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Supporting Information

Lewis acid-promoted formation of Benzoselenazole Derivatives using SeO_2 as a selenium source

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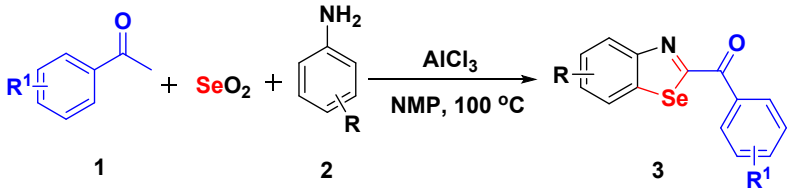
General Information

All reactions were carried out in round-bottom flasks; stirring was achieved with an oven-dried magnetic stirring bar. Solvents were purified by standard methods unless otherwise noted. Commercially available reagents were purchased from Aladdin Company in China and used throughout without further purification other than those detailed below. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis. Deuterated solvents were purchased from Cambridge Isotope laboratories. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz respectively. HRMS spectrometry (LC-HRMS) was recorded on a LXQ Spectrometer (Thermo Scientific) operating on ESI-TOF (MeOH as a solvent).

Experimental Procedure

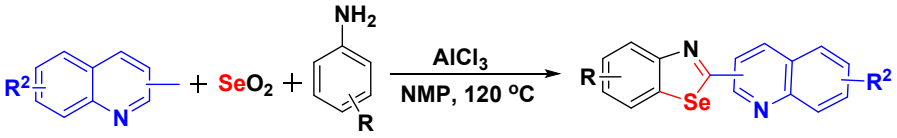
General procedure for selenization of SeO_2 as a selenium source without metal catalyst



1 2 3

Aryl ketone (0.5 mmol, 1.0 equiv.), SeO_2 (1.2 equiv.), arylaniline (1.2 equiv.) and $AlCl_3$ (0.5 equiv.) were added to a round bottom flask with anhydrous NMP (0.5 mL). The mixture was stirred at 100 °C under reflux. After 12 hrs, the reaction was cooled to room temperature, extracted with ethyl acetate, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by silica gel flash chromatography (petroleum ether : EtOAc) to give product **3**.

General procedure for selenization of SeO_2 as a selenium source without metal catalyst



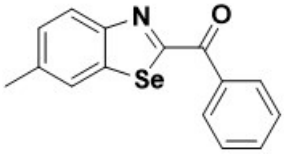
4 2 5

Quinoline (0.5 mmol, 1.0 equiv.), SeO_2 (1.2 equiv.), arylaniline (1.2 equiv.) and $AlCl_3$(0.5 equiv.) were added to a round bottom flask with anhydrous NMP (0.5 mL). The mixture was stirred at 120 °C under reflux. After 12 hrs, the reaction was cooled to room temperature, extracted with ethyl acetate, dried over anhydrous Na_2SO_4 and

concentrated in vacuo. The residue was purified by silica gel flash chromatography (petroleum ether : EtOAc) to give product **5**.

Characterization data of the products

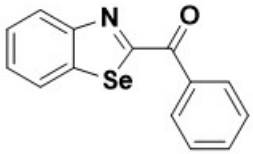
(6-methylbenzo[*d*][1,3]selenazol-2-yl)(phenyl)methanone (3a)



Yield 70%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.69 - 8.48 (m, 2H), 8.19 (d, J = 8.4 Hz, 1H), 7.91 - 7.82 (m, 1H), 7.73 - 7.62 (m, 1H), 7.62 - 7.52 (m, 2H), 7.40 (dd, J = 8.4, 1.7 Hz, 1H), 2.53 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 186.26, 172.11, 154.11, 141.09, 138.13, 134.58, 133.75, 131.33, 128.57, 128.47, 126.96, 125.12, 21.70. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{12}NOSe^+$ 302.0079 $(M+H)^+$, found 302.0077.

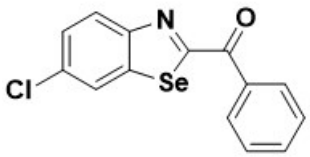
benzo[*d*][1,3]selenazol-2-yl(phenyl)methanone (3b)



Yield 74%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.66 - 8.50 (m, 2H), 8.32 (dd, J = 8.2, 1.1 Hz, 1H), 8.07 (dd, J = 8.0, 1.2 Hz, 1H), 7.80 - 7.66 (m, 1H), 7.66 - 7.55 (m, 3H), 7.51 - 7.48 (m, 1H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 186.20, 173.32, 155.96, 140.84, 134.44, 133.88, 131.39, 128.51, 127.50, 127.41, 126.84, 125.36. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_{10}NOSe^+$ 287.9922 $(M+H)^+$, found 287.9917.

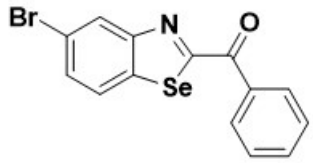
(6-chlorobenzo[*d*][1,3]selenazol-2-yl)(phenyl)methanone (3c)



Yield 68%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.64 - 8.51 (m, 2H), 8.21 (d, J = 8.7 Hz, 1H), 8.04 (d, J = 2.1 Hz, 1H), 7.74 - 7.65 (m, 1H), 7.65 - 7.49 (m, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 185.78, 173.84, 154.44, 141.84, 134.19, 134.05, 133.88, 131.35, 128.56, 128.07, 127.80, 124.96. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_9ClNOSe^+$ 321.9532 $(M+H)^+$, found 321.9537.

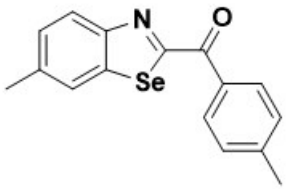
(5-bromobenzo[*d*][1,3]selenazol-2-yl)(phenyl)methanone (3d)



Yield 66%, orange solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.60 - 8.55 (m, 2H), 8.25 (dd, J = 8.2, 1.0 Hz, 1H), 7.75 - 7.67 (m, 1H), 7.60 (q, J = 7.5 Hz, 3H), 7.48 (t, J = 7.9 Hz, 1H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 185.95, 173.78, 155.05, 144.86, 134.09, 134.07, 131.41, 129.81, 128.57, 128.01, 126.16, 117.64. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_9BrNOSe^+$ 365.9027 $(M+H)^+$, found 365.9026.

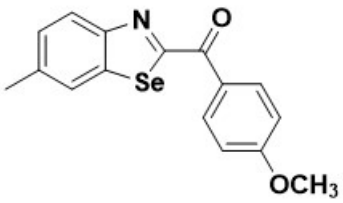
(6-methylbenzo[*d*][1,3]selenazol-2-yl)(p-tolyl)methanone (3e)



Yield 73%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.59 - 8.39 (m, 2H), 8.18 (d, J = 8.3 Hz, 1H), 7.84 (d, J = 1.6 Hz, 1H), 7.47 - 7.31 (m, 3H), 2.51 (s, 3H), 2.48 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 185.71, 172.50, 154.13, 144.80, 141.03, 137.96, 131.98, 131.48, 129.24, 128.48, 126.89, 125.10, 21.85, 21.69. **HRMS** (ESI-TOF) m/z calculated for $C_{16}H_{14}NOSe^+$ 316.0235 $(M+H)^+$, found 316.0235.

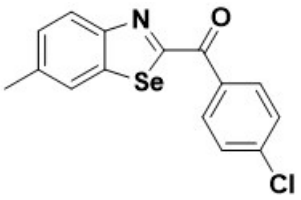
(4-methoxyphenyl)(6-methylbenzo[*d*][1,3]selenazol-2-yl)methanone (3f)



Yield 72%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.72 - 8.57 (m, 2H), 8.17 (d, J = 8.3 Hz, 1H), 7.85 (dt, J = 1.7, 0.8 Hz, 1H), 7.39 (dd, J = 8.4, 1.7 Hz, 1H), 7.12 - 6.96 (m, 2H), 3.94 (s, 3H), 2.52 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 184.29, 173.00, 164.31, 154.13, 140.92, 137.83, 133.88, 128.42, 127.32, 126.75, 125.09, 113.87, 55.56, 21.68. **HRMS** (ESI-TOF) m/z calculated for $C_{16}H_{13}NNaO_2Se^+$ 354.0004 $(M+Na)^+$, found 354.0007.

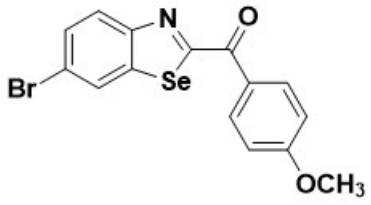
(4-chlorophenyl)(6-methylbenzo[*d*][1,3]selenazol-2-yl)methanone (3g)



Yield 64%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.65 - 8.46 (m, 2H), 8.17 (d, J = 8.4 Hz, 1H), 7.93 - 7.73 (m, 1H), 7.63 - 7.49 (m, 2H), 7.40 (dd, J = 8.4, 1.7 Hz, 1H), 2.52 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 184.89, 171.76, 154.02, 141.16, 140.44, 138.33, 132.84, 132.76, 128.82, 128.69, 126.98, 125.13, 21.72. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{11}ClNOSe^+$ 335.9689 $(M+H)^+$, found 335.9689.

(6-bromobenzo[*d*][1,3]selenazol-2-yl)(4-methoxyphenyl)methanone (3h)

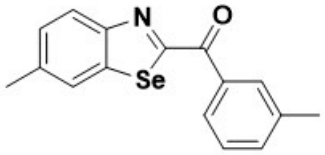


Yield 67%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.71 - 8.59 (m, 2H), 8.19 (d, J = 1.9 Hz, 1H), 8.13 (d, J = 8.7 Hz, 1H), 7.68 (dd, J = 8.7, 2.0 Hz, 1H), 7.16 - 6.98 (m, 2H), 3.95 (s,

3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 183.74, 174.85, 164.56, 154.79, 142.17, 133.94, 130.36, 128.20, 127.88, 126.92, 121.68, 113.98, 55.60. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{11}BrNO_2Se^+$ 395.9133 $(M+H)^+$, found 385.9121.

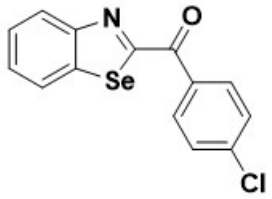
(6-methylbenzo[*d*][1,3]selenazol-2-yl)(m-tolyl)methanone (3i)



Yield 71%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.39 (dt, J = 6.8, 1.8 Hz, 1H), 8.29 (p, J = 0.9 Hz, 1H), 8.19 (d, J = 8.4 Hz, 1H), 7.90 - 7.77 (m, 1H), 7.54 - 7.43 (m, 2H), 7.39 (dd, J = 8.4, 1.7 Hz, 1H), 2.53 (s, 3H), 2.50 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 186.53, 172.24, 154.09, 141.06, 138.25, 138.06, 134.59, 131.52, 128.70, 128.53, 128.36, 126.96, 125.11, 21.70, 21.47. **HRMS** (ESI-TOF) m/z calculated for $C_{16}H_{14}NOSe^+$ 316.0235 $(M+H)^+$, found 316.0233.

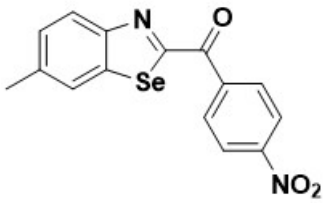
benzo[*d*][1,3]selenazol-2-yl(4-chlorophenyl)methanone (3j)



Yield 69%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.62 - 8.54 (m, 2H), 8.31 (dd, J = 8.2, 1.2 Hz, 1H), 8.10 - 8.03 (m, 1H), 7.65 - 7.53 (m, 3H), 7.49 (ddd, J = 8.3, 7.2, 1.3 Hz, 1H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 184.87, 172.98, 155.88, 140.90, 140.61, 132.81, 132.72, 128.88, 127.57, 127.53, 126.95, 125.38. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_9ClNOSe^+$ 321.9532 $(M+H)^+$, found 321.9534.

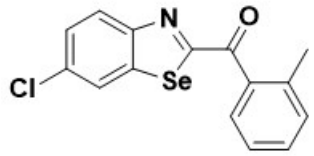
(6-methylbenzo[*d*][1,3]selenazol-2-yl)(4-nitrophenyl)methanone (3k)



Yield 47%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.87 - 8.62 (m, 2H), 8.51 - 8.30 (m, 2H), 8.20 (d, J = 8.4 Hz, 1H), 7.89 (dt, J = 1.8, 0.8 Hz, 1H), 7.44 (dd, J = 8.4, 1.7 Hz, 1H), 2.55 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 184.82, 170.67, 153.98, 150.53, 141.42, 139.45, 138.92, 132.31, 129.01, 127.20, 125.20, 123.44, 21.77. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{10}N_2NaO_3Se^+$ 368.9749 $(M+H)^+$, found 368.9742.

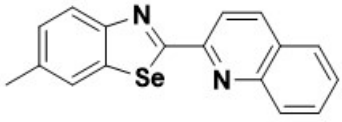
(6-chlorobenzo[d][1,3]selenazol-2-yl)(o-tolyl)methanone (3l)



Yield 57%, yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.15 (d, J = 8.7 Hz, 1H), 8.10 - 7.99 (m, 2H), 7.57 - 7.46 (m, 2H), 7.38 (ddd, J = 8.8, 5.9, 1.5 Hz, 2H), 2.55 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 189.67, 174.33, 154.34, 142.00, 139.31, 134.37, 133.90, 132.16, 131.62, 131.48, 128.16, 127.81, 125.35, 125.02, 20.79. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{11}ClNOSe^+$ 335.9689 $(M+H)^+$, found 335.9686.

6-methyl-2-(quinolin-2-yl)benzo[*d*][1,3]selenazole (5a)

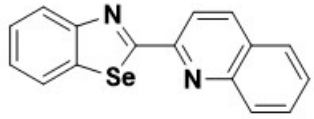


Yield 55%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.44 (d, J = 8.5 Hz, 1H), 8.33 - 8.26 (m, 1H), 8.22 - 8.16 (m, 1H), 8.07 (d, J = 8.3 Hz, 1H), 7.93 - 7.82 (m, 2H), 7.78 (ddd, J = 8.4, 6.8, 1.4 Hz, 1H), 7.61 (ddd, J = 8.0, 6.8, 1.2 Hz, 1H), 7.34 (dd, J = 8.4, 1.7 Hz, 1H), 2.52 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 174.33, 154.48, 153.12, 148.11, 139.54, 136.89, 136.12, 130.03, 129.66, 129.05, 127.81, 127.72, 127.46, 125.16,

124.87, 117.58, 21.53. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{13}N_2Se^+$ 325.0238 $(M+H)^+$, found 325.0237.

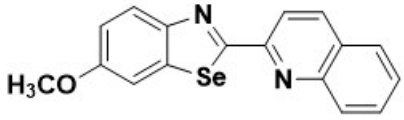
2-(quinolin-2-yl)benzo[*d*][1,3]selenazole (5b)



Yield 52%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.44 (dd, J = 19.2, 8.5 Hz, 1H), 8.31 (d, J = 8.5 Hz, 1H), 8.20 (dd, J = 8.4, 4.7 Hz, 2H), 8.04 (d, J = 7.9 Hz, 1H), 7.89 (d, J = 8.1 Hz, 1H), 7.79 (ddd, J = 8.5, 6.8, 1.6 Hz, 1H), 7.62 (t, J = 7.5 Hz, 1H), 7.59 - 7.49 (m, 1H), 7.39 (t, J = 7.7 Hz, 1H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 175.56, 156.41, 152.99, 148.12, 139.43, 136.96, 130.07, 129.70, 129.13, 127.73, 127.57, 126.25, 125.79, 125.42, 125.25, 117.61. **HRMS** (ESI-TOF) m/z calculated for $C_{16}H_{10}N_2NaSe^+$ 332.9901 $(M+H)^+$, found 332.9899.

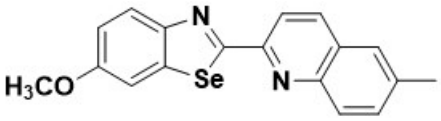
6-methoxy-2-(quinolin-2-yl)benzo[*d*][1,3]selenazole (5c)



Yield 58%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.41 (d, J = 8.5 Hz, 1H), 8.28 (dd, J = 8.6, 0.8 Hz, 1H), 8.18 (dq, J = 8.5, 0.8 Hz, 1H), 8.06 (d, J = 8.9 Hz, 1H), 7.92 - 7.84 (m, 1H), 7.77 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H), 7.60 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.51 (d, J = 2.6 Hz, 1H), 7.12 (dd, J = 8.9, 2.6 Hz, 1H), 3.94 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 172.51, 158.14, 153.11, 150.92, 148.11, 140.90, 136.84, 130.00, 129.58, 128.94, 127.72, 127.35, 125.79, 117.47, 115.25, 108.00, 55.78. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{13}N_2OSe^+$ 341.0188 $(M+H)^+$, found 341.0188.

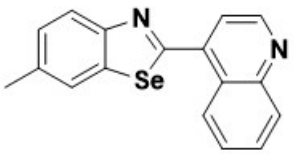
6-methoxy-2-(6-methylquinolin-2-yl)benzo[*d*][1,3]selenazole (5d)



Yield 60%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.36 (d, J = 8.5 Hz, 1H), 8.25 - 8.11 (m, 1H), 8.06 (dd, J = 8.8, 7.0 Hz, 2H), 7.67 - 7.53 (m, 2H), 7.50 (d, J = 2.6 Hz, 1H), 7.11 (dd, J = 8.9, 2.6 Hz, 1H), 3.93 (s, 3H), 2.57 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 172.71, 158.06, 152.31, 150.94, 146.71, 140.77, 137.48, 136.08, 132.28, 129.25, 128.99, 126.60, 125.68, 117.47, 115.14, 108.03, 55.77, 21.72. **HRMS** (ESI-TOF) m/z calculated for $C_{18}H_{15}N_2OSe^+$ 355.0344 $(M+H)^+$, found 355.0342.

