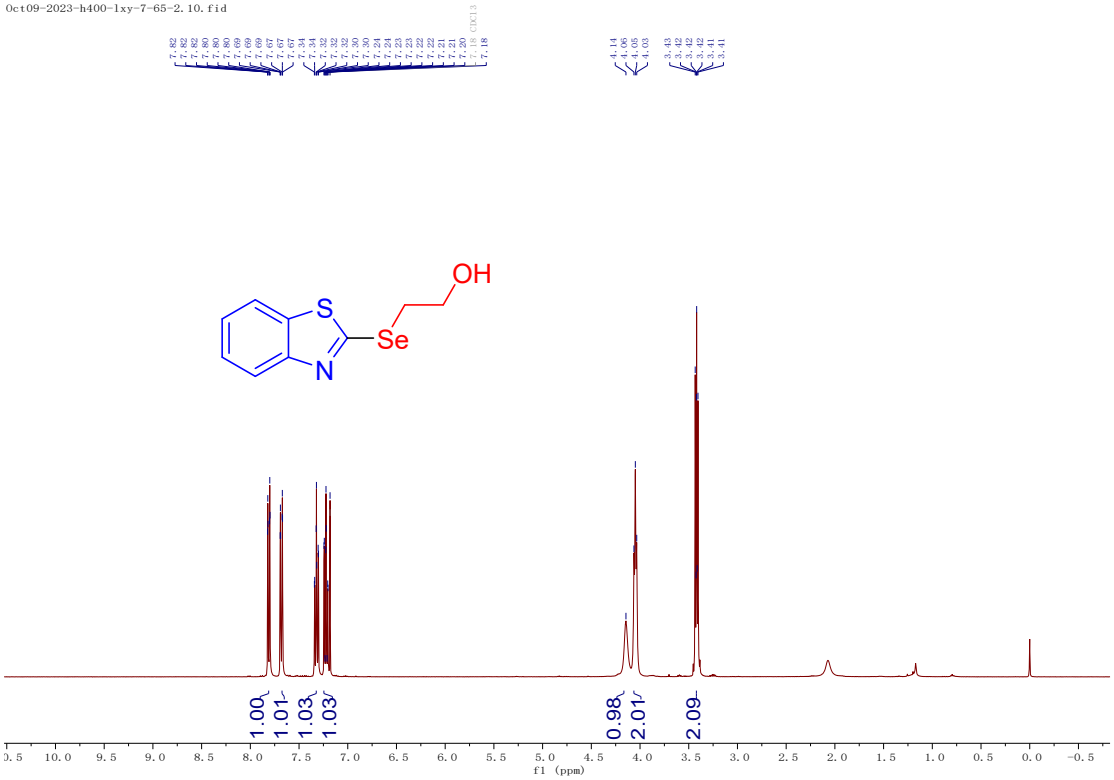
2-(octylselanyl)benzo[d]thiazole (3p)

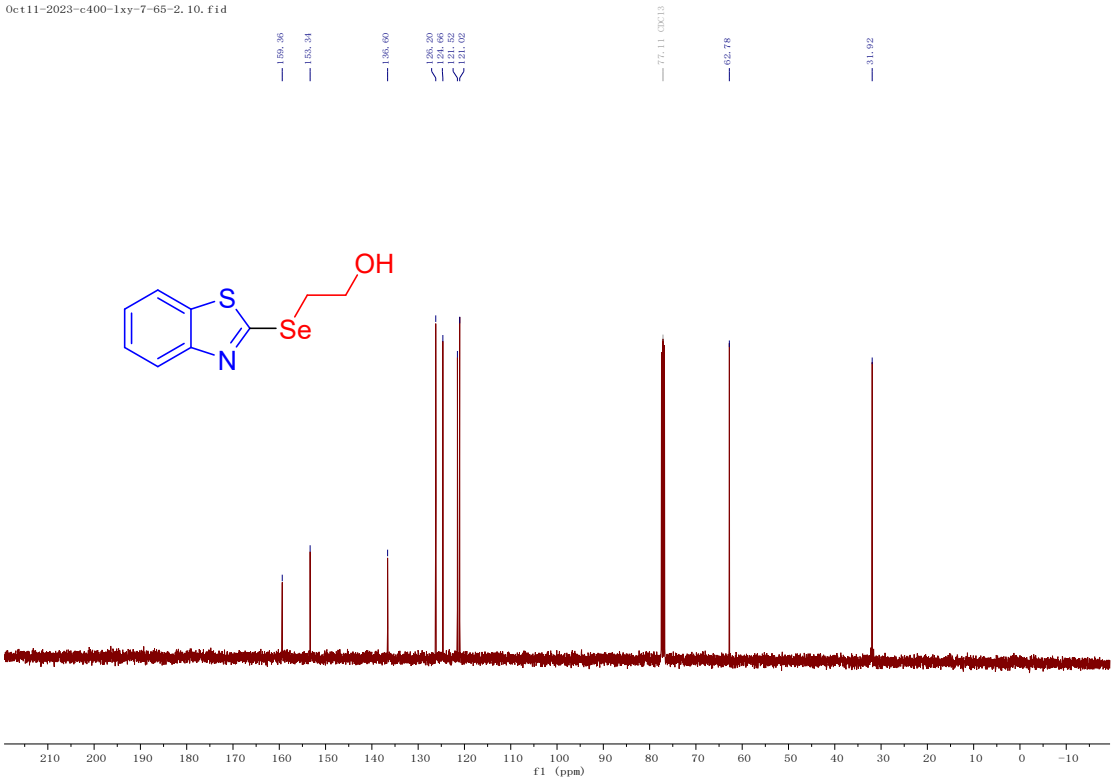

Oct30-2023-h400-lxy-7-95-1.10.fid
S
N
Se
1.00
1.01
1.02
1.02
2.01
1.99
2.13
8.11
3.16
f1 (ppm)

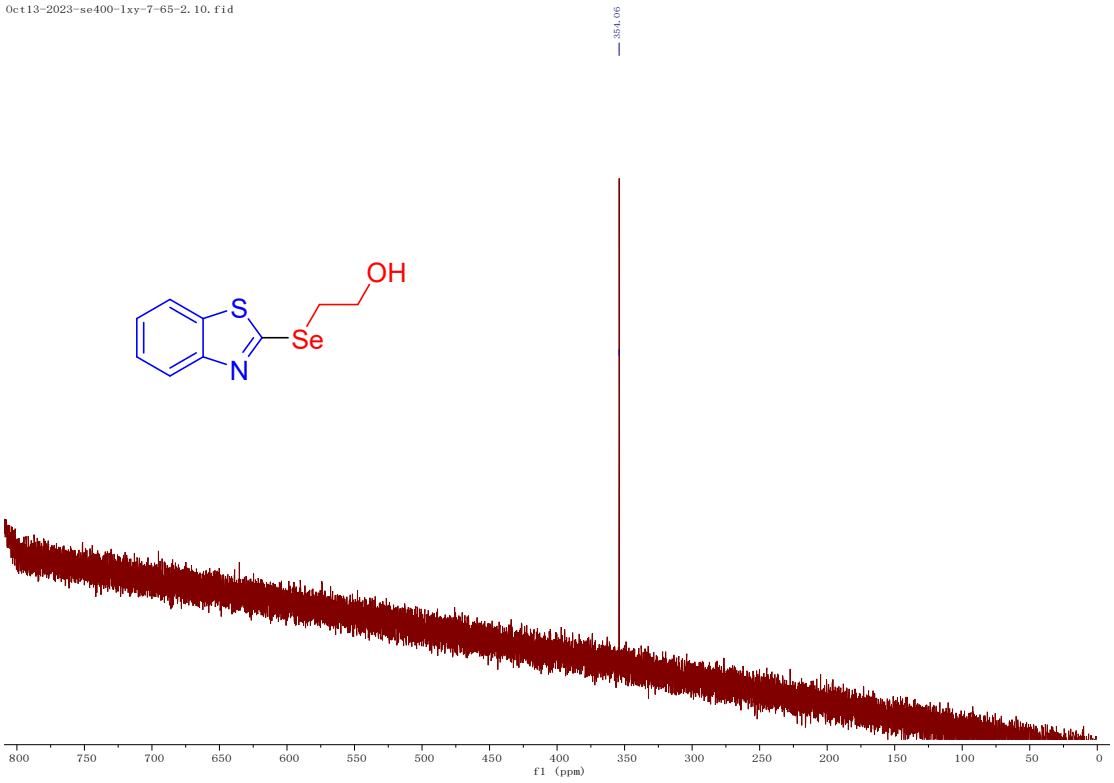

Oct30-2023-c400-lxy-7-95-1.10.fid
159.40
154.09
136.43
125.95
124.23
121.70
120.88
77.05 CDCl3
31.80
30.21
29.82
29.15
29.01
22.65
14.11
S
N
Se
f1 (ppm)



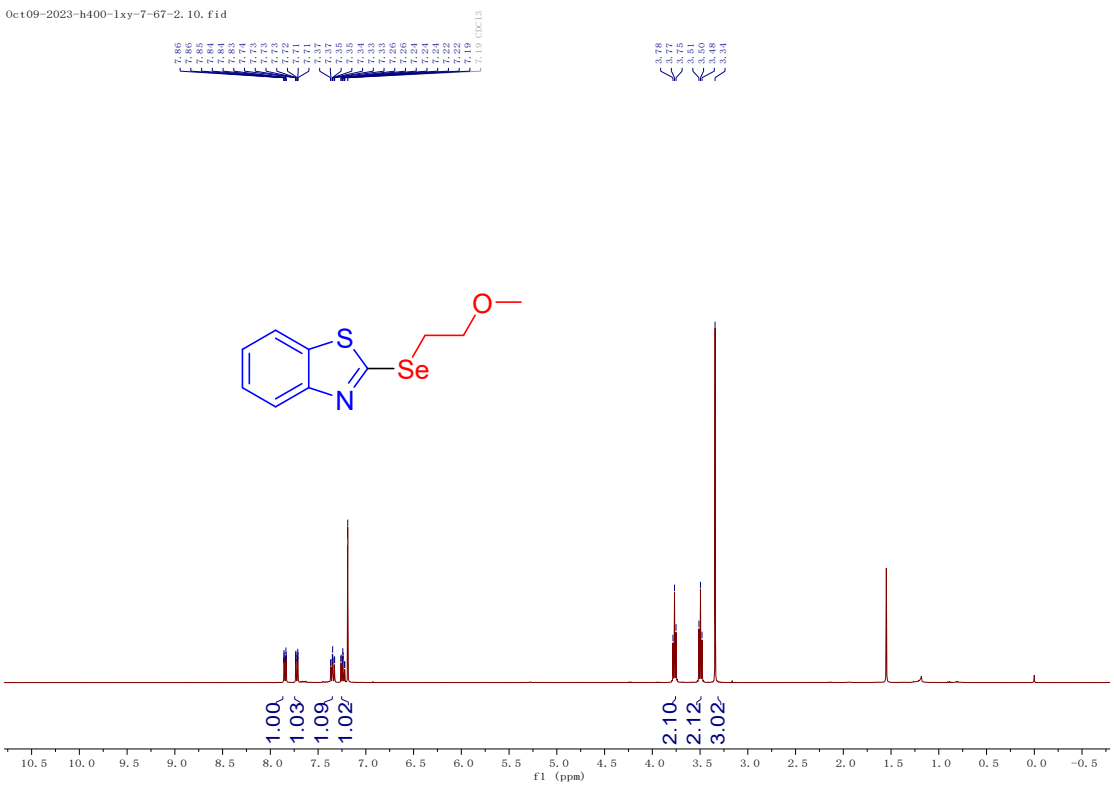
2-(benzo[*d*]thiazol-2-ylselanyl)ethan-1-ol (3q)

