

Supporting information for

Organo-Selenium Mediated Regio- and Stereoselective Iodoselenylation of Alkynes in an Aqueous Medium: A Simple Access to (*E*)- β -Iodoalkenyl Selenides

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1. General information

¹H and ¹³C NMR spectra were recorded on Varian 400 MHz NMR spectrometer using CDCl₃ as solvent and TMS as an internal standard. High-resolution mass spectra (HRMS) were recorded on a Bruker solarix FT-ICR mass spectrometer. Analysis of crude reaction mixture was done on the Varian 4000 GC/MS. Reactions were monitored using thin-layer chromatography (TLC) on commercial silica gel plates (GF254), and was performed under UV light (254 nm). All the new products were further characterized by high resolution mass spectra (HRMS). All commercial reagents and available compounds were obtained from Energy Chemical, Sinopharm Chemical Reagent Co., Ltd and TCI, and used without further purification.

2. General procedure for synthesis of β -Iodoalkenyl Selenides 3.

Optimization of the reaction conditions for the synthesis of 3a

A mixture of alkynes (0.5 mmol), iodine (0.275 mmol), diselenides (0.25 mmol) in ethanol (1.0 ml) and water (0.5 ml) was stirred at 70 °C for 0.5h under air atmosphere. After completion, the reaction mixture was cooled down to the room temperature. Then the reaction was quenched with saturated solution of sodium thiosulfate (0.5 mL) and extracted with dichloromethane for three times (3 x 3 ml). The organic layers were then combined, washed with brine, dried (anhydrous MgSO₄), and concentrated under vacuum. The residue was purified by flash chromatography (Petroleum Ether / EtOAc = 50:1) on silica gel to give the desired product.

3. Optimization of the reaction conditions for the synthesis of 3a

We commenced by studying the model reaction between phenylacetylene **1a** (1.0 equiv.) and diphenyl diselenide **2a** (0.5 equiv.) in the presence of I₂ (1.1 equiv.) as the iodine source in MeCN at 70 °C under an air atmosphere (Table S1, entry 1). The desired product, (2-iodo-2-phenylvinyl) (phenyl)selane, was obtained with good GC yield (65%) and excellent stereo-selectivity (*E*: *Z* = 90:10) after 30min. We next screened several solvents, such as THF, DMF, Dioxane, DMSO and Toluene; however, reaction in these solvent did not improve the yield of compound 3a (Table S1, entries 2-6). When EtOH was employed as the reaction solvent, the desired product was obtained in an improved yield of 84% with an *E*:*Z* ratio of 95:5. Reaction in only H₂O did not lead to an increase in yield (Table S1, entry 7 and entry 8). Gratifyingly, a mixed solvent system of EtOH and H₂O (EtOH/H₂O = 2:1) further improved the yield of the

corresponding product to 97% and the *E*:*Z* ratio to 97:3 (Table S1, entries 9-12). Additionally, we also investigated the influence of the Iodine source. The use of KI, NIS and N(Et)₄I only gave moderate to poor yields of the desired product (Table S1, entries 13-15). Further, a decrease in reaction time or temperature was detrimental to product yield (Table S1, entry 16). Finally, performing the reaction under N₂ or O₂ conditions showed that the presence of air was more efficient to promote this reaction (Table S1, entries 17 and 18)

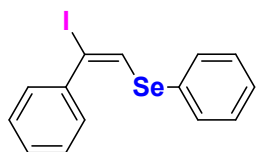
Table S1 Screening of reaction conditions^a

1a + 2a $\xrightarrow{\text{[Iodine]}}$ E-3a + Z-3a

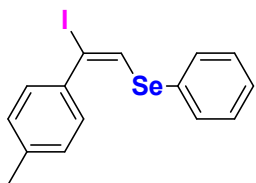
Entry	Solvent	[Iodine]	Yield[%] ^b	<i>E</i> / <i>Z</i> ^c
1	MeCN	I ₂	65	90:10
2	THF	I ₂	60	90:10
3	DMF	I ₂	70	92:8
4	Dioxane	I ₂	46	95:5
5	DMSO	I ₂	78	93:7
6	Toluene	I ₂	75	92:8
7	EtOH	I ₂	84	95:5
8	H ₂ O	I ₂	55	96:4
9	EtOH	HI	34	97:3
10	EtOH/H ₂ O (4:1)	I ₂	90	97:3
11	EtOH/H ₂ O (3:1)	I ₂	93	97:3
12	EtOH/H ₂ O (2:1)	I ₂	97 (95) ^d	97:3
13	EtOH/H ₂ O (1:1)	I ₂	91	97:3
14	EtOH/H ₂ O (2:1)	KI	56	97:3
15	EtOH/H ₂ O (2:1)	NIS	89	85:15
16	EtOH/H ₂ O (2:1)	N(Et) ₄ I	45	97:3
17 ^e	EtOH/H ₂ O (2:1)	I ₂	83	97:3
18 ^f	EtOH/H ₂ O (2:1)	I ₂	52	97:3
19 ^g	EtOH/H ₂ O (2:1)	I ₂	92	97:3

^a General reaction conditions: Phenylacetylene (0.50 mmol), 1,2-diphenyldiselenane (0.25 mmol) and iodine source (I₂ = 0.275 mmol, KI, NIS, N(Et)₄I = 0.55 mmol) in solvent (1.5 mL) at 70 °C for 30 min under an air atmosphere. ^b The GC yield of *E*-3a. ^c The *E*/*Z* ratio determined by GC on crude products. ^d The isolated yield ^e At 60 °C. ^f N₂ atmosphere ^g O₂ atmosphere

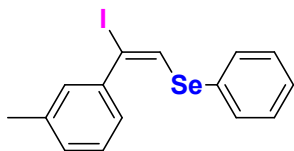
4. NMR spectra of the obtained compounds



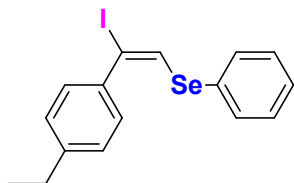
3a: light yellow oil (183.35 mg, 95%, E/Z=97:3). ^1H NMR (400 MHz, CDCl_3) δ : 7.53-7.56 (m, 2H), 7.48-7.51 (m, 2H), 7.37-7.41 (m, 2H), 7.32-7.35 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 141.76, 132.86, 130.37, 129.57, 129.45, 128.86, 128.57, 128.42, 127.99, 88.34. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{11}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 408.8968, Found 408.8965.



3b: light yellow oil (192.01 mg, 96%, E/Z=98:2). ^1H NMR (400 MHz, CDCl_3) δ : 7.53-7.56 (m, 2H), 7.39-7.41 (m, 2H), 7.32-7.35 (m, 4H), 7.19-7.21 (m, 4H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 138.93, 132.81, 130.50, 129.43, 129.07, 128.85, 128.49, 127.92, 127.36, 88.90, 21.44. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{13}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 422.9125, Found 422.9127.

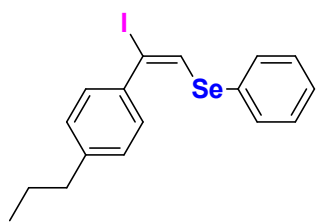


3c: light yellow oil (188.00 mg, 94%, E/Z=90:10). ^1H NMR (400 MHz, CDCl_3) δ : 7.52-7.54 (m, 2H), 7.26-7.36 (m, 7H), 7.14-7.15 (m, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 141.67, 138.17, 132.82, 131.52, 130.46, 129.68, 129.41, 129.24, 129.12, 128.27, 127.92, 125.53, 88.54, 21.43. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{13}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 422.9125, Found 422.9121.

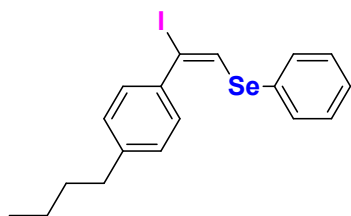


3d: light yellow oil (188.37 mg, 91%, E/Z=99:1). ^1H NMR (400 MHz, CDCl_3) δ : 7.52-7.53 (m, 2H), 7.39-7.41 (m, 2H), 7.31-7.34 (m, 4H), 7.19-7.22 (m, 2H), 2.67 (q, $J=6.0$ Hz, 2H), 1.27 (t, $J=7.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 145.12, 139.05, 132.79, 130.51, 129.40, 128.79, 128.56, 127.90, 127.83, 88.93, 28.69, 15.25. HRMS m/z (ESI): Calcd for $\text{C}_{16}\text{H}_{15}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 436.9281,

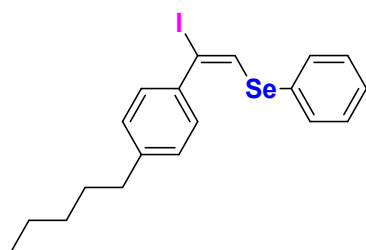
Found 436.9279.



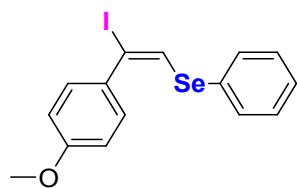
3e: light yellow oil (199.02 mg, 93%, E/Z=96:4). ^1H NMR (400 MHz, CDCl_3) δ : 7.51-7.54 (m, 1H), 7.38-7.43 (m, 2H), 7.15-7.33 (m, 7H), 2.60 (t, $J=7.6$ Hz, 2H), 1.64-1.71 (m, 2H), 0.97 (t, $J=7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 143.65, 139.03, 132.78, 132.02, 129.38, 129.17, 128.77, 128.46, 128.39, 127.88, 88.93, 37.86, 24.27, 13.90. HRMS m/z (ESI): Calcd for $\text{C}_{17}\text{H}_{17}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 450.9438, Found 450.9435.



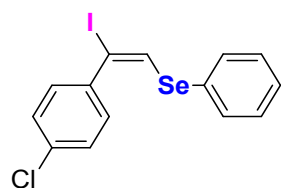
3f: light yellow oil (212.16 mg, 96%, E/Z=96:4). ^1H NMR (400 MHz, CDCl_3) δ : 7.52-7.55 (m, 2H), 7.31-7.41 (m, 6H), 7.18-7.20 (m, 2H), 2.64 (t, $J=7.6$ Hz, 2H), 1.60-1.67 (m, 2H), 1.35-1.44 (m, 2H), 0.96 (t, $J=7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 143.87, 138.99, 132.79, 131.52, 130.54, 129.40, 128.77, 128.51, 128.35, 127.89, 89.00, 35.50, 33.34, 22.44, 14.01. HRMS m/z (ESI): Calcd for $\text{C}_{18}\text{H}_{19}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 464.9694, Found 464.9692.



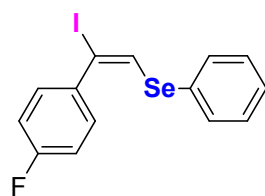
3g: light yellow oil (218.88 mg, 96%, E/Z=89:11). ^1H NMR (400 MHz, CDCl_3) δ : 7.51-7.54 (m, 2H), 7.37-7.39 (m, 2H), 7.30-7.33 (m, 4H), 7.17-7.19 (m, 2H), 2.61 (t, $J=7.6$ Hz, 2H), 1.60-1.68 (m, 2H), 1.34-1.37 (m, 4H), 0.92 (t, $J=6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 143.92, 138.96, 132.78, 131.50, 130.52, 129.38, 128.75, 128.49, 128.33, 127.88, 88.96, 35.77, 31.56, 30.88, 22.55, 14.05. HRMS m/z (ESI): Calcd for $\text{C}_{19}\text{H}_{21}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 478.9751, Found 478.9747.



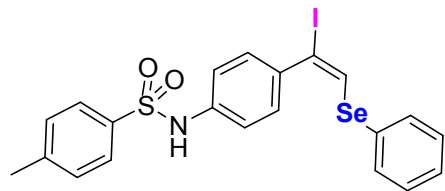
3h: light yellow oil (187.2 mg, 90%, E/Z=80:20). ^1H NMR (400 MHz, CDCl_3) δ : 7.48-7.51 (m, 2H), 7.37-7.41 (m, 2H), 7.27-7.36 (m, 4H), 7.85-7.87 (m, 2H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 161.37, 135.23, 134.43, 131.75, 131.09, 129.99, 129.57, 115.32, 90.51, 57.06. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{13}\text{IOSeNa}$ ($[\text{M}+\text{Na}]^+$): 438.9074, Found 438.9070.



3i: light yellow oil (199.5 mg, 95%, E/Z=85:15). ^1H NMR (400 MHz, CDCl_3) δ : 7.50-7.53 (m, 2H), 7.31-7.41 (m, 7H), 7.25-7.26 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 140.20, 134.52, 132.92, 131.50, 130.45, 129.90, 129.48, 128.60, 128.11, 86.30. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{10}\text{IClSeNa}$ ($[\text{M}+\text{Na}]^+$): 442.8579, Found 442.8576.

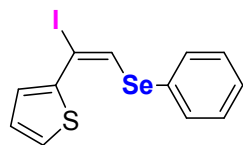


3j: light yellow oil (193.92 mg, 96%, E/Z=99:1). ^1H NMR (400 MHz, CDCl_3) δ : 7.51-7.54 (m, 2H), 7.44-7.48 (m, 2H), 7.37 (s, 1H), 7.32-7.33 (m, 3H), 7.04-7.08 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.65, 161.16, 137.88, 132.89, 130.54, 130.46, 130.02, 129.48, 128.07, 115.52, 115.31, 86.70; ^{19}F NMR (100 MHz, CDCl_3) δ : -111.43. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{10}\text{IFSeNa}$ ($[\text{M}+\text{Na}]^+$): 426.8874, Found 426.8872.

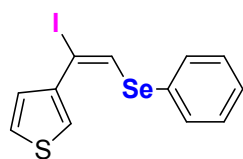


3k: white solid (241.43 mg, 87%, E/Z=99:1). ^1H NMR (400 MHz, CDCl_3) δ : 7.71-7.73 (m, 2H), 7.48-7.50 (m, 2H), 7.27-7.34 (m, 7H), 7.16 (s, 1H), 7.05-7.07 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 144.20, 136.87, 132.85, 130.14, 129.82, 129.78, 129.73, 129.44, 128.05, 127.25, 120.11, 87.08,

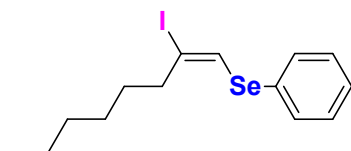
21.59. HRMS m/z (ESI): Calcd for $C_{21}H_{18}INO_2SeNa$ ($[M+Na]^+$): 577.9166, Found 577.9162.



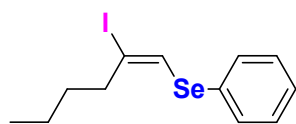
3l: light yellow oil (184.24 mg, 94%, E/Z=86:14). 1H NMR (400 MHz, $CDCl_3$) δ : 7.58-7.63 (m, 2H), 7.45-7.47 (m, 1H), 7.34-7.39 (m, 4H), 7.10-7.28 (m, 1H), 7.08-7.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 133.59, 133.14, 131.51, 130.87, 129.96, 129.19, 128.30, 127.73, 127.22, 126.96, 78.86. HRMS m/z (ESI): Calcd for $C_{12}H_9ISseNa$ ($[M+Na]^+$): 414.8533, Found 414.8530.



3m: light yellow oil (176.4 mg, 90%, E/Z=85:15). 1H NMR (400 MHz, $CDCl_3$) δ : 7.54-7.56 (m, 2H), 7.47-7.48 (m, 1H), 7.31-7.35 (m, 5H), 7.27-7.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 141.86, 132.95, 131.51, 130.39, 129.47, 129.44, 128.81, 128.10, 125.46, 125.34, 81.66. HRMS m/z (ESI): Calcd for $C_{12}H_9ISseNa$ ($[M+Na]^+$): 414.8533, Found 414.8531.

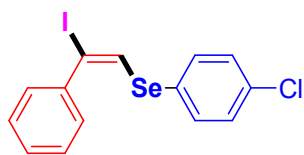


3n: light yellow oil (167.45 mg, 85%, E/Z=85:15). 1H NMR (400 MHz, $CDCl_3$) δ : 7.52-7.53 (m, 2H), 7.27-7.29 (m, 3H), 6.71(s, 1H), 2.43 (t, $J=7.2$ Hz, 2H), 1.58 (s, 2H), 1.28-1.32 (m, 6H), 0.86-0.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 134.23, 132.12, 129.35, 128.13, 127.47, 125.07, 78.06, 41.93, 31.60, 28.74, 27.95, 22.53, 14.08. HRMS m/z (ESI): Calcd for $C_{14}H_{19}ISseNa$ ($[M+Na]^+$): 416.9594, Found 416.9590.

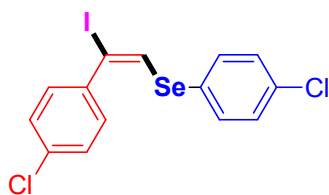


3o: light yellow oil (159.21 mg, 87%, E/Z=85:15). 1H NMR (400 MHz, $CDCl_3$) δ : 7.50-7.52 (m, 2H), 7.31-7.32 (m, 3H), 6.27(s, 1H), 2.40 (t, $J=7.2$ Hz, 2H), 1.50-1.56 (m, 2H), 1.32-1.38 (m, 2H), 0.89-0.93 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 140.34, 134.23, 129.44, 129.35, 128.14, 125.10, 77.23, 38.89, 29.95, 22.10, 13.93. HRMS m/z (ESI): Calcd for $C_{12}H_{15}ISseNa$ ($[M+Na]^+$): 388.9281, Found

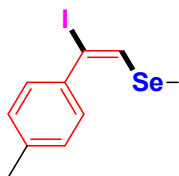
388.9278.



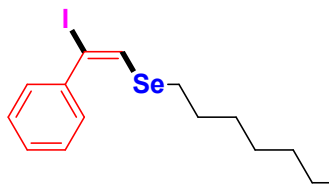
3p: light yellow oil (191.1 mg, 91%, E/Z=89:11). ^1H NMR (400 MHz, CDCl_3) δ : 7.42-7.45 (m, 2H), 7.29-7.38 (m, 4H), 7.24-7.26 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ : 141.57, 134.29, 134.13, 133.28, 129.62, 129.57, 128.95, 128.90, 128.45, 128.42, 89.19. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{10}\text{IClSeNa}$ ($[\text{M}+\text{Na}]^+$): 442.8579, Found 442.8577.



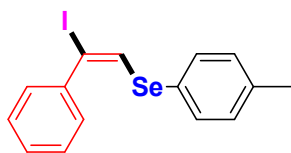
3q: light yellow solid (217.192mg, 96%, E/Z=95:5). ^1H NMR (400 MHz, CDCl_3) δ : 7.42-7.44 (m, 2H), 7.32-7.39 (m, 4H), 7.27-7.31 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 140.05, 134.23, 133.29, 129.86, 129.66, 129.64, 128.67, 128.13, 87.36. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_9\text{ICl}_2\text{SeNa}$ ($[\text{M}+\text{Na}]^+$): 476.8189, Found 476.8185.



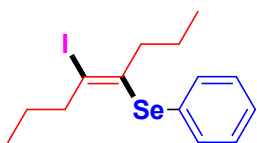
3r: light yellow oil (145.34 mg, 86%, E/Z=99:1). ^1H NMR (400 MHz, CDCl_3) δ : 7.32-7.34 (m, 2H), 7.13-7.16 (m, 3H), 2.34 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 139.01, 138.63, 129.06, 128.94, 128.47, 87.19, 21.35, 8.16. HRMS m/z (ESI): Calcd for $\text{C}_{10}\text{H}_{11}\text{ISENa}$ ($[\text{M}+\text{Na}]^+$): 360.8968, Found 360.8963.



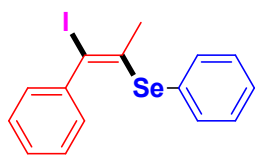
3s: light yellow oil (183.6 mg, 90%, E/Z=80:20). ^1H NMR (400 MHz, CDCl_3) δ : 7.42-7.44 (m, 2H), 7.26-7.36 (m, 3H), 7.23 (s, 1H), 2.72-2.76 (m, 2H), 1.65-1.71 (m, 2H), 1.27-1.35 (m, 8H), 0.87-0.90 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 141.95, 128.98, 128.65, 128.49, 128.22, 86.66, 31.68, 30.75, 29.54, 28.73, 28.36, 22.59, 14.08. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{21}\text{ISENa}$ ($[\text{M}+\text{Na}]^+$): 430.9751, Found 430.9749.



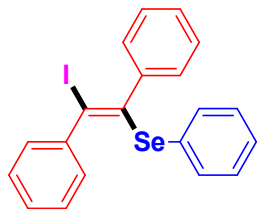
3t: light yellow oil (188.0 mg, 94%, E/Z=95:5). ^1H NMR (400 MHz, CDCl_3) δ : 7.48-7.50 (m, 2H), 7.43-7.45 (m, 2H), 7.32-7.40 (m, 4H), 7.13-7.15 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 141.77, 138.19, 133.27, 133.02, 130.34, 130.23, 130.11, 128.78, 128.59, 128.39, 126.63, 87.44, 21.21. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{13}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 422.9125, Found 422.9121.



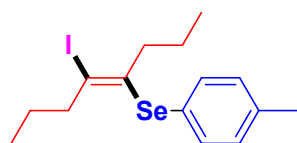
3u: light yellow oil (181.24 mg, 92%, E/Z=93:7). ^1H NMR (400 MHz, CDCl_3) δ : 7.40-7.42 (m, 2H), 7.26-7.28 (m, 3H), 2.88-2.92 (m, 2H), 2.38-2.42 (m, 2H), 1.56-1.62 (m, 2H), 1.49-1.53 (m, 2H), 0.92 (t, $J=7.2$ Hz, 3H), 0.84-0.87 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 133.15, 132.46, 130.81, 129.17, 127.23, 109.24, 47.55, 45.99, 22.73, 21.45, 13.46, 12.84. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{19}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 416.9594, Found 416.9590.



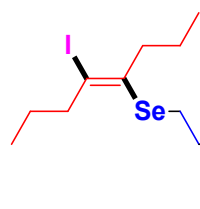
3v: light yellow oil (188.0 mg, 94%, E/Z=90:10). ^1H NMR (400 MHz, CDCl_3) δ : 7.62-7.63 (m, 1H), 7.47-7.49 (m, 2H), 7.33-7.38 (m, 2H), 7.25-7.32 (m, 5H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 145.06, 134.77, 131.51, 129.19, 129.14, 128.65, 128.31, 128.22, 128.11, 127.72, 94.16, 31.58. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{13}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 422.9125, Found 422.9123.



