

# Supporting Information for

## Visible-Light-Promoted Denitrogenative Ortho-selenylation Reaction of benzotriazinones: Synthesis of ortho-selenylated Benzamides, Ebselen Analogs

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## Contents

I. General Information.....	S2
II. Synthesis of Substrates.....	S2
III. General Procedure .....	S3
1. General Procedure A .....	S3
2. General Procedure B .....	S3
2. General Procedure C .....	S4
IV. Product Characterization.....	S4
V.	

References.....S14

VI. Copies of <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra.....S15

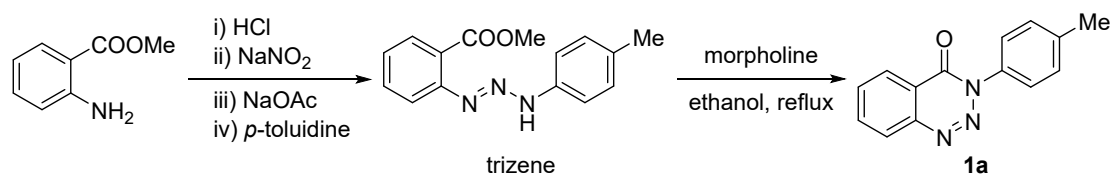
## I . General Information

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. Anhydrous DMSO, was purchased from BeiJing InnoChem Science & Technology Co., Ltd. Analytical thin-layer chromatography (TLC) was performed on silica gel, visualized by irradiation with UV light. For column chromatography, 300-400 mesh silica gel was used. <sup>1</sup>H-NMR and <sup>13</sup>C-NMR were recorded on a BRUKER 400 MHz and BRUKER 300 MHz spectrometer in CDCl<sub>3</sub> or DMSO. Chemical shifts ( $\delta$ ) were reported referenced to an internal tetramethylsilane standard, the CDCl<sub>3</sub> residual peak ( $\delta$  7.26) or the DMSO residual peak ( $\delta$  3.33) for <sup>1</sup>H NMR. Chemical shifts of <sup>13</sup>C NMR are reported relative to CDCl<sub>3</sub> ( $\delta$  77.16) or DMSO ( $\delta$  39.52). Data are reported in the following order: chemical shift ( $\delta$ ) in ppm; multiplicities are indicated s (singlet), bs (broad singlet), d (doublet), t (triplet), m (multiplet); coupling constants ( $J$ ) are in Hertz (Hz). IR spectra were recorded on a BRUKER VERTEX 70 spectrophotometer and are reported in terms of frequency of absorption (cm<sup>-1</sup>). HRMS spectra were obtained by using GCT Premier TOF-MS with EI source. The starting materials were isolated by SepaBean machine Flash Chromatography, which was purchased from Santai Technologies Inc.

## II. Synthesis of Substrates

### General procedure for the synthesis of 1,2,3-Benzotriazin-4(3H)-ones

#### (1a-n).<sup>1</sup>



To a round bottom flask containing methyl anthranilate (3.07 g, 20.3 mmol) and HCl(aq) (32 mL, 2 M) was added a solution of NaNO<sub>2</sub> (1.62 g, 23.5 mmol) in water (11 mL) at 0 °C. The reaction mixture was stirred at 0°C for 30 min. Then, a solution of NaOAc (6.33 g, 77.2 mmol) in water (25 mL) was slowly added, followed by addition of *p*-toluidine (30.4 mmol) at 0 °C. The resulting mixture was stirred at 0 °C for 3 h. The precipitate was collected by filtration, washed with cold water (50 ml), and purified by recrystallization from ethanol to give triazene as yellow solid.

The above triazene (4.85 g, 18 mmol) and morpholine (5.2 g, 60 mmol) was refluxed in ethanol (150 mL) until triazene was completely consumed. The reaction mixture was cooled to -30 °C for crystallization. The product, 1,2,3-benzotriazin-4(3*H*)-one (**1a**), was collected by filtration and washed with cold ethanol to give 3-(*p*-tolyl)benzo[d][1,2,3]triazin-4(3*H*)-one as white solid **1a** (3.74 g, 15.8 mmol) in 78 % yield (two steps).

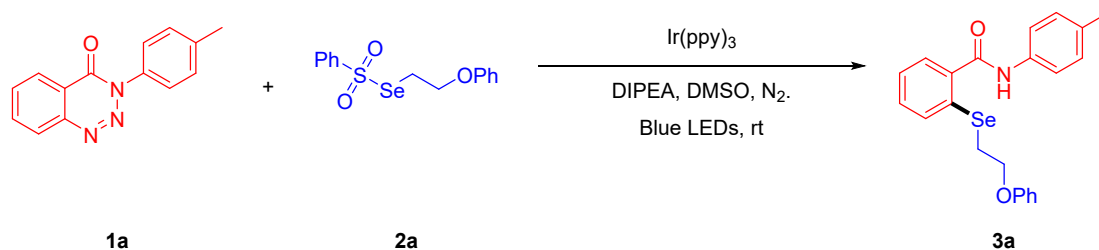
### General synthetic method for Selenium Sulfonate (**2a-J**).<sup>2</sup>

Selenium Sulfonates were prepared following the reported procedures<sup>2</sup>.

## III. General Procedure and Product Characterization

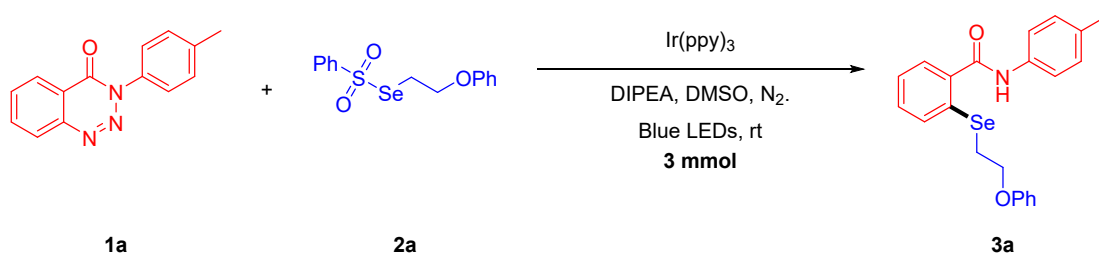
### 1. General Procedure A

A representative procedure synthesis of 2-((2-phenoxyethyl)selanyl)-*N*-(*p*-tolyl)benzamide (**3a**) is shown below.



In glovebox, an oven-dried screw-capped 8 mL vial equipped with a magnetic stir bar was charged with 3-(*p*-tolyl)benzo[d][1,2,3]triazin-4(3*H*)-one **1a** (47.4 mg, 0.2 mmol) and *Se*-(2-phenoxyethyl) benzenesulfonoselenoate **2a** (82.1 mg, 0.24 mmol), Ir(ppy)<sub>3</sub> (3.3 mg, 2.5 mol %), DIPEA (52 μL, 0.3 mmol), DMSO (2.0 mL) was added via syringe. The reaction mixture was stirred at r.t for 12 h with a 40 W LED lamp (40 W; λ = 450- 460 nm; 5 cm away; made in TanLu. Ltd; borosilicate glass;). After 12h, the crude reaction mixture was diluted with ethyl acetate (20 mL) and washed with water (20 mL × 3). The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The residue was purified by flash chromatography to afford pure product **3a**.

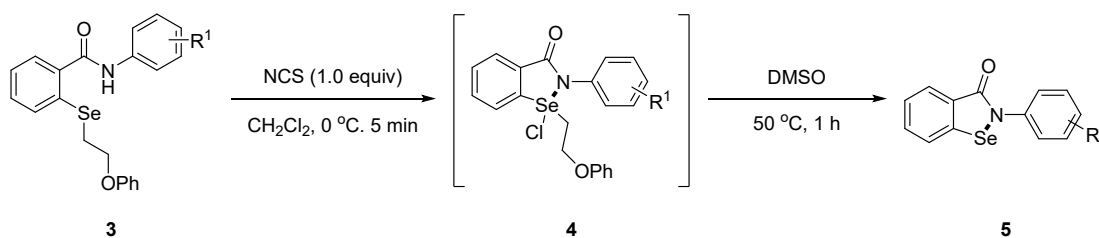
### 2. General Procedure B



**The procedure scale-up synthesis of 3a is shown below.**

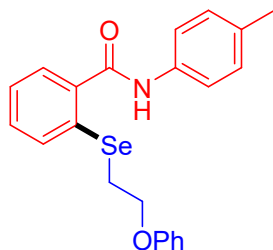
In glovebox, An oven-dried screw-capped 100-mL vial equipped with a magnetic stir bar was charged with 3-(*p*-tolyl)benzo[d][1,2,3]triazin-4(3*H*)-one **1a** and Se-(2-phenoxyethyl) benzenesulfonoselenoate **2a**, Ir(ppy)<sub>3</sub> (2.5 mol %), DMSO was added via syringe. The reaction mixture was stirred for 12 h with a 40 W LED lamp (40 W; λ = 450- 460 nm; 5 cm away; made in TanLu. Ltd; borosilicate glass;). After 12h, the crude reaction mixture was diluted with ethyl acetate (20 mL) and washed with water (20 mL × 3). The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The residue was purified by flash chromatography to afford pure product.

### 3. General Procedure C



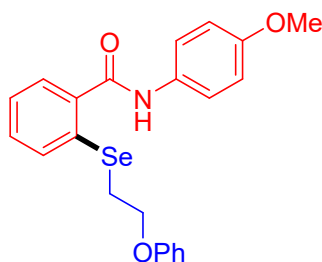
To a solution of **3a** (82.2 mg, 0.2 mmol) in dichloromethane (2.0 mL) was added N-chlorosuccinimide (267.7 mg, 0.2 mmol) mmol) at 0 °C. The mixture was stirred at 0 °C for 5 min before being concentrated *in vacuo*. DMSO (2 mL) was added to the residue and the mixture was stirred at 50 °C for 1 h. the crude reaction mixture was diluted with ethyl acetate (20 mL) and washed with water (20 mL × 3). The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The residue was purified by flash chromatography to afford pure product **5a**.

## IV. Product Characterization



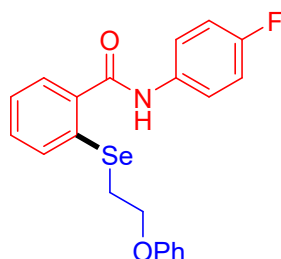
**2-((2-phenoxyethyl)selanyl)-N-(p-tolyl)benzamide (3a)**

**Yield:** 79% (64.9mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3291, 2856, 1637, 1541, 1508, 1241, 740, 689, 510.  **$^1\text{H NMR}$**  (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.28 (s, 1H), 7.70 – 7.57 (m, 4H), 7.48 – 7.40 (m, 1H), 7.35 (dd,  $J = 7.5, 1.1$  Hz, 1H), 7.25 (dd,  $J = 8.7, 7.3$  Hz, 2H), 7.14 (d,  $J = 8.2$  Hz, 2H), 6.94 – 6.85 (m, 3H), 4.19 (t,  $J = 6.9$  Hz, 2H), 3.25 (t,  $J = 6.9$  Hz, 2H), 2.27 (s, 3H).  **$^{13}\text{C NMR}$**  (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  166.5, 158.1, 137.5, 136.6, 132.6, 131.2, 130.8, 130.1, 129.5, 129.0, 128.2, 125.7, 120.7, 119.9, 114.5, 66.9, 24.4, 20.5.  **$^{77}\text{Se NMR}$**  (76 MHz,  $\text{DMSO-}d_6$ )  $\delta$  273.6. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{NO}_2\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 434.0635, found 434.0648.