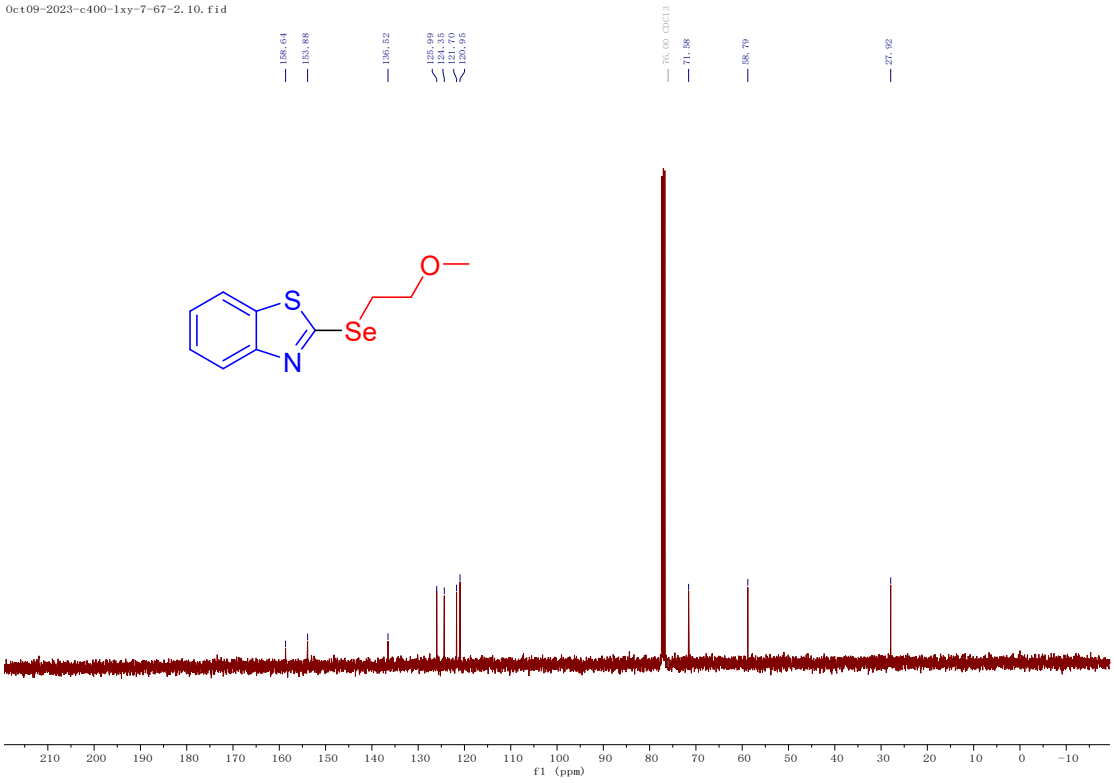


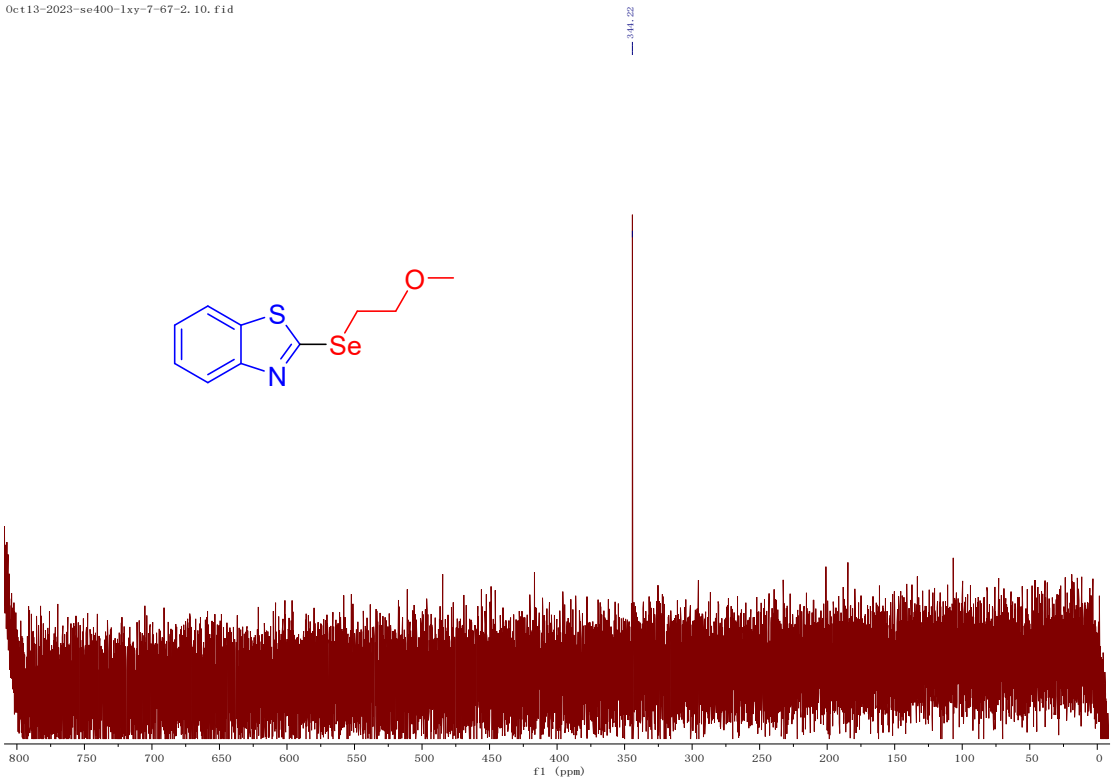




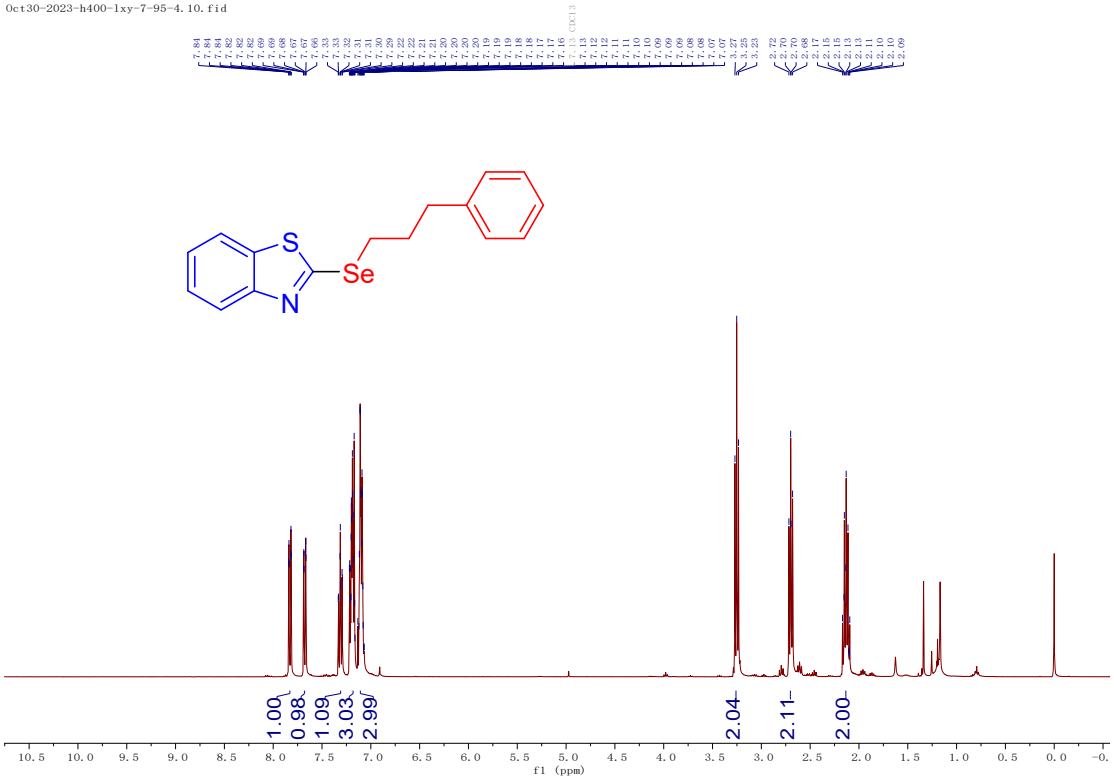
2-((2-methoxyethyl)selanyl)benzo[*d*]thiazole (3r)

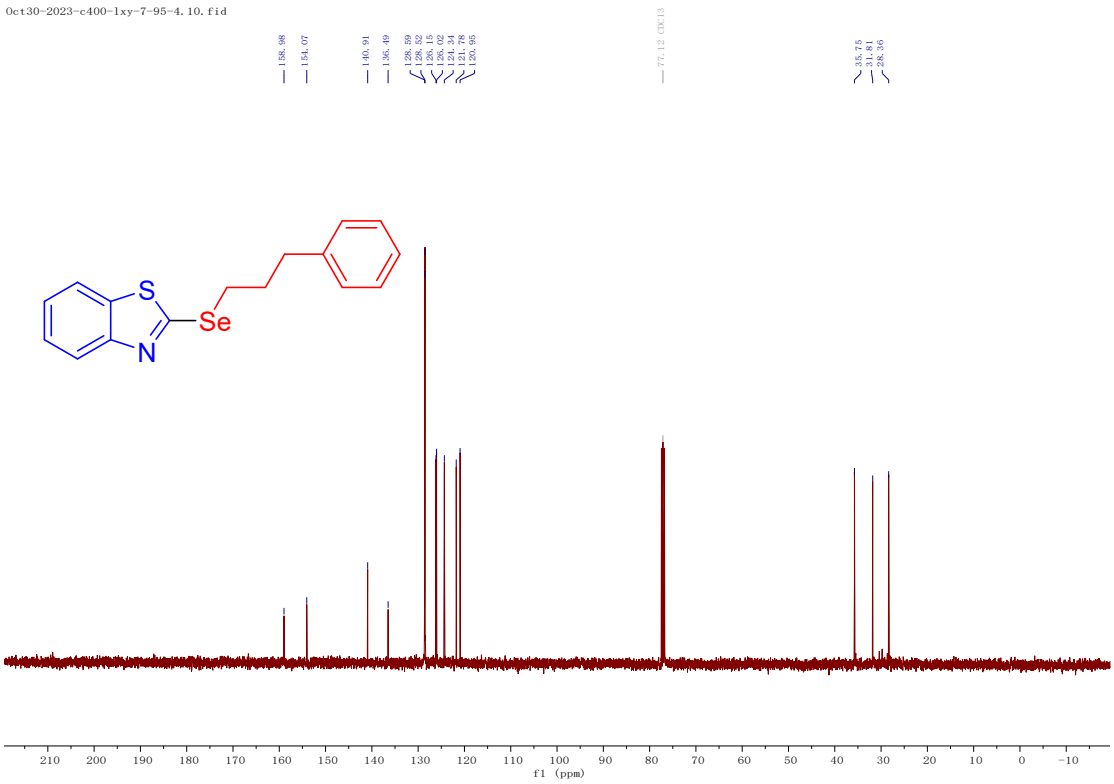

Oct09-2023-h400-lxy-7-67-2.10.fid
7.86
7.86
7.85
7.84
7.84
7.83
7.74
7.73
7.73
7.72
7.71
7.71
7.37
7.37
7.35
7.35
7.34
7.33
7.33
7.26
7.24
7.24
7.24
7.22
7.22
7.19
CDCl3
3.78
3.77
3.75
3.51
3.50
3.48
3.34
O
S
Se
N
1.00
1.03
1.09
1.02
2.10
2.12
3.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

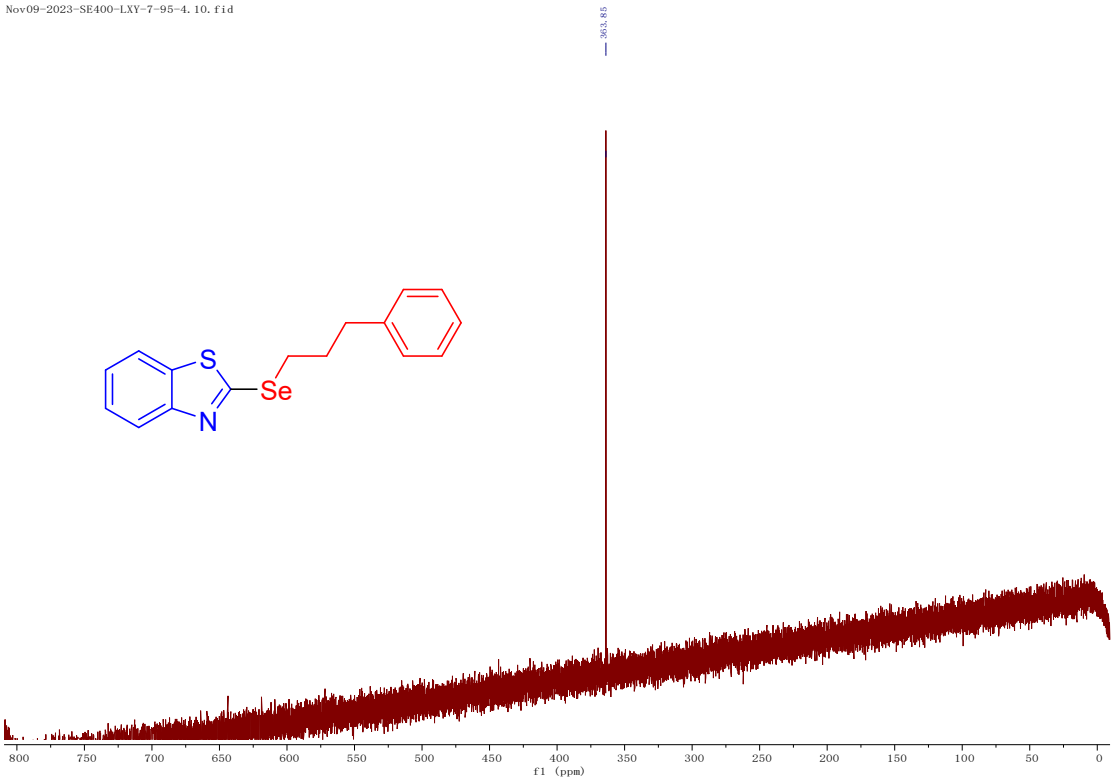

Oct09-2023-c400-lxy-7-67-2.10.fid
158.64
153.88
136.52
125.99
124.35
121.70
120.95
76.00
CDCl3
71.58
58.79
27.92
O
S
Se
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



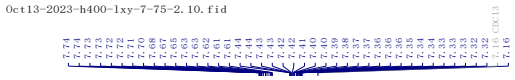
2-((3-phenylpropyl)selanyl)benzo[d]thiazole (3s)

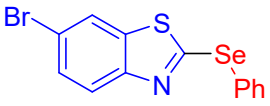


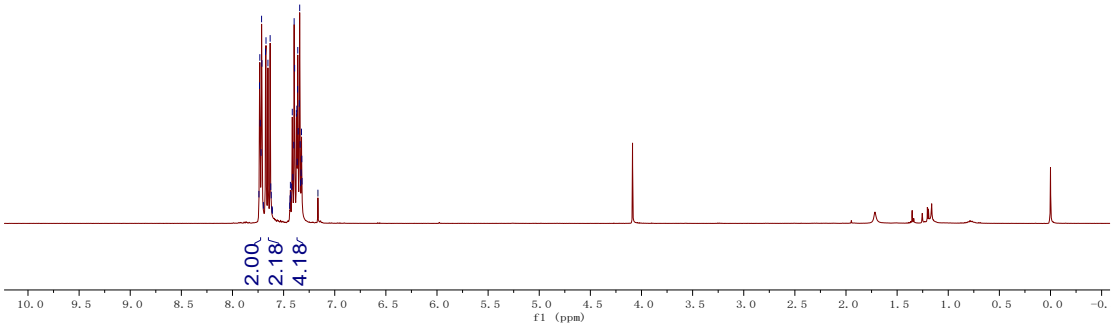




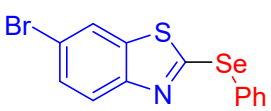
6-bromo-2-(phenylselanyl)benzo[*d*]thiazole (4a)