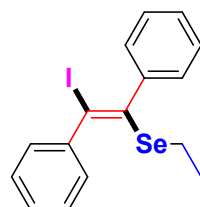
3w: light yellow solid (207.9 mg, 90%, E/Z=95:5). ^1H NMR (400 MHz, CDCl_3) δ : 7.61-7.63 (m, 1H), 7.54-7.56 (m, 4H), 7.34-7.36 (m, 6H), 7.25-7.28 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ : 132.98, 131.61, 131.51, 130.90, 129.32, 129.18, 128.34, 128.25, 127.72, 123.27, 89.38. HRMS m/z (ESI): Calcd for $\text{C}_{20}\text{H}_{15}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 484.9281, Found 484.9278.



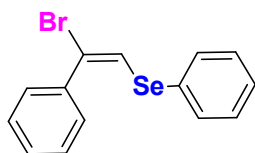
3x: light yellow oil (183.6 mg, 90%, E/Z=93:7). ^1H NMR (400 MHz, CDCl_3) δ : 7.32-7.34 (m, 2H), 7.08-7.10 (m, 2H), 2.88-2.91 (m, 2H), 2.33-2.38 (m, 5H), 1.58-1.62 (m, 2H), 1.48-1.52 (m, 2H), 0.91-0.95 (m, 3H), 0.83-0.86 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 137.51, 133.68, 133.20, 129.97, 126.72, 107.68, 47.40, 45.59, 22.68, 21.43, 21.14, 13.45, 12.85. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{21}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 430.9751, Found 430.9749.



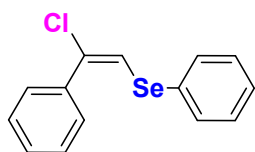
3y: light yellow oil (197.6 mg, 95%, E/Z=94:6). ^1H NMR (400 MHz, CDCl_3) δ : 2.82-2.86 (m, 1H), 2.67-2.70 (m, 2H), 2.46-2.50 (m, 1H), 1.54-1.63 (m, 6H), 1.27-1.36 (m, 10H), 0.86-0.97 (m, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ : 132.20, 101.96, 52.53, 47.20, 45.65, 31.70, 30.43, 29.74, 28.76, 27.09, 22.68, 21.55, 14.07, 13.55, 12.82. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{29}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 439.0377, Found 439.0376.



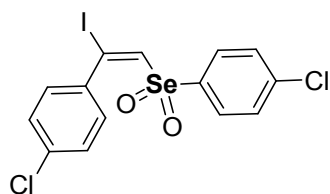
3z: light yellow oil (229.9 mg, 95%, E/Z=95:5). ^1H NMR (400 MHz, CDCl_3) δ : 7.40-7.44 (m, 6H), 7.31-7.36 (m, 4H), 2.21 (t, $J=7.6$ Hz, 2H), 1.34-1.37 (m, 2H), 1.20-1.24 (m, 2H), 1.09-1.41 (m, 6H), 0.85 (t, $J=7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 144.73, 143.61, 136.92, 131.60, 129.12, 128.76, 128.55, 128.42, 128.33, 128.31, 128.23, 127.90, 91.50, 31.57, 30.18, 29.51, 28.73, 28.60, 22.53, 14.05. HRMS m/z (ESI): Calcd for $\text{C}_{21}\text{H}_{25}\text{ISeNa}$ ($[\text{M}+\text{Na}]^+$): 507.0064, Found 507.0060.



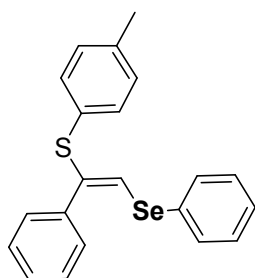
4a: light yellow oil (64.22 mg, 95%, E/Z=71:29). ^1H NMR (400 MHz, CDCl_3) δ : 7.52-7.54 (m, 2H), 7.40-7.41 (m, 2H), 7.25-7.33 (m, 6H), 7.13 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 136.32, 134.18, 132.67, 129.43, 129.36, 129.14, 129.08, 128.63, 128.33, 128.11, 127.93, 122.56, 104.21. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{11}\text{BrSeNa}$ ($[\text{M}+\text{Na}]^+$): 360.9107, Found 360.9105.



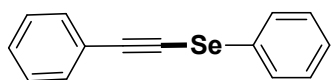
4b: light yellow oil (55.27 mg, 94%, E/Z=58:42). ^1H NMR (400 MHz, CDCl_3) δ : 7.53-7.58 (m, 2H), 7.41-7.47 (m, 3H), 7.31-7.33 (m, 5H), 6.93 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 137.08, 133.50, 132.52, 129.44, 129.32, 129.28, 129.18, 128.38, 128.30, 128.25, 128.08, 127.89, 119.62. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{11}\text{ClSeNa}$ ($[\text{M}+\text{Na}]^+$): 316.9612, Found 316.9607.



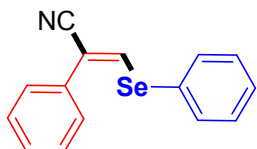
5a: light yellow solid (75.66 mg, 78%, E/Z=92:8). ^1H NMR (400 MHz, CDCl_3) δ : 8.06 (s, 2H), 7.98-8.00 (m, 2H), 7.57-7.59 (m, 3H), 7.40-7.44 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 134.68, 133.85, 131.00, 130.23, 129.82, 128.33, 128.29, 113.73. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_9\text{ISeCl}_2\text{O}_2\text{Na}$ ($[\text{M}+\text{Na}]^+$): 508.8087, Found 508.8085.



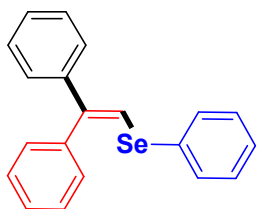
6a: light yellow oil (42.79 mg, 56%, E/Z=96:4). ^1H NMR (400 MHz, CDCl_3) δ : 7.62-7.66 (m, 1H), 7.49-7.56 (m, 3H), 7.27-7.51 (m, 9H), 7.09-7.18 (m, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 137.44, 132.86, 131.53, 130.53, 129.83, 129.57, 129.46, 129.22, 128.86, 128.58, 128.56, 128.42, 127.99, 21.13. HRMS m/z (ESI): Calcd for $\text{C}_{21}\text{H}_{18}\text{SeSNa}$ ($[\text{M}+\text{Na}]^+$): 405.0192, Found 405.0189.



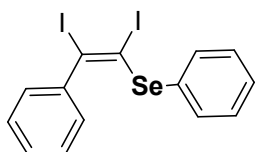
7a: light yellow oil 45.92 mg, 89%). ^1H NMR (400 MHz, CDCl_3) δ : 7.60-7.62 (m, 1H), 7.51-7.53 (m, 2H), 7.28-7.36 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ : 131.77, 129.59, 128.97, 128.61, 128.38, 127.12, 123.14, 102.99, 69.21. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{10}\text{SeNa}$ ($[\text{M}+\text{Na}]^+$): 280.9840, Found 280.9839.



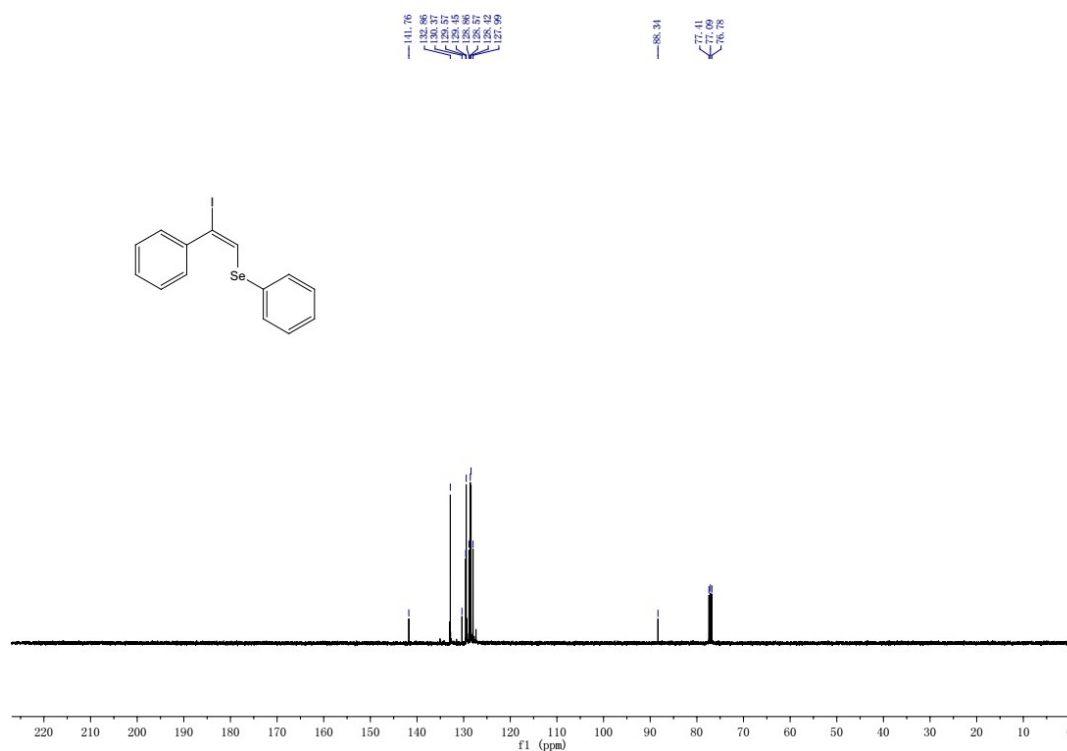
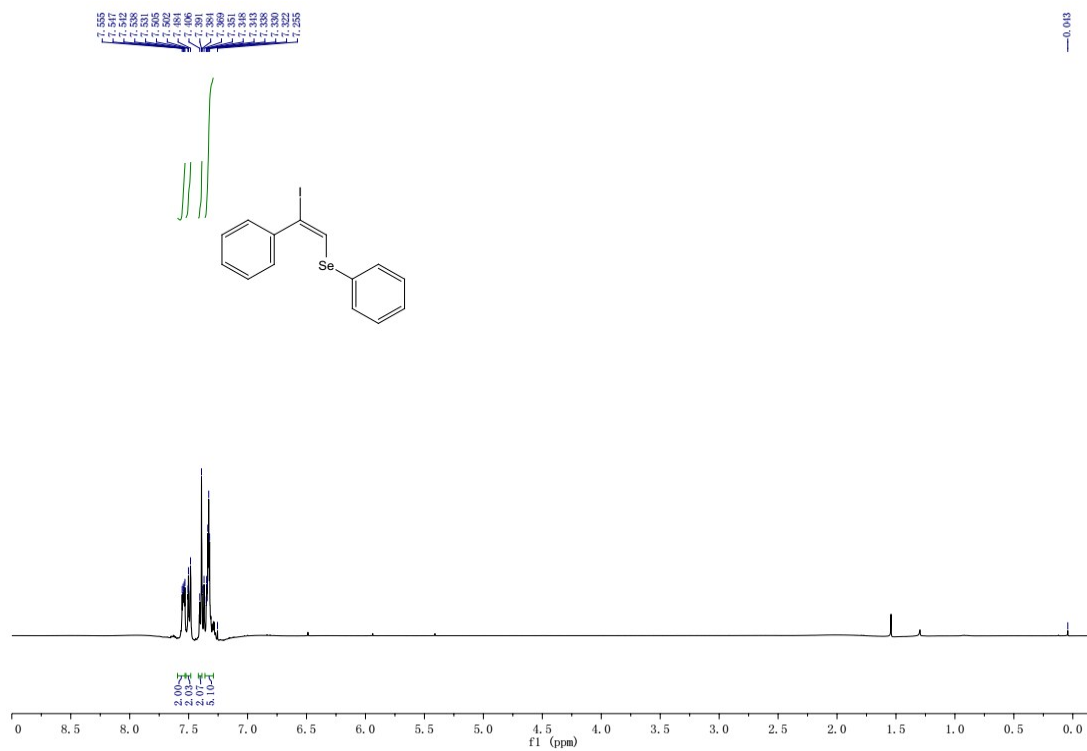
8a: white solid (29.64 mg, 52%). ^1H NMR (400 MHz, CDCl_3) δ : 7.88-7.90 (m, 2H), 7.68-7.69 (m, 2H), 7.54 (s, 1H), 7.25-7.49 (m, 5H), 7.21-7.22 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 142.27, 133.04, 132.11, 130.55, 129.26, 129.21, 129.19, 129.07, 128.96, 128.62, 128.28, 127.47, 125.99, 111.66. HRMS m/z (ESI): Calcd for $\text{C}_{15}\text{H}_{11}\text{SeNa}$ ($[\text{M}+\text{Na}]^+$): 293.9918, Found 293.9920.



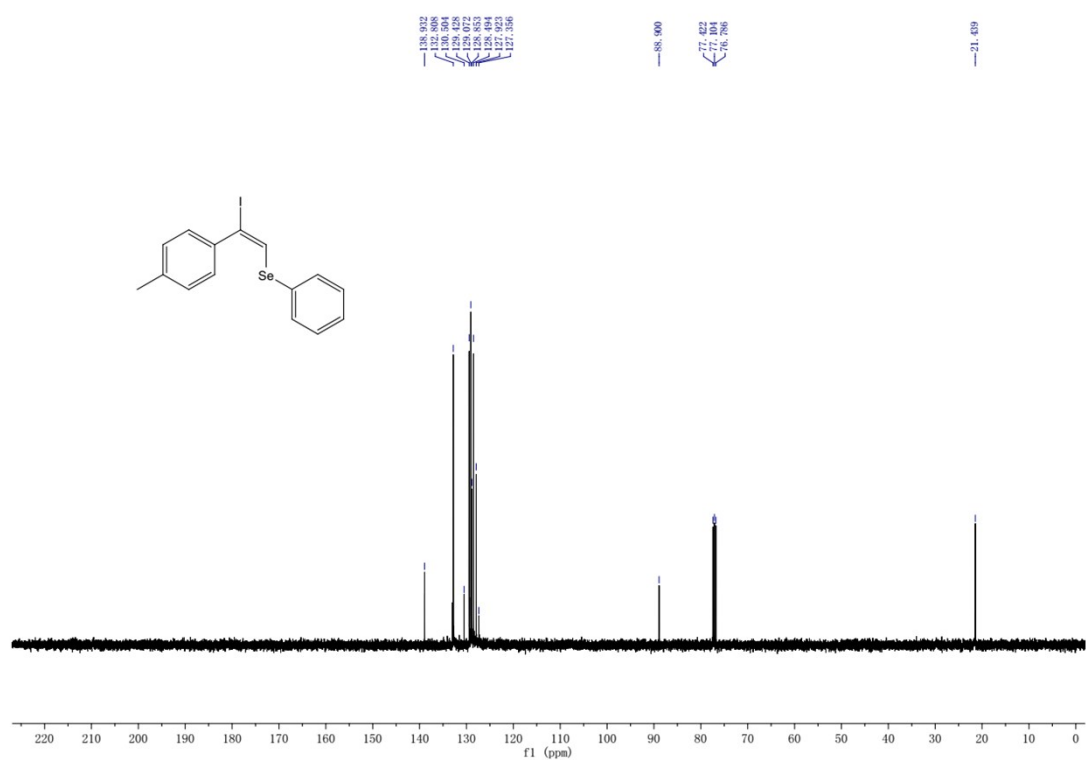
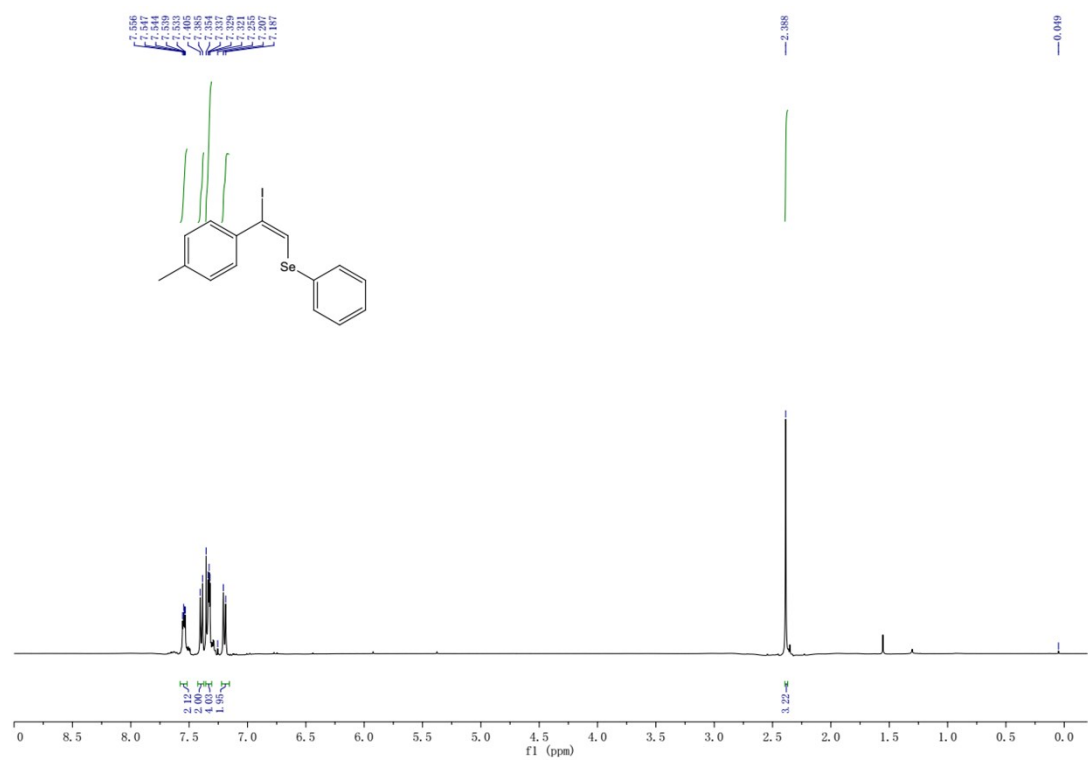
9a: light yellow oil (54.92 mg, 91%). ^1H NMR (400 MHz, CDCl_3) δ : 7.57-7.60 (m, 2H), 7.24-7.58 (m, 13H), 7.13 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 140.31, 132.50, 129.31, 128.52, 128.28, 127.42, 127.15, 122.57. HRMS m/z (ESI): Calcd for $\text{C}_{20}\text{H}_{16}\text{SeNa}$ ($[\text{M}+\text{Na}]^+$): 359.0309, Found 359.0305.



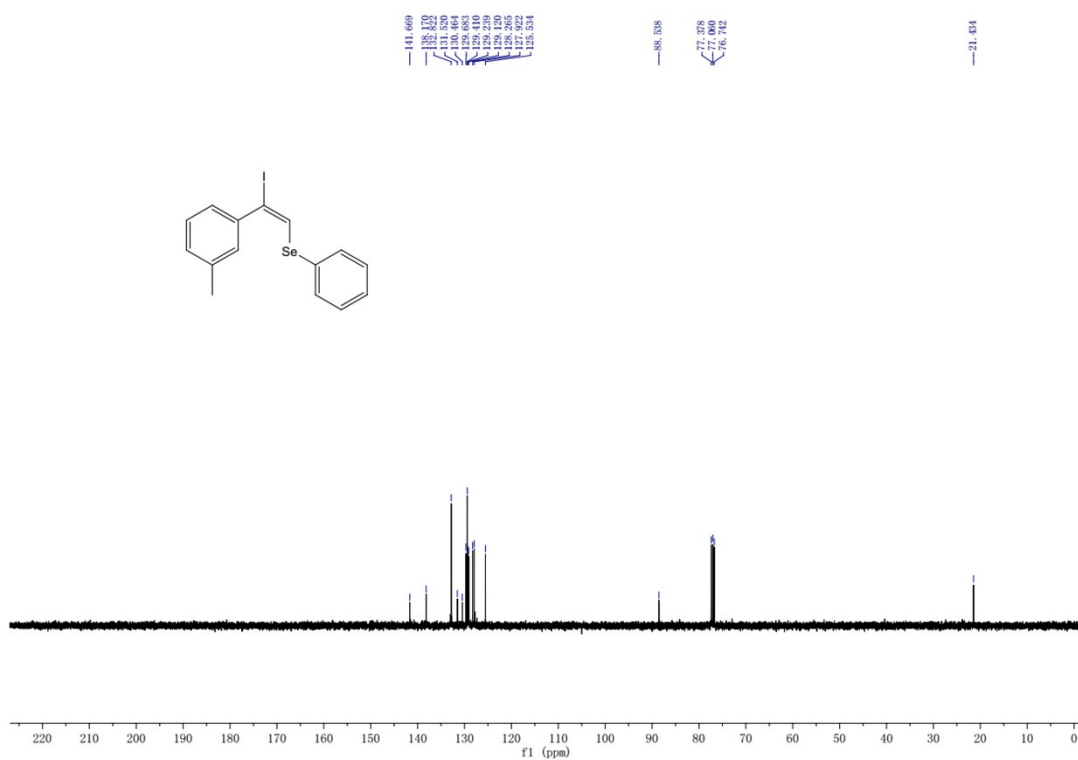
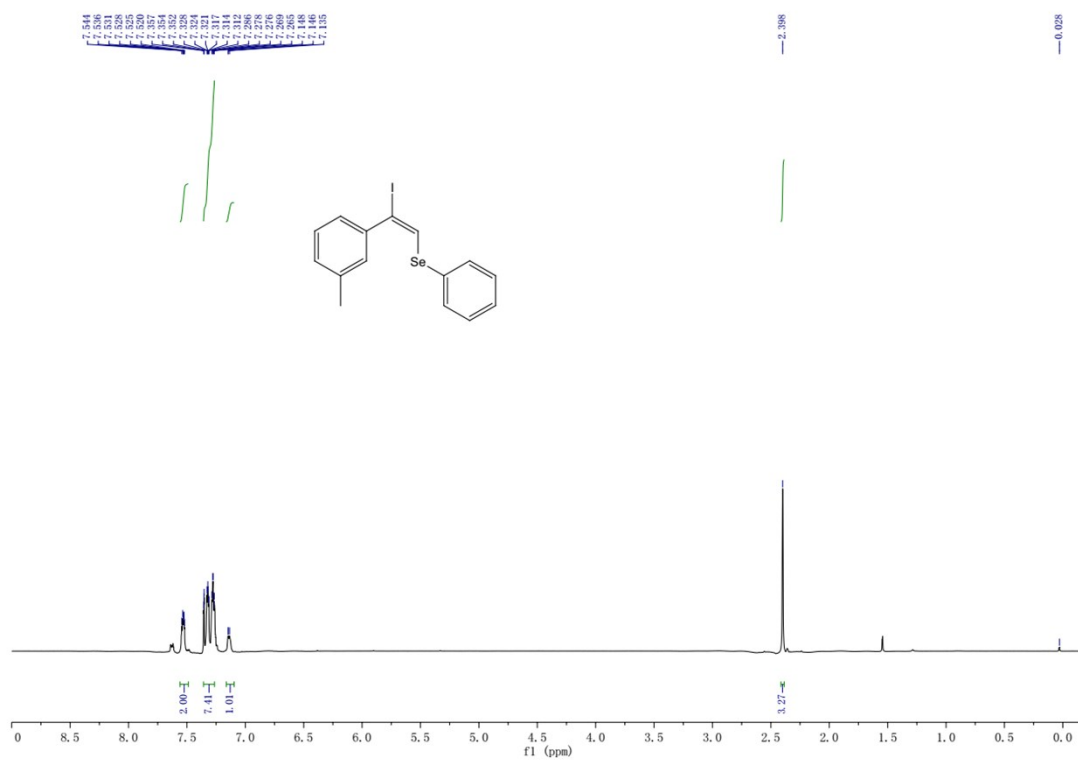
10a: light yellow oil (91.98 mg, 90%). ^1H NMR (400 MHz, CDCl_3) δ : 7.60-7.62 (m, 2H), 7.36 (s, 3H), 7.26-7.27 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 132.97, 131.51, 130.90, 129.18, 128.95, 128.48, 128.41, 127.71, 96.15, 80.78. HRMS m/z (ESI): Calcd for $\text{C}_{14}\text{H}_{10}\text{SeI}_2\text{Na}$ ($[\text{M}+\text{Na}]^+$): 534.7935, Found 534.7929



