Supporting information for

A Multicomponent Reaction of Isocyanides, Selenium Powder and 3-Aminooxetanes In Pure Water: Green and Efficient Synthesis of 1, 3-Selenazolines

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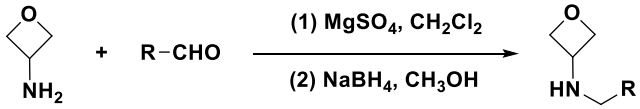
1. General Information

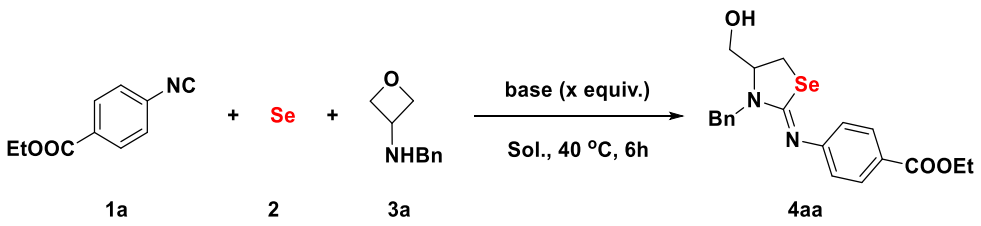
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were analytical grade and used without further purification. Tetrahydrofuran was purchased from Shanghai Lingfeng Chemical Reagent Co., Ltd. Analytical thin-layer chromatography (TLC) was performed on silica gel, visualized by irradiation with UV light. For column chromatography, 200-300 mesh silica gel was used. ^{1}H-NMR, ^{13}C-NMR, ^{77}Se-NMR and ^{19}F-NMR were recorded on a BRUKER 400 MHz or 600 MHz spectrometer in $CDCl_3$ or DMSO-d_6. Chemical shifts (δ) were reported referenced to an internal tetramethylsilane standard or the $CDCl_3$ residual peak (δ 7.26) or DMSO-d_6 residual peak (δ 2.50) for ^{1}H NMR. Chemical shifts of ^{13}C NMR are reported relative to $CDCl_3$ (δ 77.16) or DMSO-d_6 (δ 39.52). Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quarter), p (pentet), 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 ALPHA spectrophotometer and are reported in terms of frequency of absorption (cm^{-1}). HRMS spectra were obtained by using BRUKER MICROTOF-Q III instrument with ESI source.

2. Synthesis of the Starting Materials



Oxetane-3-amine (1.05 mL, 15 mmol), aryl or alkyl aldehydes (5.0 mmol), anhydrous $MgSO_4$ and dichloromethane (15 mL) was added to a 50 mL flask under argon atmosphere and allowed to react at room temperature (25 °C) for 12 h. Filtration and removal of the solvent by a rotary evaporator under reduced pressure afforded the imine intermediate. The imine intermediate was dissolved in methanol (10 mL), $NaBH_4$ (0.19 g, 5.0 mmol) was slowly added to the reaction system, and the reaction was carried out at room temperature (25 °C) for 5 h. Spin dry and purified by silica gel column chromatography (Petroleum ether/EtOAc, 5:1-2:1) to afford the desired products.

3. Optimization of the Reaction Conditions[a]

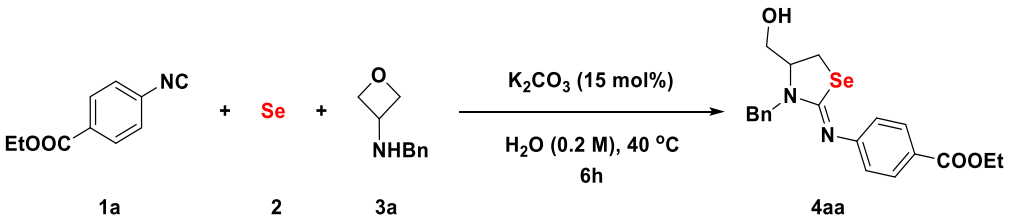


Entry	Solvent	Base (x equiv.)	T (°C)	Yield (%)[b]
1	CH_3CN	Cs_2CO_3 (1.5)	40	35
2	DMF	Cs_2CO_3 (1.5)	40	27

3	DMA	Cs_2CO_3 (1.5)	40	60
4	DMSO	Cs_2CO_3 (1.5)	40	36
5	THF	Cs_2CO_3 (1.5)	40	81
6	NMP	Cs_2CO_3 (1.5)	40	47
7	1,4-dioxane	Cs_2CO_3 (1.5)	40	85
8	CH_2Cl_2	Cs_2CO_3 (1.5)	40	72
9	DCE	Cs_2CO_3 (1.5)	40	76
10	CH_3OH	Cs_2CO_3 (1.5)	40	23
11	H_2O	Cs_2CO_3 (1.5)	40	90
12	H_2O	K_2CO_3 (1.5)	40	92
13	H_2O	Na_2CO_3 (1.5)	40	90
14	H_2O	K_3PO_4 (1.5)	40	84
15	H_2O	K_2HPO_4 (1.5)	40	91
16	H_2O	NaOH (1.5)	40	69
17	H_2O	KOH (1.5)	40	73
18	H_2O	*t*-BuONa (1.5)	40	70
19	H_2O	*t*-BuOK (1.5)	40	43
20	H_2O	*t*-BuOLi (1.5)	40	70
21	H_2O	Et_3N (1.5)	40	87
22	H_2O	DBU (1.5)	40	39
23	H_2O	--	40	67
24	H_2O	K_2CO_3 (0.2)	40	90
25	**H_2O**	**K_2CO_3 (0.15)**	**40**	**91 (84)**[c]
26	H_2O	K_2CO_3 (0.1)	40	90
27	H_2O	Na_2CO_3 (0.15)	40	80
28	H_2O	$KHCO_3$ (0.15)	40	90

[a]All reactions were performed with **1a** (0.2 mmol), **2** (0.24 mmol), **3a** (0.24 mmol) and base (0.3 mmol) in solvent (1.0 mL) at 40 °C for 6 h under air unless otherwise noted. [b]Yields were determined by LC-MS with biphenyl as the internal standard. [c]Isolated yield.

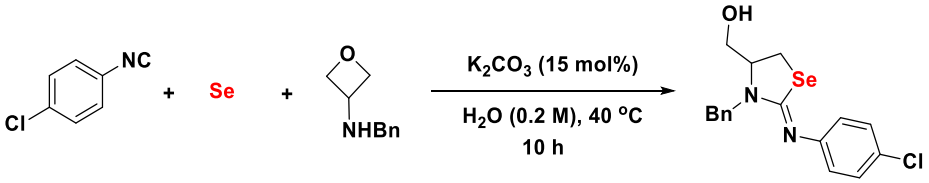
4. Typical Procedure for the Synthesis of 4aa



1a 2 3a 4aa

To a 8.0 mL scintillation vial equipped with a magnetic stirrer, isocyanide **1a** (0.20 mmol, 1.0 equiv.), selenium powder **2** (0.24 mmol, 1.2 equiv.), potassium carbonate aqueous solution (1.0 mL, 0.03 M) and N-benzyloxetan-3-amine **3a** (0.24 mmol, 1.2 equiv.) sequentially added at room temperature. The vial was sealed with a screw-top septum cap and placed in a heating block that was preheated to 40 °C for 6h. After the indicated reaction time, an aqueous saturated NH_4Cl solution and EtOAc were added and the layers were separated. The aqueous phase was extracted with EtOAc (x 3) and the combined organic layers were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (eluent: Petroleum ether/EtOAc) to give the desired product **4aa** in 84% isolated yield as a Colorless oil.

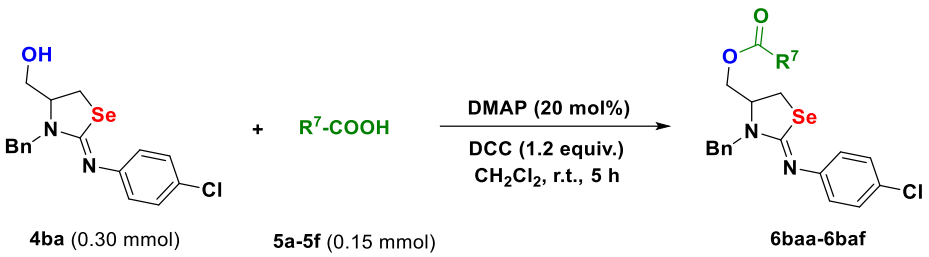
5. Typical Procedure for the Scale-up Synthesis of 4ba



1b 2 3a **4ba**, 72% (0.8259g)

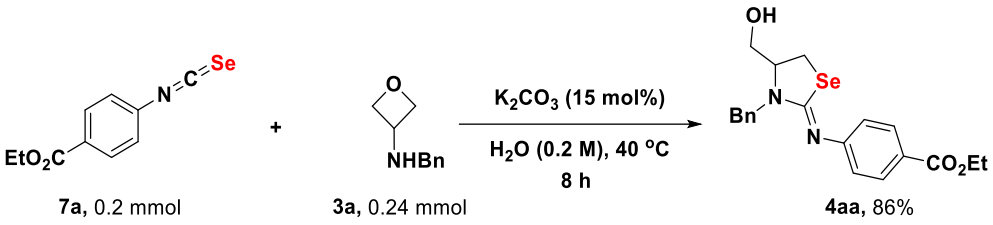
To a 50-mL round-bottomed flask equipped with a magnetic stirrer, isocyanide **1b** (3.0 mmol, 1.0 equiv.), selenium powder **2** (3.6 mmol, 1.2 equiv.), K_2CO_3 (0.45 mmol, 0.0622g), solvent H_2O (15 mL) and N-benzyloxetan-3-amine **3a** (3.6 mmol, 1.2 equiv.) sequentially added at room temperature. The flask was sealed with a rubber stopper and placed in an oil bath that was preheated to 40 °C for 10 h. After the indicated reaction time, an aqueous saturated NH_4Cl solution and EtOAc were added and the layers were separated. The aqueous phase was extracted with EtOAc (x 3) and the combined organic layers were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (eluent: Petroleum ether/EtOAc) to give the target product **4ba** as a Colorless oil in 72% isolated yield (0.83 g).

6. Typical Procedure for the synthesis of 6baa-6baf



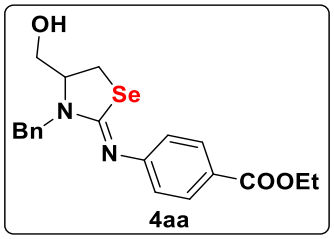
To a 8.0 mL scintillation vial equipped with a magnetic stirrer, 1, 3-selenazoline derivative **4ba** (0.30 mmol, 2.0 equiv.), bioactive acids **5a-5f** (0.15 mmol, 1.0 equiv.), 4-dimethylaminopyridine (DMAP, 0.03 mmol, 0.2 equiv.), CH_2Cl_2 (1.0 mL) and dicyclohexylcarbodiimide (DCC, 0.18 mmol, 1.2 equiv.) sequentially added at room temperature. The vial was sealed with a screw-top septum cap and the system was stirred at room temperature for 5 h. After the indicated reaction time, the reaction mixture was charged with silica gel and concentrated. The residue was purified by flash column chromatography on silica gel (eluent: Petroleum ether/EtOAc) to give the desired product **6baa-6baf** in 84%-96% isolated yield.

7. Control Experiments for Scheme 4



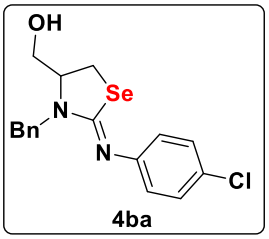
To a 8.0 mL scintillation vial equipped with a magnetic stirrer, isoselenocyanate **7a** (0.20 mmol, 1.0 equiv.), potassium carbonate aqueous solution (1.0 mL, 0.03 M) and N-benzyloxetan-3-amine **3a** (0.24 mmol, 1.2 equiv.) sequentially added at room temperature. The vial was sealed with a screw-top septum cap and placed in a heating block that was preheated to 40 °C for 8 h. After the indicated reaction time, an aqueous saturated NH_4Cl solution and EtOAc were added and the layers were separated. The aqueous phase was extracted with EtOAc (x 3) and the combined organic layers were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (eluent: Petroleum ether/EtOAc) to give the desired product **4aa** in 86% isolated yield as a Colorless oil.

8. Spectroscopic Data of Compounds



ethyl (Z)-4-((3-benzyl-4-(hydroxymethyl)-1,3-selenazolidin-2-ylidene)amino)benzoate (4aa)

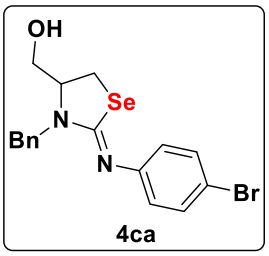
Yield = 84% (70.2 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01 – 7.93 (m, 2H), 7.38 – 7.26 (m, 5H), 7.02 – 6.94 (m, 2H), 5.19 (d, *J* = 15.4 Hz, 1H), 4.42 (d, *J* = 15.4 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.75-3.83 (m, 2H), 3.71 – 3.62 (m, 1H), 3.21-3.16 (m, 2H), 2.26 (s, 1H), 1.38 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.0, 157.4, 157.1, 137.5, 130.9, 128.9, 127.7, 127.7, 125.2, 121.6, 63.0, 61.2, 60.8, 49.7, 23.5, 14.5. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 269.0. **IR (ATR)**: ν = 3423, 2925, 1705, 1619, 1572, 1268, 1163, 1015 cm^{-1}; **HRMS** (ESI): calcd. for $C_{20}H_{22}N_2O_3Se$ $[M+H]^+$: 419.0874, found: 419.0878.



4ba

(Z)-(3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4ba)

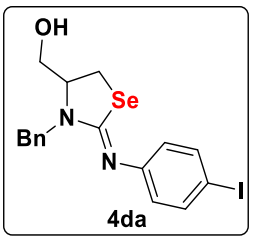
Yield = 87% (66.0 mg). White solid. **Mp**: 113.8-114.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 – 7.25 (m, 5H), 7.25 – 7.20 (m, 2H), 6.91 – 6.81 (m, 2H), 5.14 (d, *J* = 15.5 Hz, 1H), 4.38 (d, *J* = 15.5 Hz, 1H), 3.78 – 3.69 (m, 2H), 3.65 – 3.57 (m, 1H), 3.21 – 3.12 (m, 2H), 2.26 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.6, 151.7, 137.5, 129.1, 128.8, 128.7, 127.6, 123.1, 63.0, 61.3, 49.7, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.5. **IR (ATR)**: ν = 3172, 2919, 1601, 1486, 1213, 1059, 1049，837 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{17}ClN_2OSe$ $[M+H]^+$: 381.0273, found: 381.0275.



4ca

(Z)-(3-benzyl-2-((4-bromophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4ca)

Yield = 81% (68.7 mg). White solid. **Mp**: 124.8-126.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 4H), 7.32-7.25 (m, 3H), 6.85 – 6.77 (m, 2H), 5.13 (d, *J* = 15.4 Hz, 1H), 4.38 (d, *J* = 15.5 Hz, 1H), 3.77 – 3.69 (m, 2H), 3.65 – 3.57 (m, 1H), 3.21 – 3.12 (m, 2H), 2.23 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.5, 152.2, 137.4, 132.0, 128.8, 127.6, 127.6, 123.6, 116.4, 63.0, 61.3, 49.7, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.6. **IR (ATR)**: ν = 3168, 2919, 1597, 1482, 1212, 1059, 831 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{17}BrN_2OSe$ $[M+H]^+$: 424.9768, found: 424.9758.

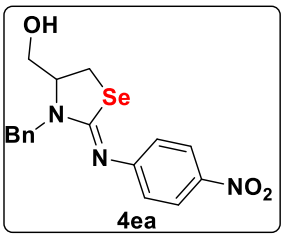


4da

(Z)-(3-benzyl-2-((4-iodophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4da)

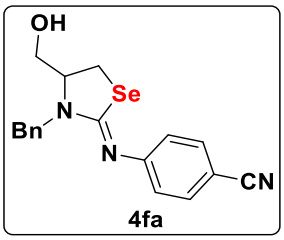
Yield = 83% (77.8 mg). White solid. **Mp**: 123.9-125.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 – 7.51 (m, 2H), 7.37 – 7.25 (m, 5H), 6.76 – 6.65 (m, 2H), 5.13 (d, *J* = 15.5 Hz, 1H), 4.41 (d, *J* = 15.4 Hz, 1H),

3.80 – 3.72 (m, 2H), 3.66-3.60 (m, 1H), 3.21-3.16 (m, 2H), 2.02 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.3, 152.8, 138.0, 137.5, 128.8, 127.6, 127.6, 124.0, 87.0, 63.0, 61.4, 49.7, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.3. **IR (ATR)**: ν = 3184, 2921, 1597, 1479, 1401, 1211, 1059, 1005, 830 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{17}IN_2OSe$ $[M+H]^+$: 472.9629, found: 472.9631.



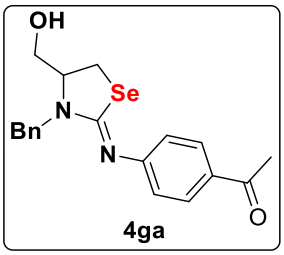
(Z)-(3-benzyl-2-((4-nitrophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4ea)

Yield = 75% (58.8 mg). Yellow solid. **Mp**: 101.3-103.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19 – 8.11 (m, 2H), 7.39 – 7.27 (m, 5H), 7.07 – 6.98 (m, 2H), 5.19 (d, *J* = 15.3 Hz, 1H), 4.47 (d, *J* = 15.4 Hz, 1H), 3.90 – 3.78 (m, 2H), 3.74-3.68 (m, 1H), 3.33-2.28 (d, *J* = 5.1 Hz, 2H), 2.08 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.0, 157.5, 143.3, 137.1, 128.9, 127.8, 127.6, 125.1, 122.1, 63.1, 61.2, 49.8, 23.7. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 274.5. **IR (ATR)**: ν =3375, 2923, 1611, 1559, 1494, 1322, 1211, 1105, 851 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{17}N_3O_3Se$ $[M+H]^+$: 392.0513, found: 392.0519.



(Z)-4-((3-benzyl-4-(hydroxymethyl)-1,3-selenazolidin-2-ylidene)amino)benzonitrile (4fa)

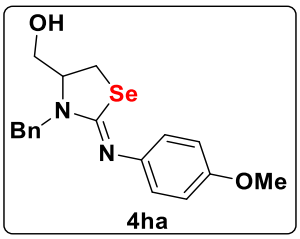
Yield = 72% (53.6 mg). White solid. **Mp**: 113.2-114.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 – 7.53 (m, 2H), 7.39 – 7.26 (m, 5H), 7.04 – 6.97 (m, 2H), 5.18 (d, *J* = 15.4 Hz, 1H), 4.44 (d, *J* = 15.4 Hz, 1H), 3.88 – 3.75 (m, 2H), 3.72-3.64 (m, 1H), 3.28 (d, *J* = 5.1 Hz, 2H), 2.23 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.3, 157.0, 137.2, 133.3, 128.9, 127.7, 127.6, 122.5, 119.7, 105.9, 63.0, 61.2, 49.7, 23.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 271.3. **IR (ATR)**: ν =3399, 2923, 2220, 1616, 1513, 1495, 1354, 1211, 1167, 1044 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{17}N_3OSe$ $[M+H]^+$: 372.0615, found: 372.0624.



(Z)-1-(4-((3-benzyl-4-(hydroxymethyl)-1,3-selenazolidin-2-ylidene)amino)phenyl)ethan-1-one (4ga)

Yield = 84% (65 mg). White solid. **Mp**: 111.4-112.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 – 7.88 (m, 2H), 7.42 – 7.33 (m, 4H), 7.33 – 7.26 (m, 1H), 7.06 – 6.98 (m, 2H), 5.23 (d, *J* = 15.4 Hz, 1H), 4.45 (d, *J* = 15.4 Hz, 1H), 3.89 – 3.77 (m, 2H), 3.76 – 3.66 (m, 1H), 3.33 – 3.21 (m, 2H), 2.73 (s, 1H), 2.58 (s, 3H).

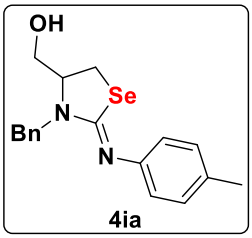
^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 157.7, 157.0, 137.4, 132.2, 129.9, 128.8, 127.7, 127.6, 121.7, 63.0, 61.1, 49.6, 26.5, 23.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 269.5. **IR (ATR)**: ν = 3193, 2915, 1673, 1609, 1574, 1357, 1269, 1214, 1059 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{20}N_2O_2Se$ $[M+H]^+$: 389.0768, found: 389.0773.



4ha

(Z)-(3-benzyl-2-((4-methoxyphenyl)imino)-1,3-selenazolidin-4-yl)methanol (4ha)

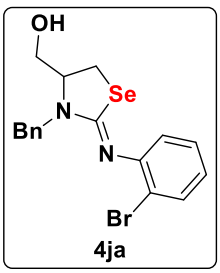
Yield = 84% (63.4 mg). White solid. **Mp**: 107.9-109.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.28 (m, 5H), 6.94 – 6.82 (m, 4H), 5.19 (d, *J* = 15.5 Hz, 1H), 4.39 (d, *J* = 15.5 Hz, 1H), 3.81 (s, 3H), 3.78 – 3.71 (m, 2H), 3.67-3.59 (m, 1H), 3.19-3.12 (m, 2H), 2.54 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.6, 156.0, 146.8, 137.7, 128.7, 127.6, 127.5, 122.6, 114.2, 62.9, 61.3, 55.5, 49.6, 23.1. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.9. **IR (ATR)**: ν = 3287, 2921, 2355, 1588, 1504, 1245, 1211, 1085, 1023 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{20}N_2O_2Se$ $[M+H]^+$: 377.0768, found: 377.0775.



4ia

(Z)-(3-benzyl-2-(p-tolylimino)-1,3-selenazolidin-4-yl)methanol (4ia)

Yield = 83% (59.6 mg). White solid. **Mp**: 124.6-126.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.23 (m, 5H), 7.12 – 7.03 (m, 2H), 6.89 – 6.76 (m, 2H), 5.15 (d, *J* = 15.5 Hz, 1H), 4.34 (d, *J* = 15.5 Hz, 1H), 3.74 – 3.65 (m, 2H), 3.62-3.54 (m, 1H), 3.14-3.07 (m, 2H), 2.51 (s, 1H), 2.30 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.3, 150.7, 137.7, 132.9, 129.6, 128.7, 127.7, 127.5, 121.5, 62.9, 61.3, 49.6, 23.1, 21.0. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 264.0. **IR (ATR)**: ν = 3162, 2914, 1616, 1594, 1505, 1212, 1198, 1050, 824 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{20}N_2OSe$ $[M+H]^+$: 361.0819, found: 361,0829.

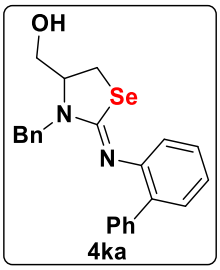


4ja

(Z)-(3-benzyl-2-((2-bromophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4ja)

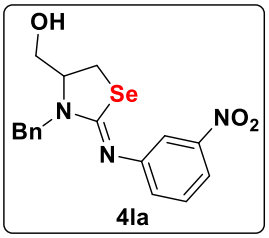
Yield = 79% (67.4 mg). White solid. **Mp**: 86.7-88.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.39-7.43 (m, 2H), 7.31-7.37 (m, 2H), 7.29 – 7.19 (m, 2H), 6.97 – 6.88 (m, 2H), 5.18 (d, *J* = 15.3 Hz, 1H), 4.45 (d, *J* = 15.3 Hz, 1H), 3.80 – 3.71 (m, 2H), 3.66 – 3.58 (m, 1H), 3.22 – 3.13 (m, 2H), 2.27 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.3, 151.4, 137.5, 132.9, 128.8, 128.2, 127.9, 127.6,

124.8, 122.5, 118.2, 63.3, 61.4, 49.8, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 279.0. **IR (ATR)**: ν = 3313, 2923, 1598, 1569, 1467, 1432, 1397, 1210, 1187, 1042, 1024 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{17}BrN_2OSe$ $[M+H]^+$: 424.9768, found: 424.9759.



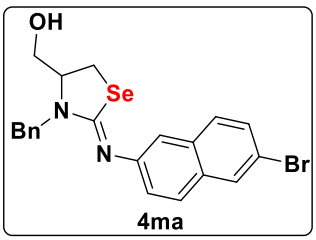
(Z)-(2-([1,1'-biphenyl]-2-ylimino)-3-benzyl-1,3-selenazolidin-4-yl)methanol (4ka)

Yield = 80% (67.7 mg). Yellow solid. **Mp**: 44.3-45.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.44 (m, 2H), 7.33 – 7.20 (m, 8H), 7.13 (td, *J* = 7.5, 1.4 Hz, 1H), 7.09 – 7.04 (m, 2H), 6.94 (dd, *J* = 7.8, 1.3 Hz, 1H), 4.93 (d, *J* = 15.3 Hz, 1H), 4.29 (d, *J* = 15.3 Hz, 1H), 3.65 – 3.55 (m, 2H), 3.52 – 3.44 (m, 1H), 3.11 – 3.03 (m, 2H), 2.01 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.8, 150.8, 140.5, 137.8, 135.1, 130.4, 129.8, 128.7, 128.2, 127.8, 127.7, 127.4, 126.5, 123.9, 121.8, 62.9, 61.3, 49.6, 23.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 277.9. **IR (ATR)**: ν = 3294, 2920, 1605, 1580, 1558, 1474, 1430, 1209, 1184, 1045 cm^{-1}; **HRMS** (ESI): calcd. for $C_{23}H_{22}N_2OSe$ $[M+H]^+$: 423.0976, found: 423.0981.



(Z)-(3-benzyl-2-((3-nitrophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4la)

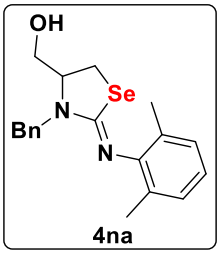
Yield = 71% (55.6 mg). Yellow solid. **Mp**: 85.7-86.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (ddd, *J* = 8.1, 2.2, 1.1 Hz, 1H), 7.80 (t, *J* = 2.2 Hz, 1H), 7.44 – 7.25 (m, 7H), 5.17 (d, *J* = 15.4 Hz, 1H), 4.47 (d, *J* = 15.4 Hz, 1H), 3.88 – 3.77 (m, 2H), 3.74 – 3.65 (m, 1H), 3.33 – 3.23 (m, 2H), 2.16 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.2, 154.2, 148.7, 137.2, 129.6, 128.9, 128.5, 127.7, 127.6, 118.0, 116.7, 63.1, 61.3, 49.7, 23.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 270.4. **IR (ATR)**: ν = 3358, 2922, 1619, 1588, 1567, 1345, 1210, 1188, 1043, 1029 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{17}N_3O_3Se$ $[M+H]^+$: 392.0513, found: 392.0520.



(Z)-(3-benzyl-2-((6-bromonaphthalen-2-yl)imino)-1,3-selenazolidin-4-yl)methanol (4ma)

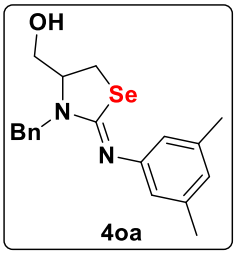
Yield = 84% (80.0 mg). Pale orange solid. **Mp**: 144.2-145.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 1.9 Hz, 1H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.47 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.37 – 7.25 (m, 6H), 7.16 (dd, *J* = 8.6, 2.1 Hz, 1H), 5.19 (d, *J* = 15.4 Hz, 1H), 4.43 (d, *J* = 15.5 Hz, 1H), 3.80 –

3.72 (m, 2H), 3.67-3.59 (m, 1H), 3.19-3.12 (m, 2H), 2.19 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.5, 151.5, 137.5, 132.7, 131.7, 129.7, 129.4, 129.0, 128.9, 127.9, 127.7, 127.6, 124.4, 118.0, 117.1, 63.0, 61.4, 49.8, 23.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 269.7. **IR (ATR)**: ν = 3148, 2920, 1596, 1492, 1406, 1351, 1217, 1196, 1060, 1049 cm^{-1}; **HRMS** (ESI): calcd. for $C_{21}H_{19}BrN_2OSe$ $[M+H]^+$: 474.9924, found: 474.9914.



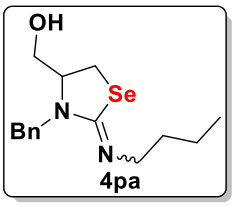
(Z)-(3-benzyl-2-((2,6-dimethylphenyl)imino)-1,3-selenazolidin-4-yl)methanol (4na)

Yield = 90% (67.0 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37-7.28 (m, 4H), 7.28 – 7.22 (m, 1H), 7.04 – 6.92 (m, 2H), 6.91-6.83 (m, 1H), 5.05 (d, *J* = 15.6 Hz, 1H), 4.43 (d, *J* = 15.5 Hz, 1H), 3.73-3.66 (m, 1H), 3.65-3.59 (m, 1H), 3.54 (dd, *J* = 10.8, 4.0 Hz, 1H), 3.17-3.11 (m, 1H), 3.08-3.02 (m, 1H), 2.55 (s, 1H), 2.14 (s, 3H), 2.08 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.2, 150.8, 137.8, 129.8, 129.6, 128.7, 128.1, 127.5, 123.4, 63.7, 61.3, 49.5, 23.0, 18.4, 18.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 288.9. **IR (ATR)**: ν = 3245, 2917, 1608, 1580, 1469, 1453, 1390, 1354, 1209, 1184, 1048 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{22}N_2OSe$ $[M+H]^+$: 375.0976, found: 375.0969.



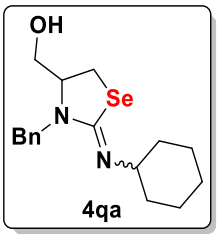
(Z)-(3-benzyl-2-((3,5-dimethylphenyl)imino)-1,3-selenazolidin-4-yl)methanol (4oa)

Yield = 88% (65.8 mg). Pale yellow solid. **Mp**: 122.8-124.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.22 (m, 5H), 6.71 (s, 1H), 6.57 (s, 2H), 5.14 (d, *J* = 15.4 Hz, 1H), 4.35 (d, *J* = 15.4 Hz, 1H), 3.76 – 3.65 (m, 2H), 3.63-3.55 (m, 1H), 3.14-3.06 (m, 2H), 2.48 (s, 1H), 2.27 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.0, 153.1, 138.6, 137.7, 128.8, 127.7, 127.5, 125.3, 119.4, 62.9, 61.3, 49.6, 23.0, 21.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.2. **IR (ATR)**: ν = 3280, 2921, 1603, 1576, 1454, 1214, 1046, 935, 845 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{22}N_2OSe$ $[M+H]^+$: 375.0976, found: 375.0975.



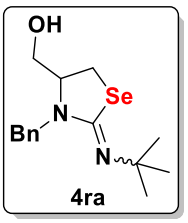
(3-benzyl-2-(butylimino)-1,3-selenazolidin-4-yl)methanol (4pa)

Yield = 73% (47.3 mg). Yellow oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42 – 7.34 (m, 2.2H), 7.33 – 7.28 (m, 1.1H), 7.28 – 7.21 (m, 2.2H), 5.95 – 5.81 (m, 1H, major), 5.57 – 5.48 (m, 0.1H, minor), 4.54 (s, 2H, major), 4.51 (s, 0.2H, minor), 4.35 – 4.30 (m, 0.1H, minor), 4.28 – 4.15 (m, 1H, major), 3.64 – 3.56 (m, 2H, major), 3.51 – 3.44 (m, 0.2H, minor), 3.40 – 3.33 (m, 0.2H, minor), 3.17 – 3.05 (m, 4.2H), 1.3 (dd, *J* = 7.4, 5.0 Hz, 2H), 1.16 – 1.06 (m, 2.2H), 0.81 (t, *J* = 7.3 Hz, 3.3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.2, 137.8, 129.1, 127.8, 125.9, 52.8, 46.3, 40.4, 32.0, 23.0, 19.8, 13.7. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 92.3. **IR (ATR)**: ν = 3351, 2954, 2927, 2860, 1624, 1523, 1452, 1323, 1222, 1127, 970 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{22}N_2OSe$ $[M+Na]^+$: 349.0795, found: 349.0796.



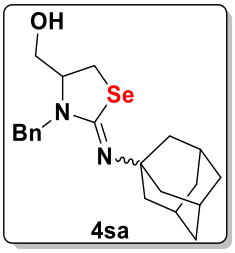
(3-benzyl-2-(cyclohexylimino)-1,3-selenazolidin-4-yl)methanol (4qa)

Yield = 67% (47.4 mg). Pale yellow solid. **Mp**: 83.4-85.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 2.16H), 7.32 – 7.27 (m, 1.08H), 7.27 – 7.19 (m, 2.16H), 5.91 – 5.78 (m, 1H, major), 5.54 – 5.44 (m, 0.1H, minor), 4.52 (s, 2H, major), 4.48 (s, 0.16H, minor), 4.22 (d, *J* = 7.7 Hz, 0.16H, minor), 4.11 (d, *J* = 7.8 Hz, 1H, major), 3.66 – 3.52 (m, 3.08H, major), 3.49 – 3.43 (m, 0.16H, minor), 3.39 – 3.32 (m, 0.16H, minor), 3.13 – 3.02 (m, 2H), 1.78 – 1.68 (m, 2.16H), 1.53 – 1.41 (m, 3.24H), 1.29 – 1.22 (m, 2.16H), 1.09 – 1.00 (m, 1.08H), 0.94 – 0.84 (m, 2.16H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.4, 137.9, 129.1, 127.8, 126.0, 52.8, 49.0, 46.4, 33.3, 25.5, 24.5, 23.1. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 91.8. **IR (ATR)**: ν = 3297, 2923, 2850, 1614, 1531, 1496, 1478, 1391, 1218, 1121, 1069 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{24}N_2OSe$ $[M+Na]^+$: 375.0952, found: 375.0947.



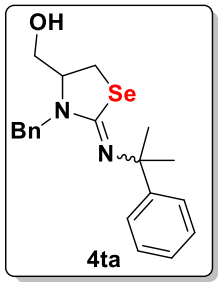
(3-benzyl-2-(tert-butylimino)-1,3-selenazolidin-4-yl)methanol (4ra)

Yield = 63% (40.9 mg). White solid. **Mp**: 100.1-101.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 2H), 7.32 – 7.27 (m, 1H), 7.26 – 7.19 (m, 2H), 5.95 – 5.79 (m, 1H, major), 5.57 – 5.48 (m, 0.03H, minor), 4.50 (s, 2H, major), 4.45 (s, 0.06H, minor), 4.19 (s, 0.03H, minor), 4.09 (s, 1H, major), 3.64 – 3.52 (m, 2H, major), 3.49 – 3.43 (m, 0.06H, minor), 3.36 – 3.30 (m, 0.06H, minor), 3.15 – 3.03 (m, 2H, major), 1.16 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.2, 138.0, 129.1, 127.8, 126.0, 52.2, 50.8, 46.5, 29.2, 23.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 90.5. **IR (ATR)**: ν = 3444, 2922, 1644, 1524, 1477, 1452, 1384, 1228, 1212, 1100, 966 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{22}N_2OSe$ $[M+Na]^+$: 349.0795, found: 349.0790.



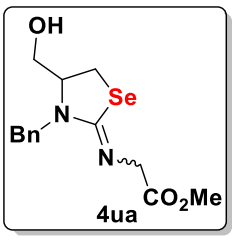
(2-(adamantan-1-ylimino)-3-benzyl-1,3-selenazolidin-4-yl)methanol (4sa)

Yield = 63% (51.1 mg). Yellow solid. **Mp**: 69.8-71.6. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 2.4H), 7.32 – 7.27 (m, 1.2H), 7.26 – 7.19 (m, 2.4H), 5.89 – 5.75 (m, 1H, major), 5.52 – 5.42 (m, 0.2H, minor), 4.50 (s, 2H, major), 4.45 (s, 0.4H, minor), 4.10 (s, 0.2H, minor), 3.99 (s, 1H, major), 3.62 – 3.53 (m, 2H, major), 3.49 – 3.42 (m, 0.4H, minor), 3.36 – 3.30 (m, 0.4H, minor), 3.13 – 3.02 (m, 2H, major), 2.01 – 1.95 (m, 3.6H), 1.81 – 1.74 (m, 7.2H), 1.63 – 1.54 (m, 7.2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.9, 138.0, 129.07 (129.14), 127.7 (127.8), 126.02 (125.95), 52.3, 51.5, 46.6, 42.1, 36.4, 32.0, 29.5, 23.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 90.8. **IR (ATR)**: ν = 3394, 2902, 2847, 1641, 1512, 1452, 1358, 1218, 1077, 967 cm^{-1}; **HRMS** (ESI): calcd. for $C_{21}H_{28}N_2OSe$ $[M+Na]^+$: 427.1265, found: 427.1269.



(3-benzyl-2-((2-phenylpropan-2-yl)imino)-1,3-selenazolidin-4-yl)methanol (4ta)

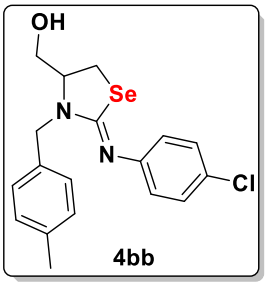
Yield = 61% (46.9 mg). Pale yellow solid. **Mp**: 52.2-53.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 2.14H), 7.36 – 7.33 (m, 1.07H), 7.32 – 7.26 (m, 2.14H), 7.24 – 7.19 (m, 2.14H), 7.17 – 7.13 (m, 1.07H), 7.11 – 7.04 (m, 2.14H), 5.93 – 5.77 (m, 1H, major), 5.56 – 5.47 (m, 0.07H, minor), 4.71 (s, 0.07H, minor), 4.59 (s, 1H, major), 4.55 (s, 2H, major), 4.51 (s, 0.14H, minor), 3.62 – 3.52 (m, 2H, major), 3.46 – 3.41 (m, 0.14H, minor), 3.35 – 3.30 (m, 0.14H, minor), 3.10 – 3.04 (m, 2H, major), 1.49 (s, 6.42H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.5, 147.6, 138.0, 129.2, 128.2, 128.0, 126.4, 126.2, 124.6, 55.5, 52.2, 46.5, 29.4, 23.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 90.7. **IR (ATR)**: ν = 3429, 3374, 2969, 1642, 1509, 1493, 1447, 1382, 1262, 1219, 1163, 967 cm^{-1}; **HRMS** (ESI): calcd. for $C_{20}H_{24}N_2OSe$ $[M+H]^+$: 389.1132, found: 389.1141.



methyl 2-((3-benzyl-4-(hydroxymethyl)-1,3-selenazolidin-2-ylidene)amino)acetate (4ua)

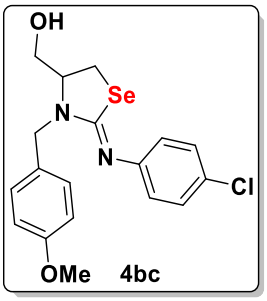
Yield = 35% (23.9 mg). Yellow oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2.4 H), 7.32 – 7.25 (m, 3.6 H), 5.83 – 5.71 (m, 1 H, major), 5.43 – 5.34 (m, 0.2 H, minor), 4.92 (t, *J* = 4.7 Hz, 0.2 H, minor), 4.81 (t, *J* = 5.4 Hz, 1H, major), 4.60 (s, 2H, major), 4.57 (s, 0.4 H, minor), 3.94 (d, *J* = 5.4 Hz,

0.4 H, minor), 3.91 (d, *J* = 5.3 Hz, 2H, major), 3.70 (s, 0.6 H, minor), 3.69 (s, 3 H, major), 3.64 – 3.59 (m, 2H, major), 3.47 – 3.41 (m, 0.4 H, minor), 3.40 – 3.34 (m, 0.4 H, minor), 3.09 – 3.02 (m, 2 H, major). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.2, 157.0 (157.7), 137.4, 129.2 (129.1), 127.84 (127.80), 126.0 (125.9), 53.2, 52.2, 46.5 (47.6), 42.5 (42.6), 22.7 (31.8). **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 96.9. **IR (ATR)**: ν = 3366, 2920, 2850, 1742, 1632, 1516, 1394, 1199, 971 cm^{-1}; **HRMS** (ESI): calcd. for $C_{14}H_{18}N_2O_3Se$ $[M+Na]^+$: 365.0380, found: 365.0385.



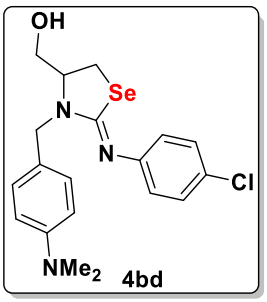
(Z)-(2-((4-chlorophenyl)imino)-3-(4-methylbenzyl)-1,3-selenazolidin-4-yl)methanol (4bb)

Yield = 84% (66.3 mg). White solid. **Mp**: 83.2-84.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.18 (m, 4H), 7.17 – 7.11 (m, 2H), 6.90 – 6.82 (m, 2H), 5.09 (d, *J* = 15.3 Hz, 1H), 4.34 (d, *J* = 15.3 Hz, 1H), 3.78 – 3.68 (m, 2H), 3.65 – 3.55 (m, 1H), 3.21 – 3.09 (m, 2H), 2.33 (s, 3H), 2.29 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.6, 151.8, 137.3, 134.4, 129.5, 129.0, 128.6, 127.7, 123.1, 62.9, 61.3, 49.4, 23.2, 21.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 268.1. **IR (ATR)**: ν = 3236, 2928, 2860, 1599, 1483, 1433, 1210, 1183, 1086, 1063, 1011, 838 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{19}ClN_2OSe$ $[M+H]^+$: 395.0429, found: 395.0420.



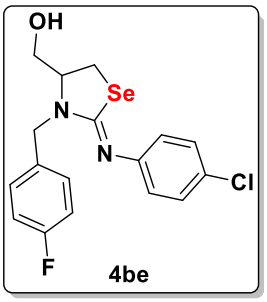
(Z)-(2-((4-chlorophenyl)imino)-3-(4-methoxybenzyl)-1,3-selenazolidin-4-yl)methanol (4bc)

Yield = 85% (70.0 mg). White solid. **Mp**: 134.8-136.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 4H), 6.93 – 6.87 (m, 4H), 5.10 (d, *J* = 15.1 Hz, 1H), 4.35 (d, *J* = 15.2 Hz, 1H), 3.82 (s, 3H), 3.80 – 3.73 (m, 2H), 3.68 – 3.62 (m, 1H), 3.22 – 3.15 (m, 2H), 2.37 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1, 157.6, 151.8, 129.5, 129.1, 129.0, 128.6, 123.1, 114.2, 62.9, 61.3, 55.3, 49.1, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 268.9. **IR (ATR)**: ν = 3268, 2927, 1599, 1509, 1485, 1305, 1247, 1207, 1175, 1054, 1029, 1012 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{19}ClN_2O_2Se$ $[M+H]^+$: 411.0379, found: 411.0384.



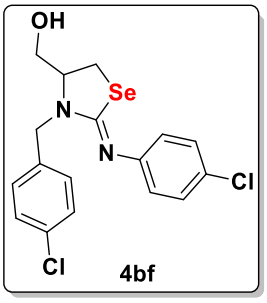
(Z)-(2-((4-chlorophenyl)imino)-3-(4-(dimethylamino)benzyl)-1,3-selenazolidin-4-yl)methanol (4bd)

Yield = 72% (61.3 mg). Yellow solid. **Mp**: 53.4-54.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25 – 7.19 (m, 4H), 6.91 – 6.86 (m, 2H), 6.72 – 6.67 (m, 2H), 5.04 (d, *J* = 15.0 Hz, 1H), 4.29 (d, *J* = 15.0 Hz, 1H), 3.79 – 3.72 (m, 2H), 3.65 – 3.59 (m, 1H), 3.19 – 3.11 (m, 2H), 2.93 (s, 6H), 2.25 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.6, 151.9, 150.1, 129.0, 128.9, 128.5, 125.0, 123.1, 112.8, 62.8, 61.2, 49.3, 40.6, 23.2. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 270.0. **IR (ATR)**: ν = 3319, 2923, 2852, 1604, 1520, 1484, 1346, 1184, 1163, 1087, 1048, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{22}ClN_3OSe$ $[M+H]^+$: 424.0695, found: 424.0690.



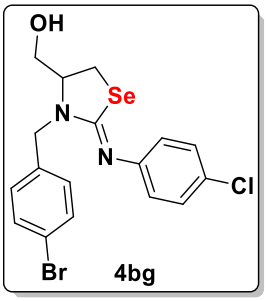
(Z)-(2-((4-chlorophenyl)imino)-3-(4-fluorobenzyl)-1,3-selenazolidin-4-yl)methanol (4be)

Yield = 73% (57.8 mg). White solid. **Mp**: 118.2-120.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.26 – 7.22 (m, 2H), 7.06 – 7.00 (m, 2H), 6.90 – 6.82 (m, 2H), 5.10 (d, *J* = 15.3 Hz, 1H), 4.39 (d, *J* = 15.4 Hz, 1H), 3.80 – 3.73 (m, 2H), 3.69 – 3.62 (m, 1H), 3.24 – 3.16 (m, 2H), 2.08 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.2 (d, $J_{C\text{-}F}$ = 244.4 Hz), 157.4, 151.6, 133.3 (d, $J_{C\text{-}F}$ = 3.2 Hz), 129.4 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.1, 128.7, 123.0, 115.6 (d, $J_{C\text{-}F}$ = 21.2 Hz), 62.9, 61.5, 49.0, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -114.7. **IR (ATR)**: ν = 3186, 2924, 2850, 1599, 1506, 1482, 1221, 1155, 1085, 1065, 1010 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}ClFN_2OSe$ $[M+H]^+$: 399.0179, found: 399.0171.



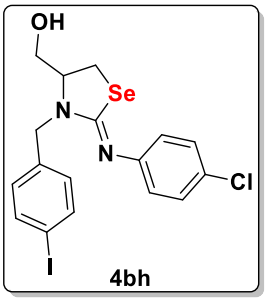
(Z)-(3-(4-chlorobenzyl)-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4bf)

Yield = 76% (62.6 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 2H), 7.26 – 7.21 (m, 4H), 6.89 – 6.81 (m, 2H), 5.10 (d, *J* = 15.5 Hz, 1H), 4.38 (d, *J* = 15.6 Hz, 1H), 3.78 – 3.70 (m, 2H), 3.68 – 3.60 (m, 1H), 3.23 – 3.14 (m, 2H), 2.19 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.4, 151.5, 136.0, 133.4, 129.1, 129.0, 128.9, 128.8, 123.0, 62.9, 61.5, 49.1, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.7. **IR (ATR)**: ν = 3318, 2923, 2852, 1602, 1574, 1485, 1394, 1211, 1187, 1088, 1011 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}Cl_2N_2OSe$ $[M+H]^+$: 414.9883, found: 414.9876.



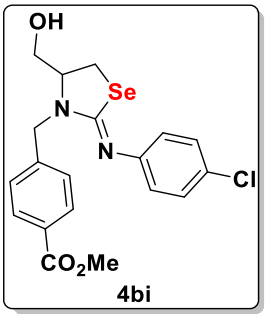
(Z)-(3-(4-bromobenzyl)-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4bg)

Yield = 70% (63.9 mg). White solid. **Mp**: 42.1-43.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 – 7.43 (m, 2H), 7.26 – 7.17 (m, 4H), 6.90 – 6.81 (m, 2H), 5.08 (d, *J* = 15.5 Hz, 1H), 4.36 (d, *J* = 15.5 Hz, 1H), 3.78 – 3.70 (m, 2H), 3.68 – 3.60 (m, 1H), 3.24 – 3.14 (m, 2H), 2.15 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.4, 151.5, 136.6, 131.9, 129.4, 129.1, 128.8, 123.0, 121.4, 62.9, 61.5, 49.1, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.7. **IR (ATR)**: ν = 3295, 2925, 2854, 1603, 1578, 1484, 1393, 1210, 1185, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}BrClN_2OSe$ $[M+H]^+$: 458.9378, found: 458.9382.



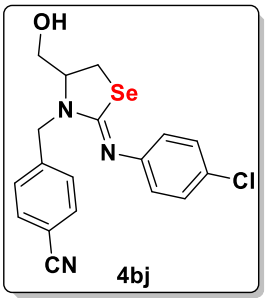
(Z)-(2-((4-chlorophenyl)imino)-3-(4-iodobenzyl)-1,3-selenazolidin-4-yl)methanol (4bh)

Yield = 87% (88.4 mg). Yellow solid. **Mp**: 42.2-43.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 – 7.63 (m, 2H), 7.25 – 7.21 (m, 2H), 7.09 – 7.04 (m, 2H), 6.89 – 6.81 (m, 2H), 5.09 (d, *J* = 15.5 Hz, 1H), 4.35 (d, *J* = 15.5 Hz, 1H), 3.78 – 3.71 (m, 2H), 3.69 – 3.62 (m, 1H), 3.23 – 3.15 (m, 2H), 2.64 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.4, 151.5, 137.8, 137.2, 129.6, 129.1, 128.8, 123.0, 93.0, 62.9, 61.5, 49.2, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 268.0. **IR (ATR)**: ν =3304, 2923, 2859, 1603, 1578, 1482, 1392, 1210, 1184, 1087, 1047, 1005 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}ClIN_2OSe$ $[M+H]^+$: 506.9239, found: 506.9237.



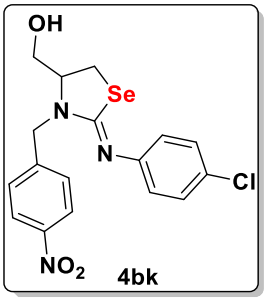
methyl (Z)-4-((2-((4-chlorophenyl)imino)-4-(hydroxymethyl)-1,3-selenazolidin-3-yl)methyl)benzoate (4bi)

Yield = 75% (65.9 mg). White solid. **Mp**: 48.7-50.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.04 – 7.98 (m, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.20 (m, 2H), 6.88 – 6.81 (m, 2H), 5.18 (d, *J* = 15.8 Hz, 1H), 4.48 (d, *J* = 15.9 Hz, 1H), 3.91 (s, 3H), 3.80 – 3.72 (m, 2H), 3.70 – 3.62 (m, 1H), 3.26 – 3.16 (m, 2H), 2.35 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.0, 157.3, 151.5, 143.0, 130.1, 129.3, 129.1, 128.7, 127.5, 123.0, 63.1, 61.5, 52.2, 49.4, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 265.9. **IR (ATR)**: ν = 3392, 2924, 1716, 1607, 1485, 1433, 1276, 1187, 1103, 1047 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{19}ClN_2O_3Se$ $[M+H]^+$: 439.0328, found: 439.0341.



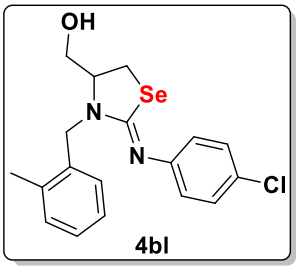
(Z)-4-((2-((4-chlorophenyl)imino)-4-(hydroxymethyl)-1,3-selenazolidin-3-yl)methyl)benzonitrile (4bj)

Yield = 70% (57.3 mg). White solid. **Mp**: 40.8-42.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 – 7.62 (m, 2H), 7.46 – 7.42 (m, 2H), 7.26 – 7.21 (m, 2H), 6.86 – 6.80 (m, 2H), 5.18 (d, *J* = 16.0 Hz, 1H), 4.56 (d, *J* = 16.0 Hz, 1H), 3.84 – 3.77 (m, 2H), 3.76 – 3.70 (m, 1H), 3.32 – 3.21 (m, 2H), 1.85 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.8, 151.3, 143.4, 132.5, 129.1, 128.8, 128.2, 122.8, 118.7, 111.3, 63.1, 61.9, 49.4, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 265.9. **IR (ATR)**: ν = 3353, 2922, 2228, 1737, 1604, 1484, 1393, 1212, 1185, 1086, 1048 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{16}ClN_3OSe$ $[M+Na]^+$: 406.0225, found: 406.0220.



(Z)-(2-((4-chlorophenyl)imino)-3-(4-nitrobenzyl)-1,3-selenazolidin-4-yl)methanol (4bk)

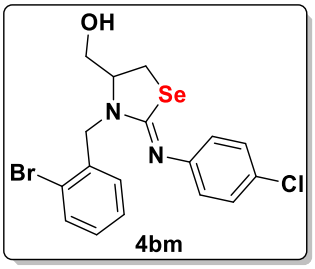
Yield = 67% (56.7 mg). Yellow solid. **Mp**: 56.7-58.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 – 8.16 (m, 2H), 7.51 – 7.45 (m, 2H), 7.26 – 7.20 (m, 2H), 6.88 – 6.79 (m, 2H), 5.20 (d, *J* = 16.1 Hz, 1H), 4.60 (d, *J* = 16.1 Hz, 1H), 3.85 – 3.77 (m, 2H), 3.76 – 3.70 (m, 1H), 3.34 – 3.27 (m, 1H), 3.26 – 3.18 (m, 1H), 2.09 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.0, 151.4, 147.3, 145.5, 129.2, 128.9, 128.3, 124.0, 122.9, 63.3, 62.0, 49.3, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 266.0. **IR (ATR)**: ν = 3329, 2922, 1600, 1577, 1514, 1484, 1339, 1211, 1185, 1086, 1046, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}ClN_3O_3Se$ $[M+H]^+$: 426.0124, found: 426.0136.



4bl

(Z)-(2-((4-chlorophenyl)imino)-3-(2-methylbenzyl)-1,3-selenazolidin-4-yl)methanol (4bl)

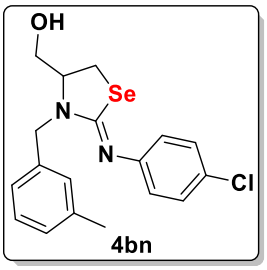
Yield = 86% (68.1 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.17 (m, 6H), 6.88 – 6.80 (m, 2H), 5.18 (d, *J* = 15.5 Hz, 1H), 4.32 (d, *J* = 15.5 Hz, 1H), 3.73 – 3.62 (m, 3H), 3.22 – 3.15 (m, 1H), 3.15 – 3.09 (m, 1H), 2.36 (s, 1H), 2.31 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.9, 151.8, 136.5, 134.9, 130.8, 129.0, 128.7, 128.0, 127.7, 126.2, 123.1, 62.3, 61.2, 47.9, 23.3, 19.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 265.9. **IR (ATR)**: ν = 3301, 2923, 1600, 1575, 1484, 1194, 1178, 1087, 1048, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{19}ClN_2OSe$ $[M+H]^+$: 395.0429, found: 395.0419.



4bm

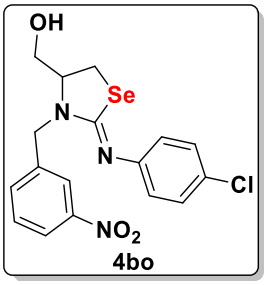
(Z)-(3-(2-bromobenzyl)-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4bm)

Yield = 84% (77.3 mg). White solid. **Mp**: 121.3-122.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.24 – 7.19 (m, 2H), 7.18 – 7.12 (m, 1H), 6.87 – 6.79 (m, 2H), 5.13 (d, *J* = 16.1 Hz, 1H), 4.57 (d, *J* = 16.1 Hz, 1H), 3.82 – 3.67 (m, 3H), 3.32 – 3.25 (m, 1H), 3.25 – 3.18 (m, 1H), 2.16 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.9, 151.6, 136.2, 133.1, 129.2, 129.1, 129.0, 128.7, 127.7, 123.3, 123.0, 63.1, 61.4, 49.8, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.2. **IR (ATR)**: ν = 3329, 2917, 2855, 1600, 1485, 1437, 1348, 1306, 1208, 1062, 1028, 1011 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}BrClN_2OSe$ $[M+H]^+$: 458.9378, found: 458.9370.



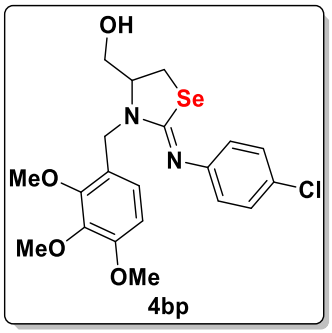
(Z)-(2-((4-chlorophenyl)imino)-3-(3-methylbenzyl)-1,3-selenazolidin-4-yl)methanol (4bn)

Yield = 77% (60.8 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25 – 7.20 (m, 3H), 7.13 – 7.06 (m, 3H), 6.91 – 6.83 (m, 2H), 5.11 (d, *J* = 15.4 Hz, 1H), 4.35 (d, *J* = 15.3 Hz, 1H), 3.79 – 3.71 (m, 2H), 3.66 – 3.58 (m, 1H), 3.17 (d, *J* = 4.8 Hz, 2H), 2.35 (s, 3H), 2.21 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.6, 151.8, 138.5, 137.4, 129.0, 128.7, 128.6, 128.4, 124.6, 123.1, 62.9, 61.3, 49.6, 23.2, 21.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.3. **IR (ATR)**: ν = 3328, 2920, 1602, 1576, 1484, 1395, 1200, 1087, 1044, 1009, 831 cm^{-1}; **HRMS** (ESI): calcd. for $C_{18}H_{19}ClN_2OSe$ $[M+H]^+$: 395.0429, found: 395.0421.