Oct13-2023-h400-lxy-7-75-2.10.fid

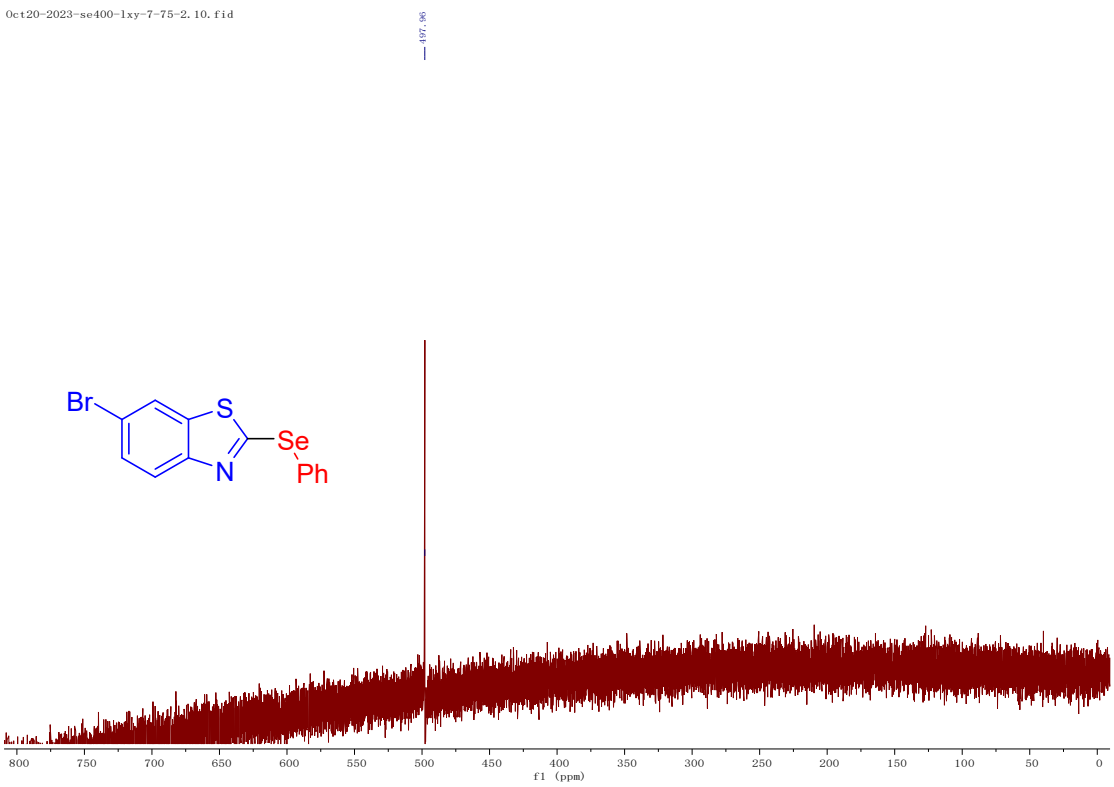

Br
S
Se
N
Ph


2.00
2.18
4.18
f1 (ppm)

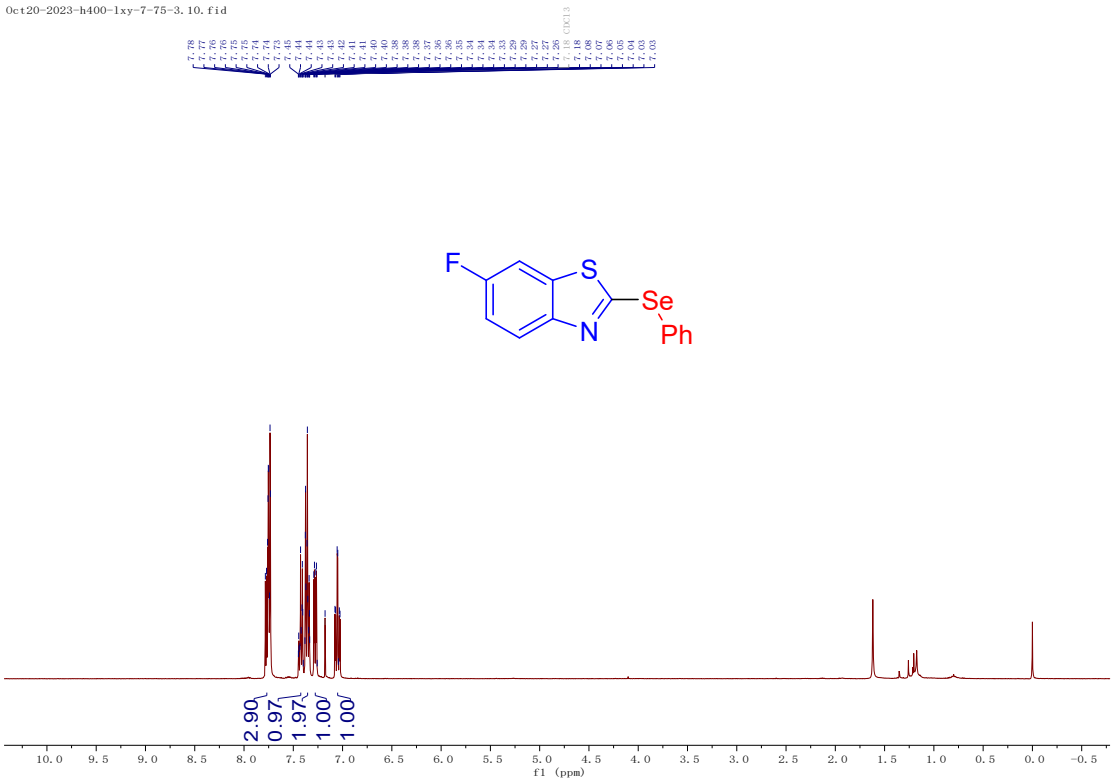

Oct13-2023-c400-lxy-7-75-2.10.fid


Br
S
Se
N
Ph

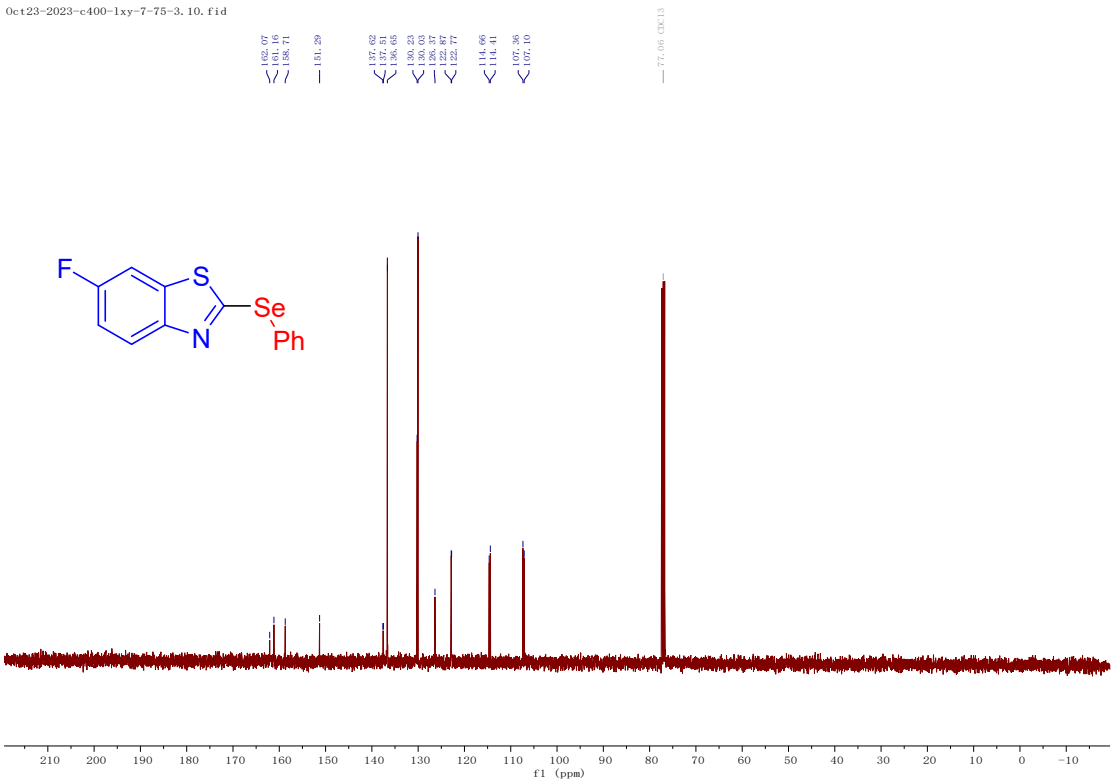
f1 (ppm)



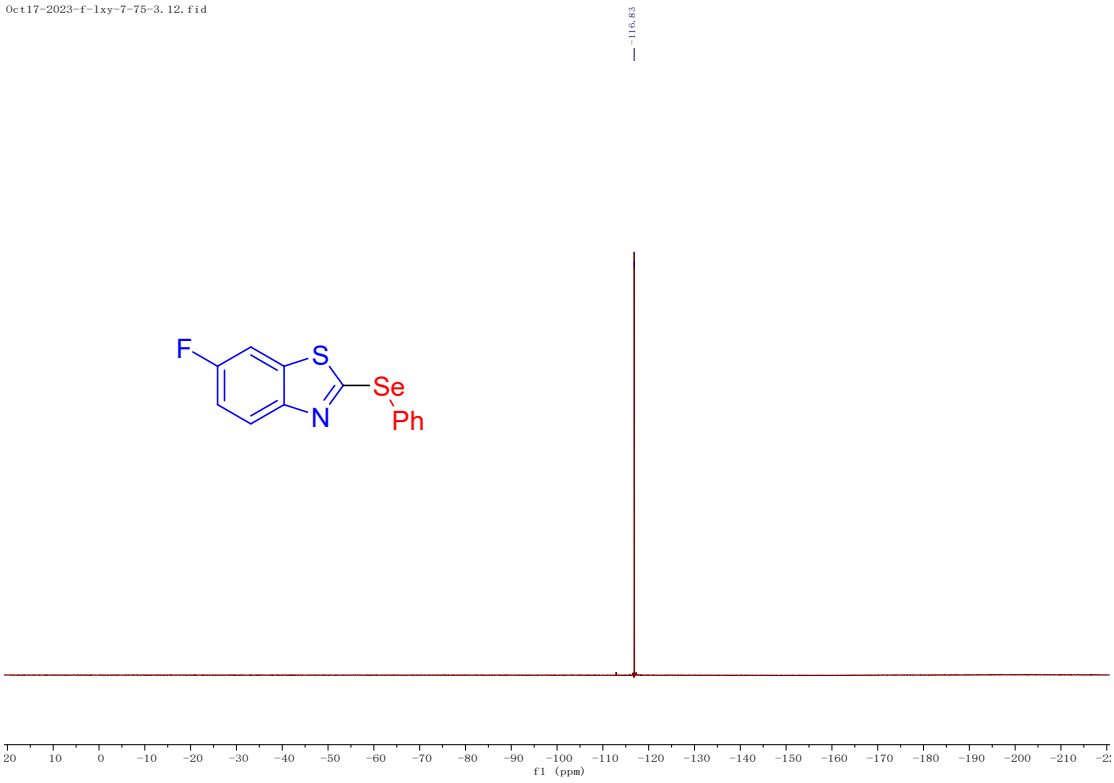
6-fluoro-2-(phenylselanyl)benzo[*d*]thiazole (4b)