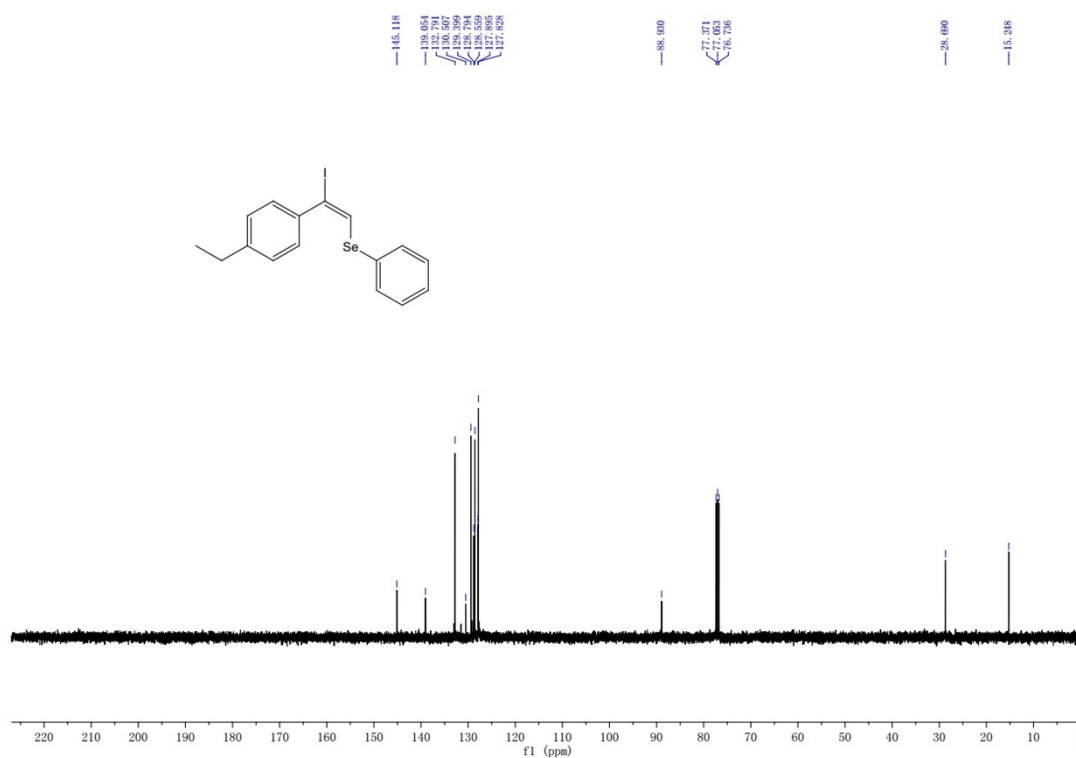
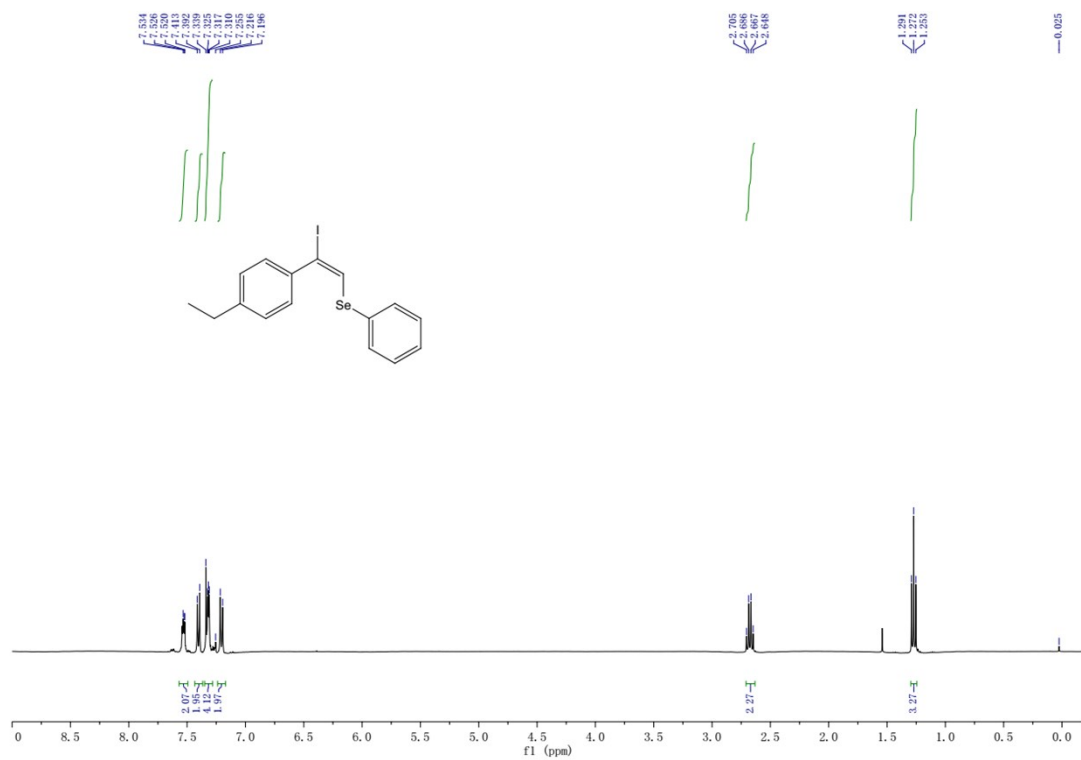
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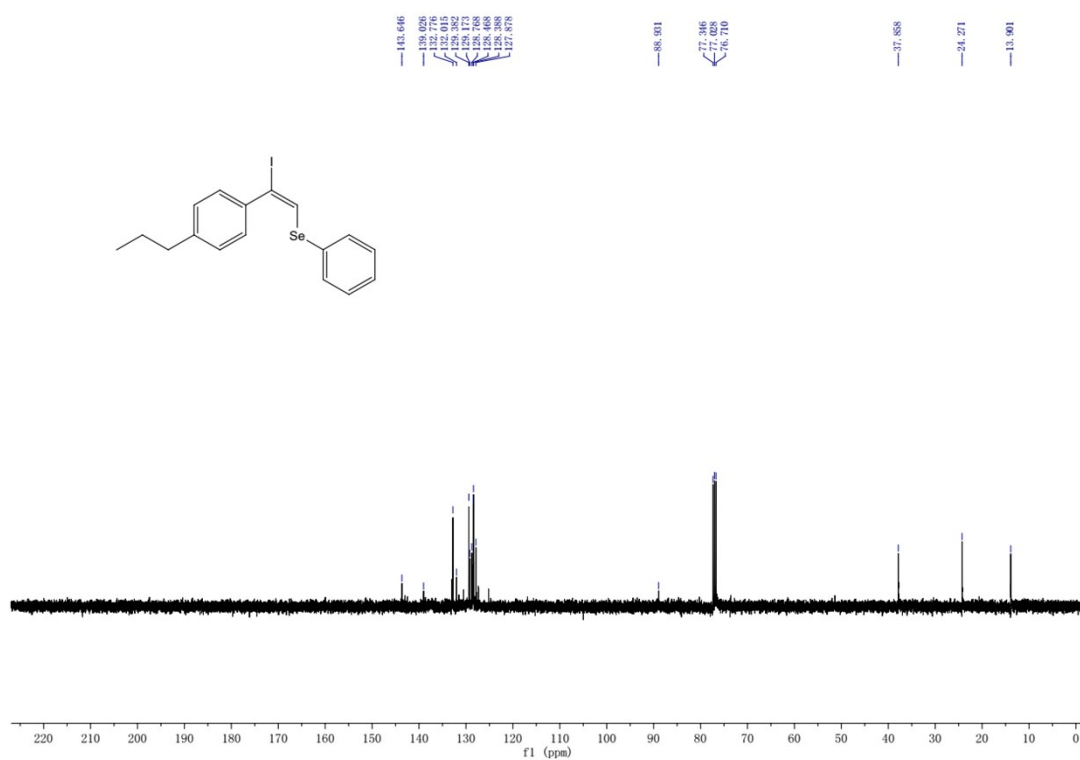
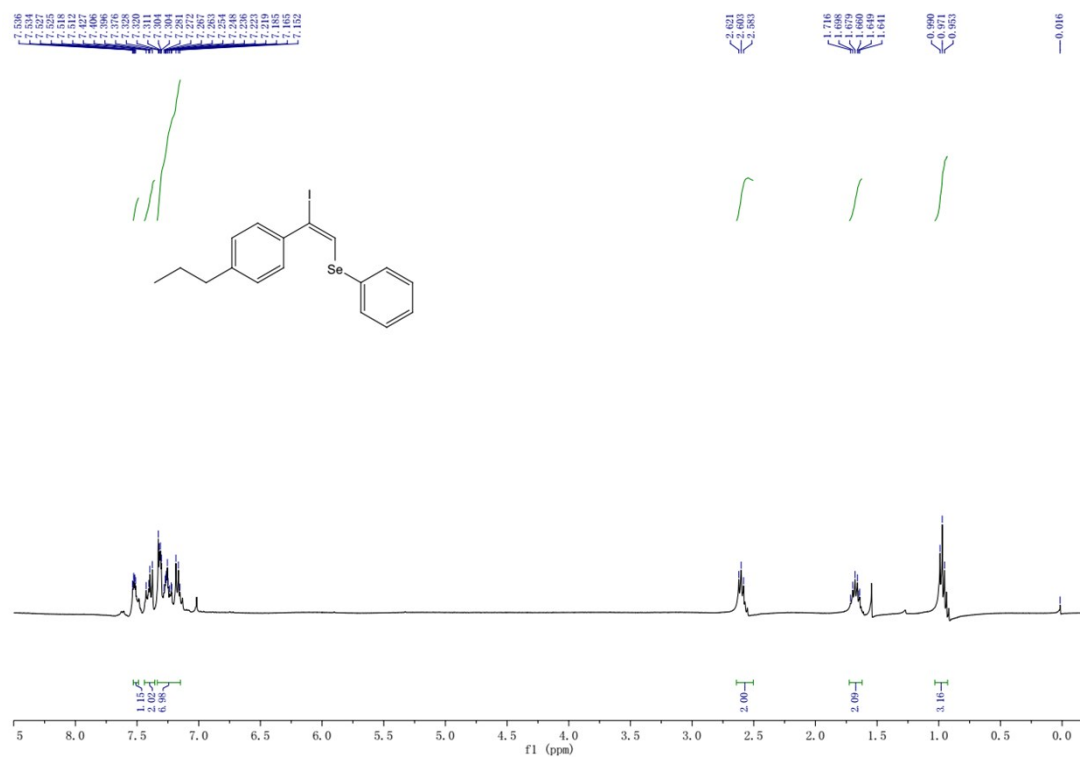
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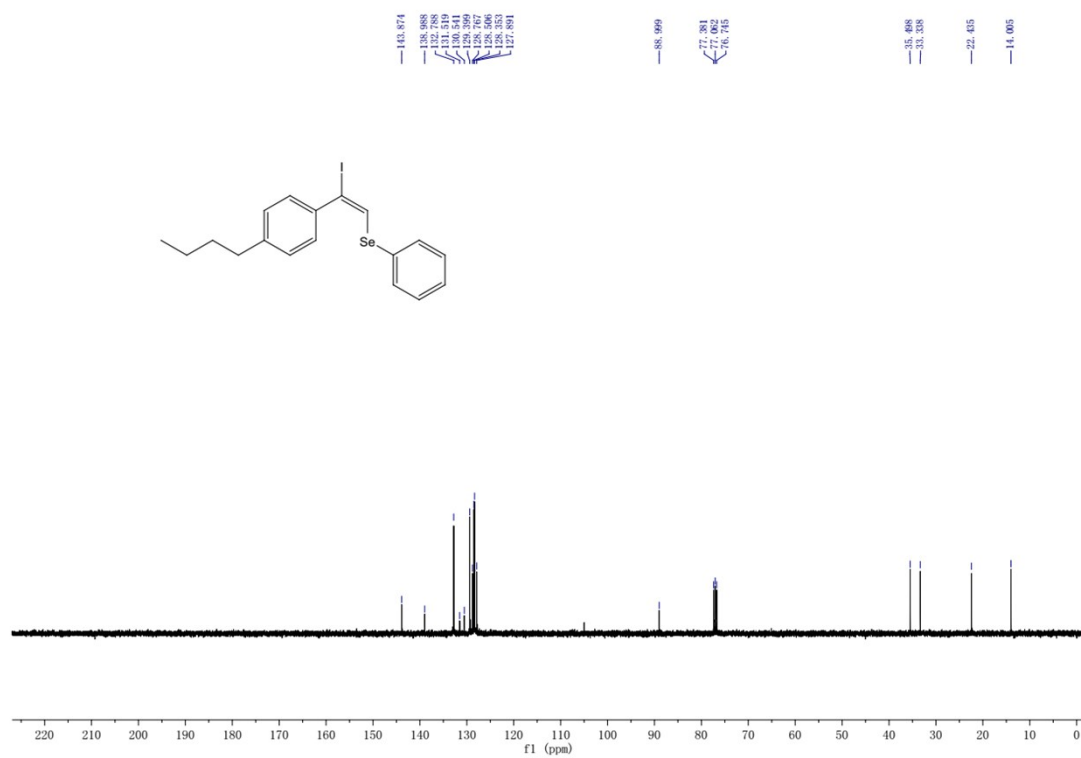
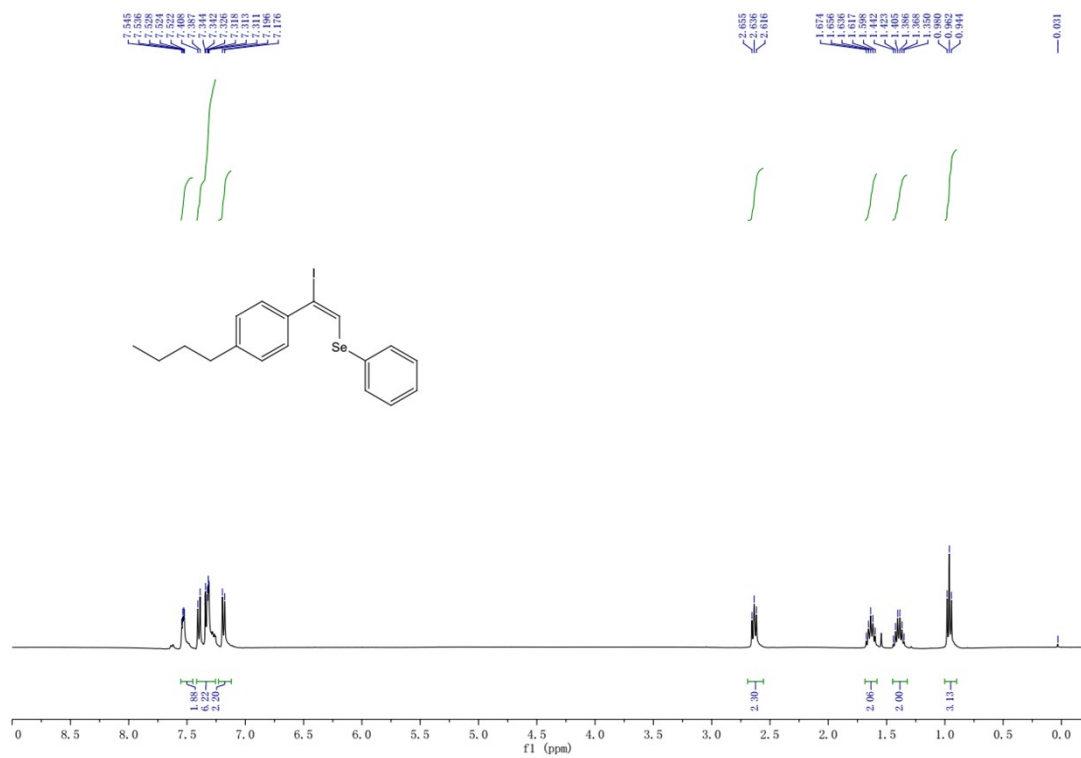
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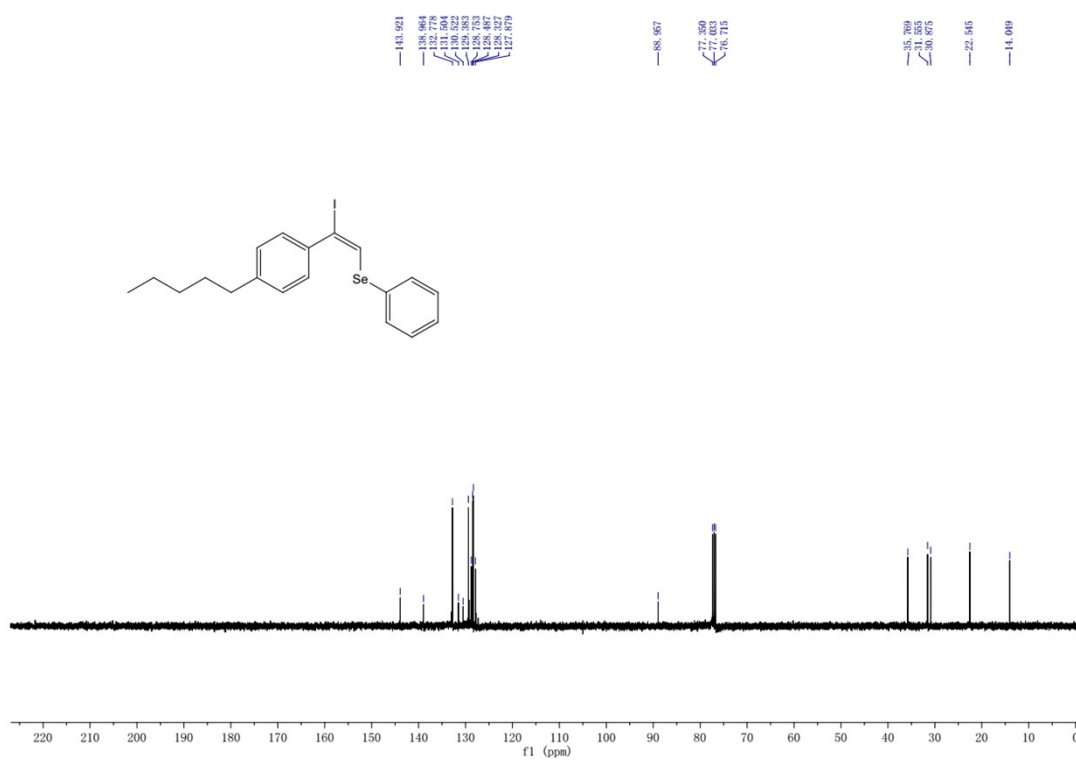
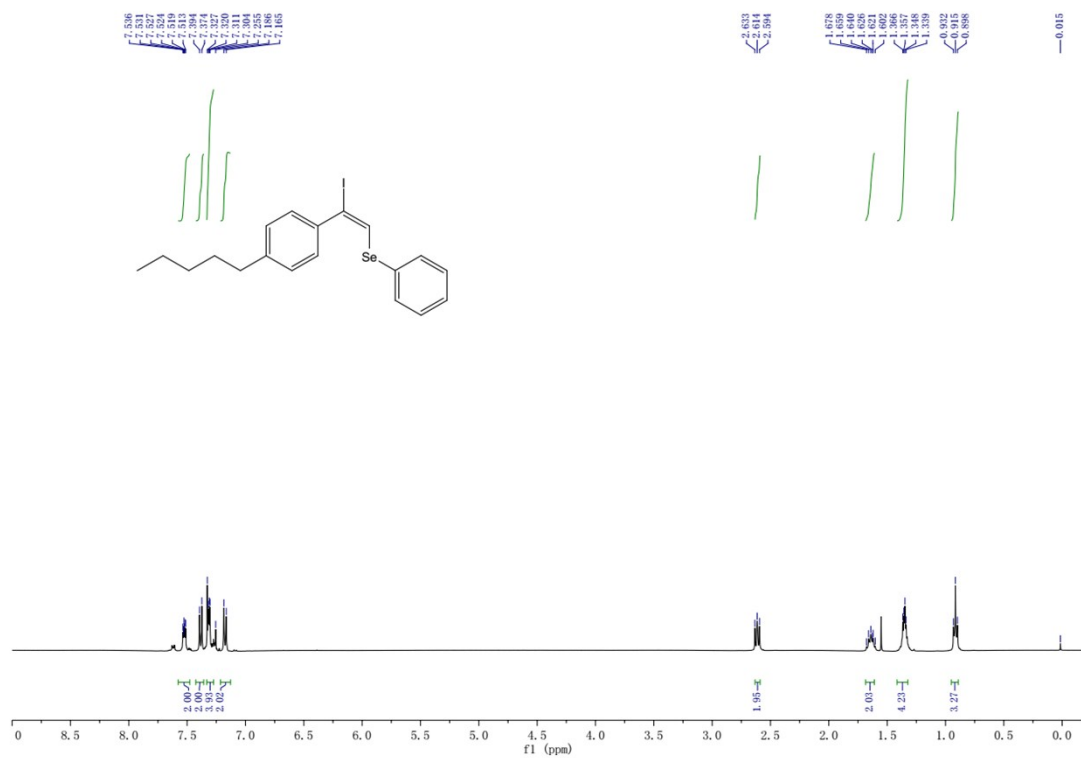
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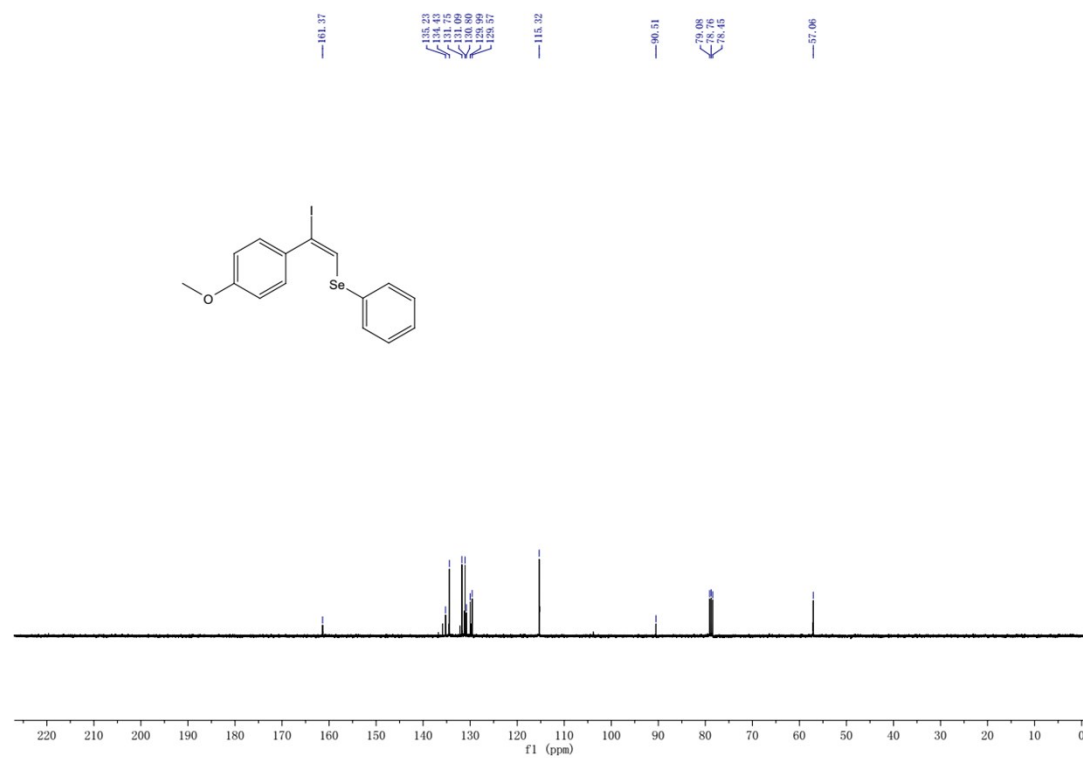
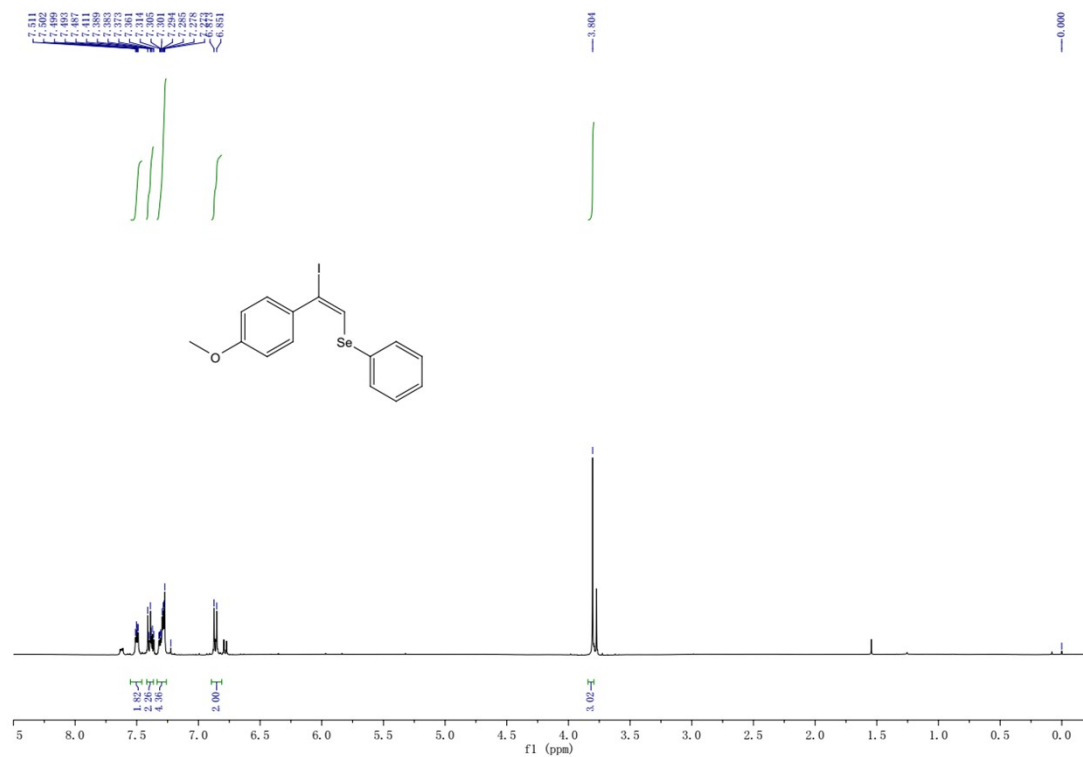
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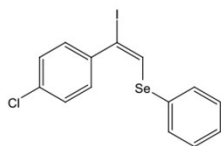
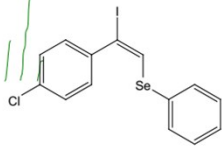