(Z)-(2-((4-chlorophenyl)imino)-3-(3-nitrobenzyl)-1,3-selenazolidin-4-yl)methanol (4bo)

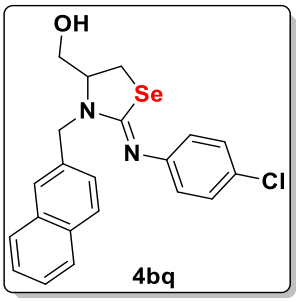
Yield = 76% (64.3 mg). Yellow oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25 – 8.19 (m, 1H), 8.16 – 8.10 (m, 1H), 7.71 – 7.65 (m, 1H), 7.55 – 7.50 (m, 1H), 7.26 – 7.20 (m, 2H), 6.89 – 6.81 (m, 2H), 5.20 (d, *J* = 15.8 Hz, 1H), 4.57 (d, *J* = 15.8 Hz, 1H), 3.86 – 3.71 (m, 3H), 3.32 – 3.26 (m, 1H), 3.25 – 3.17 (m, 1H), 2.18 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.2, 151.4, 148.4, 140.0, 133.8, 129.7, 129.1, 128.86, 122.9, 122.6, 122.6, 63.2, 61.9, 49.0, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.0. **IR (ATR)**: ν = 3340, 2923, 1604, 1577, 1523, 1484, 1344, 1213, 1192, 1087, 1045, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{17}H_{16}ClN_3O_3Se$ $[M+H]^+$: 426.0124, found: 426.0105.



(Z)-(2-((4-chlorophenyl)imino)-3-(2,3,4-trimethoxybenzyl)-1,3-selenazolidin-4-yl)methanol (4bp)

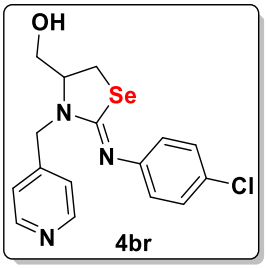
Yield = 80% (75.6 mg). White solid. **Mp**: 85.1-86.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25 – 7.20 (m, 2H), 7.04 (d, *J* = 8.6 Hz, 1H), 6.90 – 6.83 (m, 2H), 6.66 (d, *J* = 8.6 Hz, 1H), 5.06 (d, *J* = 15.2 Hz, 1H),

4.43 (d, *J* = 15.1 Hz, 1H), 3.90 (s, 3H), 3.87 (s, 3H), 3.85 (s, 3H), 3.82 – 3.75 (m, 2H), 3.72 – 3.66 (m, 1H), 3.23 – 3.15 (m, 2H), 2.42 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.1, 153.4, 151.9, 151.8, 142.2, 129.0, 128.5, 123.9, 123.1, 123.0, 107.6, 63.0, 61.4, 61.3, 60.9, 56.1, 44.1, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 266.8. **IR (ATR)**: ν = 3384, 2927, 1603, 1578, 1485, 1464, 1276, 1197, 1092, 1040, 1009 cm^{-1}; **HRMS** (ES): calcd. for $C_{20}H_{23}ClN_2O_4Se$ $[M+H]^+$: 471.0590, found: 471.0585.



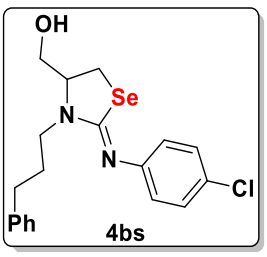
(Z)-(2-((4-chlorophenyl)imino)-3-(naphthalen-2-ylmethyl)-1,3-selenazolidin-4-yl)methanol (4bq)

Yield = 78% (67.5 mg). Pale yellow solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 – 7.77 (m, 3H), 7.69 (s, 1H), 7.50 – 7.42 (m, 3H), 7.24 – 7.21 (m, 2H), 6.93 – 6.85 (m, 2H), 5.30 (d, *J* = 15.0 Hz, 1H), 4.52 (d, *J* = 15.4 Hz, 1H), 3.78 – 3.70 (m, 2H), 3.66 – 3.58 (m, 1H), 3.18 – 3.10 (m, 2H), 2.24 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.7, 151.8, 135.0, 133.4, 132.9, 129.1, 128.8, 128.7, 127.8, 127.8, 126.5, 126.1, 125.8, 123.1, 63.0, 61.4, 50.0, 23.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 268.4. **IR (ATR)**: ν = 3292, 2921, 1600, 1574, 1484, 1191, 1086, 1044, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{21}H_{19}ClN_2OSe$ $[M+H]^+$: 431.0429, found: 431.0427.



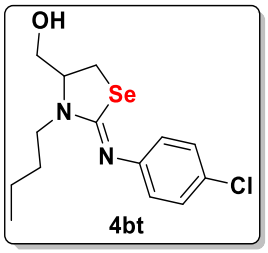
(Z)-(2-((4-chlorophenyl)imino)-3-(pyridin-4-ylmethyl)-1,3-selenazolidin-4-yl)methanol (4br)

Yield = 73% (55.2 mg). Pale yellow solid. **Mp**: 132.1-133.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.27 – 7.20 (m, 4H), 6.86 – 6.79 (m, 2H), 5.13 (d, *J* = 16.3 Hz, 1H), 4.53 (d, *J* = 16.3 Hz, 1H), 3.83 – 3.71 (m, 3H), 3.35– 3.29 (m, 1H), 3.28 – 3.22 (m, 1H), 3.13 (s, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 156.9, 151.4, 149.5, 147.6, 129.1, 128.8, 122.8, 122.6, 63.4, 61.7, 48.8, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.1. **IR (ATR)**: ν = 3141, 2922, 1602, 1485, 1416, 1390, 1316, 1214, 1185, 1052, 1005 cm^{-1}; **HRMS** (ESI): calcd. for $C_{16}H_{16}ClN_3OSe$ $[M+H]^+$: 382.0225, found: 382.0226.



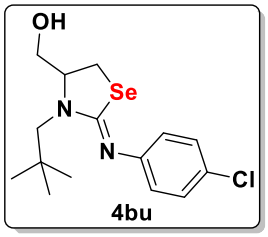
(Z)-(2-((4-chlorophenyl)imino)-3-(3-phenylpropyl)-1,3-selenazolidin-4-yl)methanol (4bs)

Yield = 83% (67.7 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 2H), 7.23 – 7.16 (m, 5H), 6.87 – 6.79 (m, 2H), 3.95 – 3.86 (m, 1H), 3.84 – 3.76 (m, 1H), 3.75 – 3.68 (m, 1H), 3.67–3.60 (m, 1H), 3.23 – 3.12 (m, 3H), 2.71 – 2.62 (m, 2H), 2.35 (s, 1H), 2.04 – 1.94 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.7, 152.0, 141.6, 129.0, 128.6, 128.5, 128.3, 126.1, 123.1, 63.6, 61.3, 46.0, 33.2, 29.1, 23.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 267.1. **IR (ATR)**: ν = 3292, 2922, 1600, 1575, 1484, 1206, 1086, 1045, 831 cm^{-1}; **HRMS** (ESI): calcd. for $C_{19}H_{21}ClN_2OSe$ $[M+H]^+$: 409.0586, found: 409.0582.



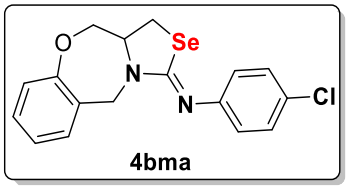
(Z)-(3-butyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methanol (4bt)

Yield = 65% (45.1 mg). White solid. **Mp**: 89.5-91.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.19 (m, 2H), 6.87 – 6.79 (m, 2H), 3.92 – 3.84 (m, 2H), 3.82 – 3.75 (m, 1H), 3.73 – 3.68 (m, 1H), 3.29 – 3.24 (m, 1H), 3.22 – 3.11 (m, 2H), 2.28 (s, 1H), 1.67 – 1.59 (m, 2H), 1.40 – 1.31 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.6, 152.1, 129.0, 128.5, 123.1, 63.4, 61.3, 46.0, 29.7, 23.4, 20.1, 14.0. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 265.9. **IR (ATR)**: ν = 3225, 2927, 1597, 1575, 1485, 1402, 1349, 1205, 1094, 1051, 1012 cm^{-1}; **HRMS** (ESI): calcd. for $C_{14}H_{19}ClN_2OSe$ $[M+H]^+$: 347.0429, found: 347.0437.



(Z)-(2-((4-chlorophenyl)imino)-3-neopentyl-1,3-selenazolidin-4-yl)methanol (4bu)

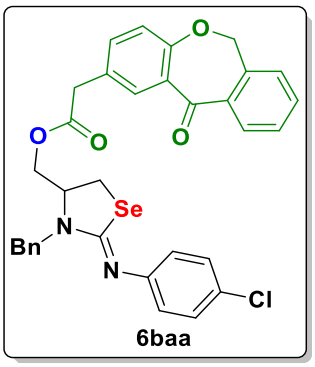
Yield = 79% (57.0 mg). White solid. **Mp**: 135.8-136.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.17 (m, 2H), 6.83 – 6.76 (m, 2H), 4.01 – 3.92 (m, 2H), 3.76 – 3.67 (m, 2H), 3.36 – 3.30 (m, 1H), 3.22 – 3.15 (m, 1H), 2.79 (d, *J* = 14.0 Hz, 1H), 2.48 (s, 1H), 0.98 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.7, 152.1, 129.0, 128.5, 123.0, 64.7, 60.5, 56.1, 34.7, 28.2, 23.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 261.9. **IR (ATR)**: ν = 3208, 2953, 1597, 1576, 1484, 1395, 1205, 1125, 1047, 837 cm^{-1}; **HRMS** (ESI): calcd. for $C_{15}H_{21}ClN_2OSe$ $[M+H]^+$: 361.0586, found: 361.0585.



(Z)-N-(4-chlorophenyl)-11,11a-dihydro-1H,3H,5H-benzo[f][1,3]selenazolo[4,4-c][1,4]oxazepin-3-imine (4bma)

Yield = 42% (32.0 mg). White solid. **Mp**: 62.9-64.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.66 (m, 1H), 7.54 – 7.51 (m, 1H), 7.47 – 7.43 (m, 2H), 7.32 – 7.28 (m, 1H), 7.26 – 7.22 (m, 2H), 7.19 – 7.15 (m, 1H), 4.95 (d, *J* = 14.5 Hz, 1H), 4.49 (d, *J* = 14.6 Hz, 1H), 4.28 – 4.21 (m, 1H), 4.01 (t, *J* = 9.2 Hz, 1H),

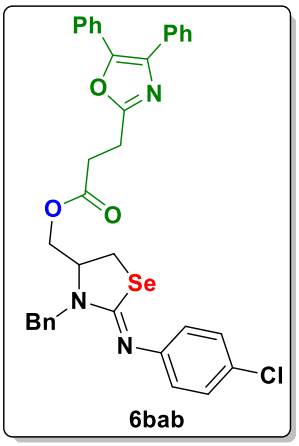
3.39 – 3.35 (m, 1H), 2.95 – 2.84 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.2, 143.1, 138.7, 134.7, 131.2, 130.6, 128.8, 128.8, 128.0, 127.4, 118.3, 57.3, 50.1, 50.0, 30.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 269.8. **IR (ATR)**: ν = 2920, 2851, 1658, 1584, 1488, 1434, 1358, 1226, 1087, 1042, 1008 cm^{-1}; **HRMS** (ES): calcd. for $C_{17}H_{15}ClN_2OSe$ $[M+H]^+$: 379.0116, found: 379.0119.



6baa

(Z)-(3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methyl 2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (6baa)

Yield = 86% (80.9 mg). White solid. **Mp**: 52.6-54.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 2.4 Hz, 1H), 7.86 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.54 (td, *J* = 7.4, 1.4 Hz, 1H), 7.44 (td, *J* = 7.6, 1.3 Hz, 1H), 7.38 (dd, *J* = 8.4, 2.5 Hz, 1H), 7.35 – 7.32 (m, 2H), 7.31 – 7.20 (m, 6H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.90 – 6.82 (m, 2H), 5.25 (d, *J* = 15.4 Hz, 1H), 5.14 (s, 2H), 4.30 – 4.19 (m, 3H), 3.95 – 3.87 (m, 1H), 3.63 (s, 2H), 3.26 – 3.19 (m, 1H), 3.03 (dd, *J* = 10.5, 2.7 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.1, 160.6, 151.8, 137.3, 136.3, 135.6, 132.9, 132.5, 129.5, 129.4, 129.0, 128.8, 128.6, 127.9, 127.8, 127.6, 127.3, 125.2, 122.9, 121.3, 73.7, 63.0, 59.7, 49.4, 40.1, 23.7. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.2. **IR (ATR)**: ν = 2958, 2919, 1735, 1609, 1485, 1298, 1136, 1119, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{33}H_{27}ClN_2O_4Se$ $[M+H]^+$: 631.0903, found: 631.0911.

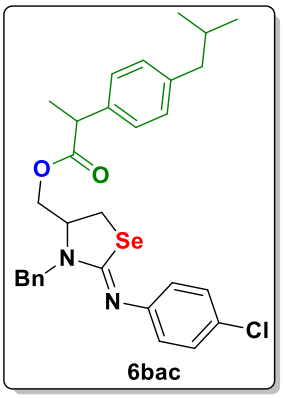


6bab

(Z)-(3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methyl 3-(4,5-diphenyloxazol-2-yl)propanoate (6bab)

Yield = 93% (91.4 mg). White solid. **Mp**: 45.5-46.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 – 7.57 (m, 4H), 7.40 – 7.31 (m, 11H), 7.29 – 7.25 (m, 2H), 6.94 – 6.88 (m, 2H), 5.31 (d, *J* = 15.3 Hz, 1H), 4.39 – 4.27 (m, 3H), 4.00 – 3.92 (m, 1H), 3.25 – 3.17 (m, 3H), 3.09 (dd, *J* = 10.5, 2.7 Hz, 1H), 2.96 (t, *J* = 7.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.7, 161.5, 156.0, 137.3, 132.4, 129.0, 128.9, 128.8, 128.7, 128.6, 128.6, 128.2, 127.9, 127.8, 127.6, 126.5, 122.9, 62.4, 59.7, 49.3, 31.0, 23.7, 23.4. **^{77}Se NMR** (76

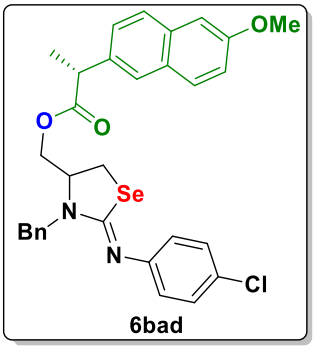
MHz, $CDCl_3$) δ 262.1. **IR (ATR)**: ν = 3059, 3027, 2949, 2920, 1738, 1612, 1485, 1434, 1387, 1355, 1214, 1153, 1087, 1056, 1025, 1008 cm^{-1}; **HRMS** (ESI): calcd. for $C_{35}H_{30}ClN_3O_3Se$ $[M+H]^+$: 656.1219, found: 656.1214.



6bac

(Z)-(3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methyl 2-(4-isobutylphenyl)propanoate (6bac)

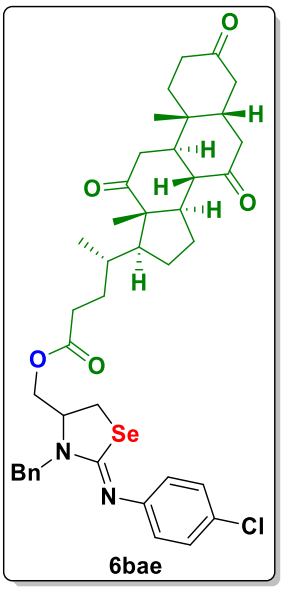
Yield = 96% (81.4 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 – 7.17 (m, 7H), 7.17 – 7.13 (m, 2H), 7.12 – 7.04 (m, 2H), 6.89 – 6.81 (m, 2H), 5.28 – 5.16 (m, 1H), 4.28 – 4.09 (m, 3H), 3.90 – 3.76 (m, 1H), 3.68 (q, *J* = 7.2 Hz, 1H), 3.16 – 3.02 (m, 1H), 2.90 – 2.79 (m, 1H), 2.45 – 2.40 (m, 2H), 1.85 – 1.79 (m, 1H), 1.48 (dd, *J* = 7.2, 2.4 Hz, 3H), 0.89 – 0.85 (m, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.4, 151.8, 140.9, 137.4, 129.5, 129.0, 128.7, 127.8, 127.8, 127.6, 127.17, 127.15, 122.9, 62.8, 62.6, 59.7, 59.6, 49.4, 49.3, 45.1, 45.1, 45.0, 30.2, 23.5, 22.4, 18.3. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 262.4. **IR (ATR)**: ν = 2952, 2928, 1736, 1613, 1583, 1486, 1453, 1152, 1088 cm^{-1}; **HRMS** (ESI): calcd. for $C_{30}H_{33}ClN_2O_2Se$ $[M+H]^+$: 569.1474, found: 569.1475.



6bad

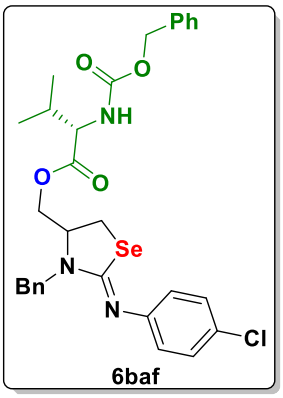
((Z)-3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methyl (2S)-2-(6-methoxynaphthalen-2-yl)propanoate (6bad)

Yield = 88% (77.8 mg). White solid. **Mp**: 44.2-45.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.61 (m, 3H), 7.37 – 7.09 (m, 10H), 6.88 – 6.78 (m, 2H), 5.26 – 5.14 (m, 1H), 4.26 – 4.13 (m, 3H), 3.88 (d, *J* = 1.0 Hz, 3H), 3.87 – 3.78 (m, 2H), 3.14 – 3.03 (m, 1H), 2.89 – 2.80 (m, 1H), 1.57 (dd, *J* = 7.1, 1.9 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.3, 157.8, 155.9, 151.8, 137.3, 129.3, 129.0, 128.7, 128.7, 128.6, 127.8, 127.7, 127.5, 127.5, 127.4, 127.4, 126.1, 126.0, 122.9, 119.3, 119.2, 105.7, 63.1, 62.8, 59.7, 59.6, 55.4, 49.3, 49.2, 45.4, 23.6, 23.5, 18.4, 18.4. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.3. **IR (ATR)**: ν = 2931, 1732, 1605, 1484, 1452, 1391, 1215, 1145, 1087, 1028 cm^{-1}; **HRMS** (ESI): calcd. for $C_{31}H_{29}ClN_2O_3Se$ $[M+H]^+$: 593.1110, found: 593.1123.



((Z)-3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methyl (4R)-4-((5R,8S,9R,10R,13S,17S)-10,13-dimethyl-3,7,12-trioxohexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanoate (6bae)

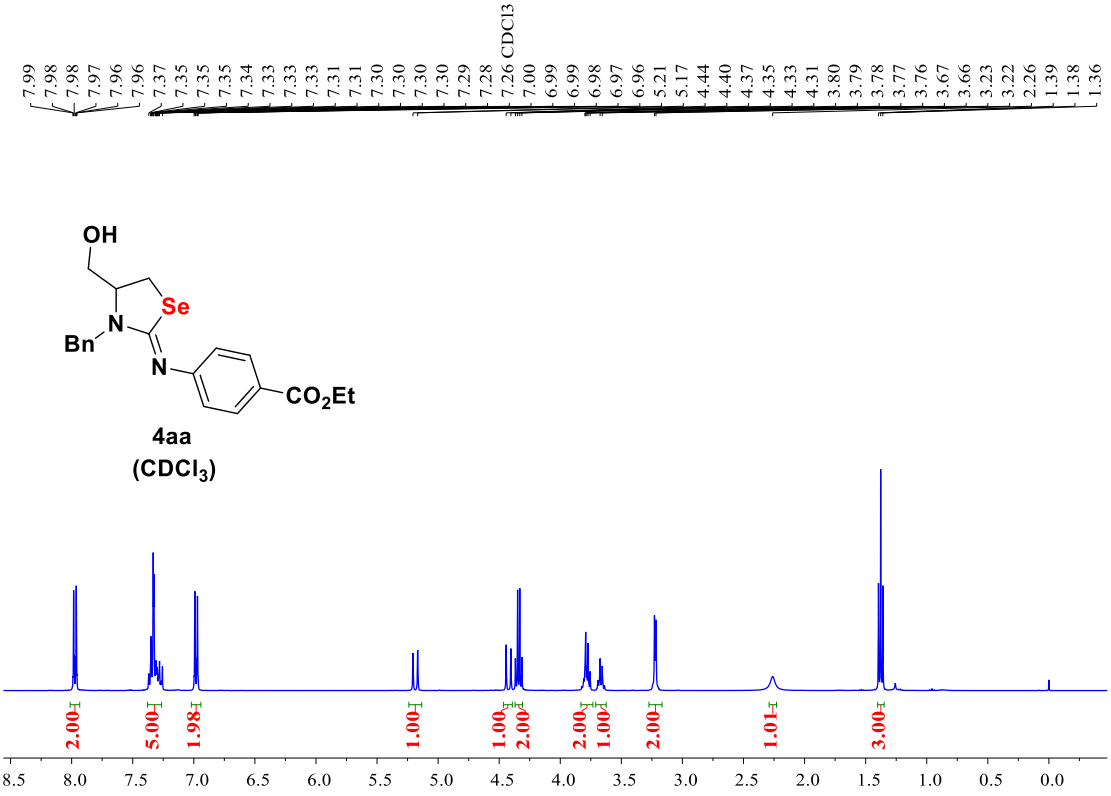
Yield = 87% (99.2 mg). Pale yellow solid. **Mp**: 92.6-94.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 – 7.28 (m, 5H), 7.26 – 7.20 (m, 2H), 6.91 – 6.83 (m, 2H), 5.31 (dd, *J* = 15.3, 2.2 Hz, 1H), 4.31 (d, *J* = 15.4 Hz, 1H), 4.27 – 4.17 (m, 2H), 3.96 – 3.89 (m, 1H), 3.31 – 3.24 (m, 1H), 3.13 – 3.06 (m, 1H), 2.93 – 2.80 (m, 3H), 2.44 – 2.21 (m, 8H), 2.20 – 2.17 (m, 1H), 2.16 – 2.08 (m, 2H), 2.05 – 1.94 (m, 4H), 1.86 – 1.77 (m, 2H), 1.71 – 1.64 (m, 1H), 1.39 (s, 3H), 1.33 – 1.23 (m, 4H), 1.05 (s, 3H), 0.84 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 212.0, 209.1, 208.7, 173.7, 137.3, 129.0, 128.7, 127.8, 127.6, 122.9, 59.7, 56.9, 51.8, 49.3, 48.9, 46.8, 45.5, 45.0, 42.8, 38.6, 36.5, 36.0, 35.5, 35.2, 33.9, 31.2, 30.3, 27.7, 25.1, 24.9, 23.8, 21.9, 18.7, 11.8. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 263.3. **IR (ATR)**: ν = 2931, 1705, 1614, 1486, 1433, 1384, 1187, 1144, 1089, 1008 cm^{-1}; **HRMS** (ES): calcd. for $C_{41}H_{49}ClN_2O_5Se$ $[M+H]^+$: 765.2573, found: 765.2575.

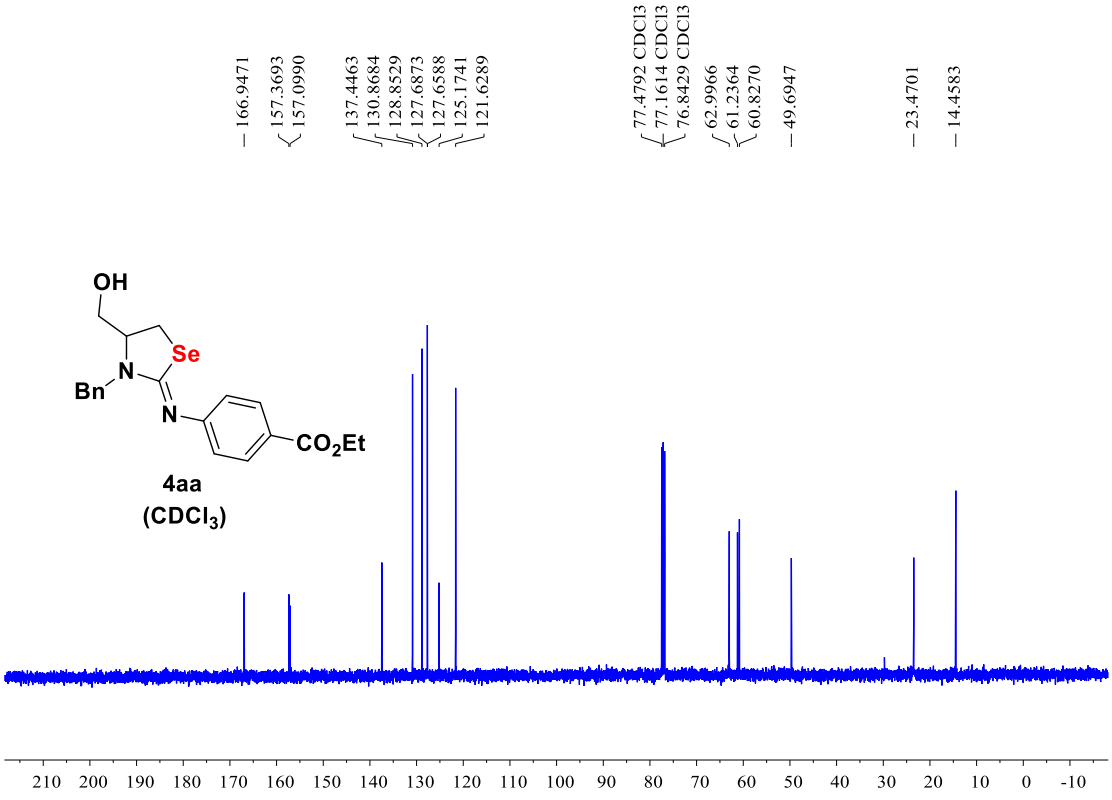


((Z)-3-benzyl-2-((4-chlorophenyl)imino)-1,3-selenazolidin-4-yl)methyl ((benzyloxy)carbonyl)-D-valinate (6baf)

Yield = 84% (77.5 mg). Colorless oil liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.27 (m, 10H), 7.25 – 7.21 (m, 2H), 6.89 – 6.84 (m, 2H), 5.34 – 5.21 (m, 2H), 5.10 (s, 2H), 4.33 – 4.19 (m, 4H), 4.01 – 3.83 (m, 1H), 3.30 – 3.16 (m, 1H), 3.09 – 2.96 (m, 1H), 2.16 – 2.10 (m, 1H), 0.98 – 0.94 (m, 3H), 0.88 (t, *J* = 6.3 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.3, 151.7, 136.2, 129.1, 128.8, 128.7, 128.6, 128.3, 128.2, 127.9, 127.8, 127.7, 122.9, 67.2, 62.8, 59.6, 59.5, 59.2, 49.4, 49.3, 31.2, 31.1, 23.7, 19.1, 17.6. **^{77}Se NMR** (76 MHz, $CDCl_3$) δ 261.9. **IR (ATR)**: ν = 3342, 2961, 2928, 1715, 1612, 1582, 1485, 1213, 1183, 1157, 1088, 1026, 1009 cm^{-1}; **HRMS** (ESI): calcd. for $C_{30}H_{32}ClN_3O_4Se$ $[M+H]^+$: 614.1325, found: 614.1301.

9. Copies of ^{1}H NMR, ^{13}C NMR, ^{77}Se NMR and ^{19}F NMR Spectra for Compounds

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77.1614 CDCl3
76.8429 CDCl3
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Bn
N
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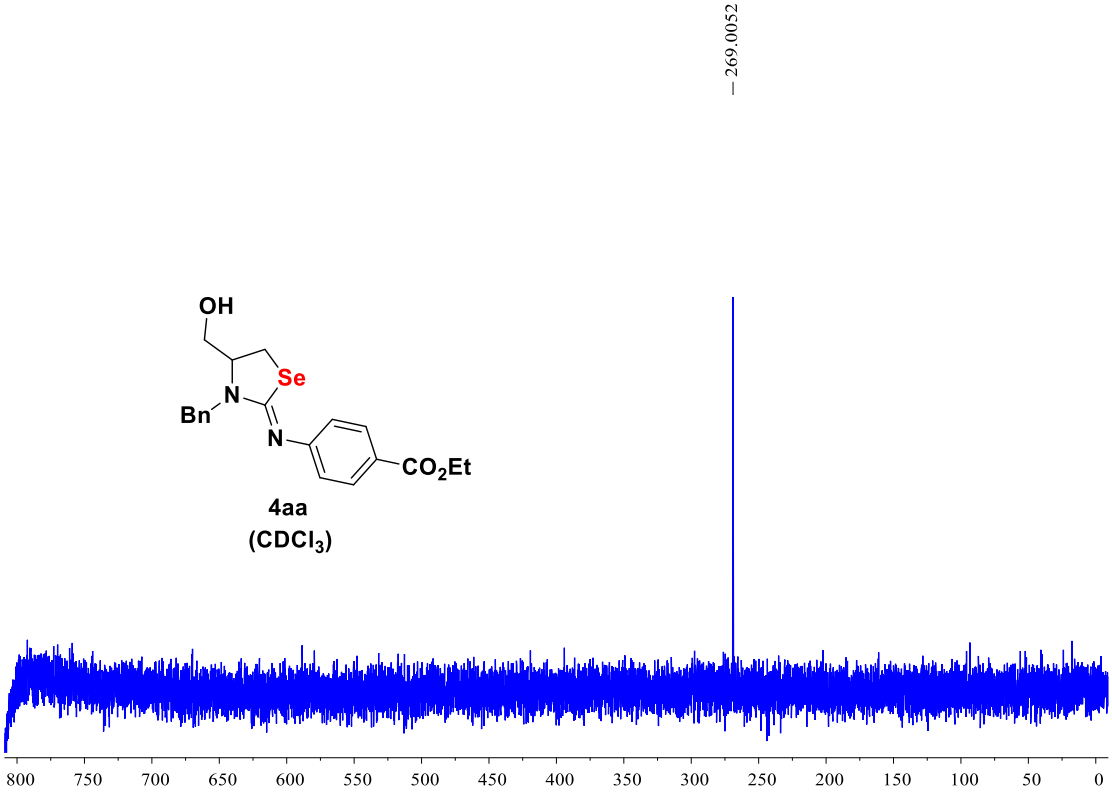
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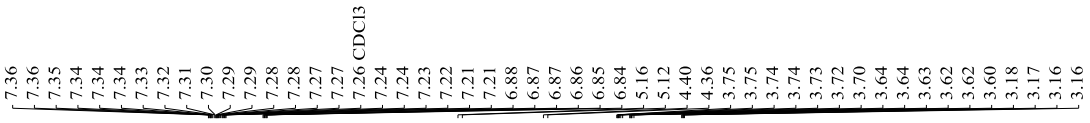
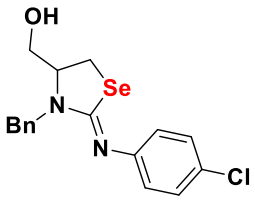
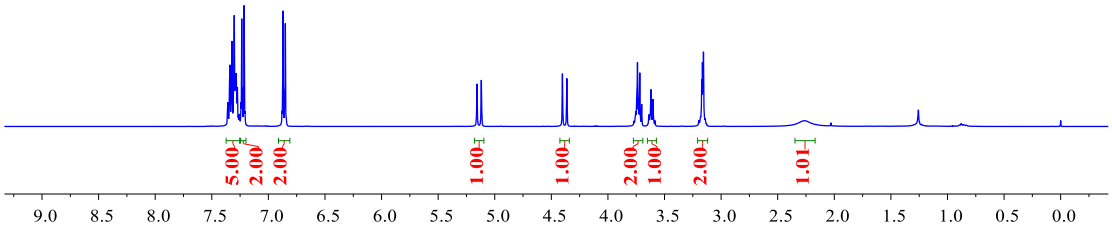
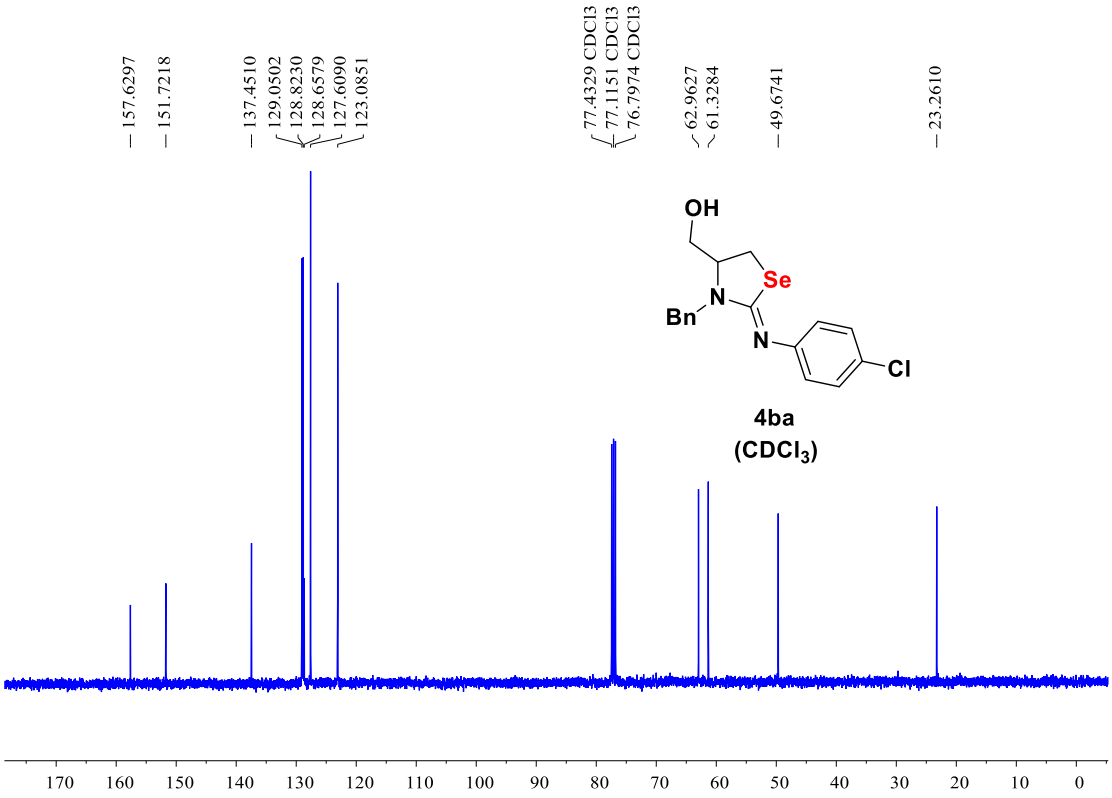


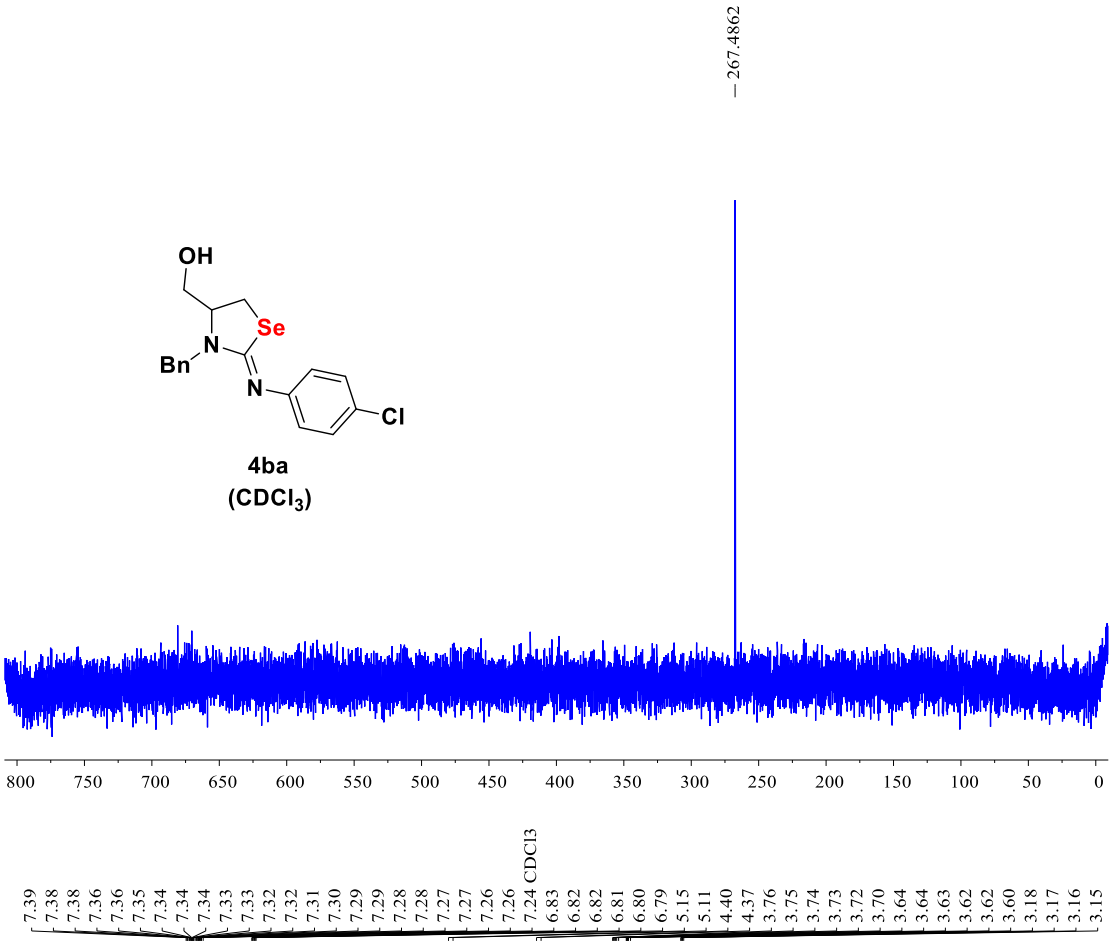


4ba
($CDCl_3$)





4ba
($CDCl_3$)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Se
Bn
N
N
Cl
4ba
(CDCl3)
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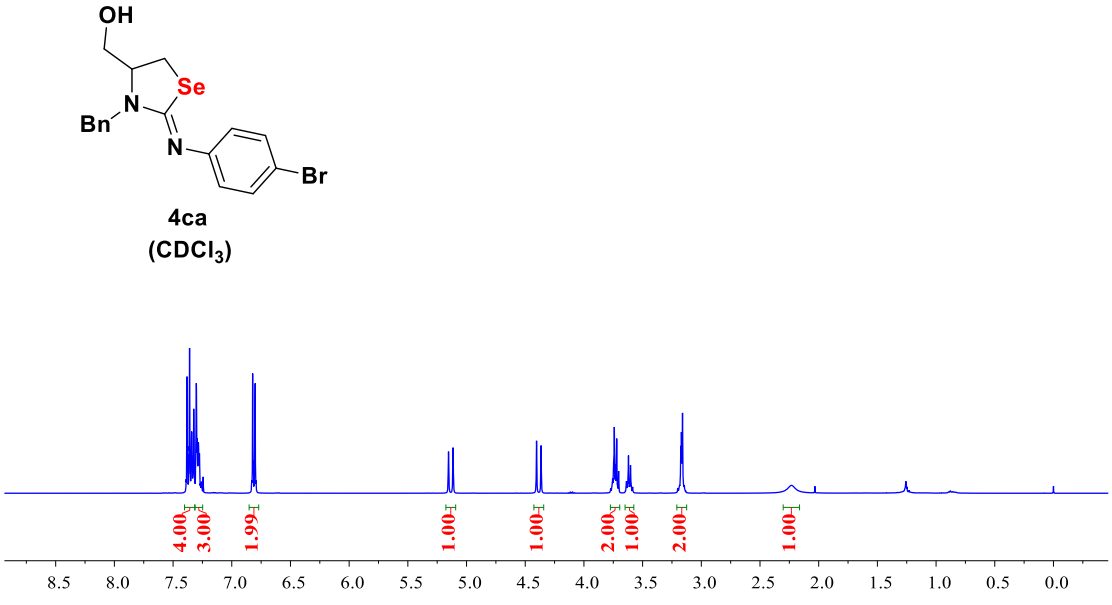
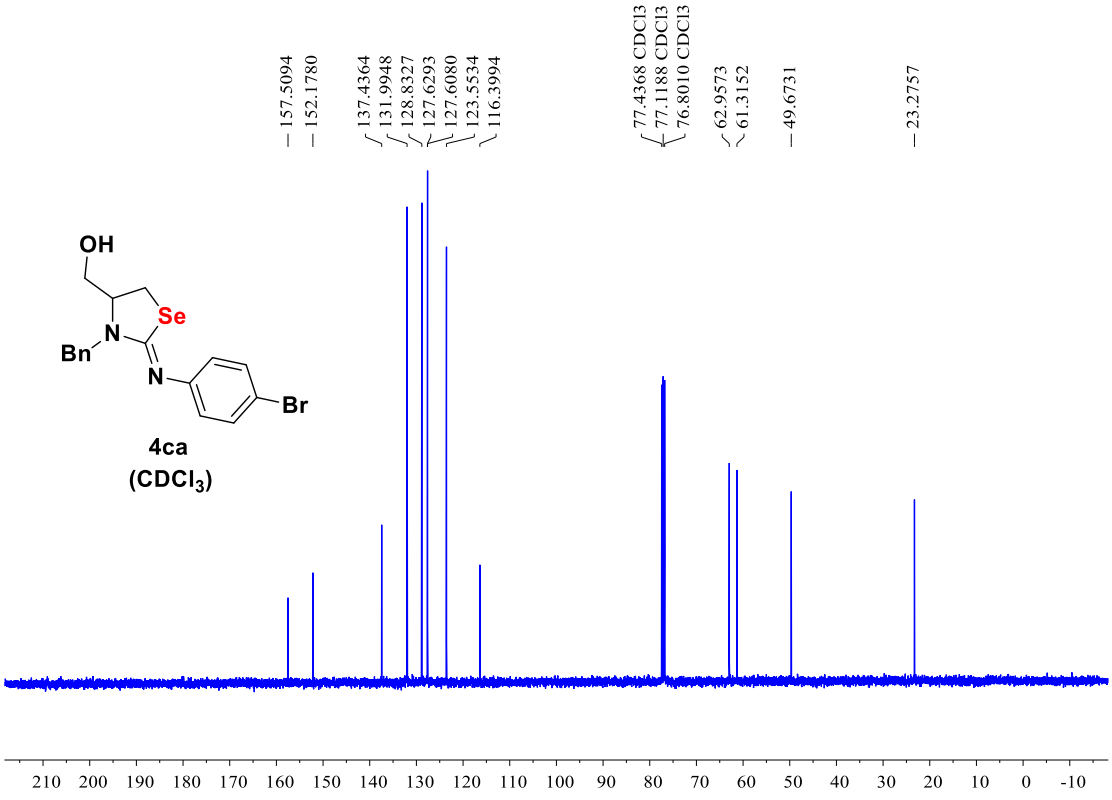

OH
Se
Bn
N
N
Br
4ca
(CDCl3)
4.00 3.00 1.99 1.00 1.00 2.00 1.00 2.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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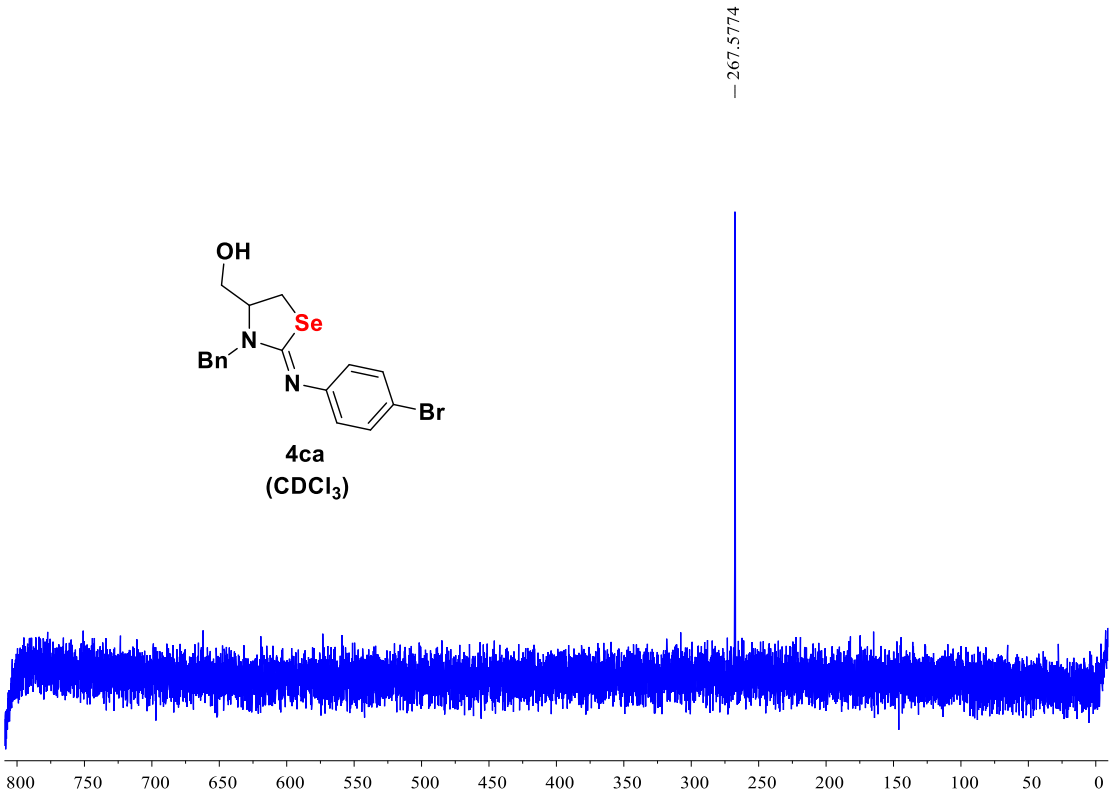
137.4364
131.9948
128.8327
127.6293
127.6080
123.5534
116.3994
77.4368 CDCl3
77.1188 CDCl3
76.8010 CDCl3
62.9573
61.3152
49.6731
23.2757
OH
Se
N
Bn
N
Br
4ca
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Bn
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Br
4ca
(CDCl3)
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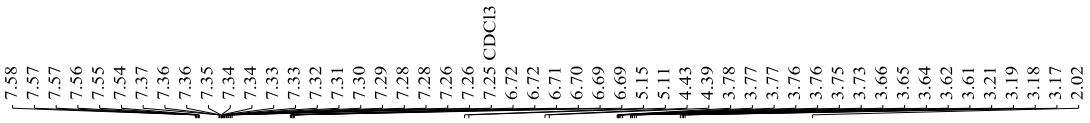
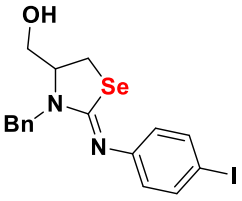
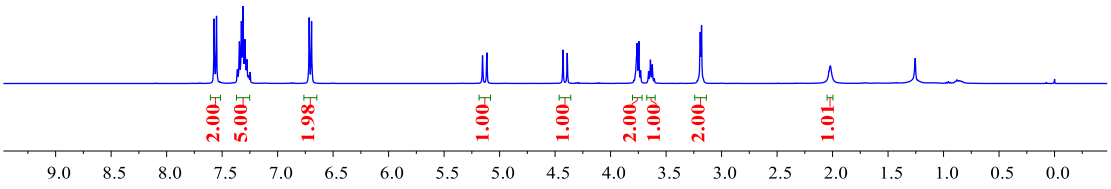
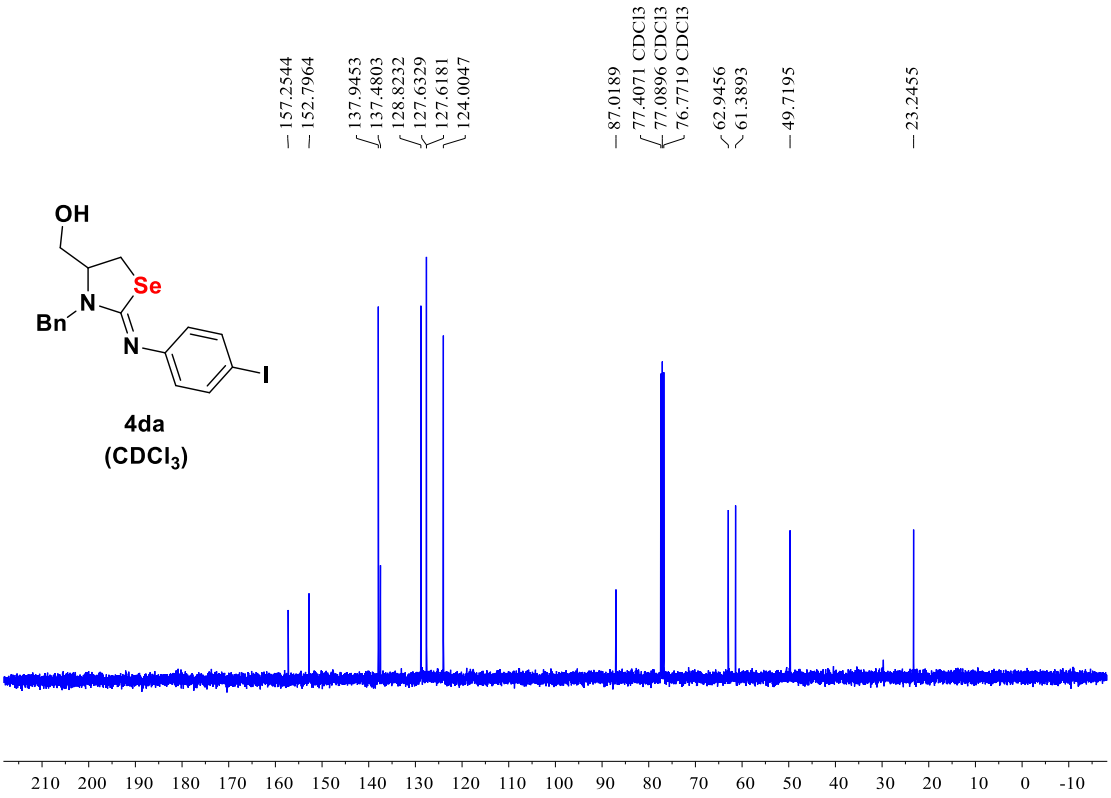




4da
($CDCl_3$)





4da
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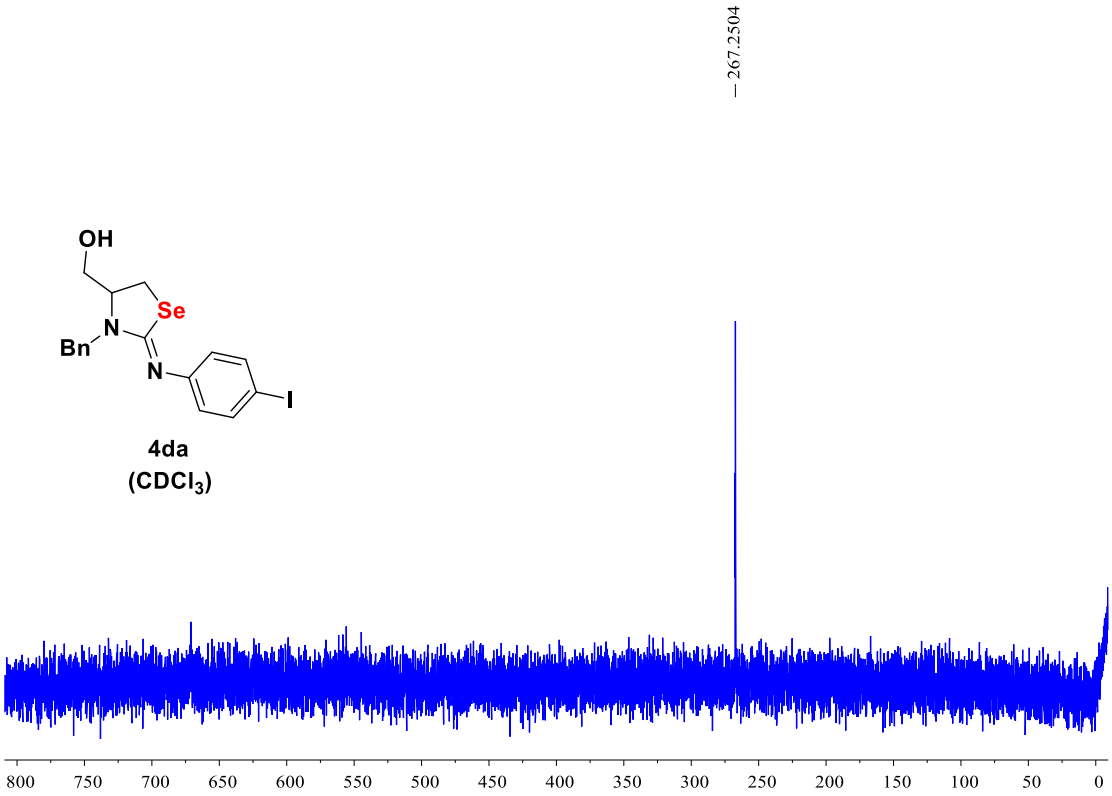
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Se
N
Bn
N
I
4da
(CDCl3)
267.2504
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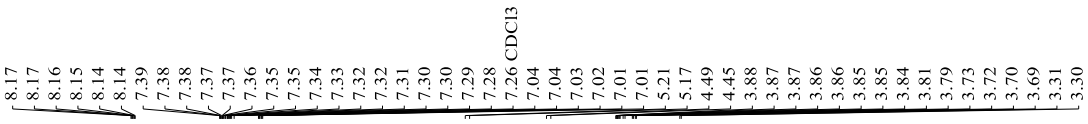
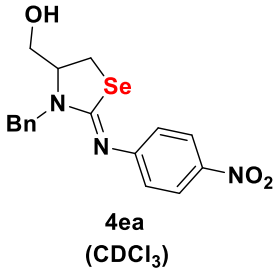