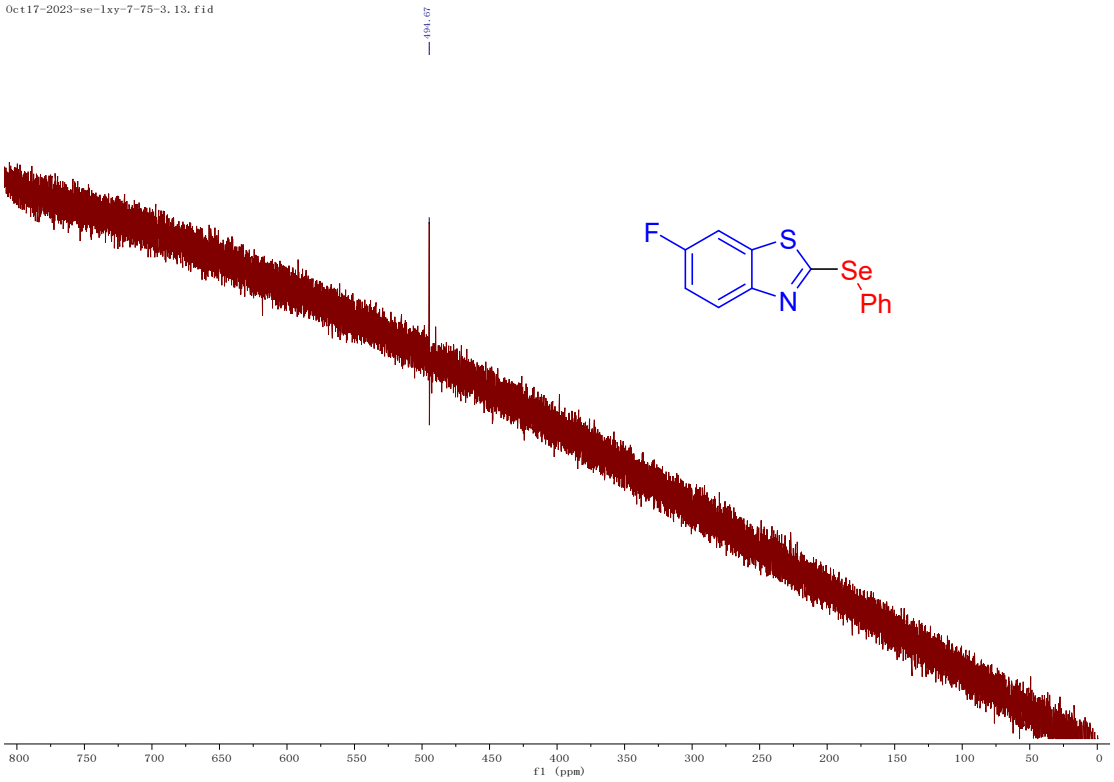


Oct23-2023-c400-lxy-7-75-3.10.fid

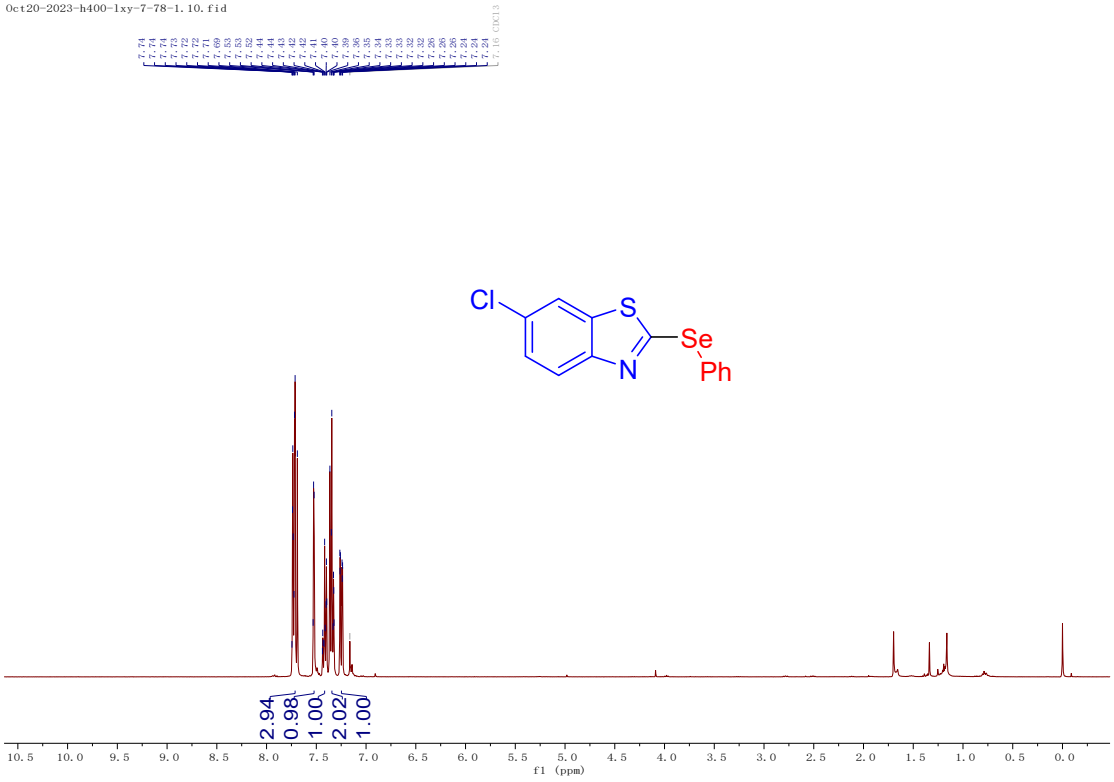


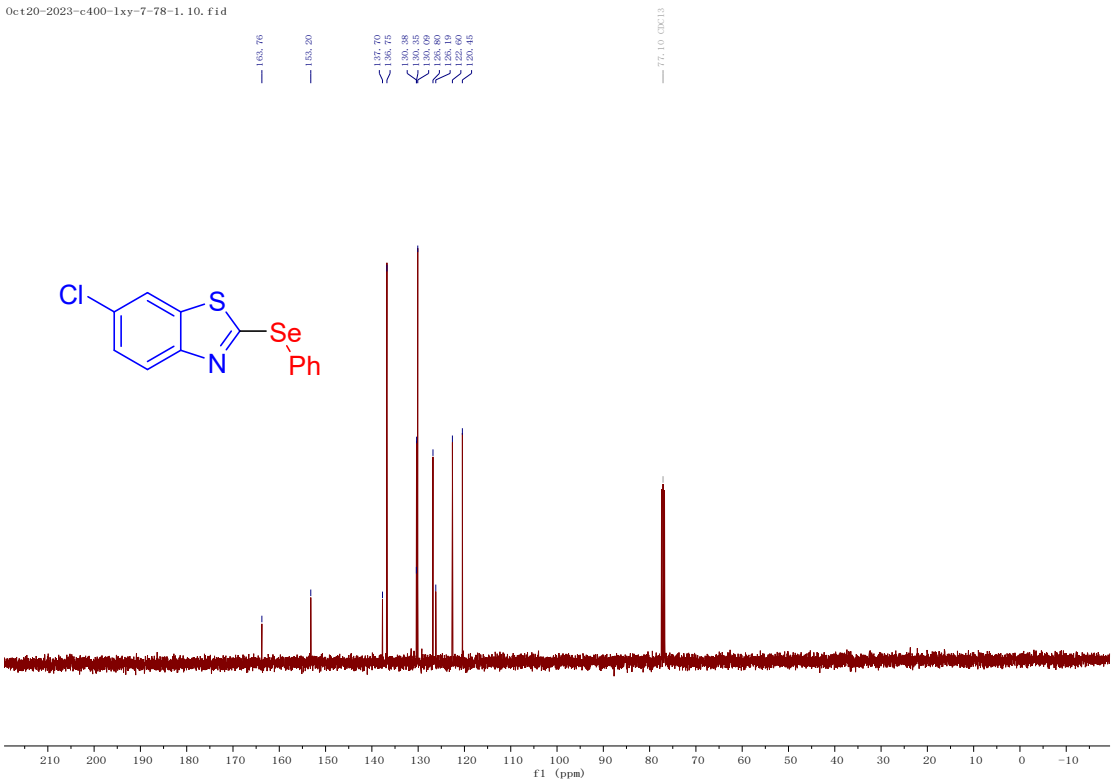
Oct17-2023-f-lxy-7-75-3.12.fid

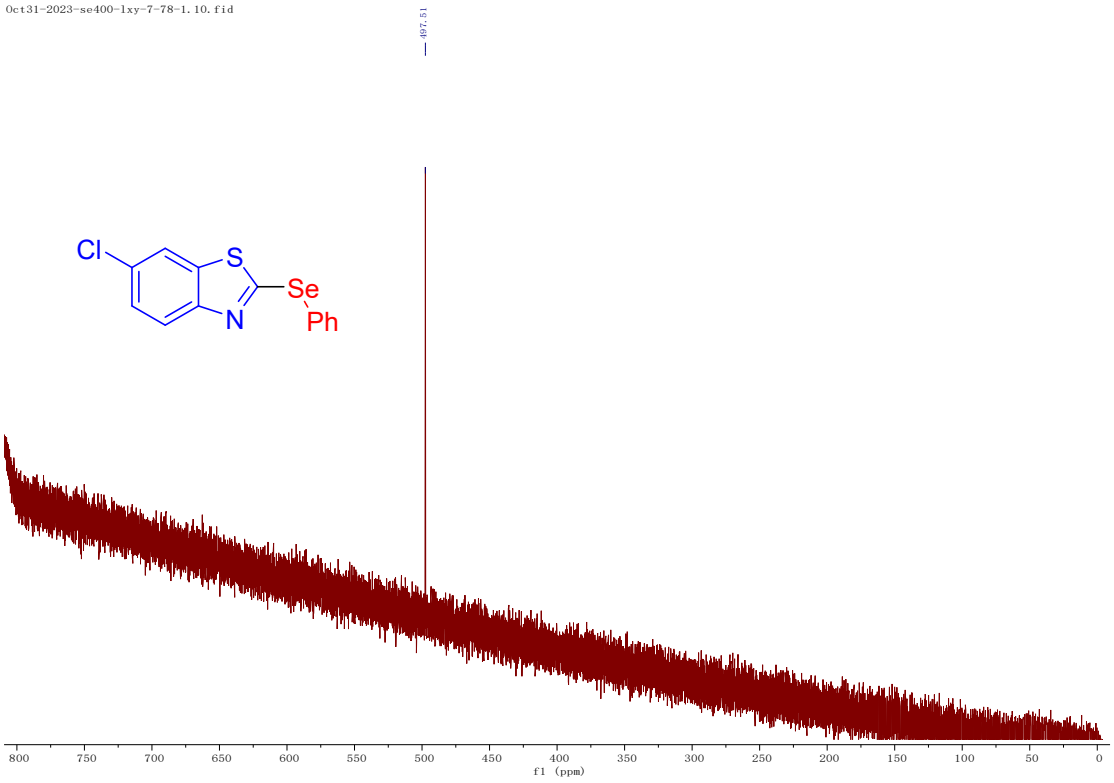




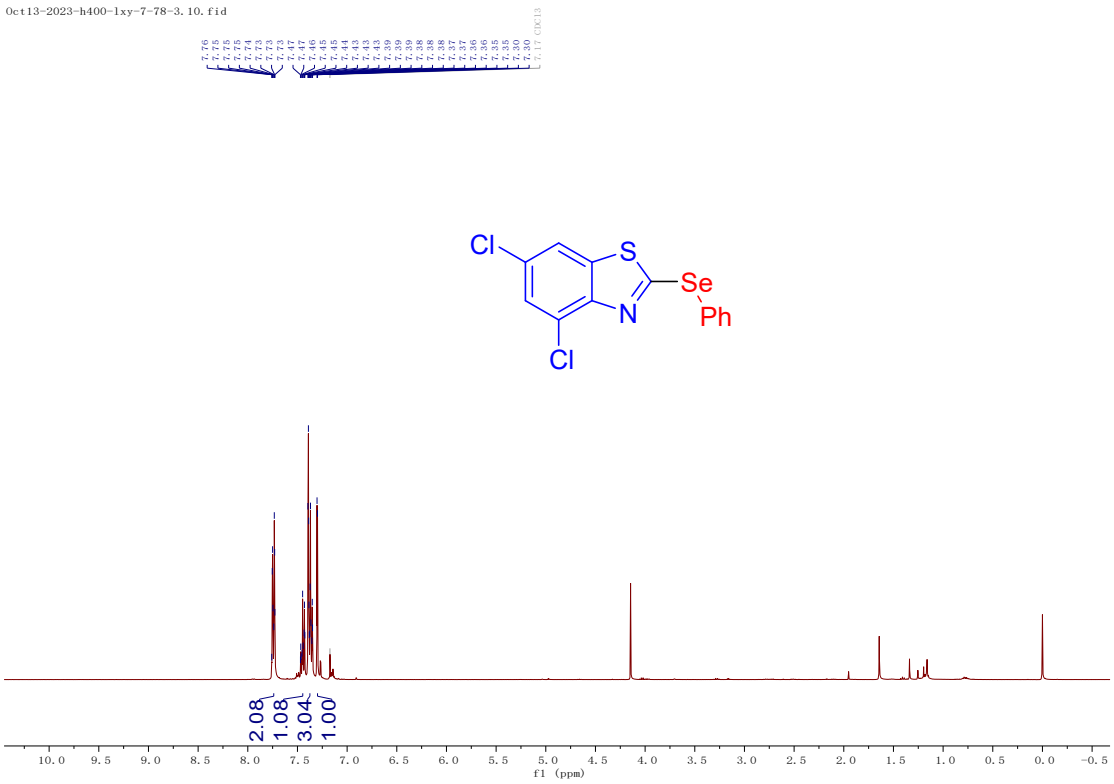
6-chloro-2-(phenylselanyl)benzo[*d*]thiazole (4c)