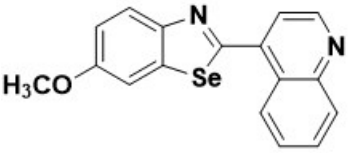
6-methyl-2-(quinolin-4-yl)benzo[*d*][1,3]selenazole (5e)



Yield 90%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 9.09 - 8.94 (m, 2H), 8.22 (dd, J = 8.4, 1.2 Hz, 1H), 8.16 (d, J = 8.3 Hz, 1H), 7.87 - 7.75 (m, 2H), 7.76 - 7.64 (m, 2H), 7.39 (dd, J = 8.3, 1.7 Hz, 1H), 2.53 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 167.72, 153.92, 149.84, 149.26, 140.75, 139.40, 136.53, 129.92, 129.88, 128.26, 128.04, 126.13, 125.17, 124.60, 124.45, 122.49, 21.54. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{13}N_2Se^+$ 325.0238 $(M+H)^+$, found 325.0234.

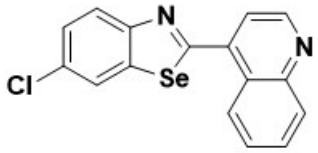
6-methoxy-2-(quinolin-4-yl)benzo[*d*][1,3]selenazole (5f)



Yield 96%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 9.15 - 8.95 (m, 2H), 8.29 - 8.10 (m, 2H), 7.80 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.77 - 7.60 (m, 2H), 7.48 (d, J = 2.6 Hz, 1H), 7.17 (dd, J = 8.9, 2.6 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 165.85, 158.31, 150.36, 149.85, 149.27, 140.66, 140.61, 129.90, 129.87, 128.01, 126.17, 126.07, 124.41, 122.43, 115.62, 107.55, 55.85. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{13}N_2OSe^+$ 341.0188 $(M+H)^+$, found 341.0185.

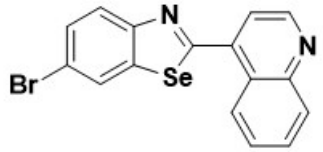
6-chloro-2-(quinolin-4-yl)benzo[*d*][1,3]selenazole (5g)



Yield 85%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 9.05 (d, J = 4.5 Hz, 1H), 8.97 (dd, J = 8.5, 1.4 Hz, 1H), 8.33 - 8.11 (m, 2H), 8.02 (d, J = 2.1 Hz, 1H), 7.84 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.79 - 7.66 (m, 2H), 7.56 (dd, J = 8.7, 2.1 Hz, 1H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 169.47, 154.28, 149.83, 149.27, 140.23, 140.19, 132.30, 130.09, 129.98, 128.25, 127.56, 126.28, 125.89, 124.40, 124.23, 122.57. **HRMS** (ESI-TOF) m/z calculated for $C_{16}H_{10}ClN_2Se^+$ 344.9692 $(M+H)^+$, found 344.9692.

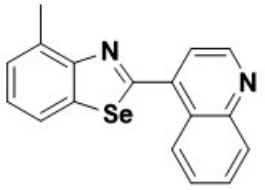
6-bromo-2-(quinolin-4-yl)benzo[*d*][1,3]selenazole (5h)



Yield 87%, pale yellow solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 9.05 (d, J = 4.5 Hz, 1H), 8.96 (dd, J = 8.5, 1.4 Hz, 1H), 8.31 - 7.96 (m, 3H), 7.83 (ddd, J = 8.4, 6.8, 1.3 Hz, 1H), 7.79 - 7.50 (m, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 169.58, 154.58, 149.83, 149.28, 140.71, 140.15, 130.29, 130.09, 129.99, 128.26, 127.30, 126.66, 125.89, 124.22, 122.56, 120.18. **HRMS** (ESI-TOF) m/z calculated for $C_{16}H_{10}BrN_2Se^+$ 388.9187$(M+H)^+$, found 388.9185.

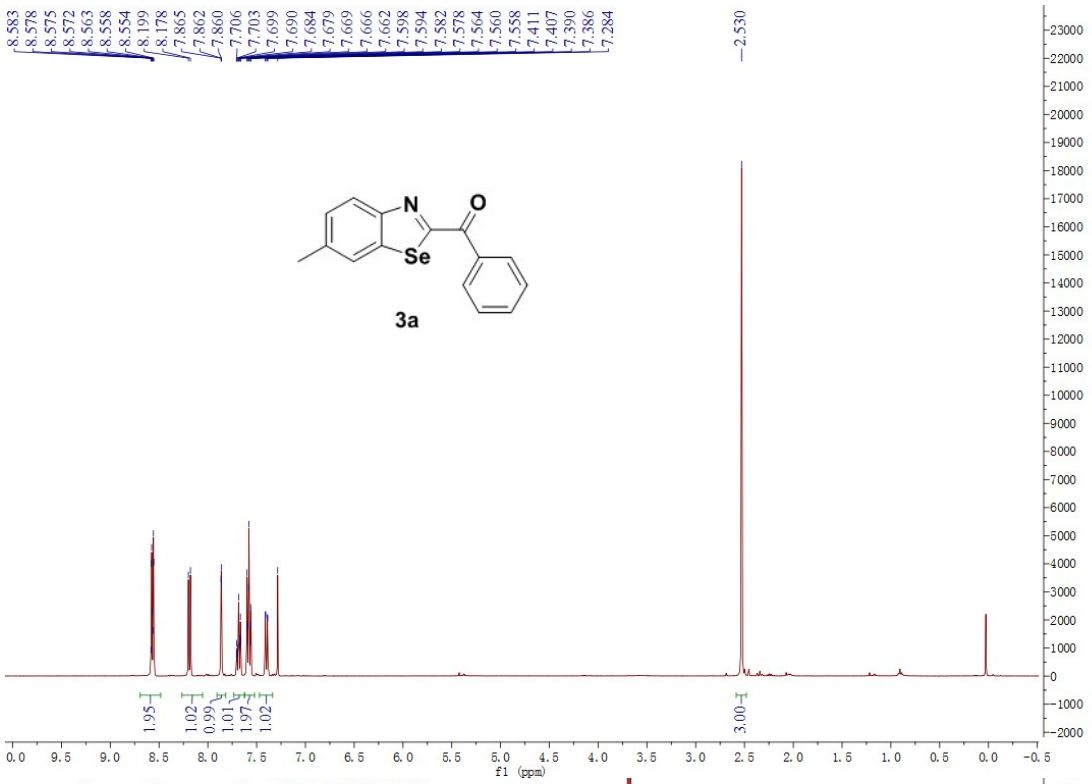
4-methyl-2-(quinolin-4-yl)benzo[*d*][1,3]selenazole (5i)

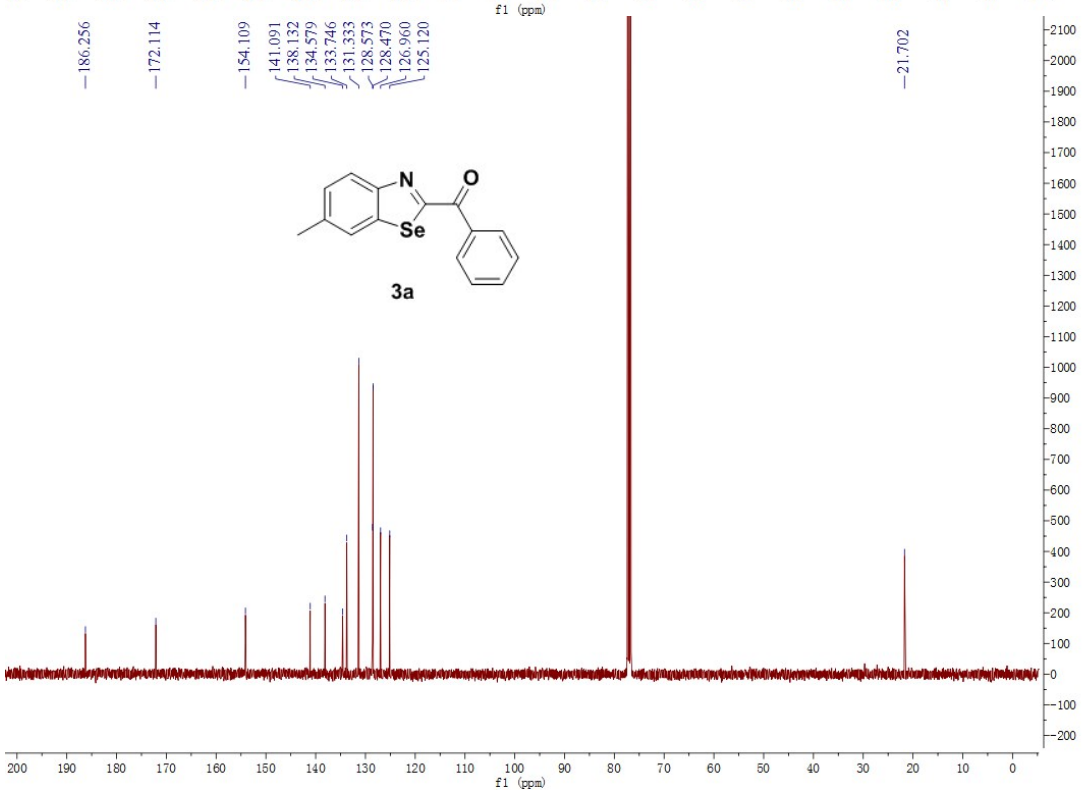


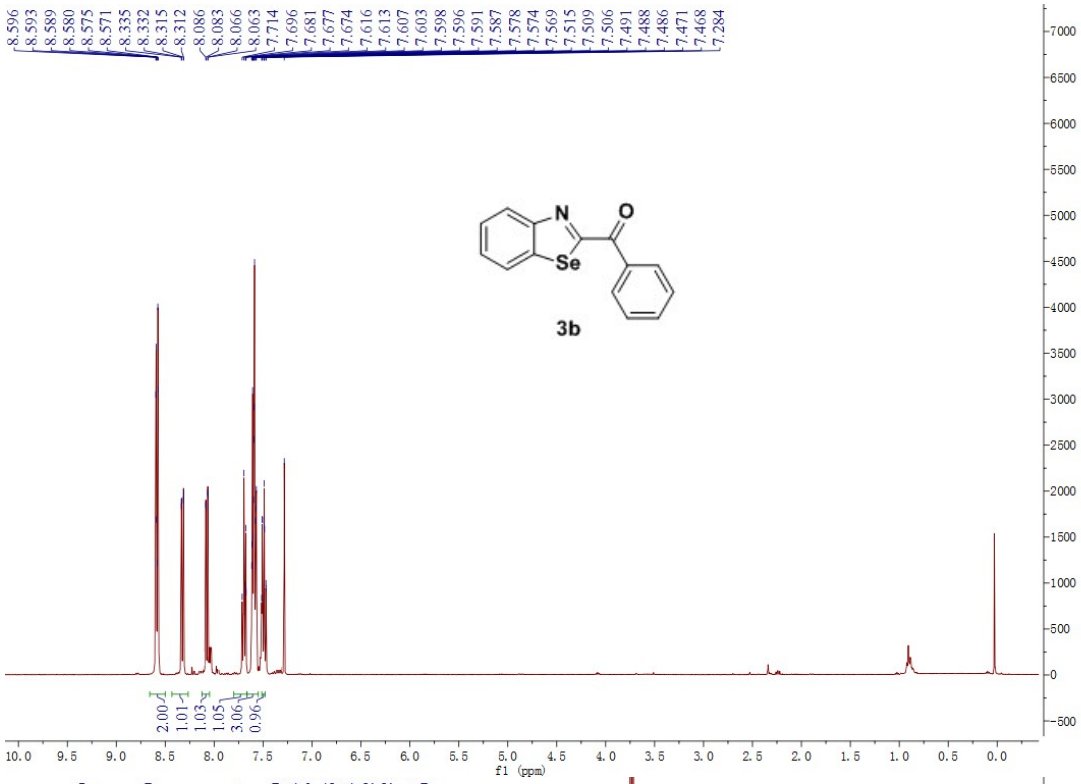
Yield 88%, white solid.

^{1}H NMR (400 MHz, Chloroform-d) δ 9.16 - 8.98 (m, 2H), 8.23 (dd, J = 8.4, 1.3 Hz, 1H), 7.94 - 7.78 (m, 2H), 7.80 - 7.64 (m, 2H), 7.46 - 7.29 (m, 2H), 2.92 (s, 3H).**^{13}C NMR** (101 MHz, Chloroform-d) δ 167.53, 155.15, 149.87, 149.34, 140.81, 139.25, 135.80, 129.90, 129.89, 128.05, 127.36, 126.25, 126.21, 124.45, 122.64, 122.15, 19.44. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{13}N_2Se^+$ 325.0238 $(M+H)^+$, found 325.0241.

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



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8.589
8.580
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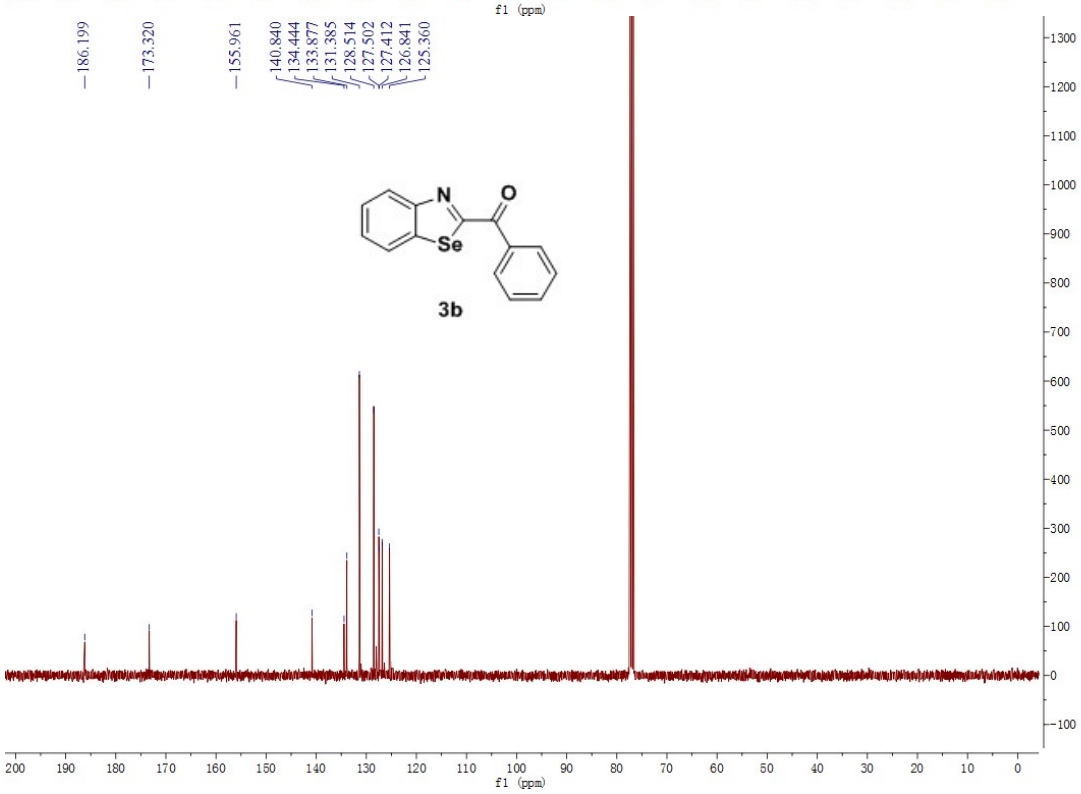
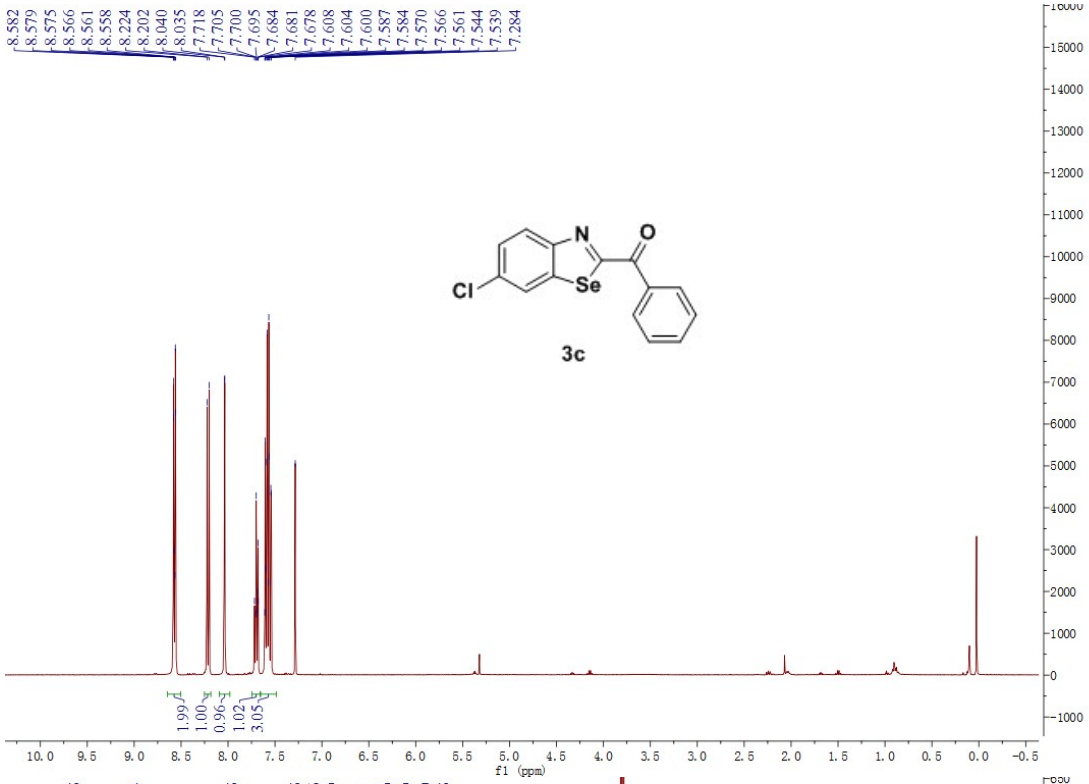
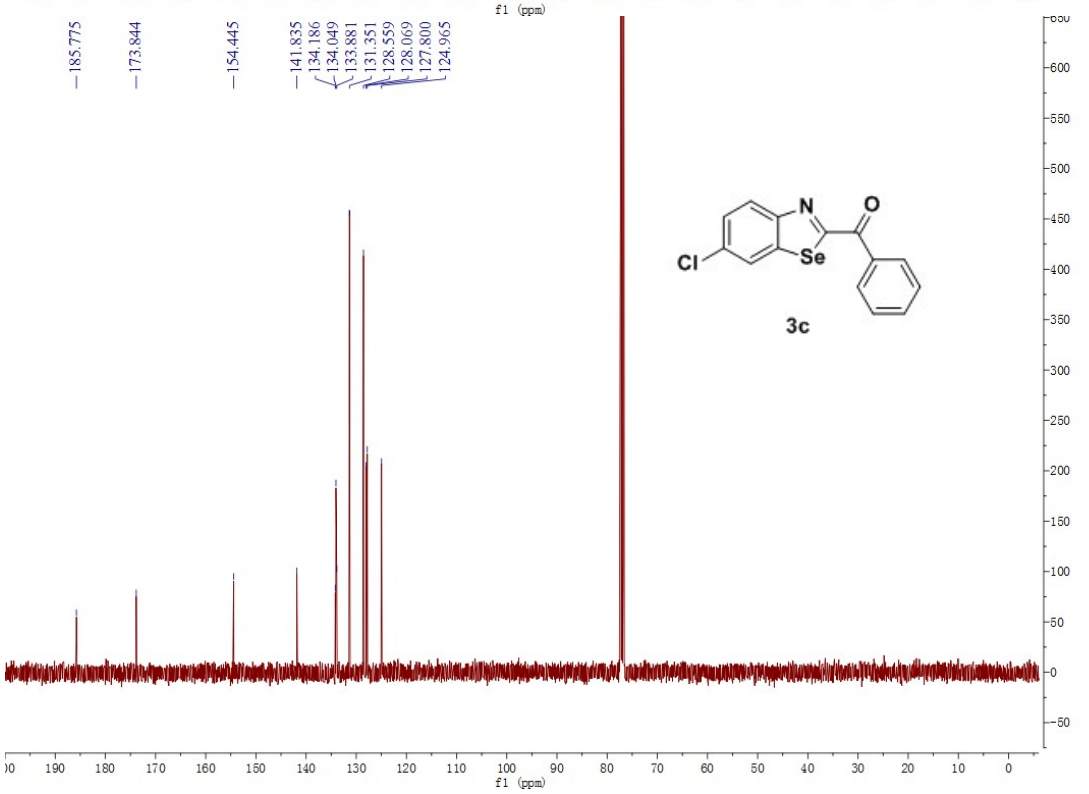
8.571
8.335
8.332
8.315
8.312
8.086
8.083
8.066
8.063
7.714
7.696
7.681
7.677
7.674
7.616
7.613
7.607
7.603
7.598
7.596
7.591
7.587
7.578
7.574
7.569
7.515
7.509
7.506
7.491
7.488
7.486
7.471
7.468
7.284
N
O
Se
3b
2.00
1.01
1.03
1.05
3.06
0.96
f1 (ppm)