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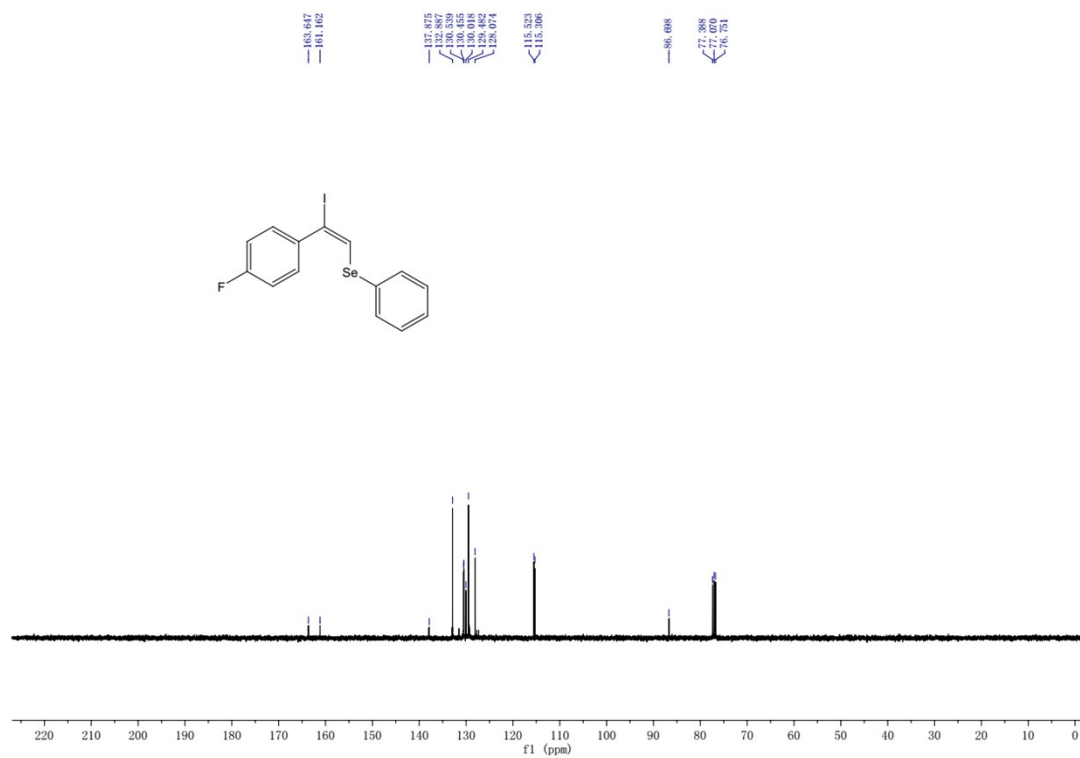
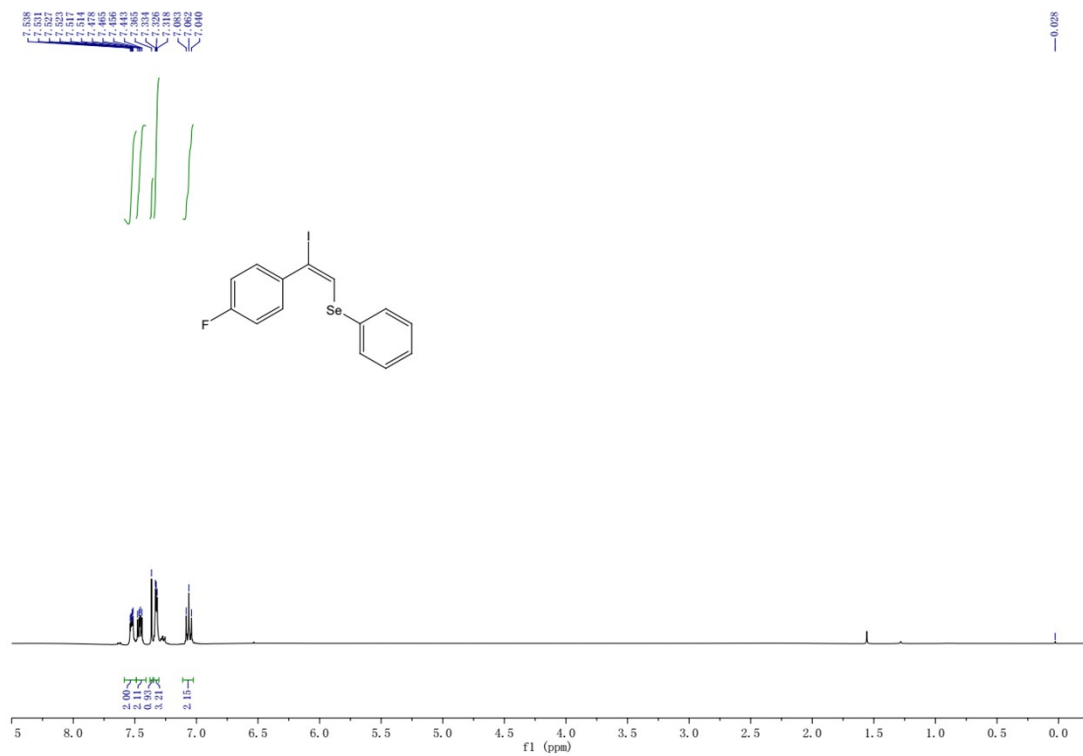


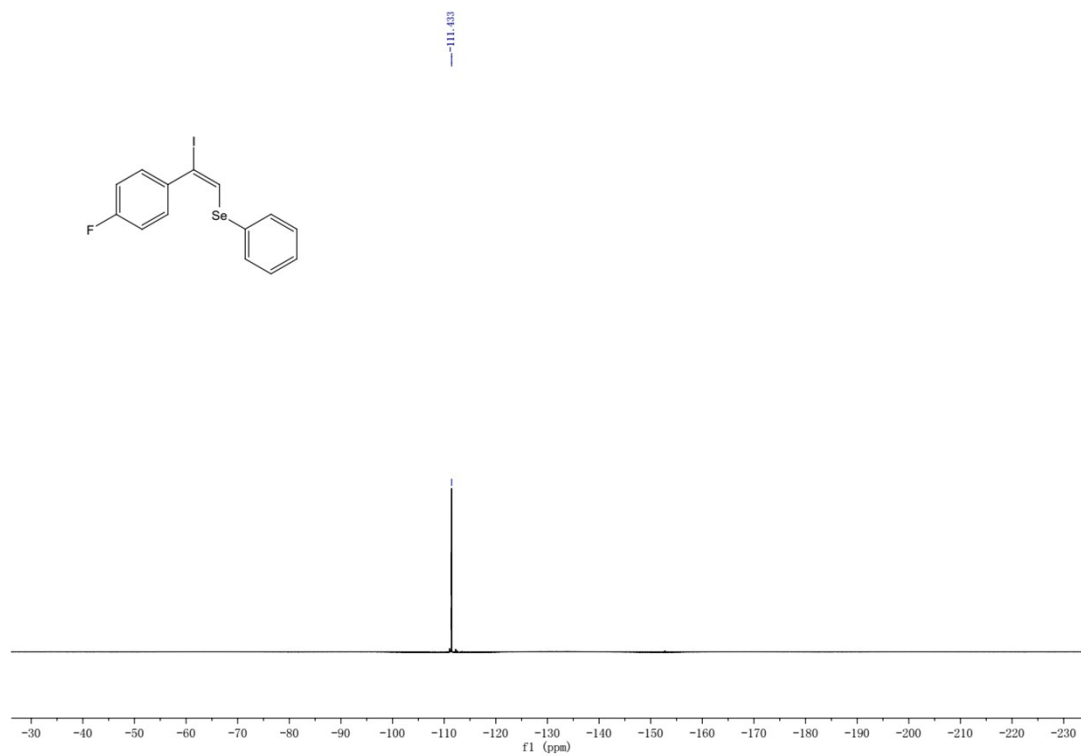
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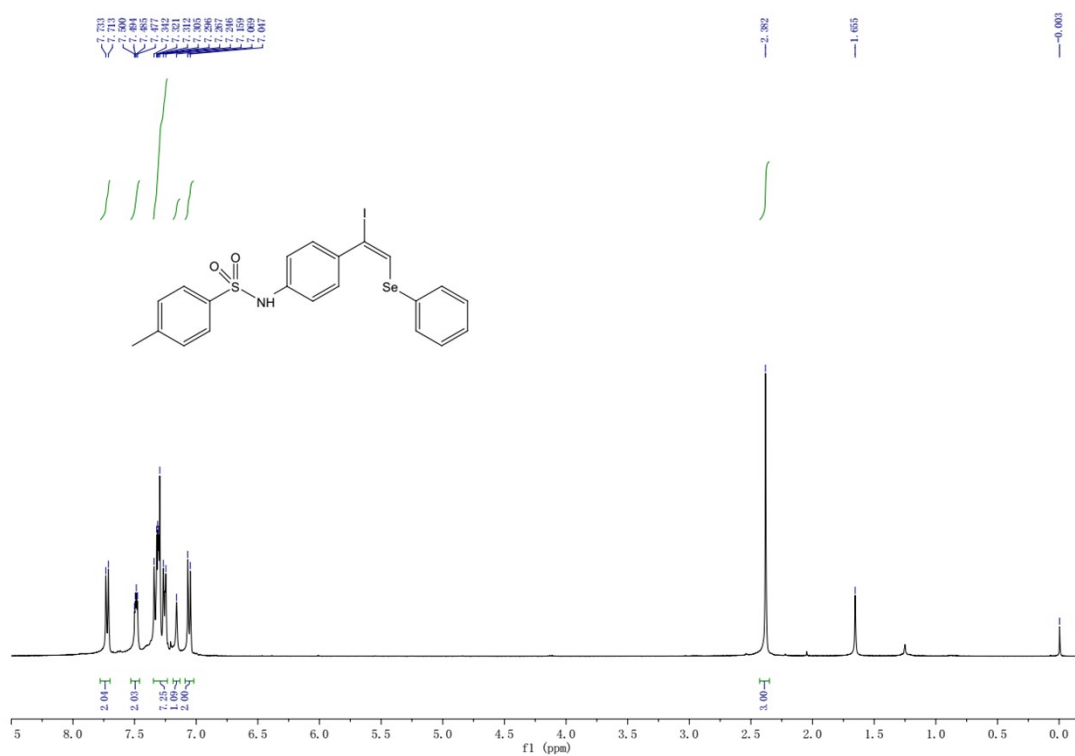


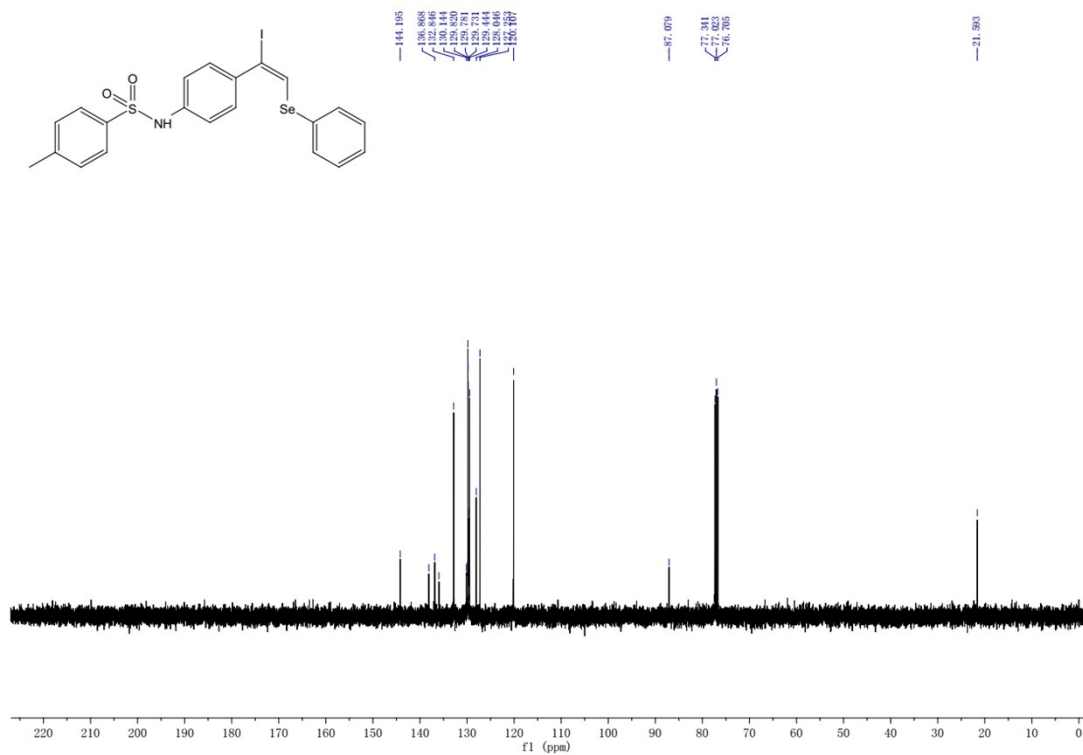
21 / 47



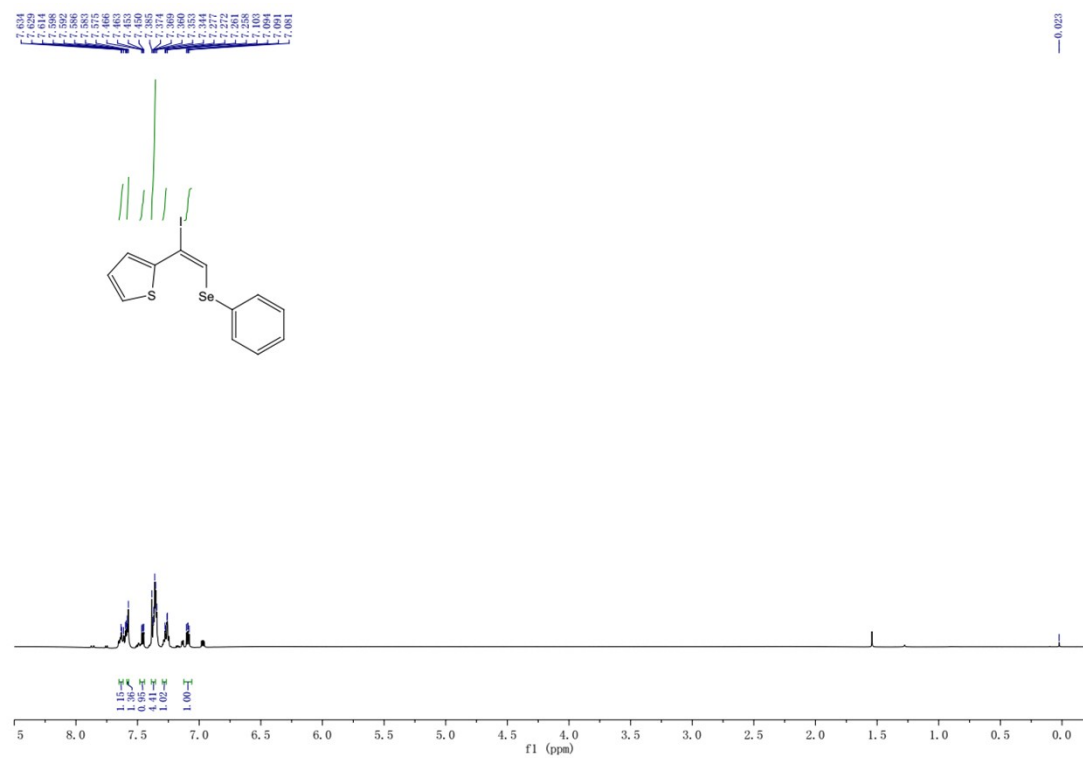


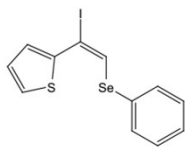
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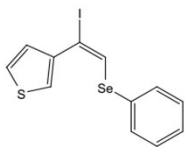