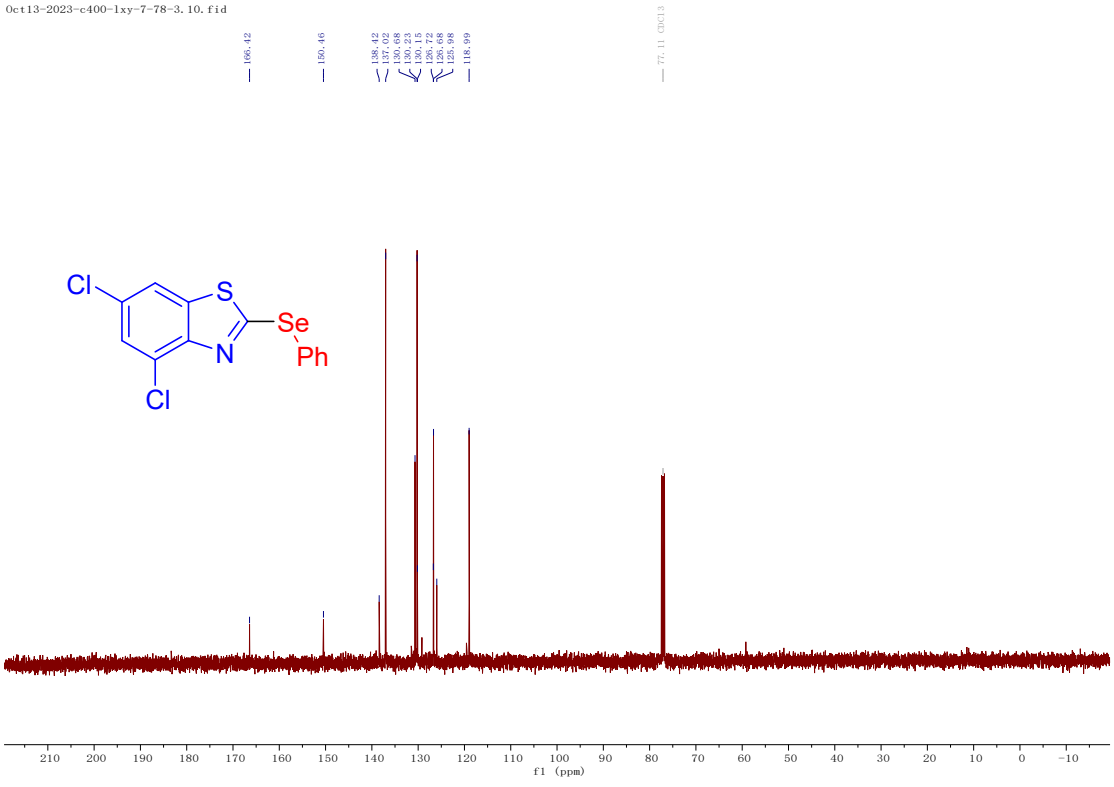


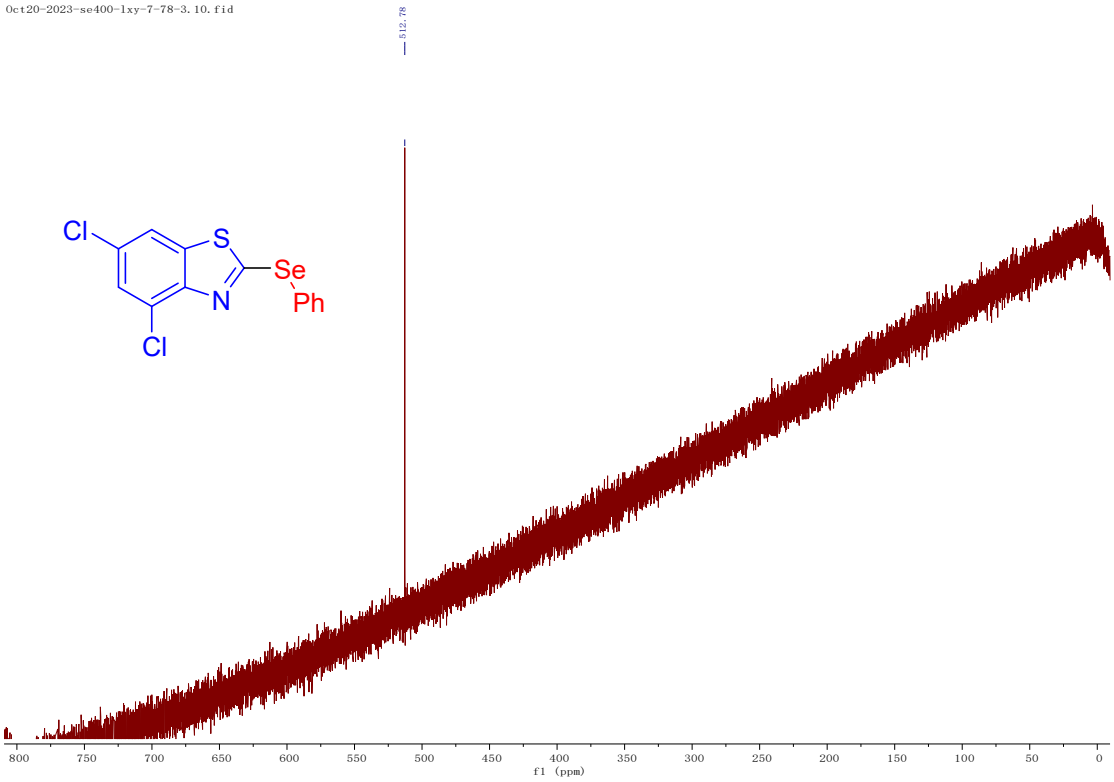




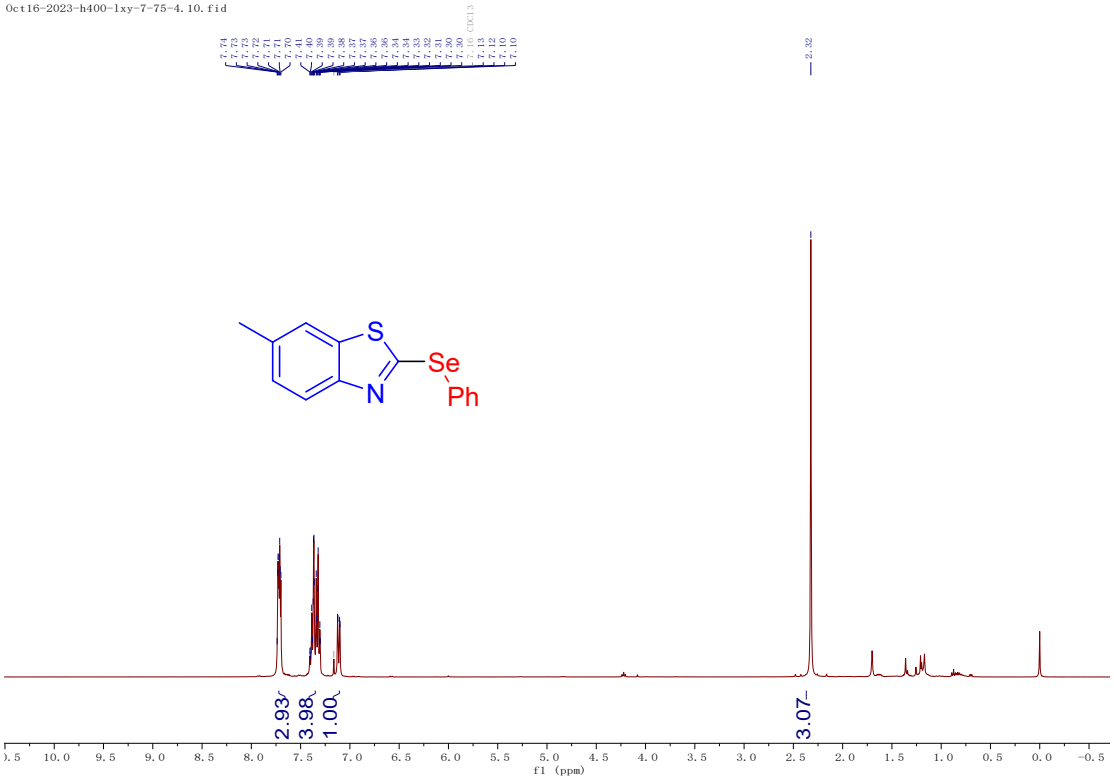
4,6-dichloro-2-(phenylselanyl)benzo[*d*]thiazole (4d)

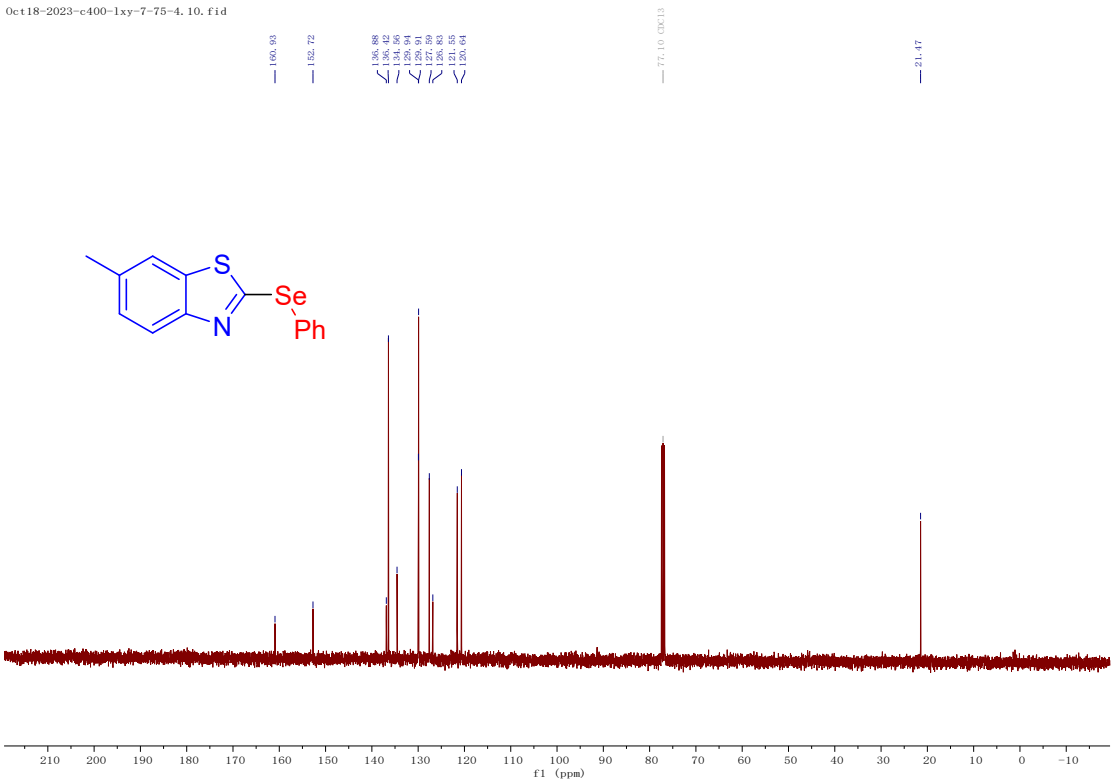

Oct13-2023-h400-lxy-7-78-3.10.fid
Cl
S
Se
Ph
N
Cl
2.08
1.08
3.04
1.00
f1 (ppm)

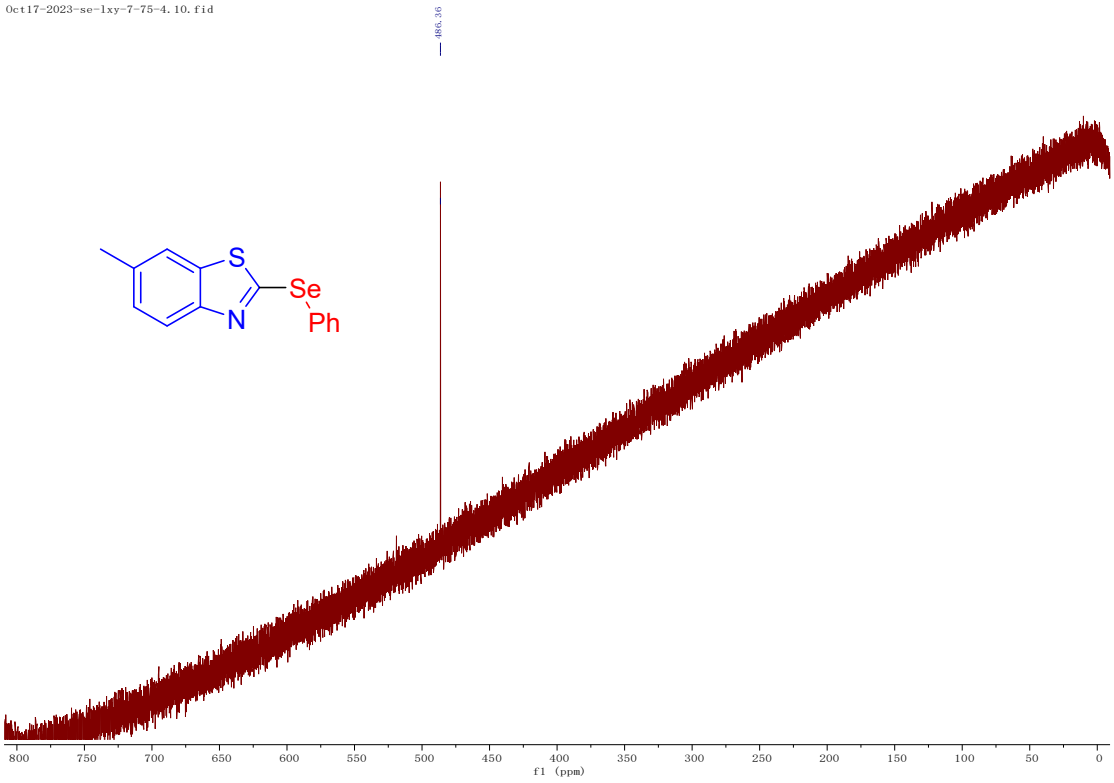

Oct13-2023-c400-lxy-7-78-3.10.fid
166.42
150.46
138.42
137.02
130.68
130.23
130.15
128.72
125.68
125.98
118.99
77.11 CDCl3
Cl
S
Se
Ph
N
Cl
f1 (ppm)