8.17 8.17 8.16 8.15 8.14 8.14 7.39 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.34 7.33 7.32 7.32 7.31 7.30 7.30 7.29 7.28 7.26 CDCl3 7.04 7.04 7.03 7.02 7.01 7.01 5.21 5.17 4.49 4.45 3.88 3.87 3.87 3.86 3.86 3.85 3.85 3.84 3.81 3.79 3.73 3.72 3.70 3.69 3.31 3.30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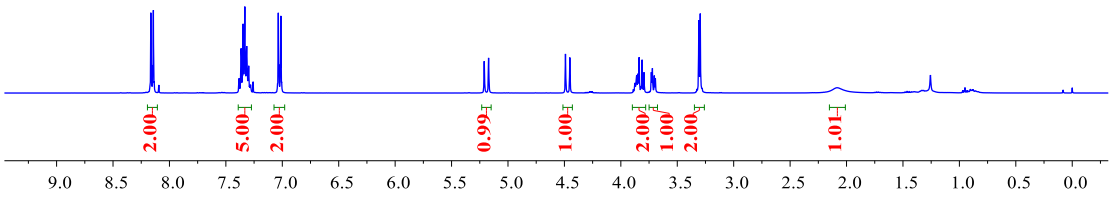
Se
N
Bn
N
NO2
4ea
(CDCl3)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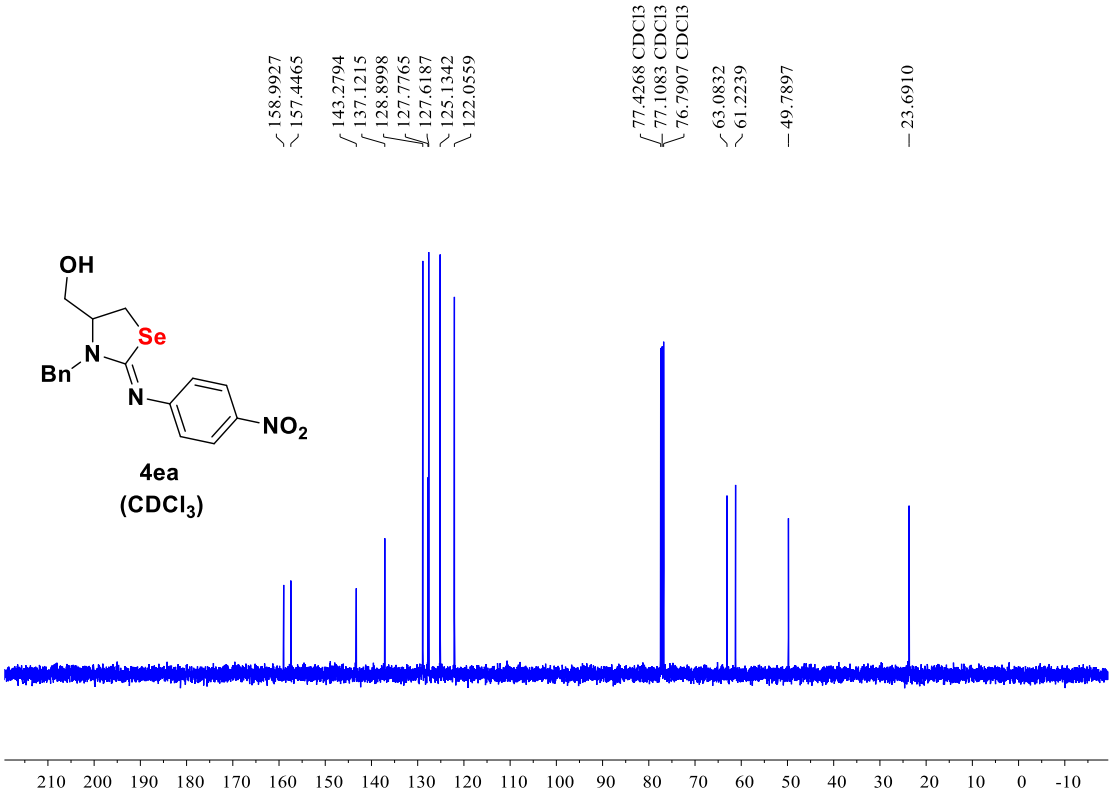
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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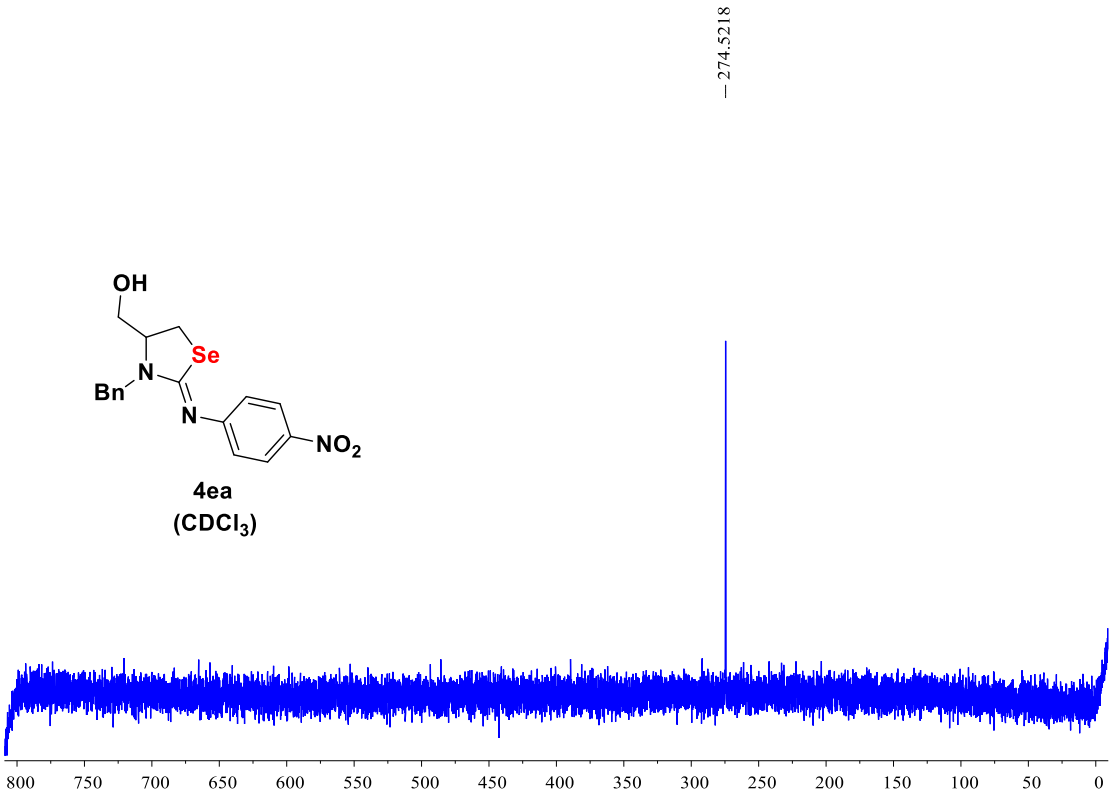
137.1215
128.8998
127.7765
127.6187
125.1342
122.0559
77.4268 CDCl3
77.1083 CDCl3
76.7907 CDCl3
63.0832
61.2239
49.7897
23.6910
OH
Se
N
Bn
N
NO2
4ea
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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N
Bn
N
NO2
4ea
(CDCl3)
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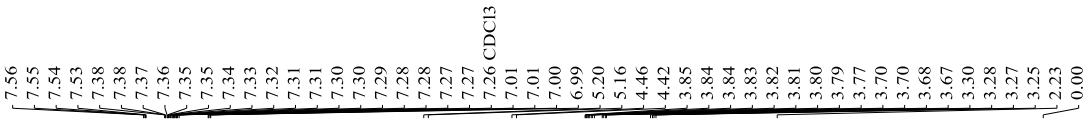
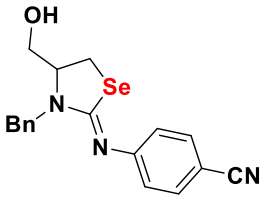
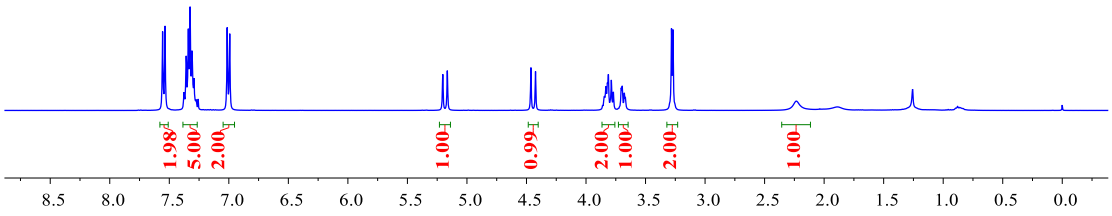
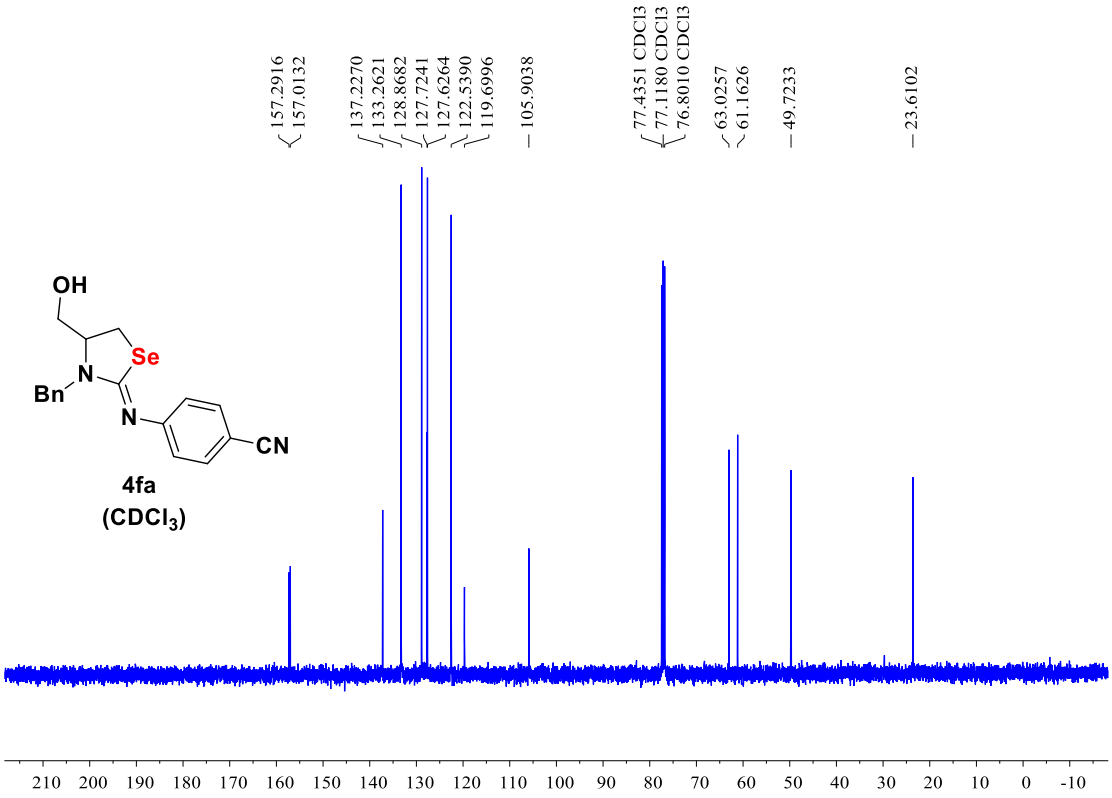


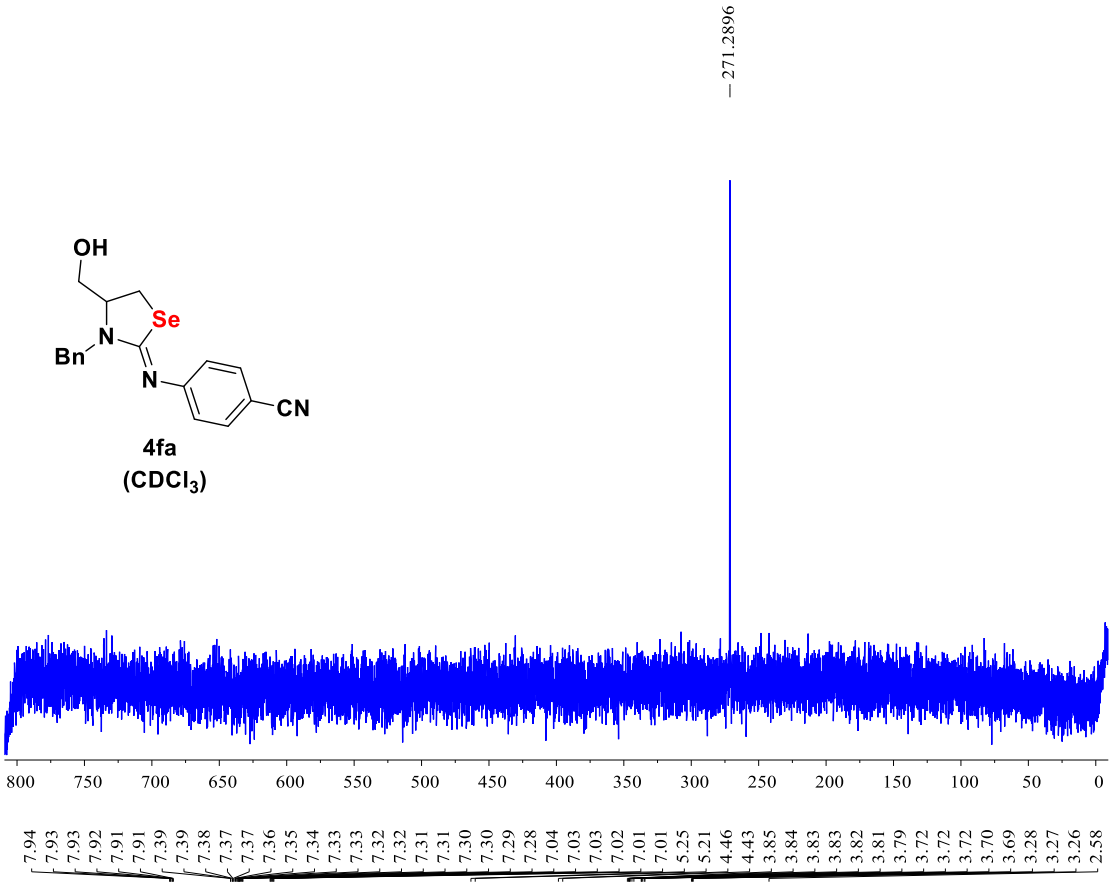


4fa
($CDCl_3$)





4fa
($CDCl_3$)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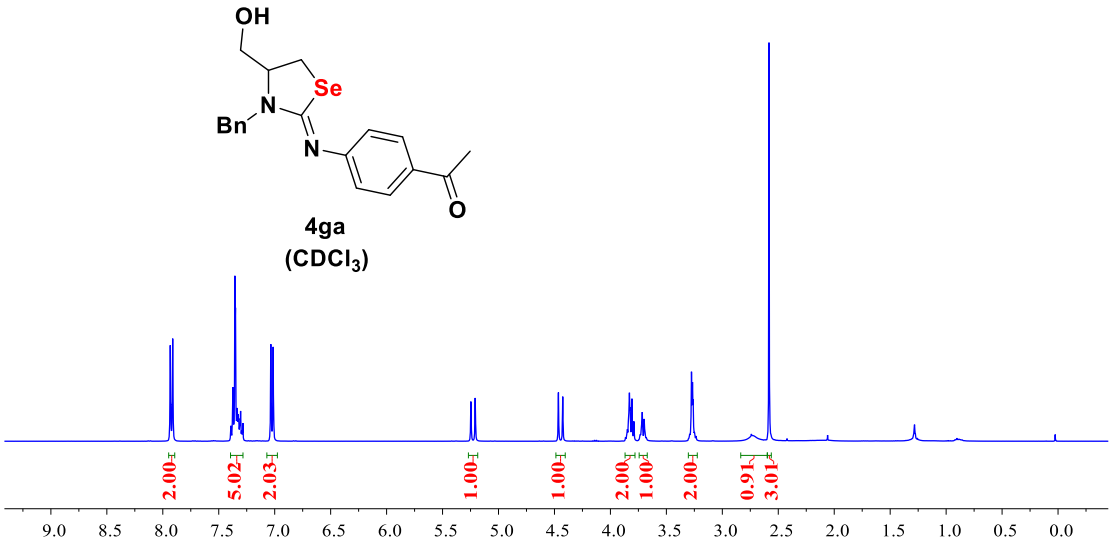
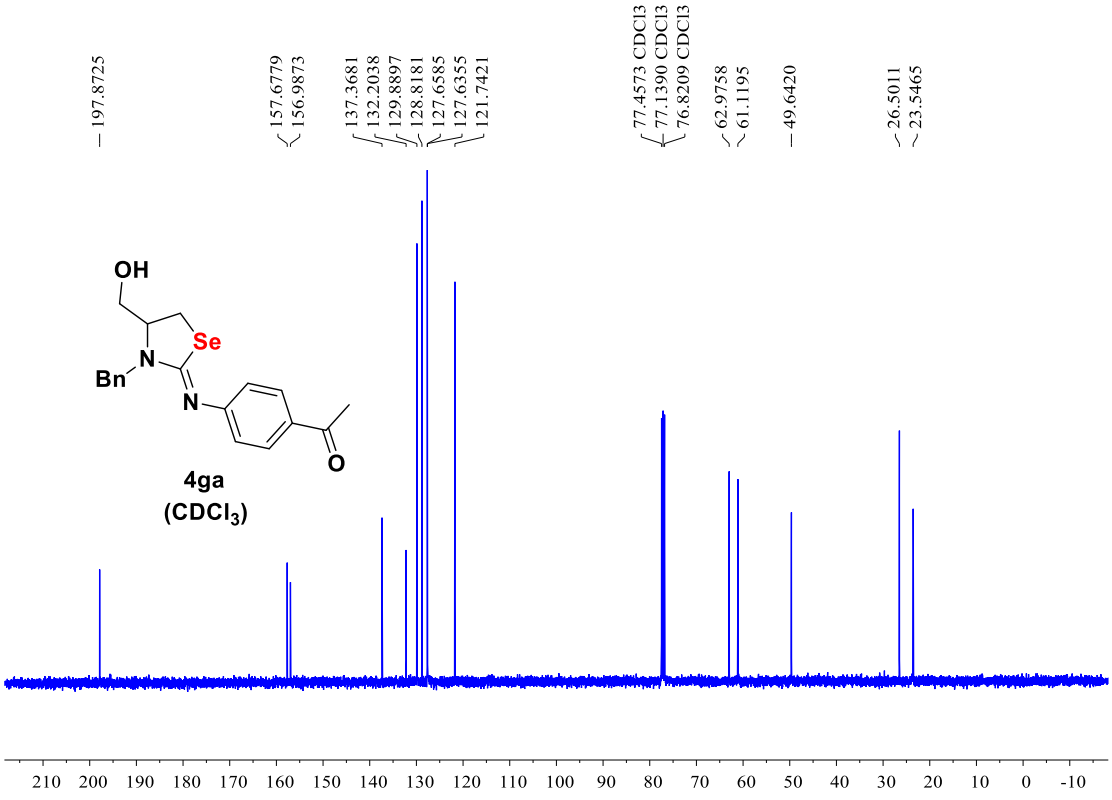
Bn
N
CN
4fa
(CDCl3)
800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0
7.94 7.93 7.93 7.92 7.91 7.91 7.39 7.39 7.38 7.37 7.37 7.36 7.35 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.04 7.03 7.03 7.02 7.01 7.01 5.25 5.21 4.46 4.43 3.85 3.84 3.83 3.83 3.82 3.81 3.79 3.72 3.72 3.72 3.70 3.69 3.28 3.27 3.26 2.58


OH
Se
N
Bn
N
O
4ga
(CDCl3)
2.00 5.02 2.03 1.00 1.00 2.00 1.00 2.00 0.91 3.01
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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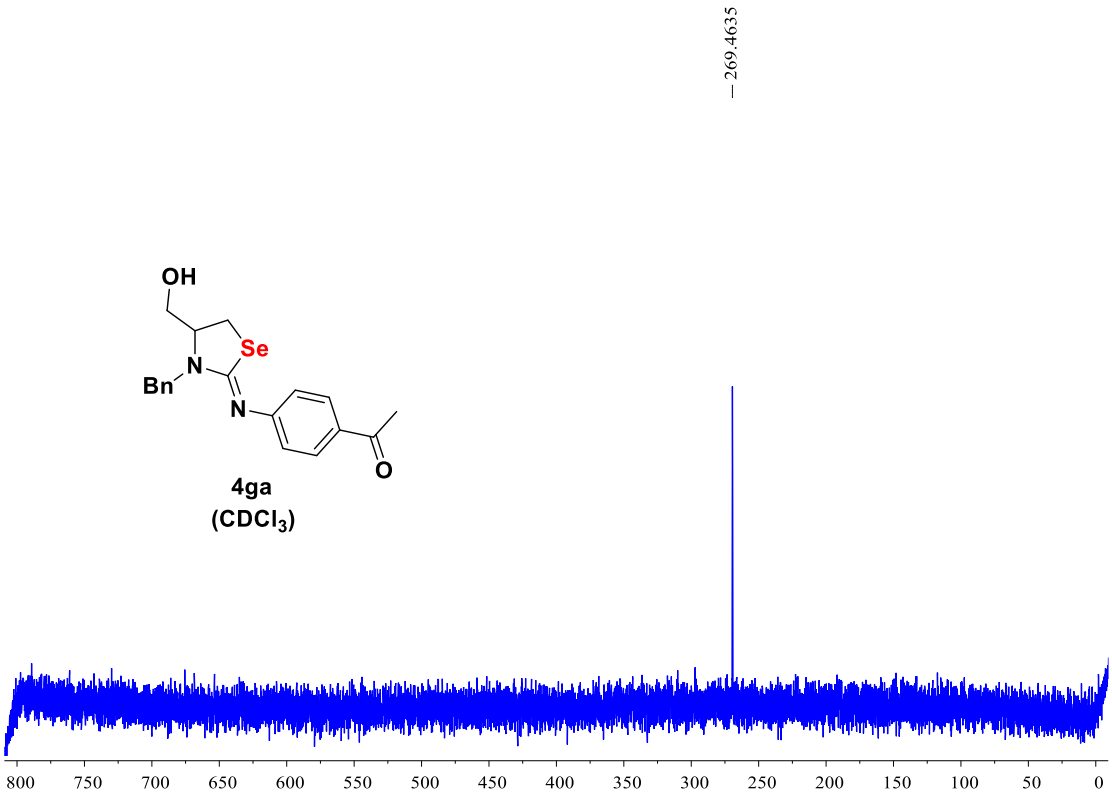
132.2038
129.8897
128.8181
127.6585
127.6355
121.7421
77.4573 CDCl3
77.1390 CDCl3
76.8209 CDCl3
62.9758
61.1195
49.6420
26.5011
23.5465
OH
Se
N
Bn
N
O
4ga
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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O
4ga
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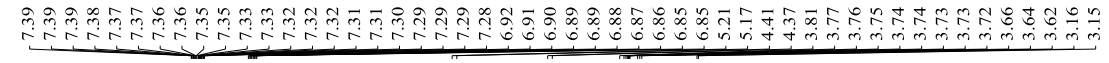
7.39
7.39
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7.37
7.36
7.36
7.35
7.35
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7.33
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7.32
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7.31
7.31
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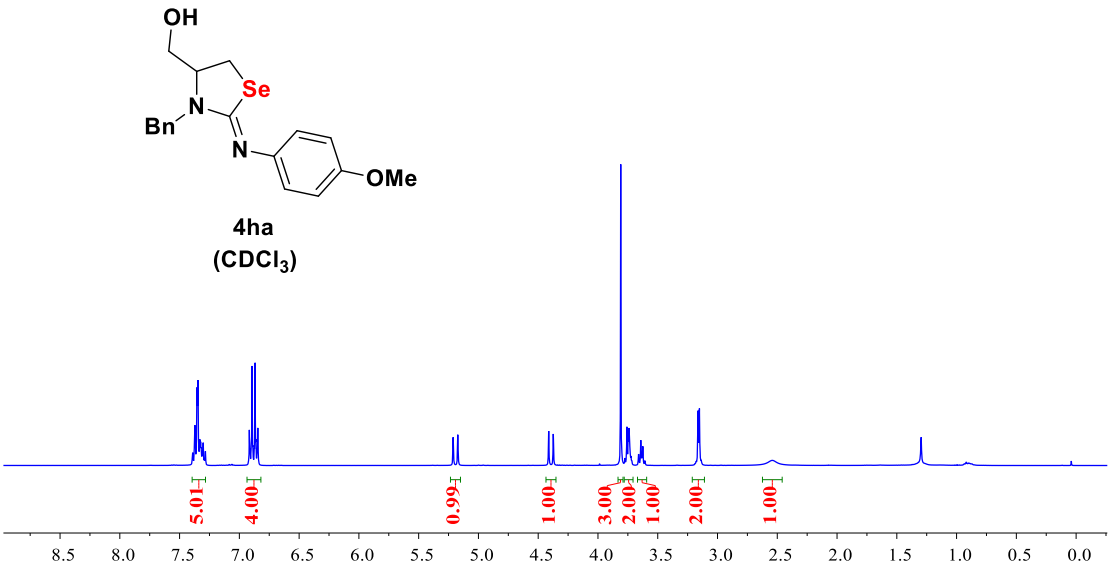
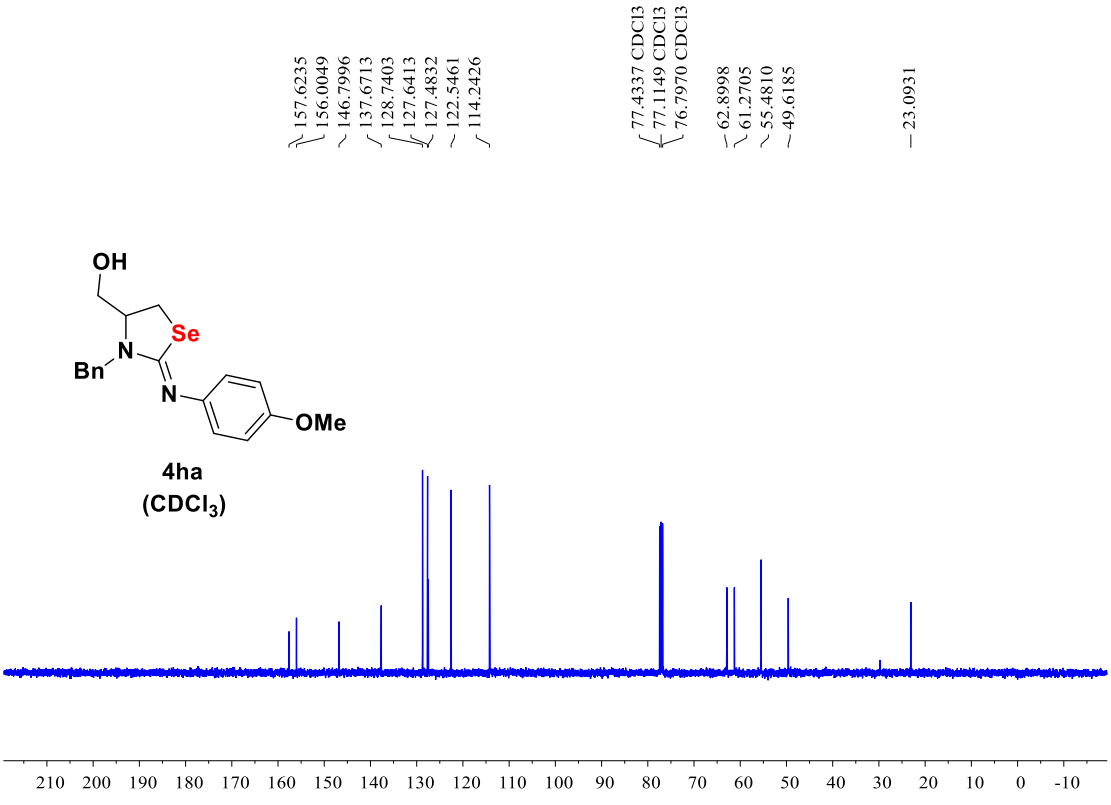
7.29
7.28
6.92
6.91
6.90
6.89
6.89
6.88
6.87
6.86
6.85
6.85
5.21
5.17
4.41
4.37
3.81
3.77
3.76
3.75
3.74
3.74
3.73
3.73
3.72
3.66
3.64
3.62
3.16
3.15


OH
Se
N
Bn
N
OMe
4ha
(CDCl3)
5.01
4.00
0.99
1.00
3.00
2.00
1.00
2.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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146.7996
137.6713
128.7403
127.6413
127.4832
122.5461
114.2426
77.4337 CDCl3
77.1149 CDCl3
76.7970 CDCl3
62.8998
61.2705
55.4810
49.6185
23.0931
OH
Se
N
Bn
N
OMe
4ha
(CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
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80
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60
50
40
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20
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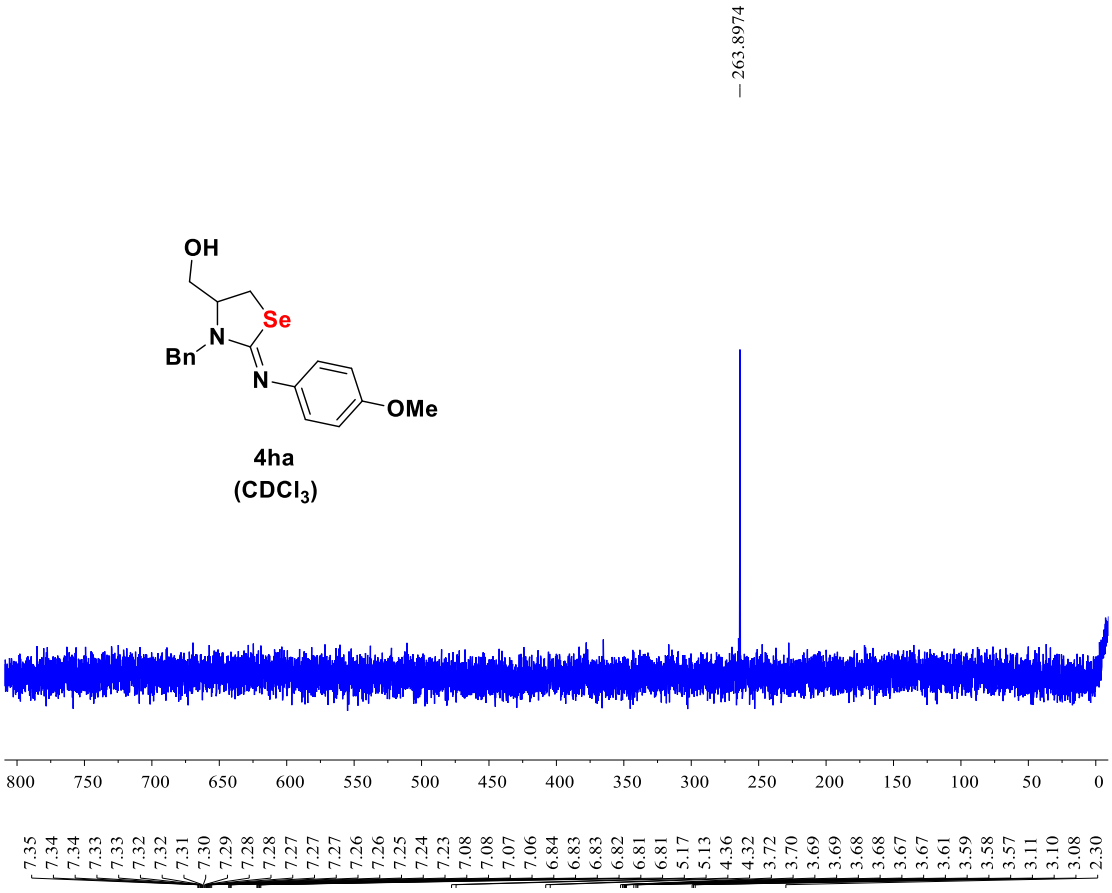
0
-10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N
Bn
N
OMe
4ha
(CDCl3)
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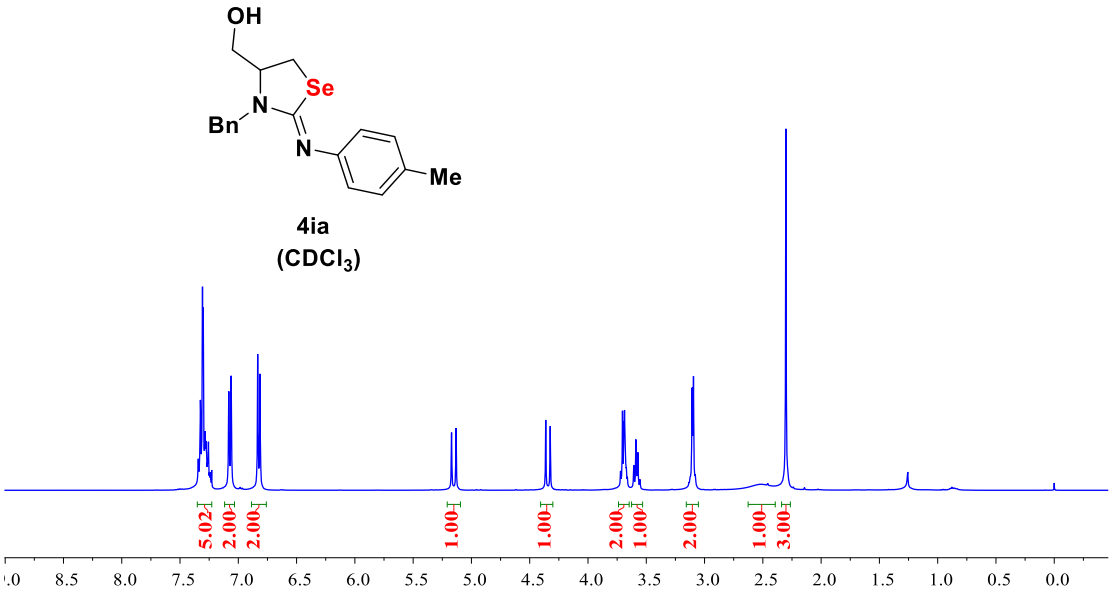
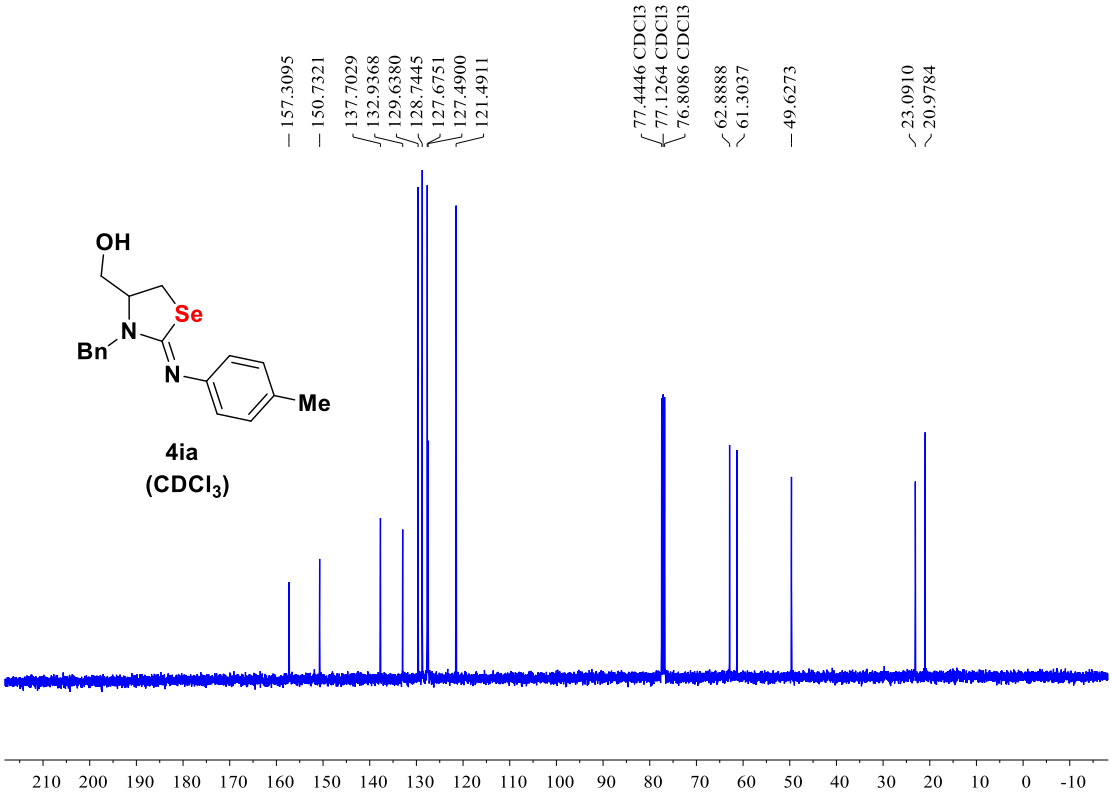
7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.27 7.27 7.26 7.26 7.25 7.24 7.23 7.08 7.08 7.07 7.06 6.84 6.83 6.83 6.82 6.81 6.81 5.17 5.13 4.36 4.32 3.72 3.70 3.69 3.69 3.68 3.68 3.67 3.67 3.61 3.59 3.58 3.57 3.11 3.10 3.08 2.30


OH
Se
N
Bn
N
Me
4ia
(CDCl3)
5.02
2.00
2.00
1.00
1.00
2.00
1.00
2.00
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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129.6380
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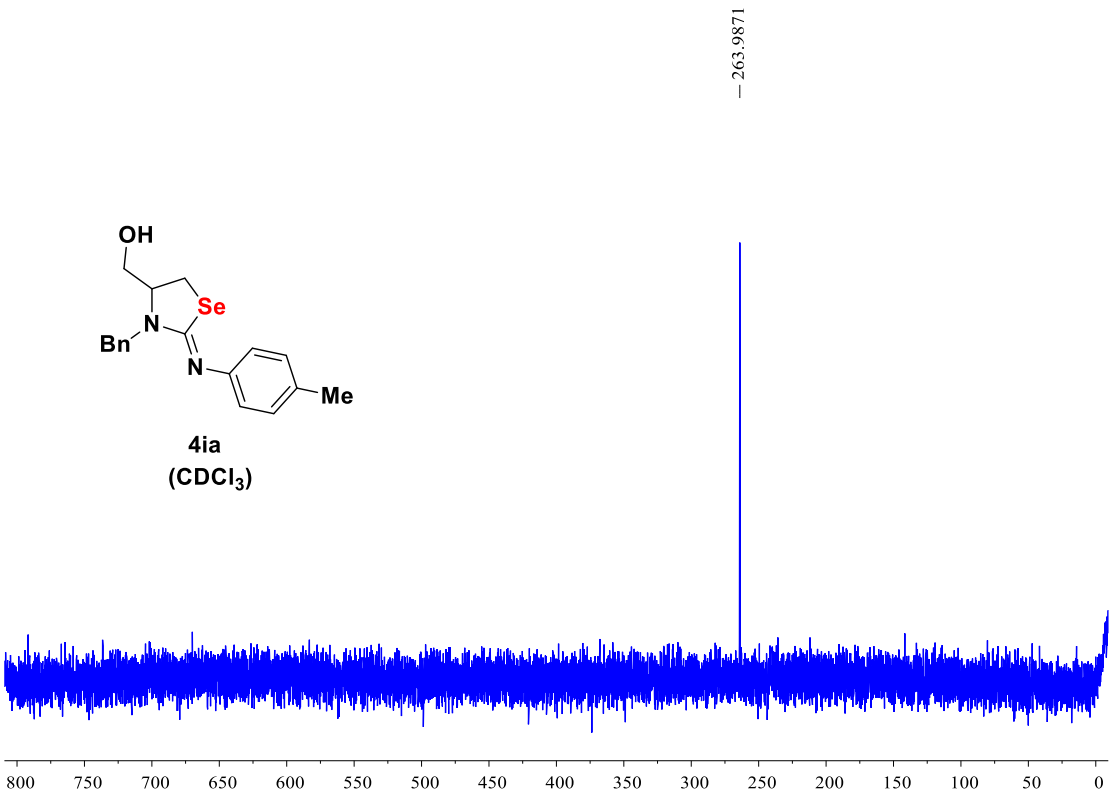
127.6751
127.4900
121.4911
77.4446 CDCl3
77.1264 CDCl3
76.8086 CDCl3
62.8888
61.3037
49.6273
23.0910
20.9784
OH
Se
N
Bn
N
Me
4ia
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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4ia
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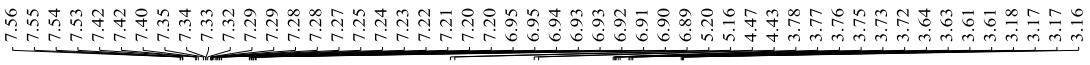
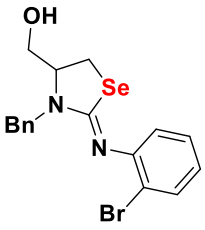
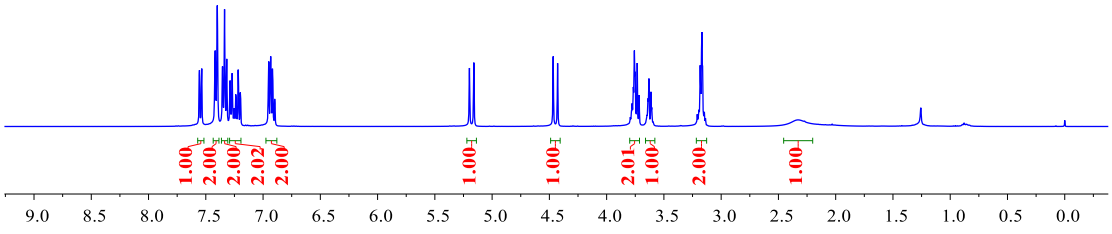
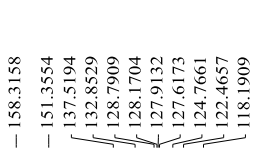




4ja

($CDCl_3$)





4ja

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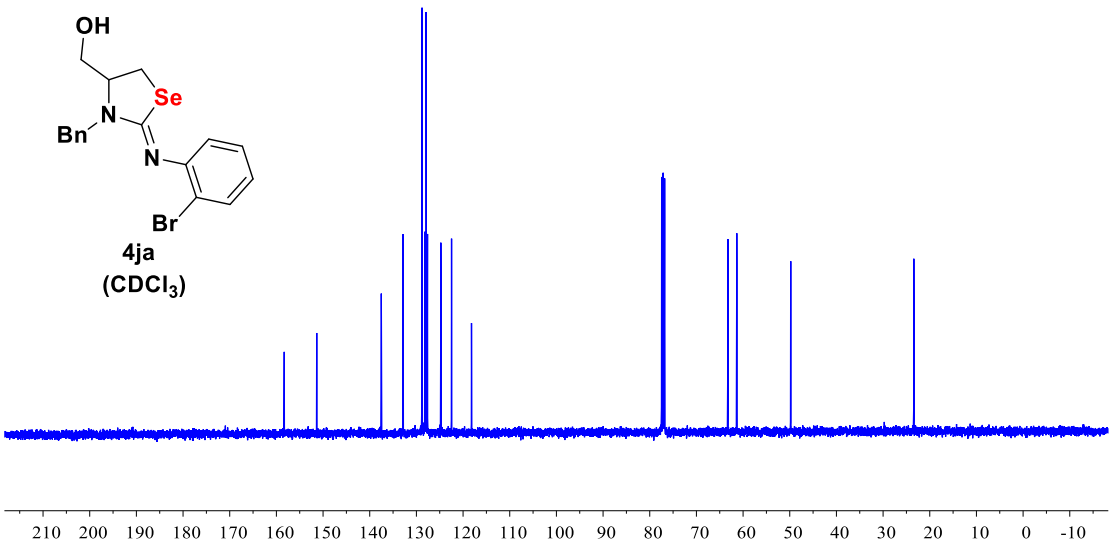

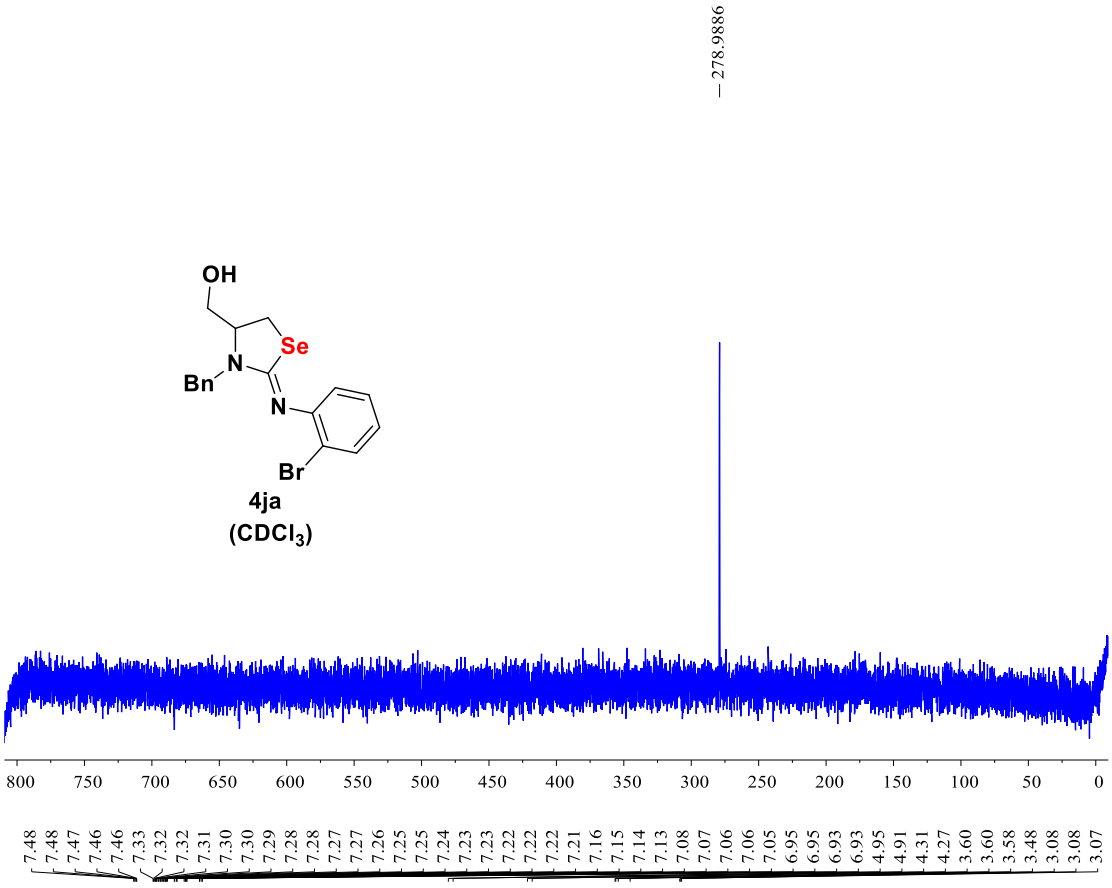
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Bn
N
Br
4ja
(CDCl3)
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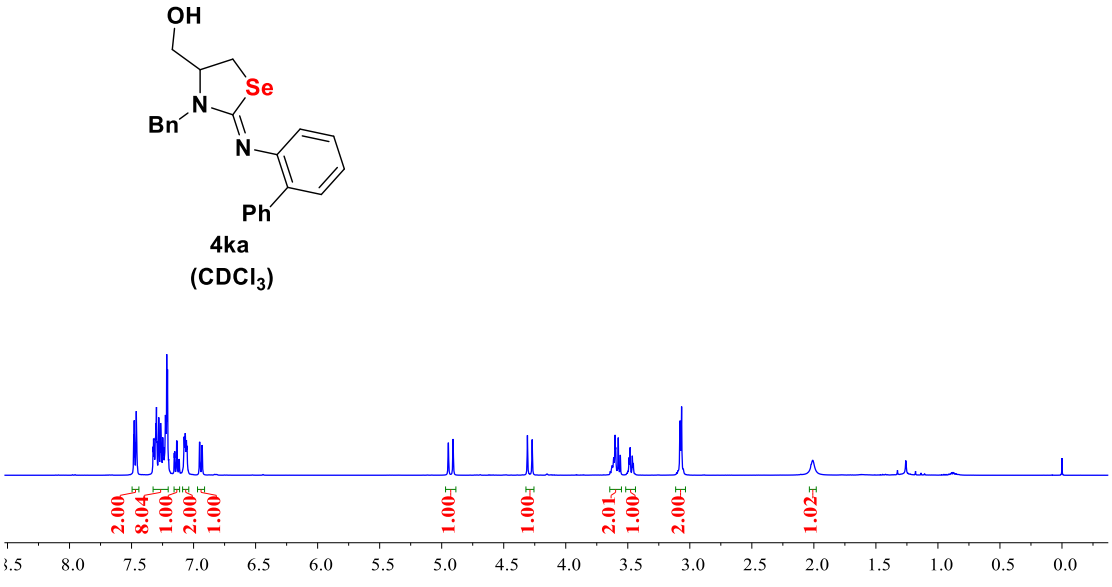
OH
Se
N
Bn
N
Ph
4ka
(CDCl3)
2.00 8.04 1.00 2.00 1.00 1.00 1.00 2.01 1.00 2.00 1.02
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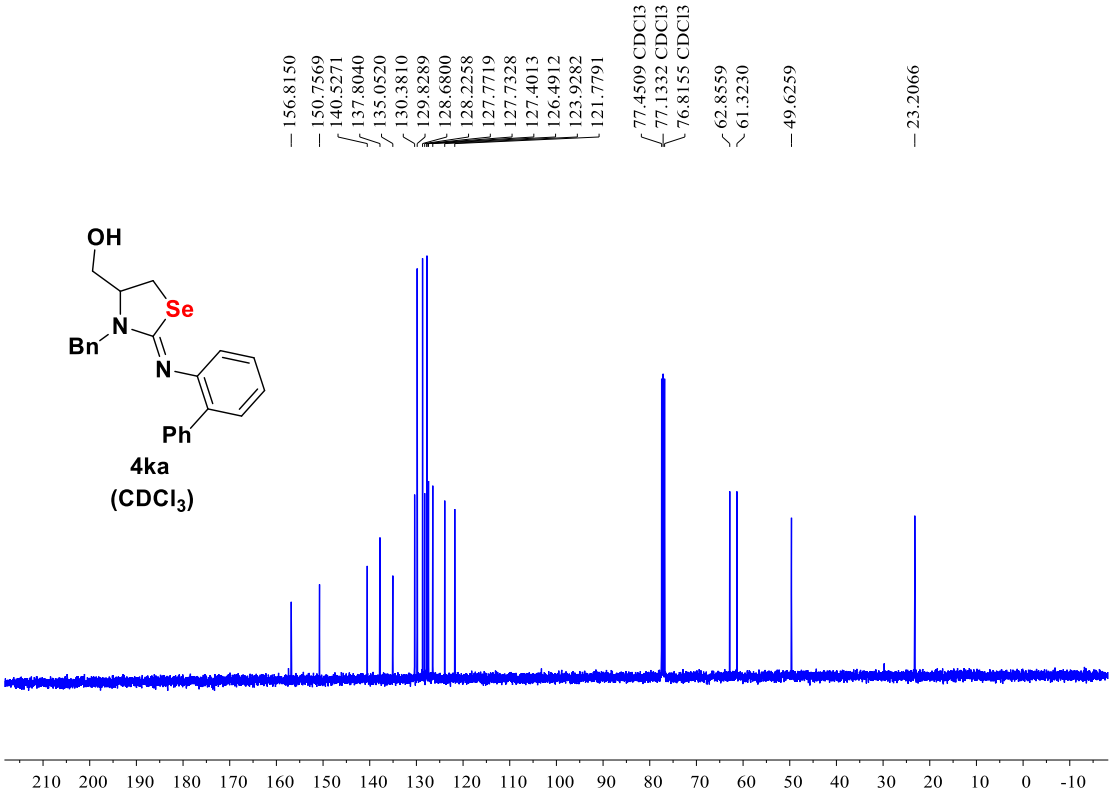
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130.3810
129.8289
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127.7328
127.4013
126.4912
123.9282
121.7791
77.4509 CDCl3
77.1332 CDCl3
76.8155 CDCl3
62.8559
61.3230
49.6259
23.2066
OH
Se
N
Bn
N
Ph
4ka
(CDCl3)
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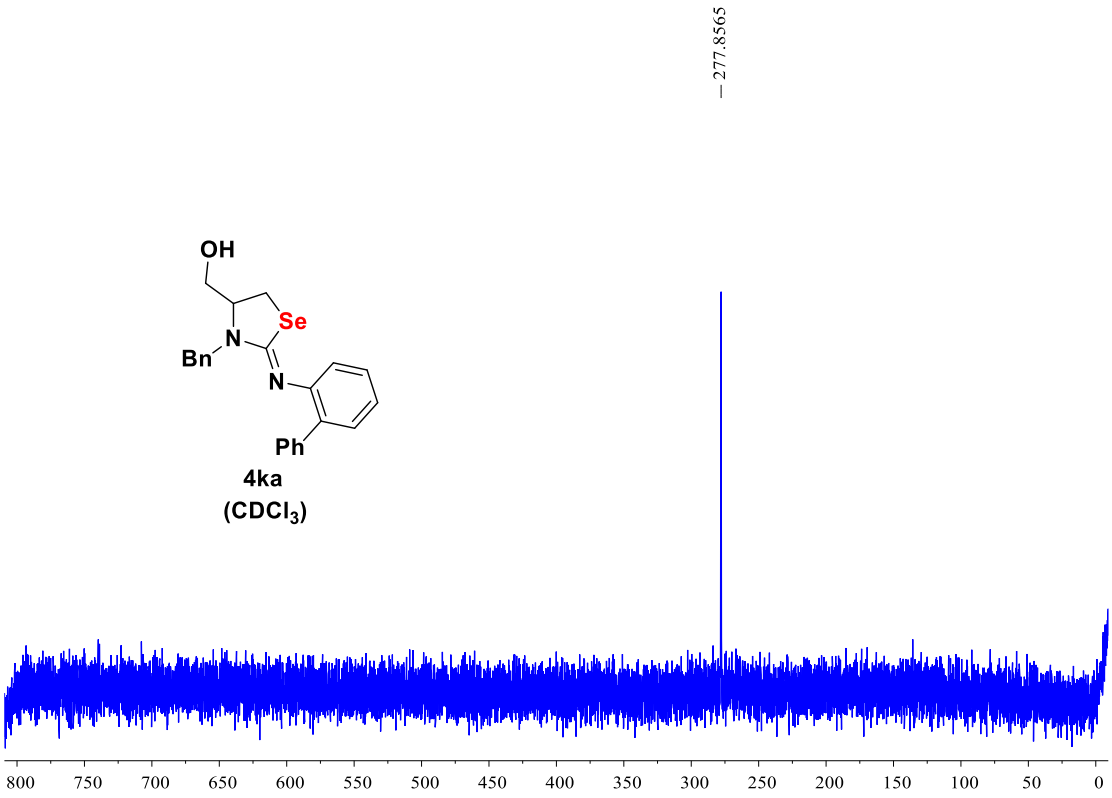
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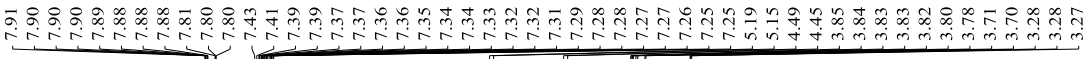
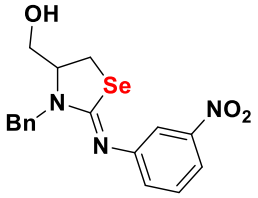
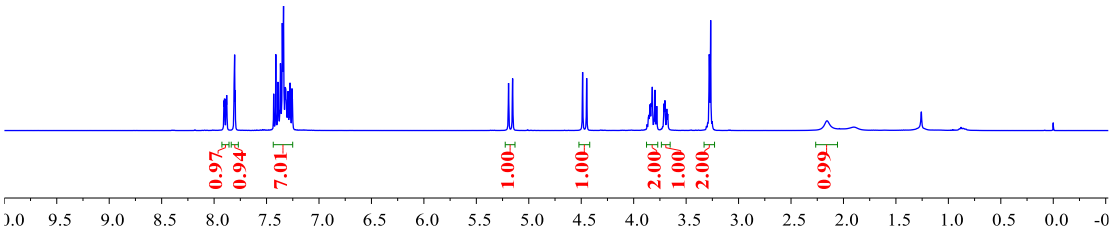
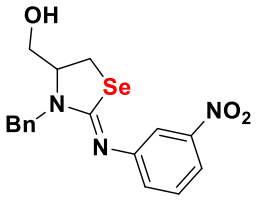




4la
($CDCl_3$)





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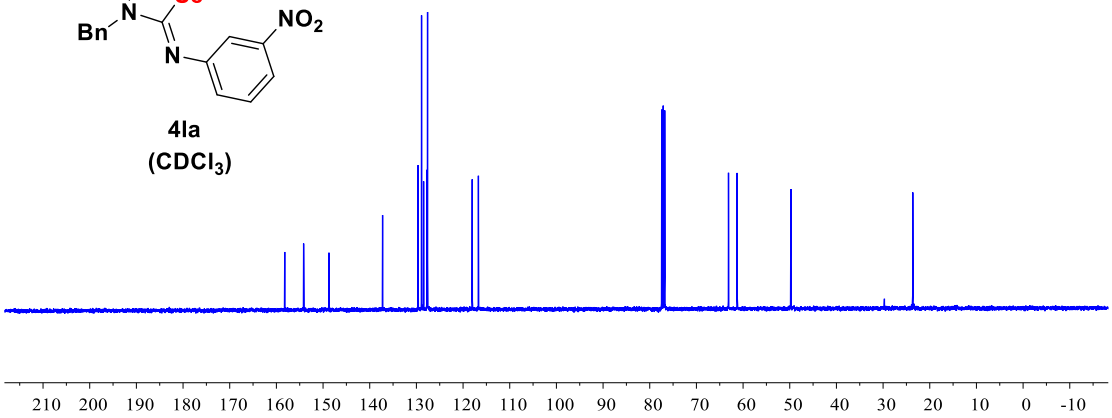