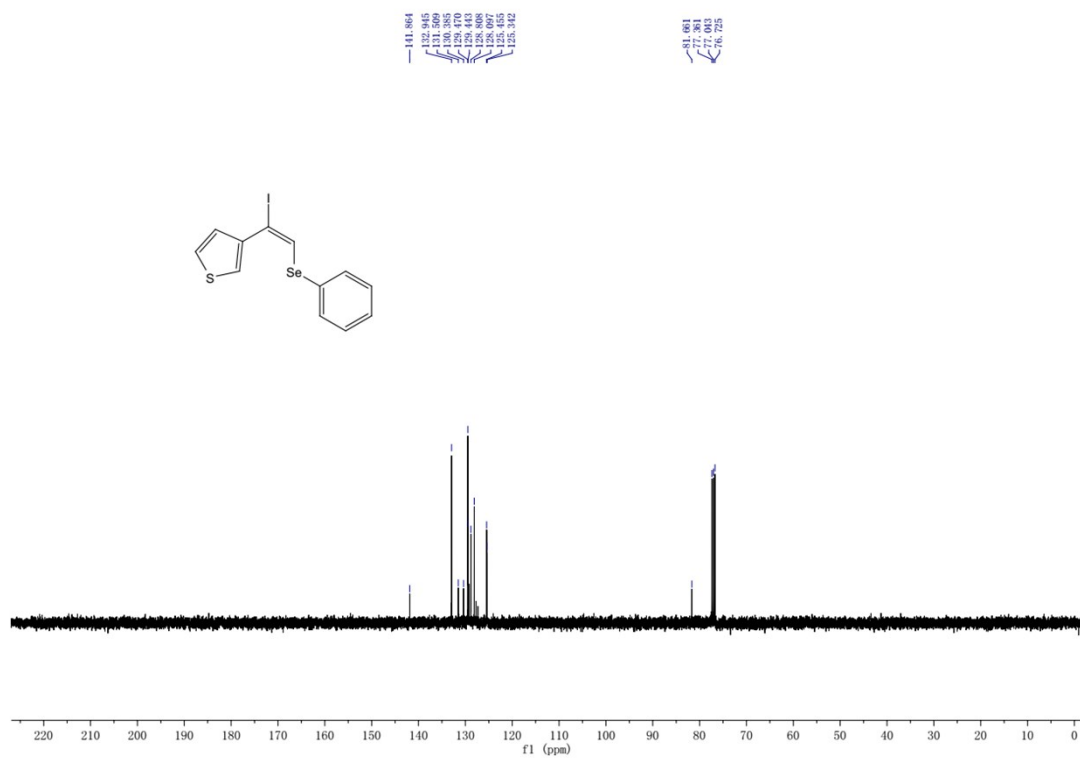
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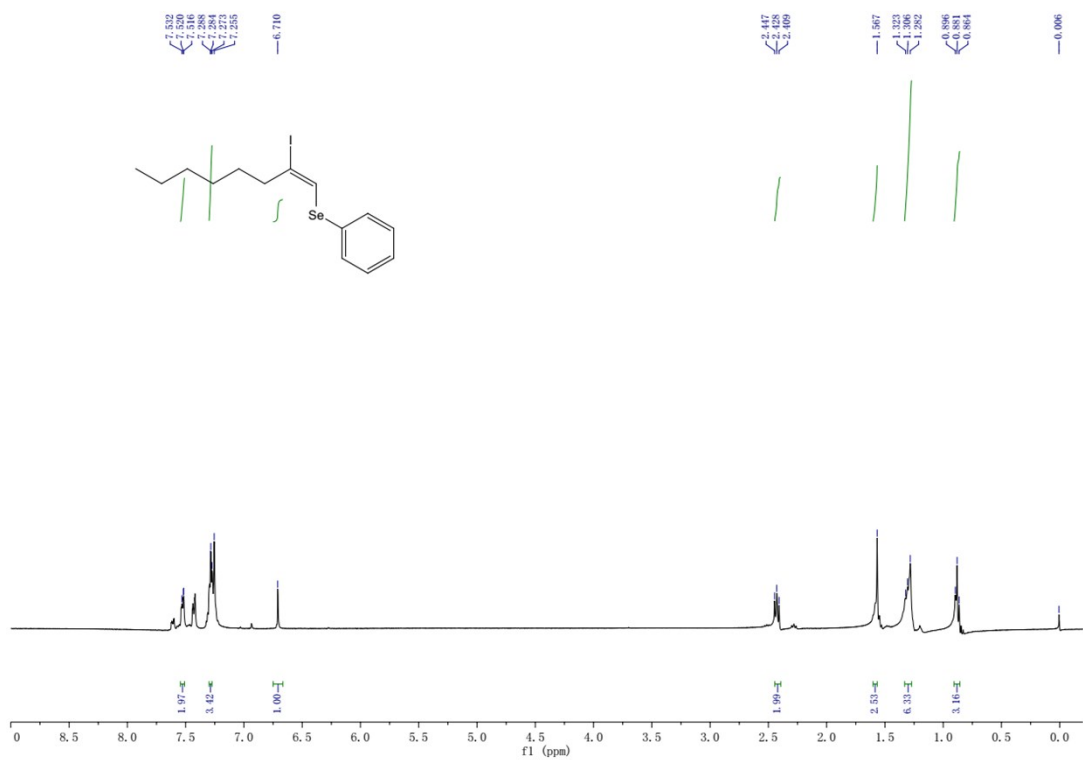


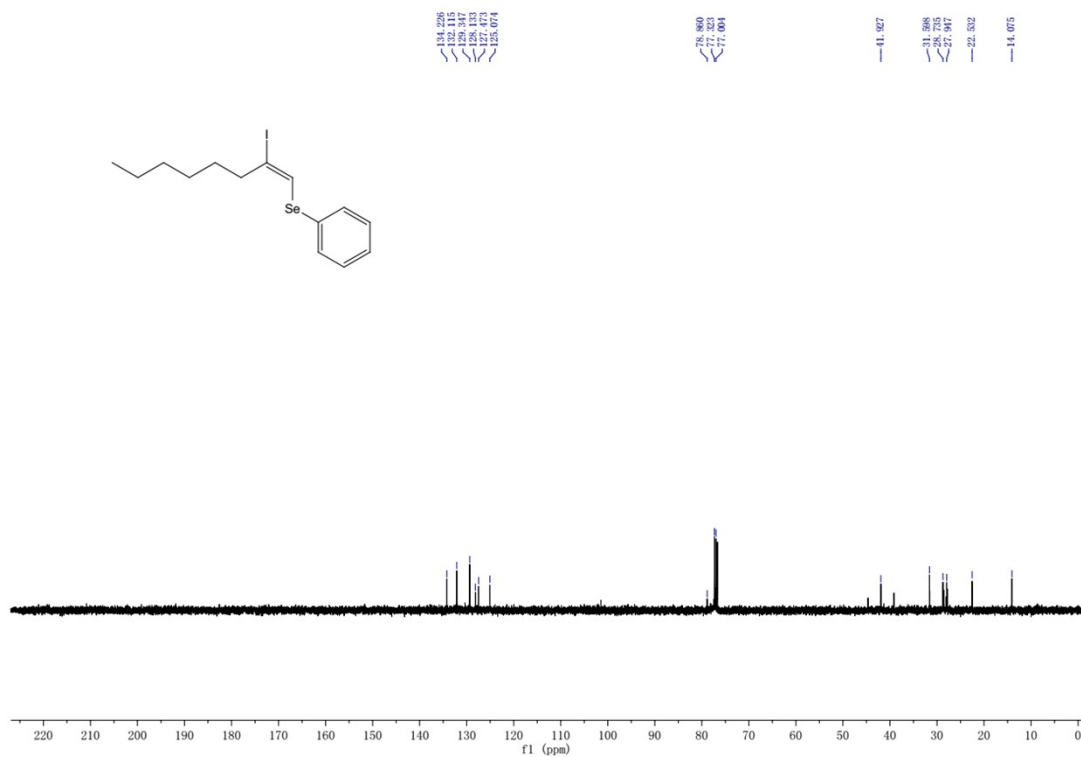
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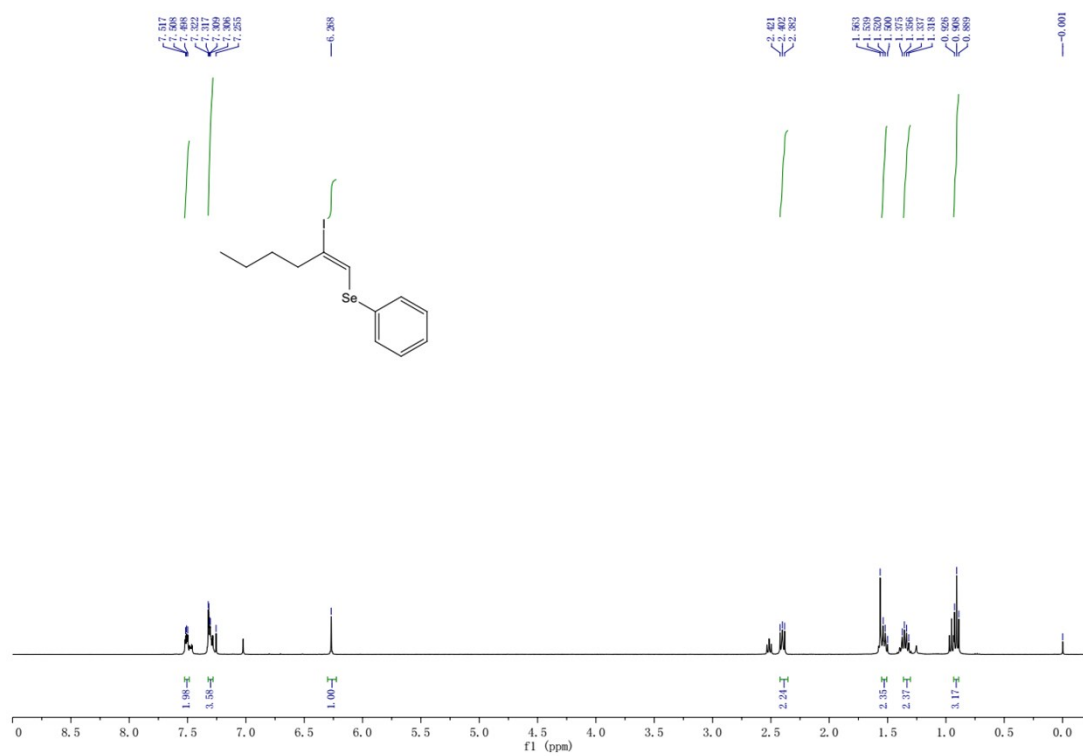


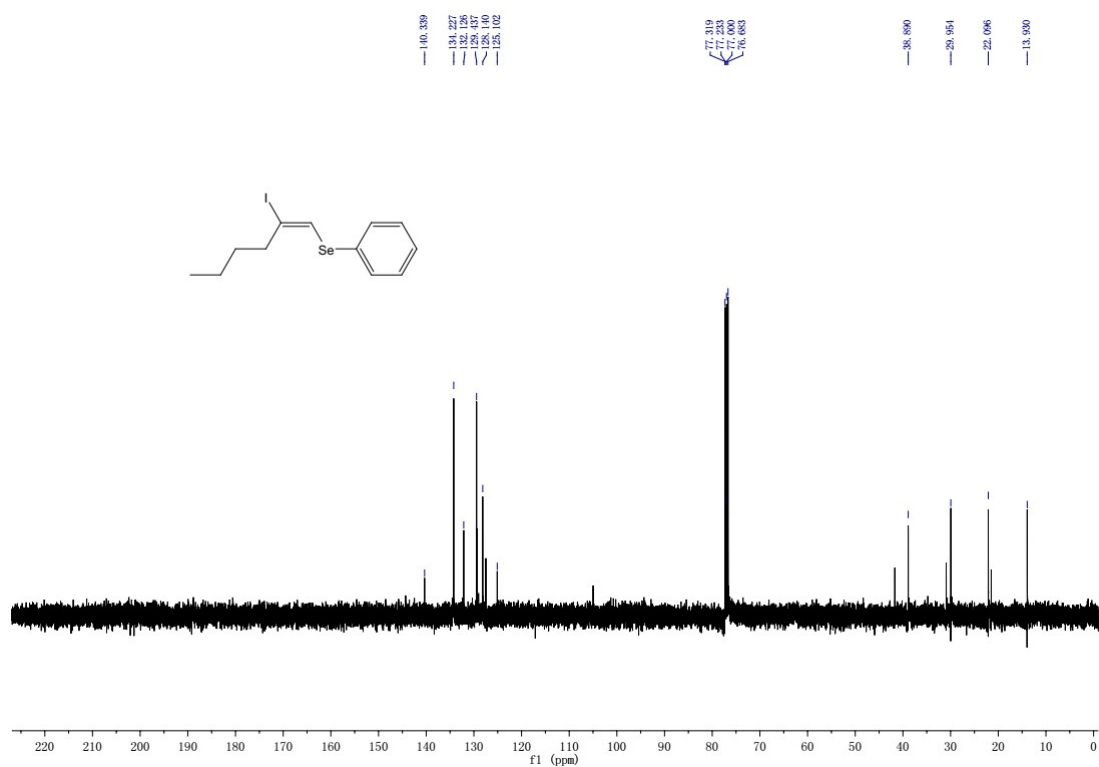
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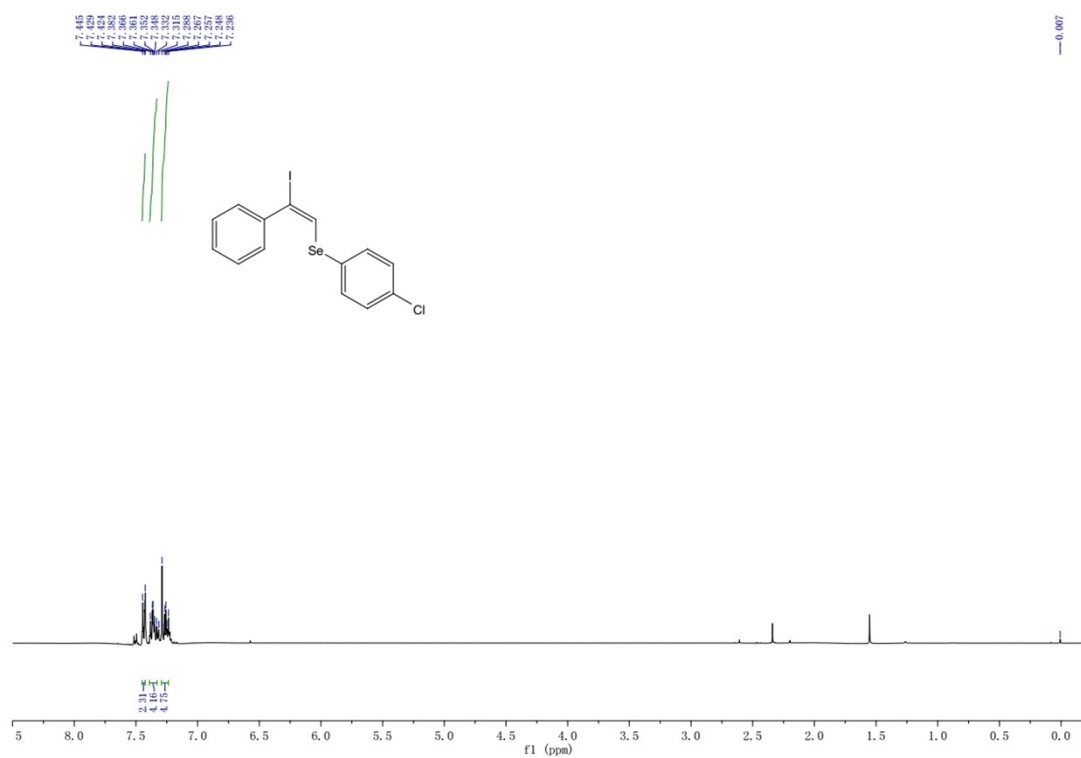


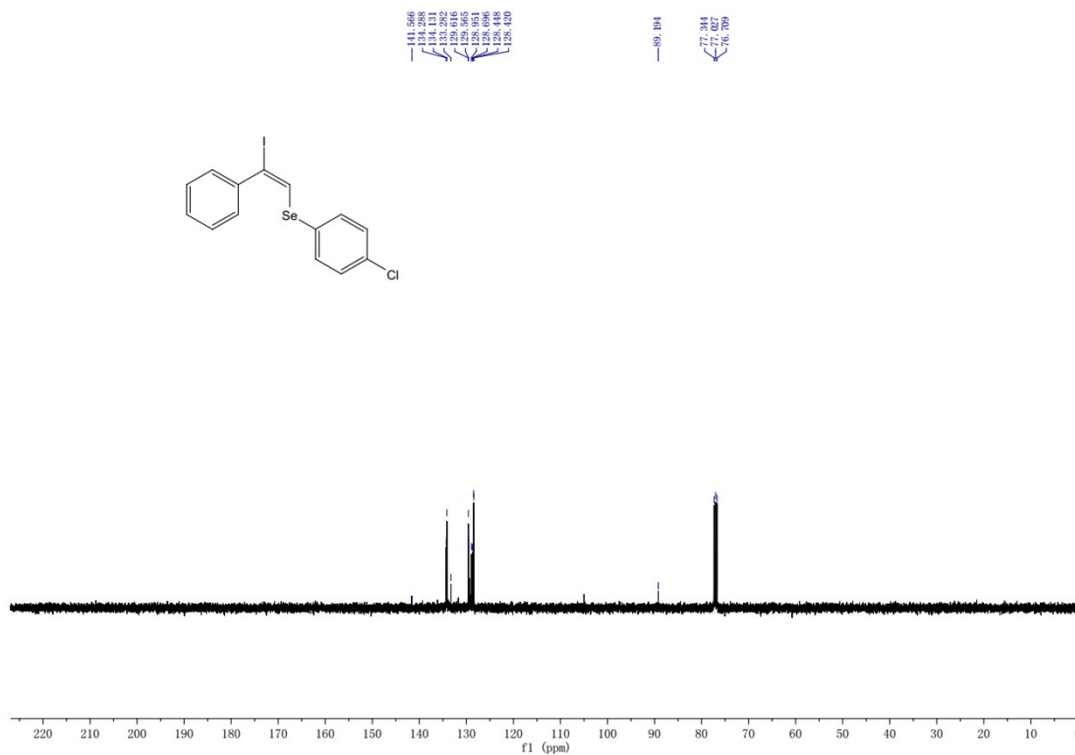
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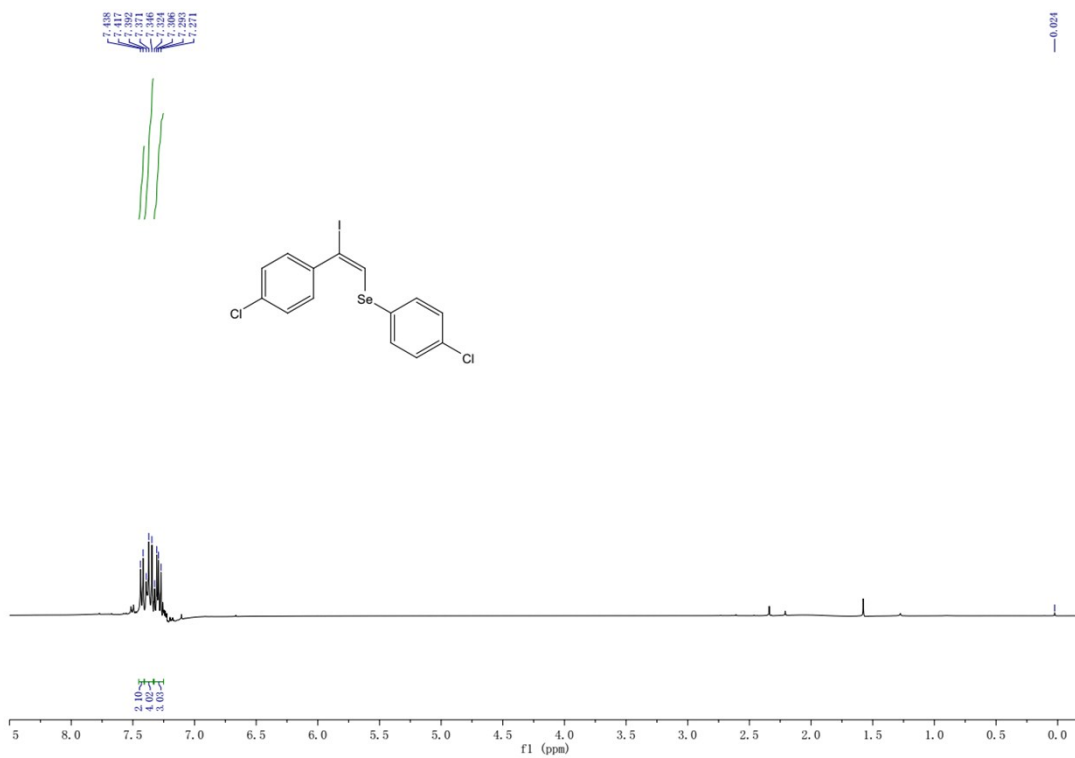