**N-(4-methoxyphenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3b)**

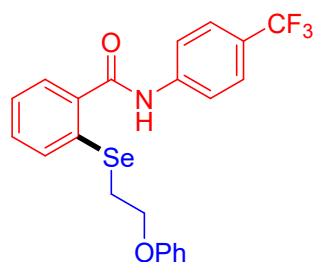
**Yield:** 57% (48.1mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3310, 2926, 1639, 1598, 1515, 1497, 1463, 1239, 1176, 1029, 1013, 823, 745, 689, 559, 521.  **$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (s, 1H), 7.72 – 7.61 (m, 2H), 7.53 (d,  $J = 8.5$  Hz, 2H), 7.42 – 7.30 (m, 2H), 7.26 (dd,  $J = 8.5, 7.2$  Hz, 2H), 7.00 – 6.86 (m, 3H), 6.81 (d,  $J = 8.2$  Hz, 2H), 4.25 (t,  $J = 6.9$  Hz, 2H), 3.82 (s, 3H), 3.28 (t,  $J = 6.9$  Hz, 2H).  **$^{13}\text{C NMR}$**  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.4, 158.2, 156.7, 137.9, 132.5, 131.0, 130.9, 129.8, 129.5, 128.4, 126.9, 121.9, 121.1, 114.6, 114.2, 67.2, 55.5, 26.0.  **$^{77}\text{Se NMR}$**  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  273.7. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{NO}_3\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 450.0584, found 450.0580.



**N-(4-fluorophenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3c)**

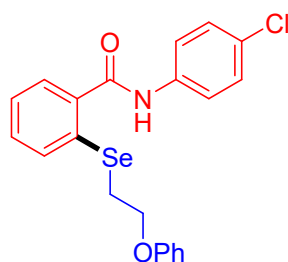
**Yield:** 78% (64.7mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3340, 2924, 1643, 1519, 1497,

1404, 1244, 1206, 1034, 828, 741, 689, 511, 489.  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.46 (s, 1H), 7.77 (dd,  $J = 8.8, 5.1$  Hz, 2H), 7.68 (td,  $J = 7.9, 1.3$  Hz, 2H), 7.46 (td,  $J = 7.6, 1.6$  Hz, 1H), 7.36 (td,  $J = 7.4, 1.1$  Hz, 1H), 7.31 – 7.23 (m, 2H), 7.20 (t,  $J = 8.9$  Hz, 2H), 6.96 – 6.85 (m, 3H), 4.21 (t,  $J = 6.9$  Hz, 2H), 3.27 (t,  $J = 6.8$  Hz, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  167.1, 158.8 ( $J = 238.7$ ), 158.5, 137.8, 135.9 ( $J = 2.5$ ), 131.6, 131.4, 130.8, 130.0, 128.7, 126.2, 122.2 ( $J = 7.9$ ), 121.2, 115.7 ( $J = 22.0$ ), 115.0, 67.3, 25.0.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{DMSO-}d_6$ )  $\delta$  274.1. **HRMS** (CI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{18}\text{FNO}_2\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 438.0384, found 438.0399.



**2-((2-phenoxyethyl)selanyl)-N-(4-(trifluoromethyl)phenyl)benzamide (3d)**

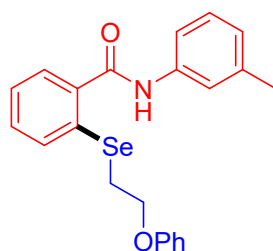
**Yield:** 71% (66.0mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3255, 2928, 1667, 1597, 1497, 1329, 1241, 1115, 1068, 834, 749, 690, 509, 468.  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.58 (s, 1H), 7.77 (d,  $J = 8.5$  Hz, 2H), 7.58 – 7.48 (m, 4H), 7.30 (td,  $J = 7.6, 1.5$  Hz, 1H), 7.20 (td,  $J = 7.5, 1.1$  Hz, 1H), 7.11 – 7.03 (m, 2H), 6.81 – 6.61 (m, 3H), 4.02 (t,  $J = 6.8$  Hz, 2H), 3.10 (t,  $J = 6.8$  Hz, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  167.2, 158.1, 142.7, 137.1, 131.3, 131.2, 130.5, 129.5, 128.4, 126.0 ( $J = 3.4$ ), 125.8, 124.4 ( $J = 269.6$ ), 123.7 ( $J = 31.8$ ), 120.8, 119.8, 114.5, 66.8, 24.7.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{DMSO-}d_6$ )  $\delta$  274.5. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{18}\text{F}_3\text{NO}_2\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 488.0353, found 488.0351.



**N-(4-chlorophenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3e)**

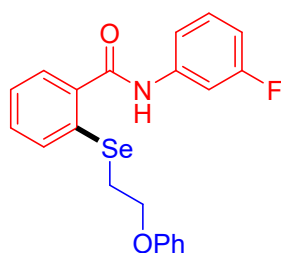
**Yield:** 73% (62.9mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3242, 2927, 1654, 1589, 1512, 1491, 1397, 1310, 1234, 1010, 818, 749, 689, 507, 469.  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.53 (s, 1H), 7.83 – 7.75 (m, 2H), 7.73 – 7.64 (m, 2H), 7.50 – 7.33 (m, 4H), 7.30 – 7.22 (m, 2H), 6.96 – 6.85 (m, 3H), 4.21 (t,  $J = 6.8$  Hz, 2H), 3.27 (t,  $J = 6.8$  Hz, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  167.3, 158.5, 138.5, 137.7, 131.6, 131.5, 130.8, 130.0, 129.1, 128.7, 127.8, 126.3, 121.9, 121.2, 115.0, 67.3, 25.0.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{DMSO-}d_6$ )  $\delta$  274.0. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{18}\text{ClNO}_2\text{Se}$

(M+Na)<sup>+</sup>: 454.0089, found 454.0089.



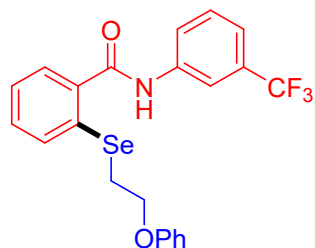
**2-((2-phenoxyethyl)selanyl)-N-(m-tolyl)benzamide (3f)**

**Yield:** 71% (58.4mg). White solid. **IR** (neat, v, cm<sup>-1</sup>): 3289, 2928, 1635, 1583, 1542, 1489, 1312, 1229, 1032, 1008, 876, 787, 728, 685, 505. **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.21 (s, 1H), 7.58 (ddd, *J* = 8.9, 7.7, 1.4 Hz, 2H), 7.43 (s, 1H), 7.39 – 7.27 (m, 2H), 7.26 – 7.15 (m, 4H), 6.96 – 6.87 (m, 2H), 6.80 – 6.73 (m, 2H), 4.18 (t, *J* = 6.9 Hz, 2H), 3.20 (t, *J* = 6.9 Hz, 2H), 2.30 (s, 3H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 166.7, 158.2, 139.00, 137.8, 137.8, 132.4, 131.1, 130.1, 129.6, 128.9, 128.4, 126.8, 125.4, 121.2, 120.8, 117.3, 114.6, 67.3, 26.0, 21.5. **<sup>77</sup>Se NMR** (76 MHz, CDCl<sub>3</sub>) δ 274.7. **HRMS** (ESI<sup>+</sup>, MeCN) *m/z* calcd for C<sub>22</sub>H<sub>21</sub>NO<sub>2</sub>Se (M+Na)<sup>+</sup>: 434.0635, found 434.0642.



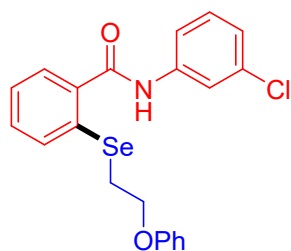
**N-(3-fluorophenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3g)**

**Yield:** 76% (63.1mg). White solid. **IR** (neat, v, cm<sup>-1</sup>): 3263, 2925, 1661, 1598, 1521, 1491, 1425, 1242, 1152, 1008, 856, 752, 676, 509. **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.40 (s, 1H), 7.66 (ddd, *J* = 8.9, 7.6, 1.5 Hz, 2H), 7.42 – 7.20 (m, 6H), 7.01 – 6.93 (m, 1H), 6.90 – 6.75 (m, 3H), 4.26 (t, *J* = 6.8 Hz, 2H), 3.28 (t, *J* = 6.8 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 166.8, 163.1 (*J* = 243.3), 158.1, 139.4 (*J* = 6.2), 137.6, 132.9, 131.4, 130.2 (*J* = 9.3), 130.0, 129.6, 128.6, 127.1, 121.3, 115.4 (*J* = 3.0), 114.6, 111.4 (*J* = 21.4), 107.6 (*J* = 26.2), 67.3, 26.4. **<sup>77</sup>Se NMR** (76 MHz, CDCl<sub>3</sub>) δ 274.7. **HRMS** (EI) (ESI<sup>+</sup>, MeCN) *m/z* calcd for C<sub>21</sub>H<sub>18</sub>FNO<sub>2</sub>Se (M+Na)<sup>+</sup> : 438.0384, found 438.0395.



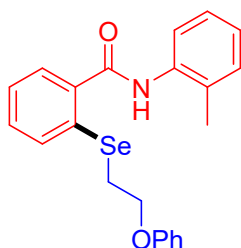
**2-((2-phenoxyethyl)selanyl)-N-(3-(trifluoromethyl)phenyl)benzamide (3h)**

**Yield:** 72% (67.0mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3246, 2946, 1655, 1519, 1496, 1331, 1240, 1121, 1009, 748, 510.  **$^1\text{H}$  NMR** (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.43 (s, 1H), 7.86 – 7.76 (m, 2H), 7.65 (td,  $J = 7.1, 1.6$  Hz, 2H), 7.49 – 7.27 (m, 4H), 7.22 (dd,  $J = 8.5, 7.2$  Hz, 2H), 6.93 (t,  $J = 7.4$  Hz, 1H), 6.75 (d,  $J = 8.1$  Hz, 2H), 4.24 (t,  $J = 6.6$  Hz, 2H), 3.26 (t,  $J = 6.7$  Hz, 2H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  167.1, 158.1, 138.4, 137.3, 132.8, 131.5, 131.4 ( $J = 32.2$ ), 130.1, 129.6, 129.6, 128.6, 127.0, 123.9 ( $J = 270.7$ ), 123.3, 121.3, 121.1 ( $J = 3.7$ ), 116.9 ( $J = 3.8$ ), 114.6, 67.3, 26.4.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{CDCl}_3$ )  $\delta$  275.4. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{18}\text{F}_3\text{NO}_2\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 488.0353, found 488.0336.



**N-(3-chlorophenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3i)**

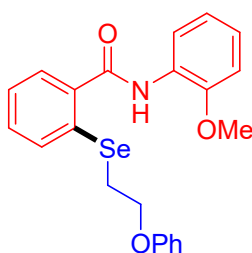
**Yield:** 63% (54.3mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3283, 2931, 1734, 1645, 1592, 1529, 1480, 1403, 1310, 1235, 1171, 870, 776, 750, 678, 592, 509.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.52 (s, 1H), 7.73 (t,  $J = 2.1$  Hz, 1H), 7.62 (td,  $J = 7.8, 1.4$  Hz, 2H), 7.44 (ddd,  $J = 8.0, 2.1, 1.0$  Hz, 1H), 7.36 (td,  $J = 7.6, 1.6$  Hz, 1H), 7.30 – 7.21 (m, 4H), 7.11 (ddd,  $J = 8.0, 2.0, 1.0$  Hz, 1H), 7.00 – 6.94 (m, 1H), 6.83 – 6.77 (m, 2H), 4.24 (t,  $J = 6.8$  Hz, 2H), 3.26 (t,  $J = 6.8$  Hz, 2H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.9, 158.1, 139.0, 137.2, 134.6, 132.5, 131.3, 130.1, 130.0, 129.6, 128.4, 126.9, 124.6, 121.2, 120.3, 118.2, 114.6, 67.2, 26.2.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{CDCl}_3$ )  $\delta$  275.3. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{18}\text{ClNO}_2\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 454.0089, found 454.0096.