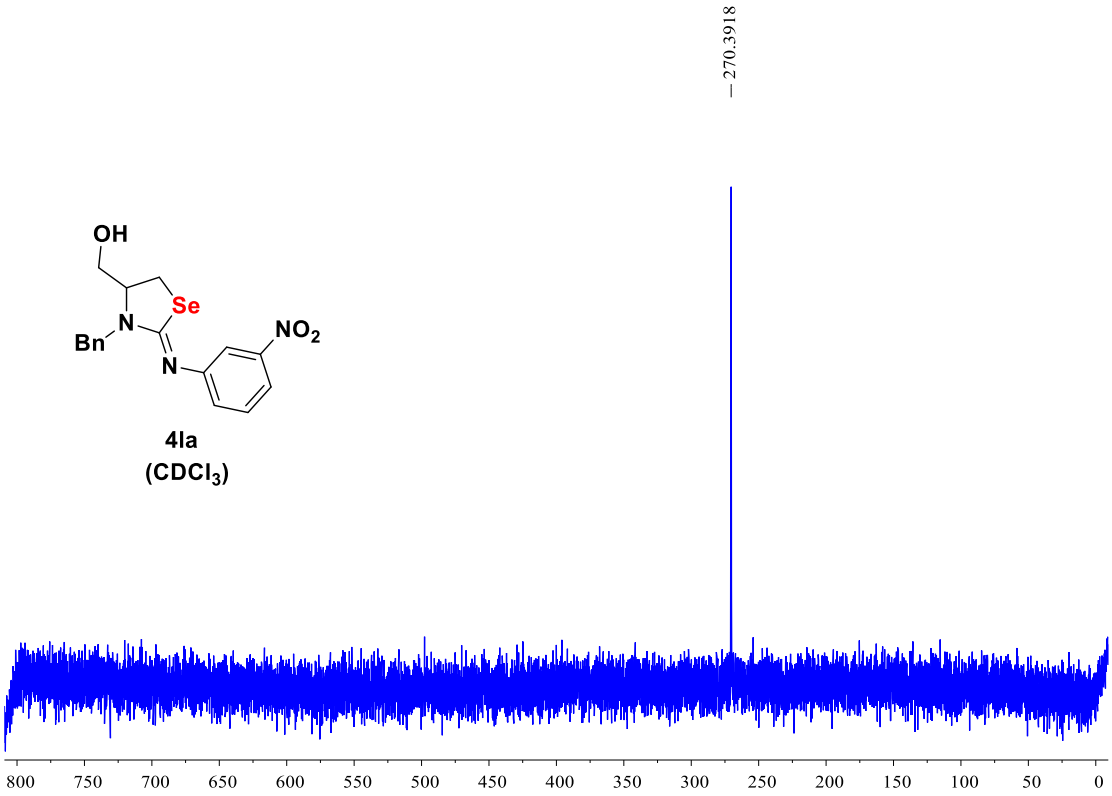
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Bn
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NO2
4la
(CDCl3)
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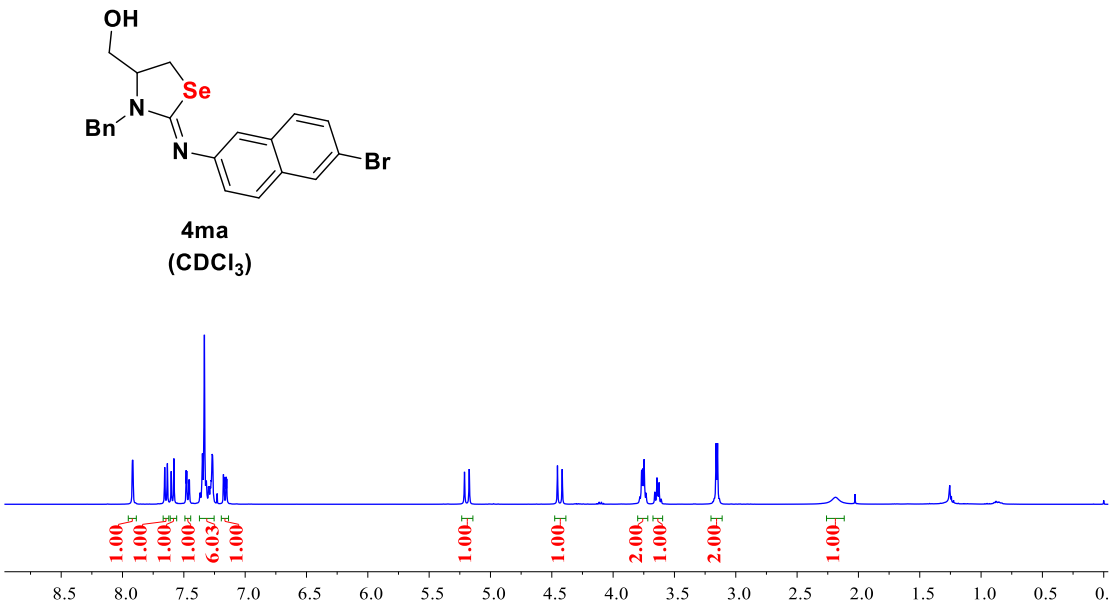
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Se
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Bn
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Br
4ma
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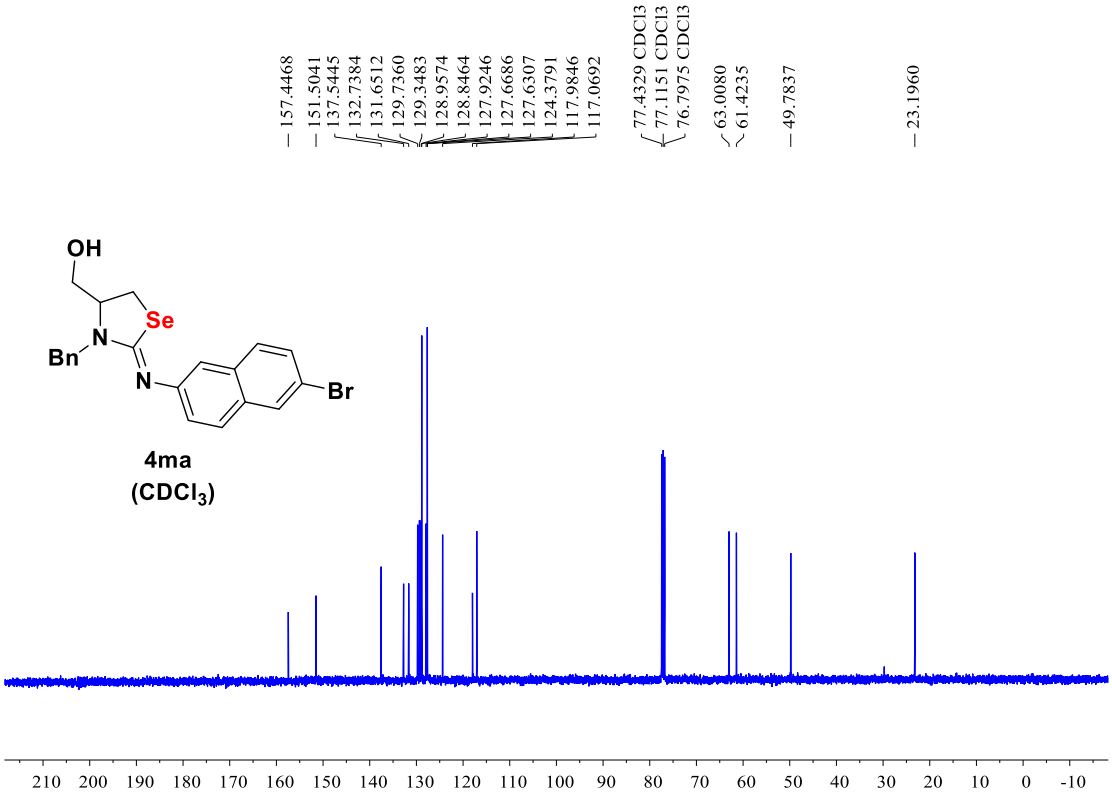
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124.3791
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77.1151 CDCl3
76.7975 CDCl3
63.0080
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49.7837
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Bn
N
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Br
4ma
(CDCl3)
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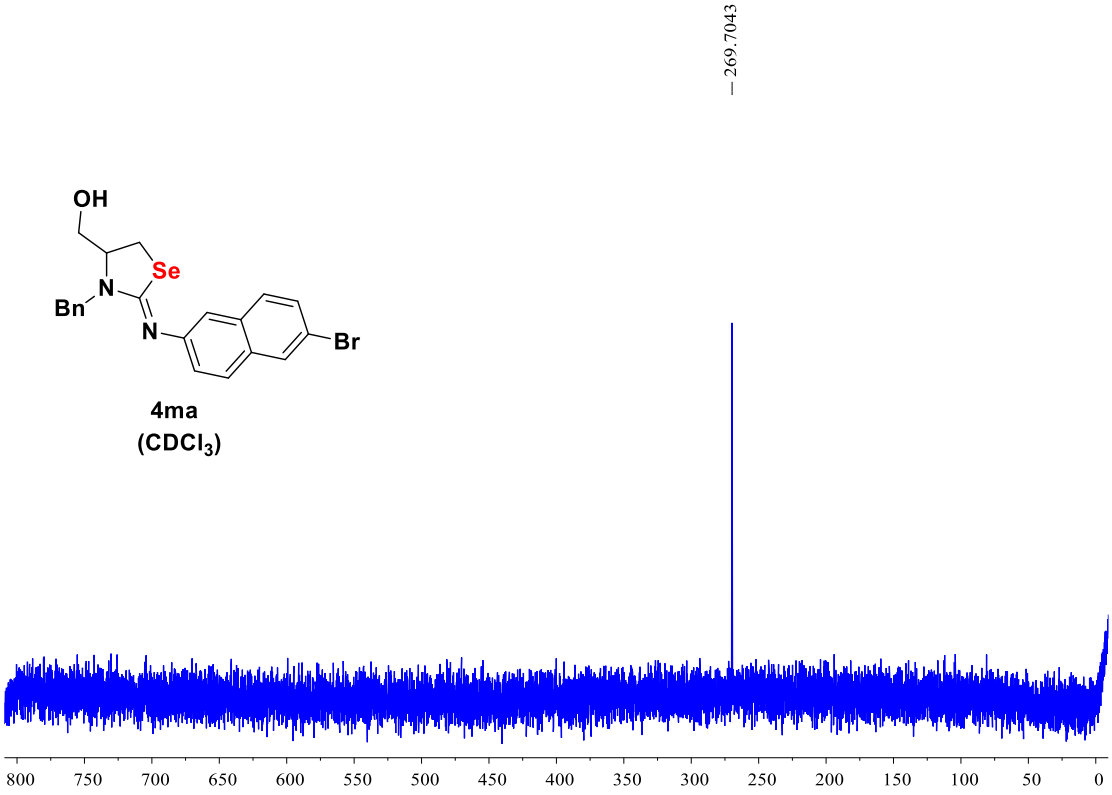
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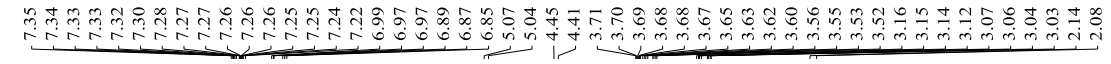
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7.24
7.22
6.99
6.97
6.97
6.89
6.87
6.85
5.07
5.04
4.45
4.41
3.71
3.70
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3.68
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3.65
3.63
3.62
3.60
3.56
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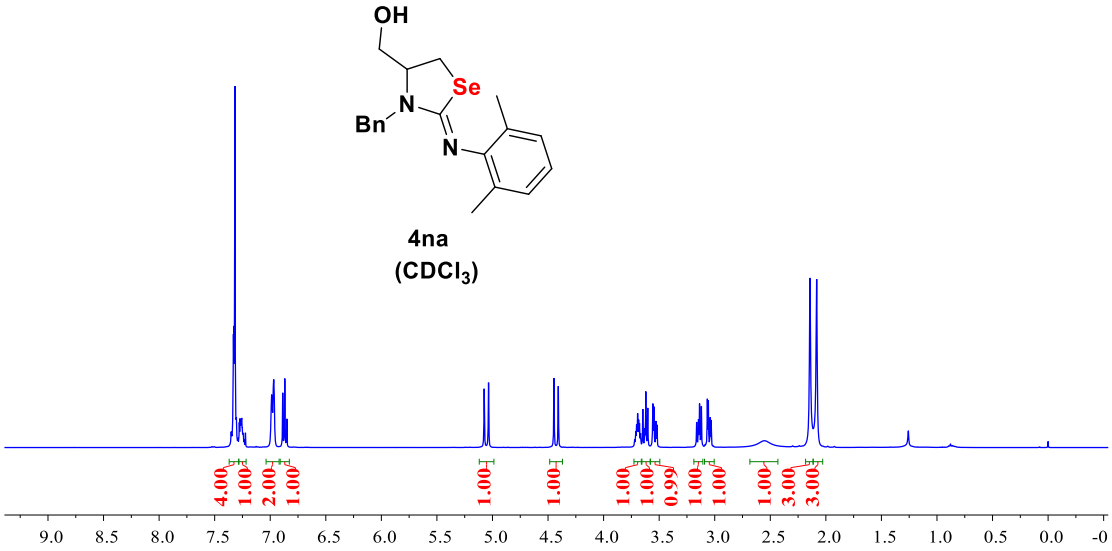
3.06
3.04
3.03
2.14
2.08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Bn
N
4na
(CDCl3)
4.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
0.99
1.00
1.00
1.00
3.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
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1.5
1.0
0.5
0.0
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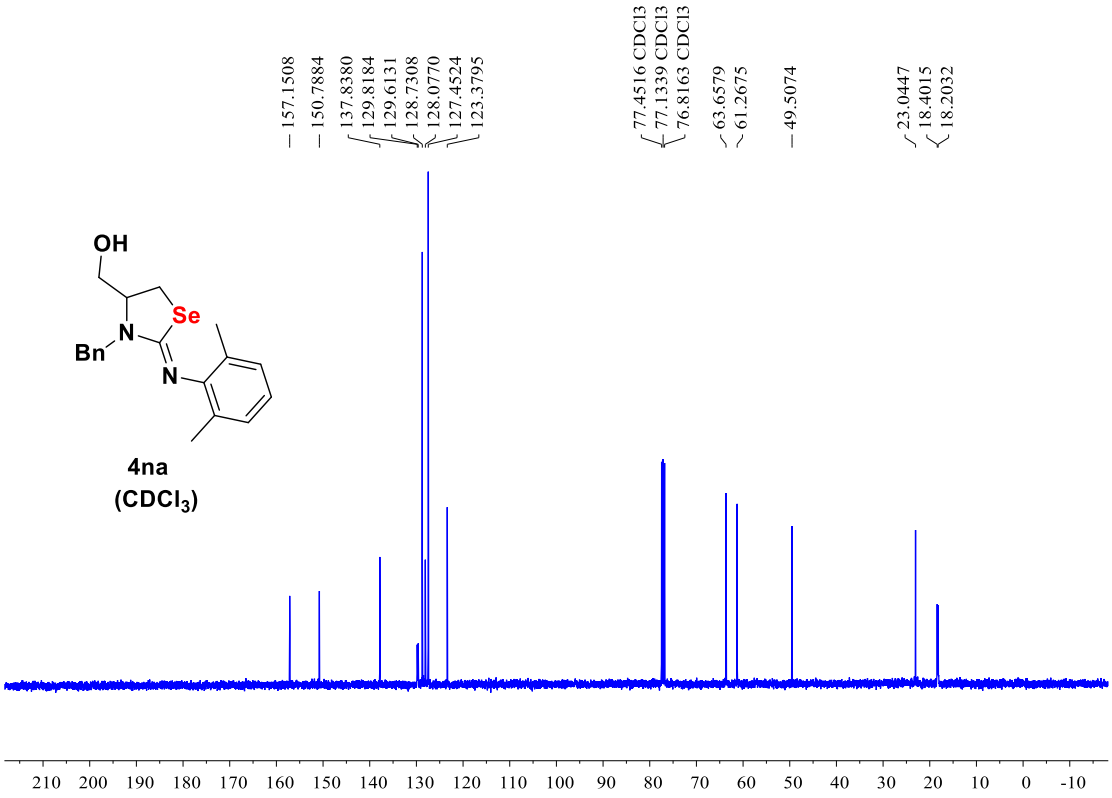
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77.1339 CDCl3
76.8163 CDCl3
63.6579
61.2675
49.5074
23.0447
18.4015
18.2032
OH
Se
N
Bn
N
4na
(CDCl3)
210
200
190
180
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140
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120
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100
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50
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20
10
0
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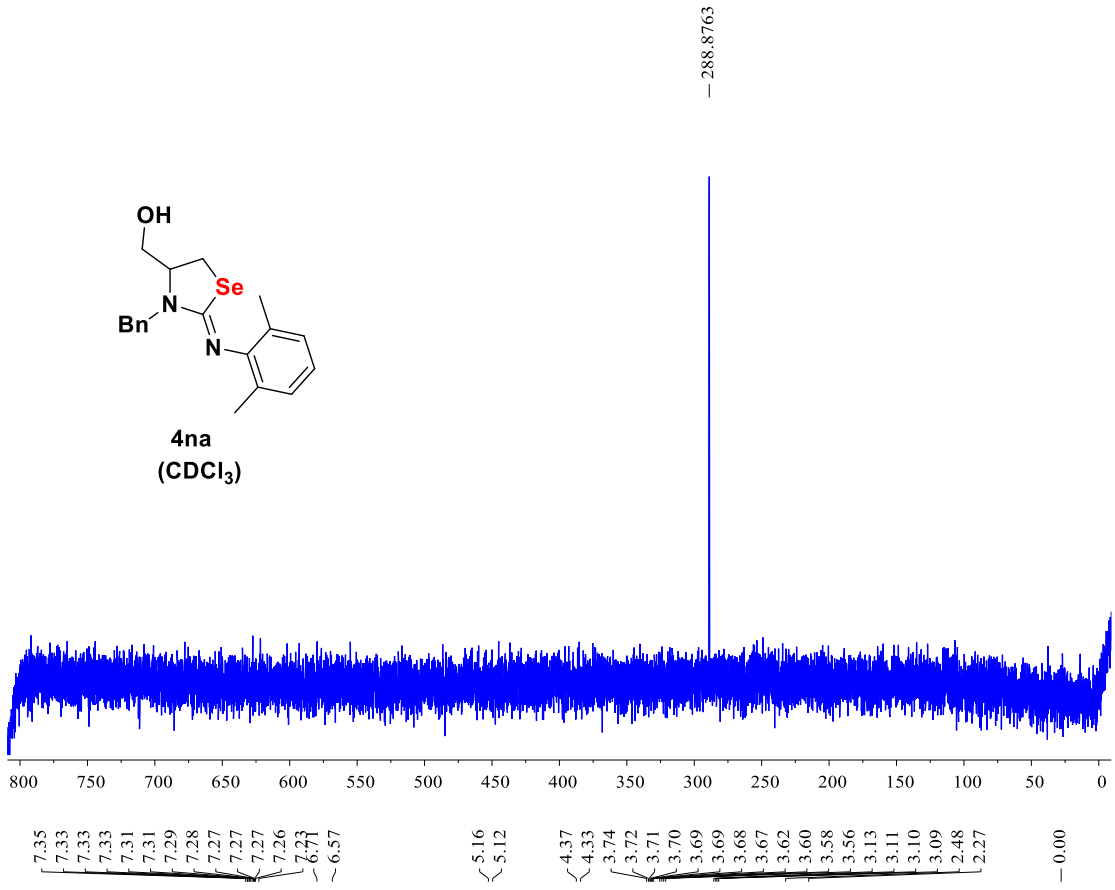
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N
Bn
N
4na
(CDCl3)
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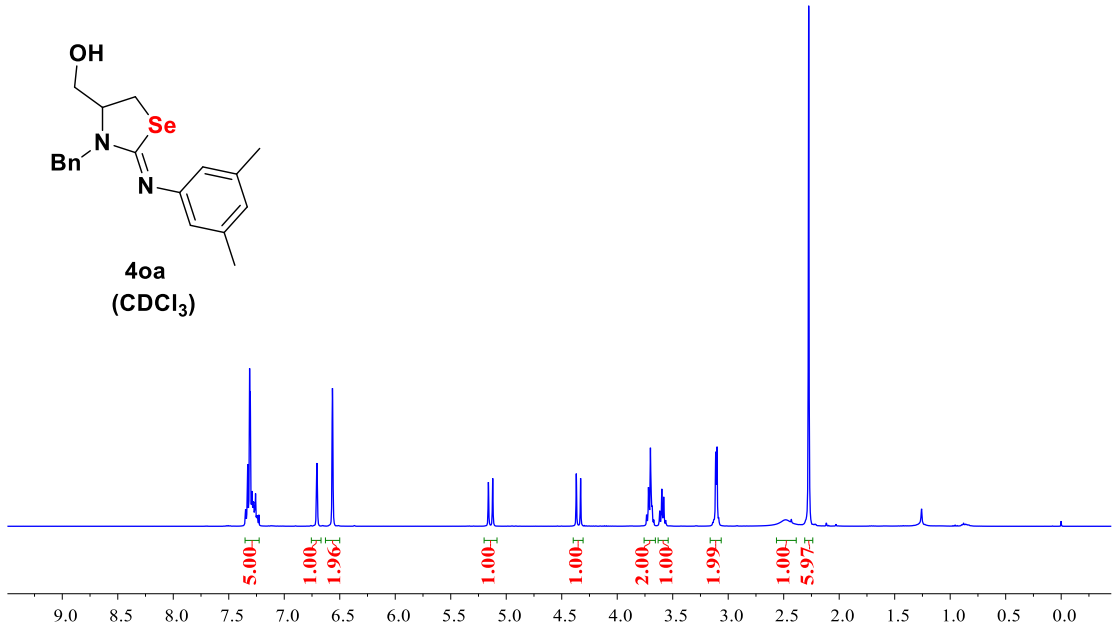
5.16 5.12
4.37 4.33 3.74 3.72 3.71 3.70 3.69 3.69 3.68 3.67 3.62 3.60 3.58 3.56 3.13 3.11 3.10 3.09 2.48 2.27
0.00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Se
N
Bn
N
4oa
(CDCl3)
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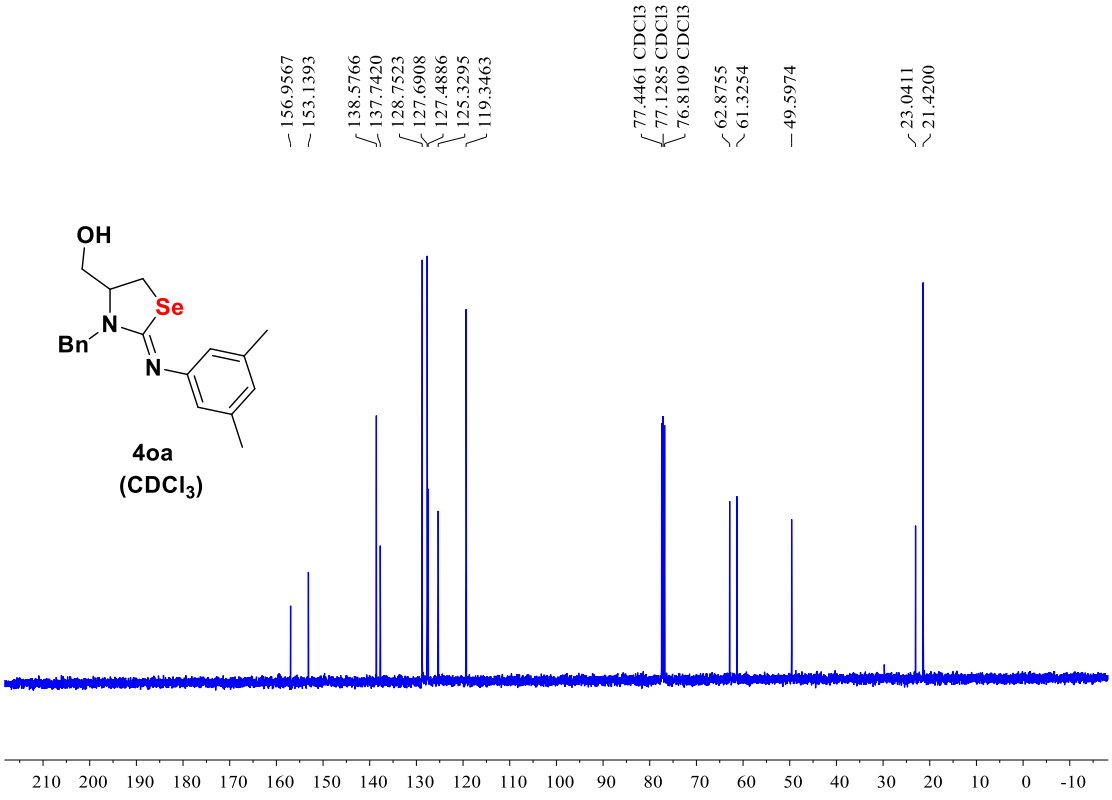
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76.8109 CDCl3
62.8755
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49.5974
23.0411
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N
Bn
N
4oa
(CDCl3)
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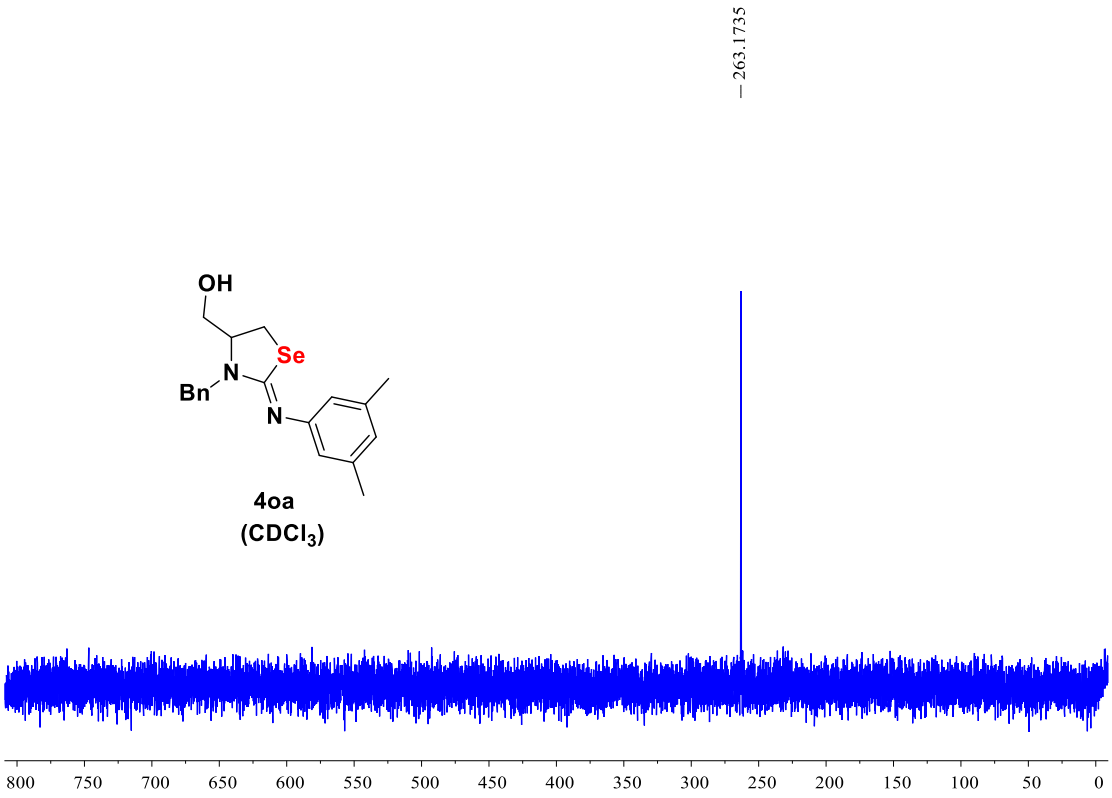
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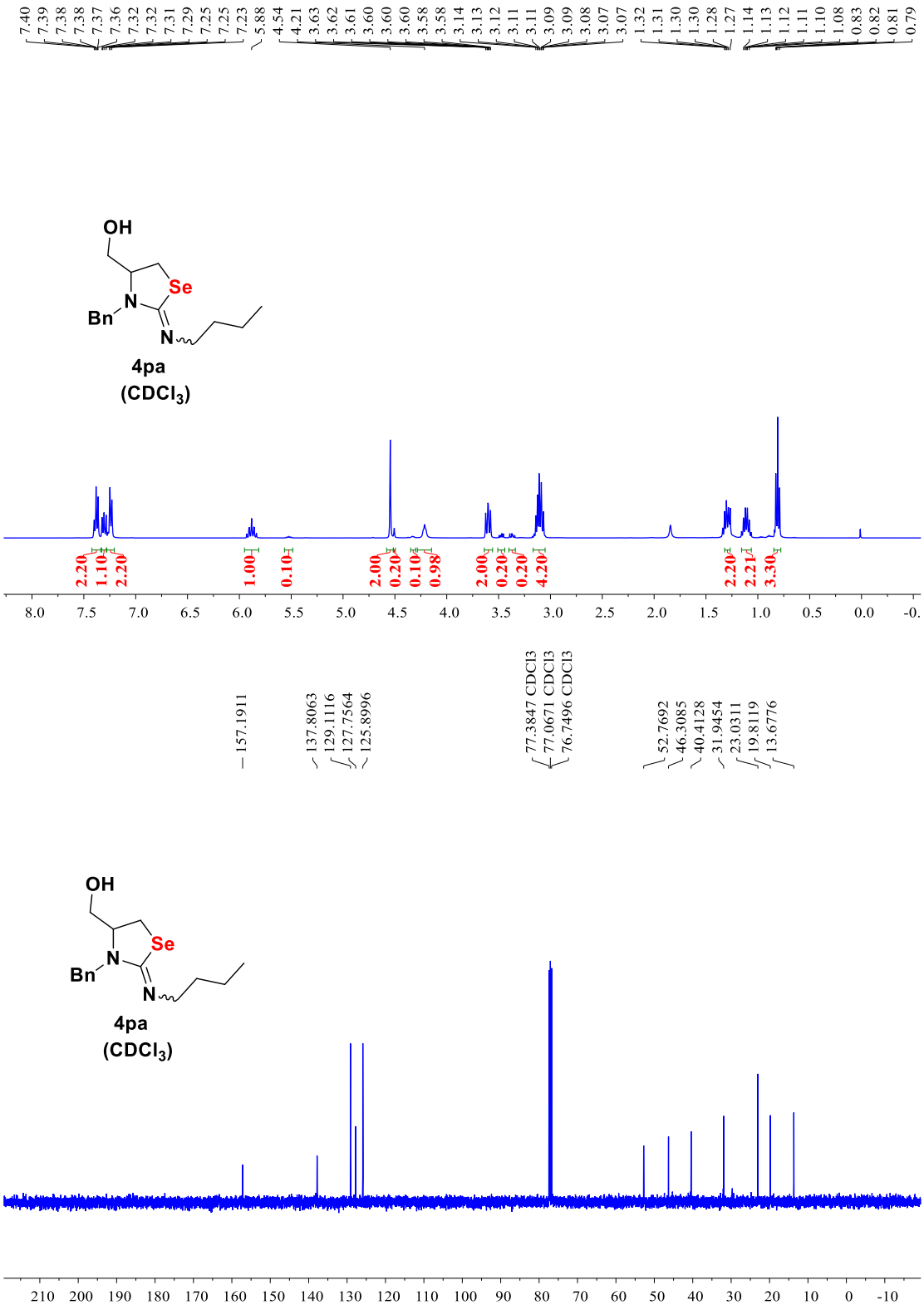
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OH
Se
Bn
N
N
4pa
(CDCl3)
2.20 1.10 2.20 1.00 0.10 2.00 0.20 0.10 0.98 2.00 0.20 0.20 4.20 2.20 2.21 3.30
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
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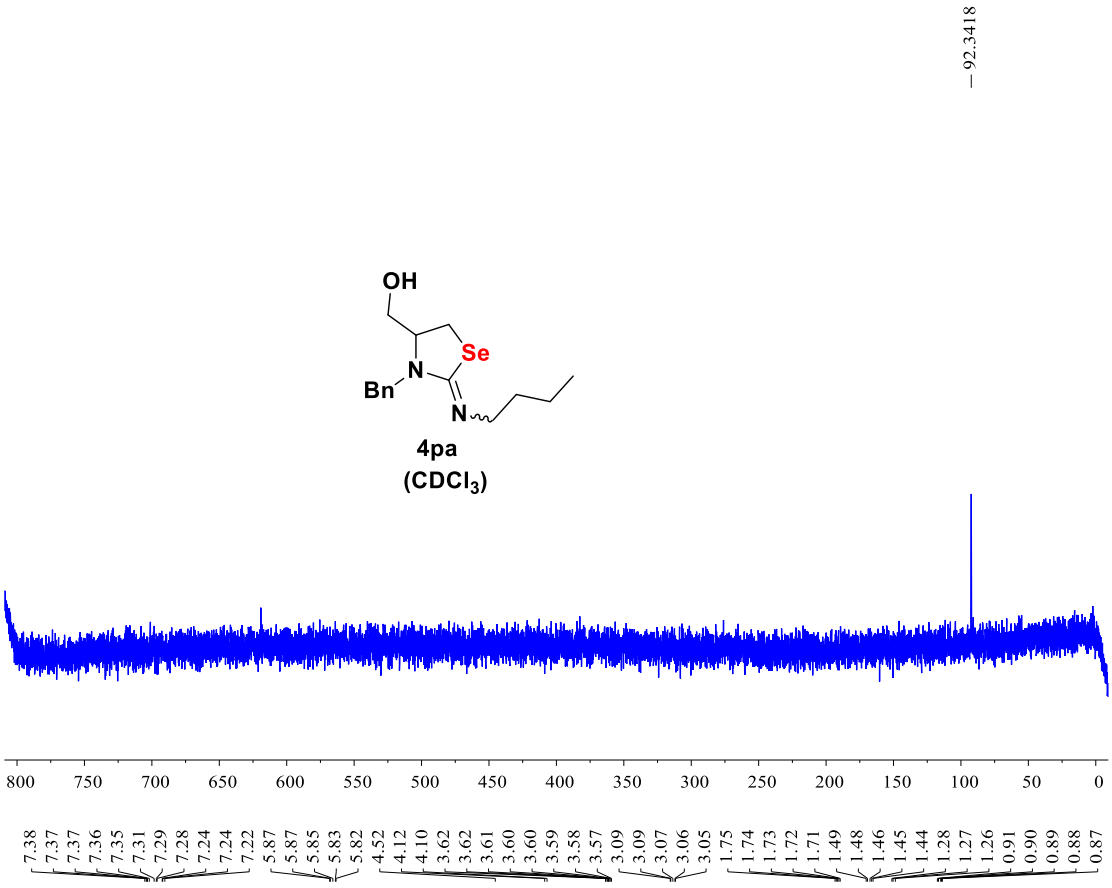
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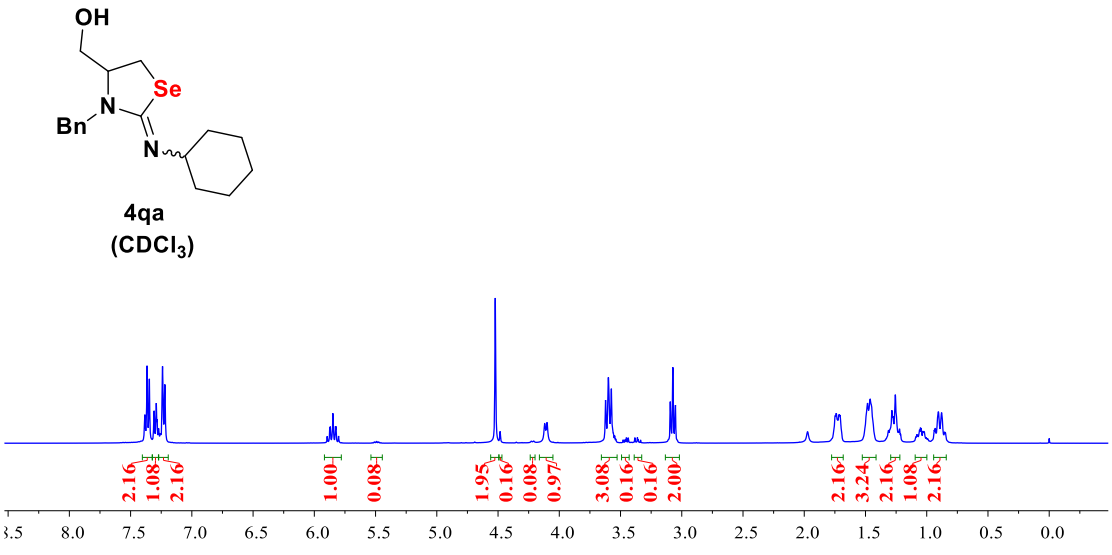
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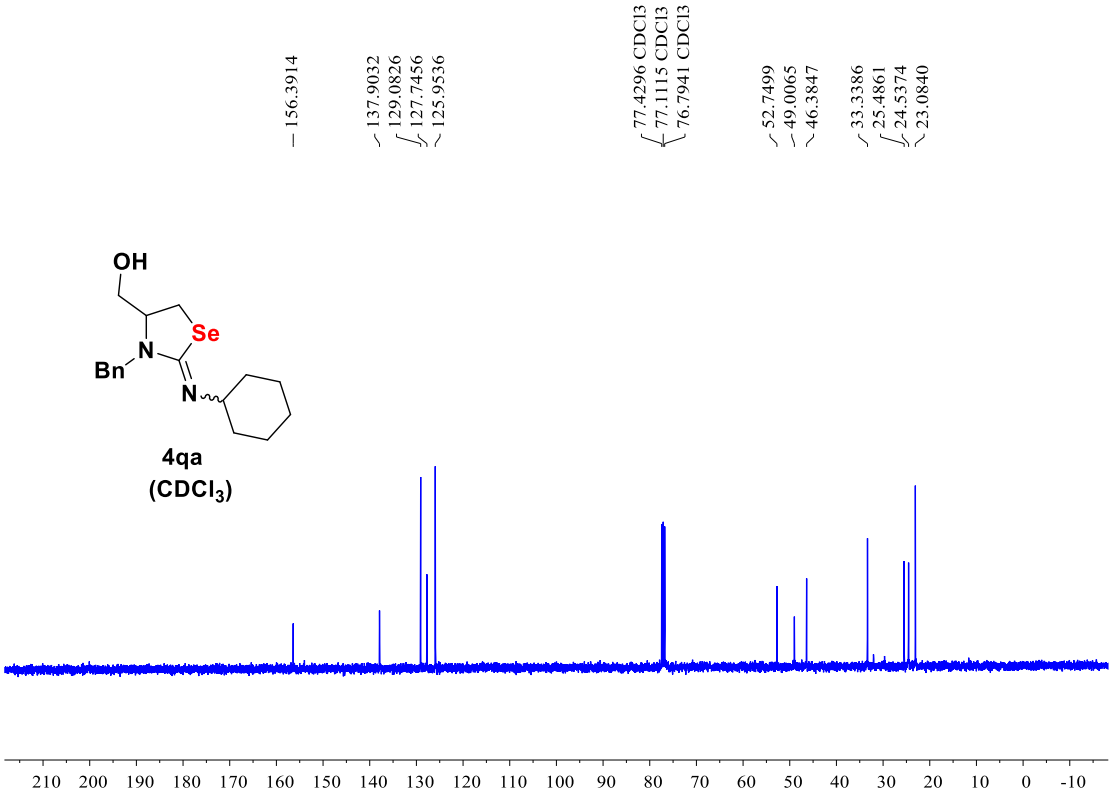
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46.3847
33.3386
25.4861
24.5374
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Se
N
Bn
N
4qa
(CDCl3)
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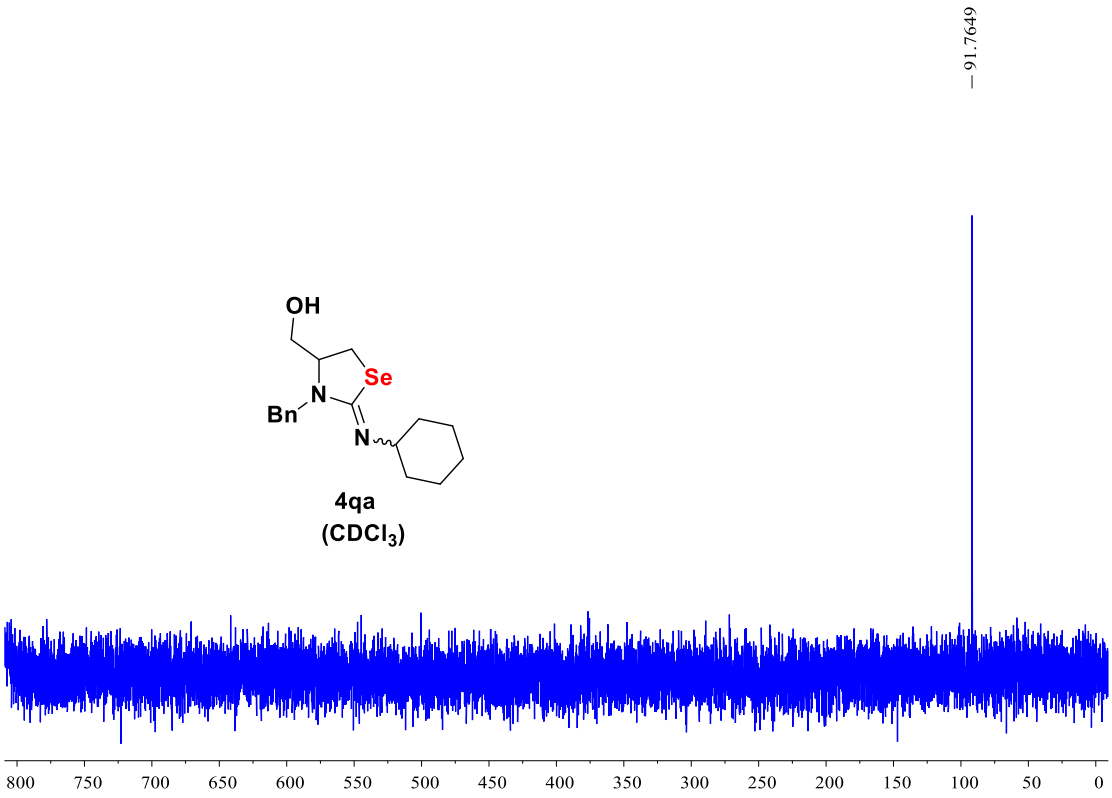
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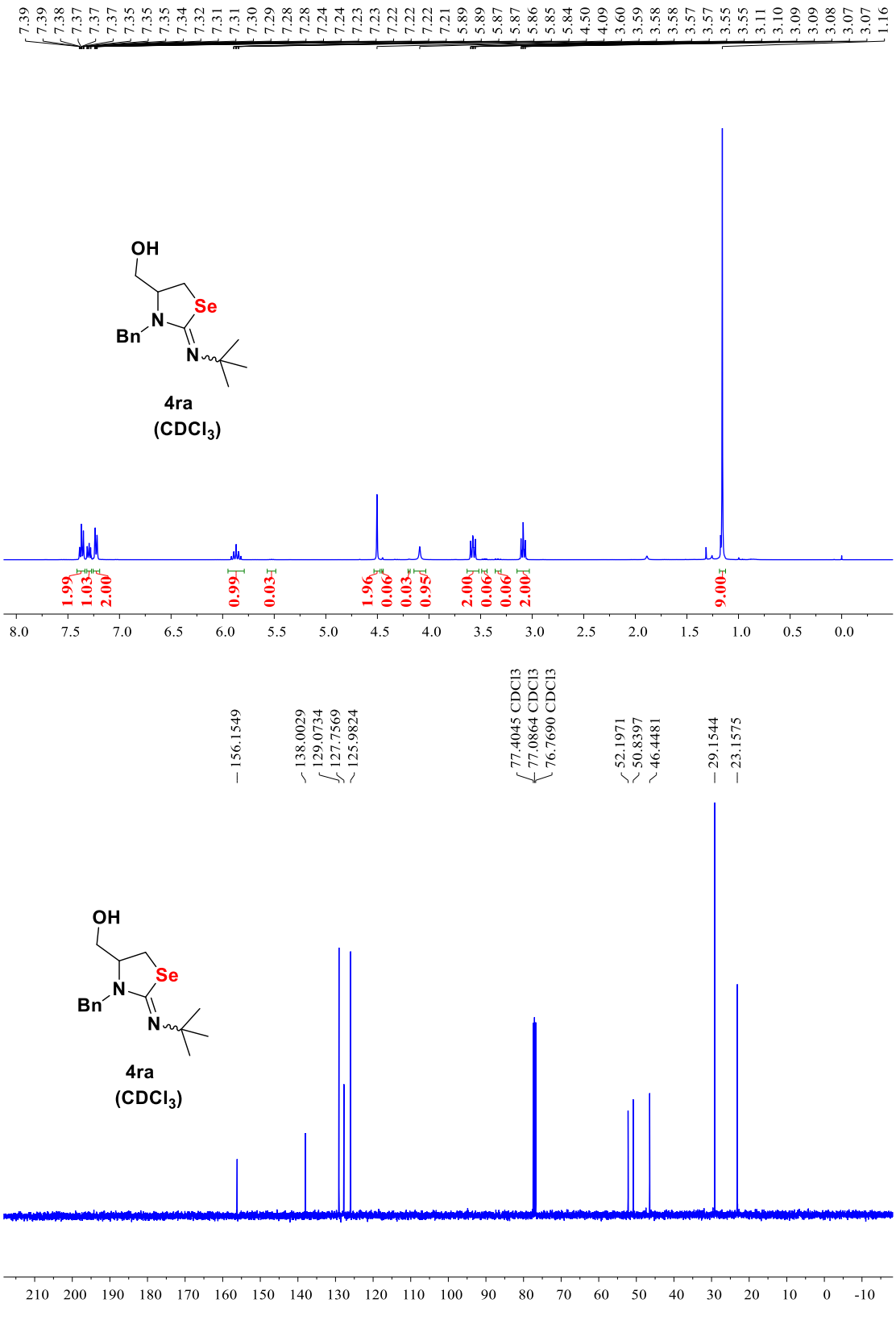
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OH
Se
N
Bn
N
4ra
(CDCl3)
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8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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Bn
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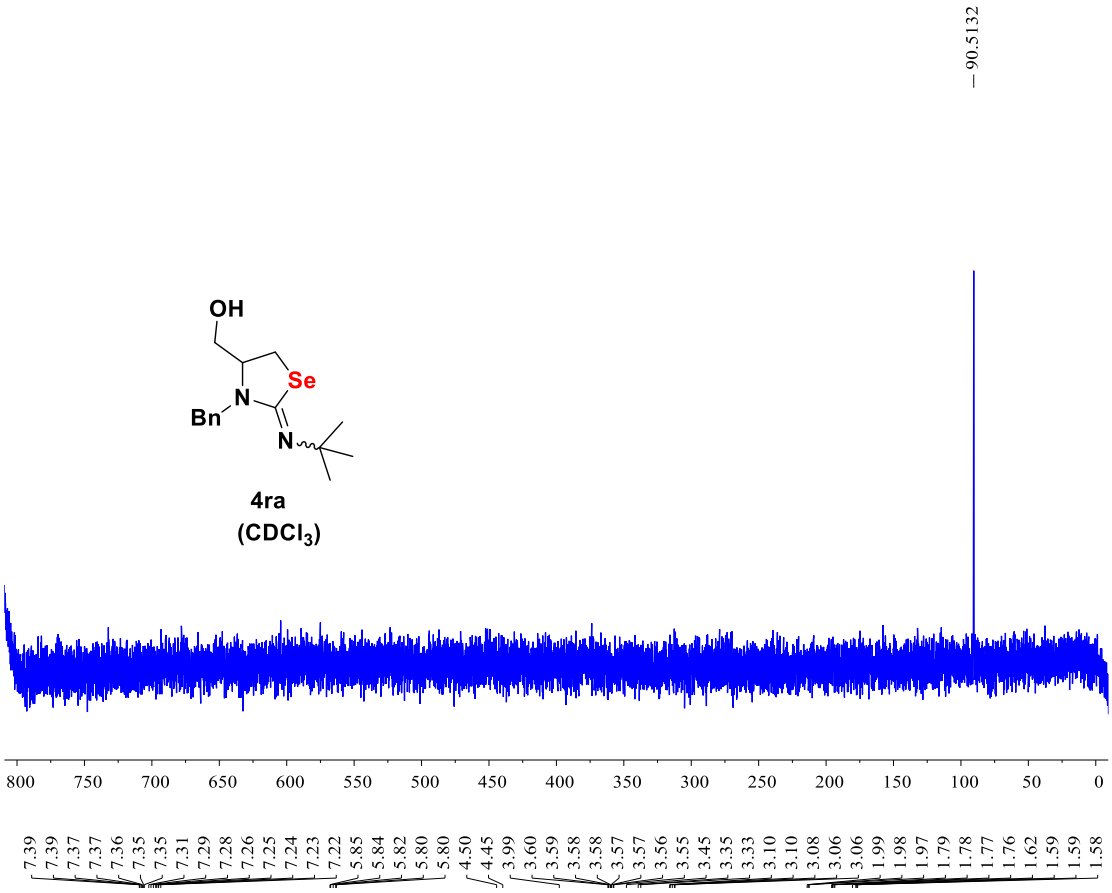
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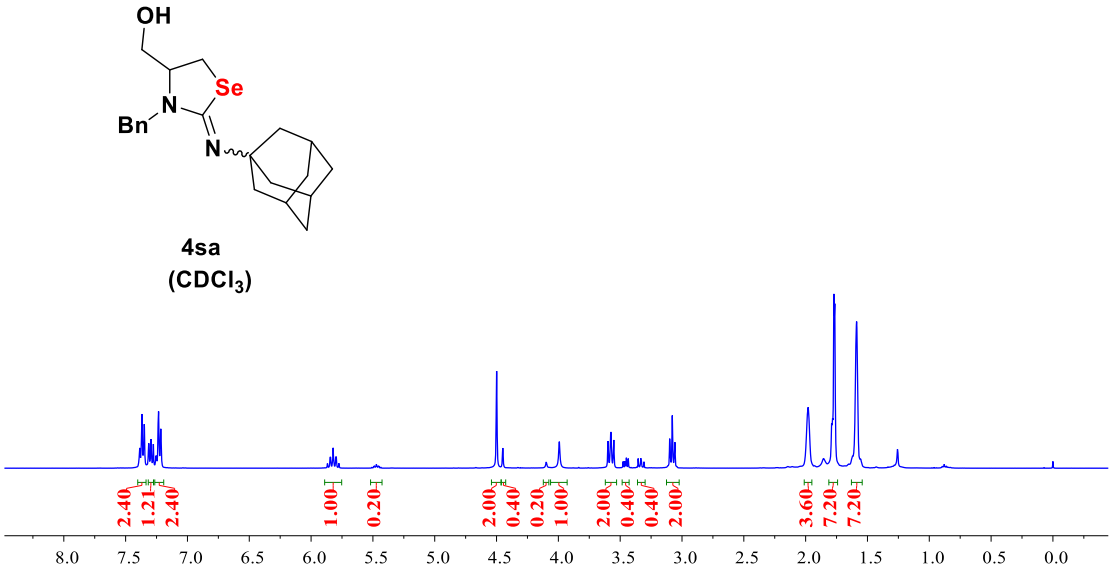
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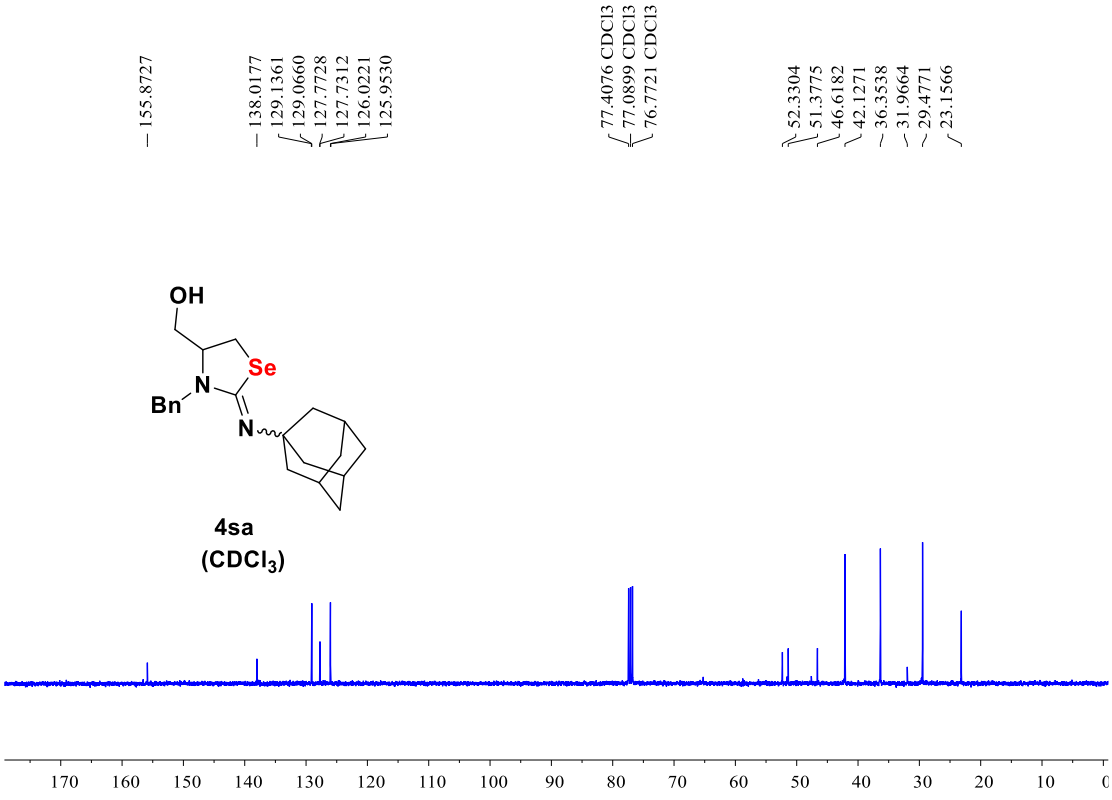
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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46.6182
42.1271
36.3538
31.9664
29.4771
23.1566
OH
Se
N
Bn
N
4sa
(CDCl3)
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80
70
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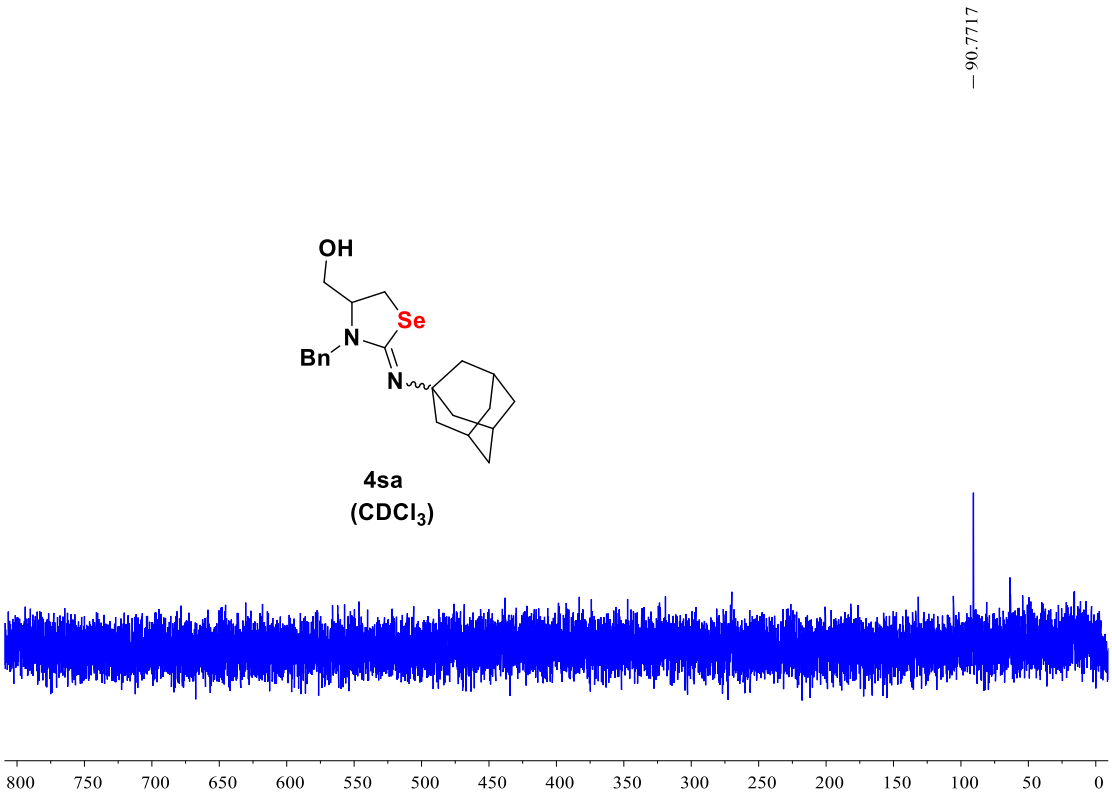
20
10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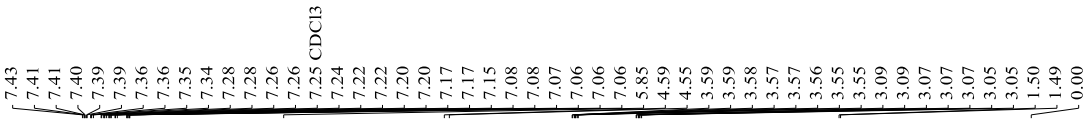
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7.25 CDCl3
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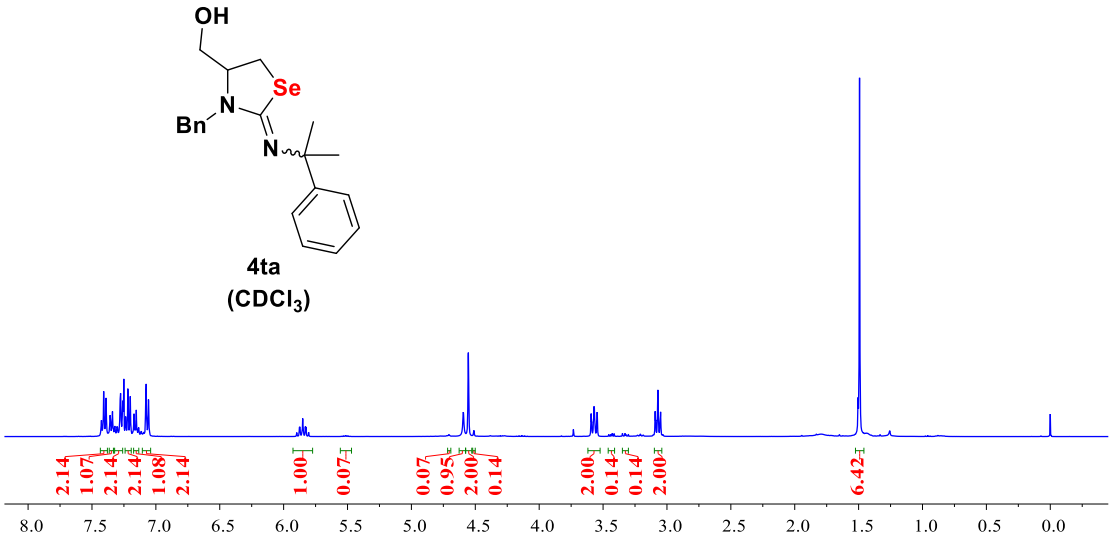
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N
Bn
N
4ta
(CDCl3)
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1.07
2.14
2.14
1.08
2.14
1.00
0.07
0.07
0.95
2.00
0.14
2.00
0.14
0.14
2.00
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6.5
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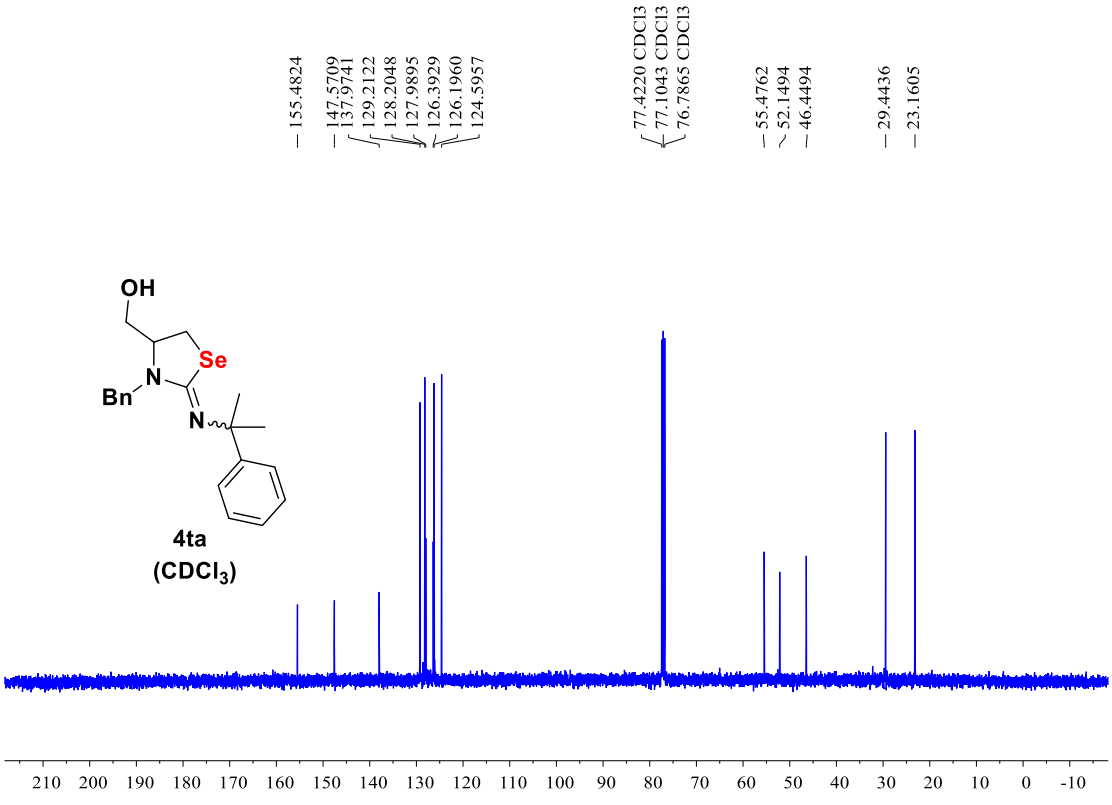
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76.7865 CDCl3
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46.4494
29.4436
23.1605
OH
Se
N
Bn
N
4ta
(CDCl3)
210
200
190
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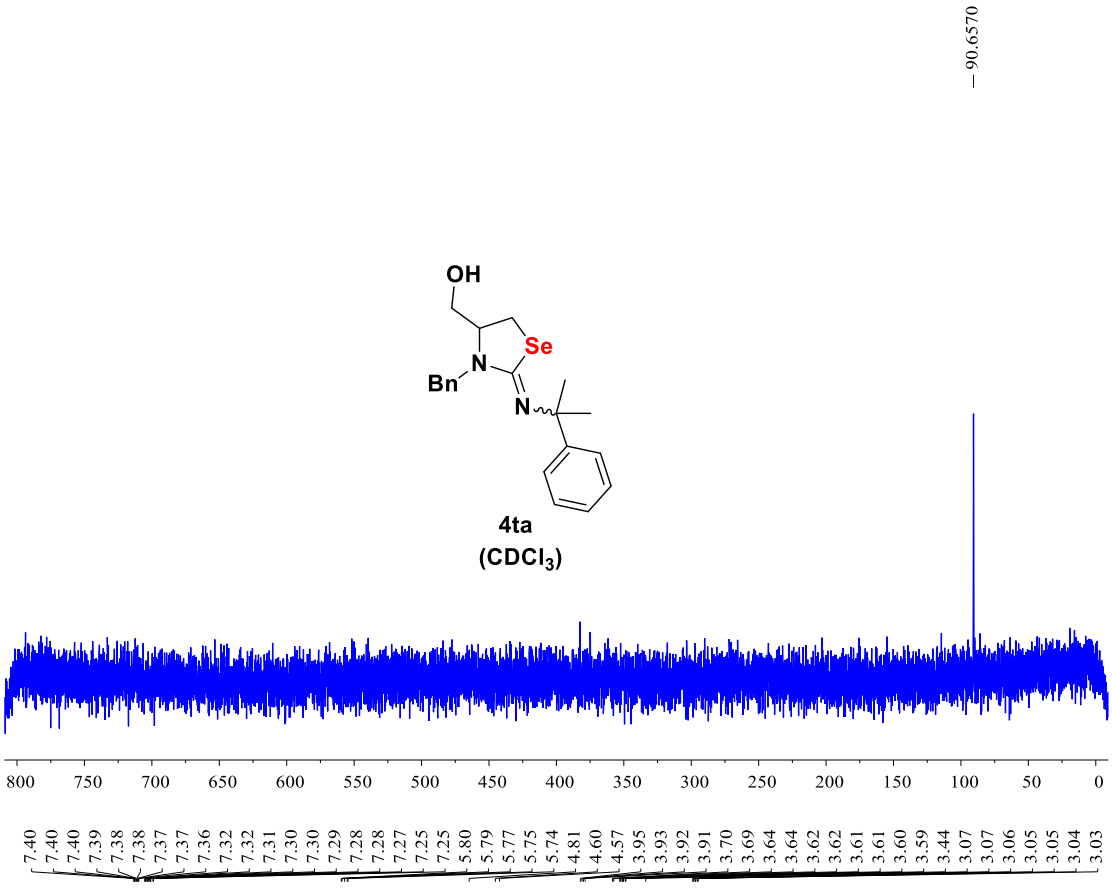
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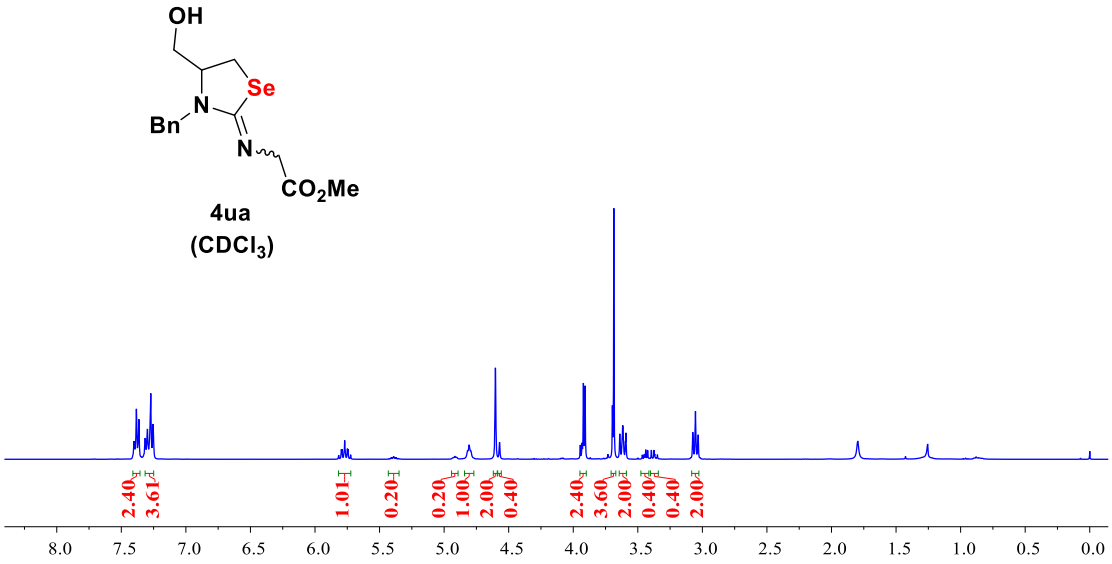
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Bn