186.199
173.320
155.961
140.840
134.444
133.877
131.385
128.514
127.502
127.412
126.841
125.360
N
O
Se
3b
f1 (ppm)


8.582
8.579
8.575
8.566
8.561
8.558
8.224
8.202
8.040
8.035
7.718
7.705
7.700
7.695
7.684
7.681
7.678
7.608
7.604
7.600
7.587
7.584
7.570
7.566
7.561
7.544
7.539
7.284
N
O
Cl
Se
3c
1.99
1.00
0.96
1.02
3.05
f1 (ppm)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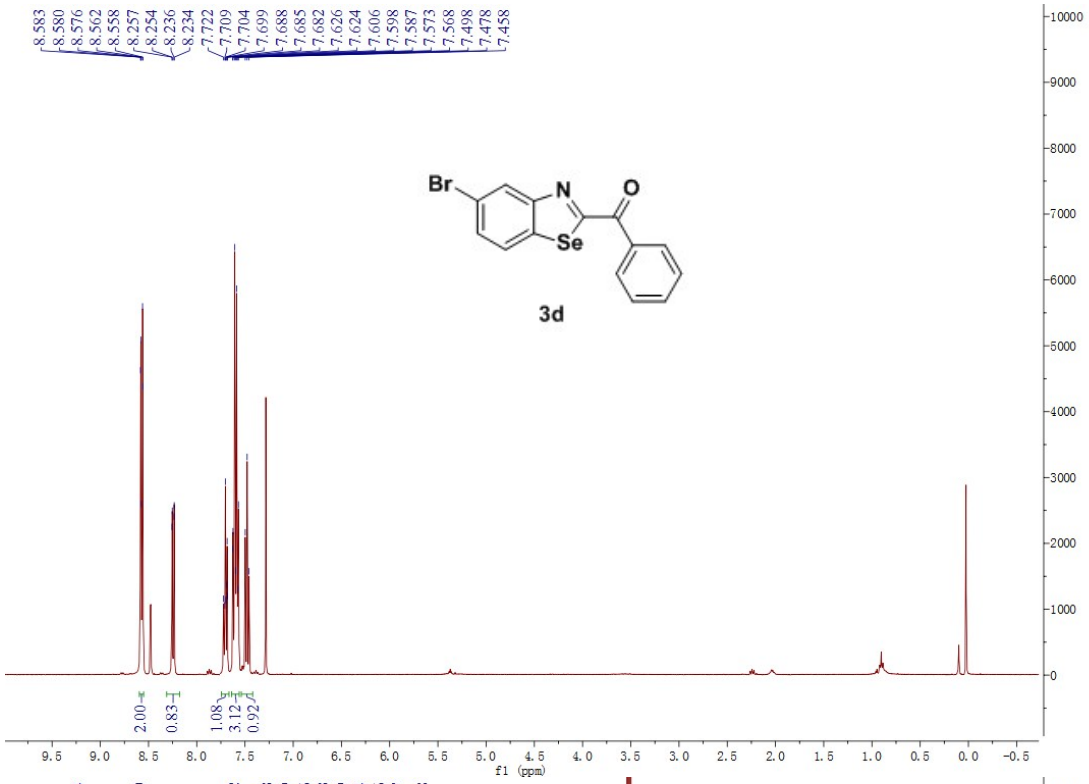
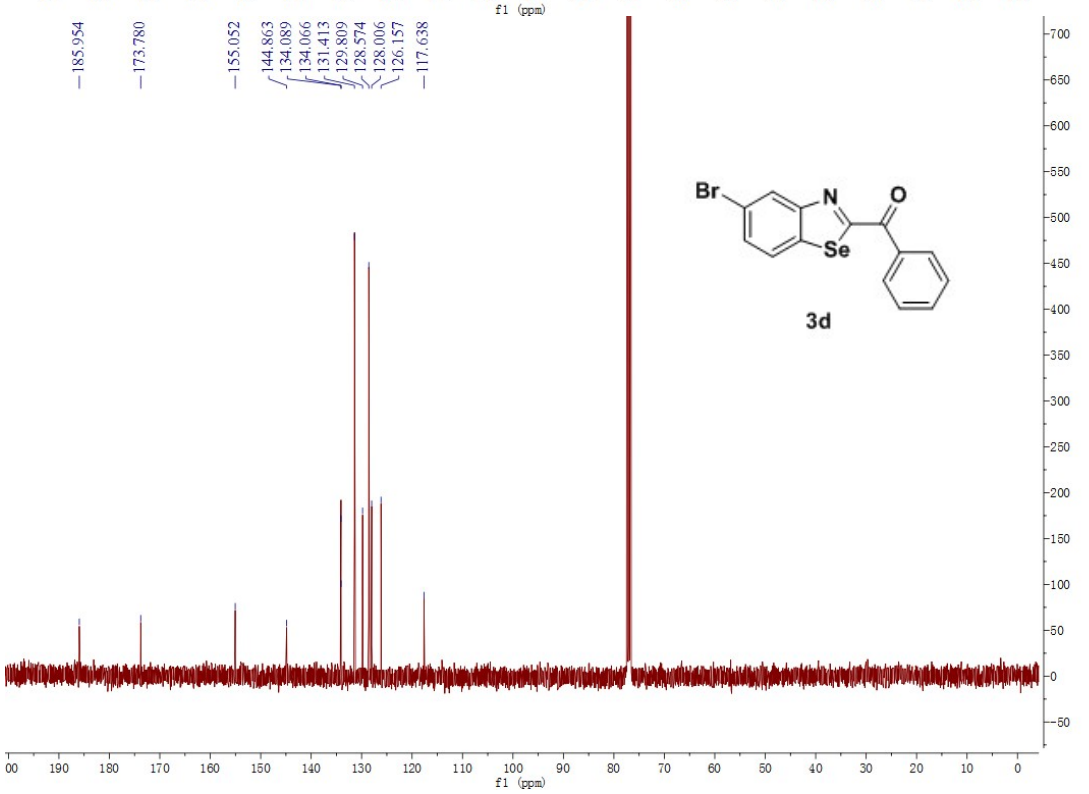
154.445
141.835
134.186
134.049
133.881
131.351
128.559
128.069
127.800
124.965
N
O
Cl
Se
3c
f1 (ppm)