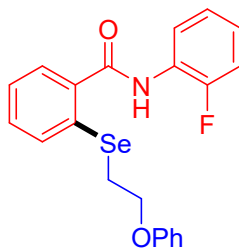
### 2-((2-phenoxyethyl)selanyl)-N-(o-tolyl)benzamide (3j)

**Yield:** 65% (53.4mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3256, 3028, 2927, 1656, 1517, 1494, 1303, 1240, 1008, 746, 688, 509, 451.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 7.8$  Hz, 1H), 7.84 (s, 1H), 7.78 – 7.66 (m, 2H), 7.41 (dtd,  $J = 21.6, 7.4, 1.5$  Hz, 2H), 7.34 – 7.26 (m, 4H), 7.17 (td,  $J = 7.5, 1.3$  Hz, 1H), 6.98 (tt,  $J = 7.3, 1.1$  Hz, 1H), 6.89 – 6.83 (m, 2H), 4.28 (t,  $J = 7.0$  Hz, 2H), 3.33 (t,  $J = 7.0$  Hz, 2H), 2.37 (s, 3H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 137.8, 135.6, 132.3, 131.1, 130.6, 130.24, 129.5, 128.3, 126.9, 126.8, 125.5, 123.2, 121.1, 114.6, 67.1, 25.9, 18.1.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{CDCl}_3$ )  $\delta$  274.2. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{NO}_2\text{Se}(\text{M}+\text{Na})^+$ : 434.0635, found 434.0649.



### 2-(2-methoxyphenyl)-1-(2-((2-phenoxyethyl)selanyl)phenyl)ethan-1-one (3k)

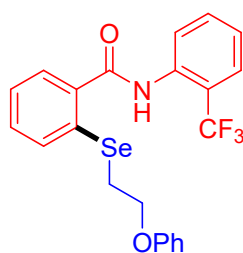
**Yield:** 46% (39.3mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3446, 2929, 2365, 1654, 1599, 1520, 1487, 1458, 1432, 1337, 1290, 1237, 1022, 744, 728, 693, 551.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.58 – 8.40 (m, 2H), 7.68 – 7.59 (m, 2H), 7.38 (td,  $J = 7.6, 1.6$  Hz, 1H), 7.31 (td,  $J = 7.5, 1.2$  Hz, 1H), 7.27 – 7.20 (m, 2H), 7.08 (td,  $J = 7.8, 1.7$  Hz, 1H), 7.01 (td,  $J = 7.8, 1.5$  Hz, 1H), 6.96 – 6.88 (m, 2H), 6.87 – 6.80 (m, 2H), 4.22 (t,  $J = 7.3$  Hz, 2H), 3.86 (s, 3H), 3.26 (t,  $J = 7.3$  Hz, 2H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.4, 158.4, 148.3, 137.5, 131.5, 131.4, 131.2, 129.6, 128.0, 127.7, 126.5, 124.2, 121.3, 121.1, 120.1, 114.7, 110.1, 67.2, 55.9, 25.2.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{CDCl}_3$ )  $\delta$  278.3. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{NO}_3\text{Se}(\text{M}+\text{Na})^+$ : 450.0584, found 450.0584.



### N-(2-fluorophenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3l)

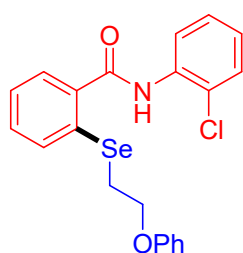
**Yield:** 67% (55.6mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3437, 2914, 1672, 1518, 1458, 1448, 1318, 1235, 1171, 757, 738, 690, 553, 456.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.36 (td,  $J = 8.1, 1.5$  Hz, 1H), 8.17 (s, 1H), 7.58 (ddd,  $J = 16.1, 7.7, 1.5$  Hz, 2H), 7.27 (dtd,  $J = 25.3, 7.5, 1.4$  Hz, 2H), 7.18 – 7.12 (m, 2H), 7.11 – 7.06 (m, 1H), 7.06 – 6.96 (m,

2H), 6.84 (tt,  $J = 7.3, 1.1$  Hz, 1H), 6.77 – 6.71 (m, 2H), 4.14 (t,  $J = 7.1$  Hz, 2H), 3.18 (t,  $J = 7.1$  Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.5, 158.3, 152.9 ( $J = 242.0$ ), 137.0, 131.9 ( $J = 64.7$ ), 131.0, 129.6, 128.4, 126.8, 126.4 ( $J = 10.1$ ), 124.8 ( $J = 7.4$ ), 124.8 ( $J = 3.6$ ), 122.1, 121.2, 115.0 ( $J = 18.9$ ), 114.7, 67.2, 25.8.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  277.1. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{18}\text{FNO}_2\text{Se}(\text{M}+\text{Na})^+$ : 438.0384, found 438.0403.



**1-(2-((2-phenoxyethyl)selanyl)phenyl)-2-(2-(trifluoromethyl)phenyl)ethan-1-one (3m)**

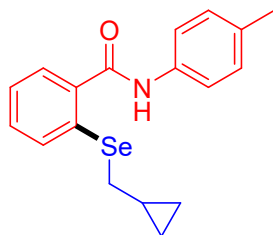
**Yield:** 64% (59.5mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3484, 3065, 2914, 2869, 2377, 2349, 1678, 1588, 1532, 1448, 1292, 1235, 1091, 1031, 764, 752, 692, 496.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.42 (d,  $J = 8.2$  Hz, 1H), 8.16 (s, 1H), 7.74 – 7.58 (m, 4H), 7.45 (td,  $J = 7.6, 1.6$  Hz, 1H), 7.40 – 7.23 (m, 4H), 6.98 (t,  $J = 7.3$  Hz, 1H), 6.89 (d,  $J = 8.1$  Hz, 2H), 4.29 (t,  $J = 7.2$  Hz, 2H), 3.32 (t,  $J = 7.2$  Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 158.4, 136.4, 135.3, 133.1, 132.2, 131.7, 131.5, 129.6, 127.6, 126.6, 126.3 ( $J = 5.3$ ), 125.0, 124.7, 124.2 ( $J = 271.3$ ), 121.2, 120.6 ( $J = 29.5$ ), 67.1, 25.3.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  281.1. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{18}\text{F}_3\text{NO}_2\text{Se}(\text{M}+\text{Na})^+$ : 488.0353, found 488.0349.



**N-(2-chlorophenyl)-2-((2-phenoxyethyl)selanyl)benzamide (3n)**

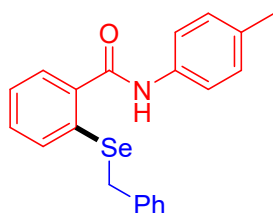
**Yield:** 62% (53.4mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3445, 2913, 1669, 1588, 1519, 1497, 1432, 1315, 1230, 1172, 1028, 879, 747, 689, 587, 511, 438.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.58 (dd,  $J = 8.3, 1.5$  Hz, 1H), 8.41 (s, 1H), 7.78 – 7.64 (m, 2H), 7.48 – 7.24 (m, 6H), 7.12 (td,  $J = 7.8, 1.4$  Hz, 1H), 6.97 (t,  $J = 7.3$  Hz, 1H), 6.88 (d,  $J = 8.2$  Hz, 2H), 4.27 (t,  $J = 7.2$  Hz, 2H), 3.32 (t,  $J = 7.2$  Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.4, 158.4, 136.6, 134.7, 131.9, 131.6, 131.5, 129.6, 129.2, 128.0, 127.9, 126.6, 125.1, 123.3, 121.8, 121.1, 114.7, 67.1, 25.4.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  280.8. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $(\text{M})^+ \text{C}_{21}\text{H}_{18}\text{ClNO}_2\text{Se}(\text{M}+\text{Na})^+$ : 454.0089,

found 454.0109.



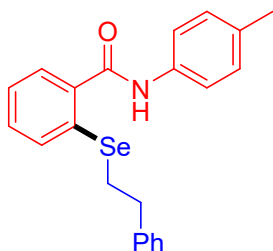
**2-((cyclopropylmethyl)selanyl)-N-(p-tolyl)benzamide (3q)**

**Yield:** 79% (54.5mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3258, 2915, 1637, 1596, 1508, 1322, 1254, 815, 739, 680, 512, 458.  **$^1\text{H}$  NMR** (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  10.24 (s, 1H), 7.59 (dd,  $J = 22.8, 8.2$  Hz, 4H), 7.36 (dt,  $J = 40.4, 7.5$  Hz, 2H), 7.15 (d,  $J = 8.0$  Hz, 2H), 2.86 (d,  $J = 7.2$  Hz, 2H), 2.28 (s, 3H), 1.08 – 0.93 (m, 1H), 0.54 (t,  $J = 6.4$  Hz, 2H), 0.23 (t,  $J = 4.9$  Hz, 2H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{DMSO}-d_6$ )  $\delta$  166.6, 137.4, 136.65, 132.6, 132.1, 130.5, 130.2, 129.0, 128.0, 125.3, 119.8, 31.3, 20.5, 10.5, 6.6.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{DMSO}-d_6$ )  $\delta$  295.1. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{18}\text{H}_{19}\text{NOSe}(\text{M}+\text{Na})^+$ : 368.0530, found 368.0530.



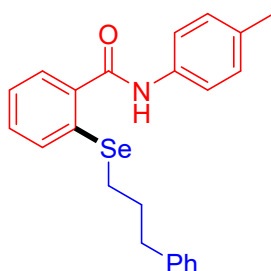
**2-(benzylselanyl)-N-(p-tolyl)benzamide (3r)**

**Yield:** 75% (57.2mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3297, 2931, 2359, 1635, 1600, 1540, 1509, 1323, 1253, 817, 764, 737, 696, 511, 468.  **$^1\text{H}$  NMR** (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  10.25 (s, 1H), 7.70 – 7.55 (m, 4H), 7.43 (td,  $J = 7.6, 1.5$  Hz, 1H), 7.39 – 7.23 (m, 5H), 7.23 – 7.11 (m, 3H), 4.18 (s, 2H), 2.27 (s, 3H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{DMSO}-d_6$ )  $\delta$  166.4, 138.1, 136.5, 136.3, 133.1, 132.6, 130.78, 130.0, 129.0, 128.4, 128.2, 126.7, 125.4, 119.9, 29.4, 20.5.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{DMSO}-d_6$ )  $\delta$  360.1. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{19}\text{NOSe}(\text{M}+\text{Na})^+$ : 404.0530, found 404.0535.



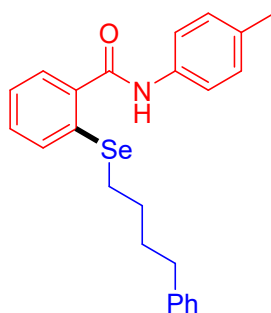
**(S)-6-(phenethylselanyl)-N-(p-tolyl)cyclohexa-1,3-diene-1-carboxamide (3s)**

**Yield:** 71% (56.4mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3263, 2922, 1637, 1598, 1523, 1509, 1323, 1253, 1032, 815, 738, 699, 512, 459.  **$^1\text{H}$  NMR** (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.28 (s, 1H), 7.62 (dd,  $J = 8.1, 3.9$  Hz, 4H), 7.45 (td,  $J = 7.6, 1.6$  Hz, 1H), 7.34 (t,  $J = 7.2$  Hz, 1H), 7.27 (p,  $J = 7.0, 6.3$  Hz, 4H), 7.22 – 7.18 (m, 1H), 7.15 (d,  $J = 8.2$  Hz, 2H), 3.14 (dd,  $J = 8.6, 6.9$  Hz, 2H), 2.93 (t,  $J = 7.8$  Hz, 2H), 2.28 (s, 3H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  166.6, 140.9, 137.7, 136.6, 132.6, 131.5, 130.7, 130.1, 129.0, 128.3, 128.1, 126.2, 125.5, 119.9, 35.1, 26.6, 20.5.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{DMSO-}d_6$ )  $\delta$  299.0. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{NOSe}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.0686, found 418.0696.



**2-((3-phenylpropyl)selanyl)-N-(p-tolyl)benzamide (3t)**

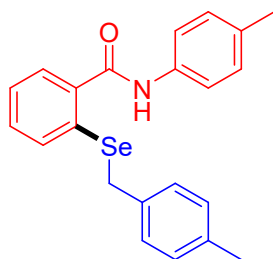
**Yield:** 44% (36.0mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3295, 2919, 1637, 1519, 1509, 1401, 1319, 1252, 896, 812, 742, 688, 493.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 (s, 1H), 7.72 – 7.63 (m, 1H), 7.59 – 7.49 (m, 3H), 7.38 – 7.26 (m, 4H), 7.25 – 7.12 (m, 5H), 2.92 (t,  $J = 7.4$  Hz, 2H), 2.75 (t,  $J = 7.5$  Hz, 2H), 2.37 (s, 3H), 2.10 – 1.99 (m, 2H).  **$^{13}\text{C}$  NMR** (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.5, 141.2, 137.4, 135.4, 134.3, 132.1, 131.0, 130.8, 129.6, 128.7, 128.6, 128.6, 128.5, 127.1, 126.5, 126.1, 120.5, 120.2, 35.9, 31.1, 26.8, 21.0.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{CDCl}_3$ )  $\delta$  290.1. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{23}\text{NOSe}$  ( $\text{M}+\text{Na}$ ) $^+$ : 432.0843, found 432.0843.