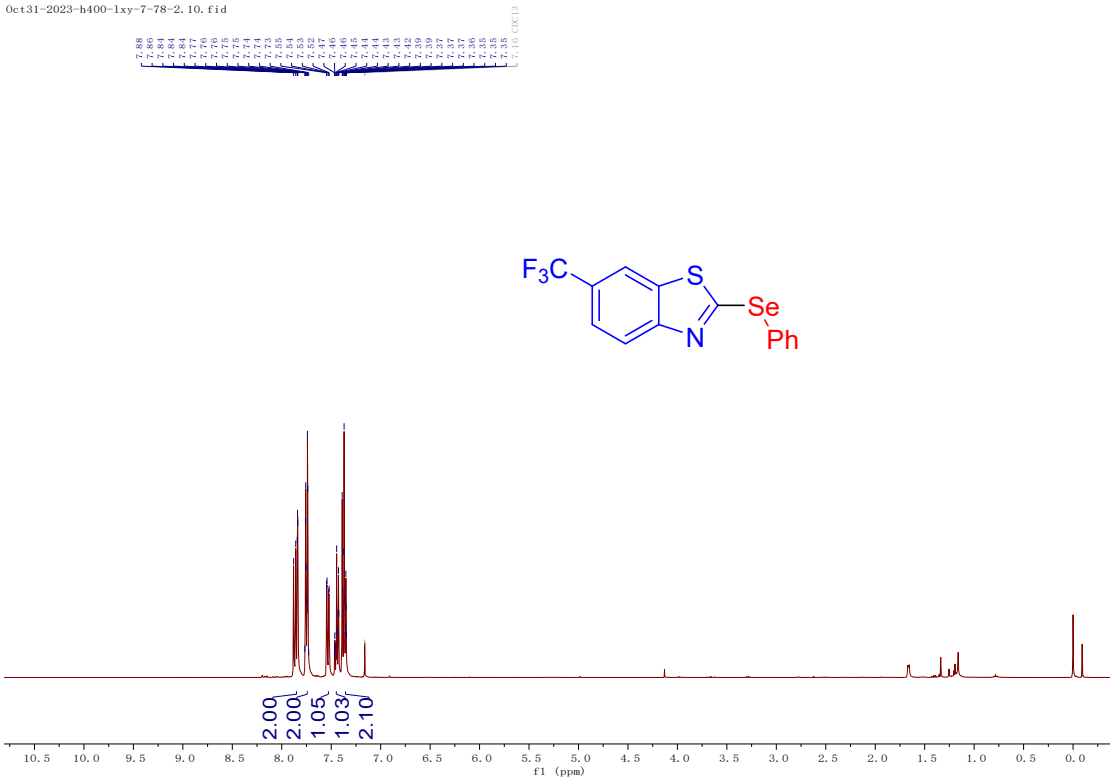
6-methyl-2-(phenylselanyl)benzo[*d*]thiazole (4e)

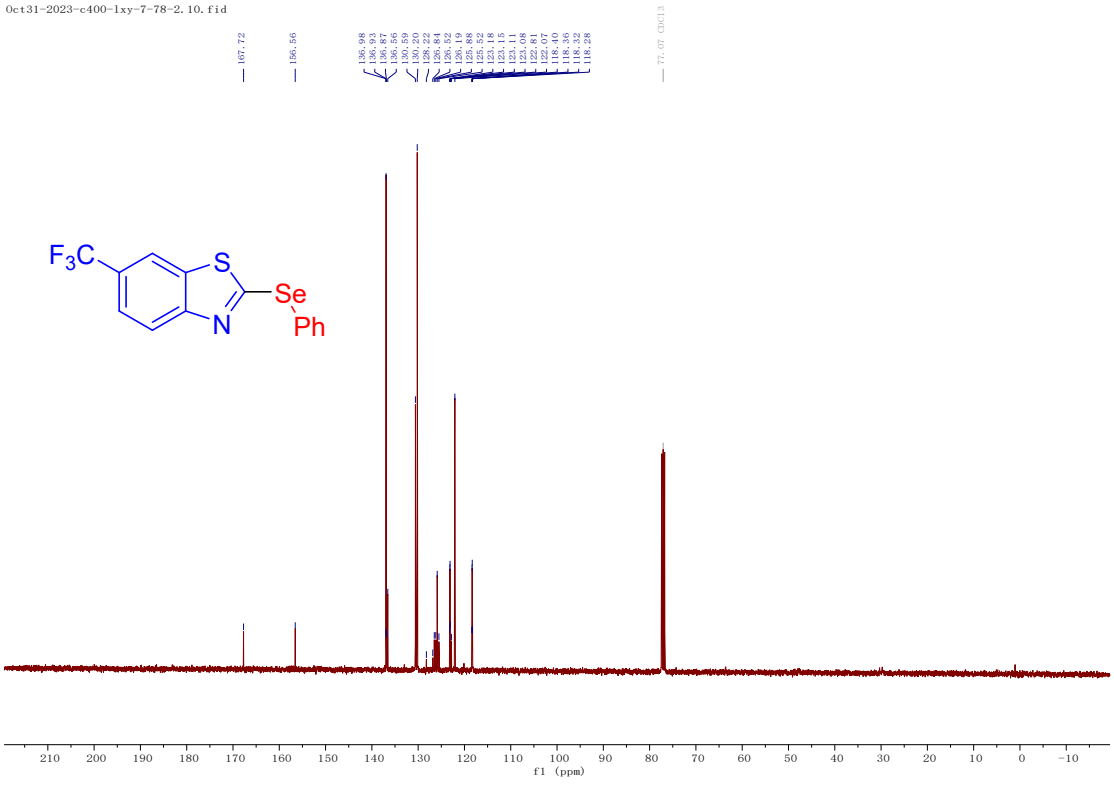


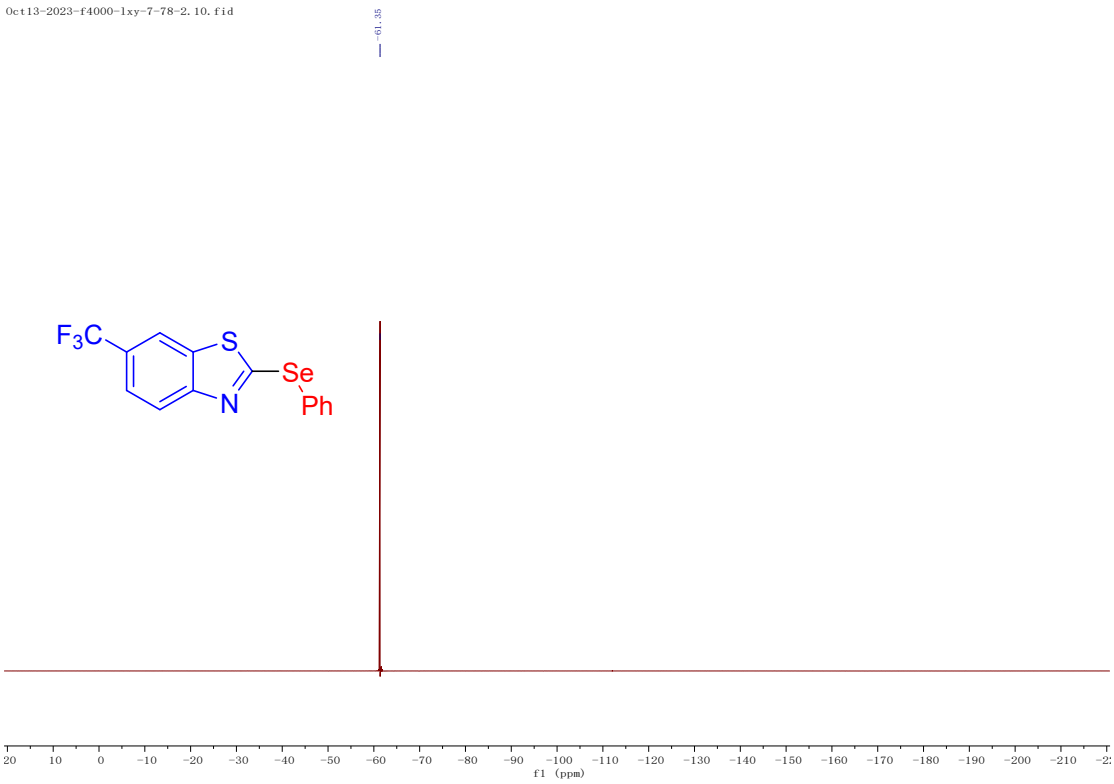


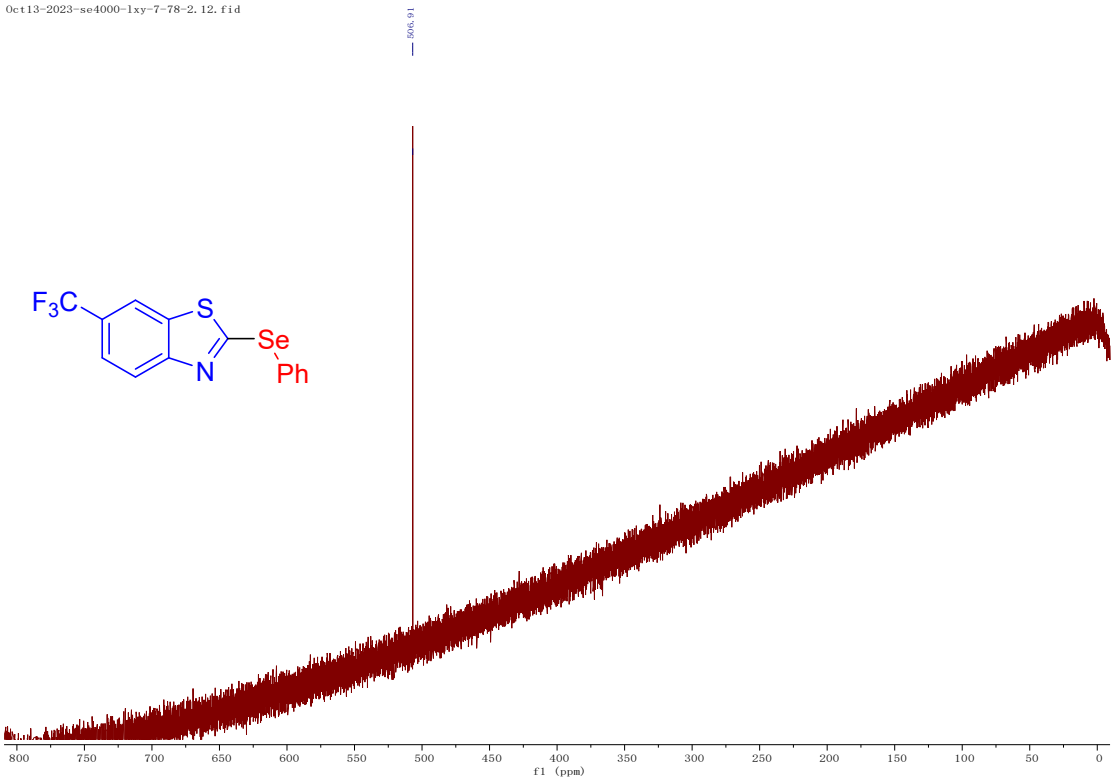


2-(phenylselanyl)-6-(trifluoromethyl)benzo[*d*]thiazole (4f)

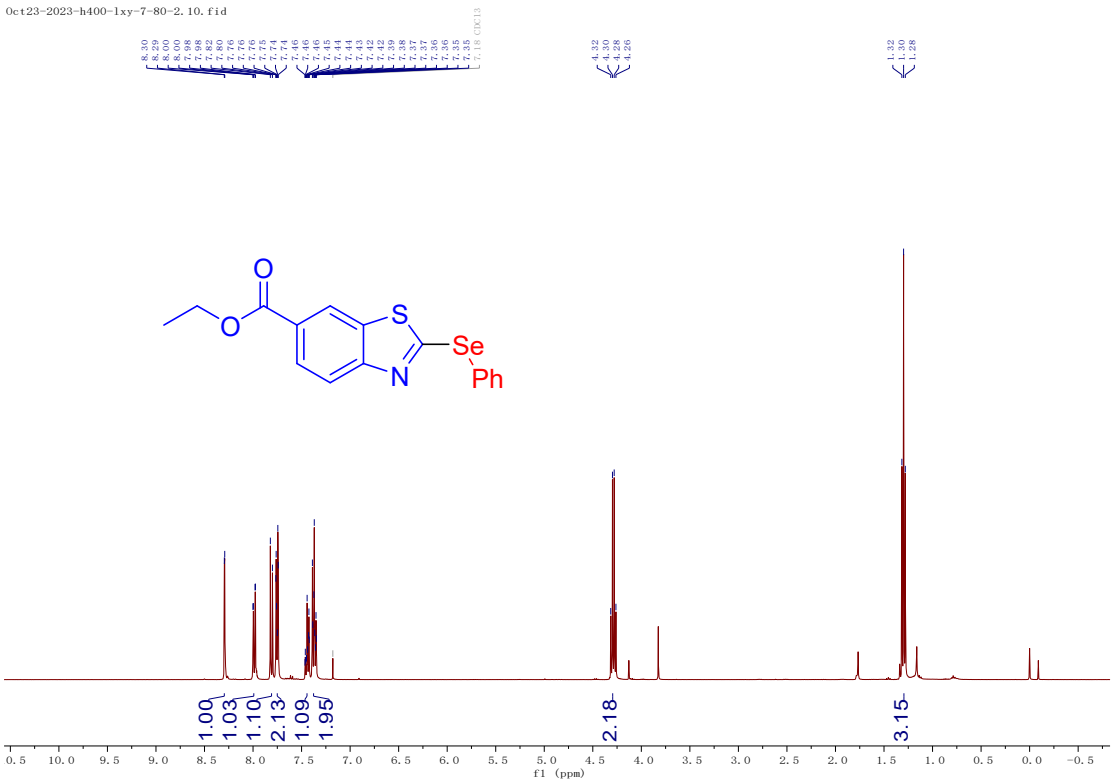

Oct31-2023-h400-lxy-7-78-2.10.fid
F3C
S
Se
N
Ph
2.00
2.00
1.05
1.03
2.10
f1 (ppm)