8.583
8.580
8.576
8.562
8.558
8.257
8.254
8.236
8.234
7.722
7.709
7.704
7.699
7.688
7.685
7.682
7.626
7.624
7.606
7.598
7.587
7.573
7.568
7.498
7.478
7.458
Br
N
O
Se
3d
2.00
0.83
1.08
3.12
0.92
f1 (ppm)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155.052
144.863
134.089
134.066
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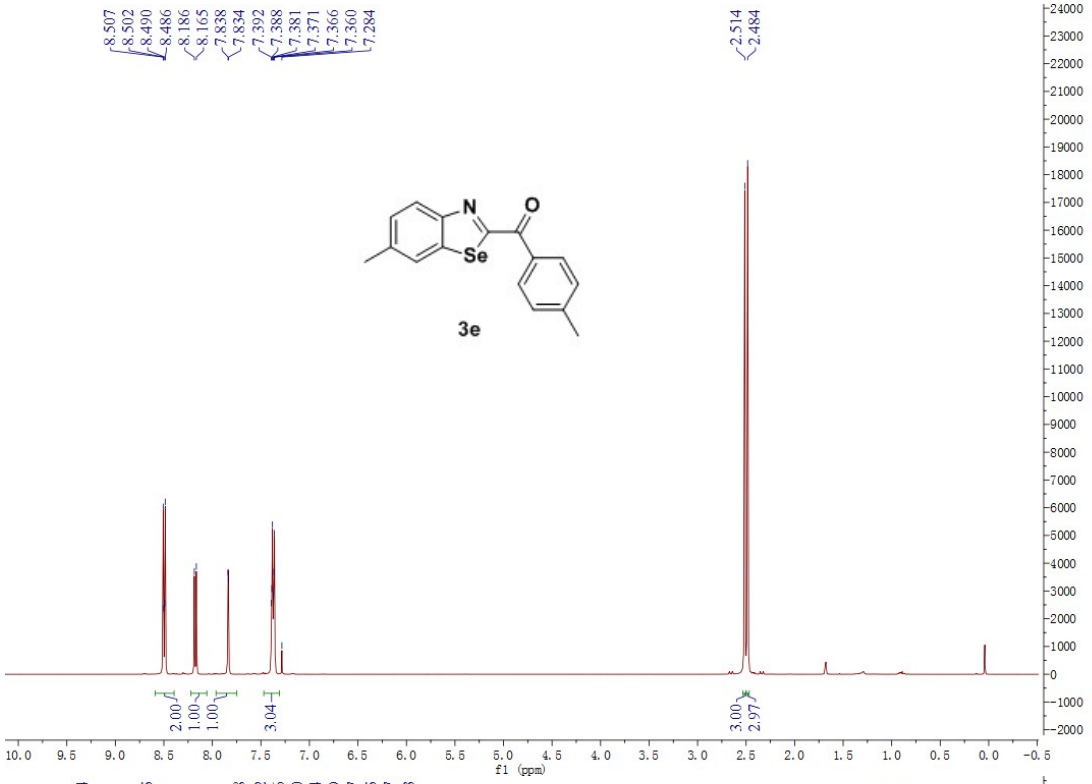
129.809
128.574
128.006
126.157
117.638
Br
N
O
Se
3d
f1 (ppm)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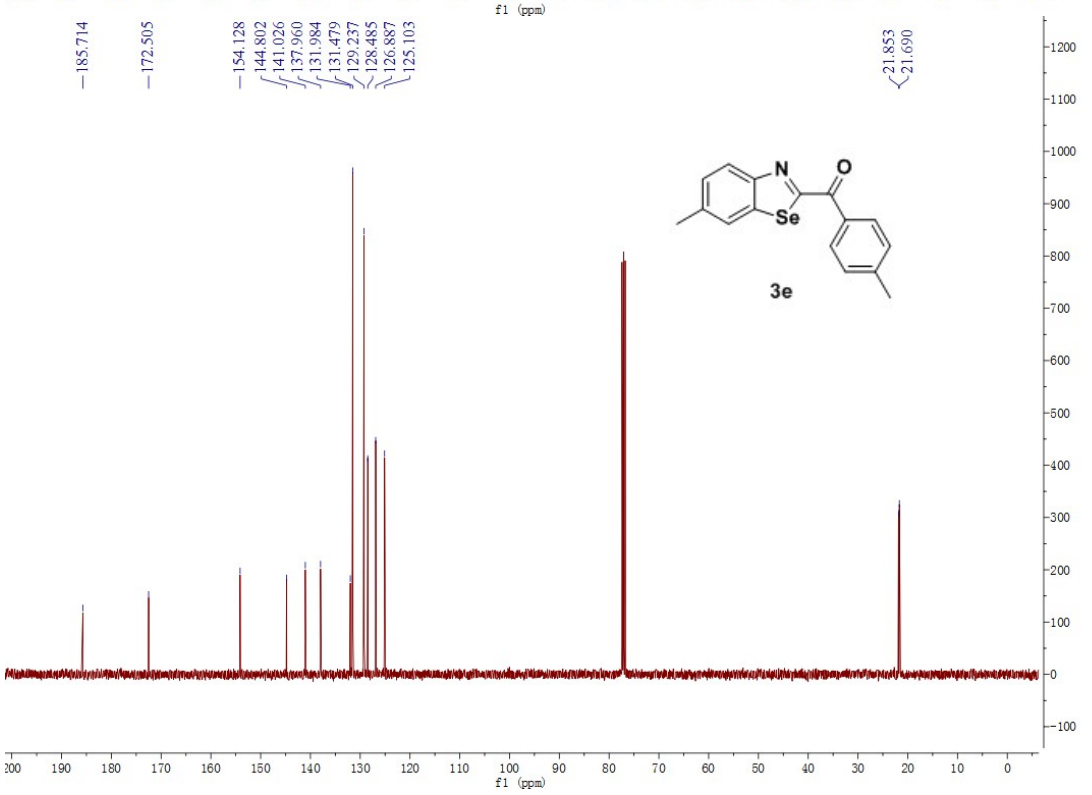
8.502
8.490
8.486
8.186
8.165
7.838
7.834
7.392
7.388
7.381
7.371
7.366
7.360
7.284
2.514
2.484
N
O
Se
3e
2.00
1.00
1.00
3.04
3.00
2.97
f1 (ppm)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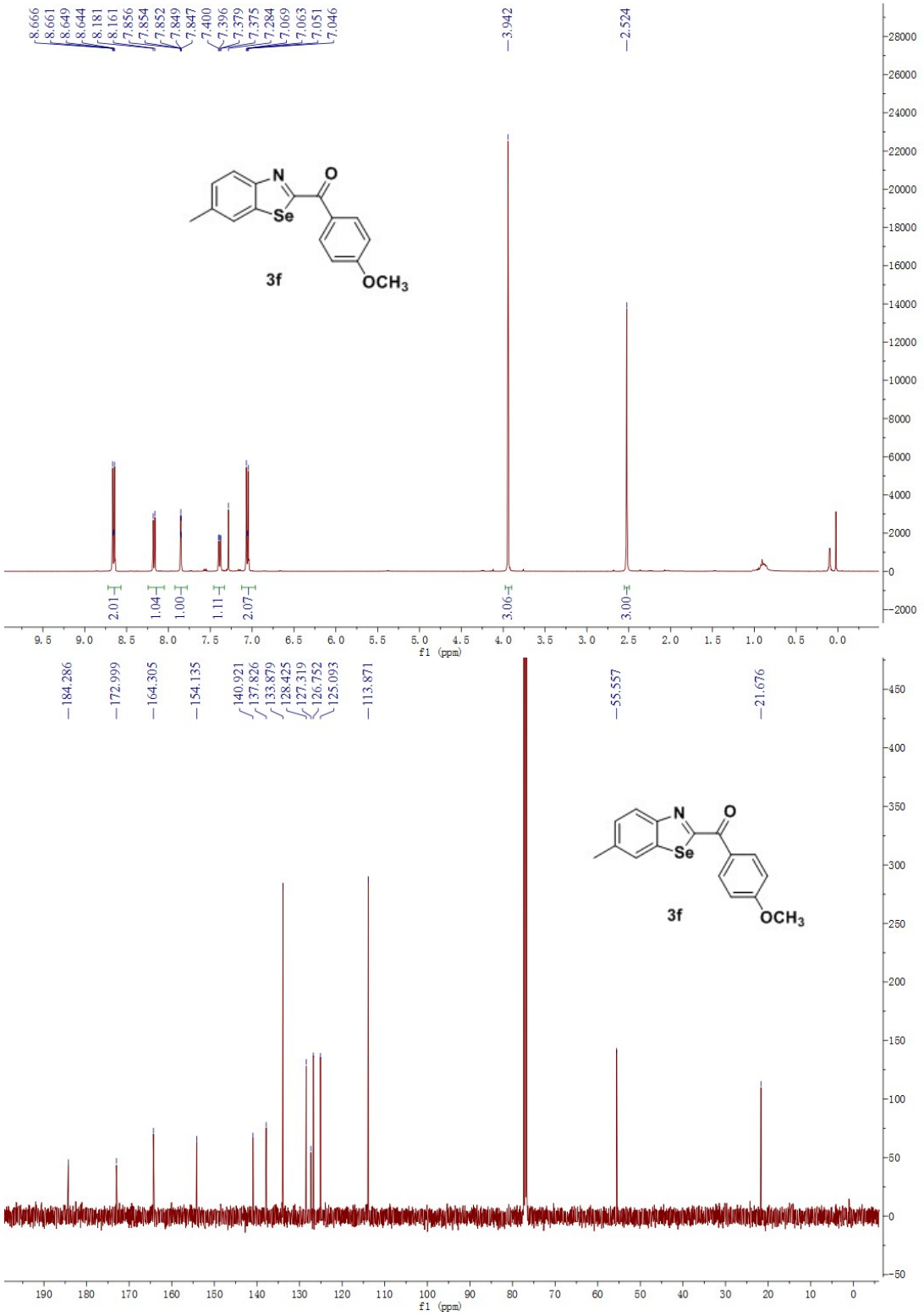
154.128
144.802
141.026
137.960
131.984
131.479
129.237
128.485
126.887
125.103
21.853
21.690
N
O
Se
3e
f1 (ppm)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8.649
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8.181
8.161
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7.854
7.852
7.849
7.847
7.400
7.396
7.379
7.375
7.284
7.069
7.063
7.051
7.046
3.942
2.524
N
O
Se
3f
OCH3
2.01
1.04
1.00
1.11
2.07
3.06
3.00
f1 (ppm)
184.286
172.999
164.305
154.135
140.921
137.826
133.879
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113.871
55.557
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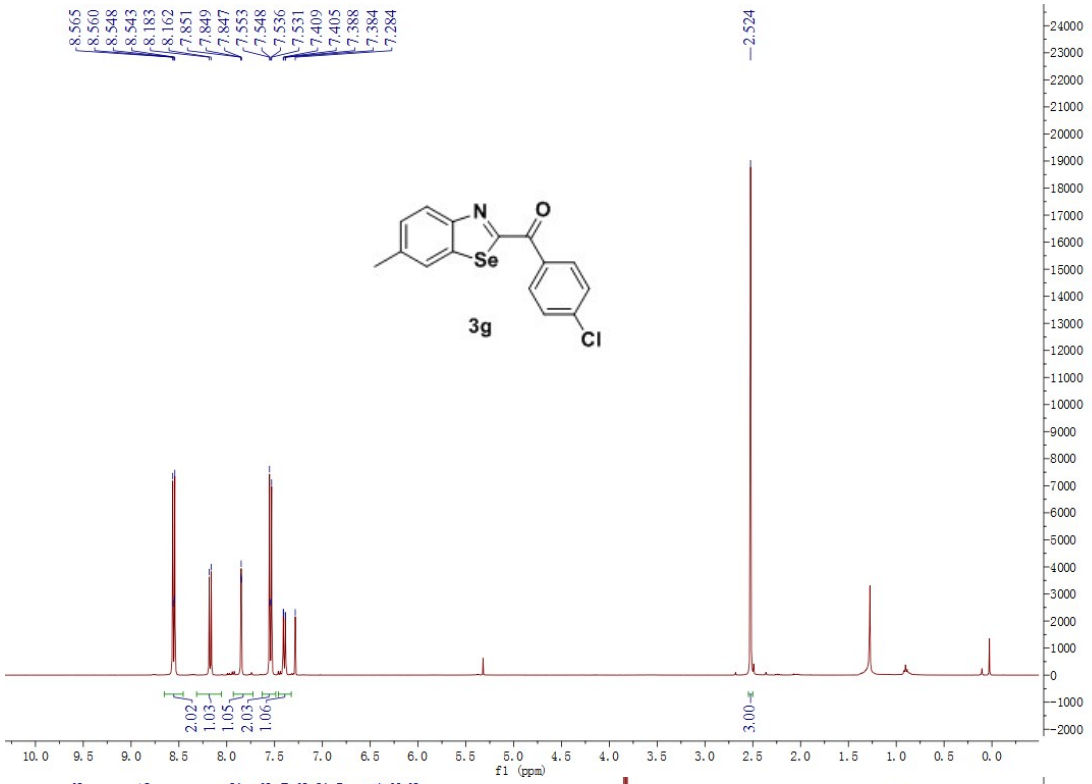
Se
3f
OCH3
f1 (ppm)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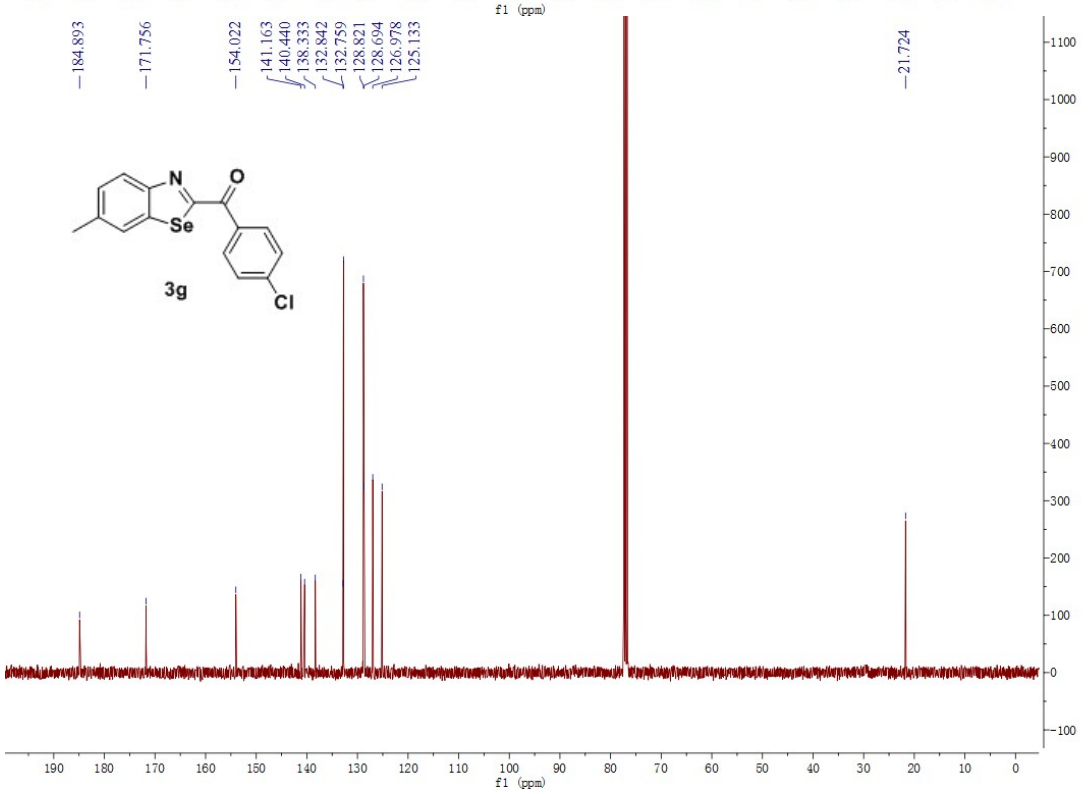
8.560
8.548
8.543
8.183
8.162
7.851
7.849
7.847
7.553
7.548
7.536
7.531
7.409
7.405
7.388
7.384
7.284
2.524
N
O
Se
Cl
3g
2.02
1.03
1.05
2.03
1.06
3.00
f1 (ppm)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141.163
140.440
138.333
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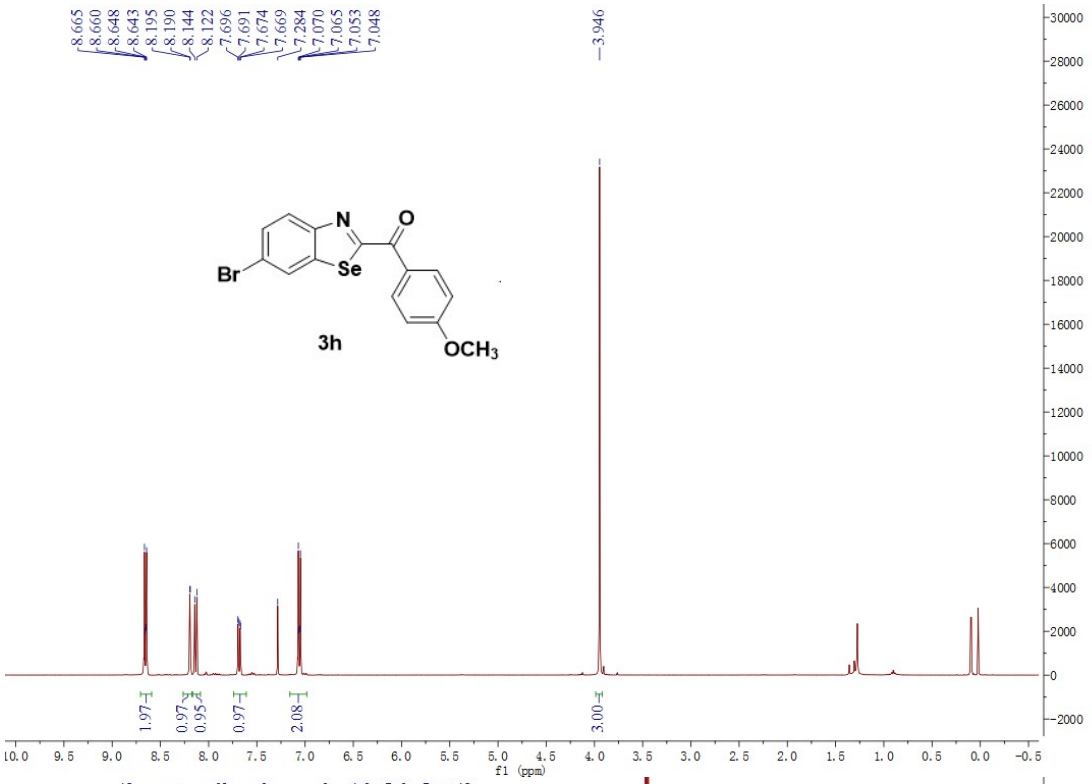
128.821
128.694
126.978
125.133
21.724
N
O
Se
Cl
3g
f1 (ppm)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8.144
8.122
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7.674
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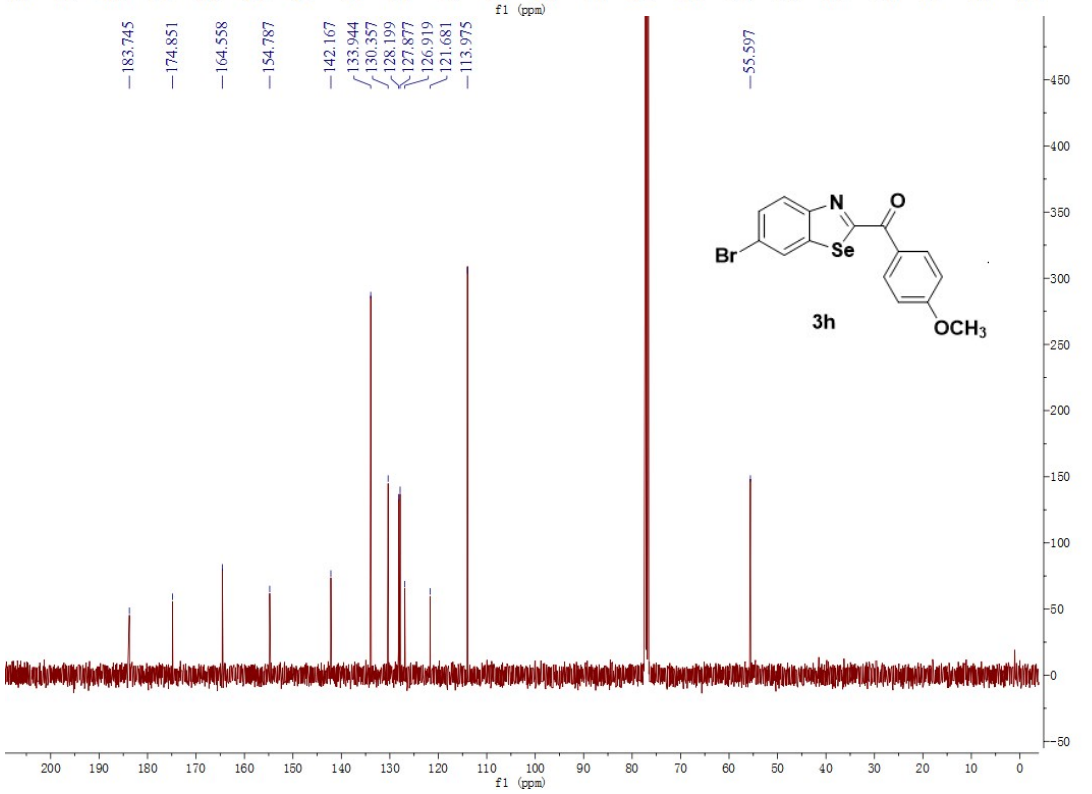
7.284
7.070
7.065
7.053
7.048
3.946
Br
N
Se
O
OCH3
3h
1.97
0.97
0.95
0.97
2.08
3.00
f1 (ppm)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130.357
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121.681
113.975
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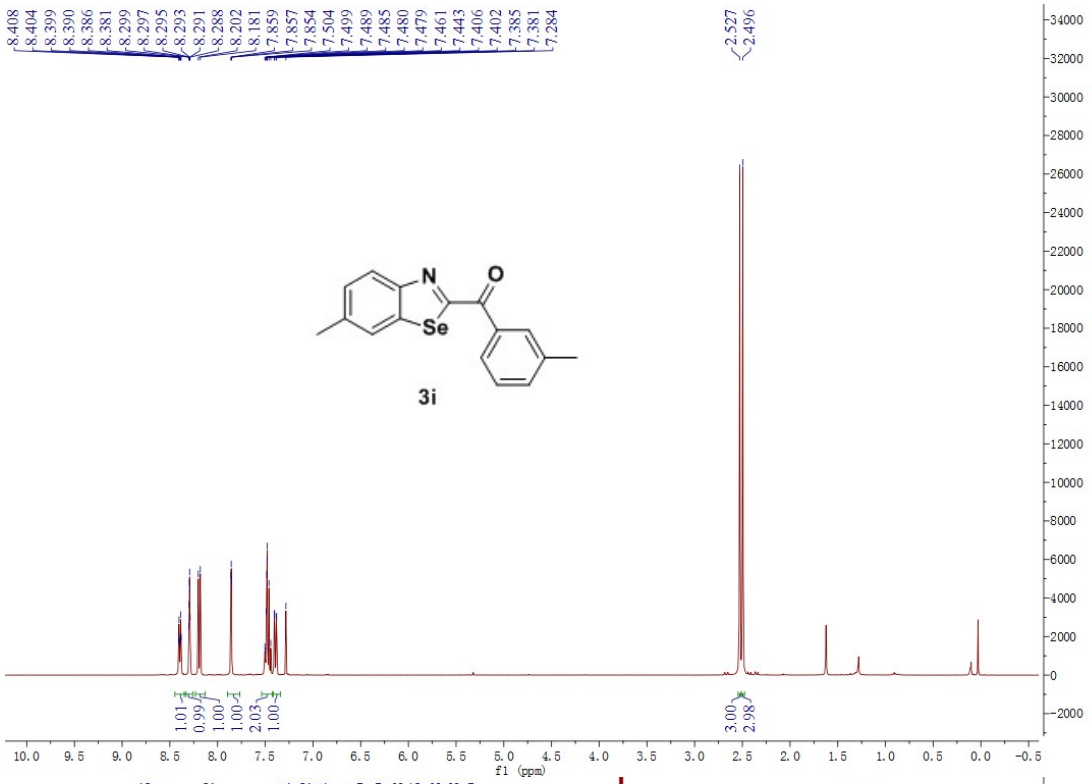
Se
O
OCH3
3h
f1 (ppm)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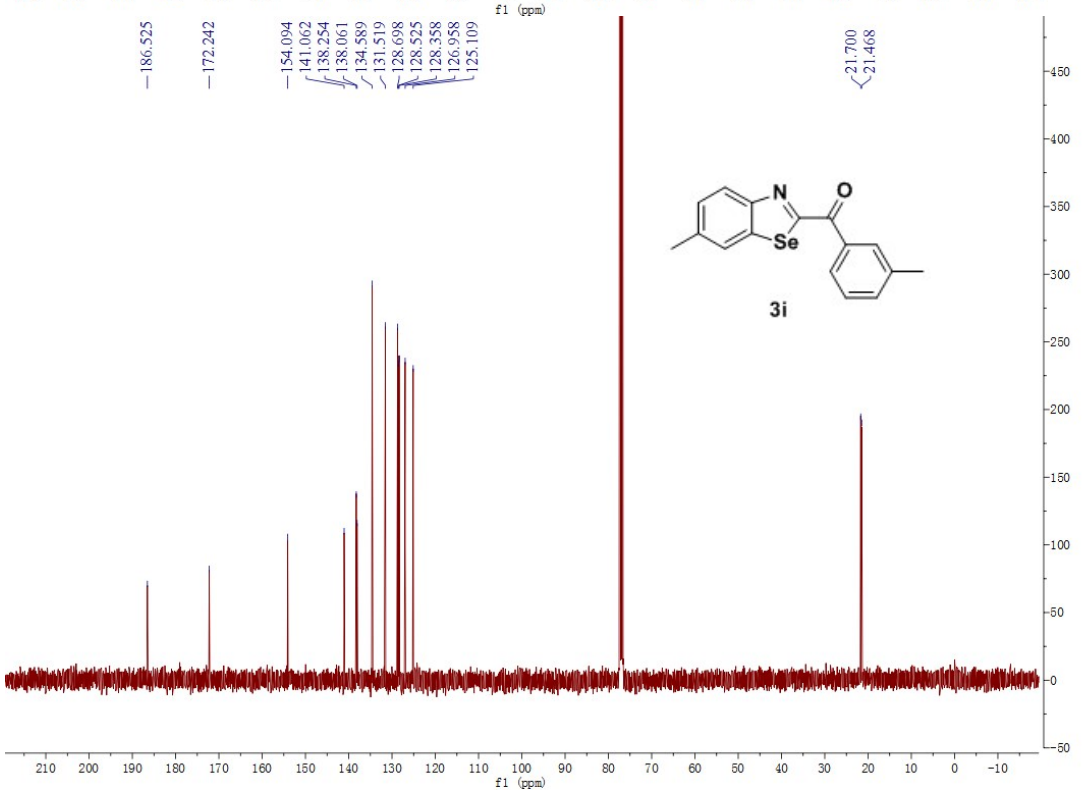
8.381
8.299
8.297
8.295
8.293
8.291
8.288
8.202
8.181
7.859
7.857
7.854
7.504
7.499
7.489
7.485
7.480
7.479
7.461
7.443
7.406
7.402
7.385
7.381
7.284
2.527
2.496
N
O
Se
3i
1.01
0.99
1.00
1.00
2.03
1.00
3.00
2.98
f1 (ppm)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154.094
141.062
138.254
138.061
134.589
131.519