**2-((4-phenylbutyl)selanyl)-N-(p-tolyl)benzamide (3u)**

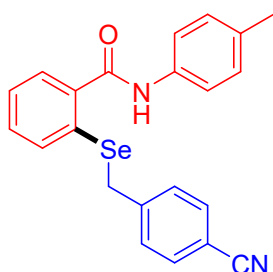
**Yield:** 52% (44.0mg). White solid. **IR** (neat, v,  $\text{cm}^{-1}$ ): 3270, 2919, 1637, 1522, 1508, 814, 685, 515, 459.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 – 7.54 (m, 1H), 7.47 – 7.37 (m, 3H), 7.28 – 7.22 (m, 1H), 7.20 (dd,  $J = 7.3, 1.4$  Hz, 1H), 7.15 (d,  $J = 7.4$  Hz, 2H), 7.09 (d,  $J = 7.4$  Hz, 2H), 7.06 – 7.01 (m, 3H), 2.81 (t,  $J = 4.3$  Hz, 2H), 2.55 – 2.44 (m, 2H), 2.25 (s, 3H), 1.68 – 1.60 (m, 4H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.4, 142.1, 137.6, 135.4, 134.3, 132.5, 131.0, 130.7, 129.7, 128.8, 128.5, 128.4, 126.7, 125.9,

120.2, 35.4, 31.6, 29.1, 27.8, 21.0.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  289.6. HRMS (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{25}\text{NOSe}$  ( $\text{M}+\text{Na}$ ) $^+$ : 446.0999, found 446.0985.



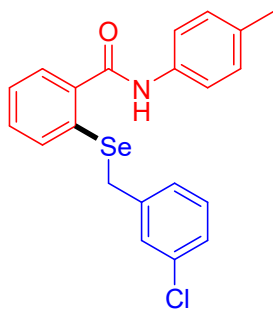
**2-((4-methylbenzyl)selanyl)-N-(p-tolyl)benzamide (3v)**

**Yield:** 67% (53.1mg). White solid. IR (neat,  $\nu$ ,  $\text{cm}^{-1}$ ): 3310, 2922, 2851, 1635, 1598, 1532, 1511, 1403, 1321, 1270, 1253, 1037, 818, 737, 684, 514, 476, 412.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  10.22 (s, 1H), 7.62 (td,  $J = 7.7, 1.3$  Hz, 2H), 7.57 (d,  $J = 8.1$  Hz, 2H), 7.40 (td,  $J = 7.6, 1.5$  Hz, 1H), 7.29 (td,  $J = 7.5, 1.2$  Hz, 1H), 7.24 – 7.17 (m, 2H), 7.11 (d,  $J = 8.2$  Hz, 2H), 7.04 (d,  $J = 7.8$  Hz, 2H), 4.11 (s, 2H), 2.24 (s, 3H), 2.21 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ )  $\delta$  166.4, 136.6, 136.4, 135.8, 134.9, 133.2, 132.7, 130.8, 130.0, 129.0, 128.9, 128.9, 128.2, 125.4, 120.0, 29.2, 20.7, 20.5.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{DMSO}-d_6$ )  $\delta$  358.3. HRMS (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{NOSe}$  ( $\text{M}+\text{Na}$ ) $^+$ : 418.0686, found 418.0680.



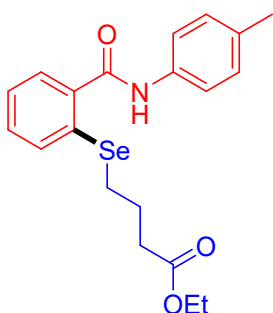
**2-((4-cyanobenzyl)selanyl)-N-(p-tolyl)benzamide (3w)**

**Yield:** 50% (40.6mg). White solid. IR (neat,  $\nu$ ,  $\text{cm}^{-1}$ ): 3246, 2921, 2852, 2225, 1630, 1598, 1526, 1510, 1404, 1326, 1254, 1031, 858, 817, 737, 684, 544, 513, 464.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (s, 1H), 7.65 (t,  $J = 4.6$  Hz, 1H), 7.47 (dt,  $J = 9.3, 5.7$  Hz, 5H), 7.31 (ddd,  $J = 8.2, 5.9, 3.2$  Hz, 4H), 7.16 (d,  $J = 8.0$  Hz, 2H), 4.11 (s, 2H), 2.35 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.4, 143.8, 137.9, 135.2, 134.5, 133.2, 132.2, 131.1, 130.3, 129.7, 129.6, 128.2, 127.3, 120.2, 118.9, 110.5, 31.3, 21.0.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  380.7. HRMS (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{18}\text{N}_2\text{OSe}$  ( $\text{M}+\text{Na}$ ) $^+$ : 429.0482, found 429.0487.



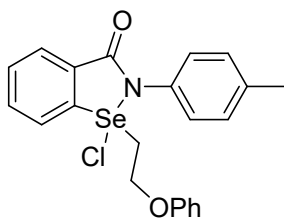
**2-((3-chlorobenzyl)selanyl)-N-(p-tolyl)benzamide (3x)**

**Yield:** 70% (58.1mg). White solid. **IR** (neat,  $\nu$ ,  $\text{cm}^{-1}$ ): 3310, 3261, 2929, 1650, 1633, 1600, 1537, 1511, 1401, 1324, 816, 791, 695, 684, 512, 491.  **$^1\text{H}$  NMR** (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.27 (s, 1H), 7.71 – 7.55 (m, 4H), 7.47 – 7.40 (m, 2H), 7.36 – 7.22 (m, 4H), 7.14 (d,  $J = 8.2$  Hz, 2H), 4.19 (s, 2H), 2.27 (s, 3H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  166.4, 141.1, 136.5, 136.4, 132.8, 132.7, 132.5, 130.8, 130.1, 129.0, 128.7, 128.3, 127.7, 126.6, 125.6, 120.0, 28.5, 20.5.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{DMSO-}d_6$ )  $\delta$  370.8. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{18}\text{ClNOSe}$  ( $\text{M}+\text{Na}$ ) $^+$ : 438.0140, found 438.0147.



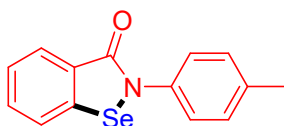
**ethyl 4-((2-(p-tolylcarbamoyl)phenyl)selanyl)butanoate (3y)**

**Yield:** 54% (43.7mg). White solid. **IR** (neat,  $\nu$ ,  $\text{cm}^{-1}$ ): 3289, 2980, 2930, 2905, 1725, 1638, 1596, 1511, 1405, 1372, 1348, 1319, 1252, 1239, 1190, 1027, 896, 813, 736, 682, 647, 511, 458.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (m,  $J = 8.7, 7.5$  Hz, 3H), 7.60 (m,  $J = 1.8$  Hz, 1H), 7.43 (m,  $J = 7.3, 6.3, 3.8$  Hz, 3H), 7.19 (m,  $J = 7.3$  Hz, 2H), 7.14 (m,  $J = 7.0$  Hz, 1H), 7.09 – 7.04 (m, 2H), 3.80 (s, 2H), 2.62 (t,  $J = 7.5$  Hz, 2H), 2.39 (t,  $J = 7.3$  Hz, 2H), 1.84 (p,  $J = 7.5$  Hz, 2H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 137.8, 135.4, 134.4, 132.4, 131.1, 130.3, 129.7, 128.6, 126.7, 120.24, 77.5, 77.2, 76.8, 60.6, 34.2, 26.7, 24.9, 21.0, 14.3.  **$^{77}\text{Se}$  NMR** (76 MHz,  $\text{CDCl}_3$ )  $\delta$  289.7. **HRMS** (ESI+, MeCN)  $m/z$  calcd for  $\text{C}_{20}\text{H}_{23}\text{NO}_3\text{Se}$  ( $\text{M}+\text{Na}$ ) $^+$ : 428.0741, found 428.0741.



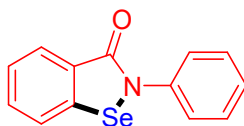
#### 4a

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 9.03 (dd, *J* = 8.2, 1.0 Hz, 1H), 8.05 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.73 (td, *J* = 7.8, 1.6 Hz, 1H), 7.65 (td, *J* = 7.4, 1.1 Hz, 1H), 7.29 – 7.18 (m, 4H), 7.11 – 7.01 (m, 2H), 6.86 – 6.75 (m, 1H), 6.31 – 6.20 (m, 2H), 4.66 (ddd, *J* = 11.2, 8.1, 3.0 Hz, 1H), 4.27 (ddd, *J* = 11.4, 5.6, 3.2 Hz, 1H), 4.18 (ddd, *J* = 11.3, 5.6, 2.9 Hz, 1H), 3.94 (ddd, *J* = 11.3, 8.0, 3.2 Hz, 1H), 2.34 (s, 3H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 165.4, 156.8, 138.1, 134.4, 133.7, 133.4, 131.4, 130.7, 130.6, 129.3, 129.3, 127.1, 121.7, 114.1, 62.7, 62.3, 21.2. **<sup>77</sup>Se NMR** (76 MHz, CDCl<sub>3</sub>) δ 610.9. **HRMS** (ESI+, MeCN) *m/z* calcd for C<sub>22</sub>H<sub>22</sub>NO<sub>2</sub>Se(M+H<sub>2</sub>O)<sup>+</sup>: 428.0765, found 428.0763.



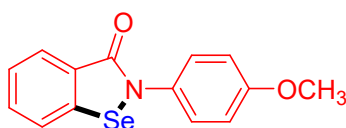
#### 2-(p-tolyl)benzo[d][1,2]selenazol-3(2H)-one (5a)

**Yield:** 90% (52.0mg). White solid. **IR** (neat, v, cm<sup>-1</sup>): 3056, 3028, 2918, 2856, 2328, 1594, 1562, 1505, 1443, 1333, 1309, 1262, 1133, 817, 788, 739, 730, 662, 552, 510, 480. **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.11 – 8.06 (m, 1H), 7.90 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.67 (ddd, *J* = 8.3, 7.2, 1.5 Hz, 1H), 7.53 – 7.45 (m, 3H), 7.29 – 7.22 (m, 2H), 2.32 (s, 3H). **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 164.9, 138.9, 137.1, 135.2, 132.1, 129.6, 128.5, 127.9, 126.2, 125.8, 124.6, 20.5. **<sup>77</sup>Se NMR** (76 MHz, DMSO-*d*<sub>6</sub>) δ 912.2. **HRMS** (ESI+, MeCN) *m/z* calcd for C<sub>14</sub>H<sub>11</sub>NOSe(M+Na)<sup>+</sup>: 311.9904, found 311.9903.



#### 2-phenylbenzo[d][1,2]selenazol-3(2H)-one (5b)

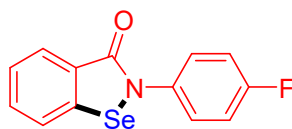
**Yield:** 84% (46.2mg). White solid. **IR** (neat, v, cm<sup>-1</sup>): 3090, 2957, 2920, 2851, 2162, 1762, 1586, 1576, 1560, 1486, 1441, 1345, 1262, 1027, 755, 735, 684, 676, 509, 479. **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.07 (d, *J* = 8.0 Hz, 1H), 7.89 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.70 – 7.60 (m, 3H), 7.45 (dt, *J* = 11.7, 7.8 Hz, 3H), 7.25 (dd, *J* = 8.1, 6.7 Hz, 1H). **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 165.0, 139.7, 138.9, 132.3, 129.2, 128.5, 128.0, 126.3, 125.8, 125.8, 124.7. **<sup>77</sup>Se NMR** (76 MHz, DMSO-*d*<sub>6</sub>) δ 912.6. **HRMS** (ESI+, MeCN) *m/z* calcd for C<sub>13</sub>H<sub>9</sub>NOSe(M+Na)<sup>+</sup>: 297.9747, found 297.9745.