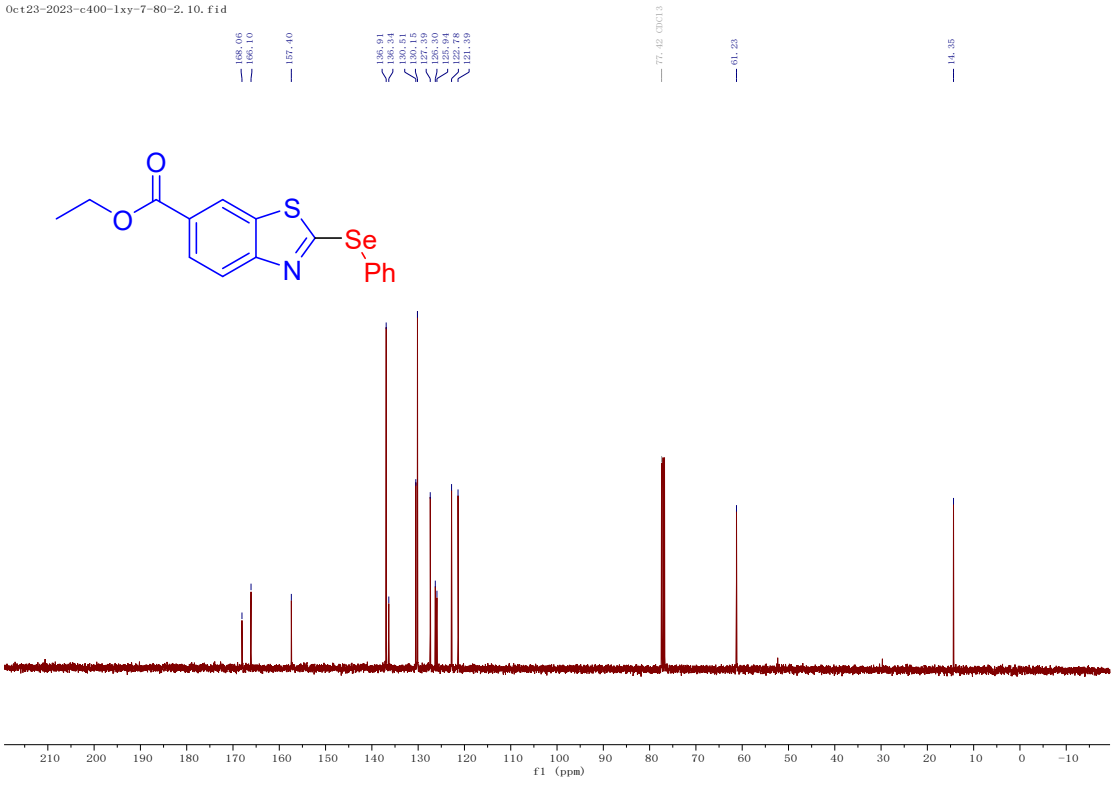

Oct31-2023-c400-lxy-7-78-2.10.fid
F3C
S
Se
N
Ph
f1 (ppm)

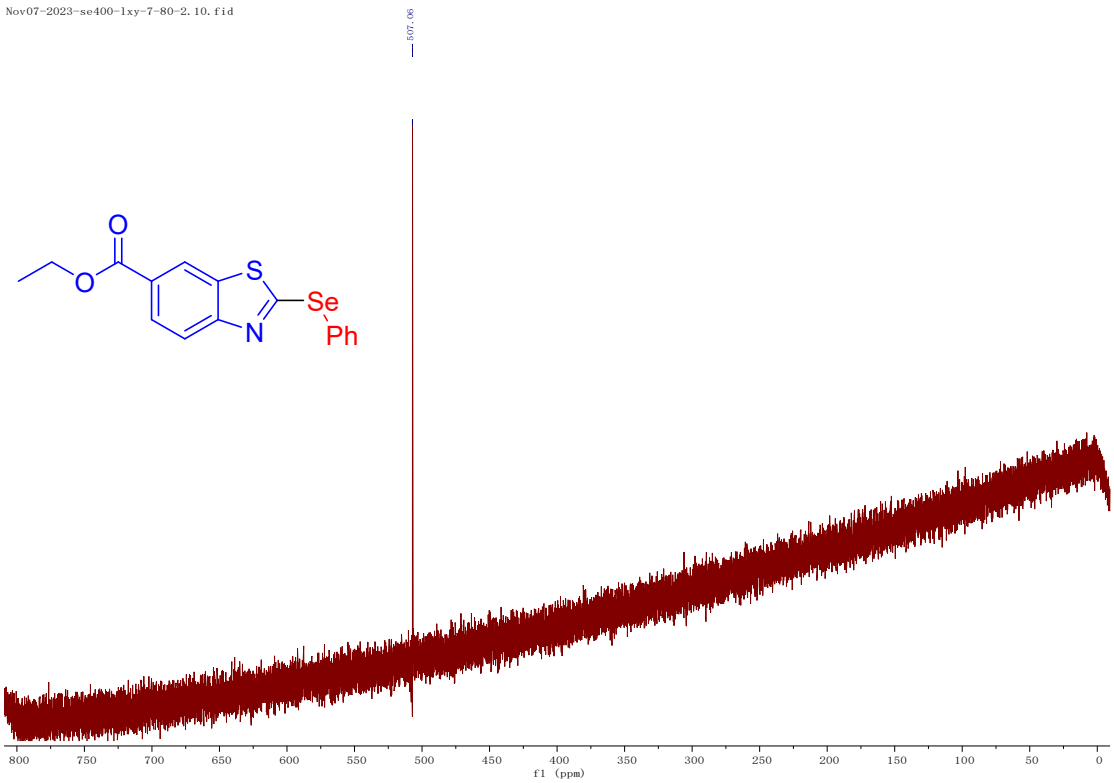




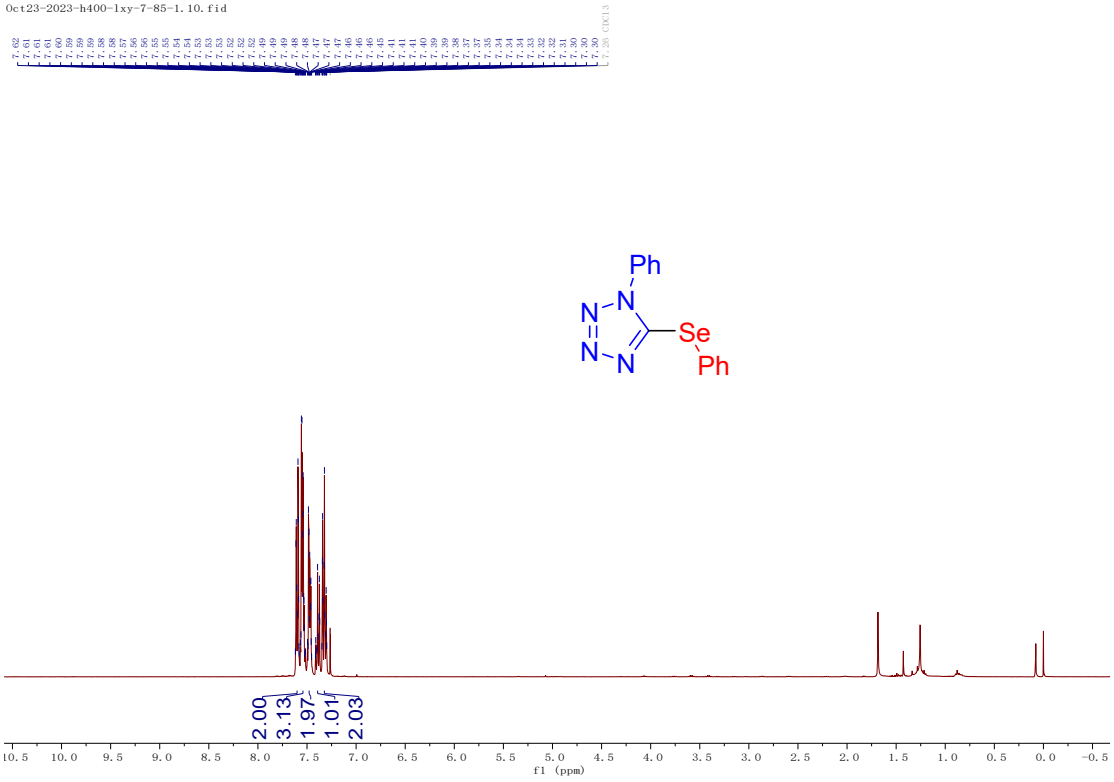
ethyl 2-(phenylselanyl)benzo[d]thiazole-6-carboxylate (4g)

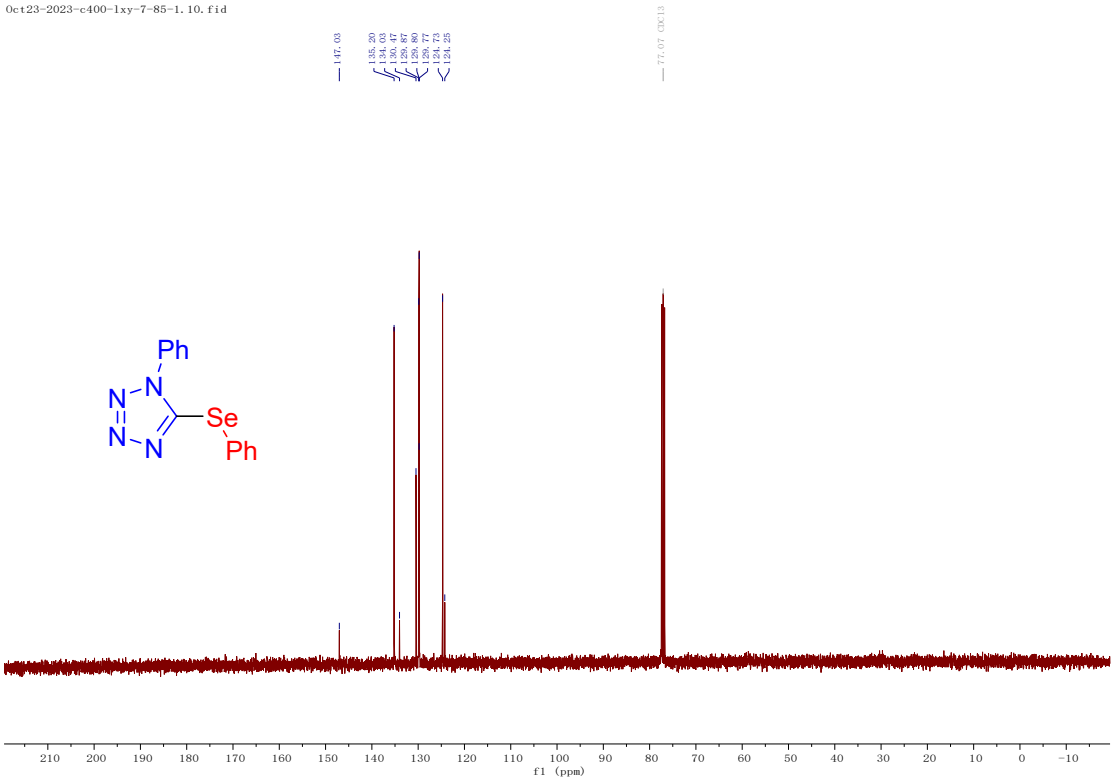

Oct23-2023-h400-lxy-7-80-2.10.fid
O
O
S
Se
N
Ph
1.00
1.03
1.10
2.13
1.09
1.95
2.18
3.15
f1 (ppm)

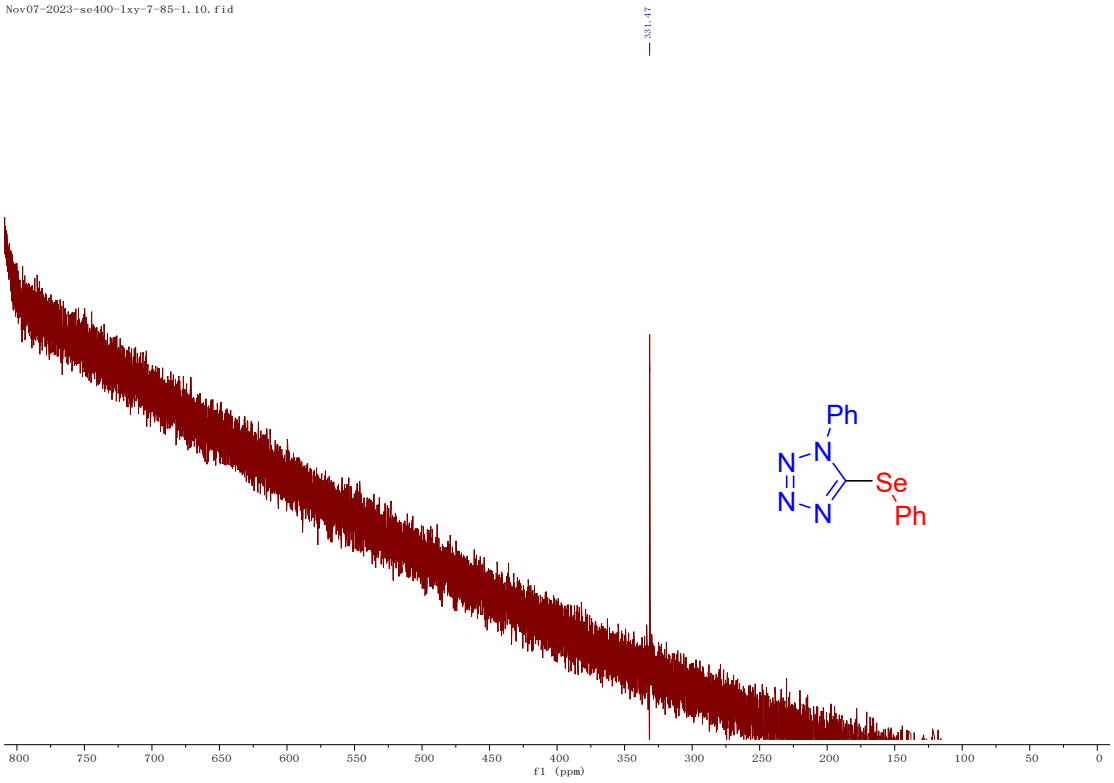

Oct23-2023-c400-lxy-7-80-2.10.fid
O
O
S
Se
N
Ph
f1 (ppm)