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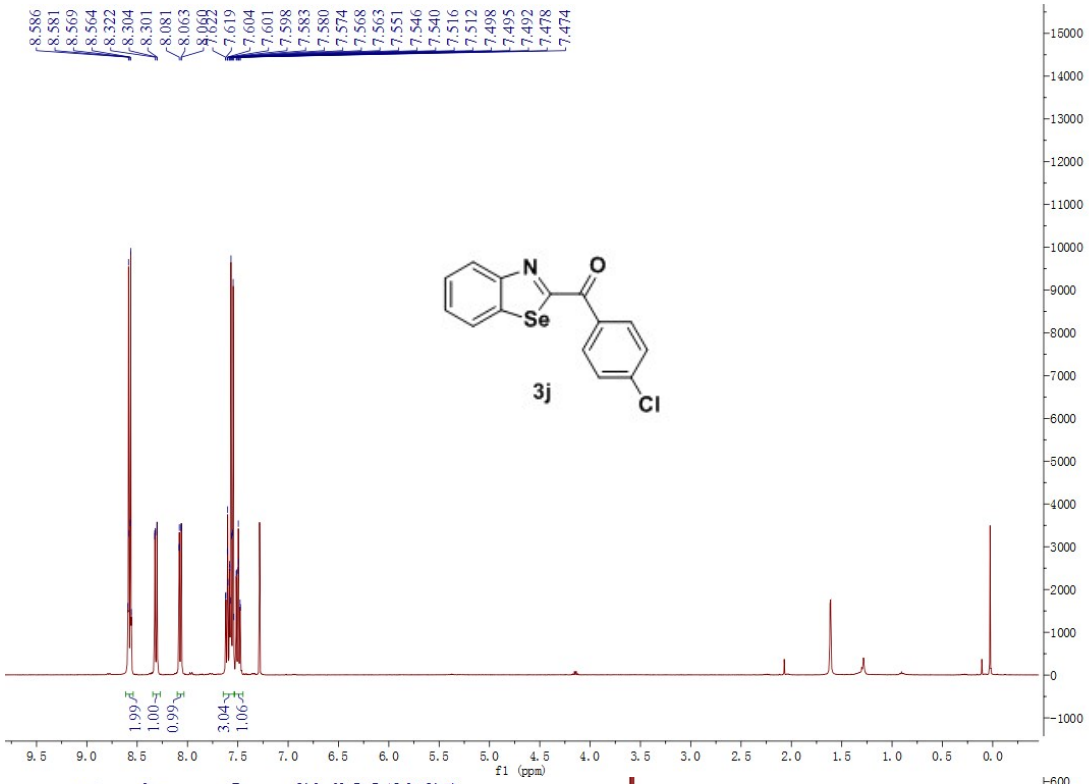
128.525
128.358
126.958
125.109
21.700
21.468
N
O
Se
3i
f1 (ppm)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8.060
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7.604
7.601
7.598
7.583
7.580
7.574
7.568
7.563
7.551
7.546
7.540
7.516
7.512
7.498
7.495
7.492
7.478
7.474
N
O
Se
Cl
3j
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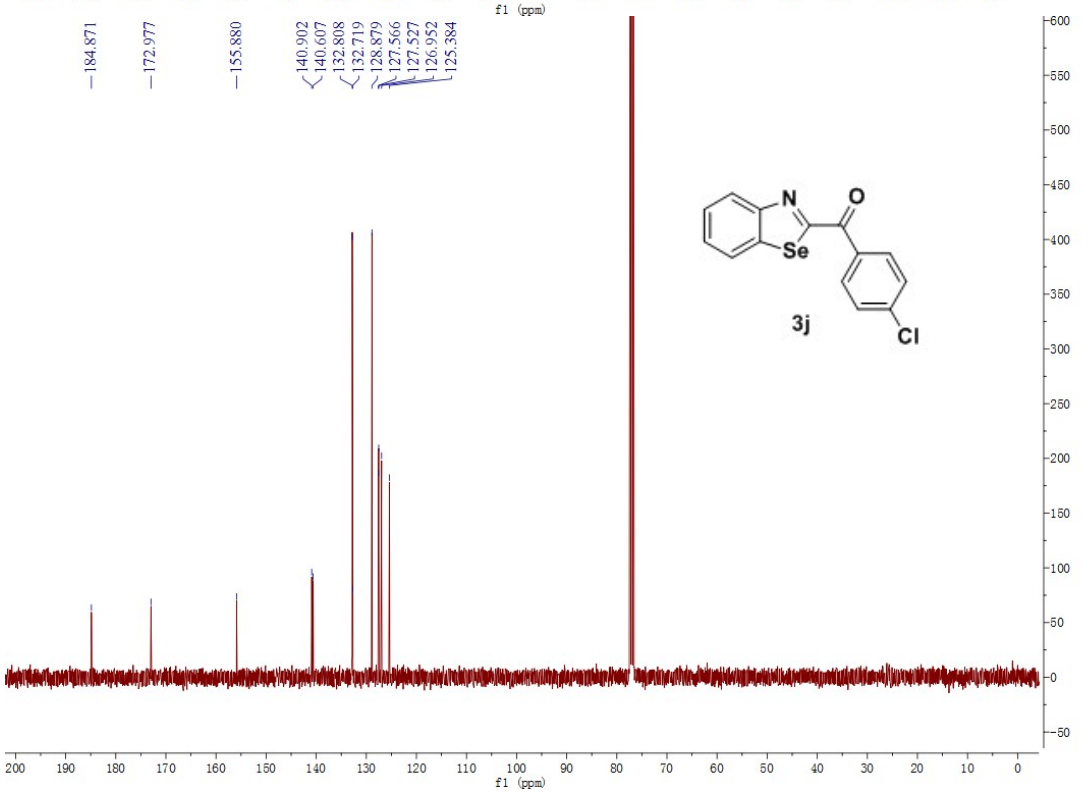
1.00
0.99
3.04
1.06
f1 (ppm)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128.879
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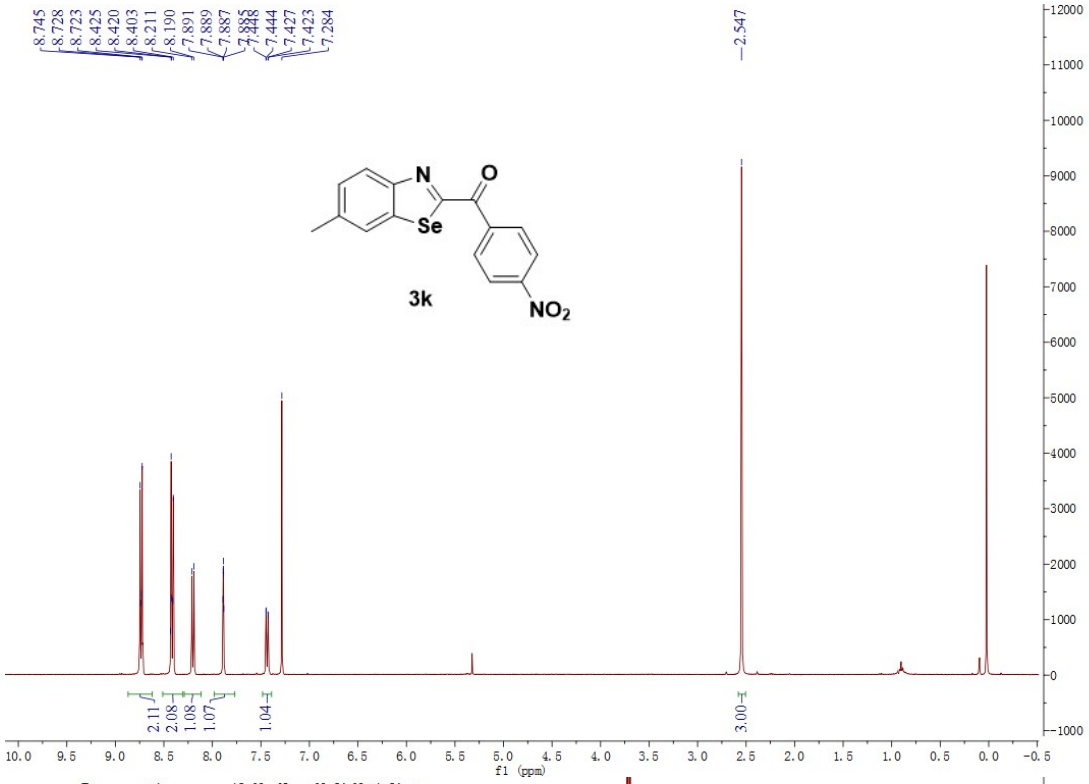
127.527
126.952
125.384
N
O
Se
Cl
3j
f1 (ppm)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8.190
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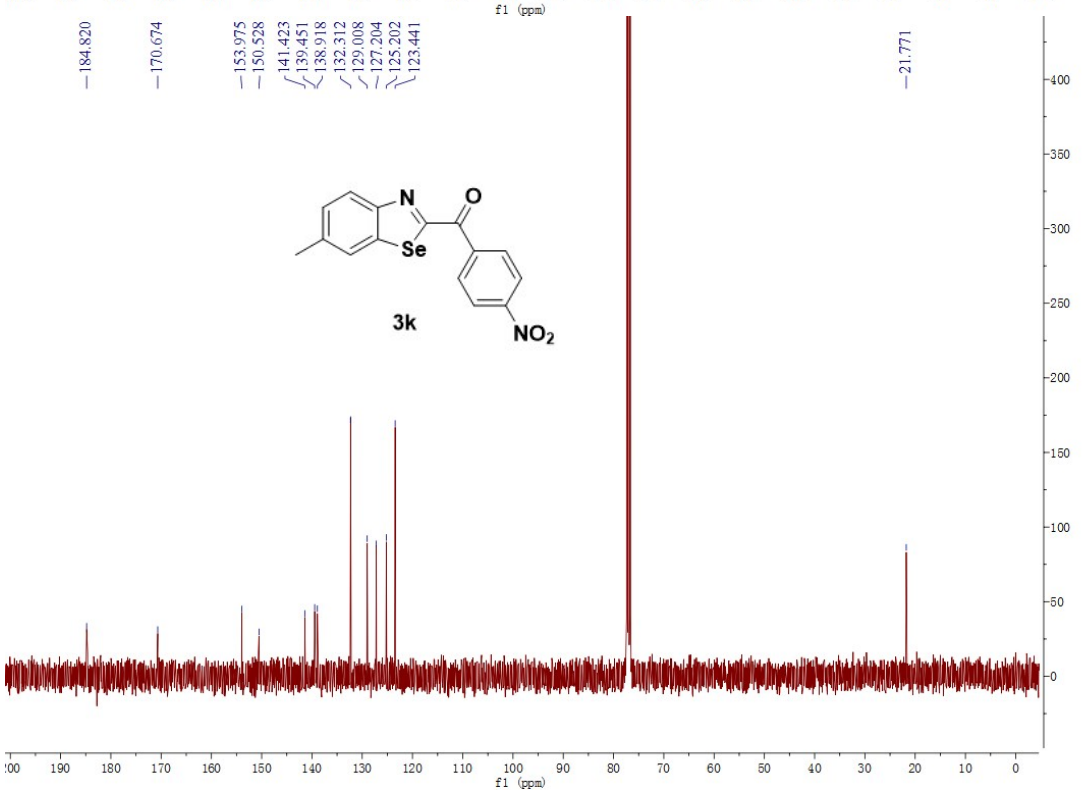
7.889
7.887
7.444
7.427
7.423
7.284
2.547
N
O
Se
3k
NO2
2.11
2.08
1.08
1.07
1.04
3.00
f1 (ppm)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123.441
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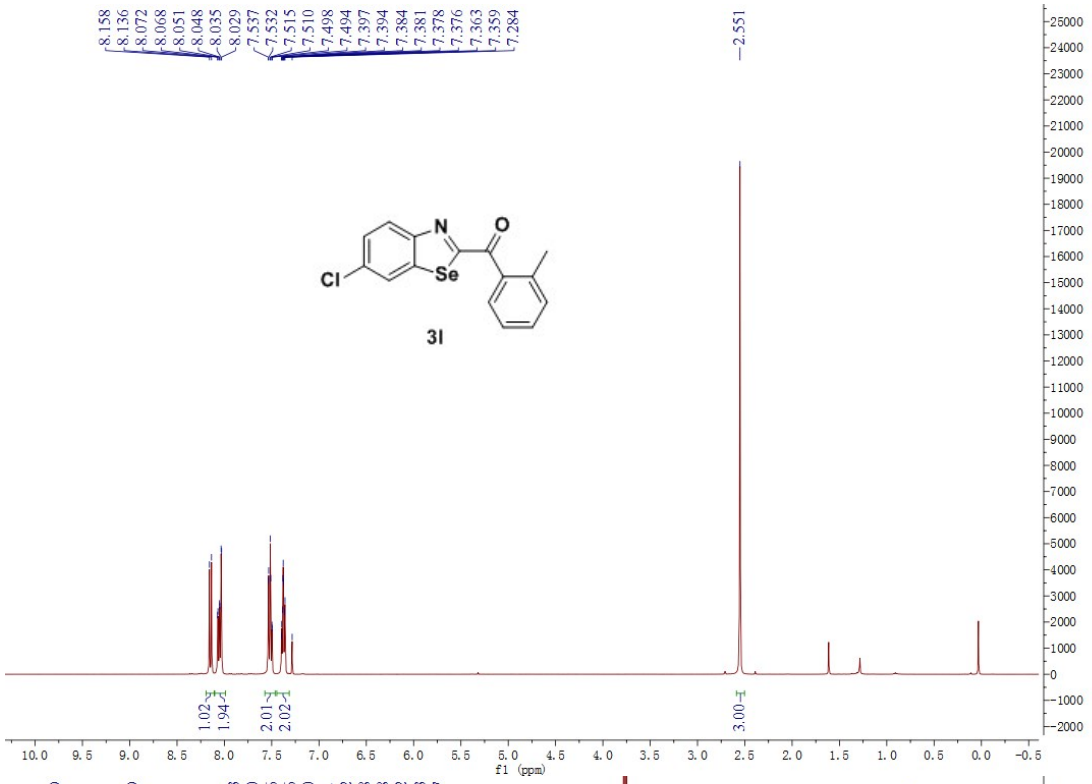
N
O
Se
3k
NO2
f1 (ppm)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8.048
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8.029
7.537
7.532
7.515
7.510
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7.494
7.397
7.394
7.384
7.381
7.378
7.376
7.363
7.359
7.284
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N
O
Cl
Se
3l
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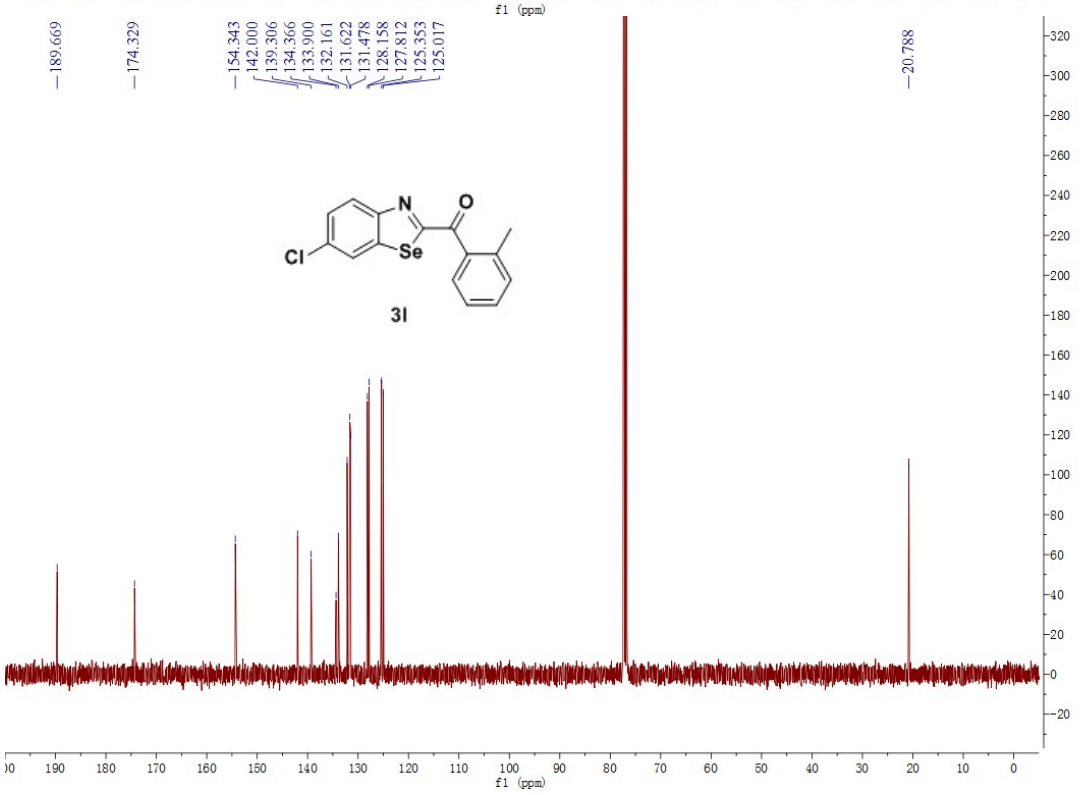
2.01
2.02
3.00
f1 (ppm)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134.366
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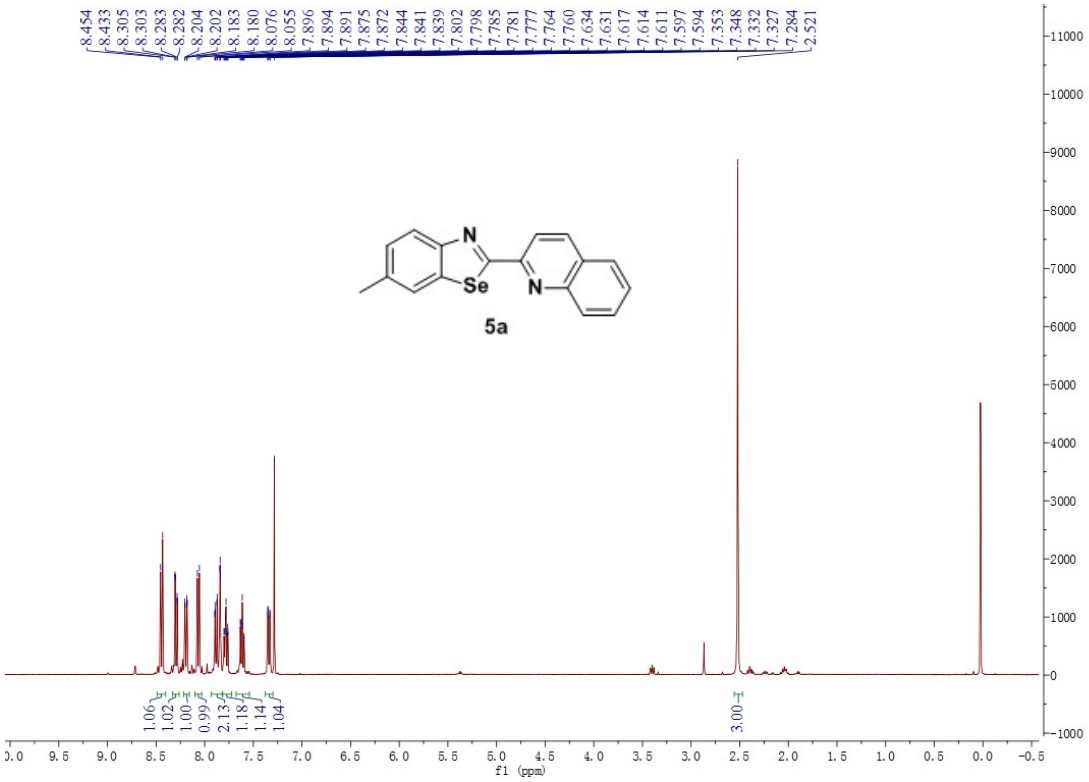
128.158
127.812
125.353
125.017
20.788
N
O
Cl
Se
3l
f1 (ppm)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8.180
8.076
8.055
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7.894
7.891
7.875
7.872
7.844
7.841
7.839
7.802
7.798
7.785
7.781
7.777
7.764
7.760
7.634
7.631
7.617
7.614
7.611
7.597
7.594
7.353
7.348
7.332
7.327
7.284
2.521
N
Se
N
5a
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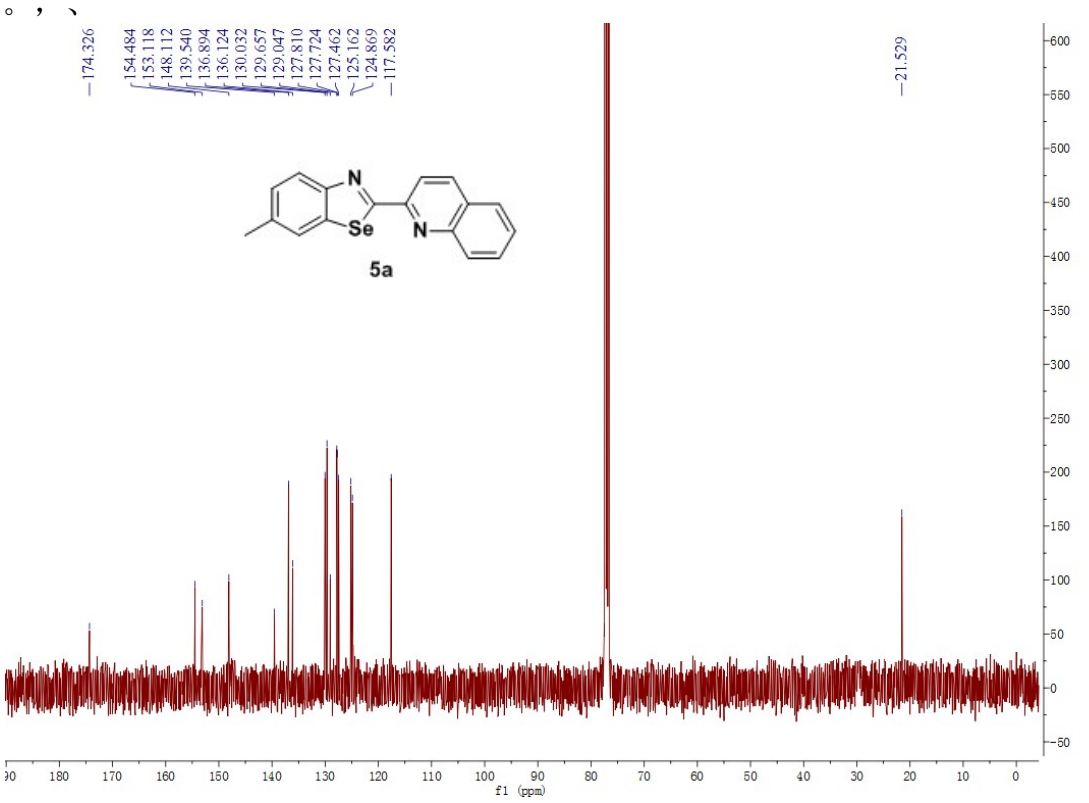
1.02
1.00
0.99
2.13
1.18
1.14
1.04
3.00
f1 (ppm)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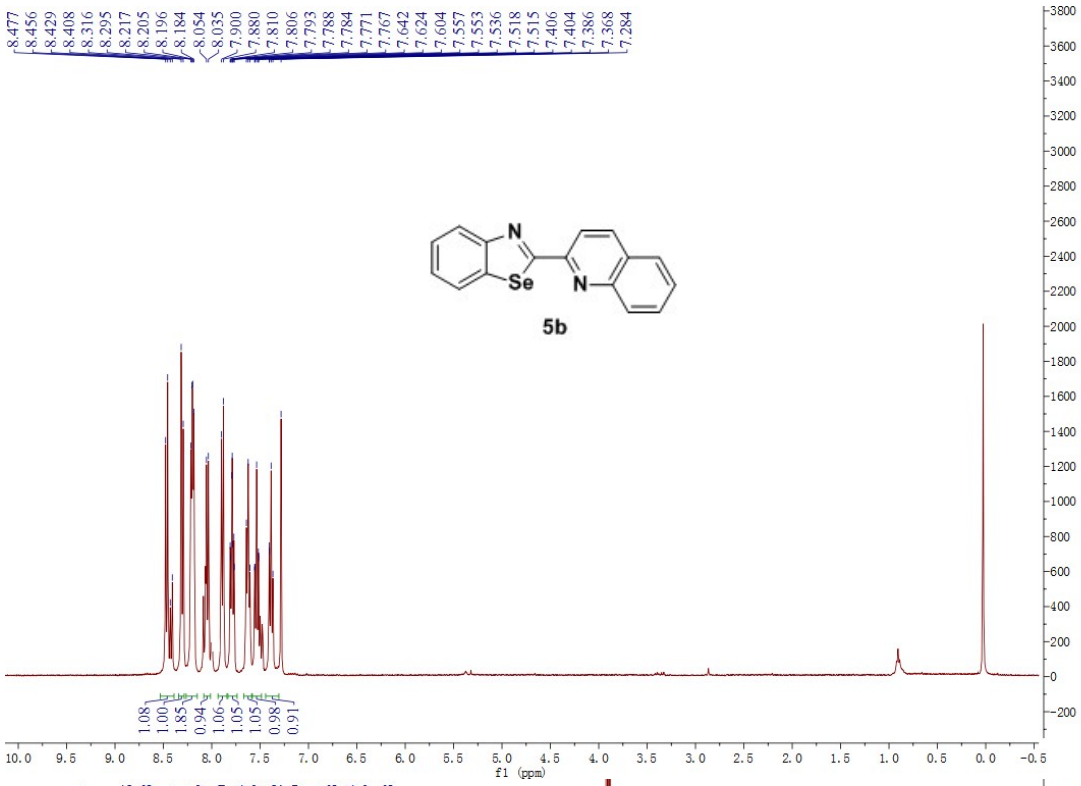
153.118
148.112
139.540
136.894
136.124
130.032
129.657
129.047
127.810
127.724
127.462
125.162
124.869
117.582
21.529
N
Se
N
5a
f1 (ppm)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8.456
8.429
8.408
8.316
8.295
8.217
8.205
8.196
8.184
8.054
8.035
7.900
7.880
7.810
7.806
7.793
7.788
7.784
7.771
7.767
7.642
7.624
7.604
7.557
7.553
7.536
7.518
7.515
7.406
7.404
7.386
7.368
7.284
N
Se
N
5b
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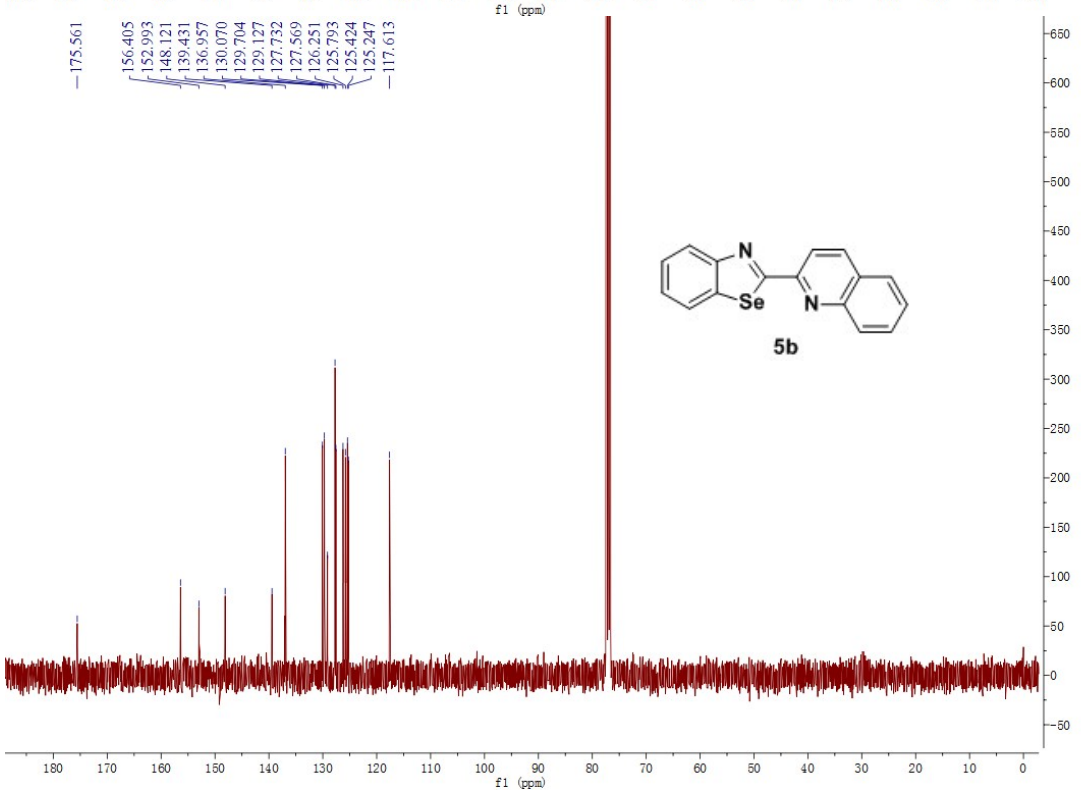
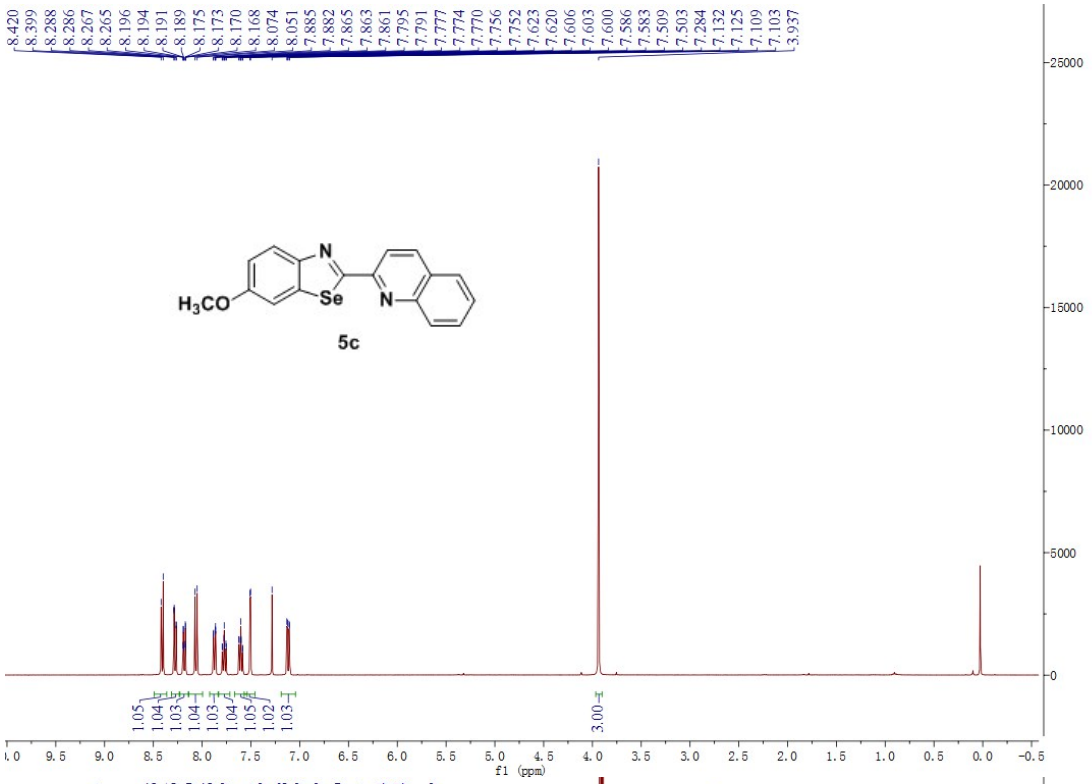
1.00
1.85
0.94
1.06
1.05
1.05
0.98
0.91
f1 (ppm)