#### 2-(4-methoxyphenyl)benzo[d][1,2]selenazol-3(2H)-one (5c)

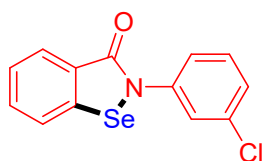
**Yield:** 93% (56.7mg). White solid. **IR** (neat, v, cm<sup>-1</sup>): 3410, 2921, 2851, 2252, 2127, 1772, 1596, 1508, 1440, 1353, 1295, 1246, 1050, 1022, 822, 761, 736, 673, 626, 562,

518, 485. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.06 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.87 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.65 (ddd, *J* = 8.3, 7.2, 1.4 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.02 – 6.95 (m, 2H), 3.76 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 165.0, 157.3, 139.0, 132.2, 132.0, 128.3, 127.9, 126.5, 126.2, 125.8, 114.3, 55.4. <sup>77</sup>Se NMR (76 MHz, DMSO-*d*<sub>6</sub>) δ 913.9. HRMS (ESI+, MeCN) *m/z* calcd for C<sub>14</sub>H<sub>11</sub>NO<sub>2</sub>Se(M+Na)<sup>+</sup>: 327.9853, found 327.9858.



#### 2-(4-fluorophenyl)benzo[d][1,2]selenazol-3(2H)-one (5d)

**Yield:** 87% (51.0mg). White solid. IR (neat, v, cm<sup>-1</sup>): 3052, 2958, 2924, 2850, 2335, 2195, 2055, 2013, 1601, 1586, 1560, 1499, 1443, 1337, 1227, 1130, 1020, 826, 795, 786, 728, 509, 435. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.89 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.70 – 7.60 (m, 3H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.27 (t, *J* = 8.8 Hz, 2H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 165.1, 159.7 (*J* = 242.2), 138.9, 135.9 (*J* = 2.8), 132.2, 128.3, 128.0, 126.9 (*J* = 8.6), 126.3, 125.9, 115.9 (*J* = 22.4). <sup>77</sup>Se NMR (76 MHz, DMSO-*d*<sub>6</sub>) δ 916.8. HRMS (ESI+, MeCN) *m/z* calcd for C<sub>13</sub>H<sub>8</sub>FNOSe(M+Na)<sup>+</sup>: 315.9653, found 315.9653.



#### 2-(3-chlorophenyl)benzo[d][1,2]selenazol-3(2H)-one (5e)

**Yield:** 85% (52.5mg). White solid. IR (neat, v, cm<sup>-1</sup>): 3056, 2920, 2855, 2335, 2194, 1599, 1563, 1551, 1474, 1443, 1333, 1309, 1255, 1133, 1022, 731, 786, 667, 519, 510, 478. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.08 (d, *J* = 8.1 Hz, 1H), 7.95 – 7.84 (m, 2H), 7.68 (ddd, *J* = 8.4, 7.2, 1.5 Hz, 1H), 7.58 – 7.41 (m, 3H), 7.31 (ddd, *J* = 7.8, 2.1, 1.1 Hz, 1H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 165.3, 141.2, 138.8, 133.3, 132.5, 130.9, 128.3, 128.1, 126.4, 125.9, 125.5, 124.0, 122.9. <sup>77</sup>Se NMR (76 MHz, DMSO-*d*<sub>6</sub>) δ 921.2. HRMS (ESI+, MeCN) *m/z* calcd for C<sub>13</sub>H<sub>8</sub>ClNOSe(M+Na)<sup>+</sup>: 331.9357, found 311.9357.

## V. References

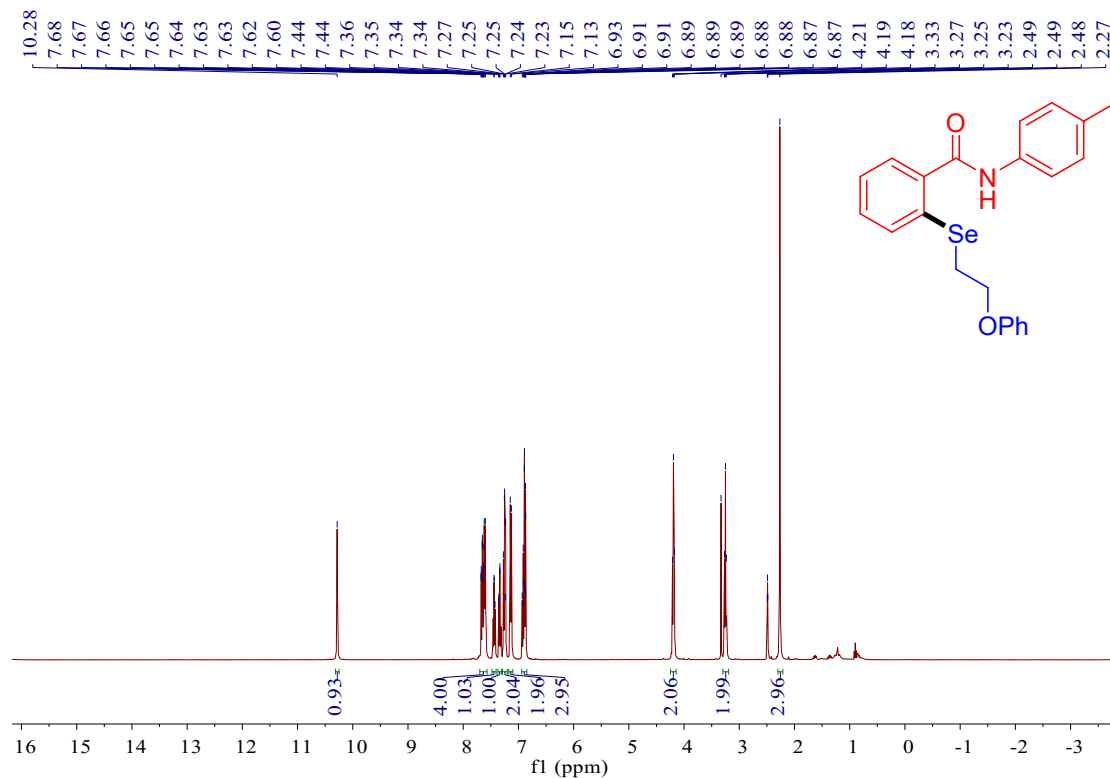
- (1) (a) Motoshi, Y.; Masao, M.; Tomoya, M.; Masahiro, M. *J. Am. Chem. Soc.* **2010**, *132*, 54–55; (b) Miura, T.; Yamauchi, M.; Murakami, M. *Org. Lett.* **2008**, *10*, 3085; (c) Kumar, K. S.; Adepu, R.; Sandra, S.; Rambabu, D.; Krishna, G. R.; Reddy, C. M.; Misra, P.; Pal, M. *Bioorg. Med. Chem. Lett.* **2012**, *22*, 1146; (d) Clark, A. S.; Deans, B.; Stevens, M. F. G.; Tisdale, M. J.; Wheelhouse, R. T.; Denny, B. J.; Hartley, J. A. *J. Med. Chem.* **1995**, *38*, 1493; (e) Miura, T.; Morimoto, M.; Yamauchi, M.; Murakami, M. *J. Org. Chem.* **2010**, *75*, 5359; (f) G. Wang, X. Chen, Y. Deng, Z. Li, X. Xu, *J. Agric. Food. Chem.* **2015**, *63*, 6883.



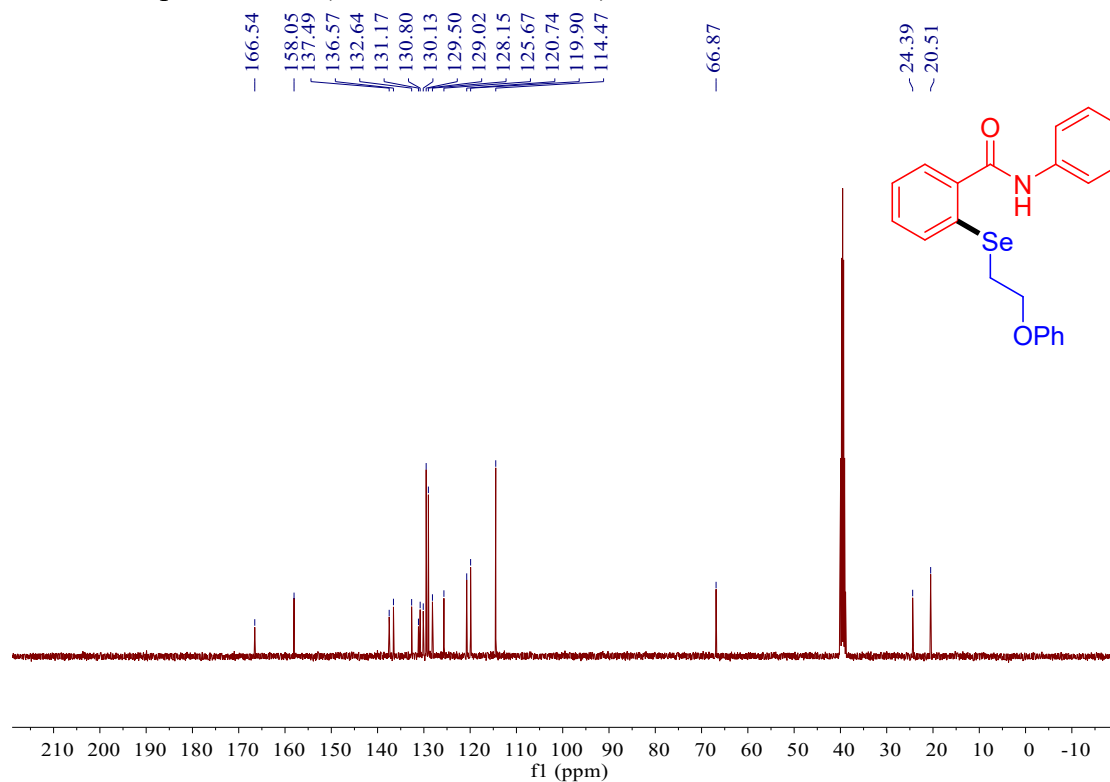
(2) (a) Li, J.; Rao, W.; Wang, S.-Y.; Ji, S.-J. *J. Org. Chem.* **2019**, *84*, 11542. (b) Fang, Y.; Rogge, T.; Ackermann, L.; Wang, S.-Y.; Ji, S.-J. *Nat. Commun.* **2018**, *9*, 2240.