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CO2Me
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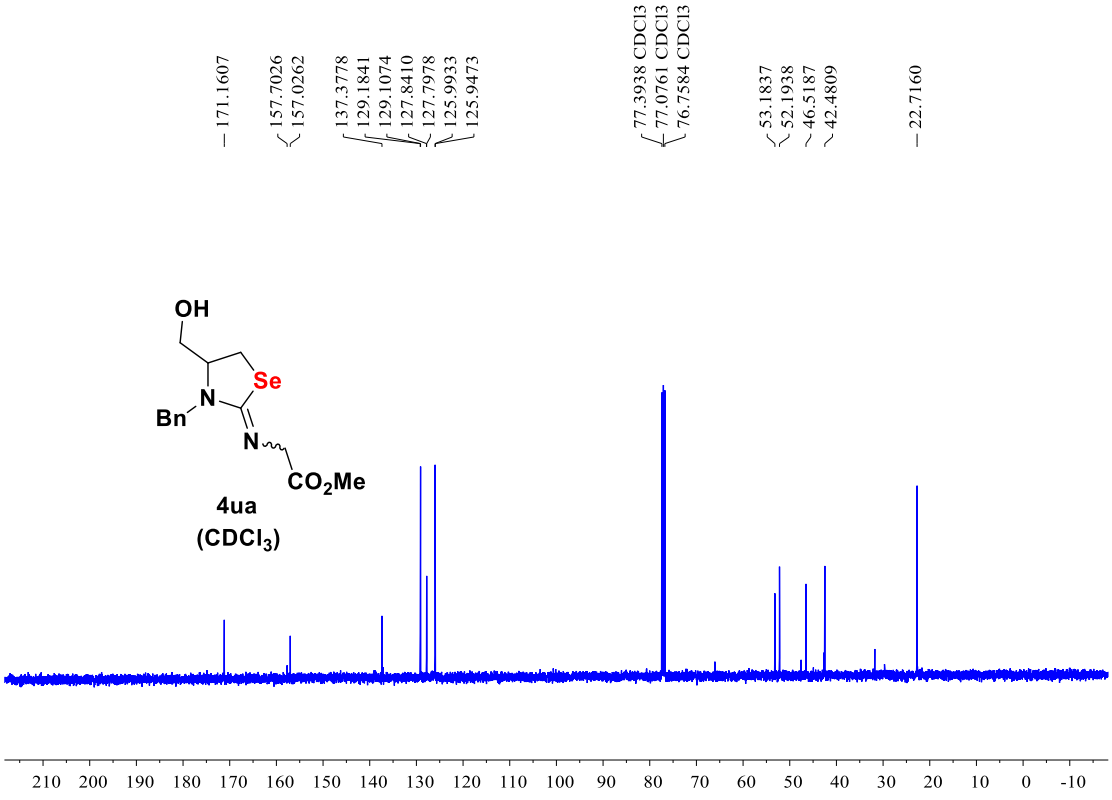
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76.7584 CDCl3
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Bn
N
CO2Me
4ua
(CDCl3)
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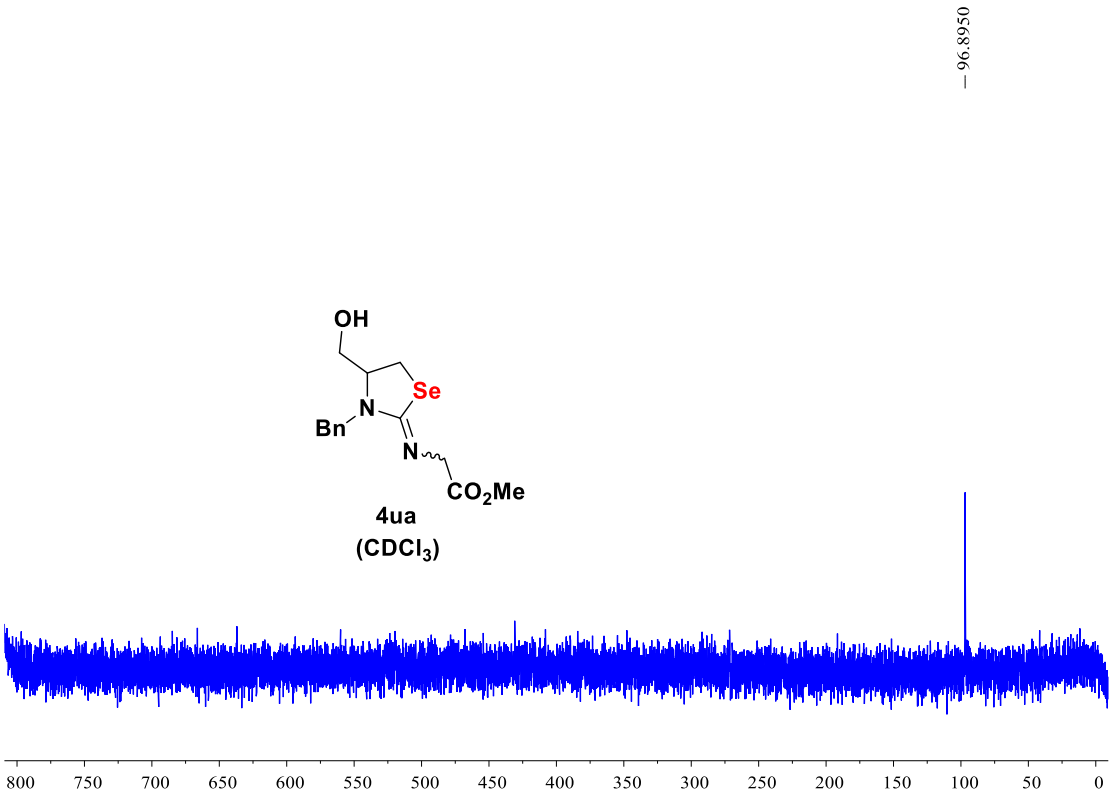
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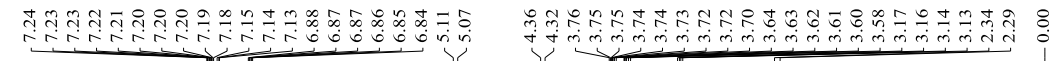
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4.36
4.32
3.76
3.75
3.75
3.74
3.74
3.73
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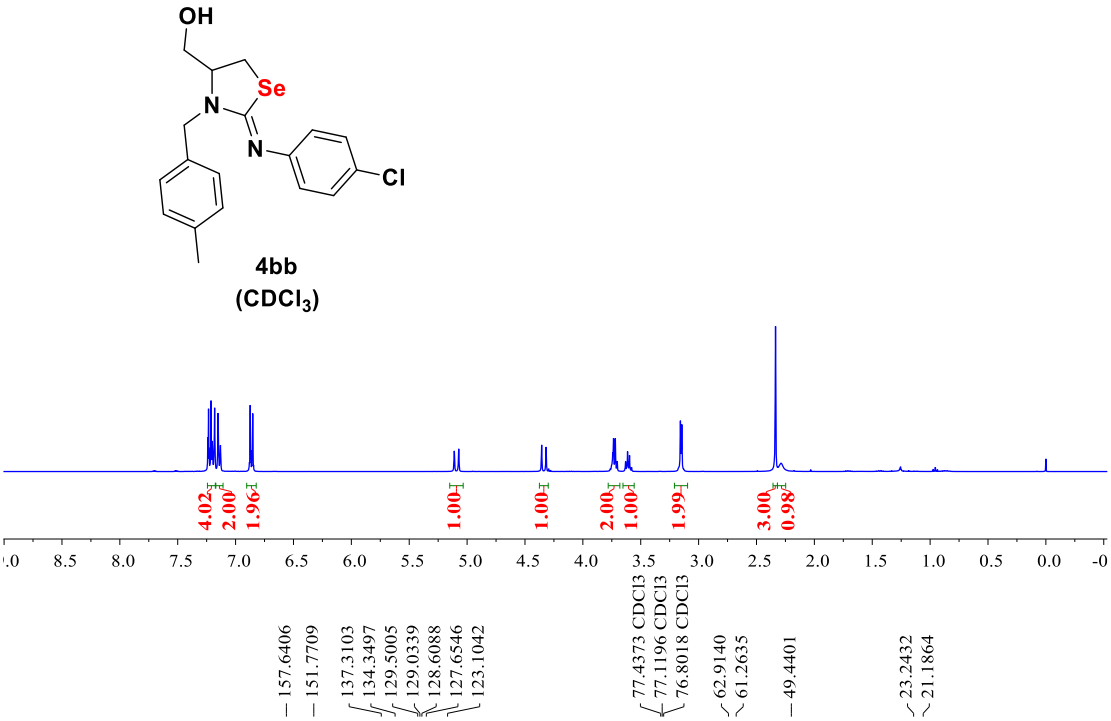
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Cl
4bb
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1.00
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1.99
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0.98
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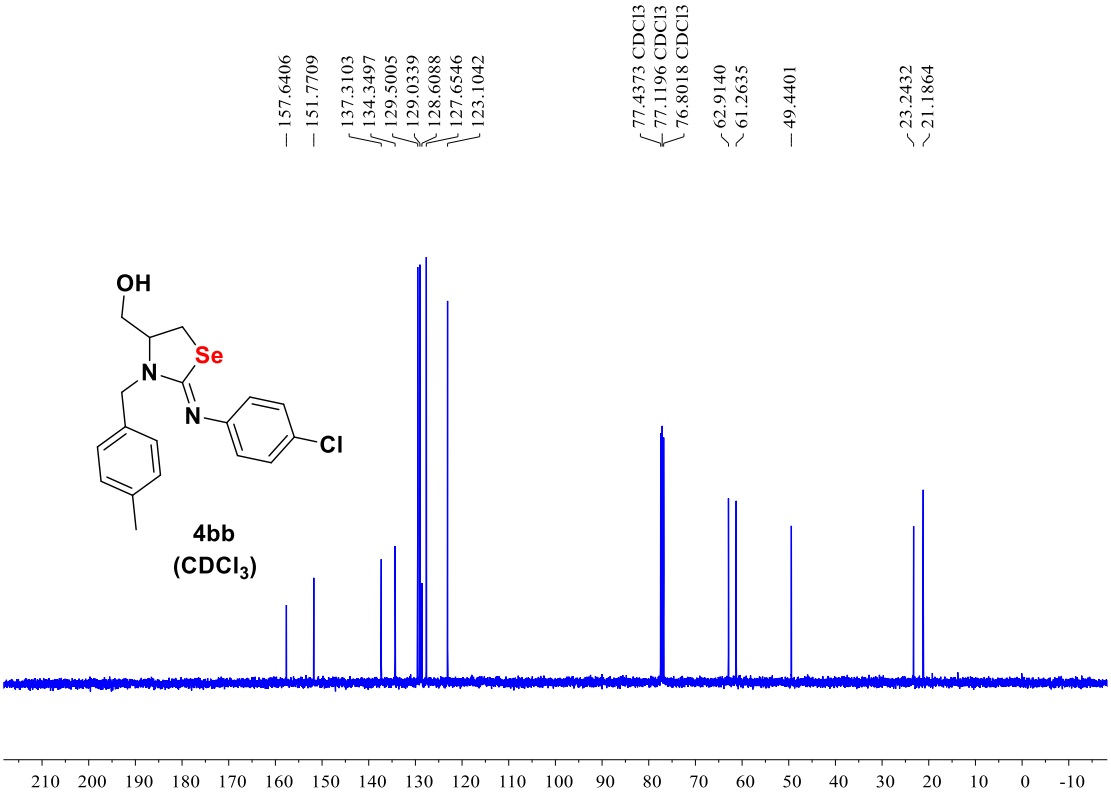
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123.1042
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77.1196 CDCl3
76.8018 CDCl3
62.9140
61.2635
49.4401
23.2432
21.1864
OH
Se
N
N
Cl
4bb
(CDCl3)
210
200
190
180
170
160
150
140
130
120
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100
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80
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60
50
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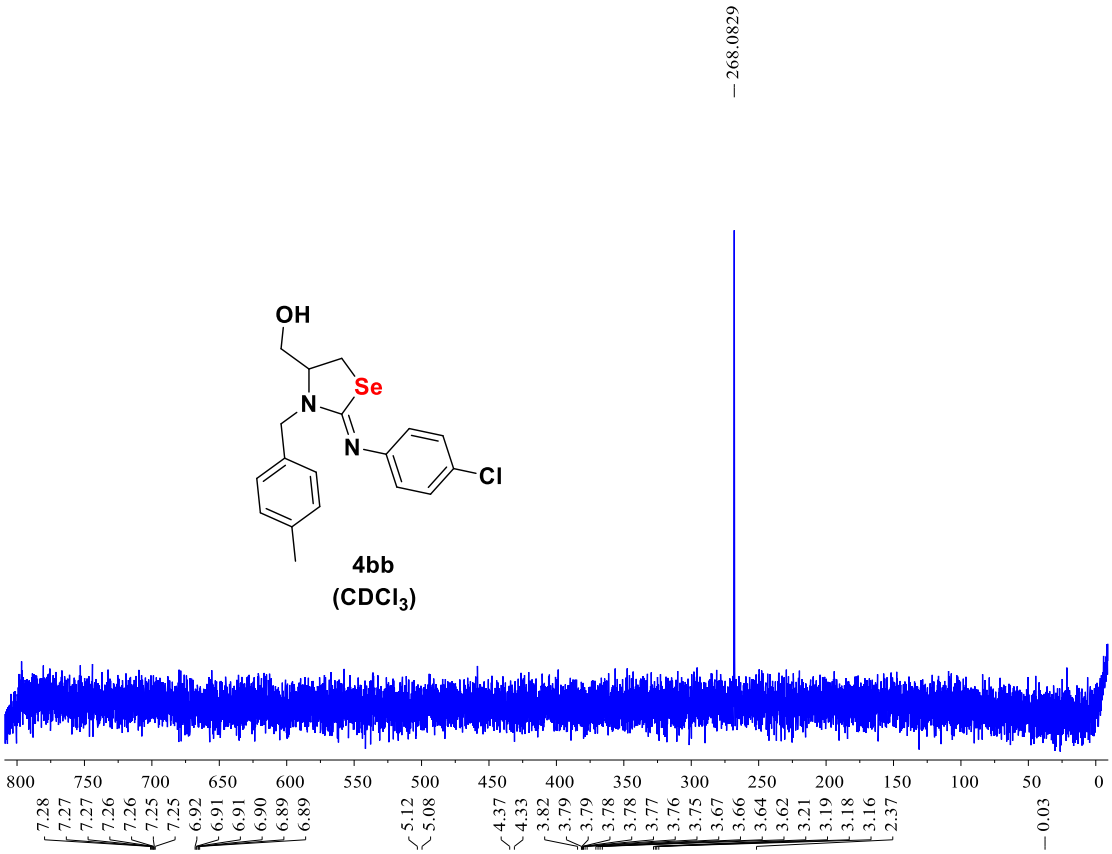
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Cl
4bb
(CDCl3)
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6.92 6.91 6.91 6.90 6.89 6.89
5.12 5.08
4.37 4.33
3.82 3.79 3.79 3.78 3.78 3.77 3.76 3.75 3.67 3.66 3.64 3.62 3.21 3.19 3.18 3.16 2.37
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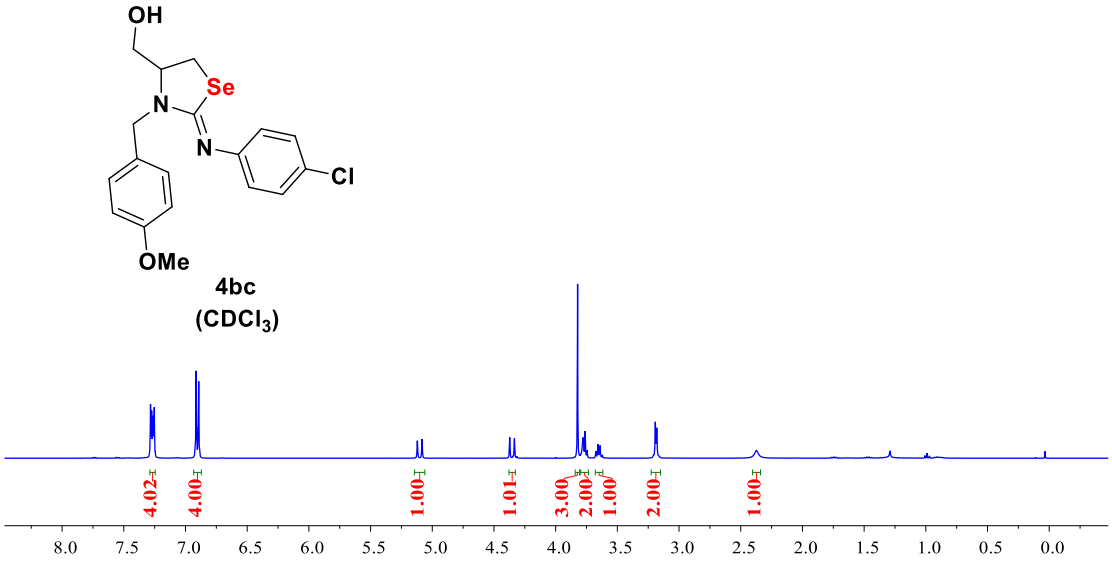
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Se
N
N
Cl
OMe
4bc
(CDCl3)
4.02
4.00
1.00
1.01
3.00
2.00
1.00
2.00
1.00
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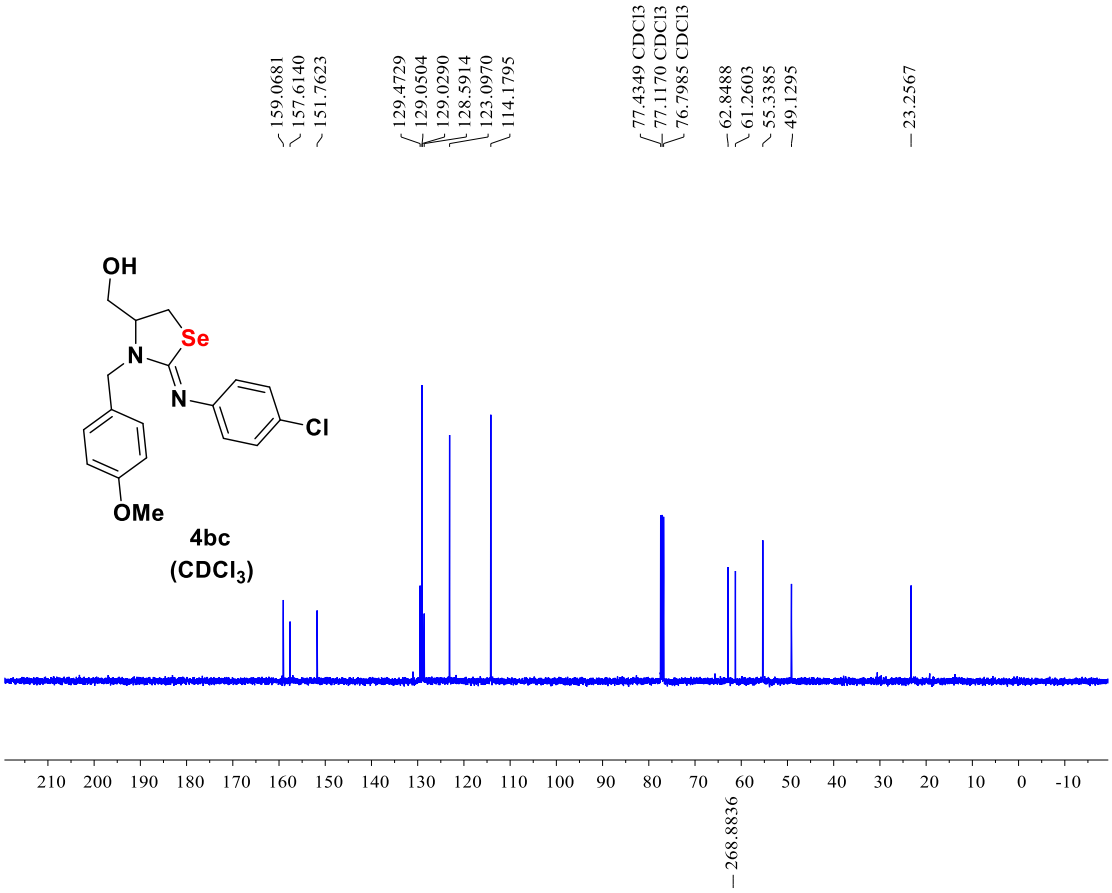
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61.2603
55.3385
49.1295
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OH
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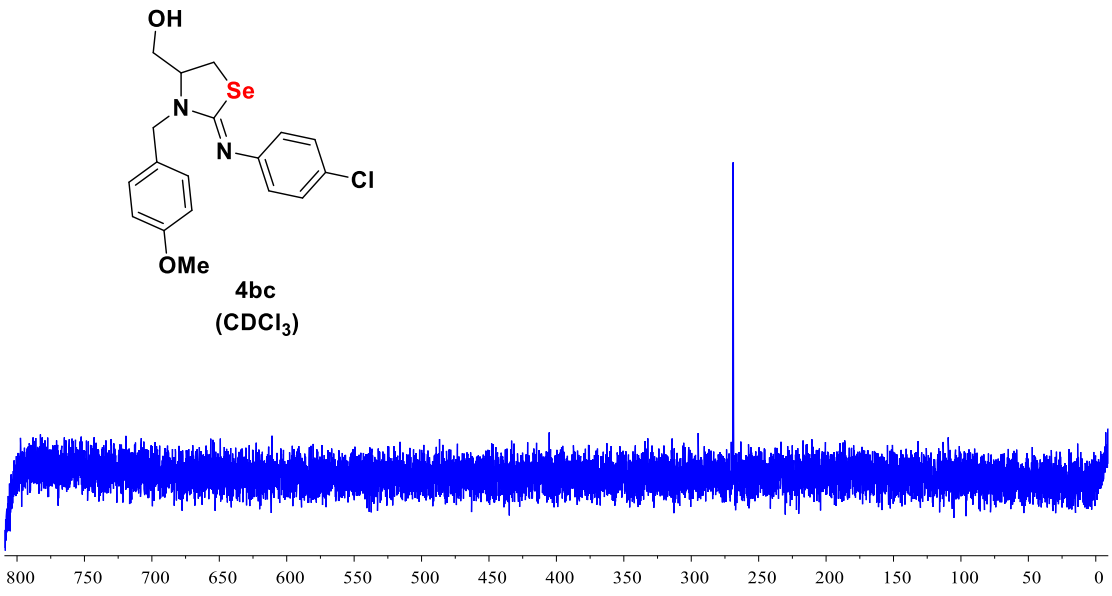
N
N
Cl
OMe
4bc
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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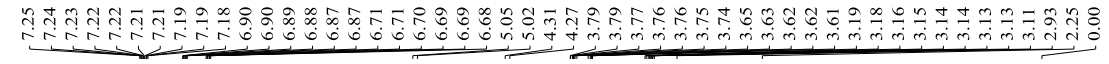
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6.88
6.87
6.87
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6.71
6.70
6.69
6.69
6.68
5.05
5.02
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4.27
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3.76
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3.75
3.74
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3.63
3.62
3.62
3.61
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3.13
3.11
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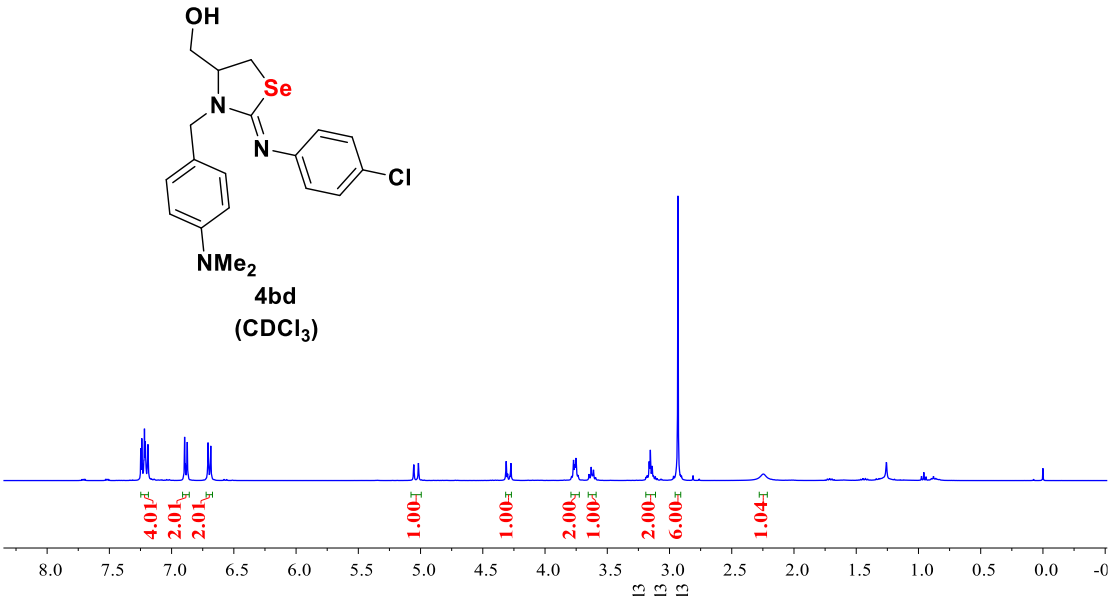
2.25
0.00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N
N
Cl
NMe2
4bd
(CDCl3)
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2.01
2.01
1.00
1.00
2.00
1.00
2.00
6.00
1.04
8.0
7.5
7.0
6.5
6.0
5.5
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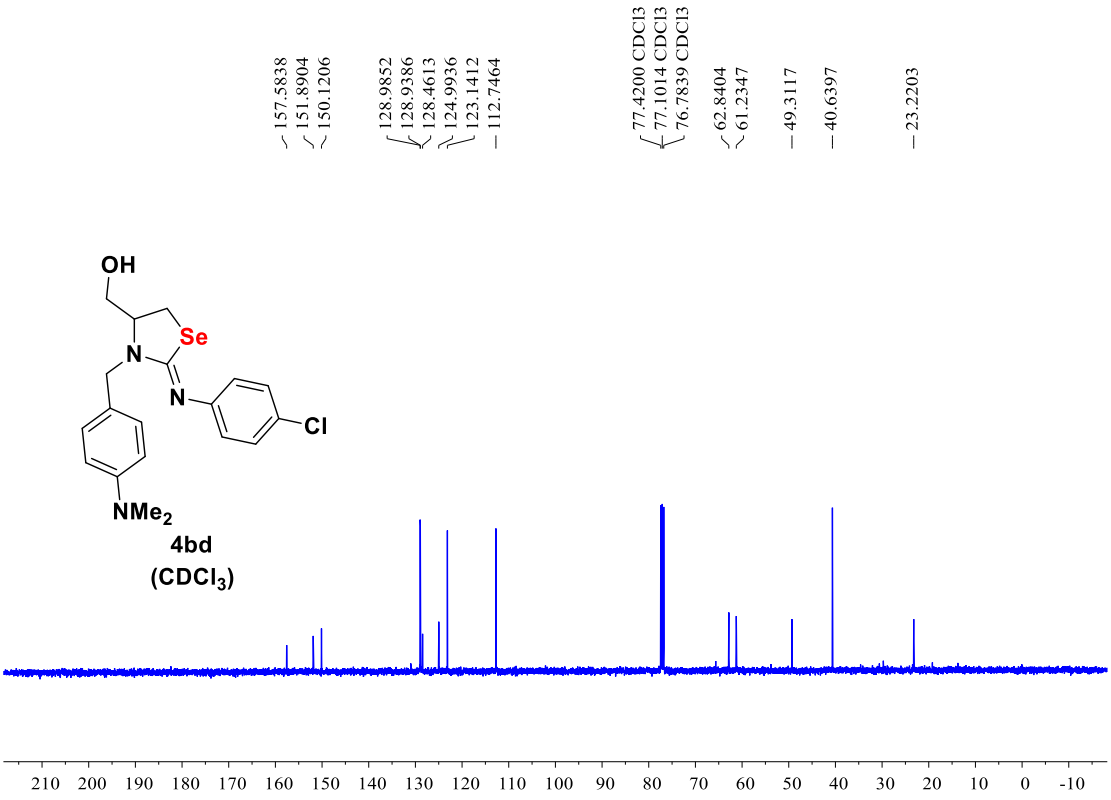
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40.6397
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OH
Se
N
N
Cl
NMe2
4bd
(CDCl3)
210
200
190
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140
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120
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100
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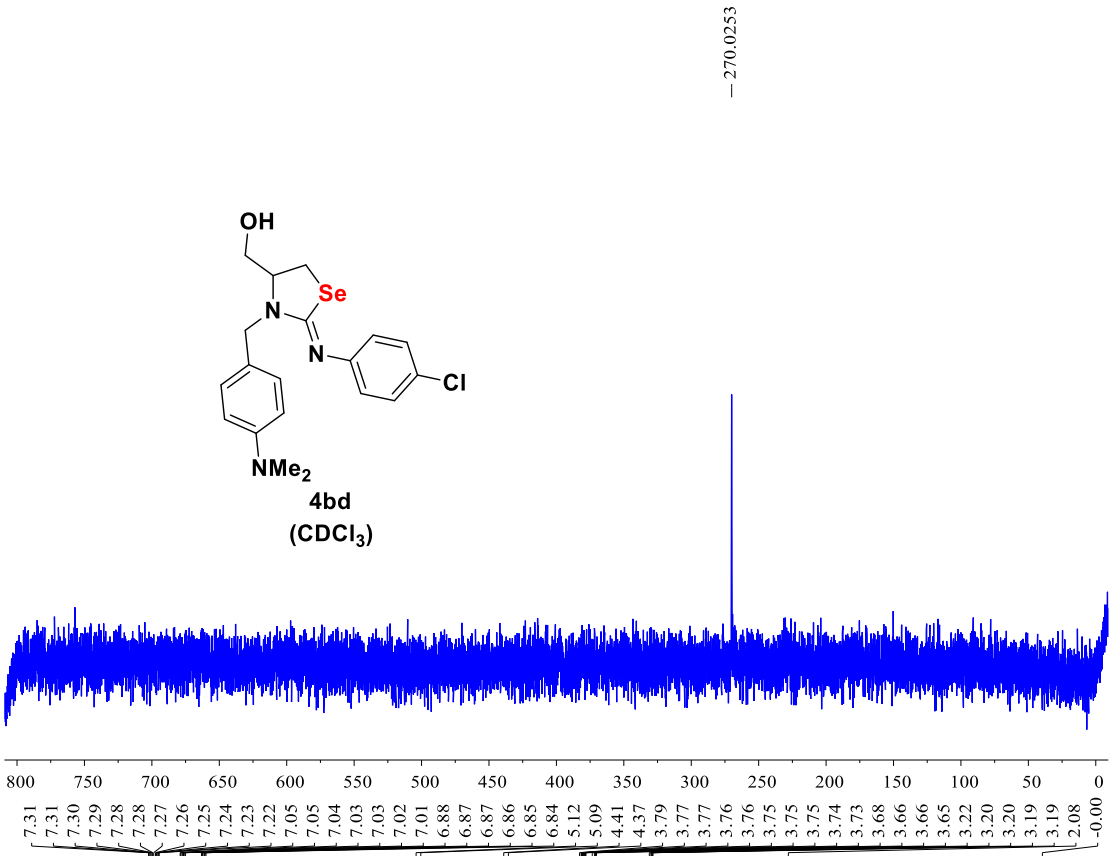
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4bd
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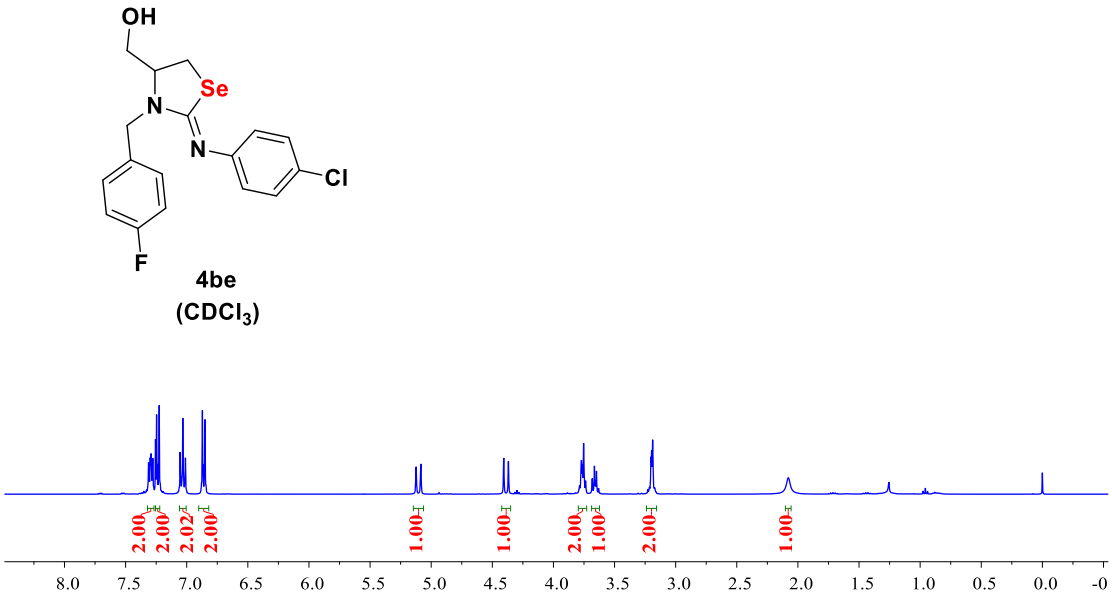
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N
Cl
F
4be
(CDCl3)
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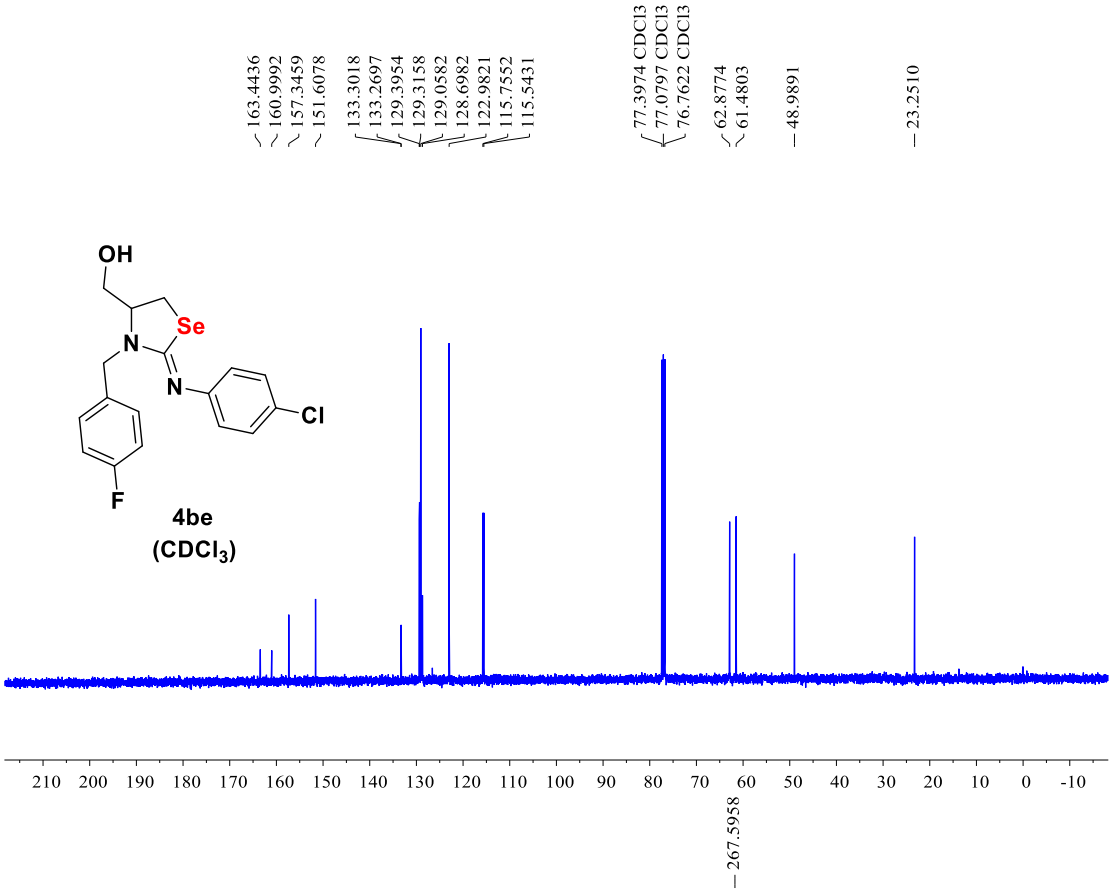
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61.4803
48.9891
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N
N
Cl
F
4be
(CDCl3)
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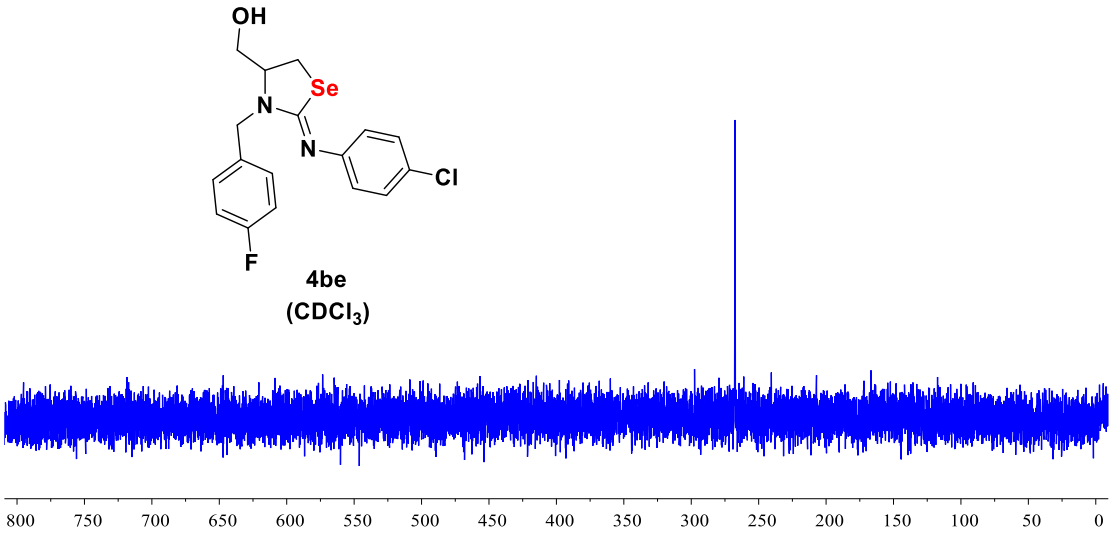
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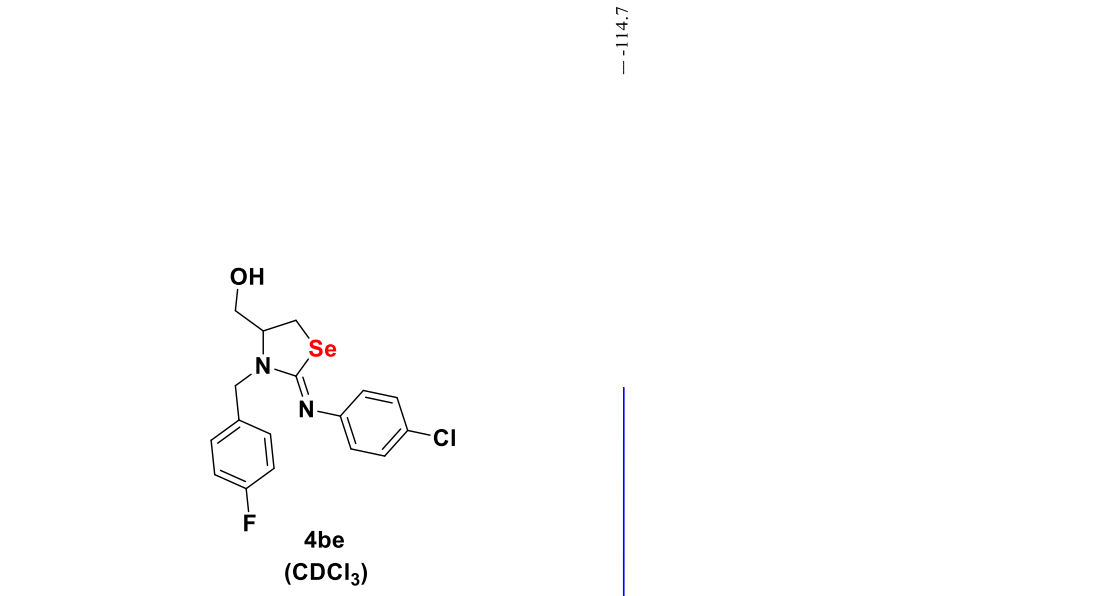
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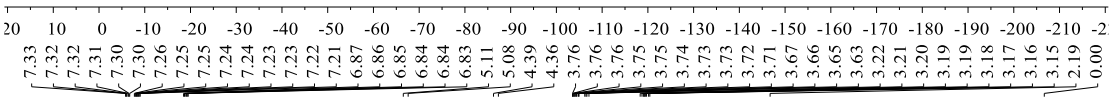
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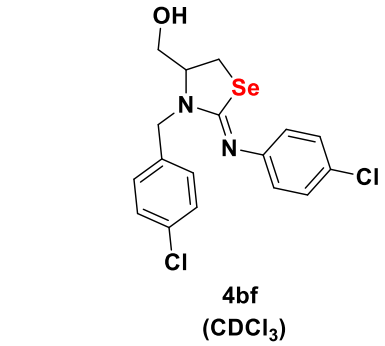
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Cl
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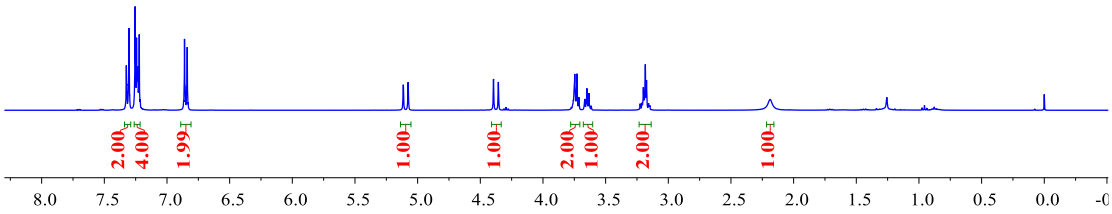
(CDCl3)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2.00
1.00
2.00
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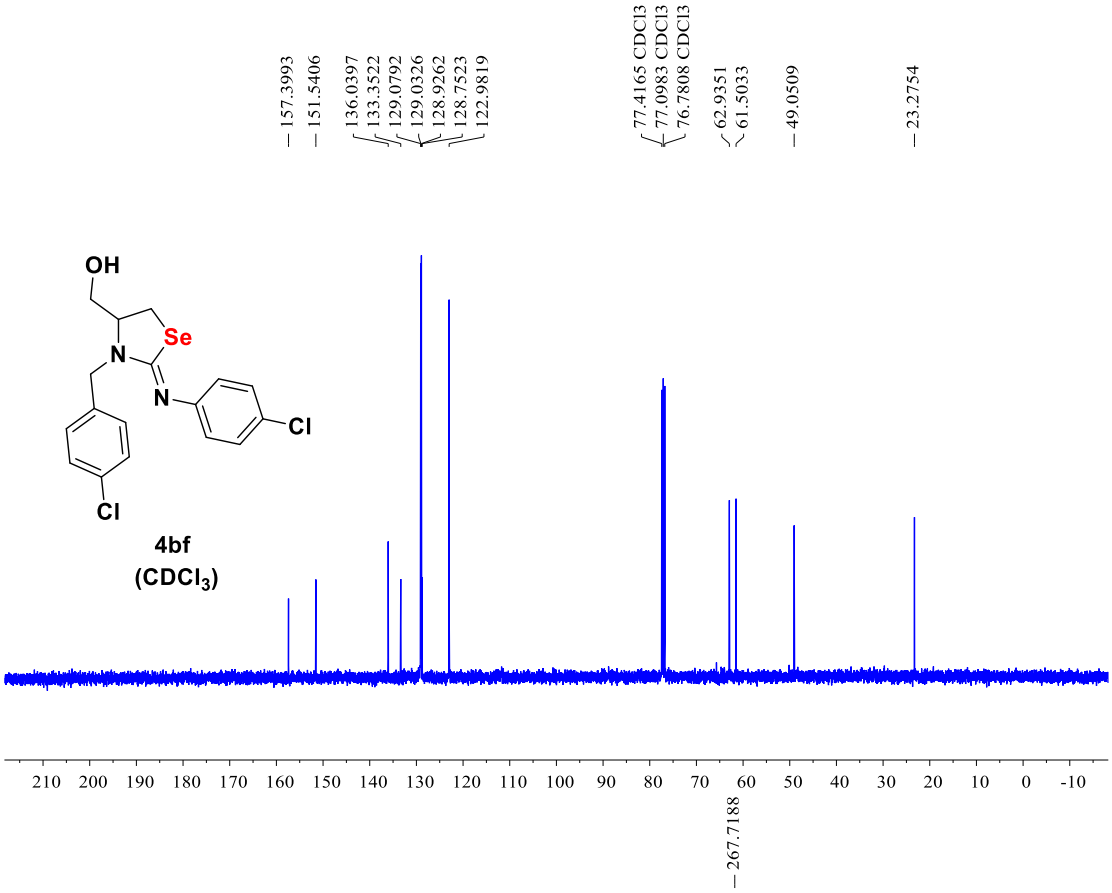
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N
Cl
Cl
4bf
(CDCl3)
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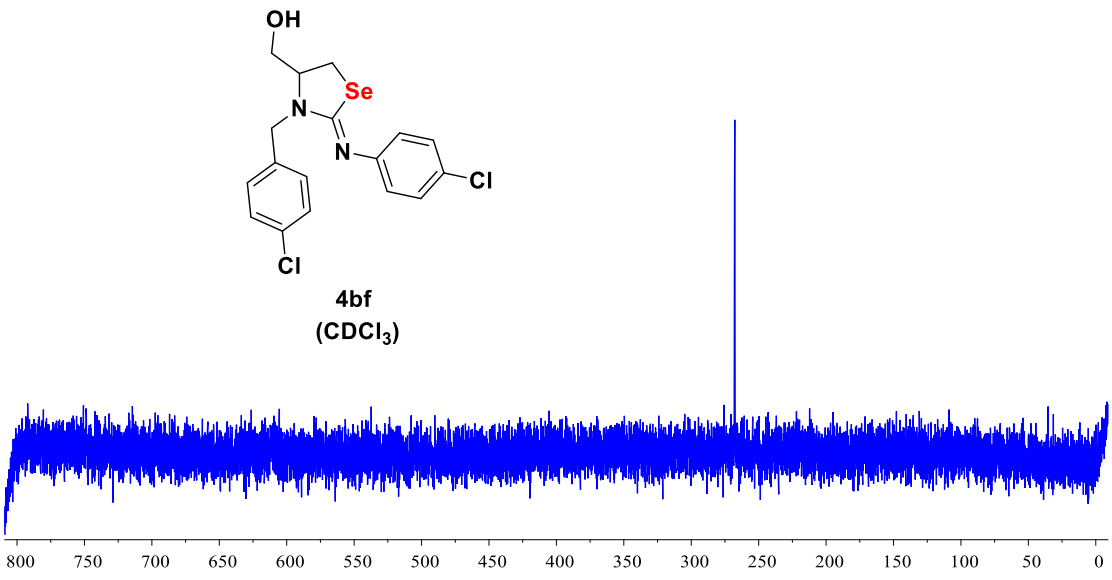
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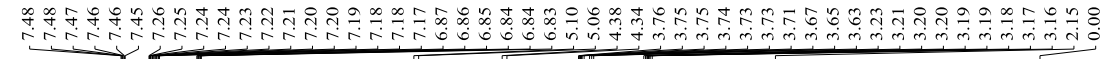
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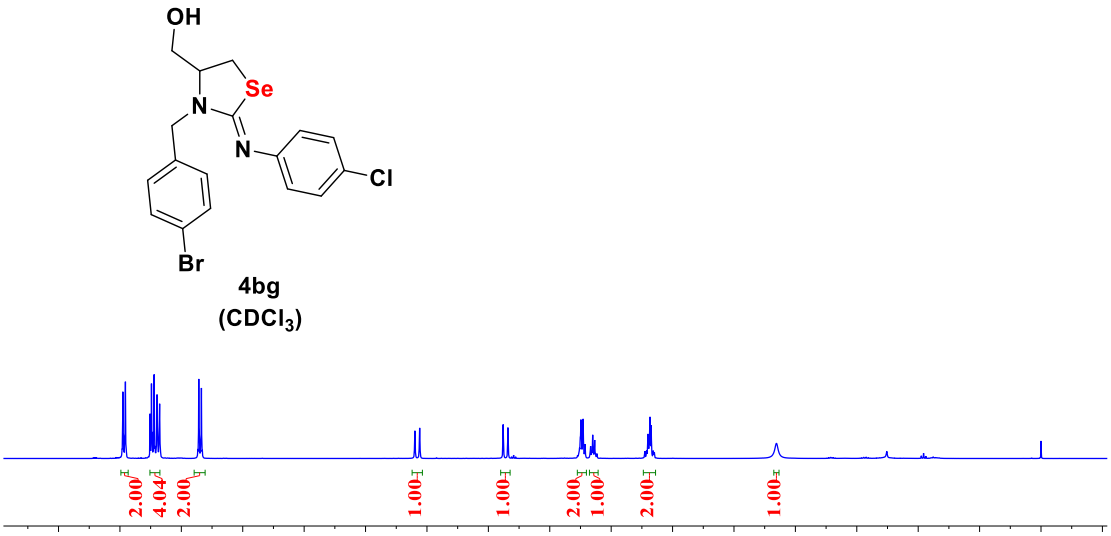
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Cl
Br
4bg
(CDCl3)
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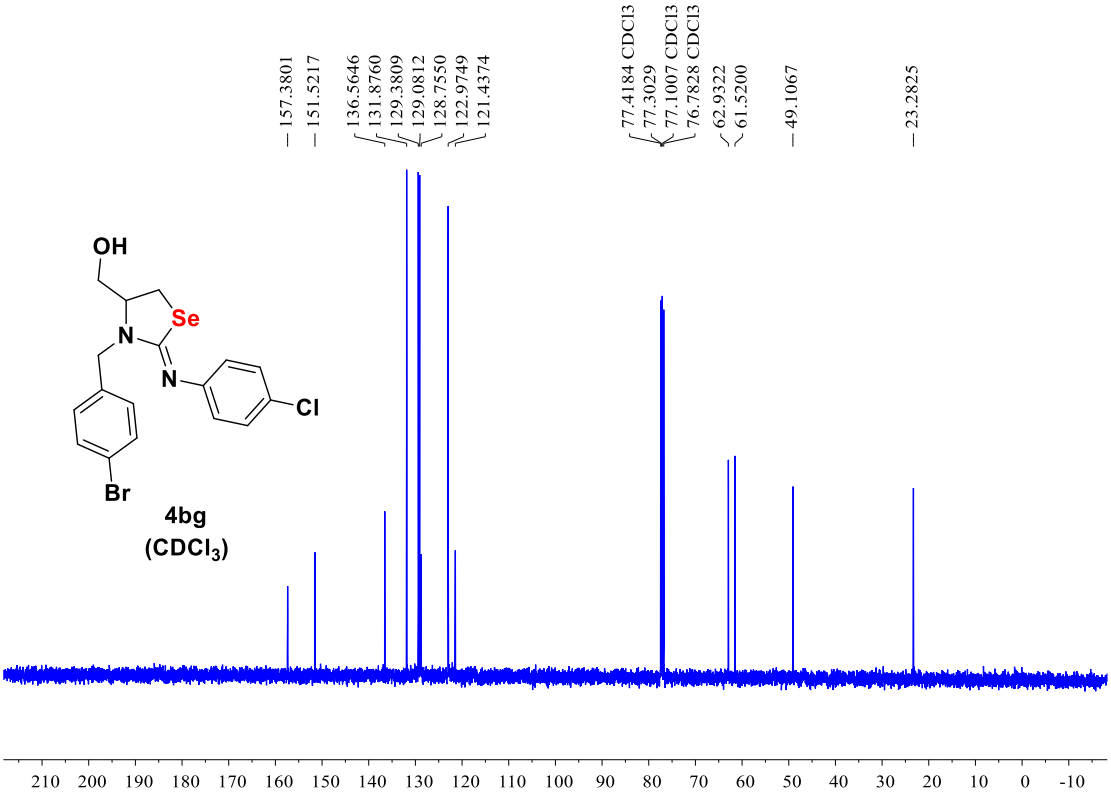
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OH
Se
N
N
Cl
Br
4bg
(CDCl3)
210
200
190
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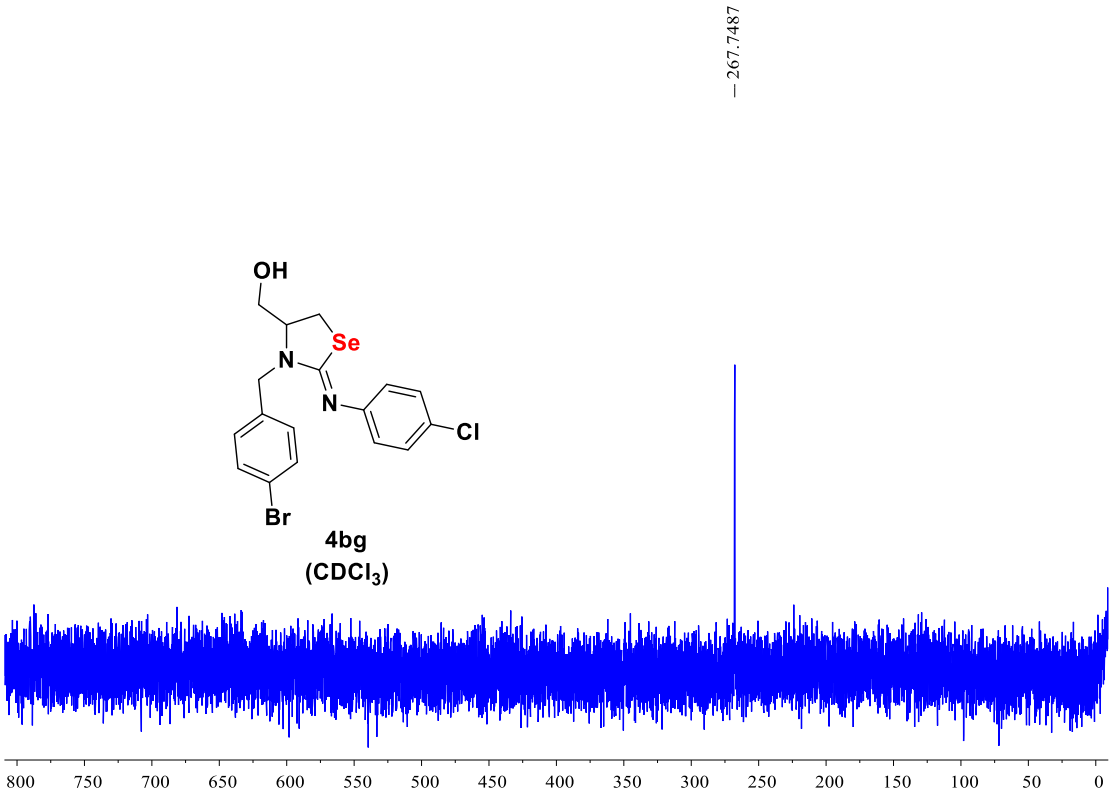
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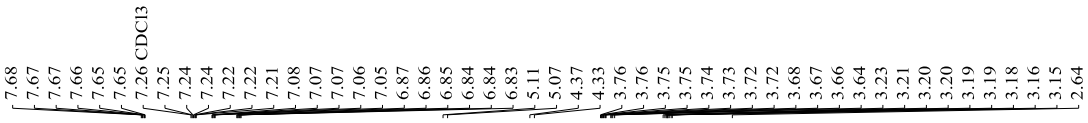
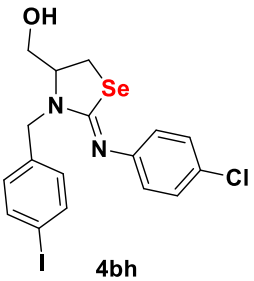
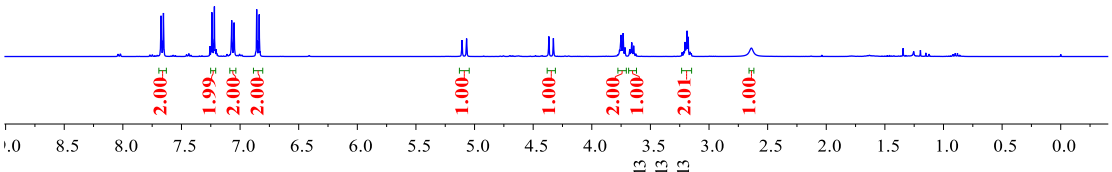
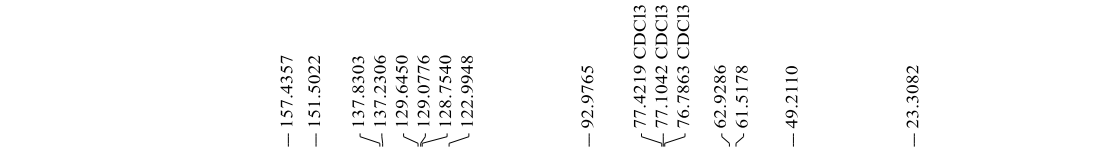
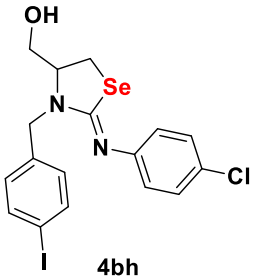