175.561
156.405
152.993
148.121
139.431
136.957
130.070
129.704
129.127
127.732
127.569
126.251
125.793
125.424
125.247
117.613
N
Se
N
5b
f1 (ppm)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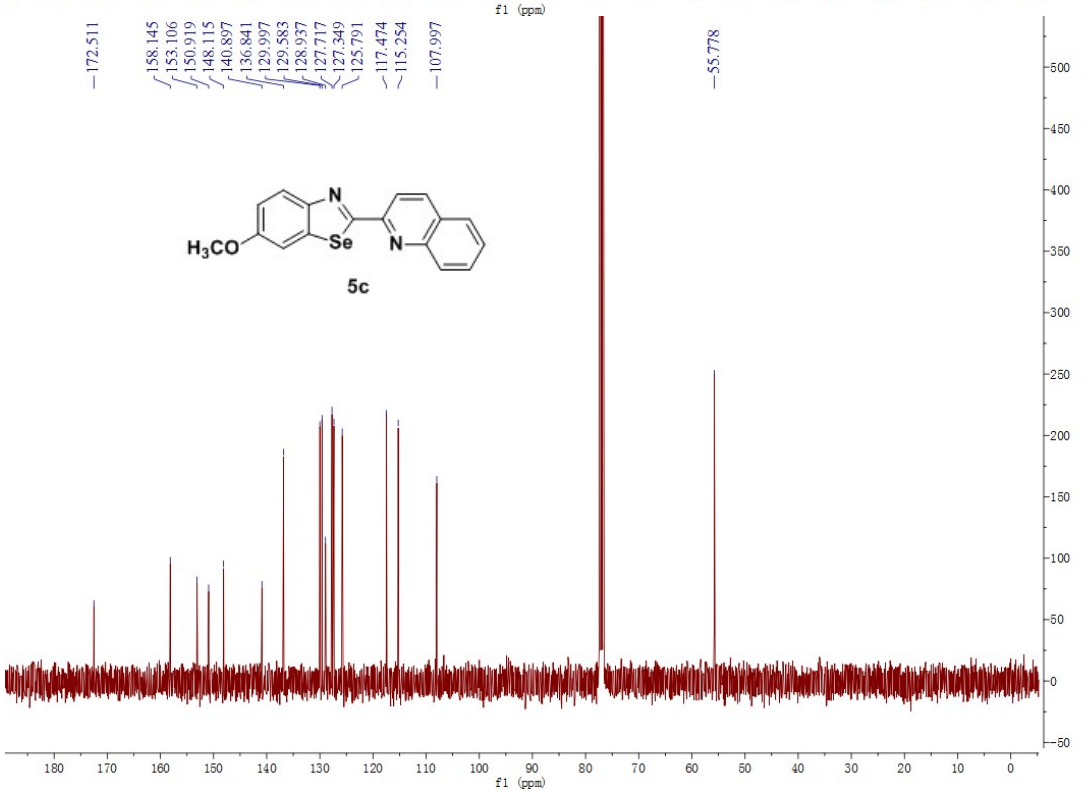
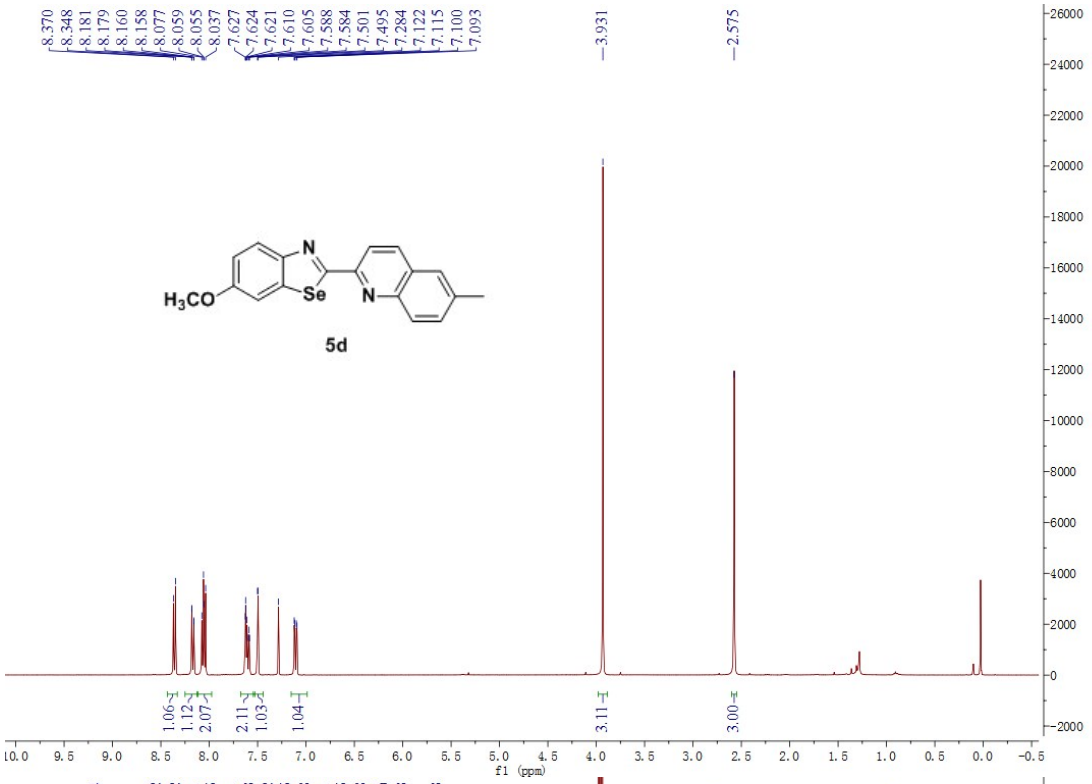
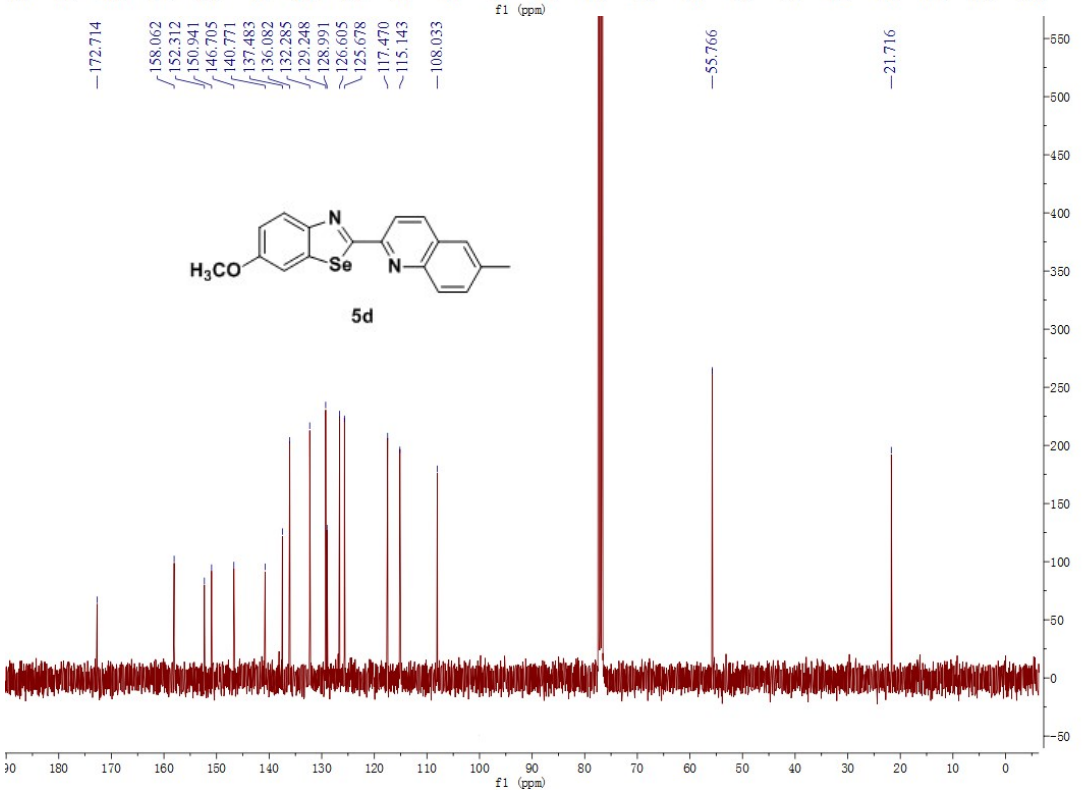
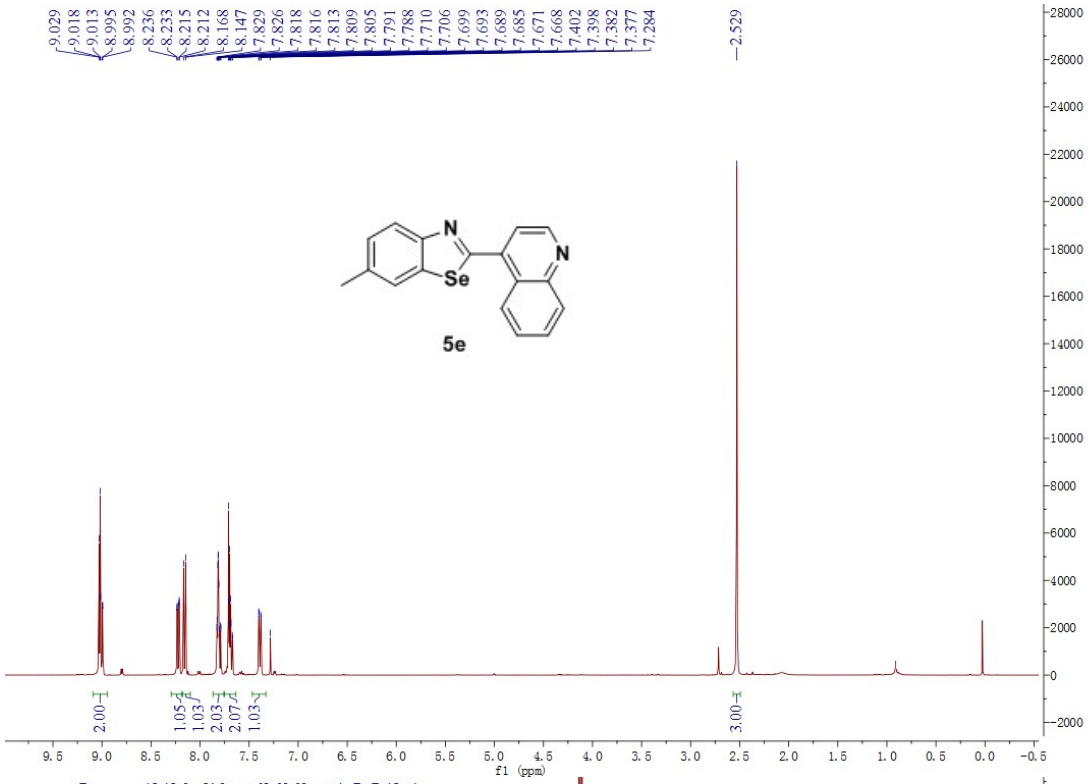
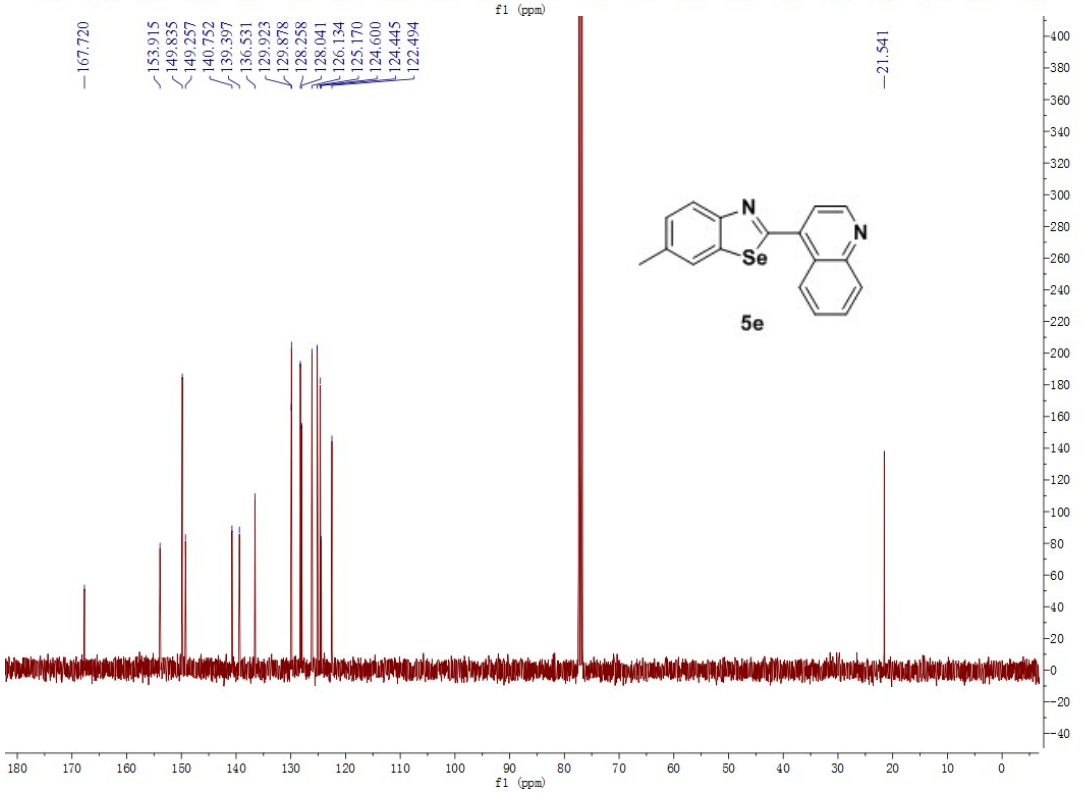
8.399
8.288
8.286
8.267
8.265
8.196
8.194
8.191
8.189
8.175
8.173
8.170
8.168
8.074
8.051
7.885
7.882
7.865
7.863
7.861
7.795
7.791
7.777
7.774
7.770
7.756
7.752
7.623
7.620
7.606
7.603
7.600
7.586
7.583
7.509
7.503
7.284
7.132
7.125
7.109
7.103
3.937
N
Se
N
H3CO
5c
1.05
1.04
1.03
1.04
1.03
1.04
1.05
1.02
1.03
3.00
f1 (ppm)