## **VI. Copies of $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra**

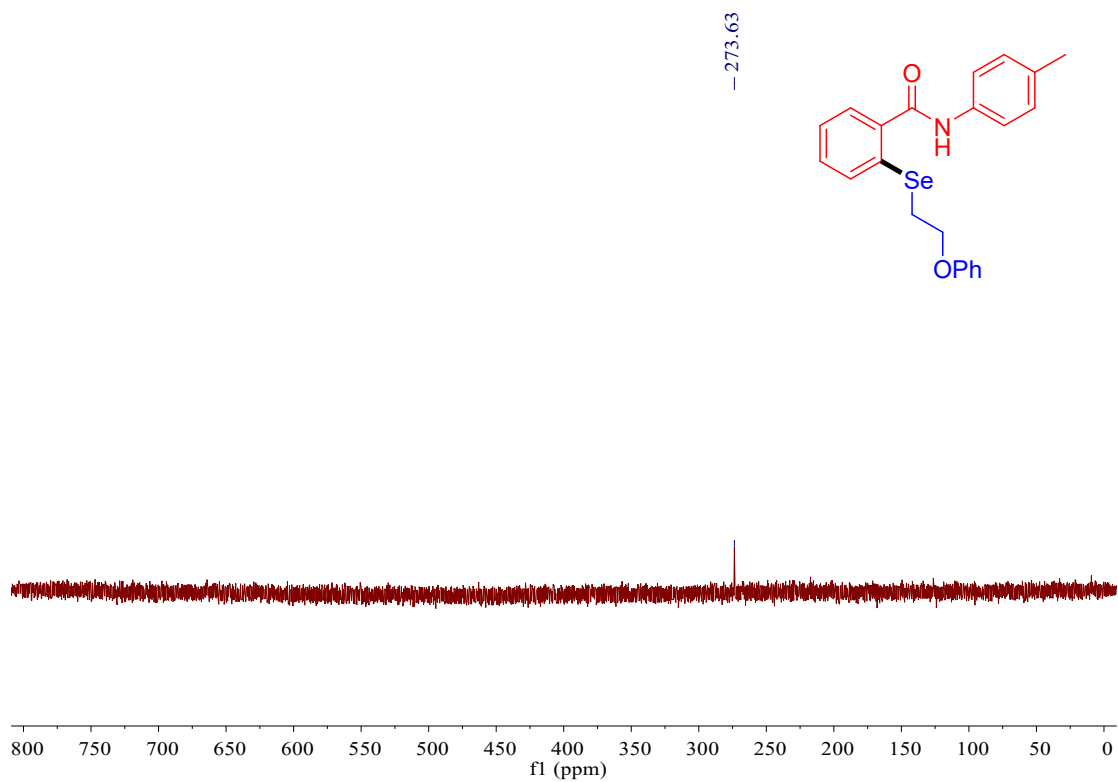
$^1\text{H}$  NMR Spectra of **3a** (400 MHz,  $\text{DMSO-}d_6$ )



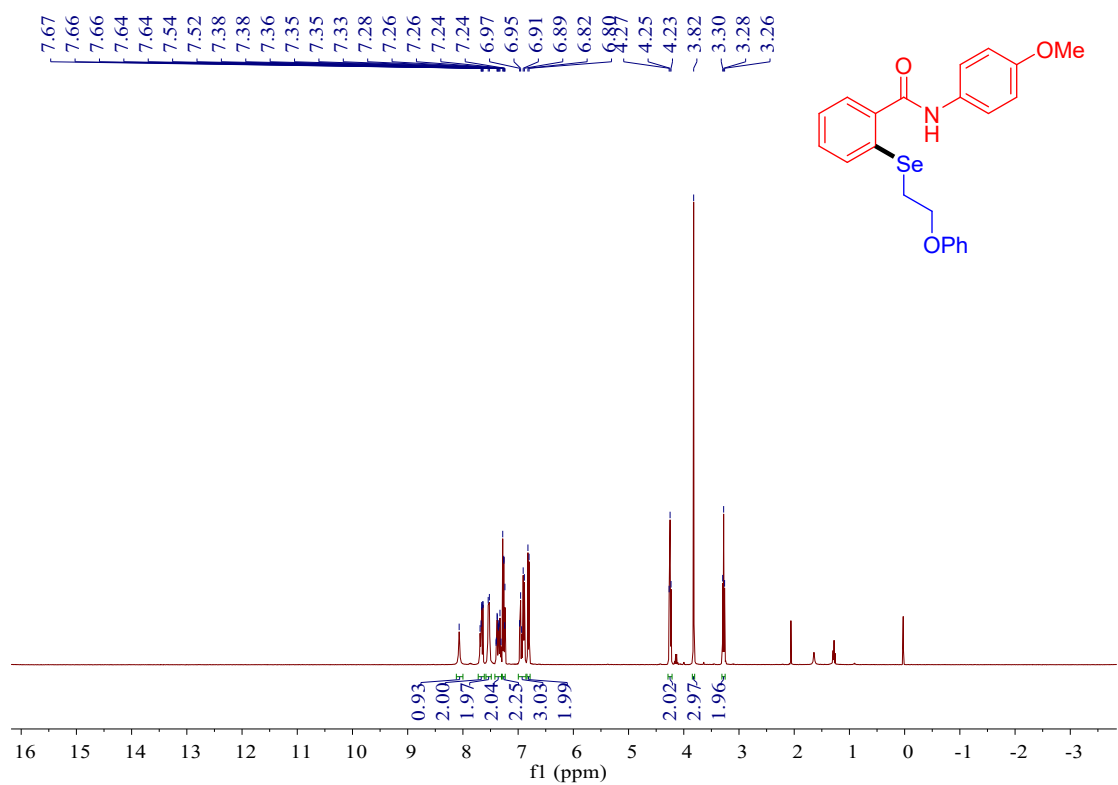
**<sup>13</sup>C NMR Spectra of **3a** (400 MHz, DMSO-*d*<sub>6</sub>)**



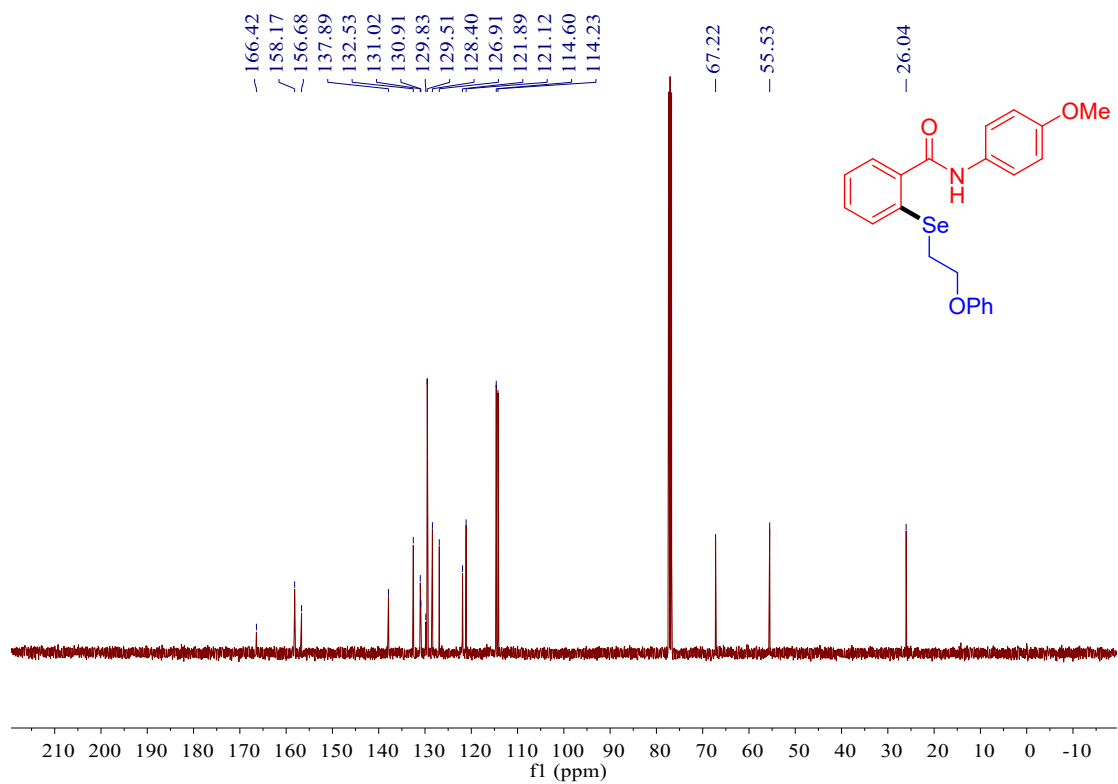
**<sup>77</sup>Se NMR Spectra of **3a** (400 MHz, DMSO-*d*<sub>6</sub>)**



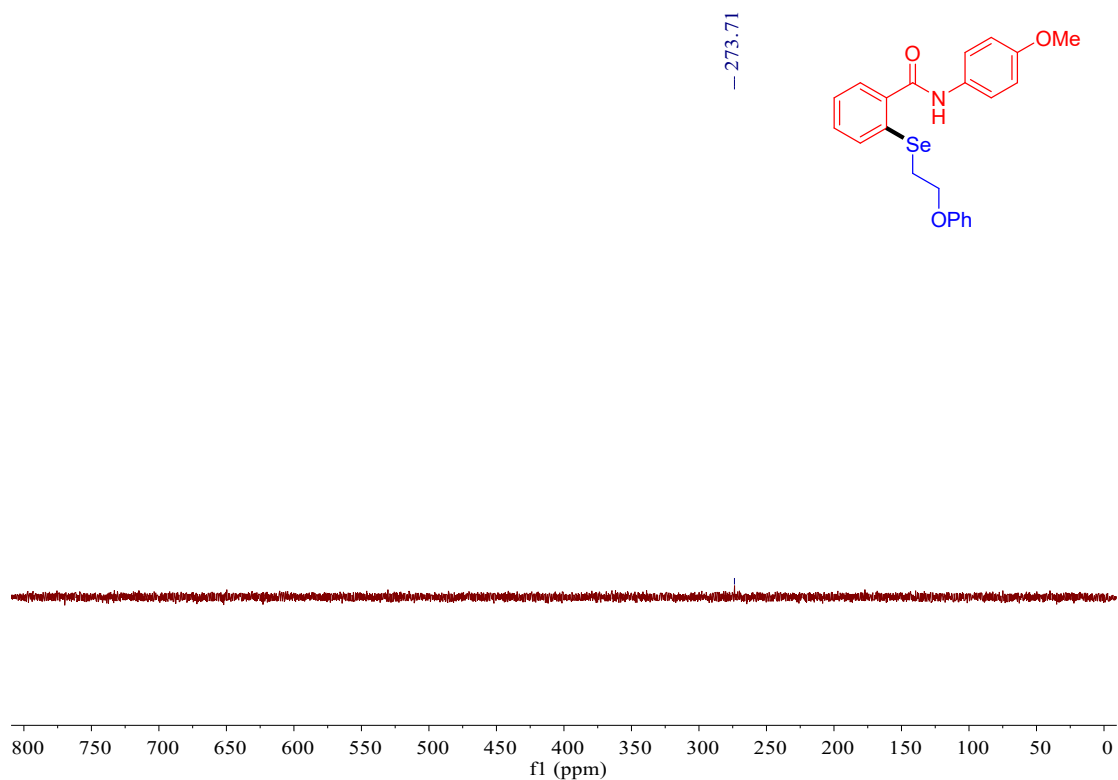
$^1\text{H}$  NMR Spectra of **3b** (400 MHz,  $\text{CDCl}_3$ )



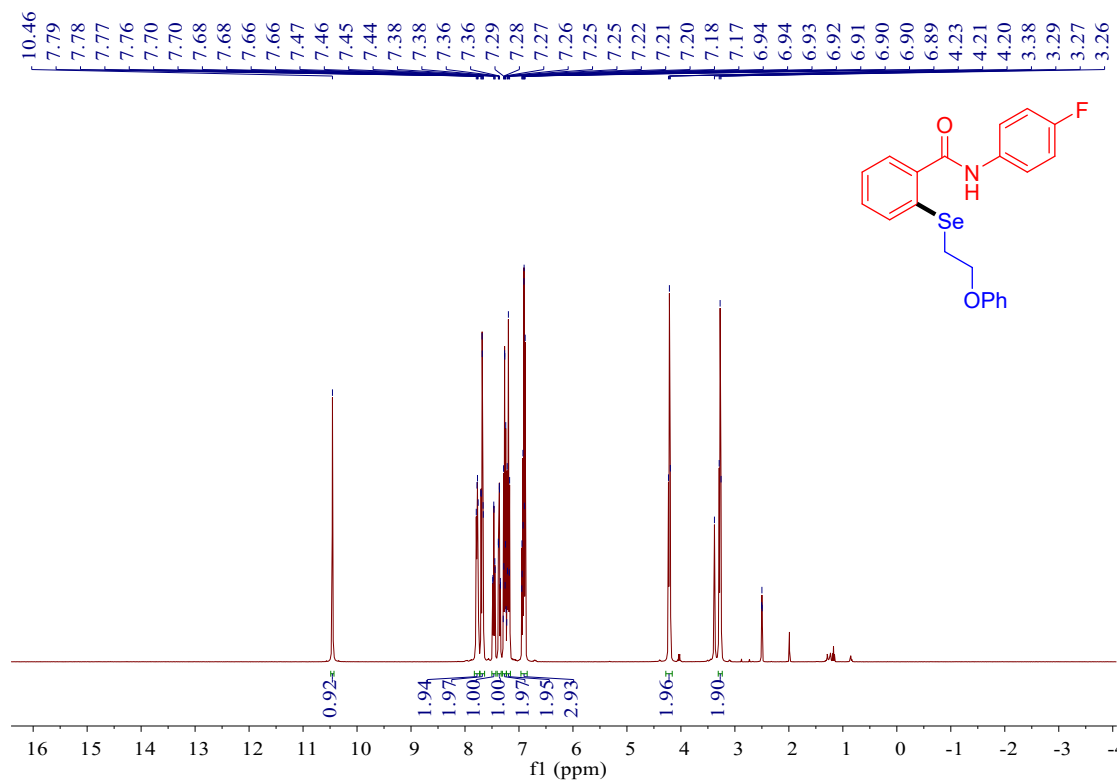
$^{13}\text{C}$  NMR Spectra of **3b** (400 MHz,  $\text{CDCl}_3$ )