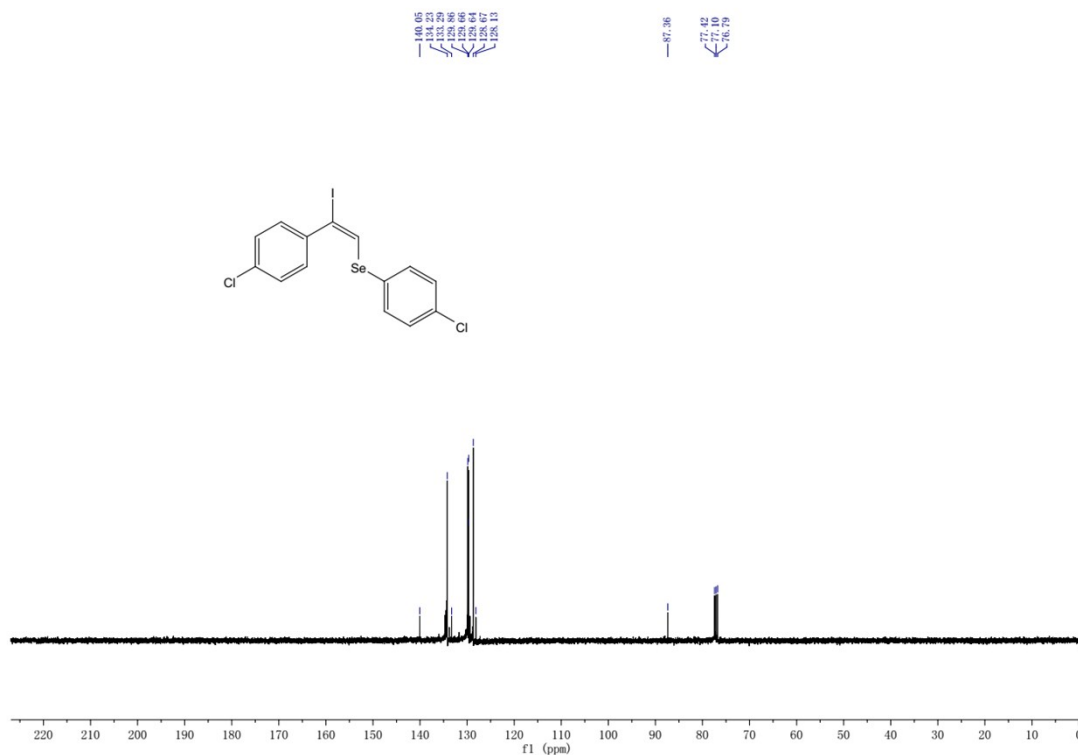
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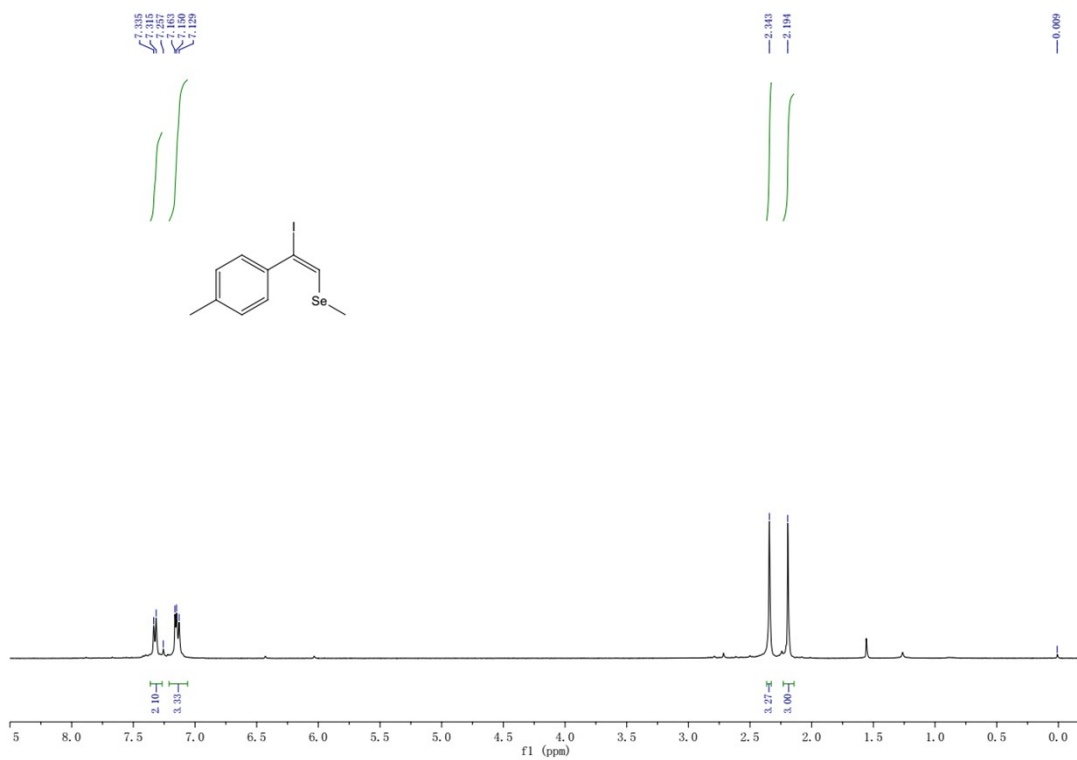


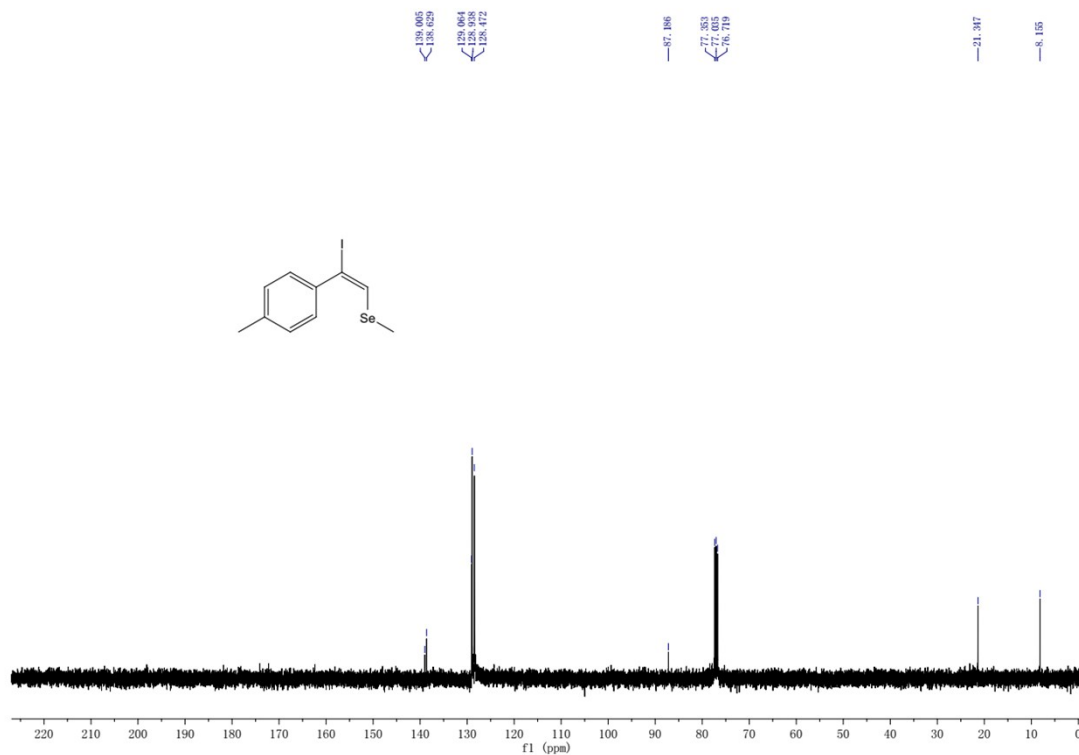
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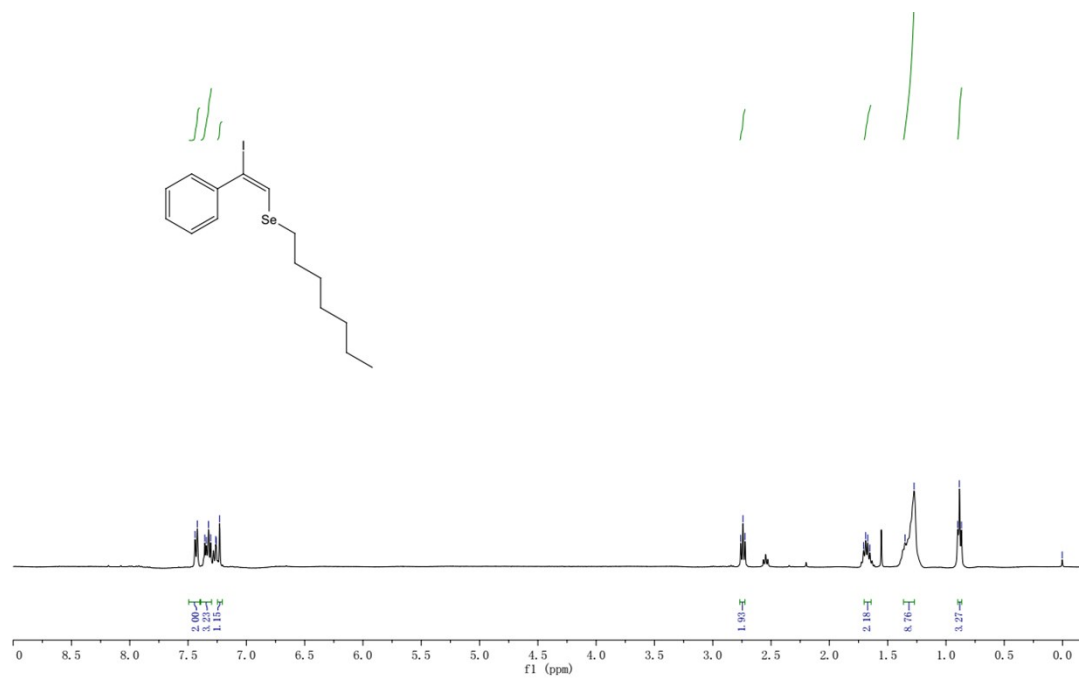


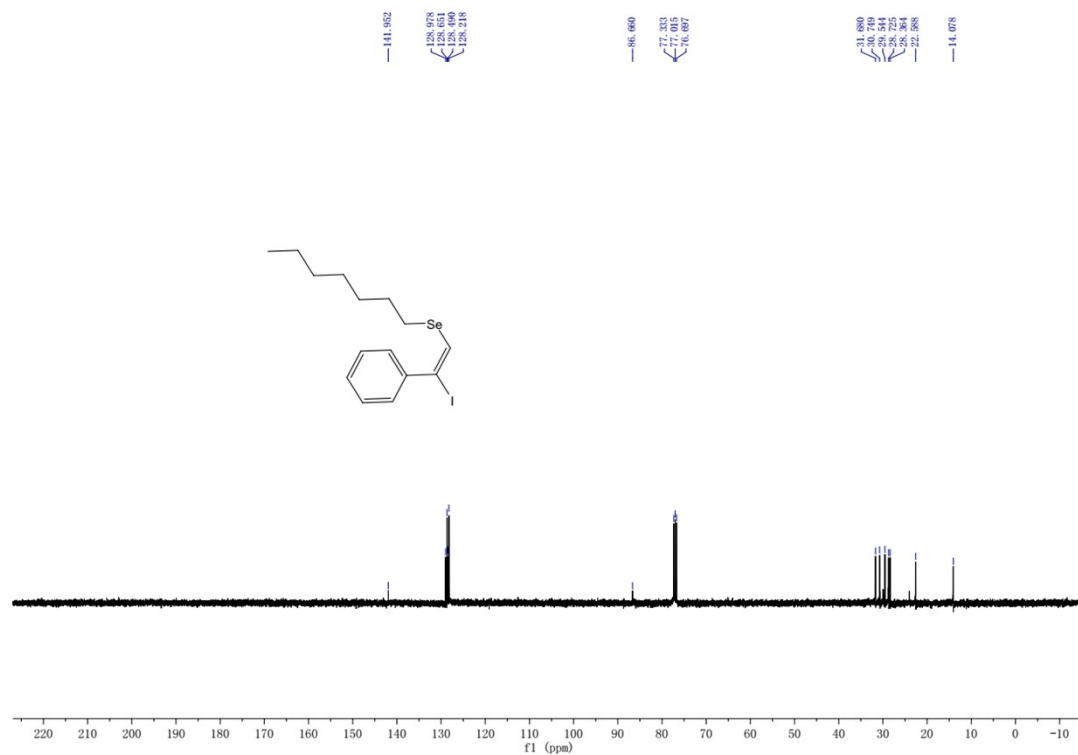
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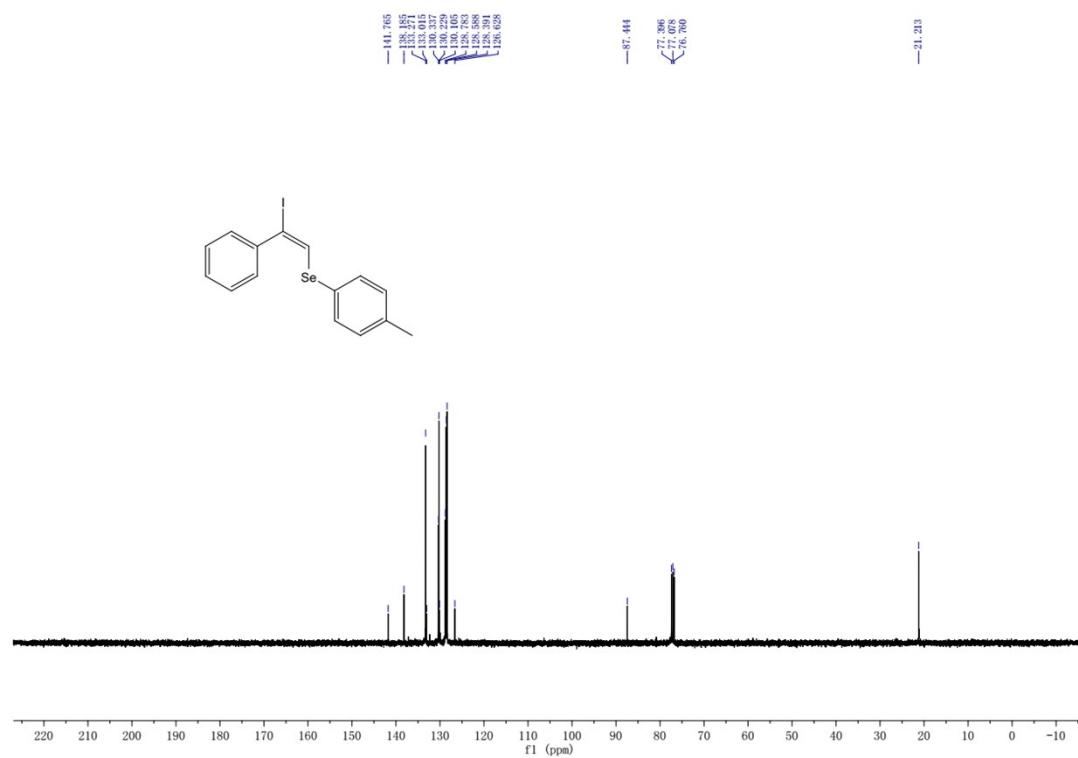
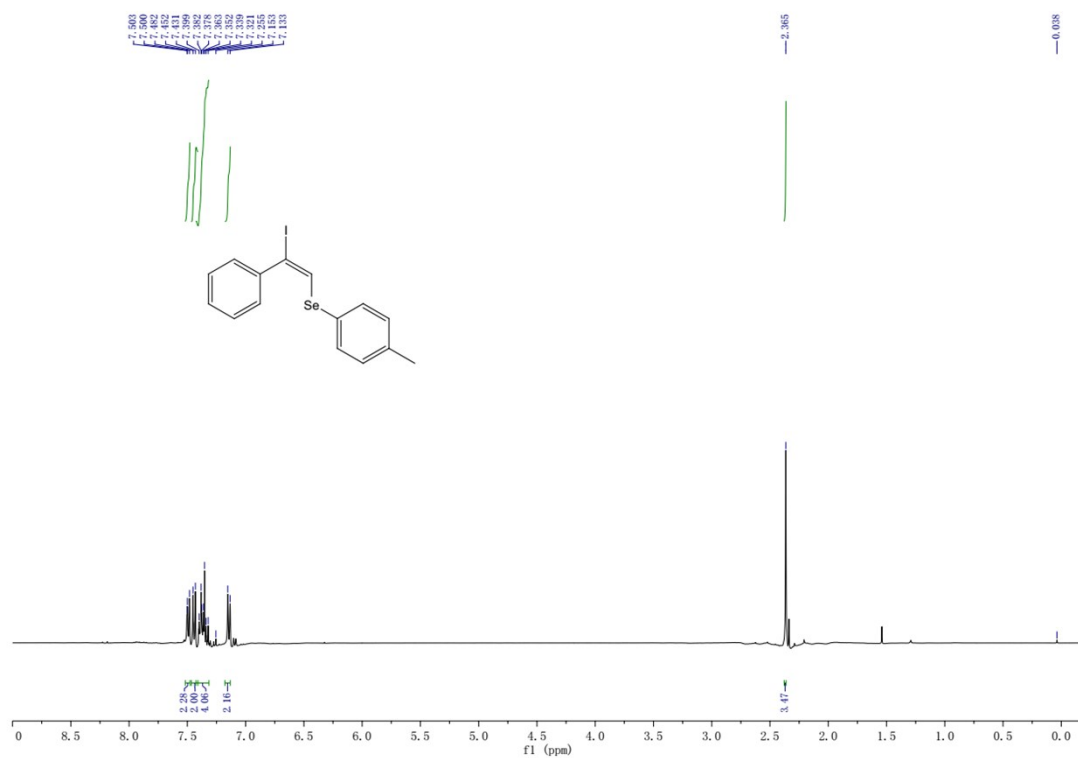


3s

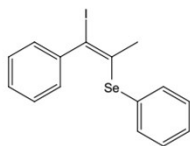
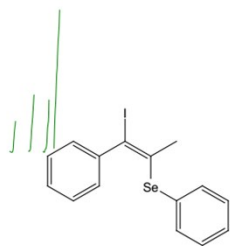