4bh
($CDCl_3$)







4bh
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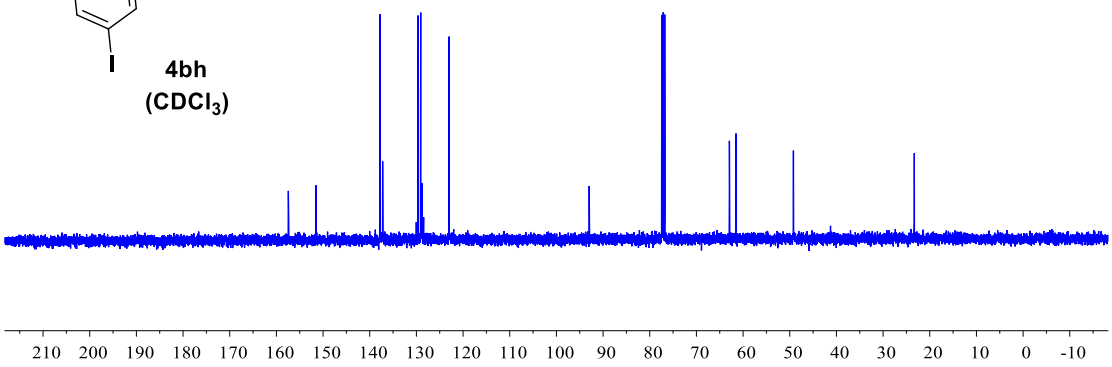

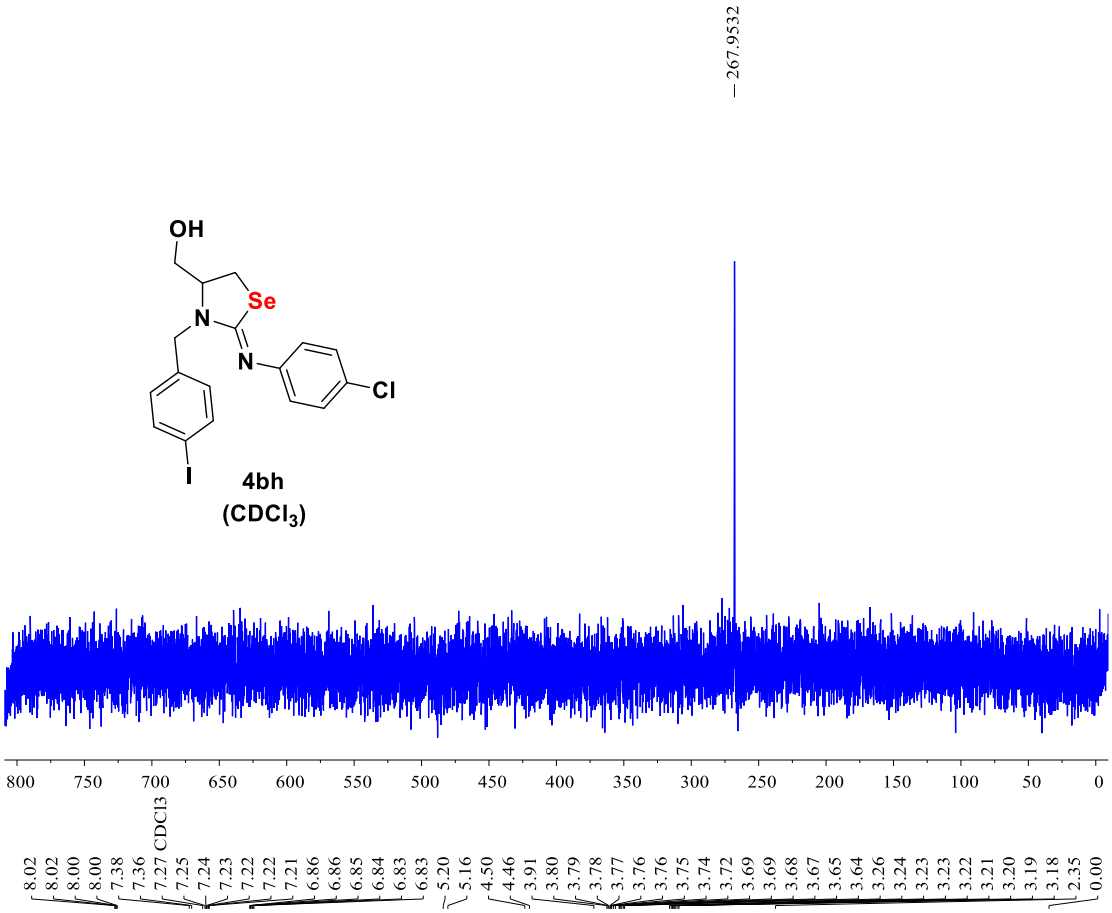
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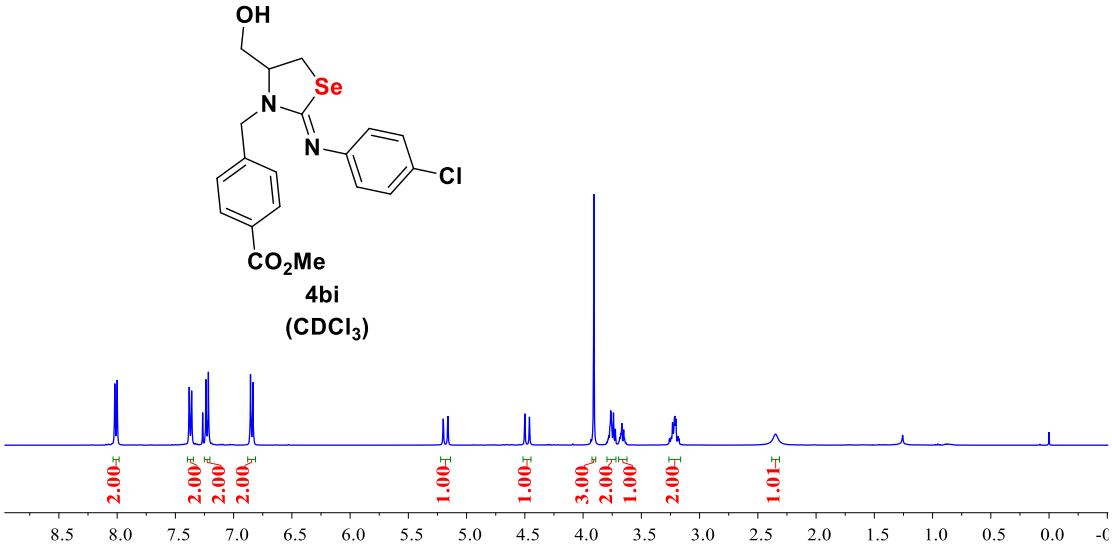
Cl
I
4bh
(CDCl3)
CDCl3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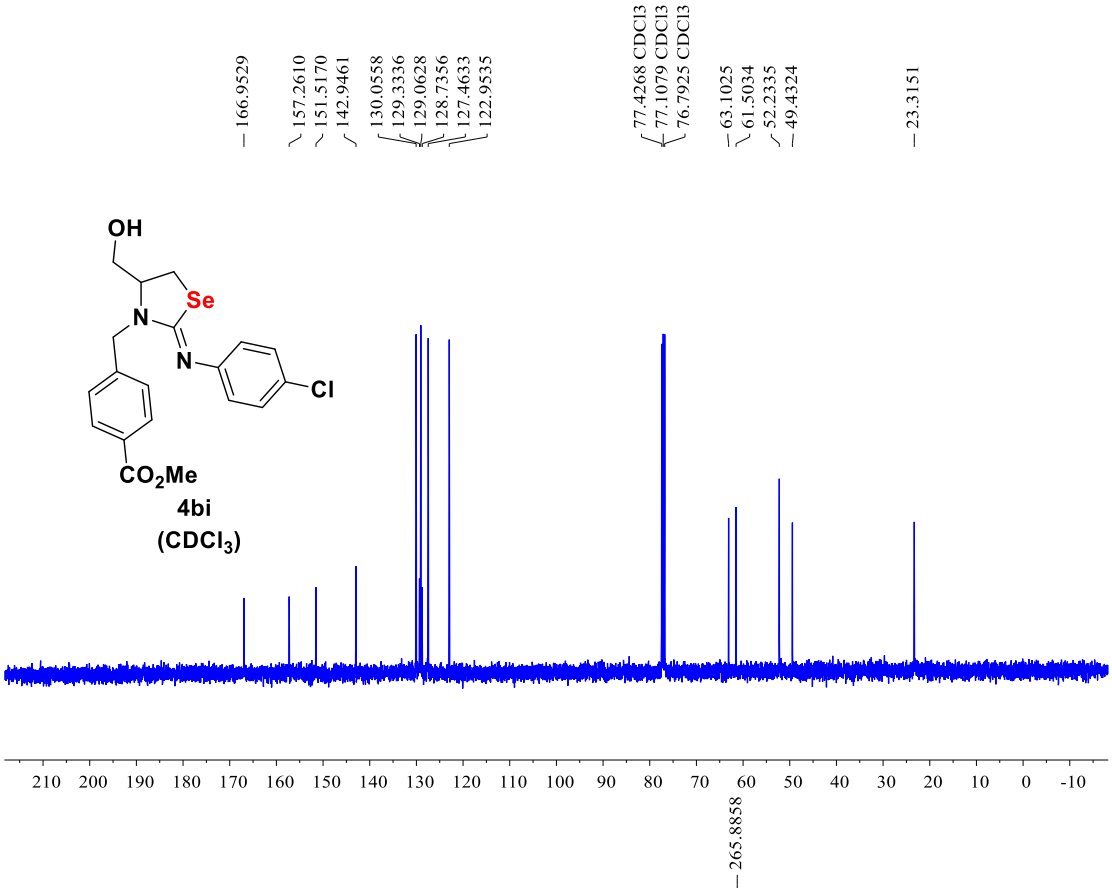
N
Cl
CO2Me
4bi
(CDCl3)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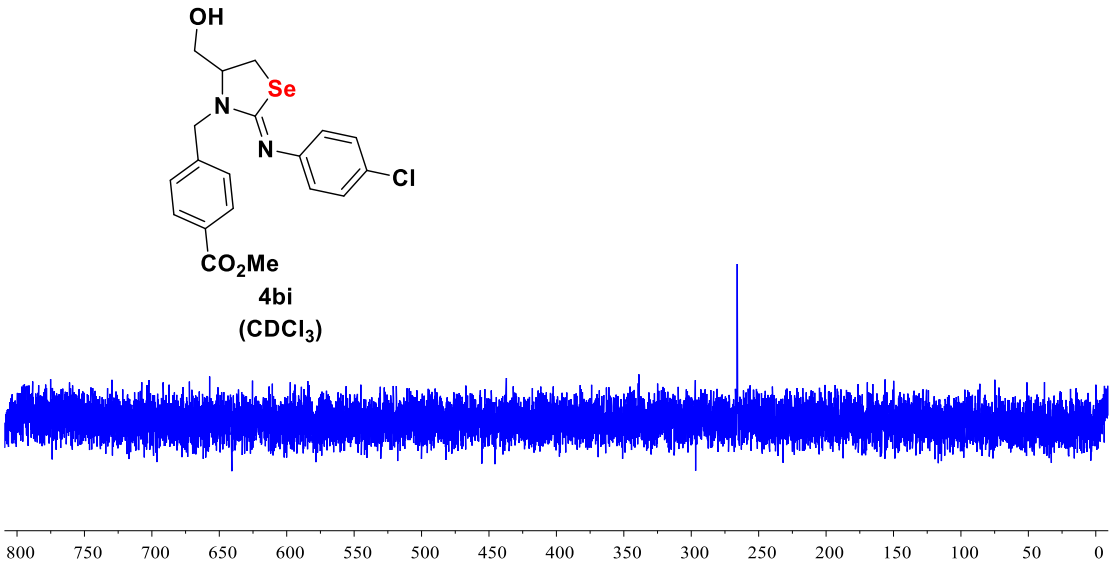
122.9535
77.4268 CDCl3
77.1079 CDCl3
76.7925 CDCl3
63.1025
61.5034
52.2335
49.4324
23.3151
OH
Se
N
N
Cl
CO2Me
4bi
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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N
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4bi
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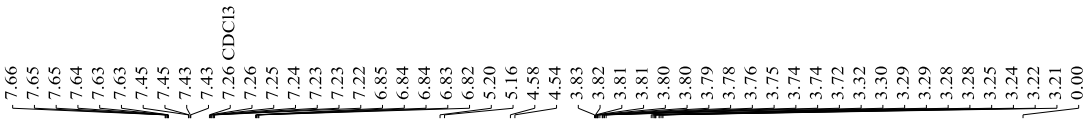
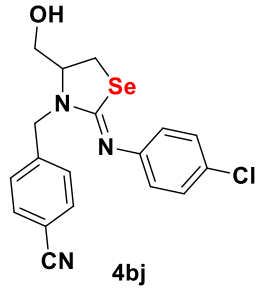
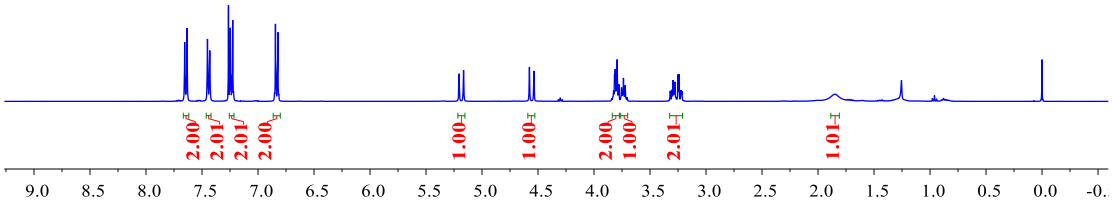




4bj
($CDCl_3$)



4bj
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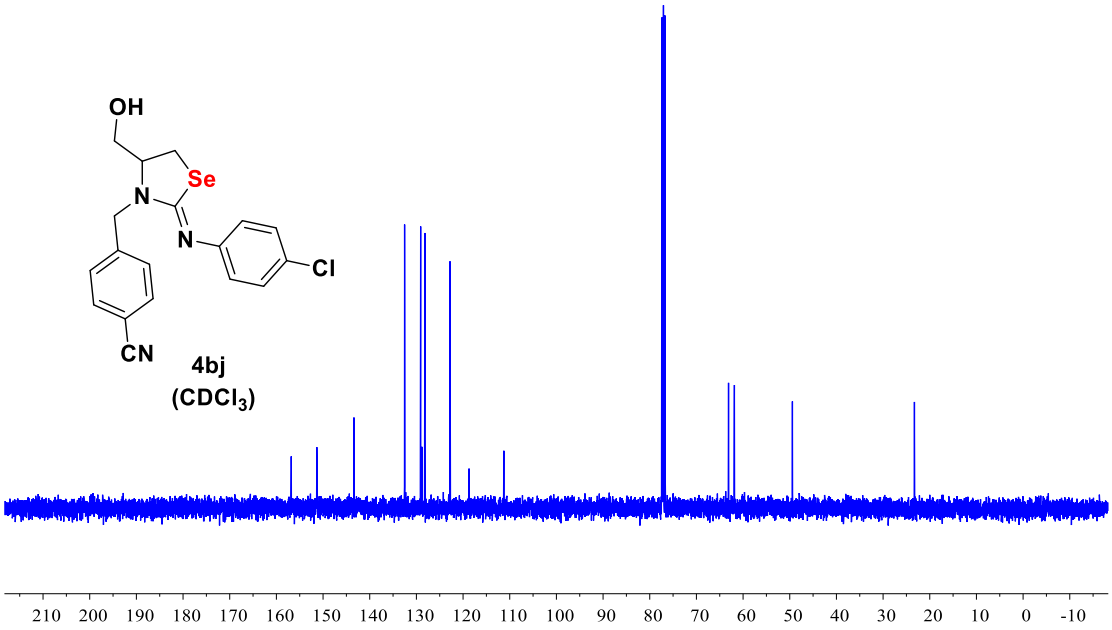

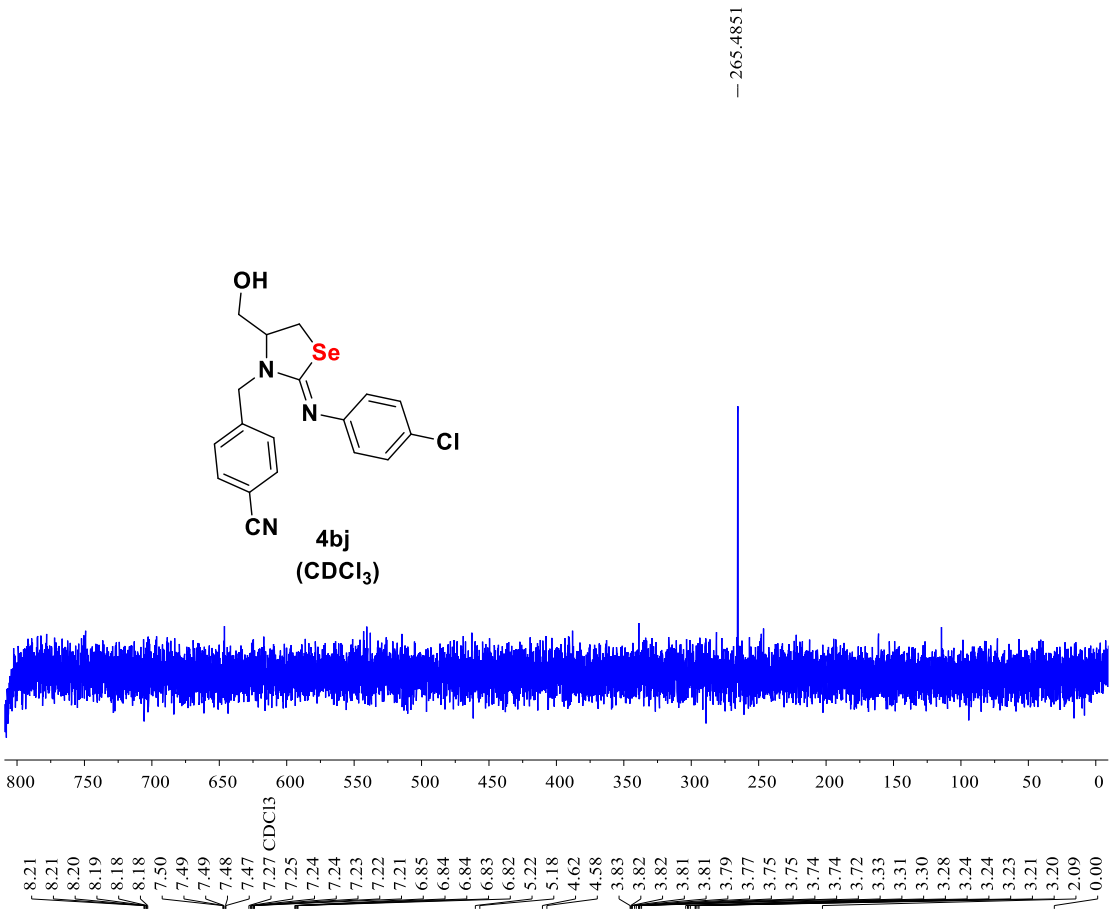
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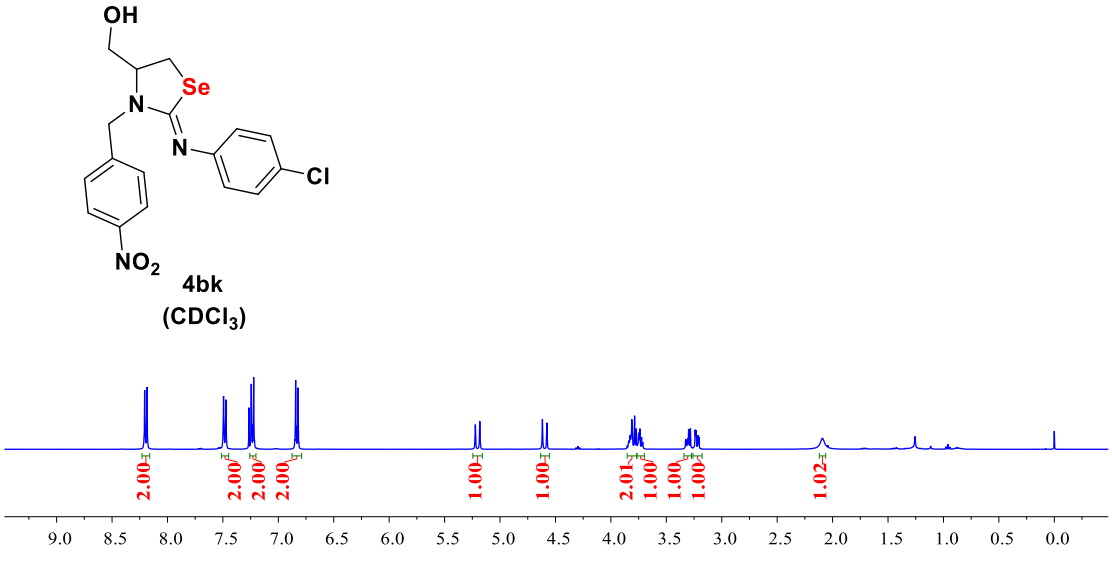
Cl
CN
4bj
(CDCl3)
CDCl3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Se
N
N
Cl
NO2
4bk
(CDCl3)
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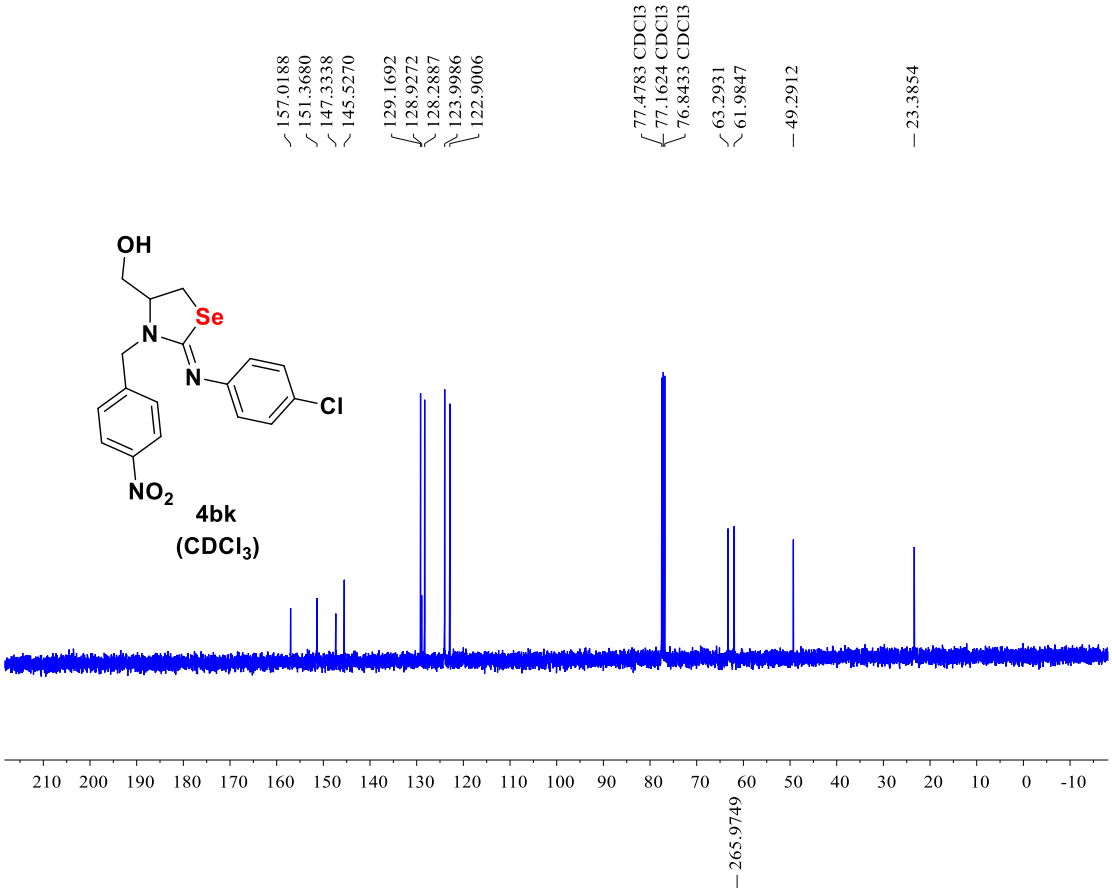
2.00
2.00
2.00
1.00
1.00
2.01
1.00
1.00
1.00
1.02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145.5270
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128.9272
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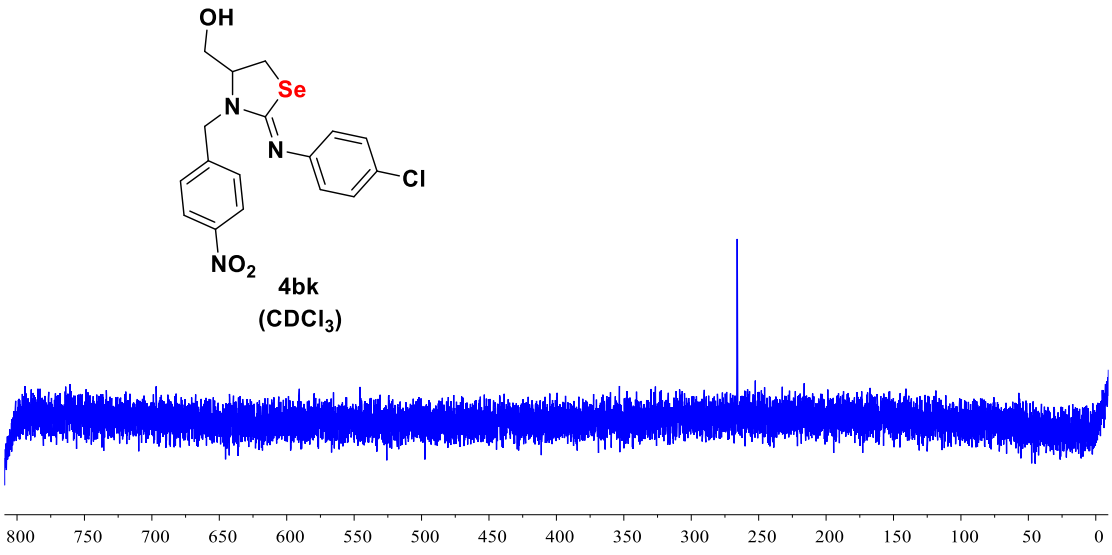
122.9006
77.4783 CDCl3
77.1624 CDCl3
76.8433 CDCl3
63.2931
61.9847
49.2912
23.3854
OH
Se
N
N
Cl
NO2
4bk
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Cl
NO2
4bk
(CDCl3)
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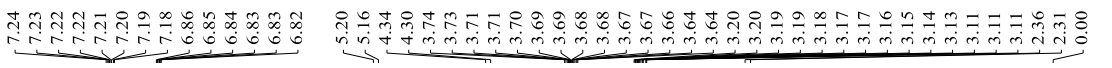
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7.22
7.22
7.21
7.20
7.19
7.18
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6.85
6.84
6.83
6.83
6.82
5.20
5.16
4.34
4.30
3.74
3.73
3.71
3.71
3.70
3.69
3.69
3.68
3.68
3.67
3.67
3.66
3.64
3.64
3.20
3.20
3.19
3.19
3.18
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3.13
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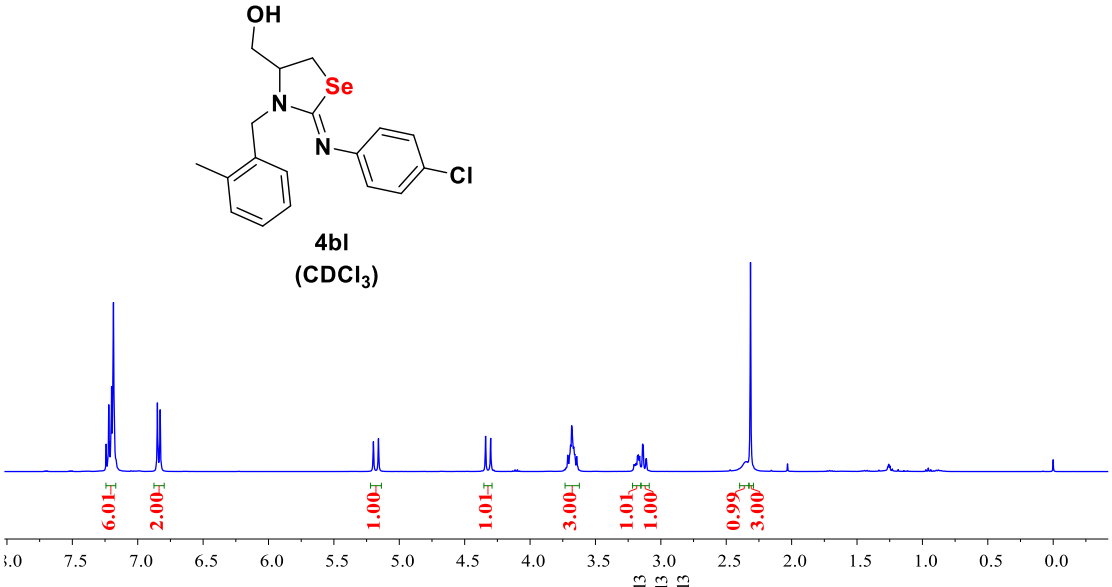
2.36
2.31
0.00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Se
N
N
Cl
4bl
(CDCl3)
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2.00
1.00
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3.00
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1.00
0.99
3.00
7.5
7.0
6.5
6.0
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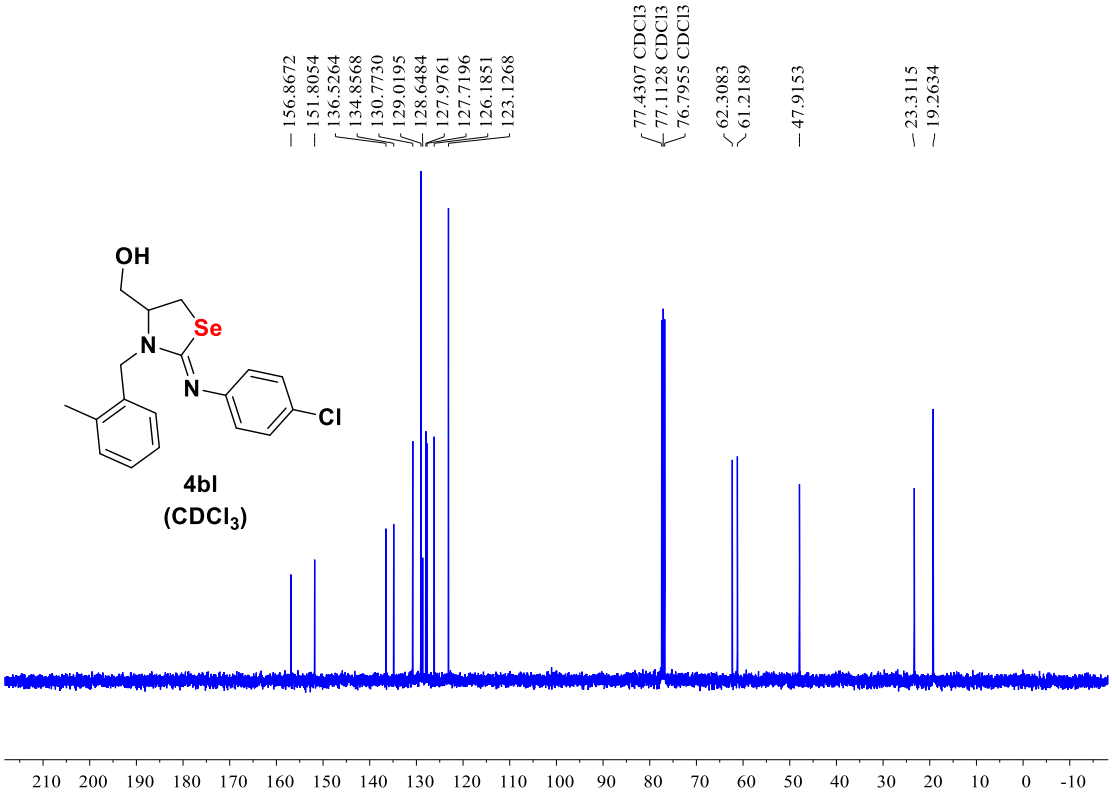
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126.1851
123.1268
77.4307 CDCl3
77.1128 CDCl3
76.7955 CDCl3
62.3083
61.2189
47.9153
23.3115
19.2634
OH
Se
N
N
Cl
4bl
(CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
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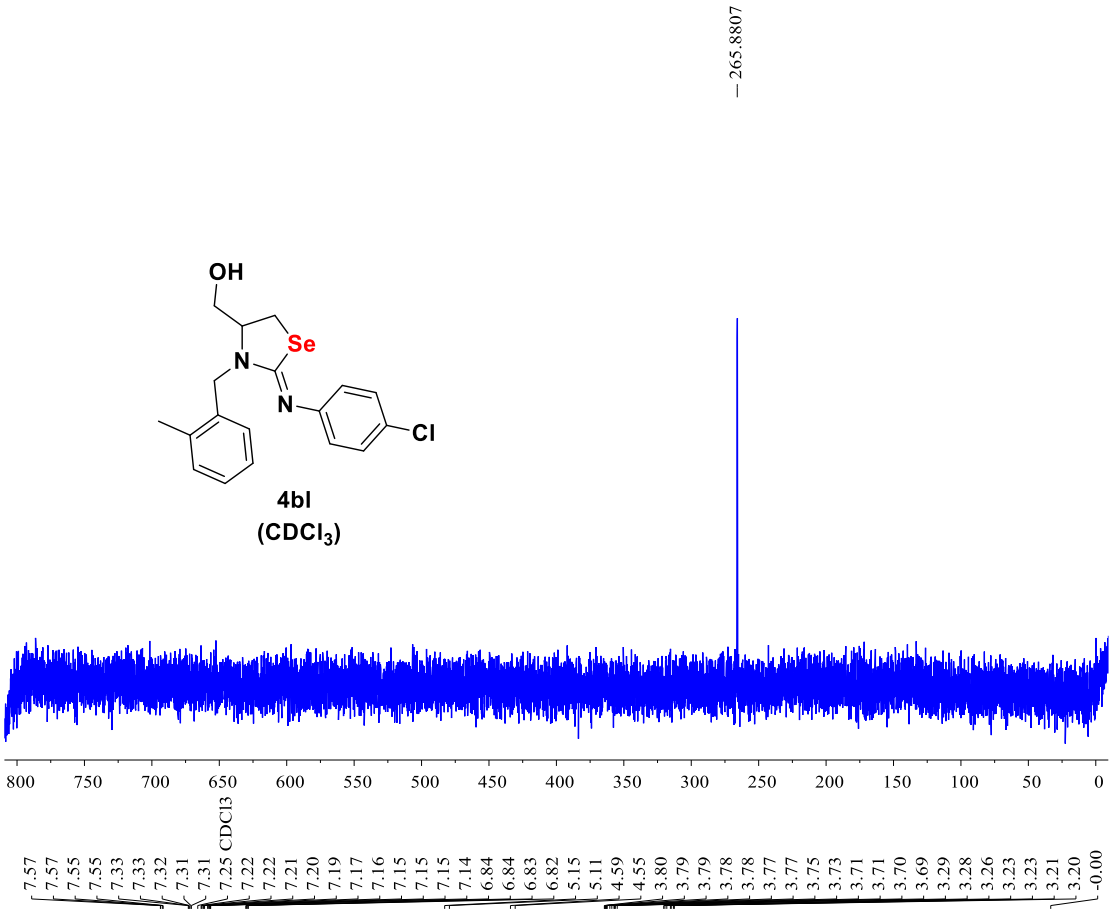
60
50
40
30
20
10
0
-10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Cl
4bl
(CDCl3)
265.8807
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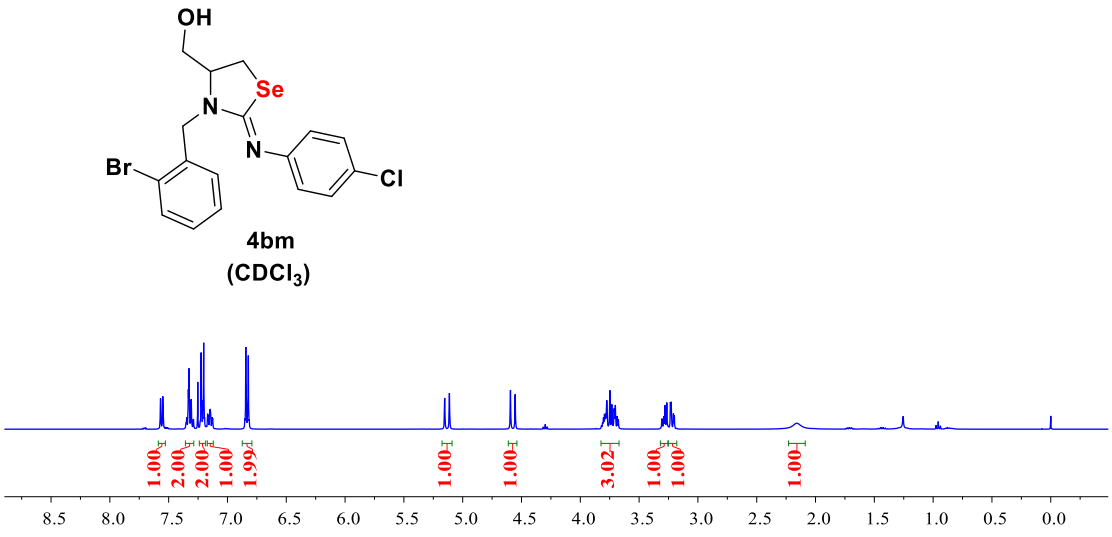
7.57 7.57 7.55 7.55 7.33 7.33 7.32 7.31 7.31 7.25 CDCl3 7.22 7.22 7.21 7.20 7.19 7.17 7.16 7.15 7.15 7.15 7.14 6.84 6.84 6.83 6.82 5.15 5.11 4.59 4.55 3.80 3.79 3.79 3.78 3.78 3.77 3.77 3.75 3.73 3.71 3.71 3.70 3.69 3.29 3.28 3.26 3.23 3.23 3.21 3.20 -0.00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Se
N
N
Br
Cl
4bm
(CDCl3)
1.00 2.00 2.00 1.00 1.99 1.00 1.00 3.02 1.00 1.00 1.00
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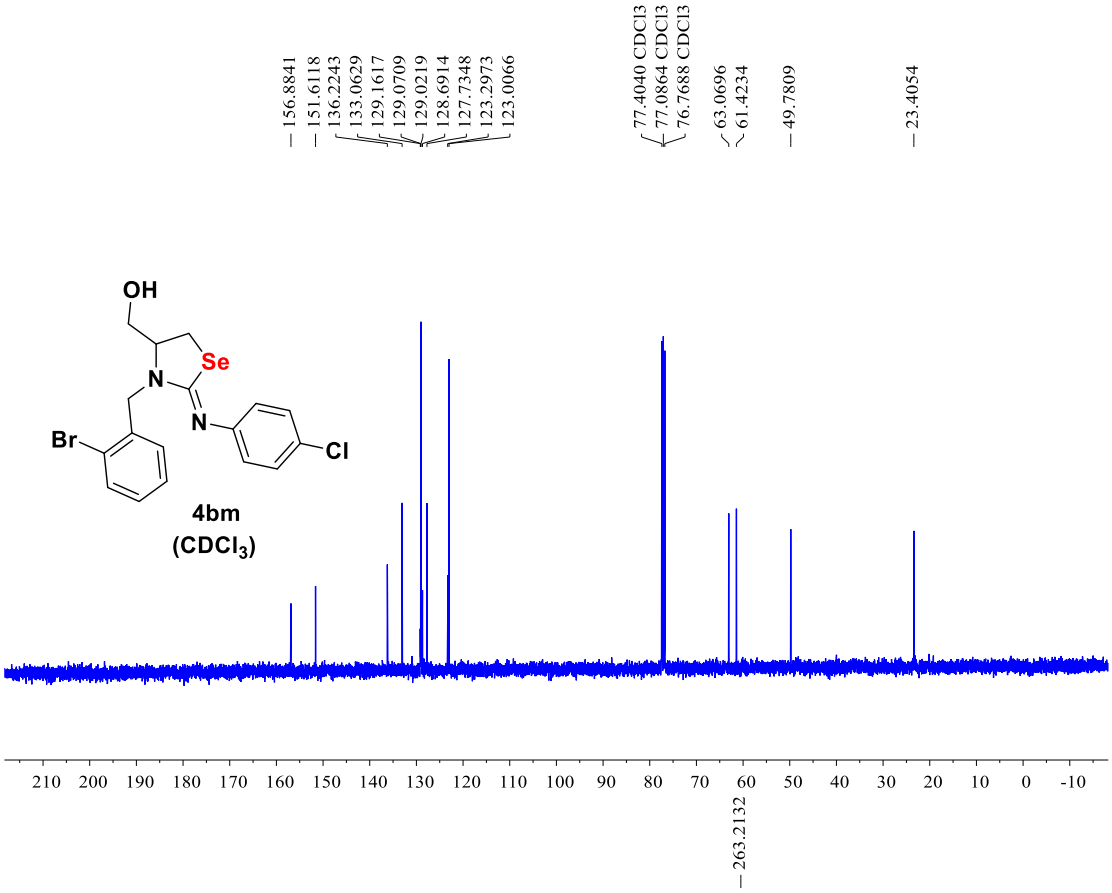
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123.0066
77.4040 CDCl3
77.0864 CDCl3
76.7688 CDCl3
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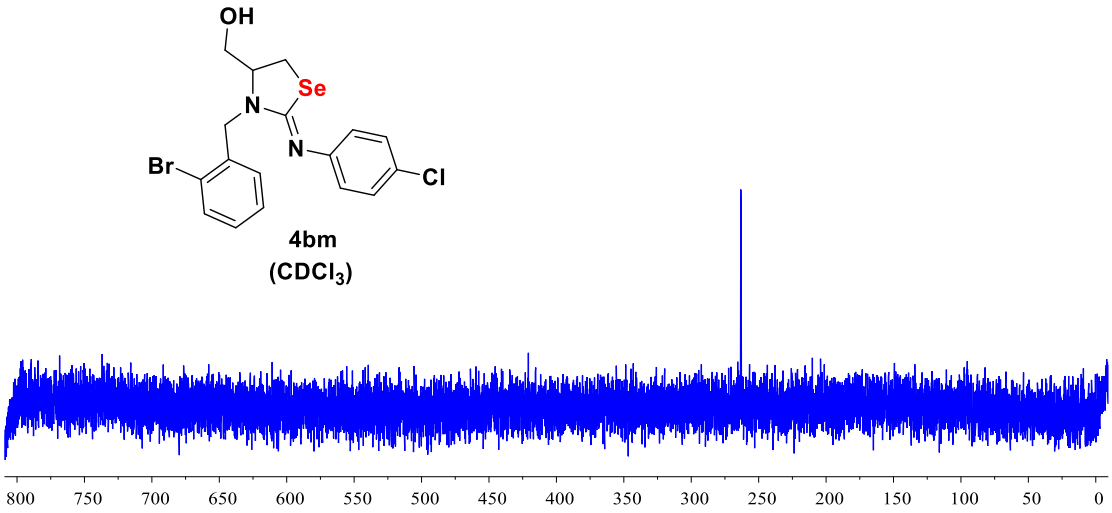
49.7809
23.4054
OH
Se
N
N
Br
Cl
4bm
(CDCl3)
263.2132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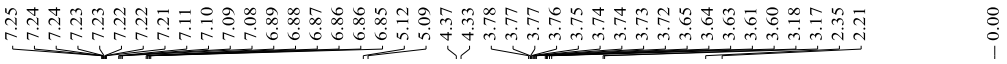
N
N
Br
Cl
4bm
(CDCl3)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7.21
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7.09
7.08
6.89
6.88
6.87
6.86
6.86
6.85
5.12
5.09
4.37
4.33
3.78
3.77
3.77
3.76
3.75
3.74
3.74
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3.60
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3.17
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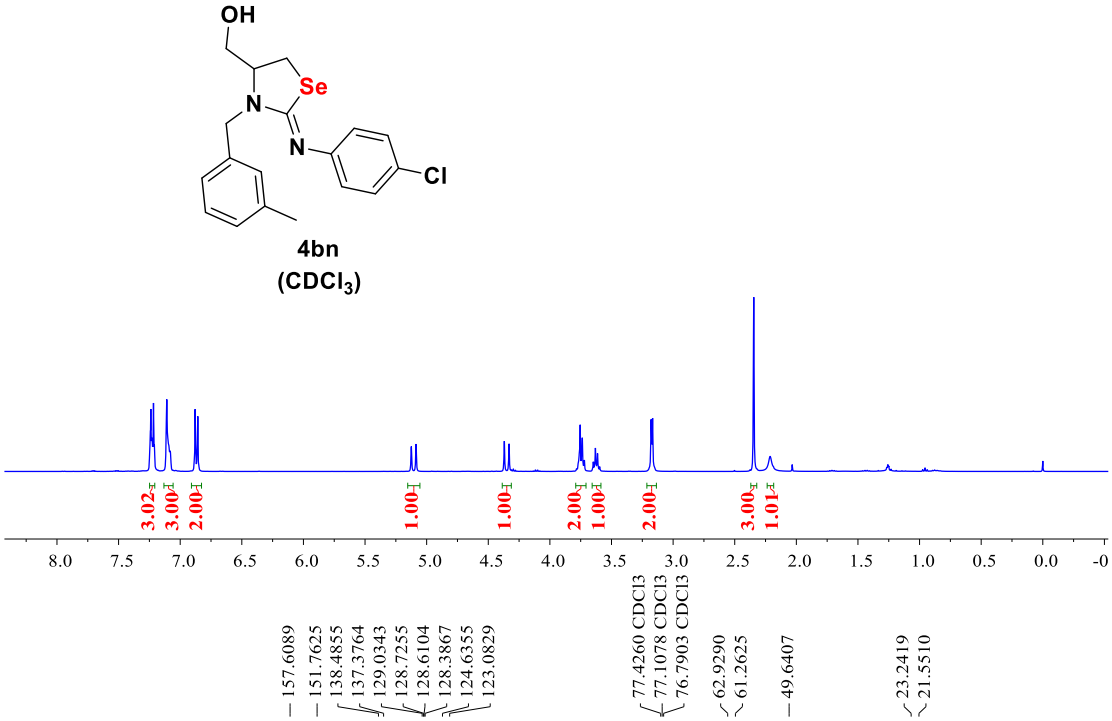
2.21
0.00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Se
N
N
Cl
4bn
(CDCl3)
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2.00
1.00
1.00
2.00
1.00
2.00
3.00
1.01
8.0
7.5
7.0
6.5
6.0
5.5
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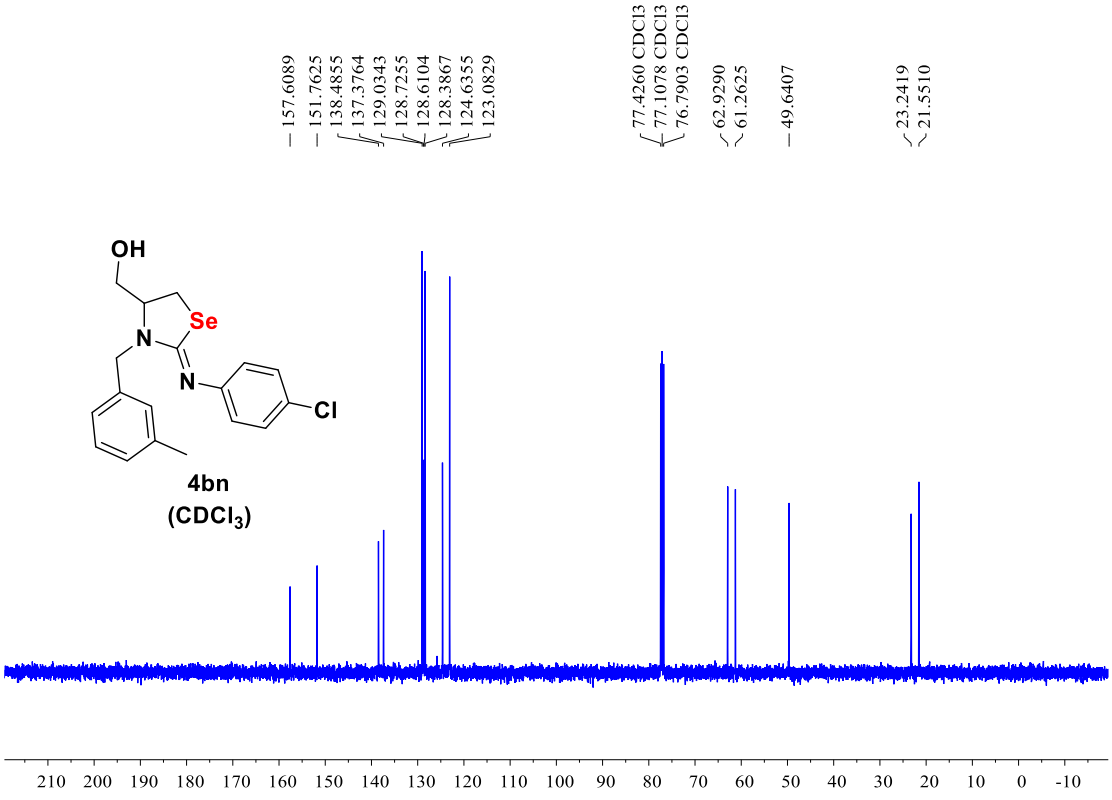
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123.0829
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76.7903 CDCl3
62.9290
61.2625
49.6407
23.2419
21.5510
OH
Se
N
N
Cl
4bn
(CDCl3)
210
200
190
180
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160
150
140
130
120
110
100
90
80
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60
50
40
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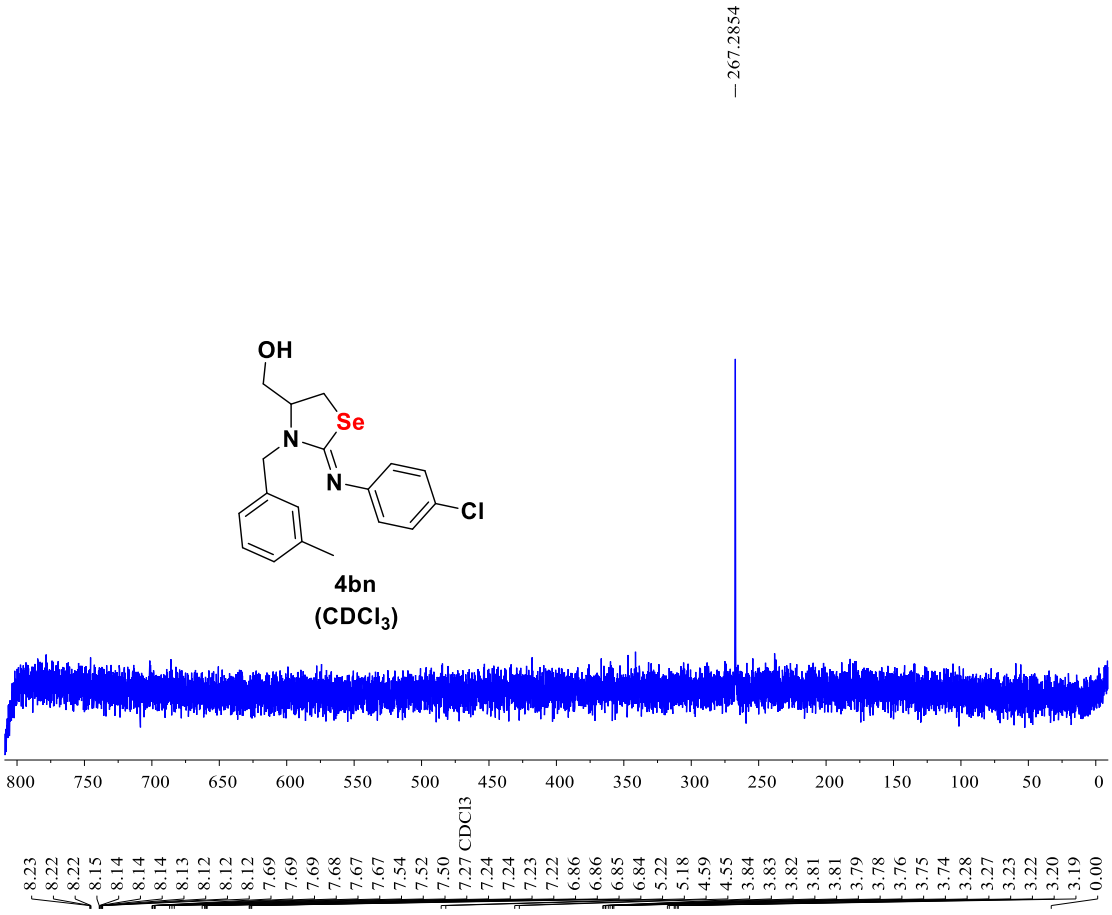
20
10
0
-10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Cl
4bn
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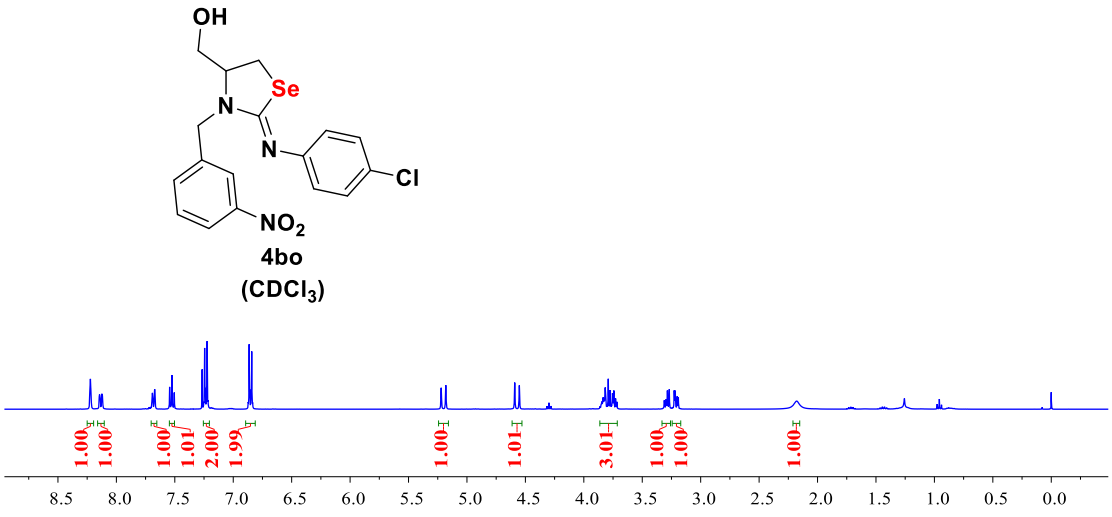
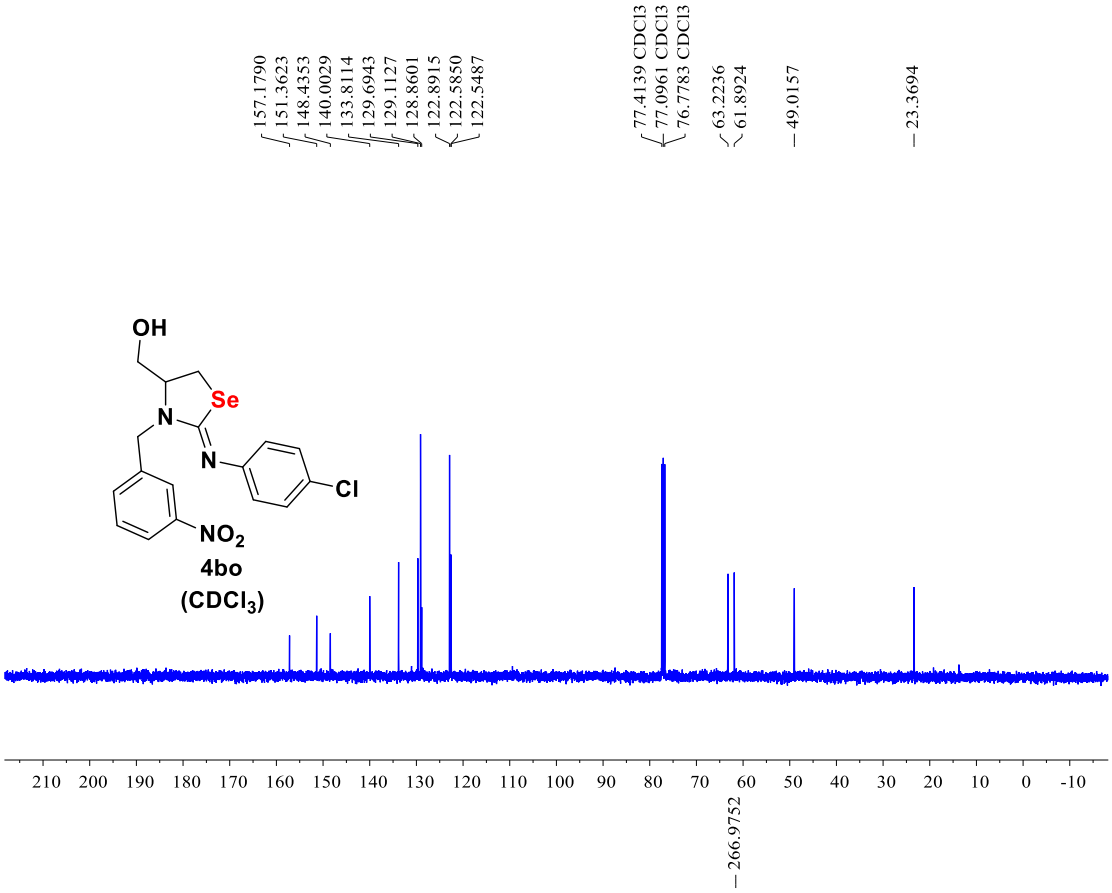