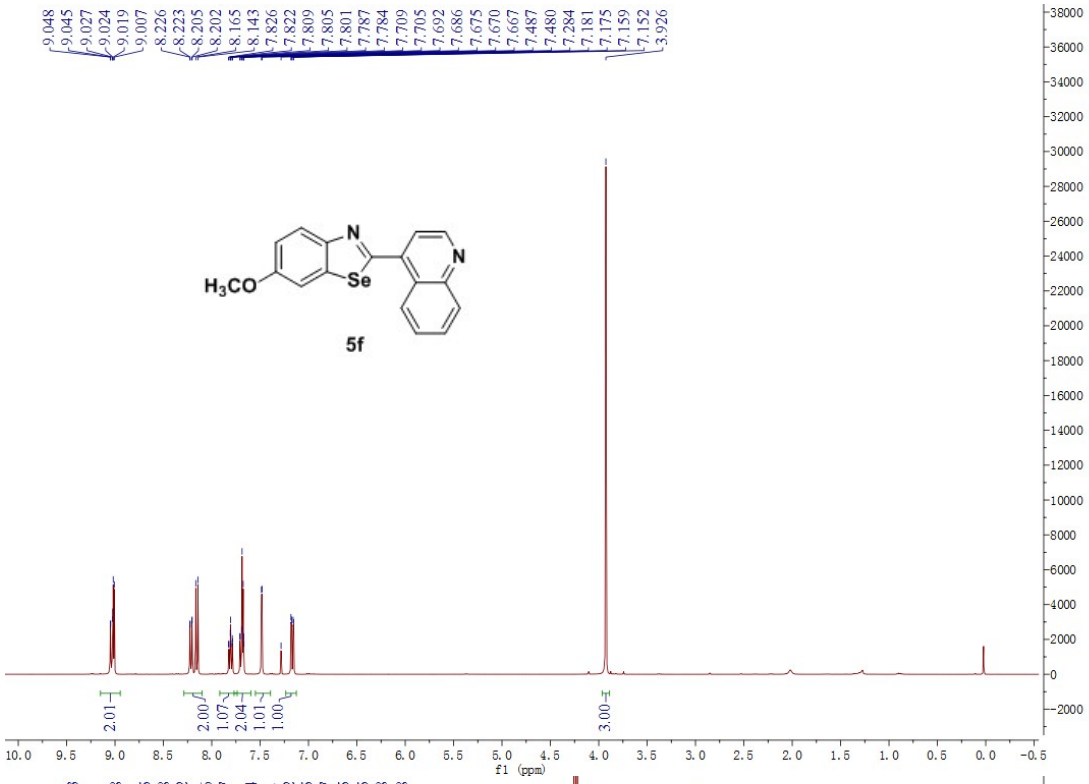

172.511
158.145
153.106
150.919
148.115
140.897
136.841
129.997
129.583
128.937
127.717
127.349
125.791
117.474
115.254
107.997
55.778
N
Se
N
H3CO
5c
f1 (ppm)

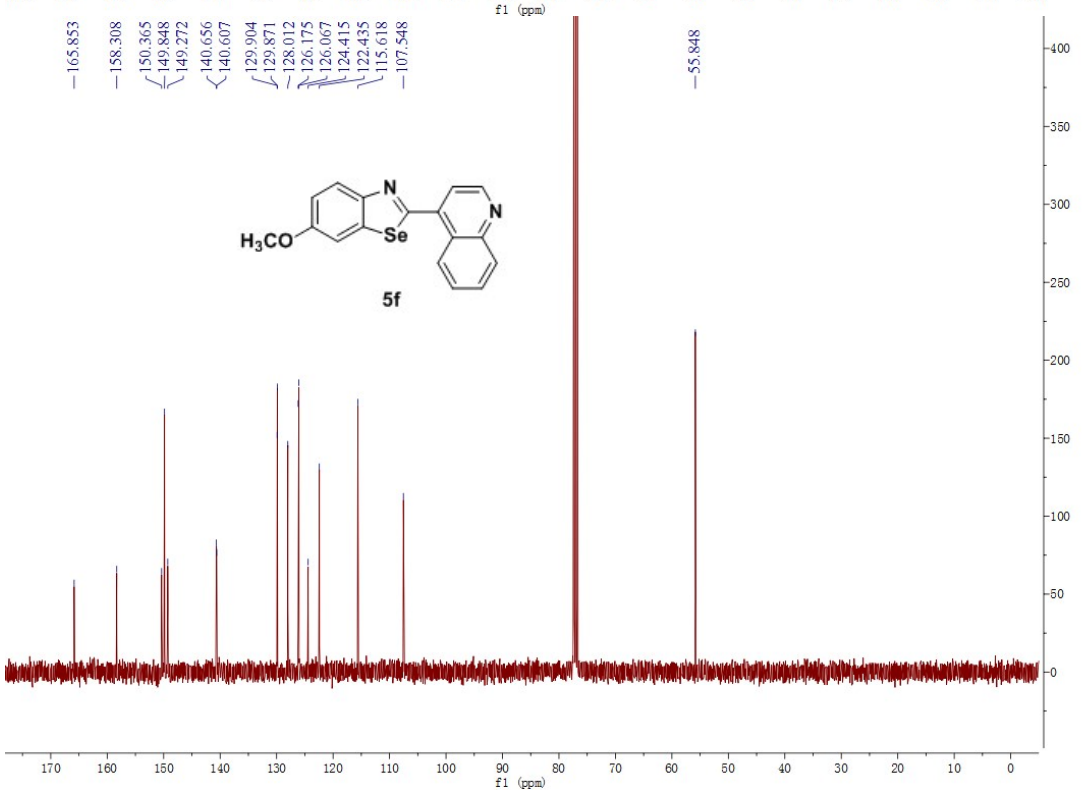

8.370
8.348
8.181
8.179
8.160
8.158
8.077
8.059
8.055
8.037
7.627
7.624
7.621
7.610
7.605
7.588
7.584
7.501
7.495
7.284
7.122
7.115
7.100
7.093
3.931
2.575
H3CO
N
Se
N
5d
1.06
1.12
2.07
2.11
1.03
1.04
3.11
3.00
f1 (ppm)


172.714
158.062
152.312
150.941
146.705
140.771
137.483
136.082
132.285
129.248
128.991
126.605
125.678
117.470
115.143
108.033
55.766
21.716
H3CO
N
Se
N
5d
f1 (ppm)


9.029
9.018
9.013
8.995
8.992
8.236
8.233
8.215
8.212
8.168
8.147
7.829
7.826
7.818
7.816
7.813
7.809
7.805
7.791
7.788
7.710
7.706
7.699
7.693
7.689
7.685
7.671
7.668
7.402
7.398
7.382
7.377
7.284
2.529
N
Se
N
5e
2.00
1.05
1.03
2.03
2.07
1.03
3.00
f1 (ppm)


167.720
153.915
149.835
149.257
140.752
139.397
136.531
129.923
129.878
128.258
128.041
126.134
125.170
124.600
124.445
122.494
21.541
N
Se
N
5e
f1 (ppm)


9.048
9.045
9.027
9.024
9.019
9.007
8.226
8.223
8.205
8.202
8.165
8.143
7.826
7.822
7.809
7.805
7.801
7.787
7.784
7.709
7.705
7.692
7.686
7.675
7.670
7.667
7.487
7.480
7.284
7.181
7.175
7.159
7.152
3.926
N
Se
H3CO
N
5f
2.01
2.00
1.07
2.04
1.01
1.00
3.00
f1 (ppm)