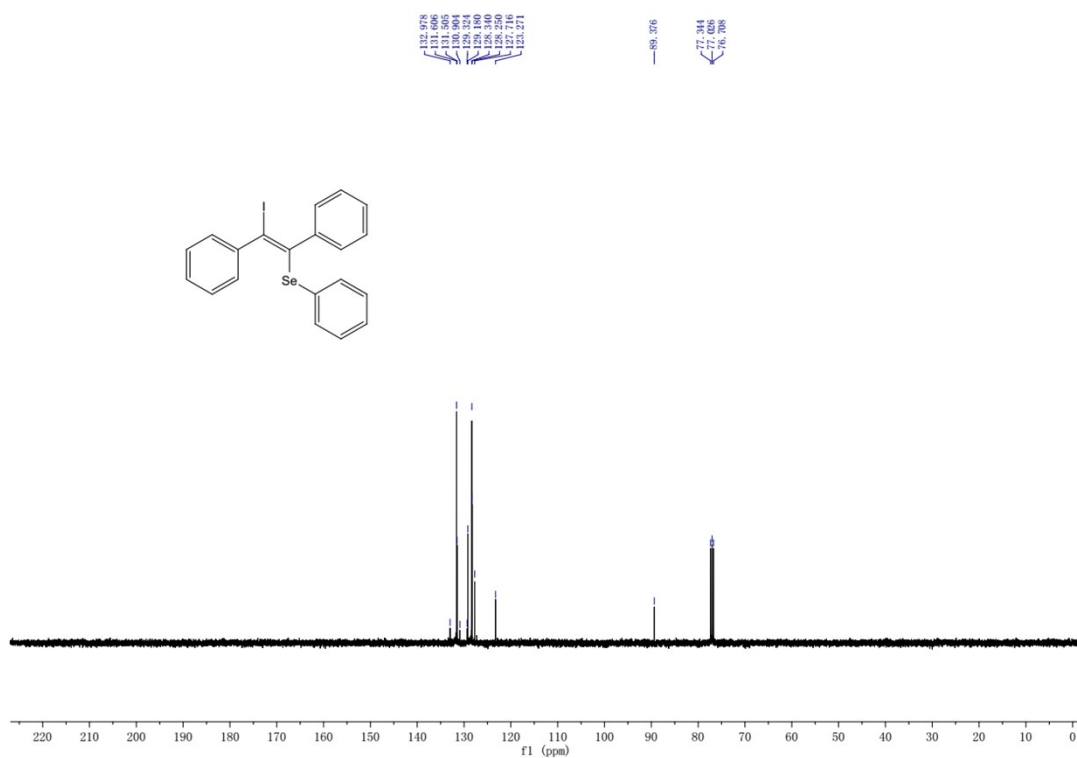
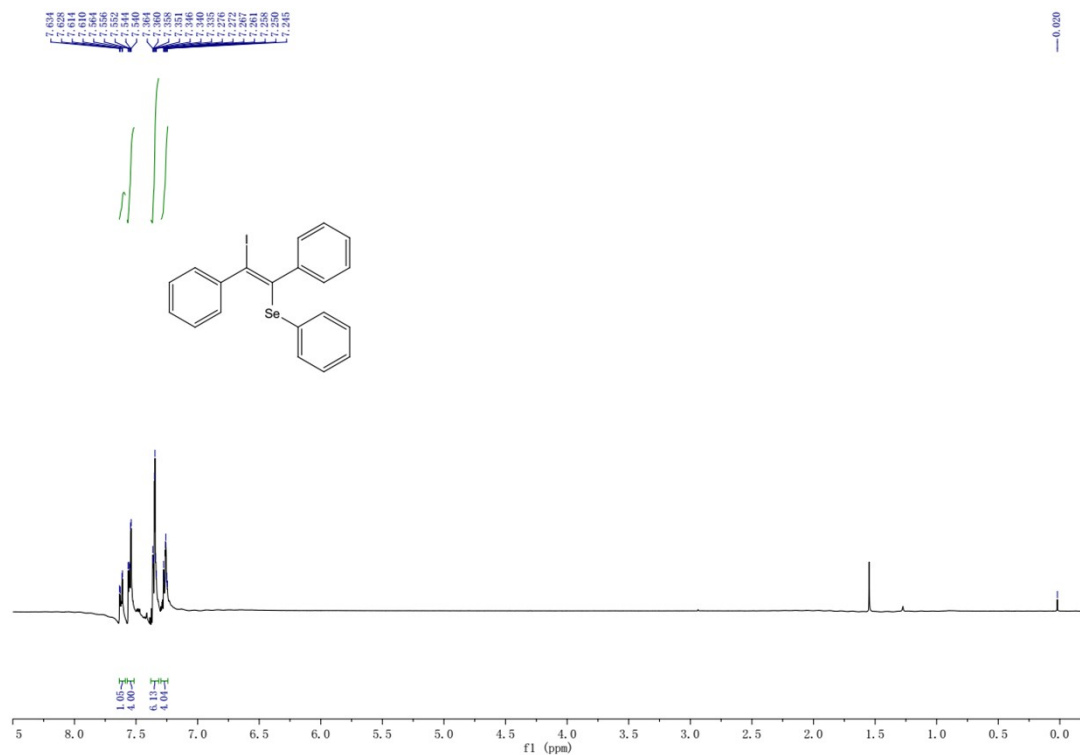
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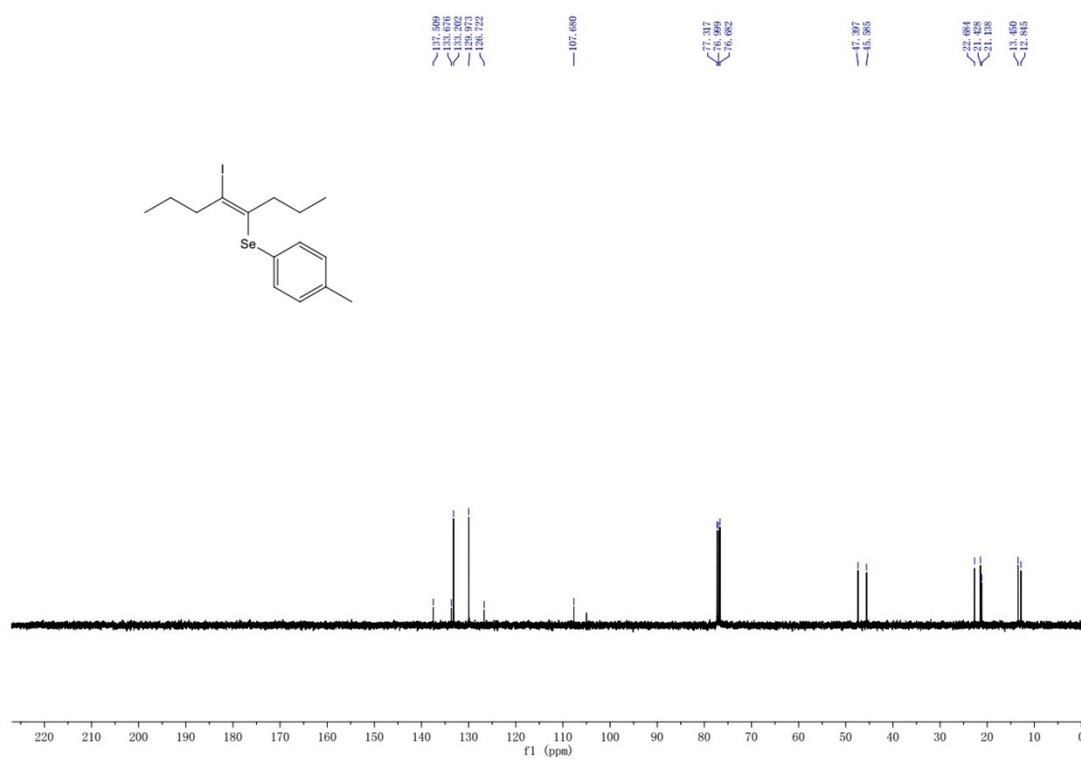
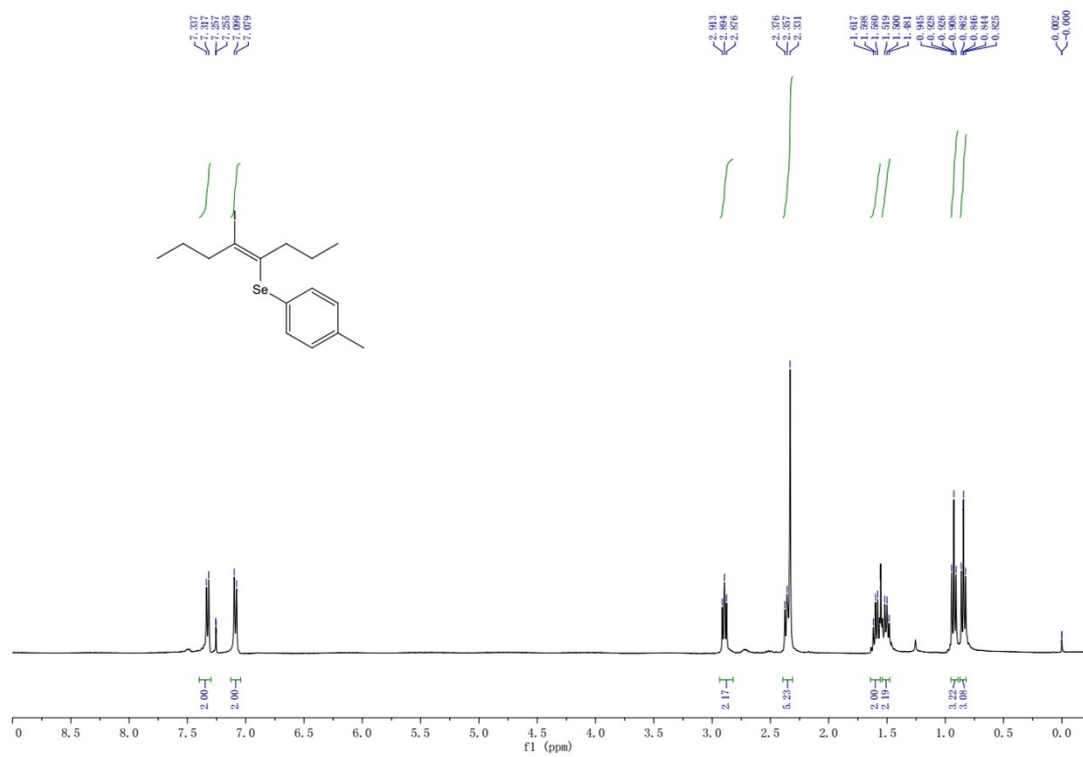
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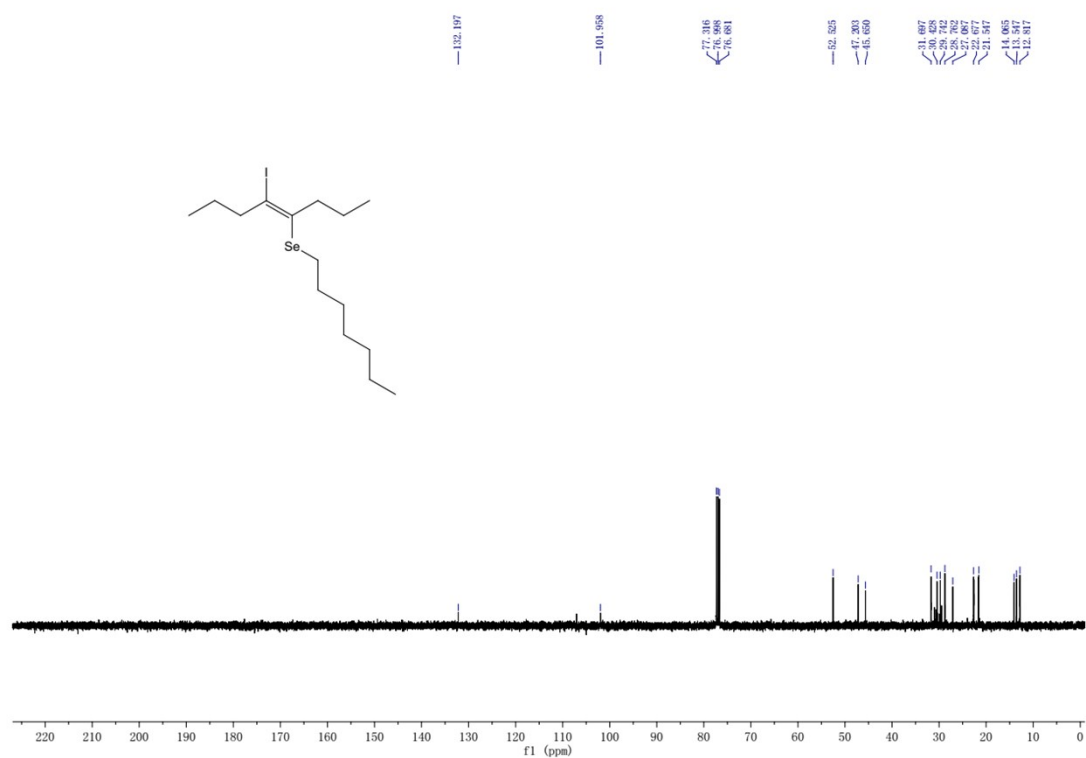
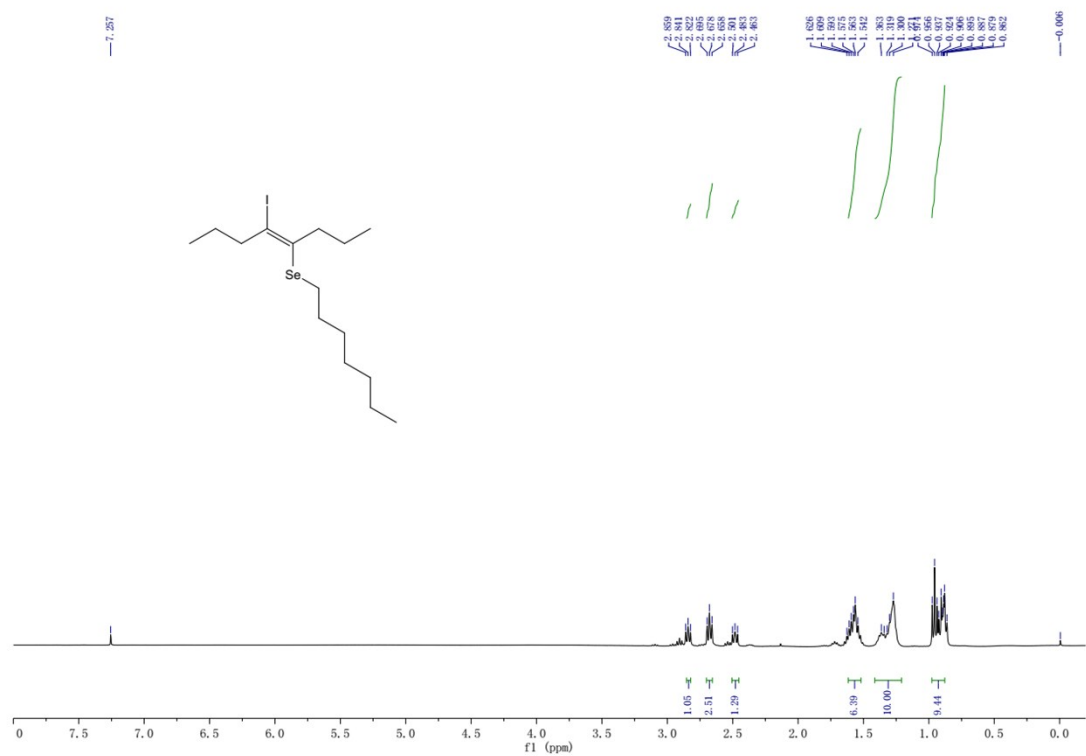
35 / 47



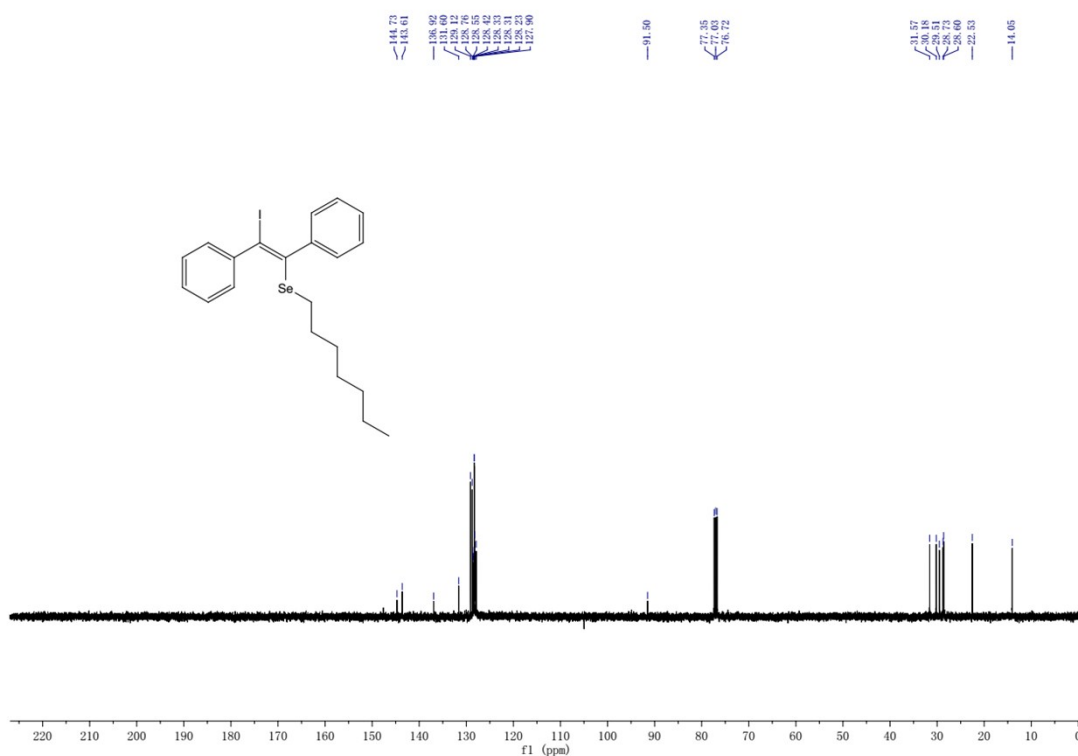
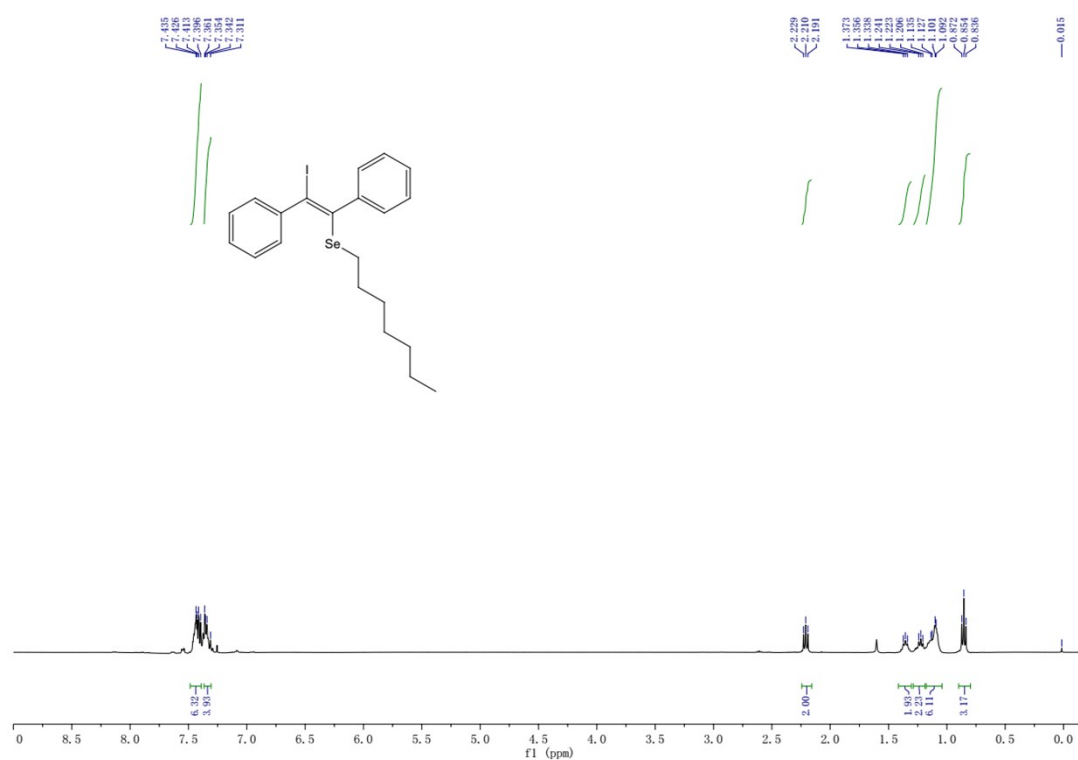
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3y



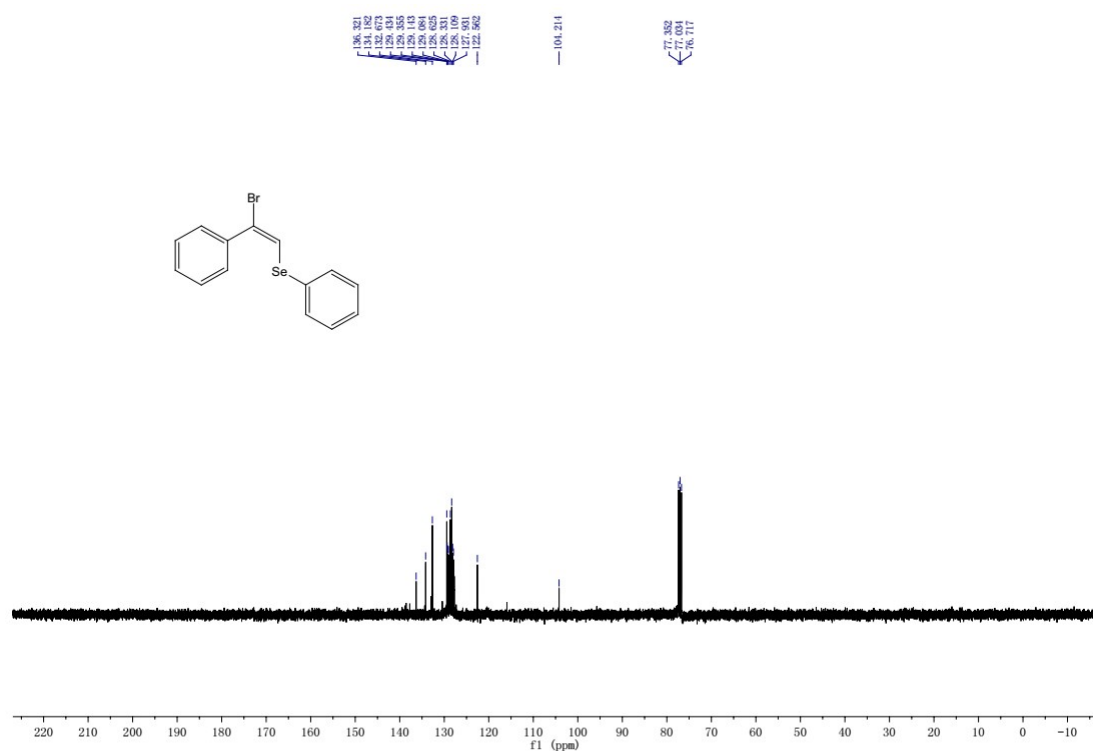
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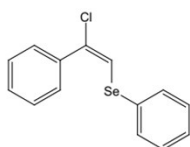
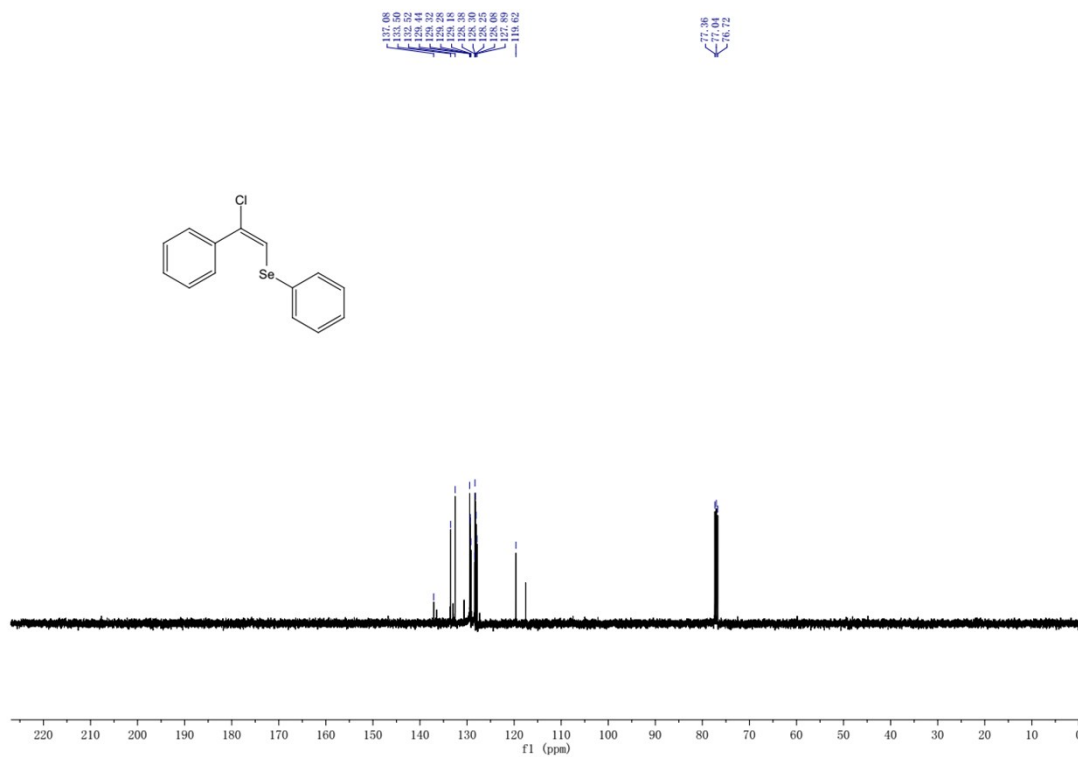
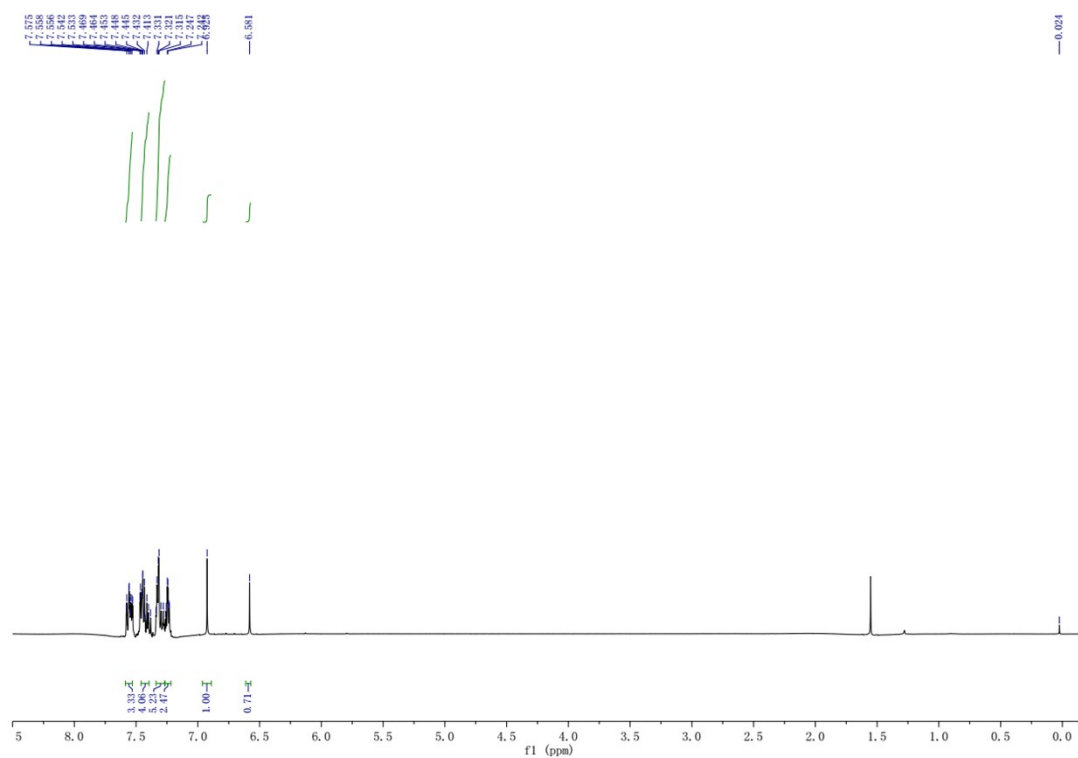
Chemical structure: BrC(=C)Se1ccccc1