OH
Se
N
N
Cl
NO2
4bo
(CDCl3)
1.00 1.00 1.00 1.01 2.00 1.99 1.00 1.01 3.01 1.00 1.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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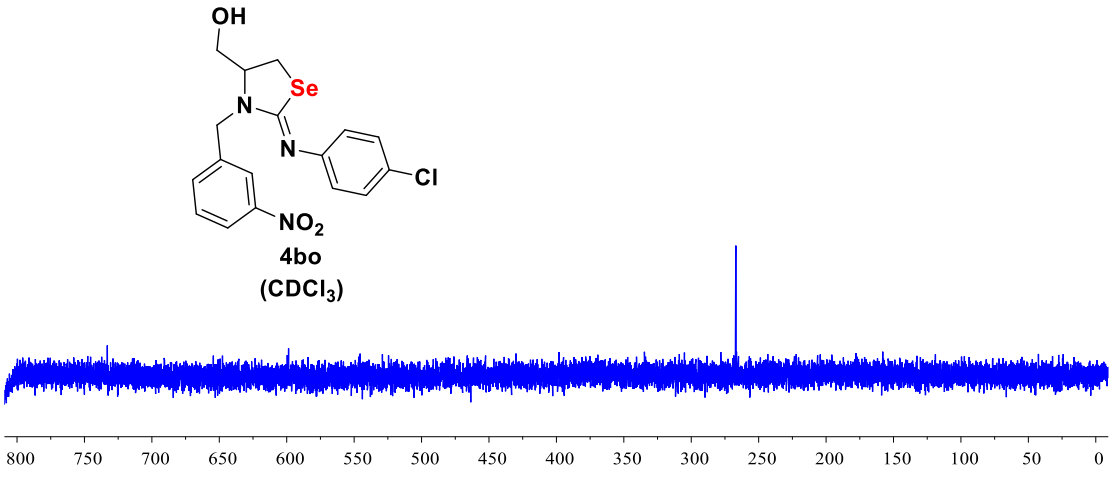
77.0961 CDCl3
76.7783 CDCl3
63.2236
61.8924
49.0157
23.3694
OH
Se
N
N
Cl
NO2
4bo
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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4bo
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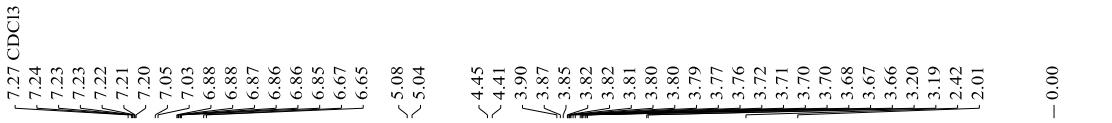
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7.03
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6.86
6.86
6.85
6.67
6.65
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5.04
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4.41
3.90
3.87
3.85
3.82
3.82
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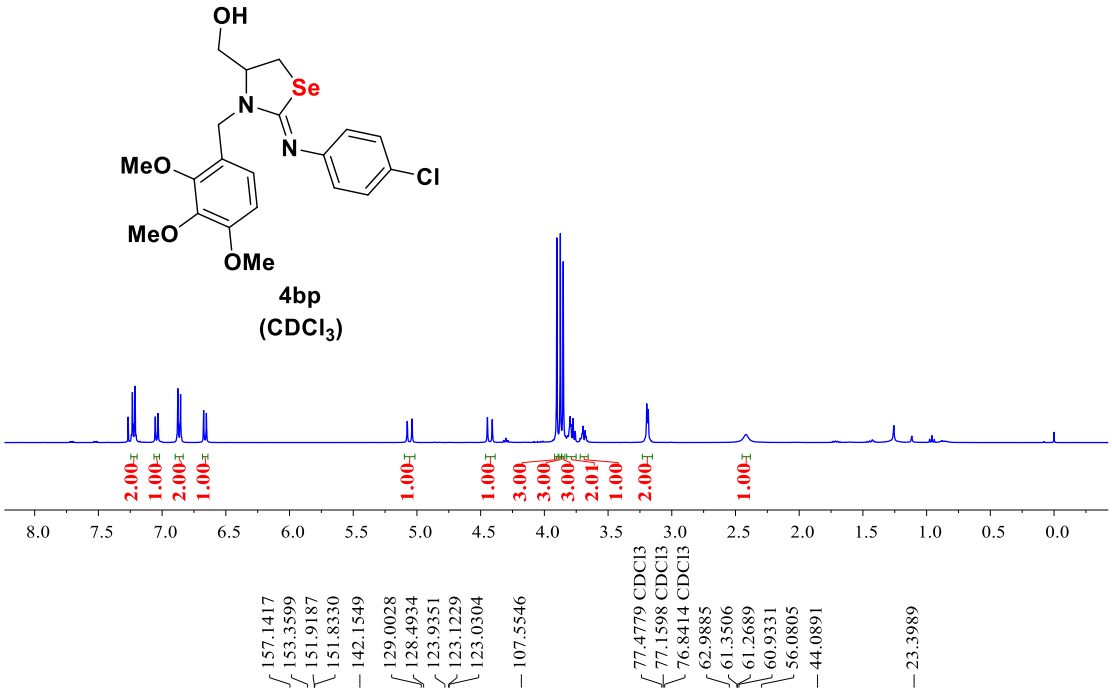
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Se
N
N
Cl
MeO
MeO
OMe
4bp
(CDCl3)
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1.00
2.00
1.00
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3.00
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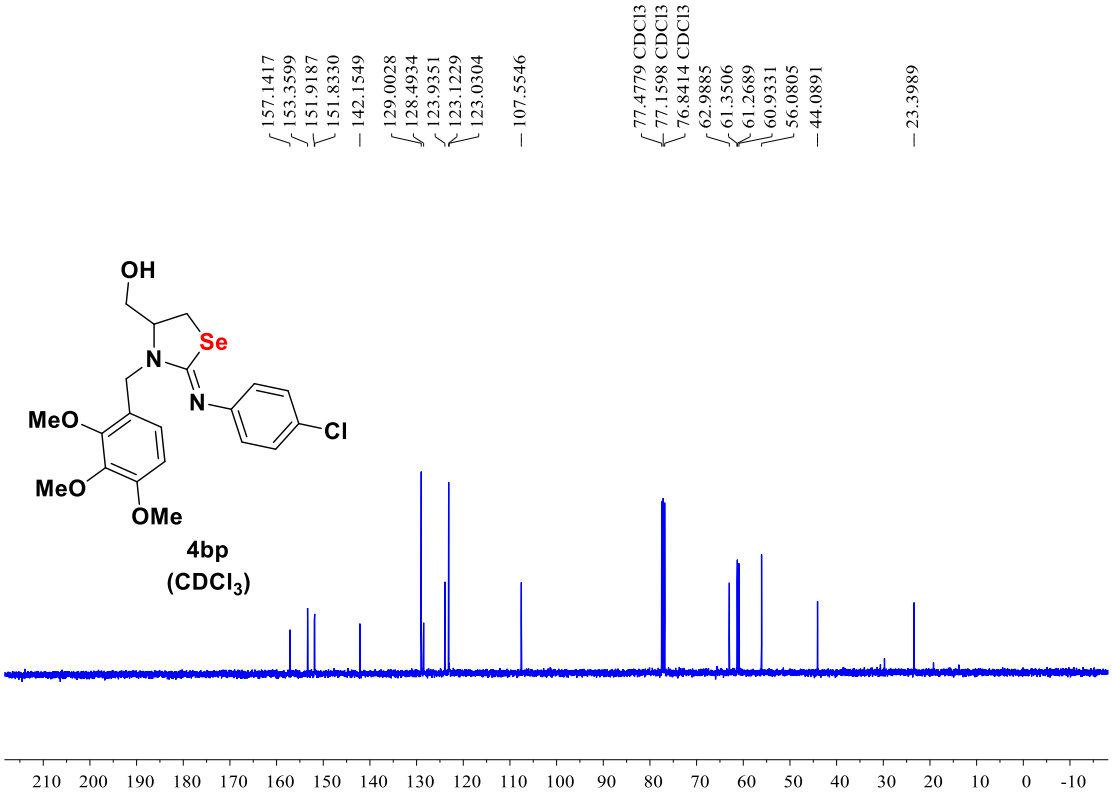
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77.1598 CDCl3
76.8414 CDCl3
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61.2689
60.9331
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44.0891
23.3989
OH
Se
N
N
Cl
MeO
MeO
OMe
4bp
(CDCl3)
210
200
190
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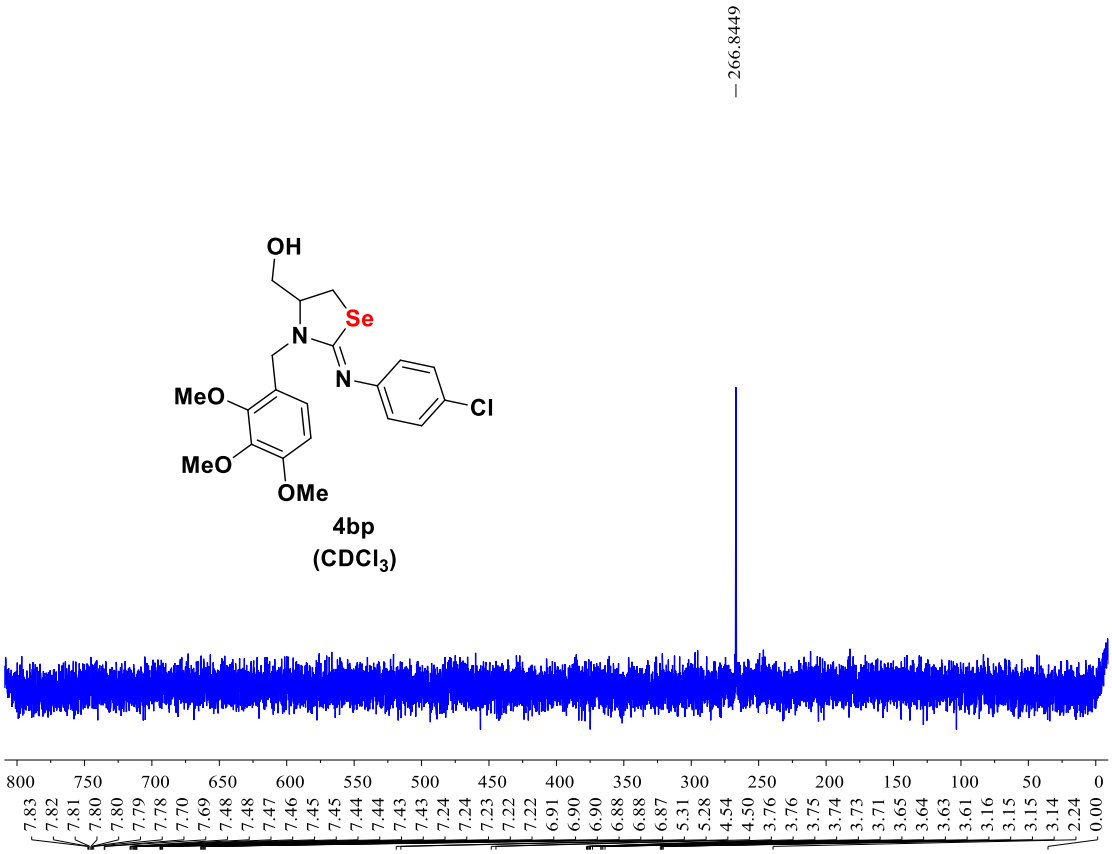
0
-10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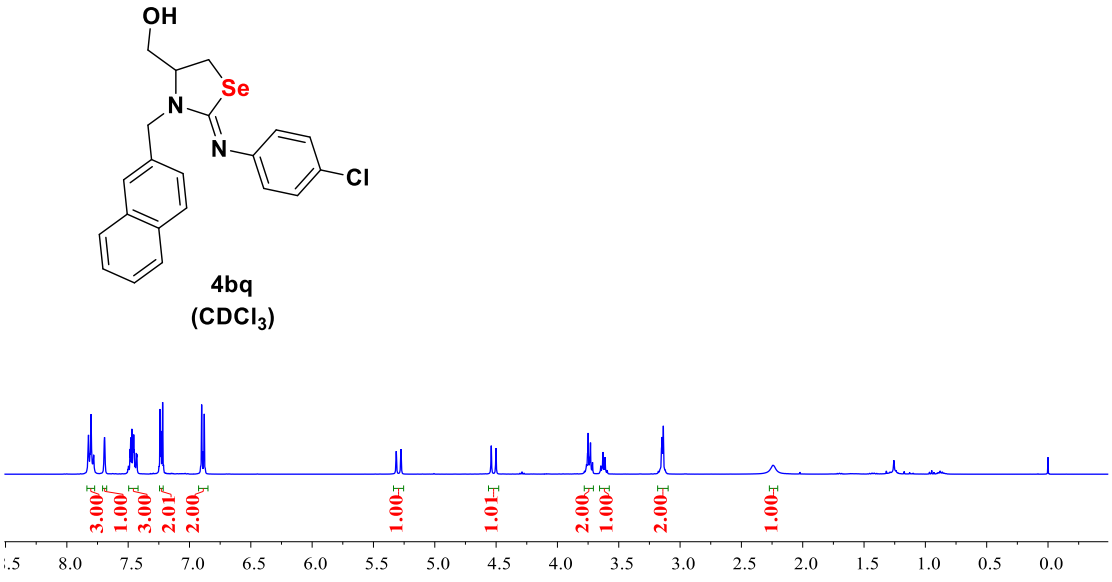
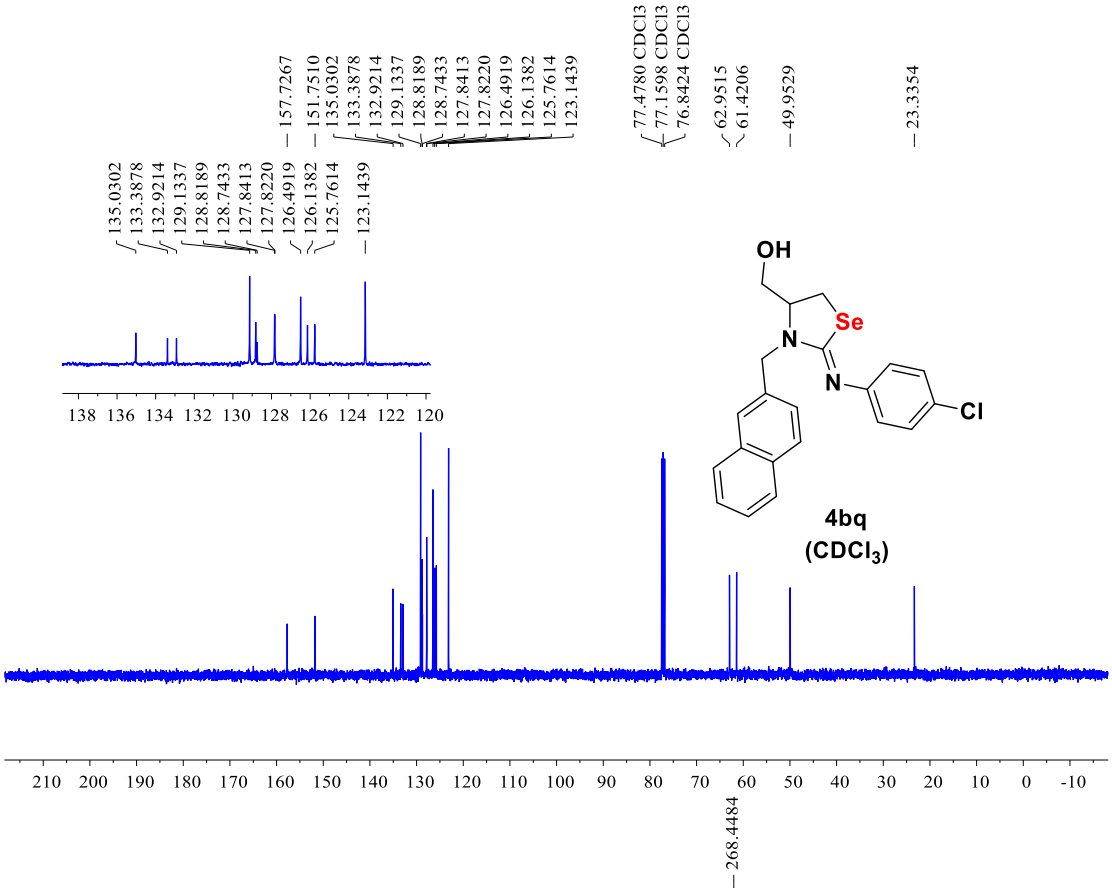
N
Cl
MeO
MeO
OMe
4bp
(CDCl3)
800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0
7.83 7.82 7.81 7.80 7.80 7.79 7.78 7.70 7.69 7.48 7.48 7.47 7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.24 7.24 7.23 7.22 7.22 6.91 6.90 6.90 6.88 6.88 6.87 5.31 5.28 4.54 4.50 3.76 3.76 3.75 3.74 3.73 3.71 3.65 3.64 3.63 3.61 3.16 3.15 3.14 2.24 0.00


OH
Se
N
N
Cl
4bq
(CDCl3)
3.00 1.00 3.00 2.01 2.00 1.00 1.01 2.00 1.00 2.00 1.00
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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132.9214
129.1337
128.8189
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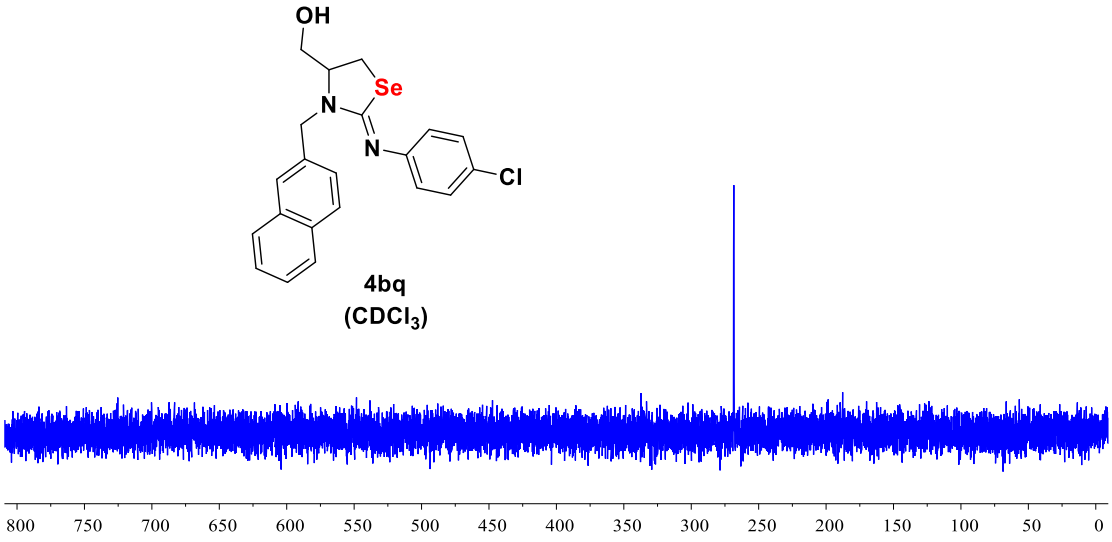
127.8413
127.8220
126.4919
126.1382
125.7614
123.1439
77.4780 CDCl3
77.1598 CDCl3
76.8424 CDCl3
62.9515
61.4206
49.9529
23.3354
OH
Se
N
N
Cl
4bq
(CDCl3)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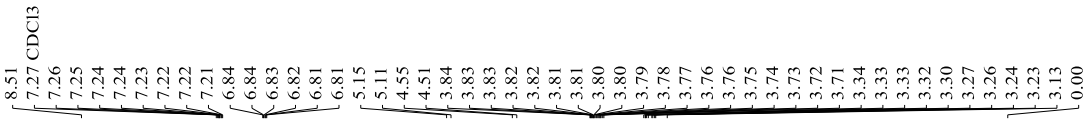
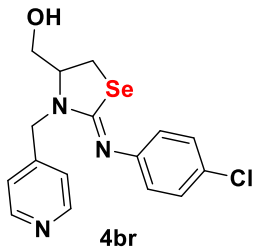
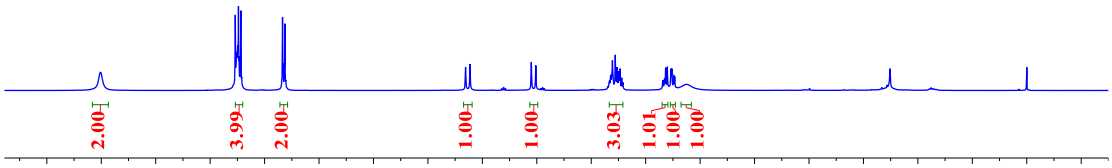
N
N
Cl
4bq
(CDCl3)





4br
($CDCl_3$)



4br
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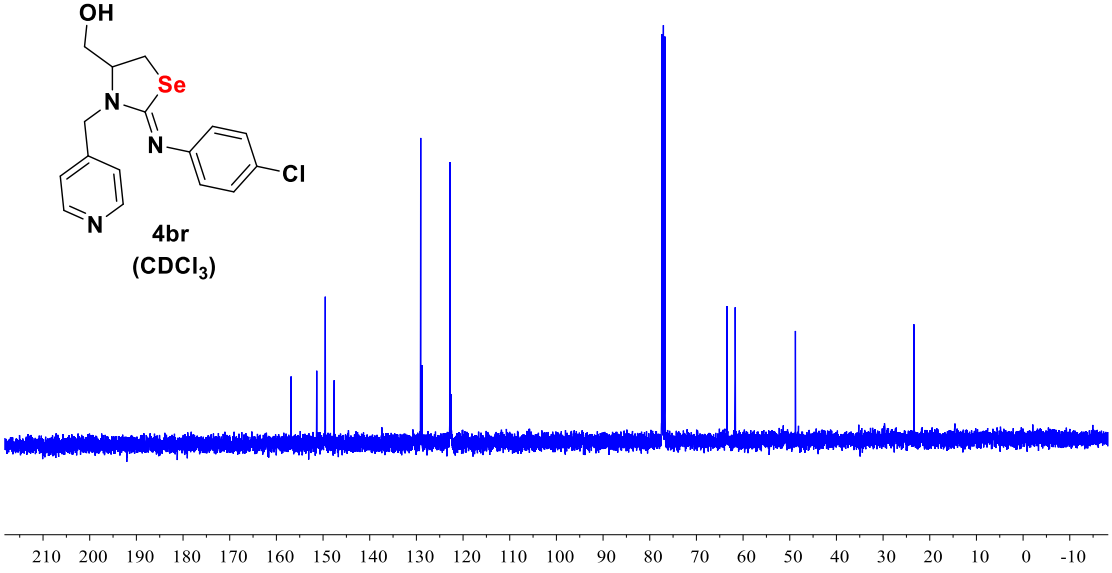

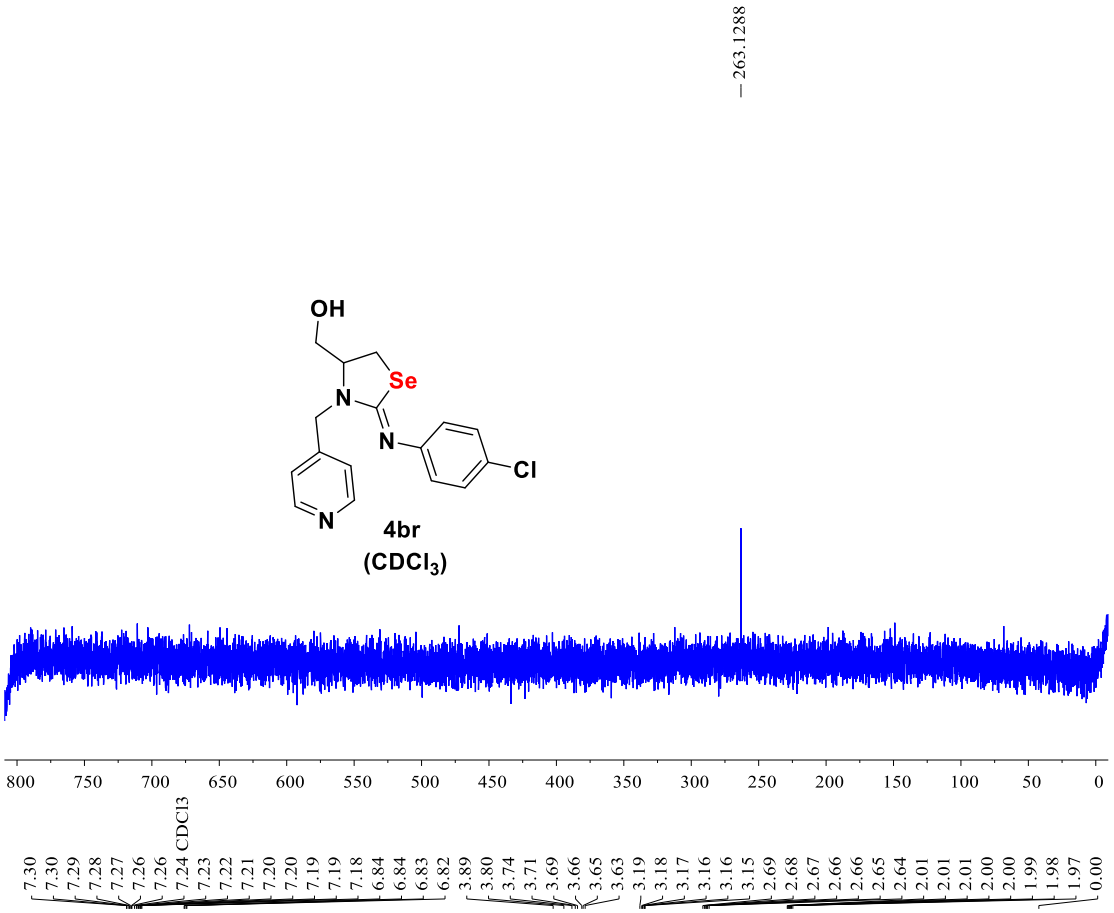
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Se
N
N
Cl
N
4br
(CDCl3)
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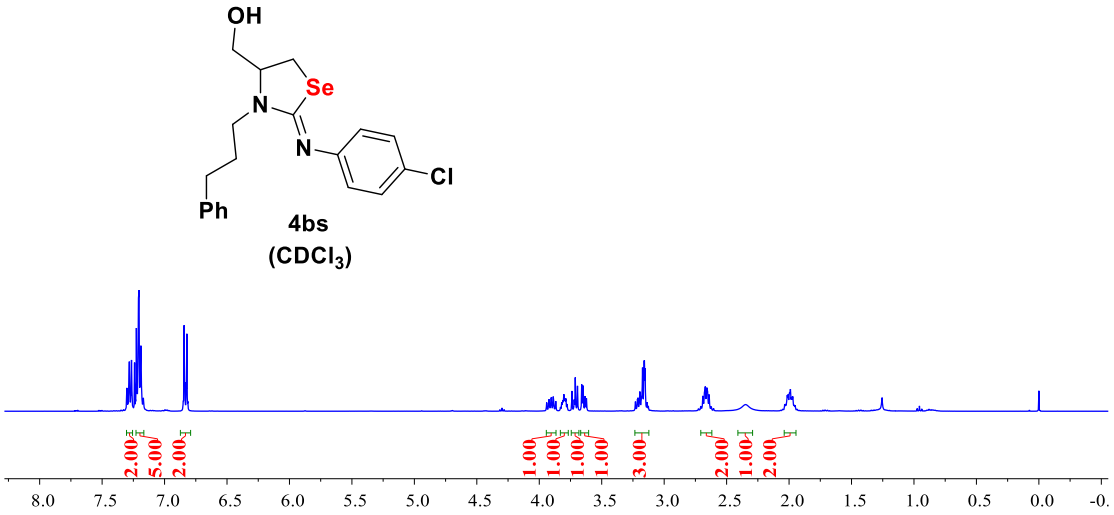
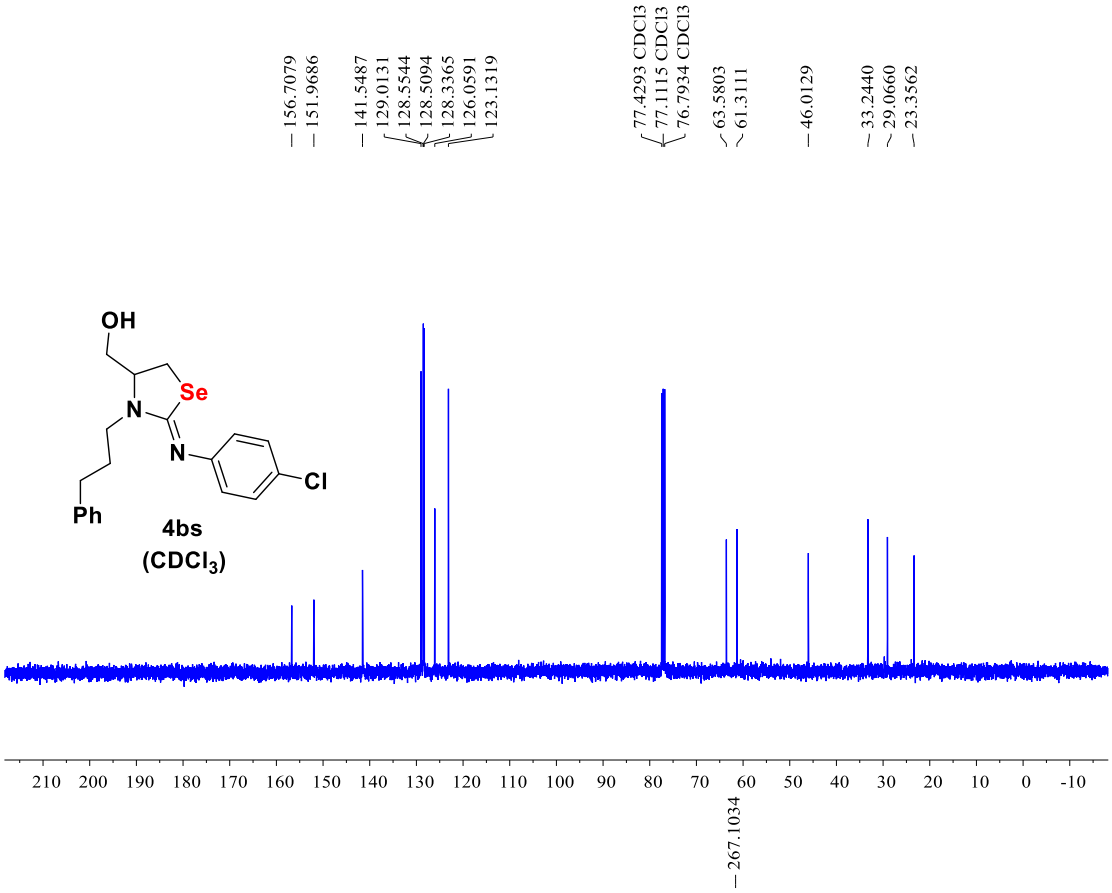
CDCl3
7.30 7.30 7.29 7.28 7.27 7.26 7.26 7.24 7.23 7.22 7.21 7.20 7.20 7.19 7.19 7.18 6.84 6.84 6.83 6.82
3.89 3.80 3.74 3.71 3.69 3.66 3.65 3.63
3.19 3.18 3.17 3.16 3.16 3.15 2.69 2.68 2.67 2.66 2.66 2.65 2.64 2.01 2.01 2.01 2.00 2.00 1.99 1.98 1.97 0.00


OH
Se
N
N
Cl
Ph
4bs
(CDCl3)
2.00 5.00 2.00 1.00 1.00 1.00 1.00 3.00 2.00 1.00 2.00
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.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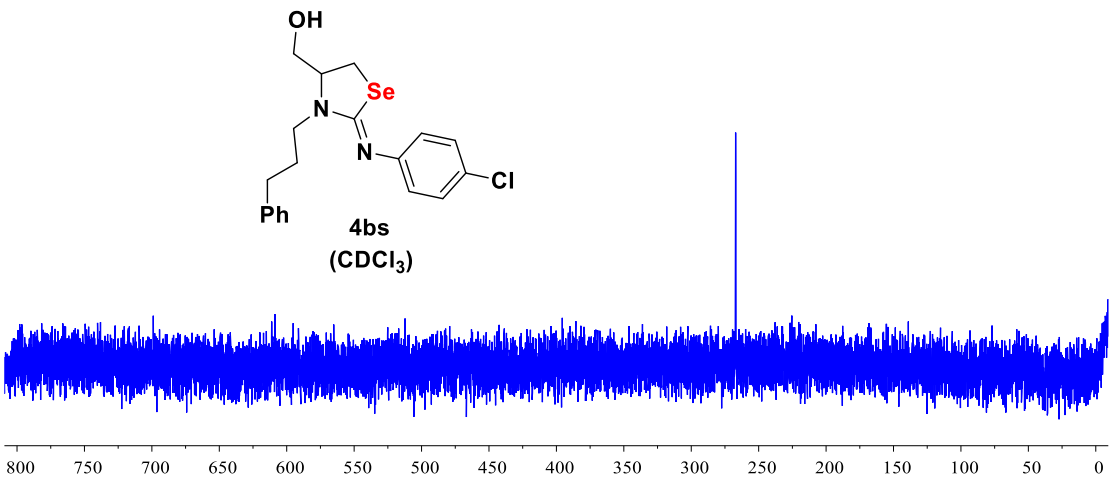
141.5487
129.0131
128.5544
128.5094
128.3365
126.0591
123.1319
77.4293 CDCl3
77.1115 CDCl3
76.7934 CDCl3
63.5803
61.3111
46.0129
33.2440
29.0660
23.3562
OH
Se
N
N
Cl
Ph
4bs
(CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Se
N
N
Cl
Ph
4bs
(CDCl3)
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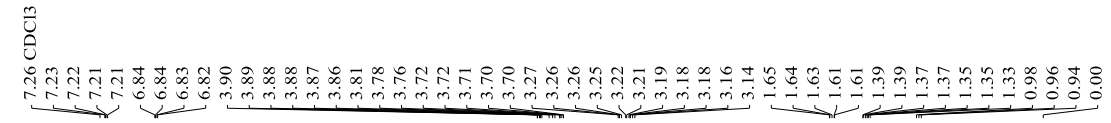
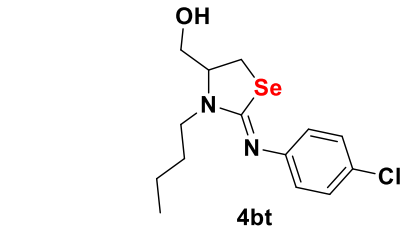
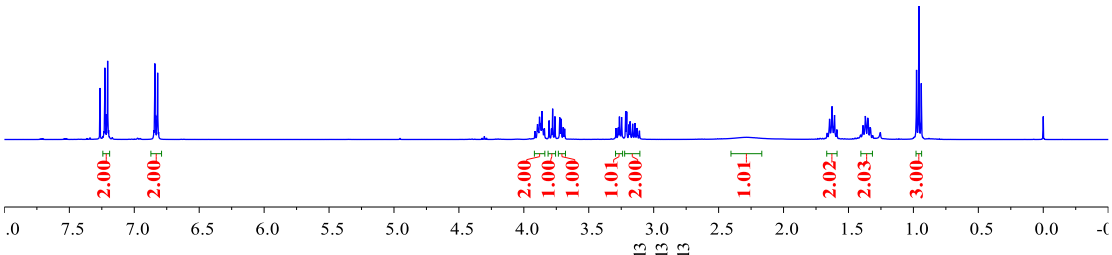
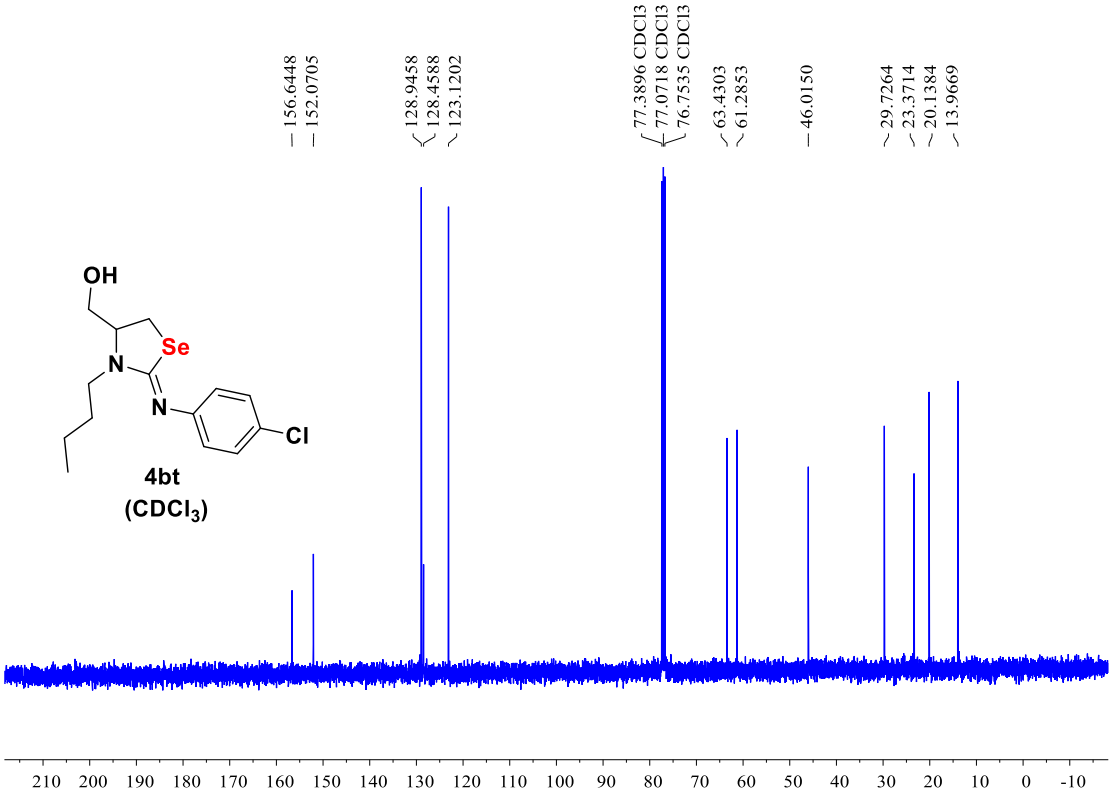




4bt
($CDCl_3$)





4bt
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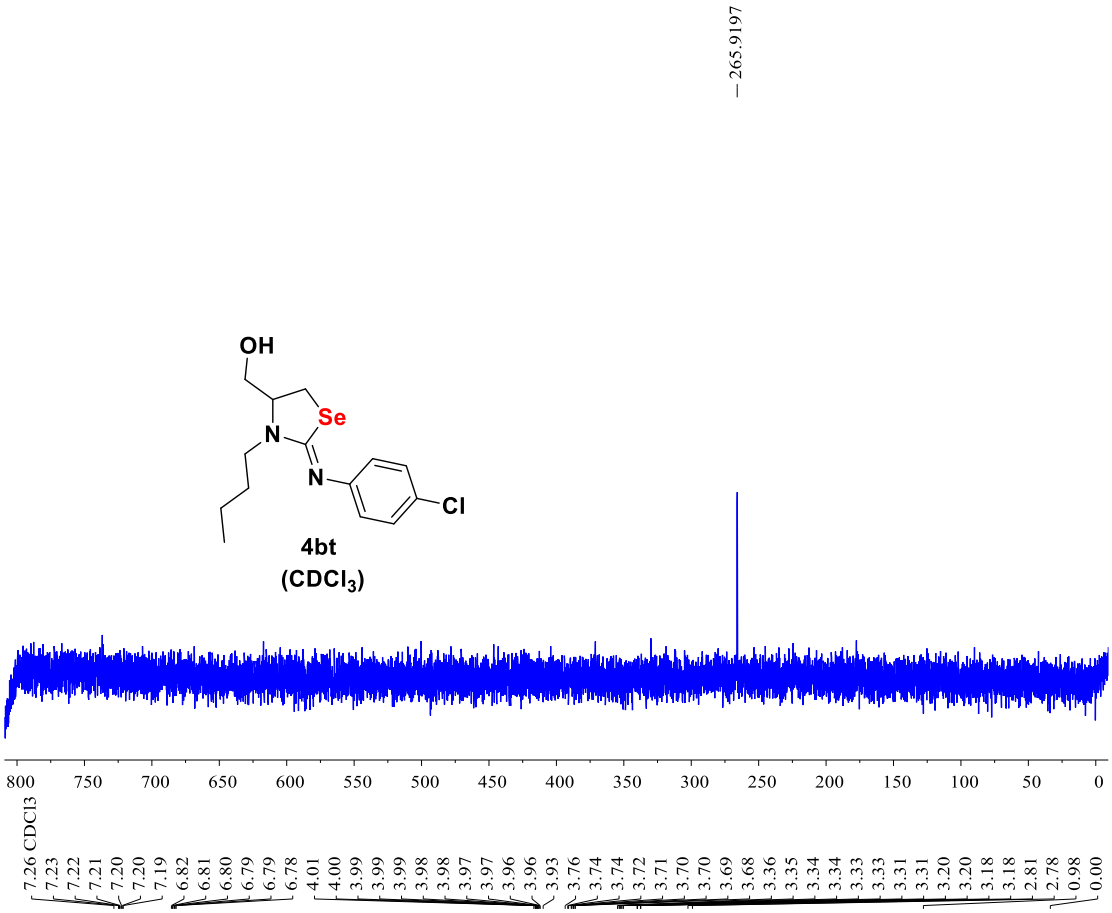
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Se
N
N
Cl
4bt
(CDCl3)
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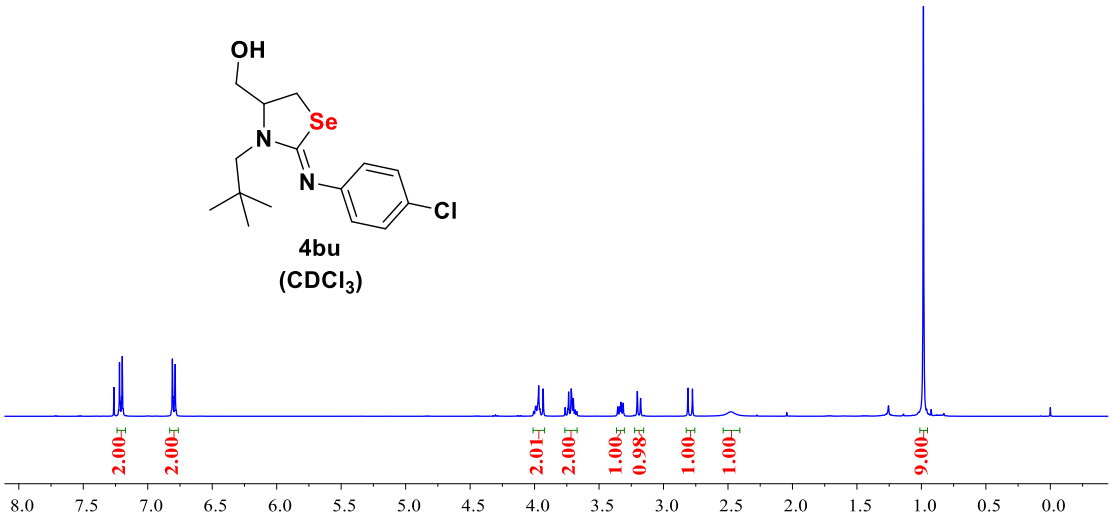
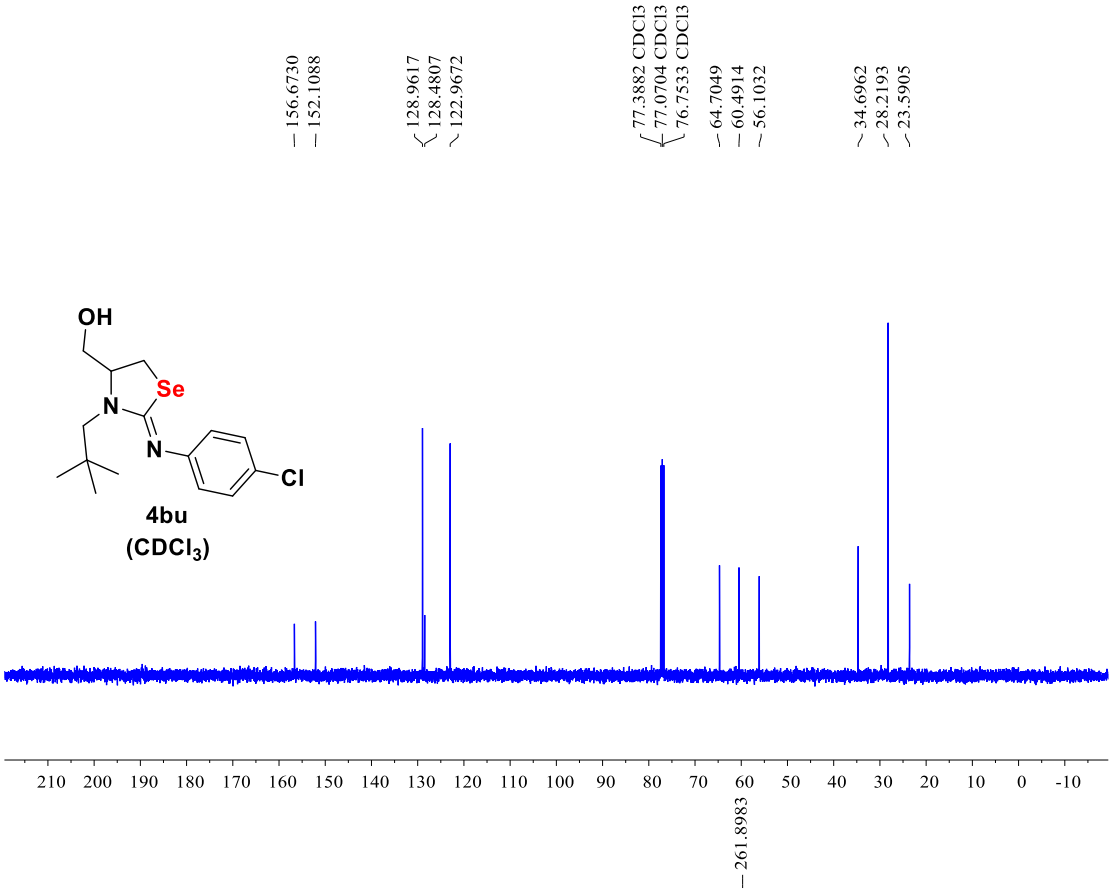
7.26 CDCl3
7.23 7.22 7.21 7.20 7.20 7.19 6.82 6.81 6.80 6.79 6.79 6.78 4.01 4.00 3.99 3.99 3.99 3.98 3.98 3.97 3.97 3.96 3.96 3.93 3.76 3.74 3.74 3.72 3.71 3.70 3.70 3.69 3.68 3.36 3.35 3.34 3.34 3.33 3.33 3.31 3.31 3.20 3.20 3.18 3.18 2.81 2.78 0.98 0.00