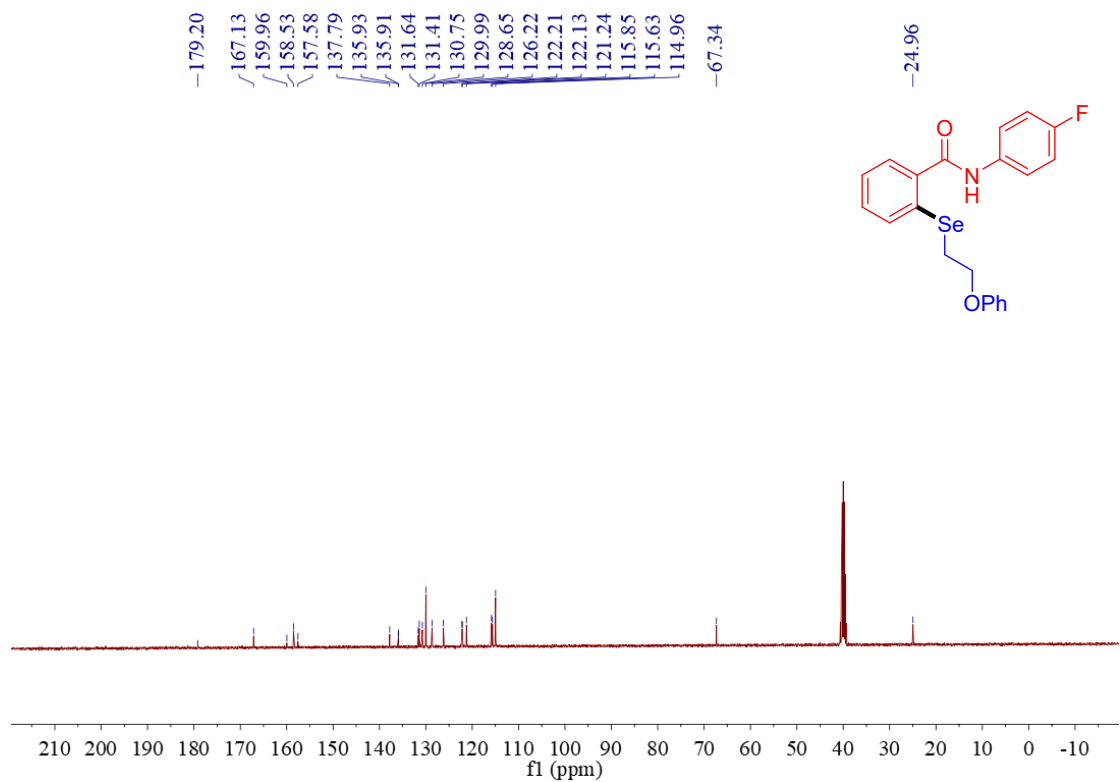
$^{77}\text{Se}$  NMR Spectra of **3b** (400 MHz,  $\text{CDCl}_3$ )



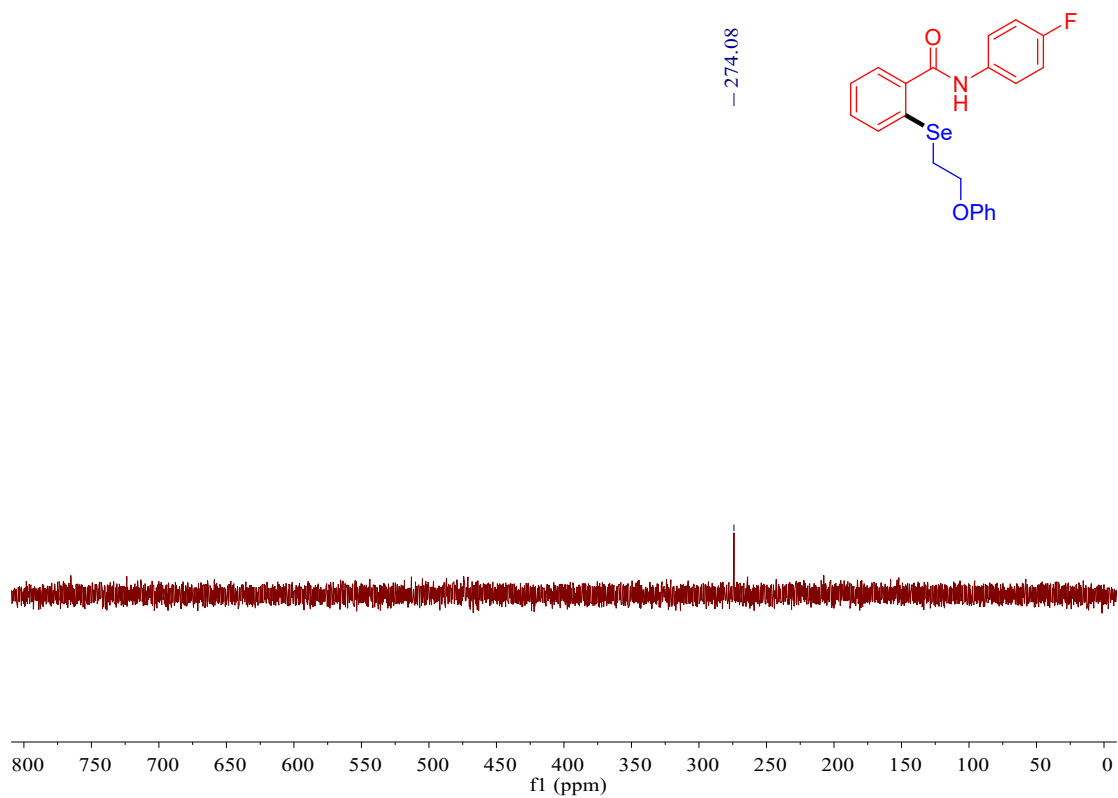
$^1\text{H}$  NMR Spectra of **3c** (400 MHz,  $\text{DMSO}-d_6$ )



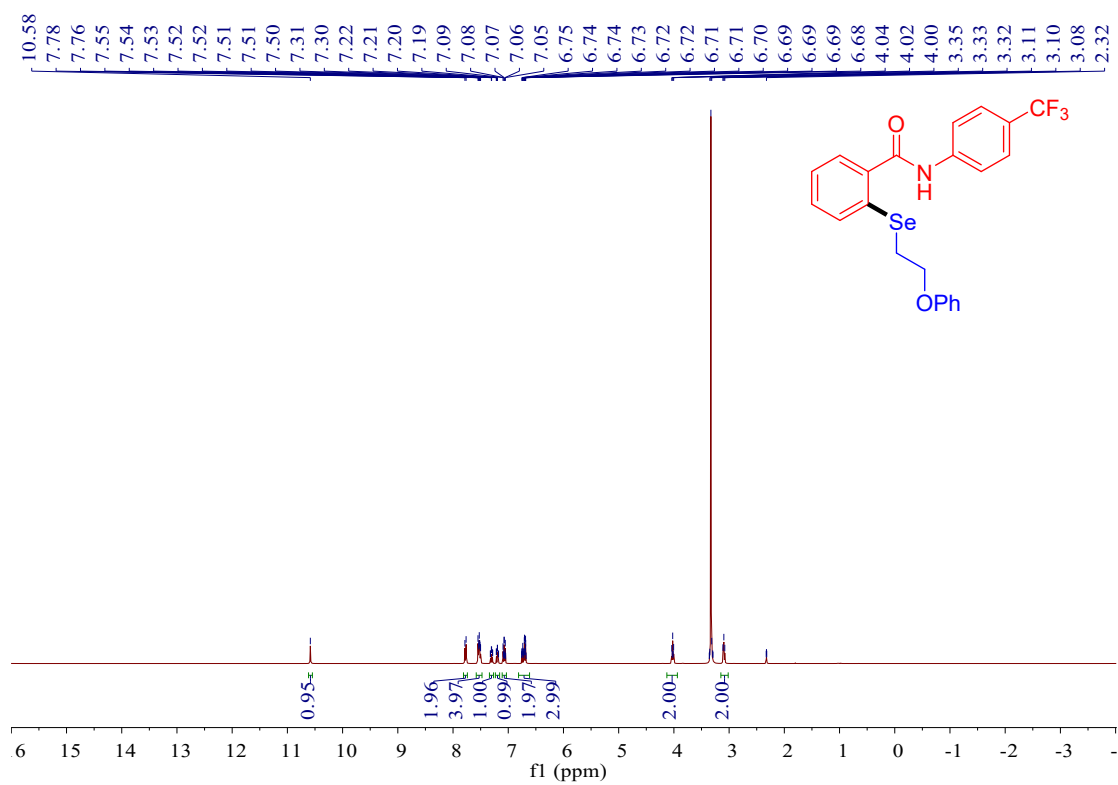
<sup>13</sup>C NMR Spectra of 3c (400 MHz, DMSO-*d*<sub>6</sub>)



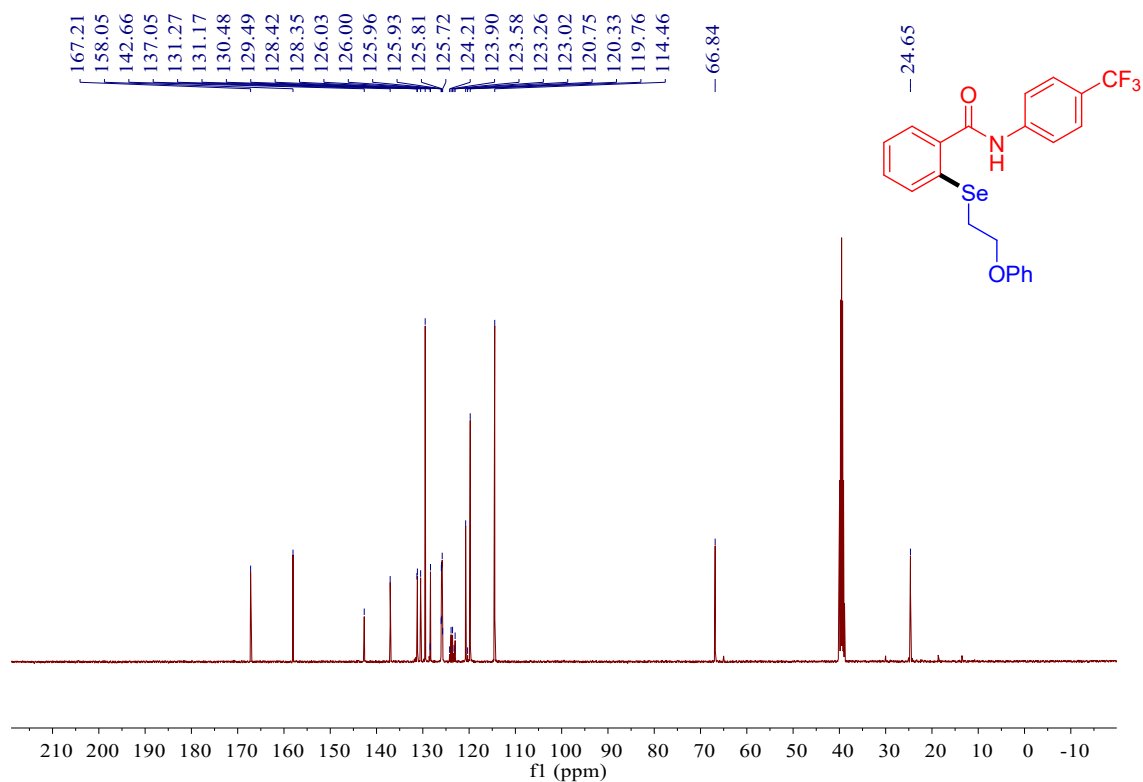
<sup>77</sup>Se NMR Spectra of 3c (400 MHz, DMSO-*d*<sub>6</sub>)