165.853
158.308
150.365
149.848
149.272
140.656
140.607
129.904
129.871
128.012
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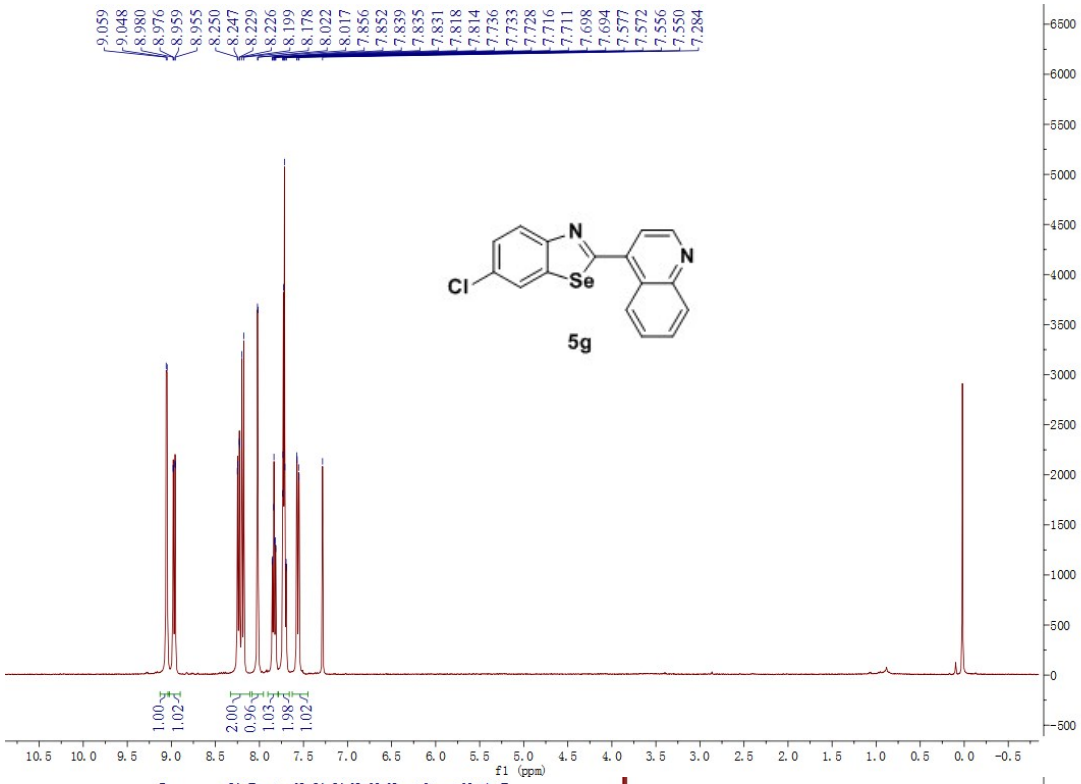
126.067
124.415
122.435
115.618
107.548
55.848
N
Se
H3CO
N
5f
f1 (ppm)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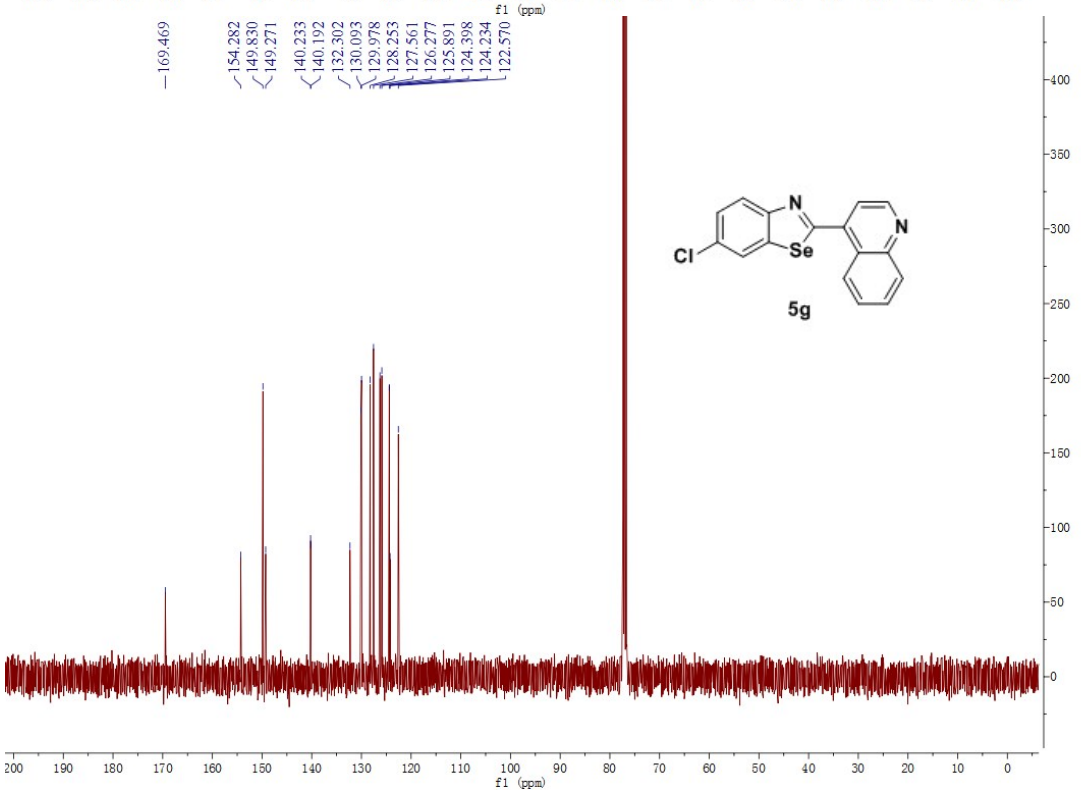
9.048
8.980
8.976
8.959
8.955
8.250
8.247
8.229
8.226
8.199
8.178
8.022
8.017
7.856
7.852
7.839
7.835
7.831
7.818
7.814
7.736
7.733
7.728
7.716
7.711
7.698
7.694
7.577
7.572
7.556
7.550
7.284
N
Se
Cl
N
5g
1.00
1.02
2.00
0.96
1.03
1.98
1.02
f1 (ppm)


169.469
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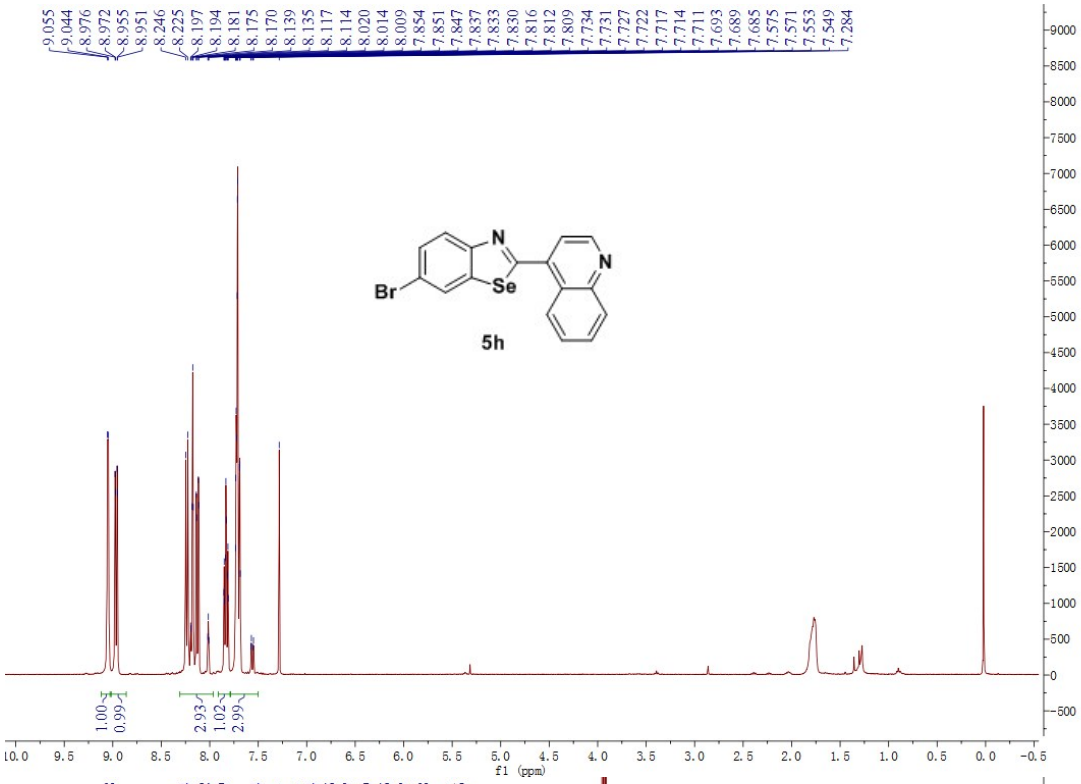
149.830
149.271
140.233
140.192
132.302
130.093
129.978
128.253
127.561
126.277
125.891
124.398
124.234
122.570
N
Se
Cl
N
5g
f1 (ppm)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9.044
8.976
8.972
8.955
8.951
8.246
8.225
8.197
8.194
8.181
8.175
8.170
8.139
8.135
8.117
8.114
8.020
8.014
8.009
7.854
7.851
7.847
7.837
7.833
7.830
7.816
7.812
7.809
7.734
7.731
7.727
7.722
7.717
7.714
7.711
7.693
7.689
7.685
7.575
7.571
7.553
7.549
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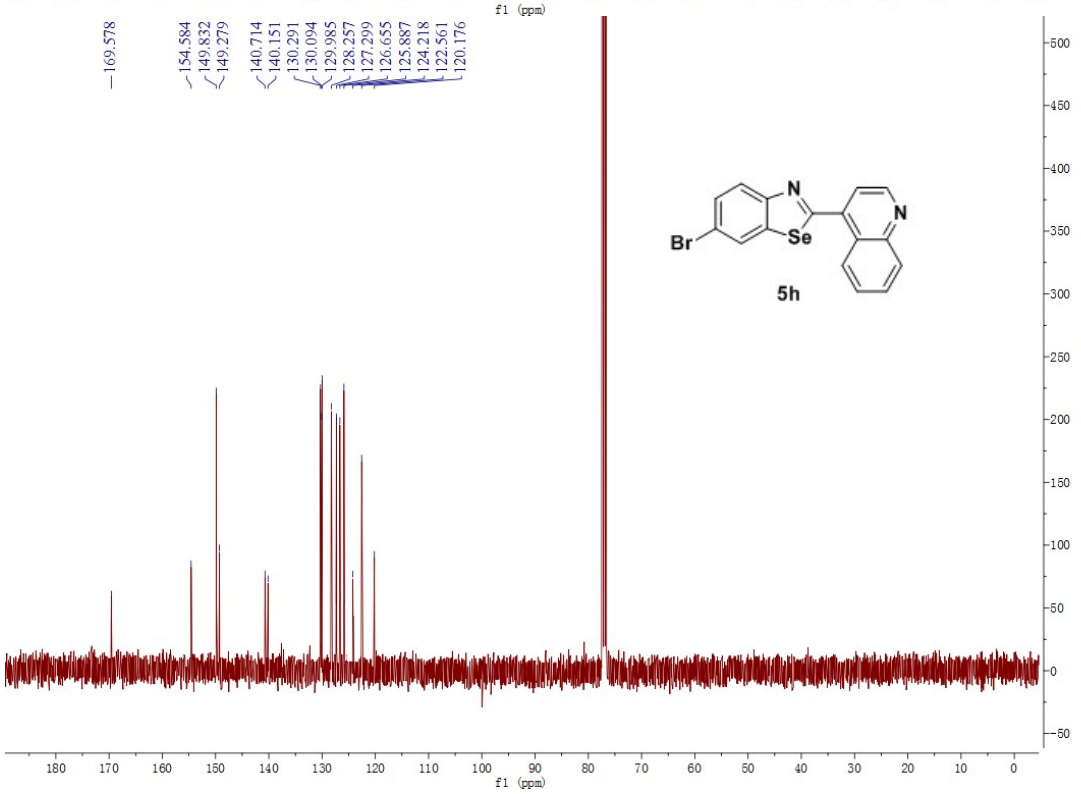
N
Se
Br
N
5h
1.00
0.99
2.93
1.02
2.99
f1 (ppm)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149.279
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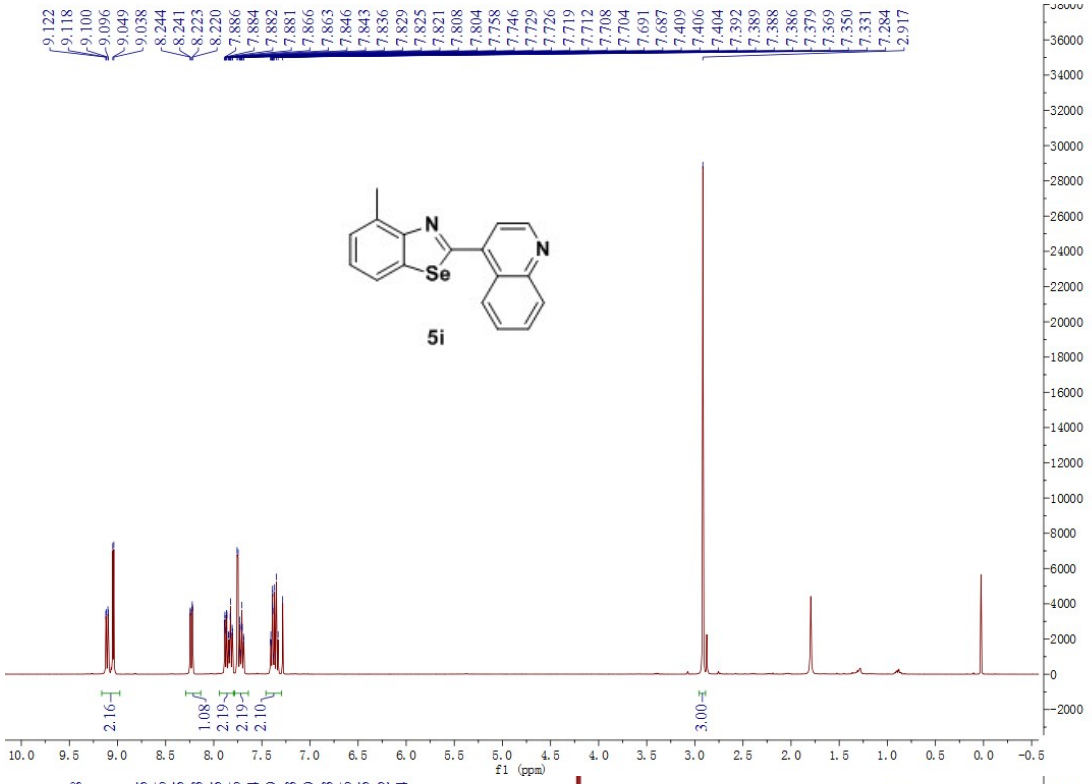
140.151
130.291
130.094
129.985
128.257
127.299
126.655
125.887
124.218
122.561
120.176
N
Se
Br
N
5h
f1 (ppm)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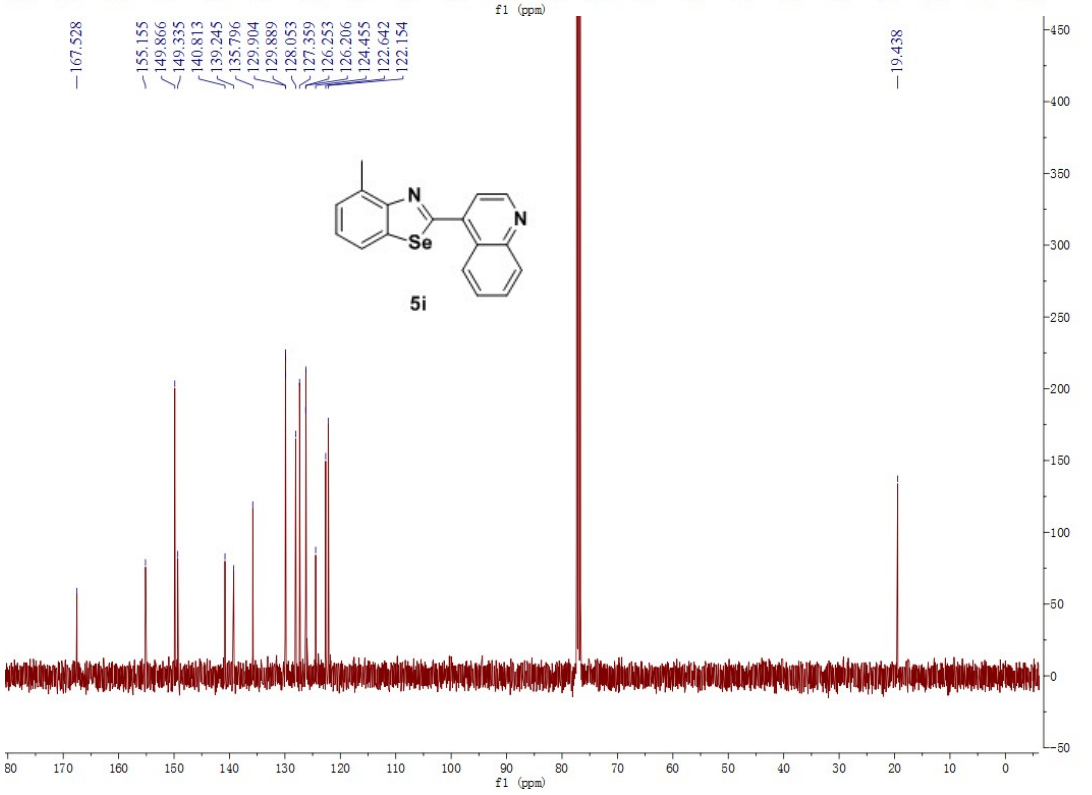
9.096
9.049
9.038
8.244
8.241
8.223
8.220
7.886
7.884
7.882
7.881
7.866
7.863
7.846
7.843
7.836
7.829
7.825
7.821
7.808
7.804
7.758
7.746
7.729
7.726
7.719
7.712
7.708
7.704
7.691
7.687
7.409
7.406
7.404
7.392
7.389
7.388
7.386
7.379
7.369
7.350
7.331
7.284
2.917
N
Se
N
5i
2.16
1.08
2.19
2.19
2.10
3.00
f1 (ppm)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155.155
149.866
149.335
140.813
139.245
135.796
129.904
129.889
128.053
127.359
126.253
126.206
124.455
122.642
122.154
19.438
N
Se
N
5i
f1 (ppm)