OH
Se
N
N
Cl
4bu
(CDCl3)
2.00 2.00 2.01 2.00 1.00 0.98 1.00 1.00 9.00
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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128.4807
122.9672
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77.0704 CDCl3
76.7533 CDCl3
64.7049
60.4914
56.1032
34.6962
28.2193
23.5905
OH
Se
N
N
Cl
4bu
(CDCl3)
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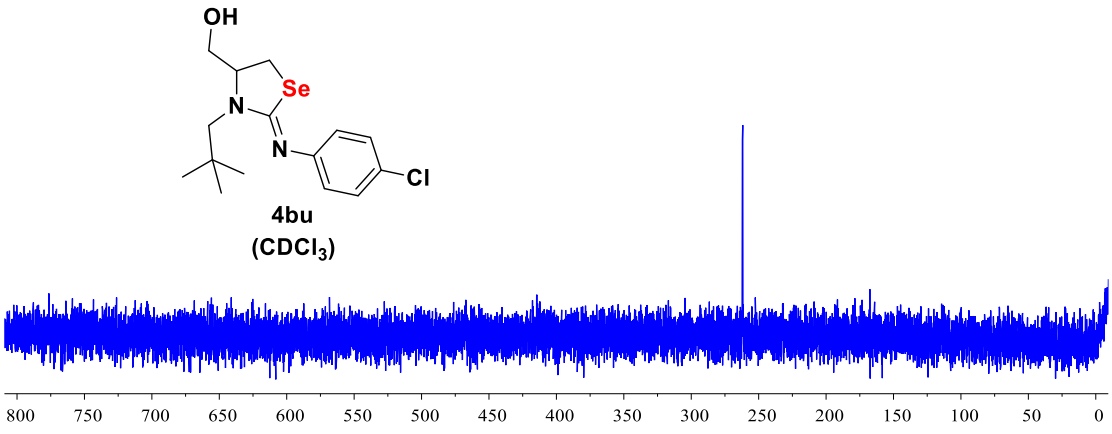
261.8983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Se
N
N
Cl
4bu
(CDCl3)
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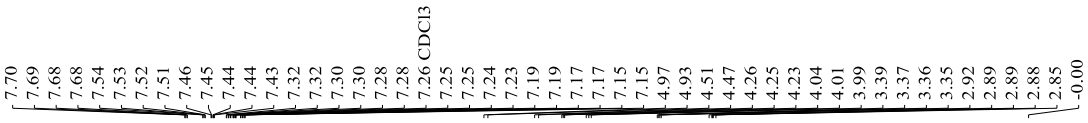

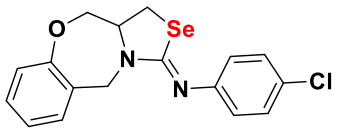

4bma
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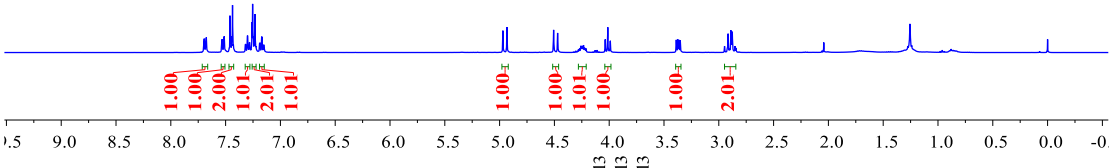
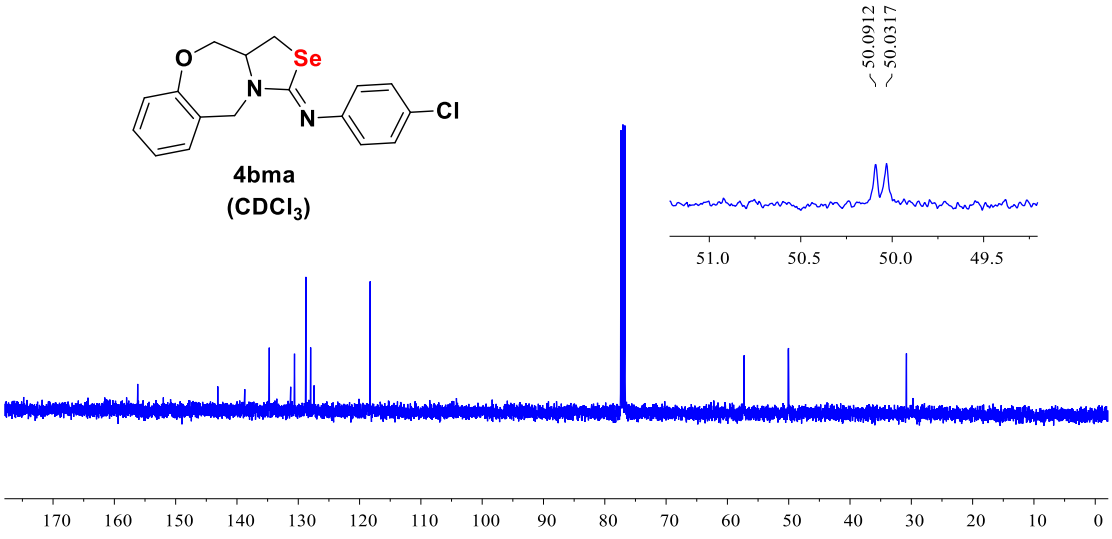
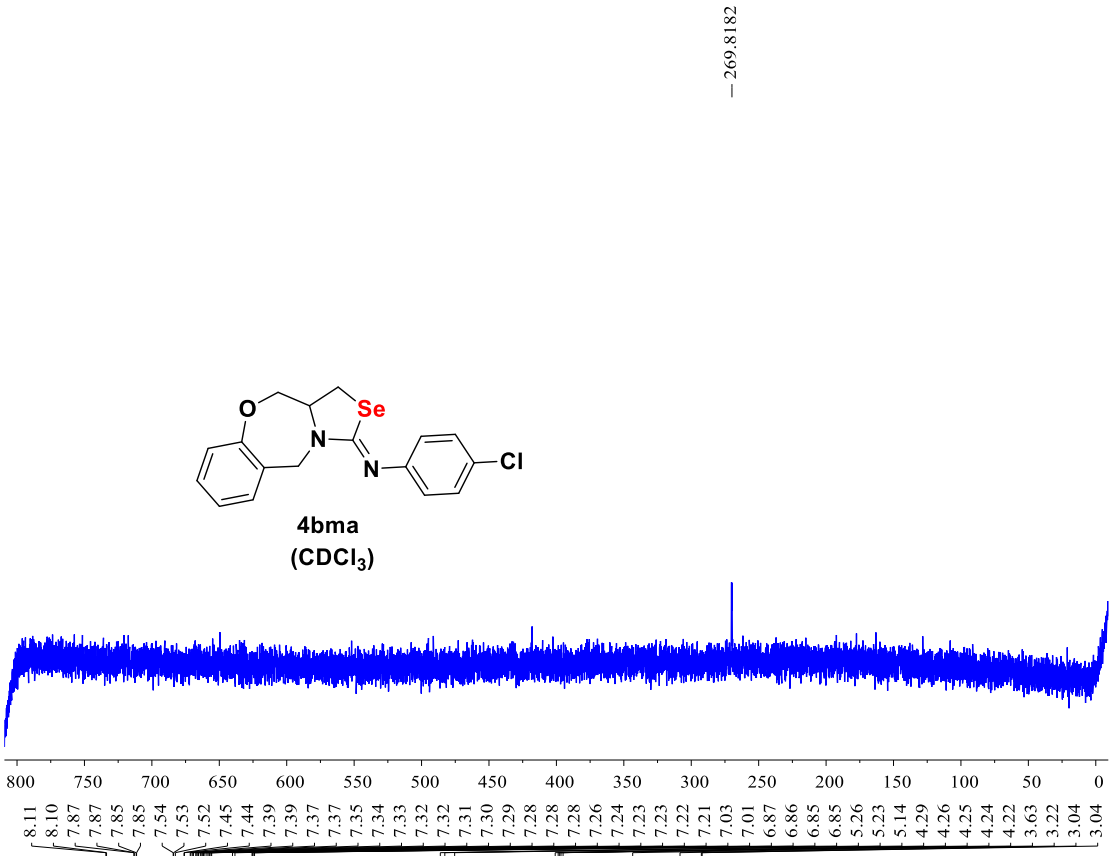


4bma
($CDCl_3$)

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Se
N
N
Cl
4bma
(CDCl3)
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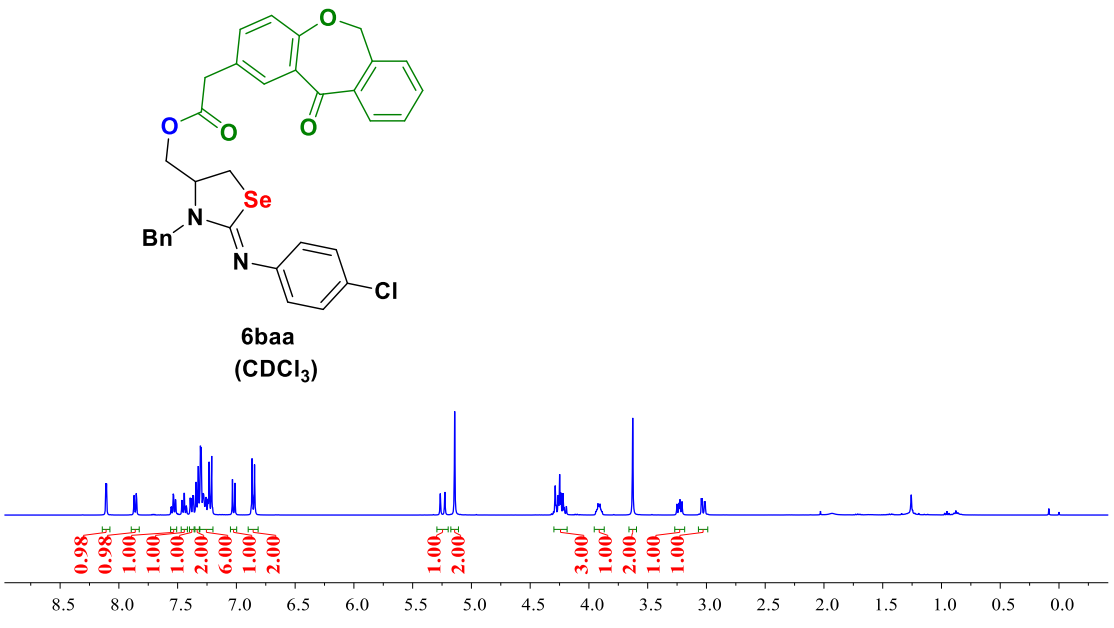
O
O
O
O
Se
N
Bn
N
Cl
6baa
(CDCl3)
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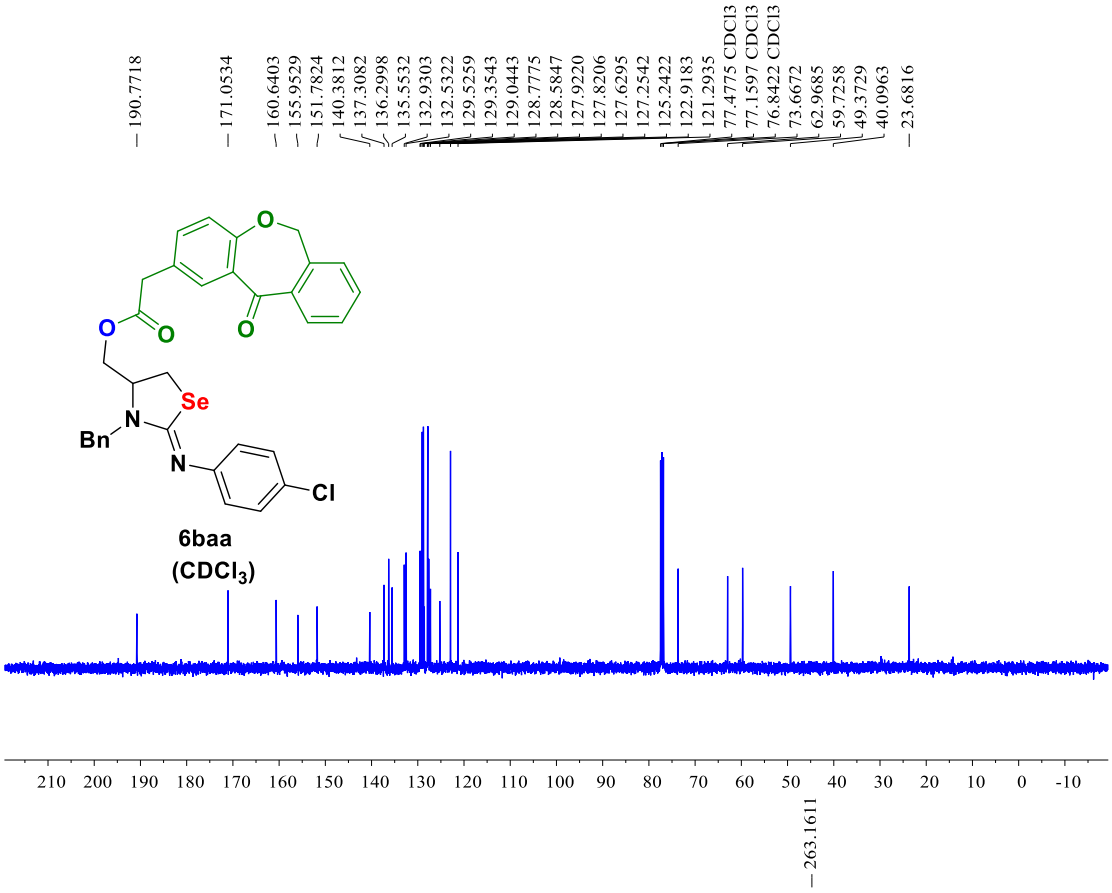
1.00 2.00
3.00 1.00 2.00 1.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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132.9303
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129.5259
129.3543
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128.7775
128.5847
127.9220
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127.6295
127.2542
125.2422
122.9183
121.2935
77.4775 CDCl3
77.1597 CDCl3
76.8422 CDCl3
73.6672
62.9685
59.7258
49.3729
40.0963
23.6816
O
O
O
O
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N
Bn
N
Cl
6baa
(CDCl3)
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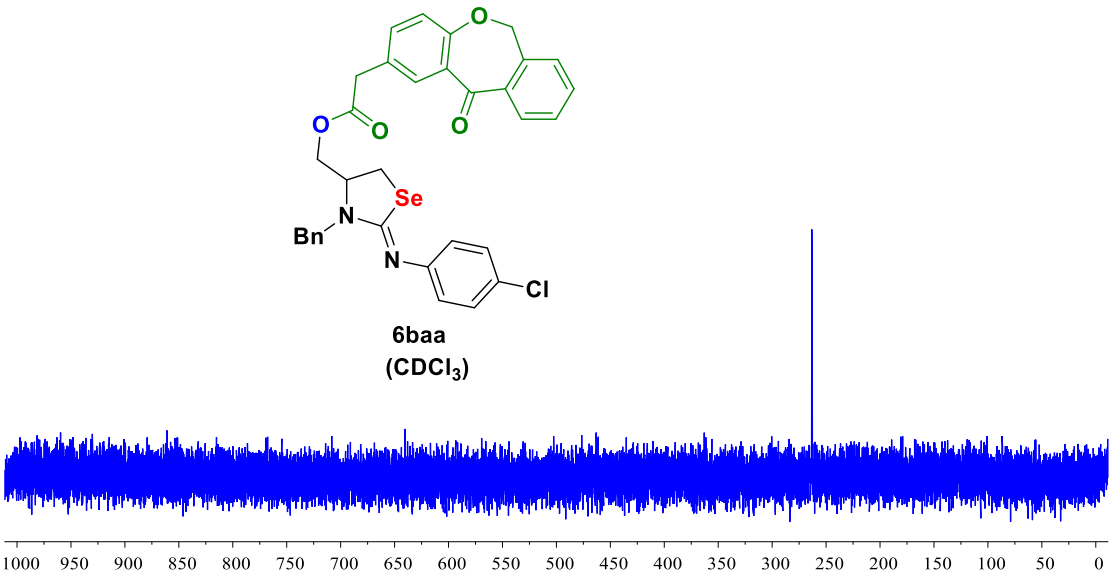
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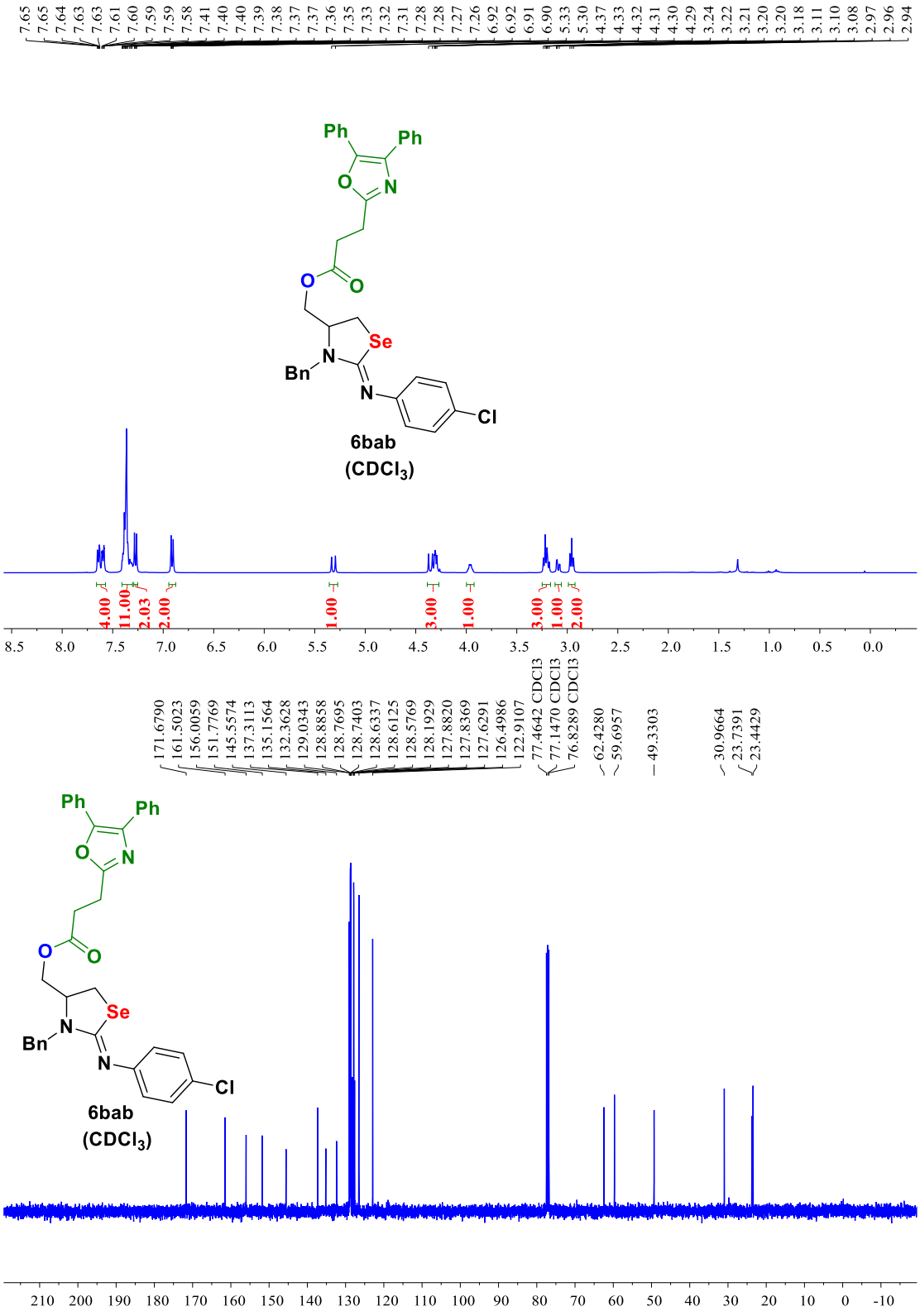
7.65 7.65 7.64 7.63 7.63 7.61 7.60 7.59 7.59 7.58 7.41 7.40 7.40 7.39 7.38 7.37 7.37 7.36 7.35 7.33 7.32 7.31 7.28 7.28 7.27 7.26 6.92 6.92 6.91 6.90 5.33 5.30 4.37 4.33 4.32 4.31 4.30 4.29 3.24 3.22 3.21 3.20 3.18 3.11 3.10 3.08 2.97 2.96 2.94
Ph
Ph
O
N
O
O
Se
Bn
N
N
Cl
6bab
(CDCl3)
4.00
11.00
2.03
2.00
1.00
3.00
1.00
3.00
1.00
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
171.6790
161.5023
156.0059
151.7769
145.5574
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135.1564
132.3628
129.0343
128.8858
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128.1929
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126.4986
122.9107
77.4642 CDCl3
77.1470 CDCl3
76.8289 CDCl3
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59.6957
49.3303
30.9664
23.7391
23.4429
Ph
Ph
O
N
O
O
Se
Bn
N
N
Cl
6bab
(CDCl3)
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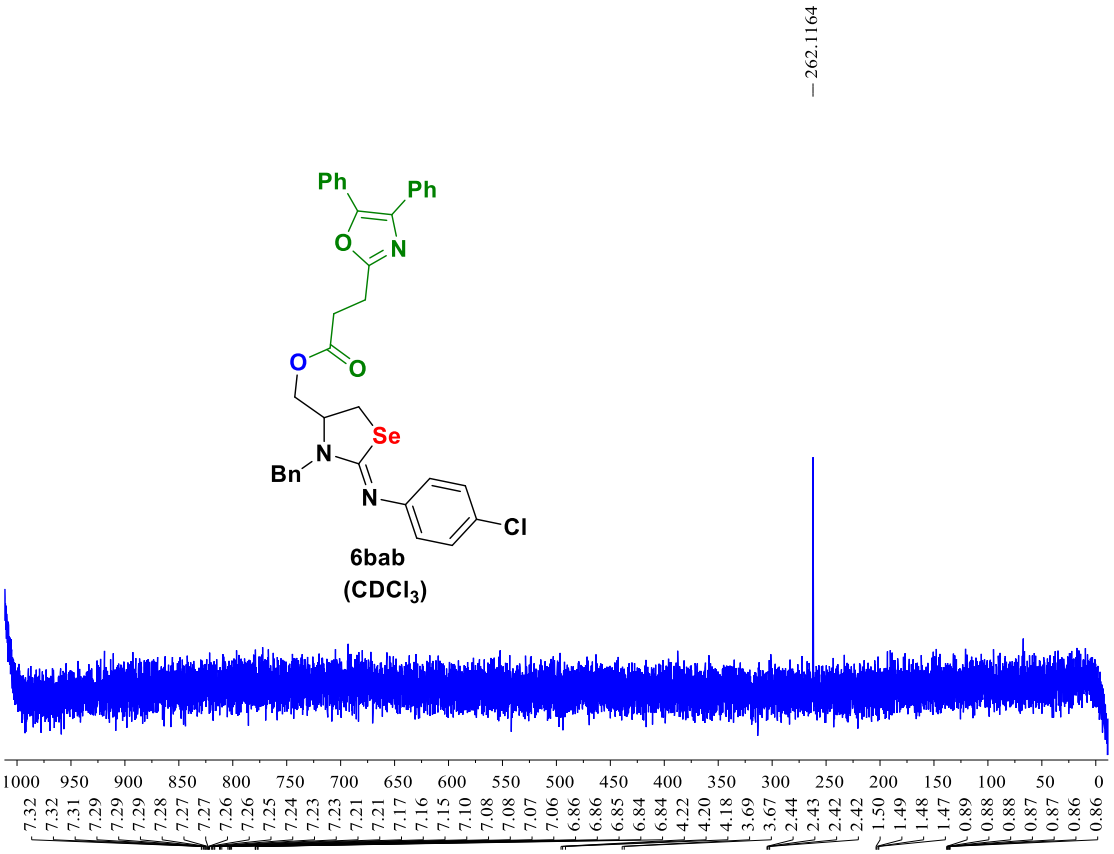
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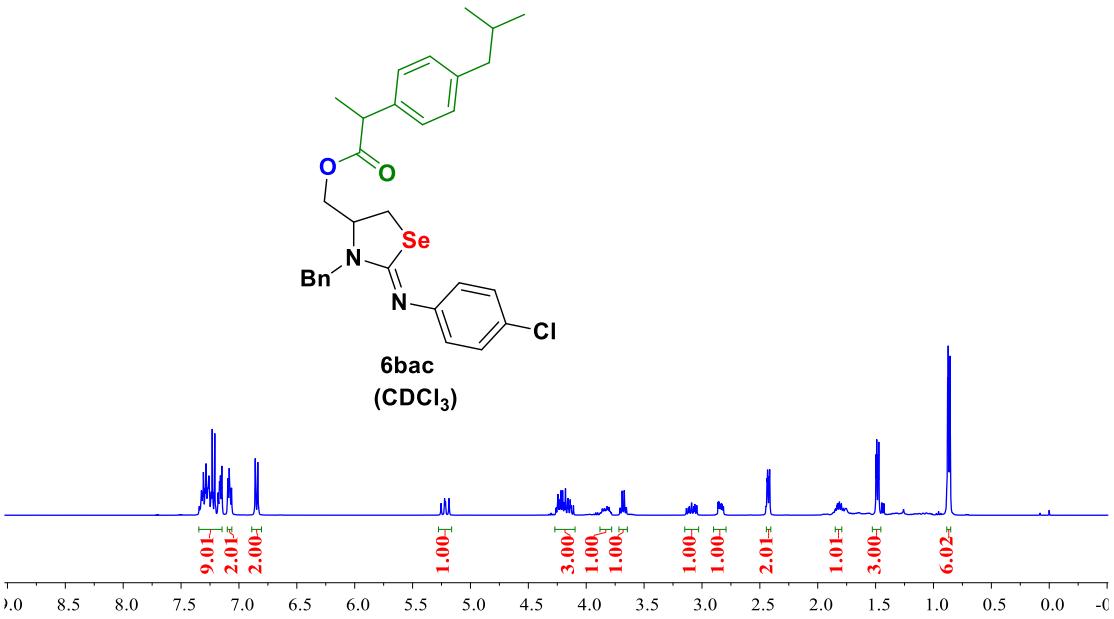
6bab
(CDCl3)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O
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Bn
N
N
Cl
6bac
(CDCl3)
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2.01
2.00
1.00
3.00
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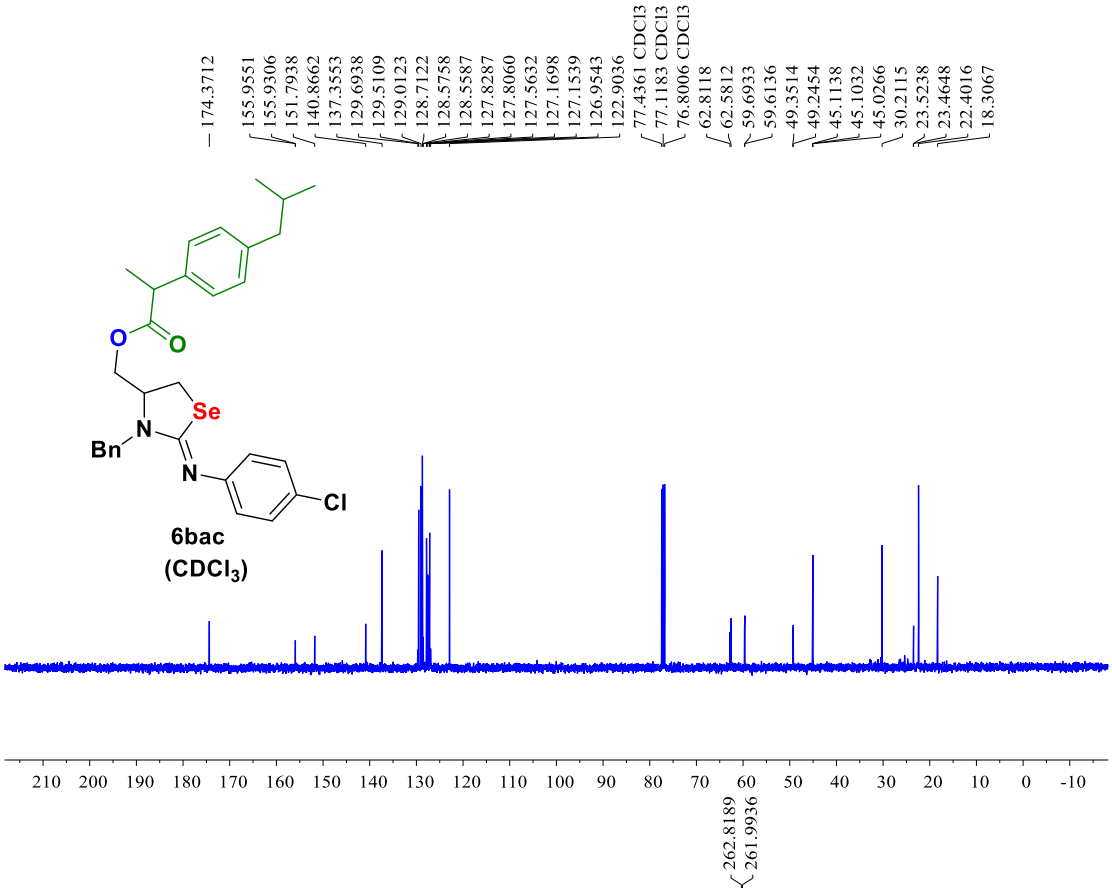
1.00
1.00
2.01
1.01
3.00
6.02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127.1698
127.1539
126.9543
122.9036
77.4361 CDCl3
77.1183 CDCl3
76.8006 CDCl3
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49.2454
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45.1032
45.0266
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23.5238
23.4648
22.4016
18.3067
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Bn
N
Cl
6bac
(CDCl3)
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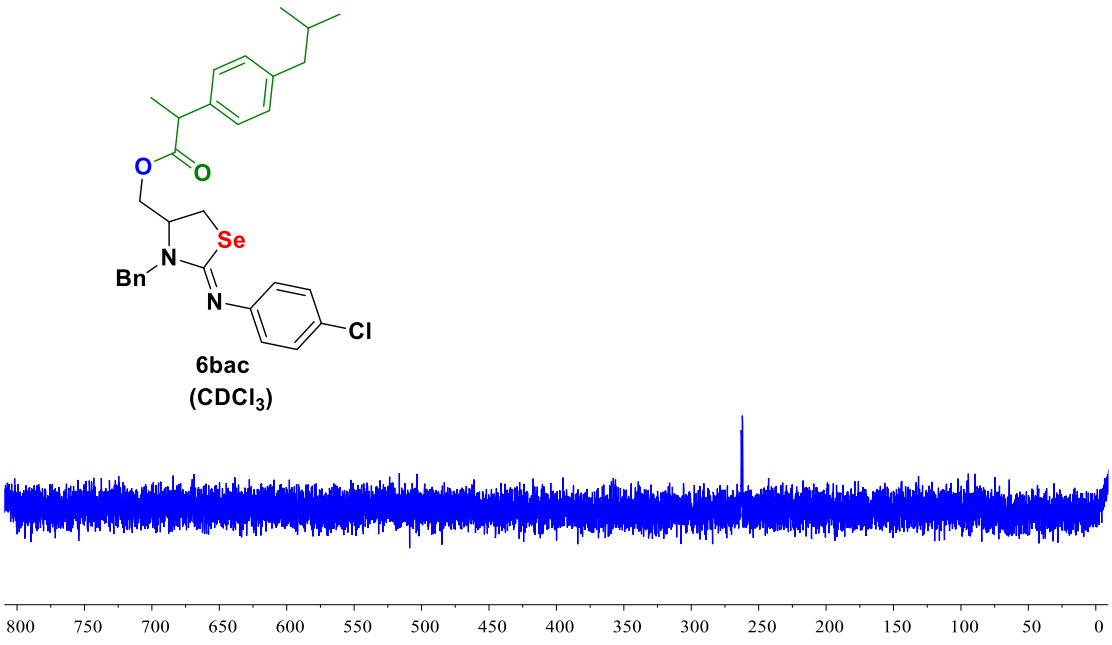
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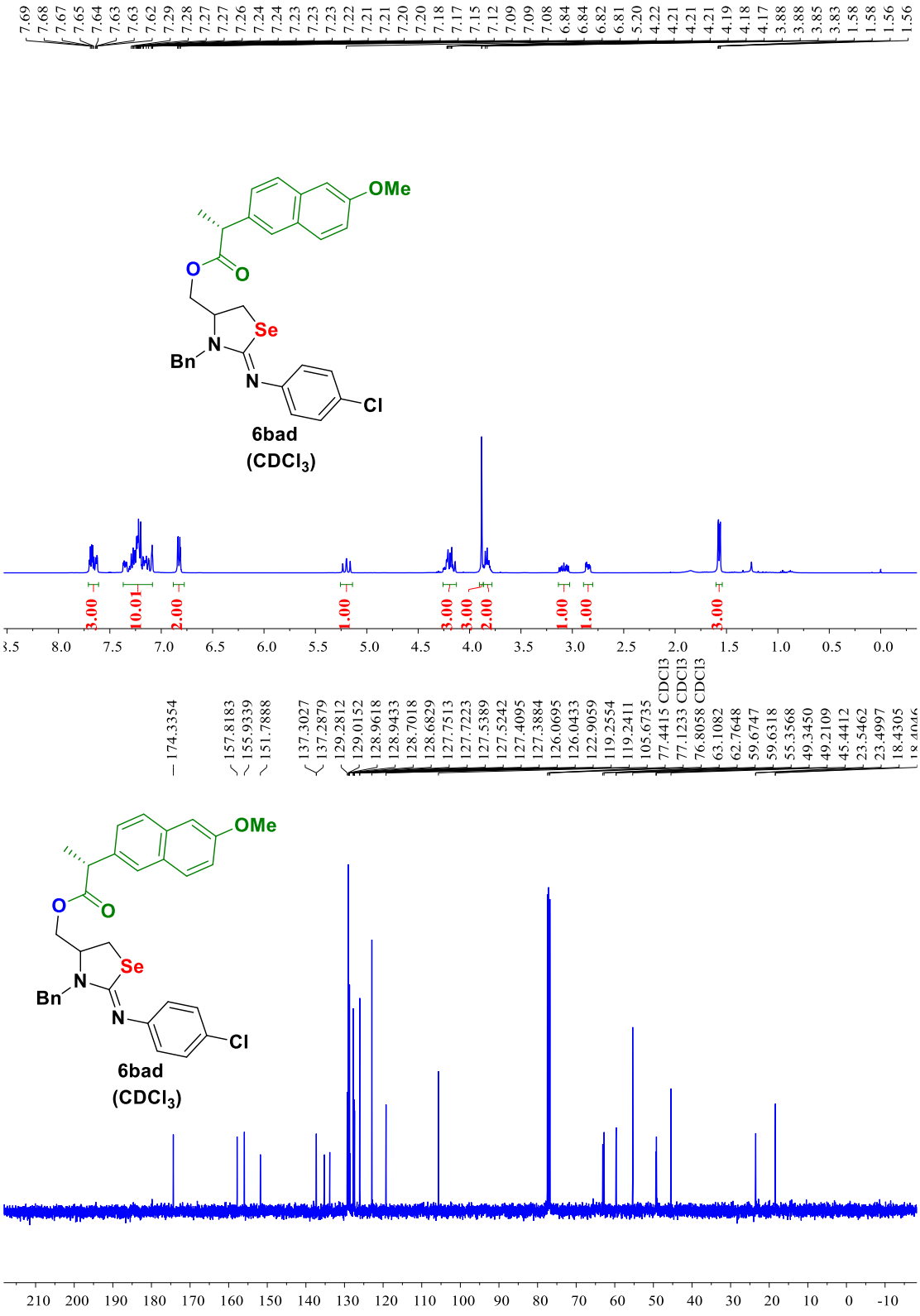
OMe
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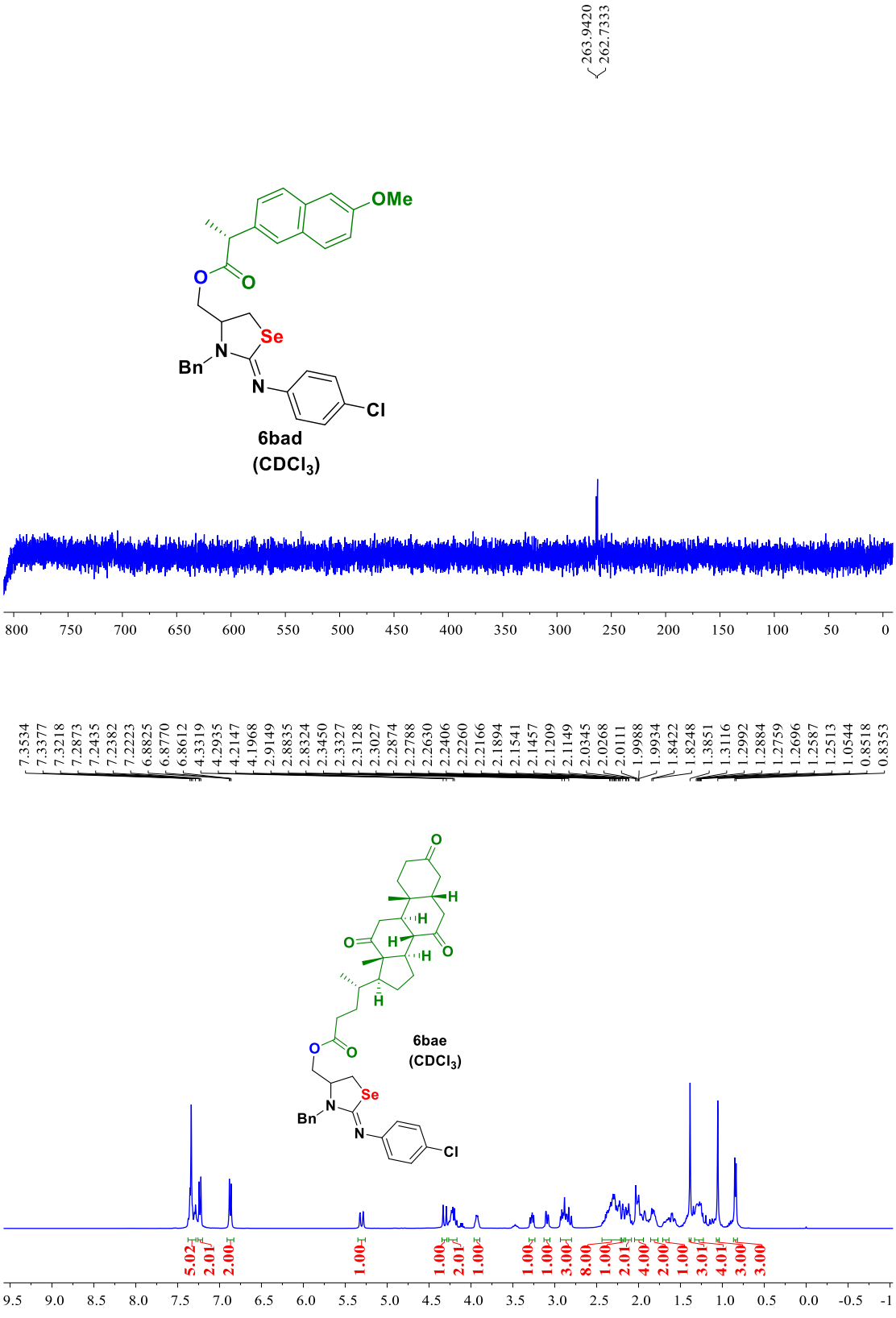
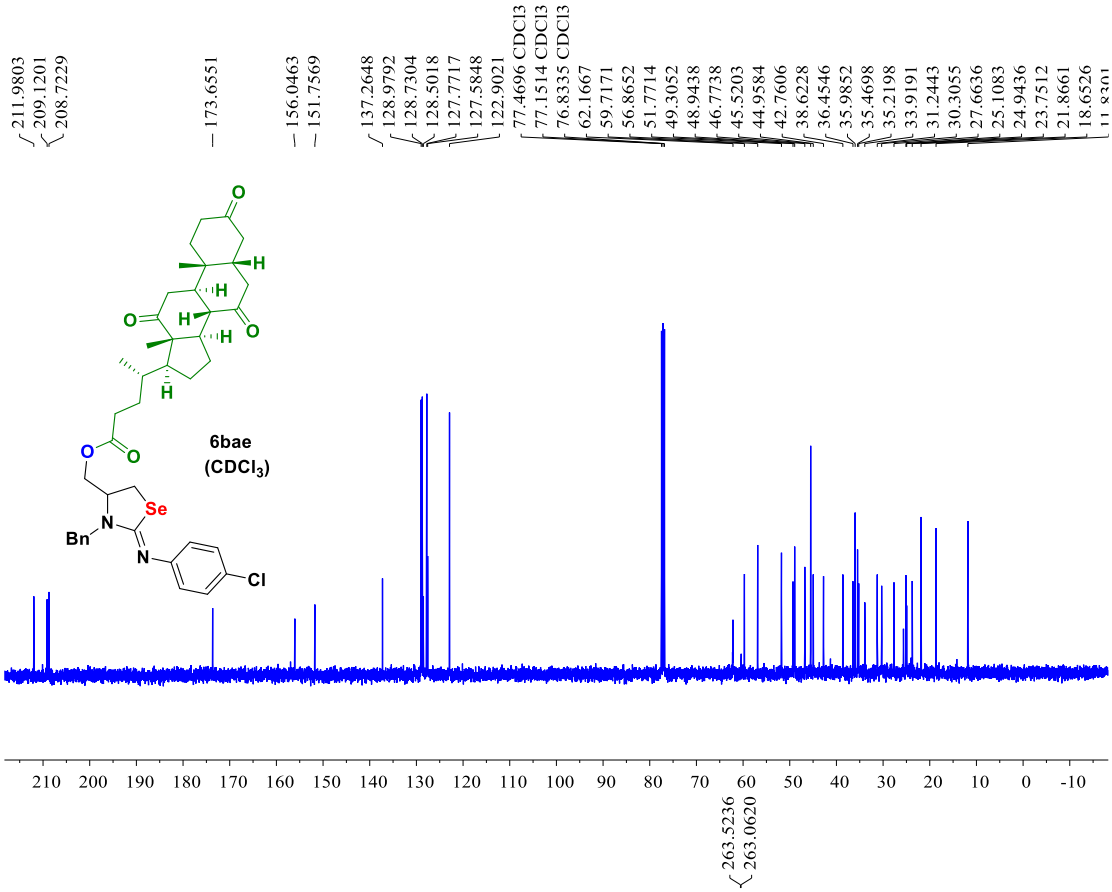
O
Se
N
Bn
N
Cl
6bad
(CDCl3)
3.00
10.01
2.00
1.00
3.00
3.00
2.00
1.00
1.00
3.00
OMe
O
O
Se
N
Bn
N
Cl
6bad
(CDCl3)


263.9420
262.7333
OMe
O
O
Se
N
Bn
N
Cl
6bad
(CDCl3)
800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0
7.3534 7.3377 7.3218 7.2873 7.2435 7.2382 7.2223 6.8825 6.8770 6.8612 4.3319 4.2935 4.2147 4.1968 2.9149 2.8835 2.8324 2.3450 2.3327 2.3128 2.3027 2.2874 2.2788 2.2630 2.2406 2.2260 2.2166 2.1894 2.1541 2.1457 2.1209 2.1149 2.0345 2.0268 2.0111 1.9988 1.9934 1.8422 1.8248 1.3851 1.3116 1.2992 1.2884 1.2759 1.2696 1.2587 1.2513 1.0544 0.8518 0.8353
O
H
H
O
H
O
H
H
O
O
6bae
(CDCl3)
Se
N
Bn
N
Cl
5.02 2.01 2.00 1.00 1.00 2.01 1.00 1.00 1.00 3.00 8.00 1.00 2.01 4.00 2.00 1.00 3.01 4.01 3.00 3.00
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 -1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N
Cl
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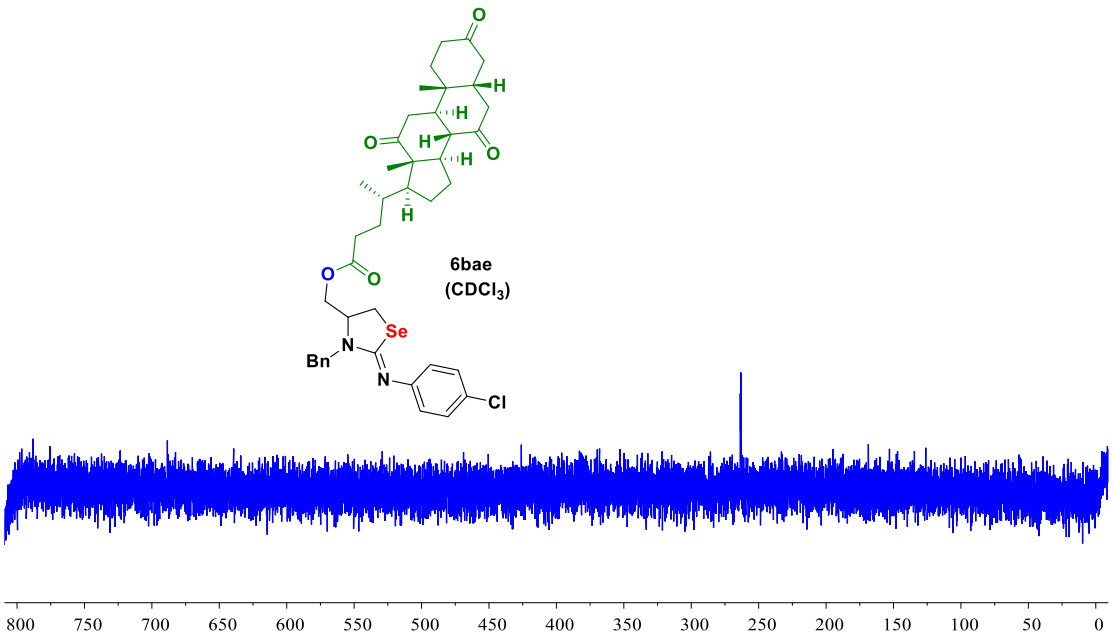
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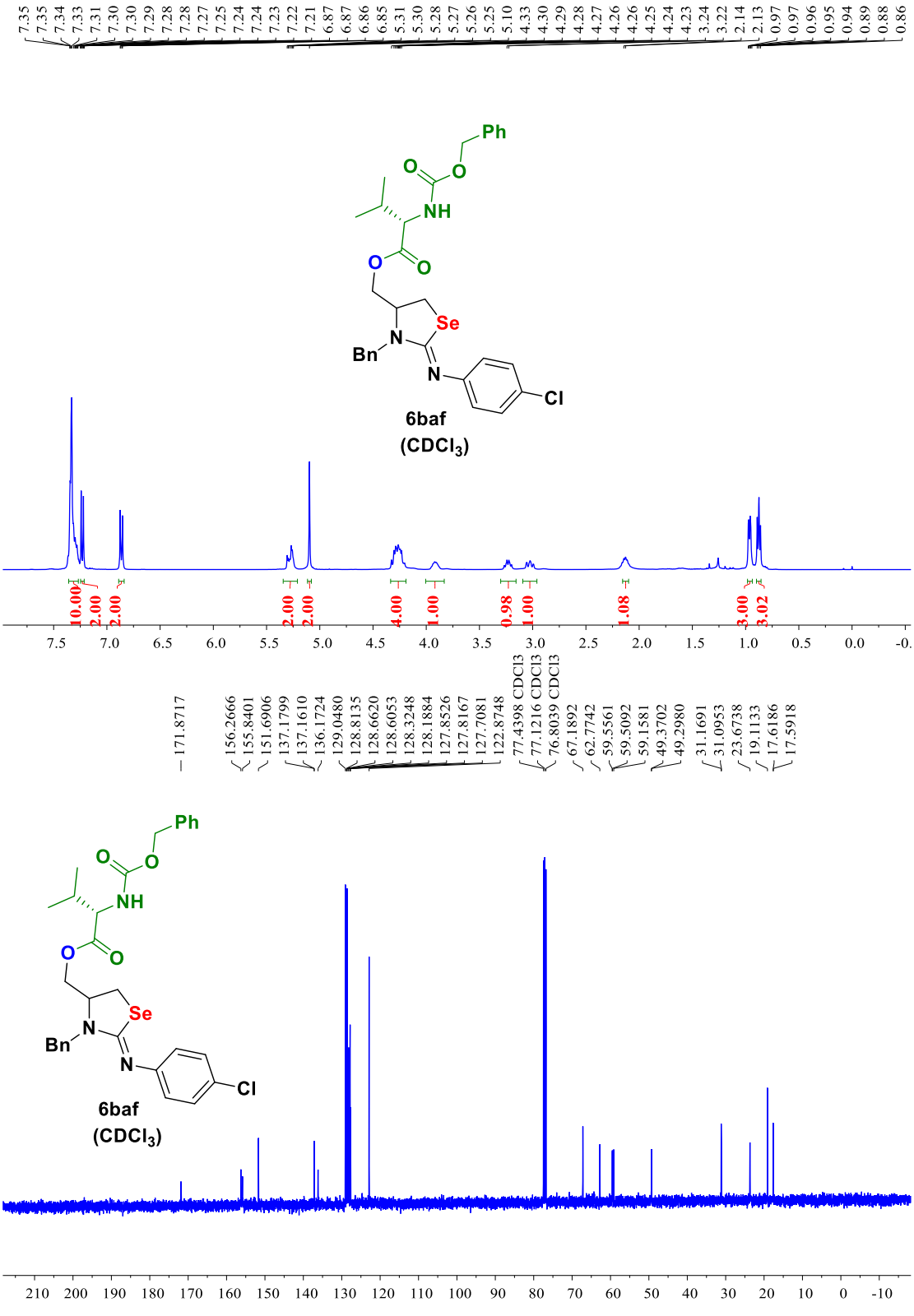
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Ph
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O
NH
O
O
Se
N
Bn
N
Cl
6baf
(CDCl3)
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2.00
2.00
2.00
2.00
4.00
1.00
0.98
1.00
1.08
3.00
3.02
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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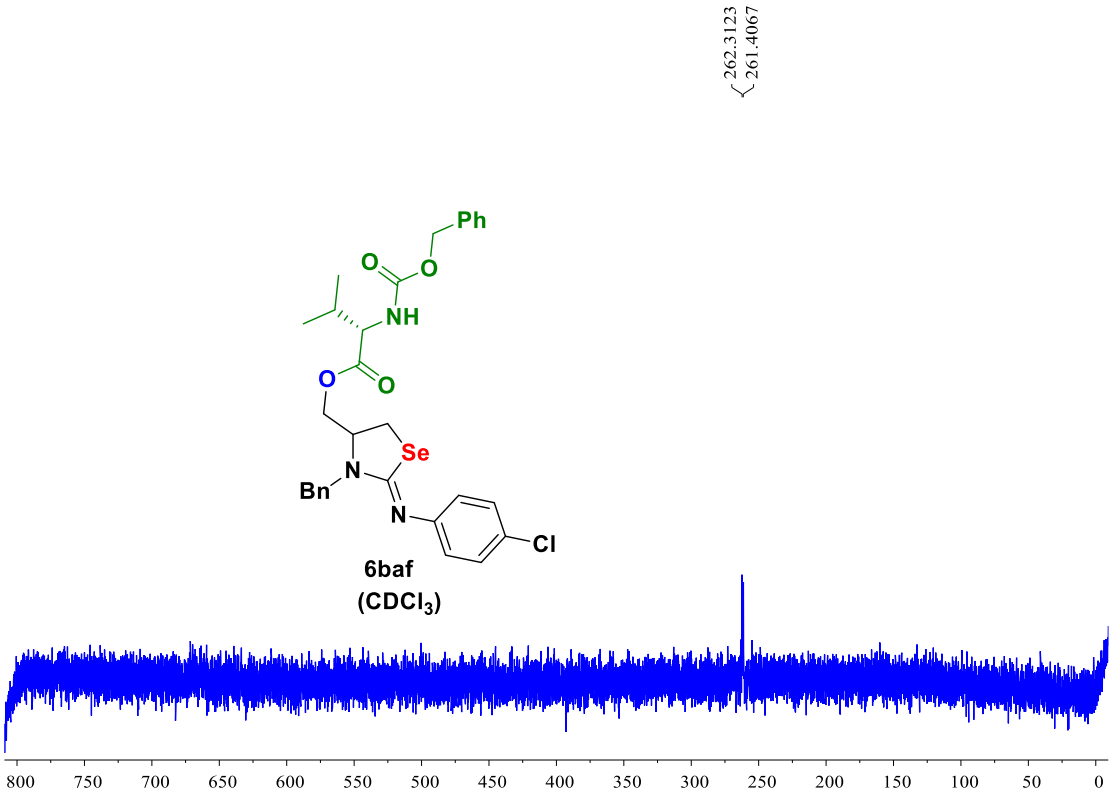
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(CDCl3)
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150
100
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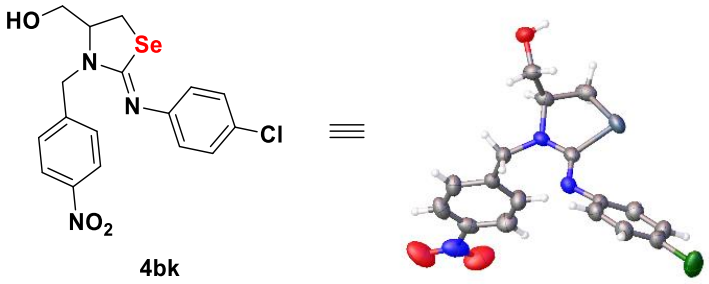
0

10. Crystal data and structure refinement for 4bk



4bk

X-Ray Crystallographic Data of **4bk**

The thermal ellipsoid was drawn at the 50% probability level.

Crystal Number: CCDC 2243152

Empirical formula: $C_{17}H_{16}ClN_3O_3Se$

Formula weight: 424.74

Unit cell parameters: a = 7.3092 (6) Å, b = 10.4613 (9) Å, c = 12.1430 (10) Å,

α = 72.439 (3), β = 87.404 (3), γ = 81.976 (3)

Temperature: 296 (2) K

Wavelength: 0.71073 Å

Crystal system: triclinic

Volume: 876.56 (13) $Å^3$

Calculated density: 1.609 Mg/m^3

Absorption coefficient: 2.316 mm^{-1}

F (000): 428.0

Crystal size: 0.20× 0.40 × 0.58 mm^3

Correction-type: multi-scan

h, k, l max: 9, 13, 15

Tmin, Tmax: 0.455/0.746

Data completeness: 0.997

Device: Bruker APEX-II CCD

Measurement method: \f and \w scans.

Crystal sample preparation of 4bk

Crystal of **4bk** was prepared using DCM and Hexane as solvent, the solution was evaporated at room temperature for about one week, single crystals were formed.