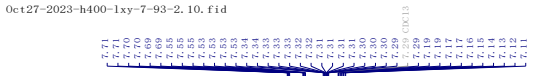
1-phenyl-5-(phenylselanyl)-1*H*-tetrazole (4h)

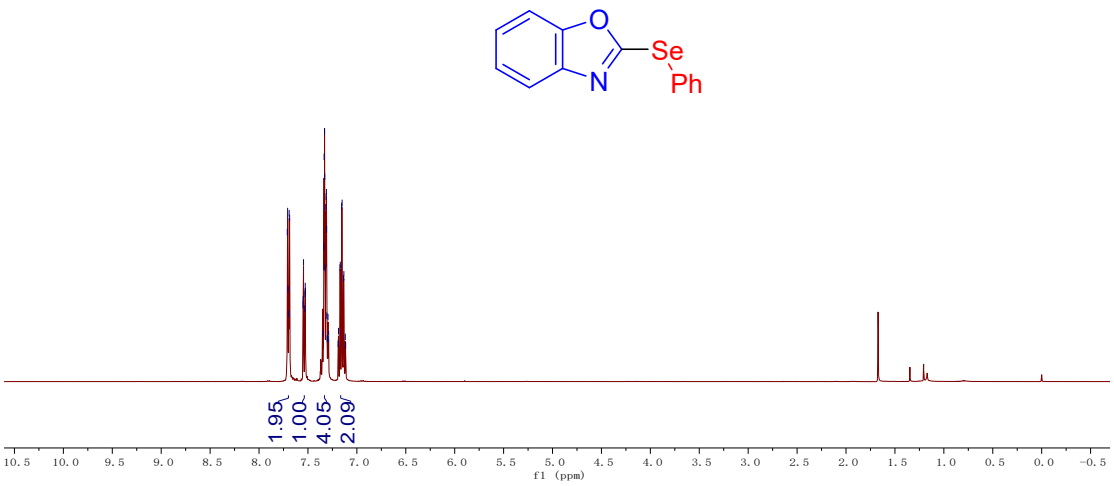


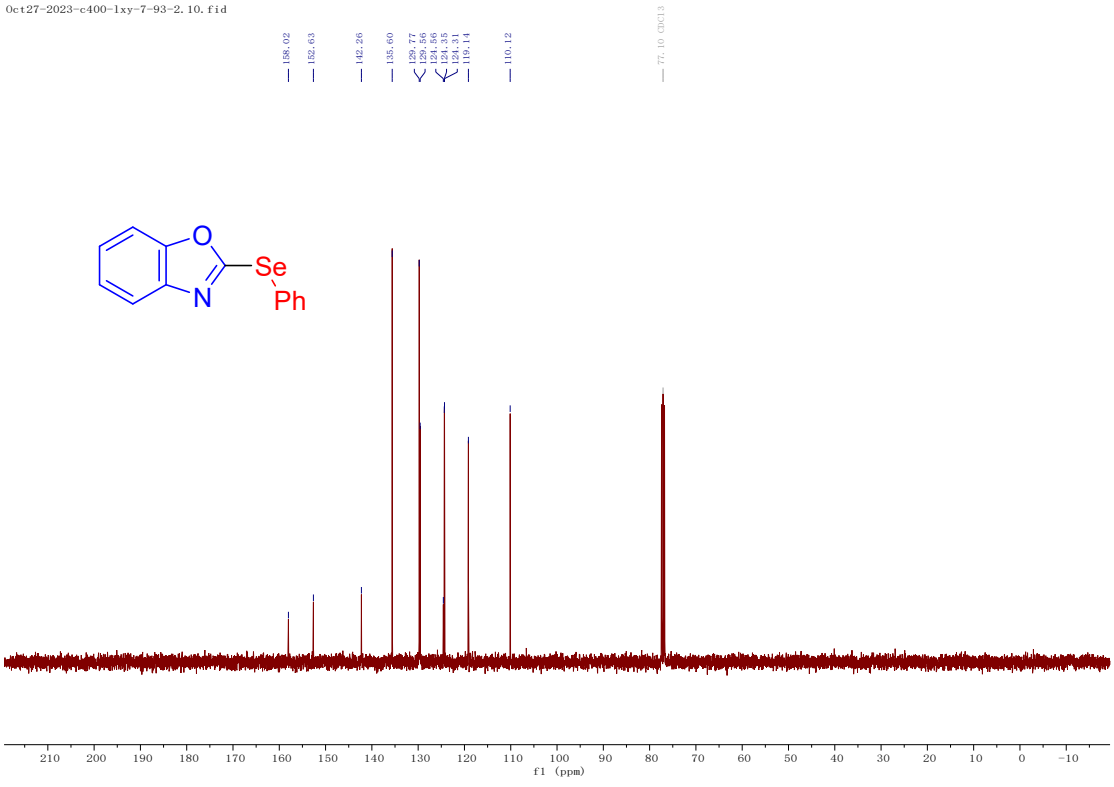


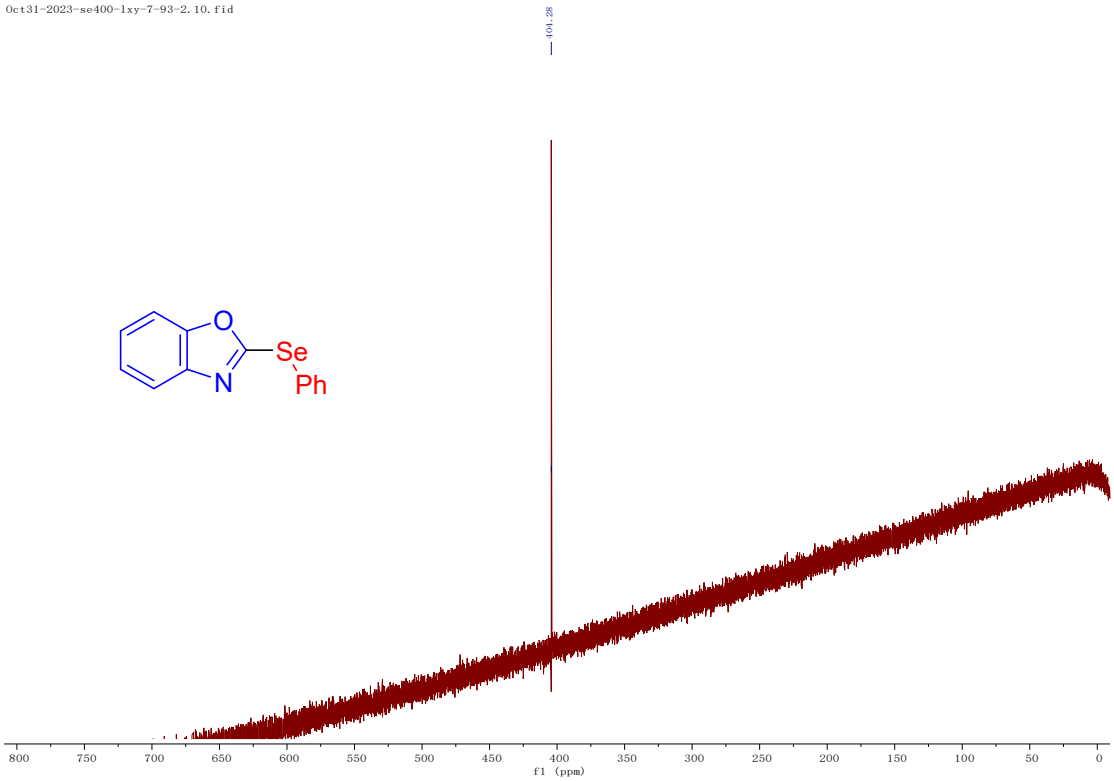


2-(phenylselanyl)benzo[*d*]oxazole (4i)

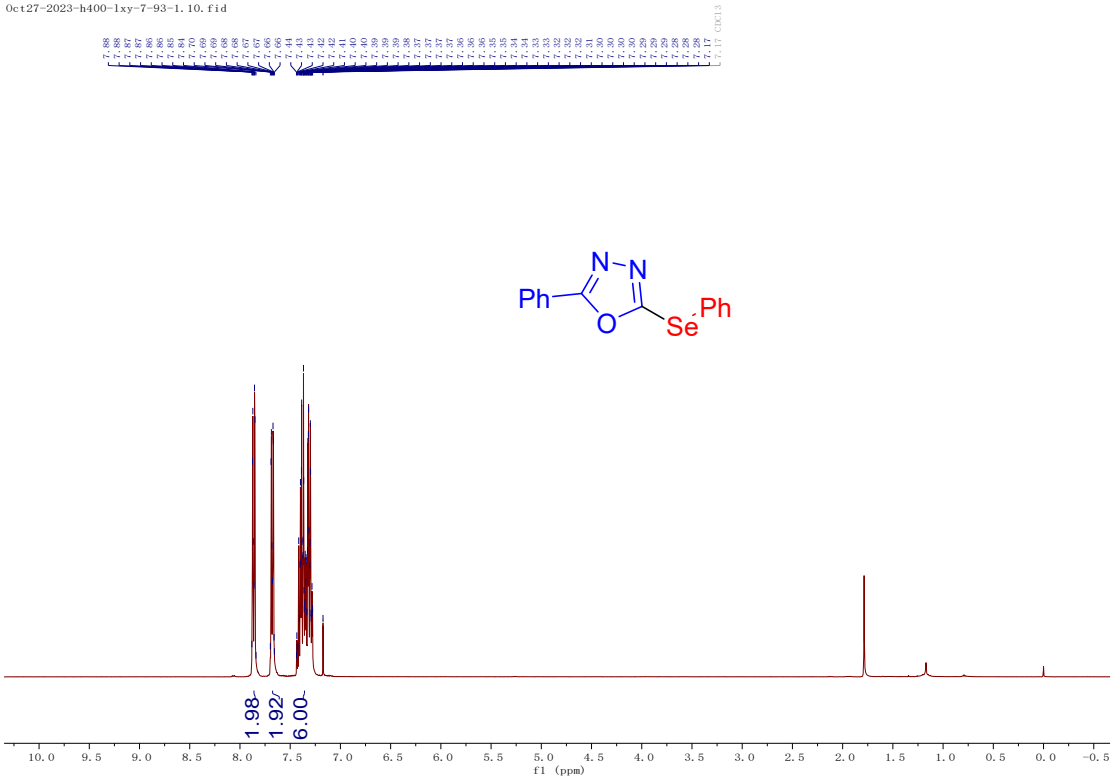

Oct27-2023-h400-1xy-7-93-2.10.fid


O
Se
N
Ph
1.95
1.00
4.05
2.09
f1 (ppm)

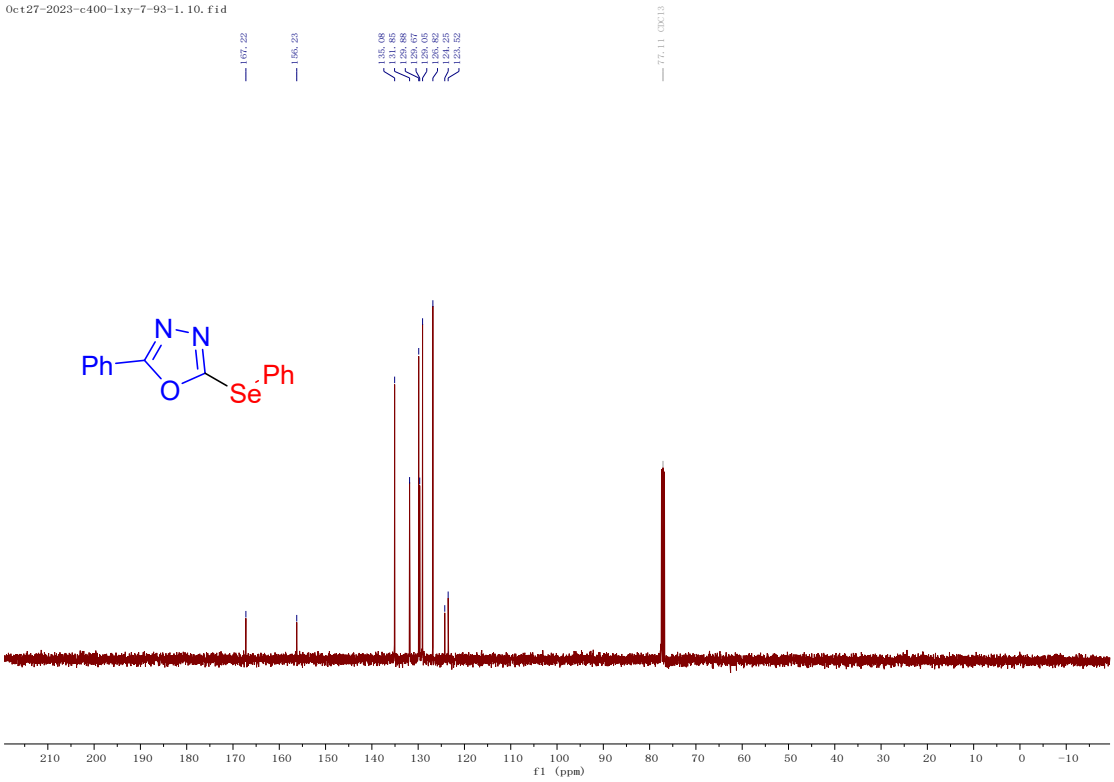

Oct27-2023-c400-1xy-7-93-2.10.fid
158.02
152.63
142.26
135.60
129.77
129.56
124.56
124.35
124.31
119.14
110.12
77.10 CDCl3
O
Se
N
Ph
f1 (ppm)



2-phenyl-5-(phenylselanyl)-1,3,4-oxadiazole (4j)



Oct27-2023-c400-lxy-7-93-1.10.fid



Oct31-2023-se400-lxy-7-93-1.10.fid