¹H NMR spectrum (CDCl₃) data:

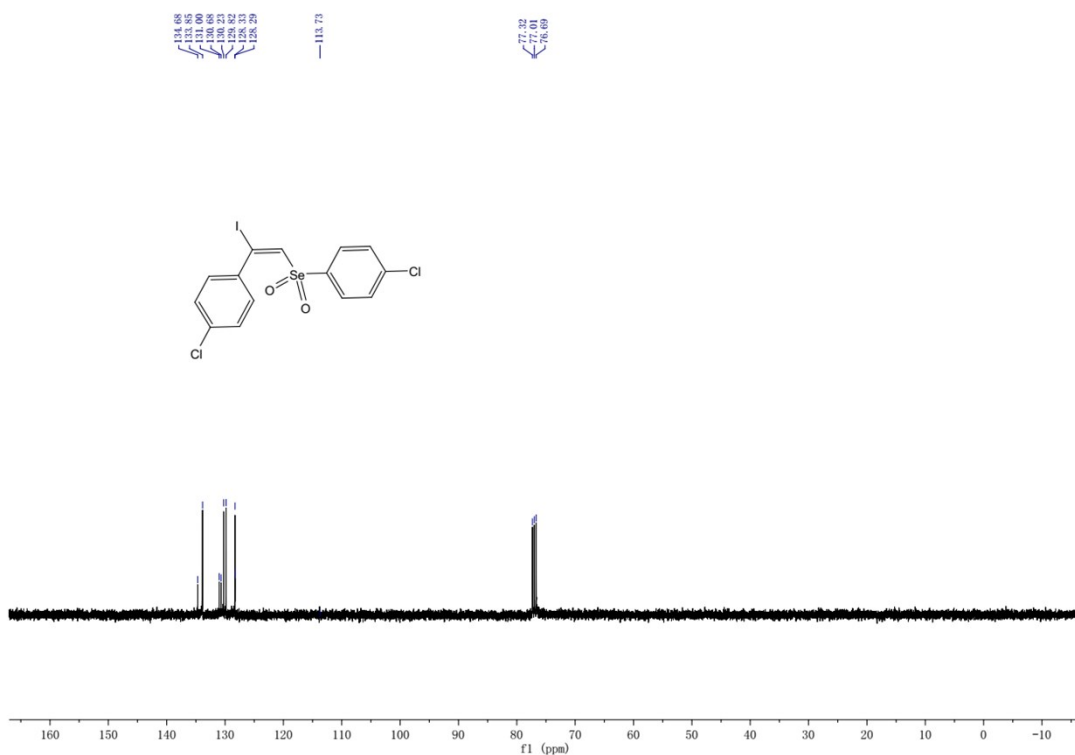
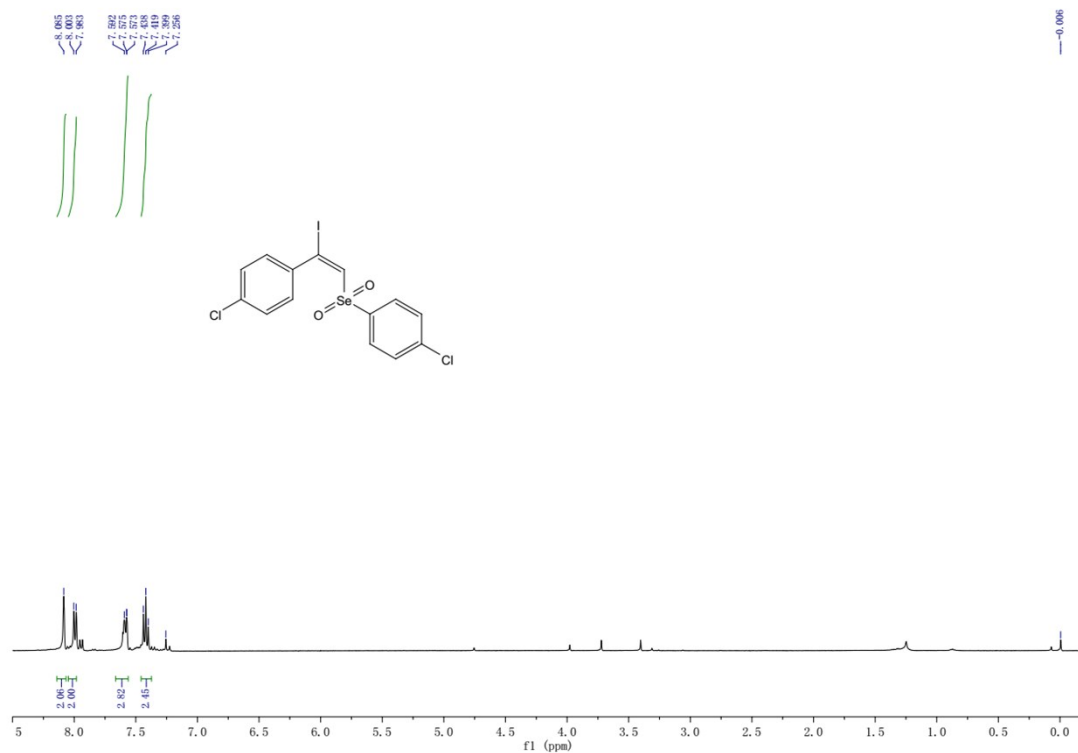
Chemical Shift (ppm)	Integration
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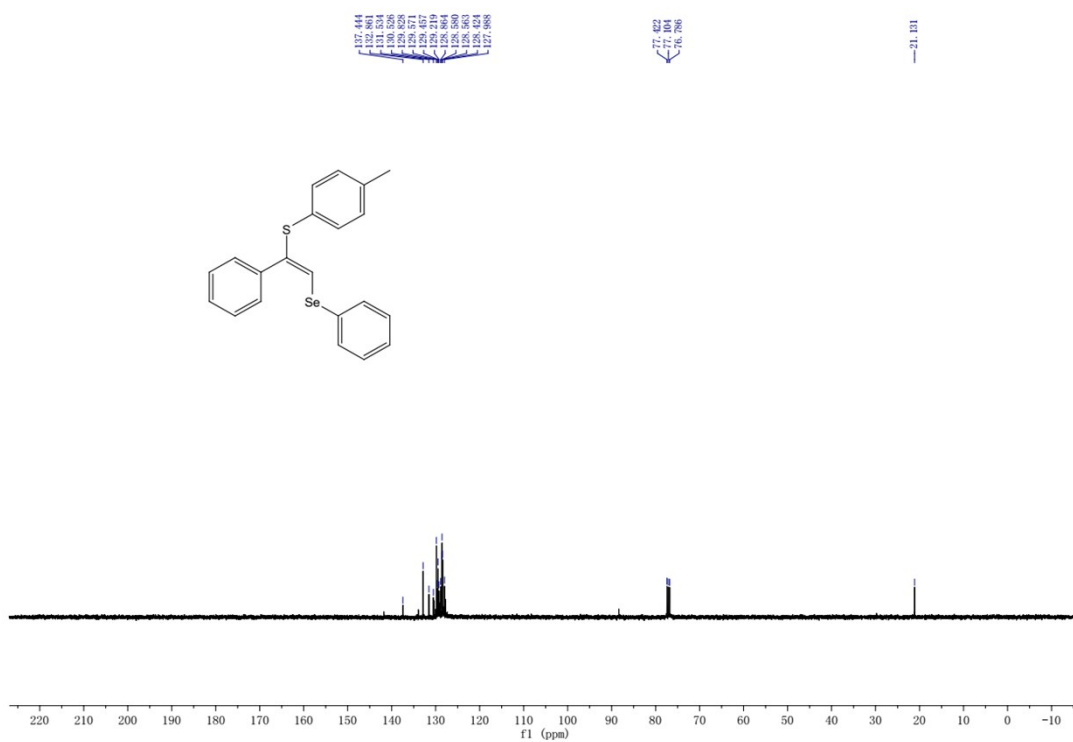
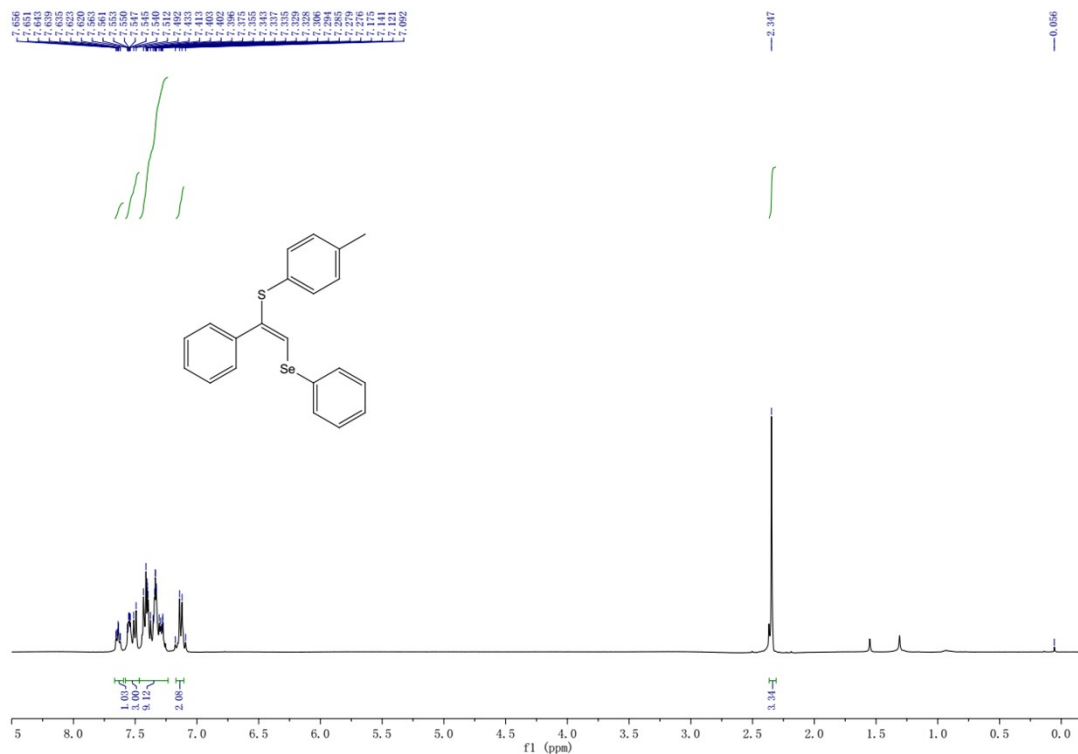
4b



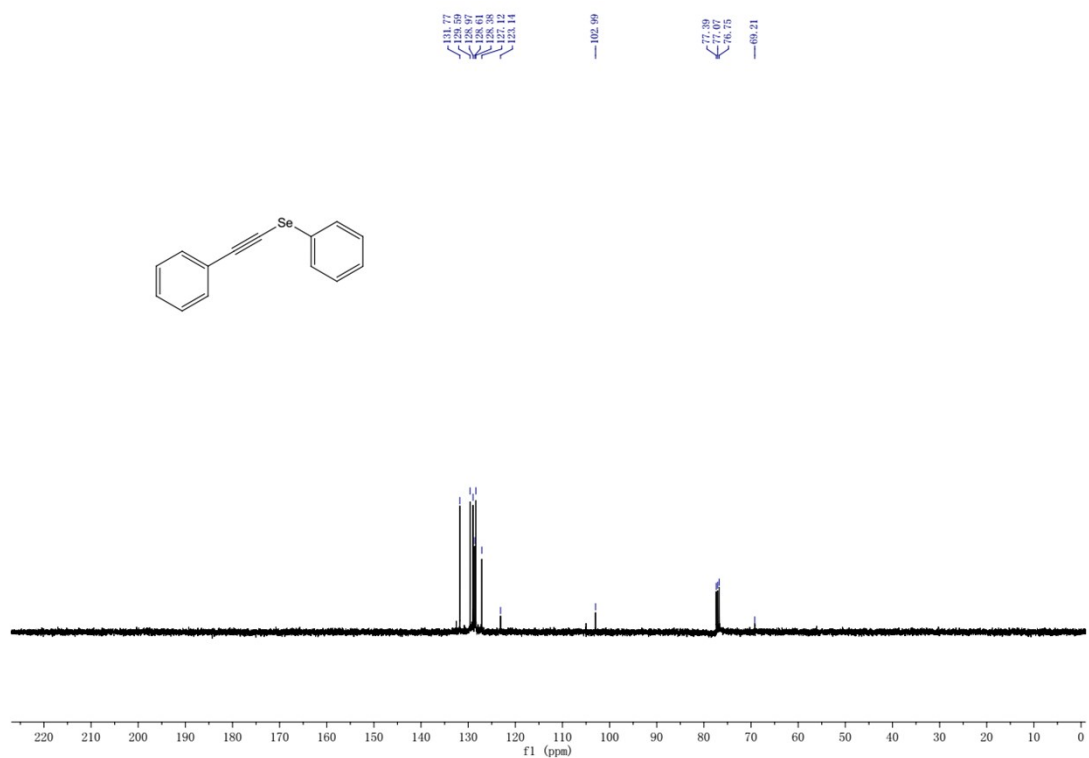
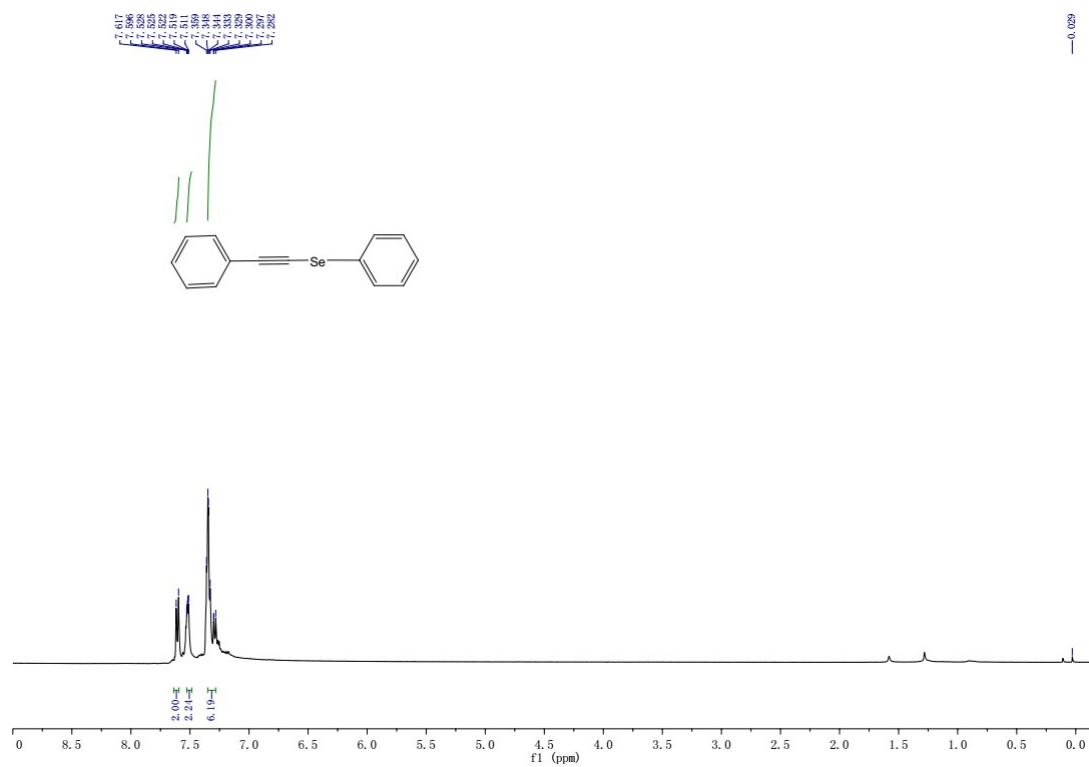
5a



6a



7a



N#CC=C(c1ccccc1)Sc2ccccc2

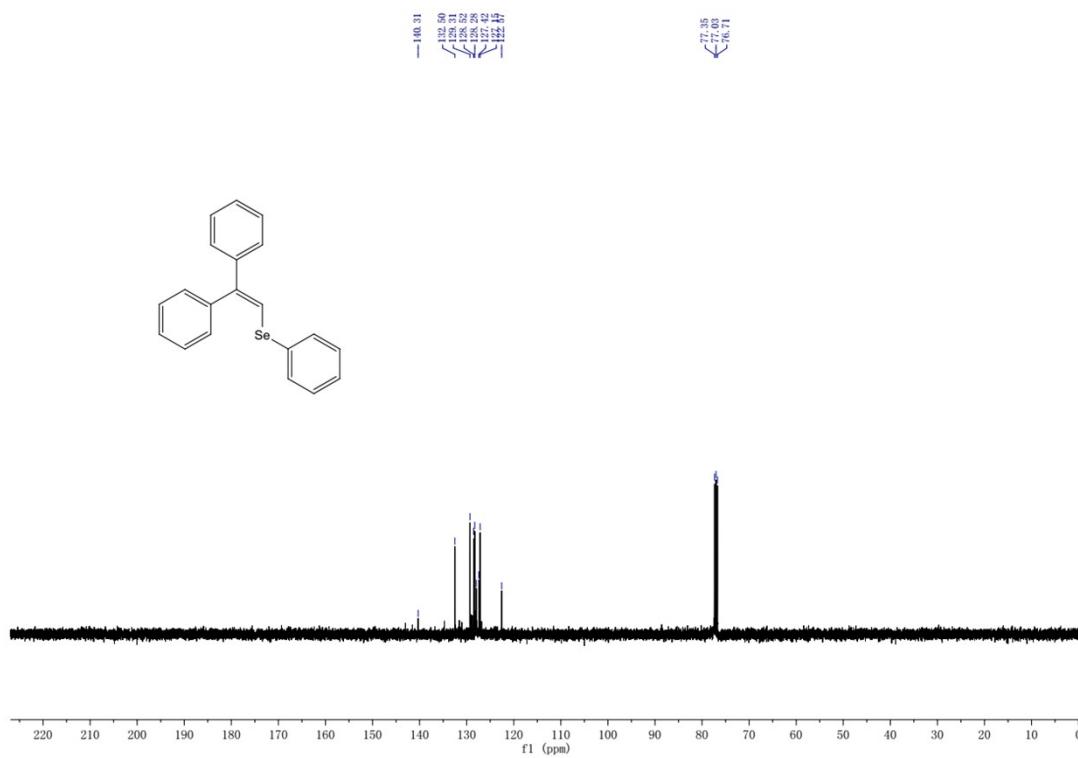
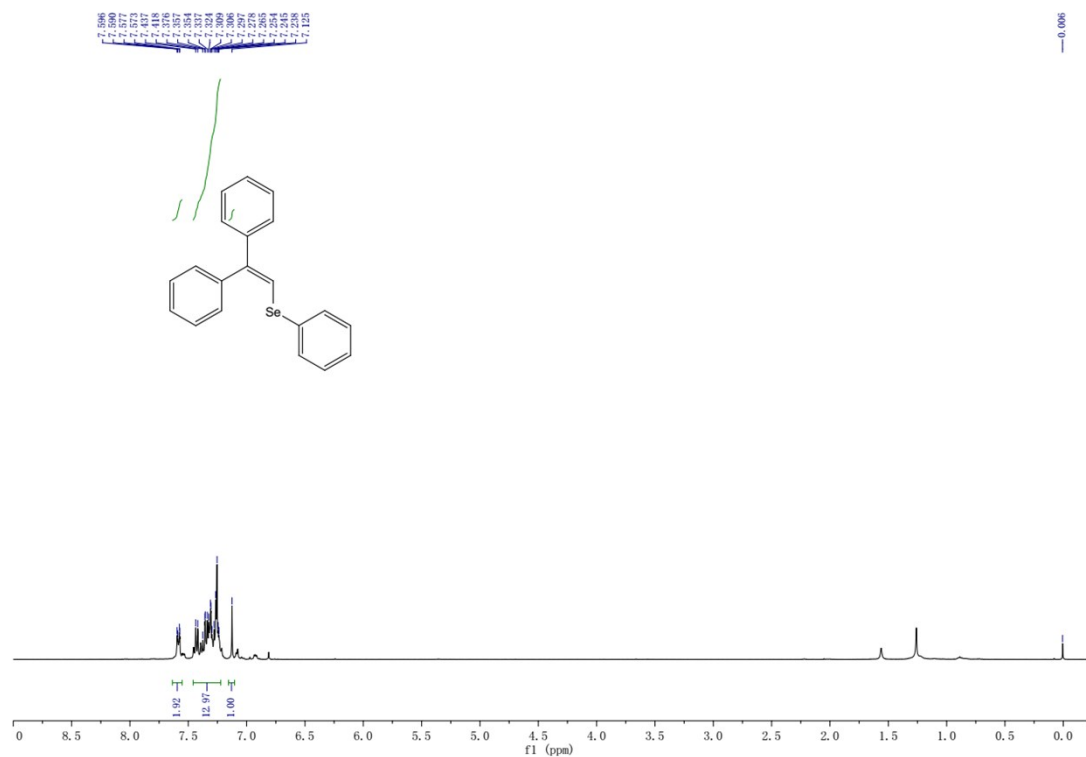
Chemical structure: (E)-1-(benzylseleno)-2-phenylvin-1-ylidene cyanide

¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (7.0-8.0 ppm) and aliphatic region (1.0-1.5 ppm). Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
7.80	2.00
7.60	2.11
7.40	2.04
7.20	1.06
1.45	1.00
1.25	1.00
1.05	1.00



9a



10a