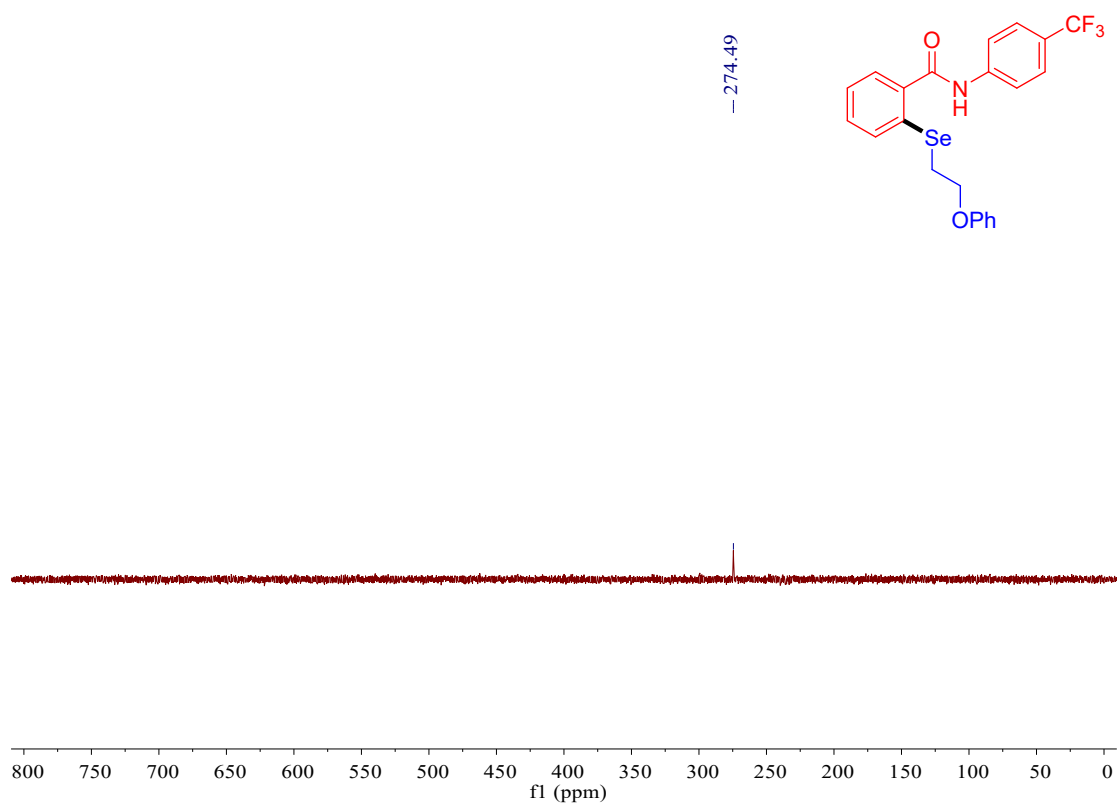
$^1\text{H}$  NMR Spectra of **3d** (400 MHz,  $\text{DMSO-}d_6$ )



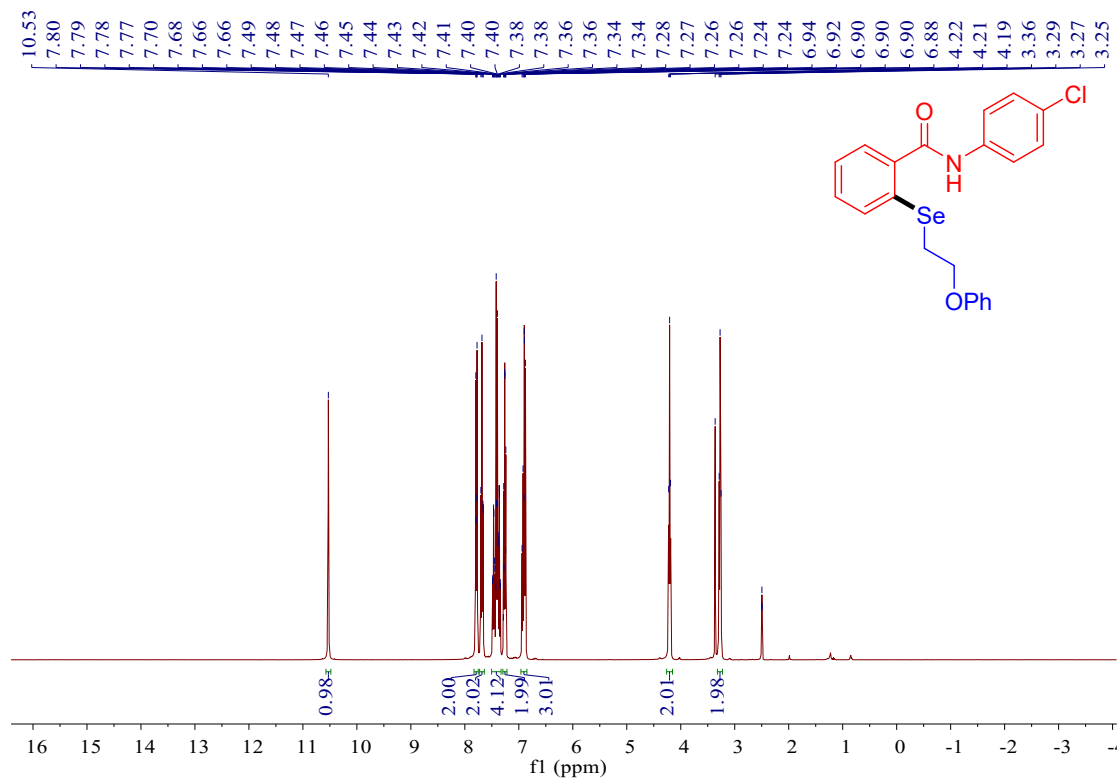
$^{13}\text{C}$  NMR Spectra of **3d** (400 MHz,  $\text{DMSO-}d_6$ )



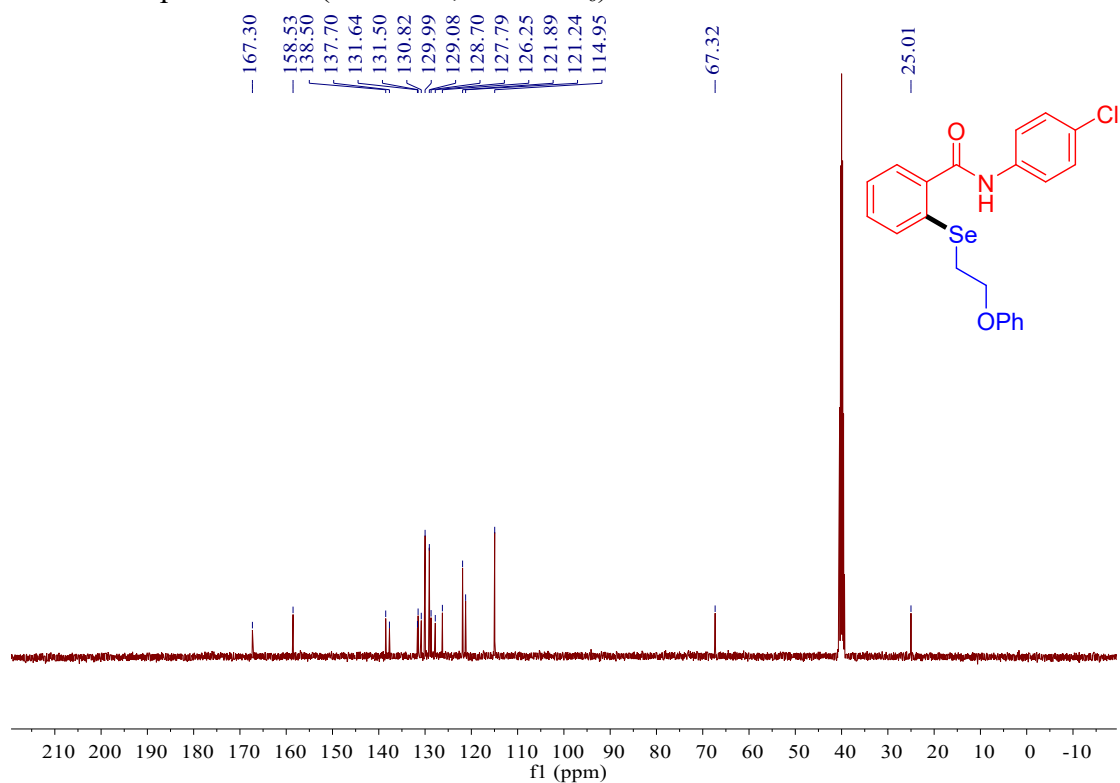
<sup>77</sup>Se NMR Spectra of **3d** (400 MHz, DMSO-*d*<sub>6</sub>)



<sup>1</sup>H NMR Spectra of **3e** (400 MHz, DMSO-*d*<sub>6</sub>)

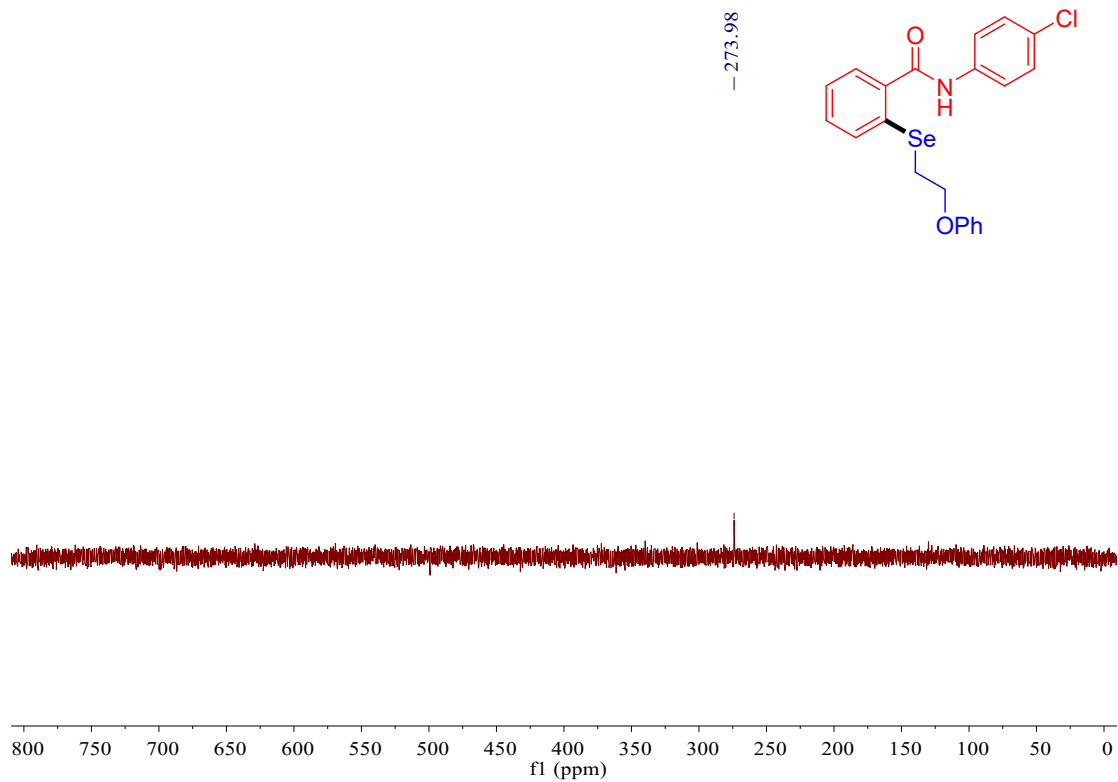


<sup>13</sup>C NMR Spectra of **3e** (400 MHz, DMSO-*d*<sub>6</sub>)

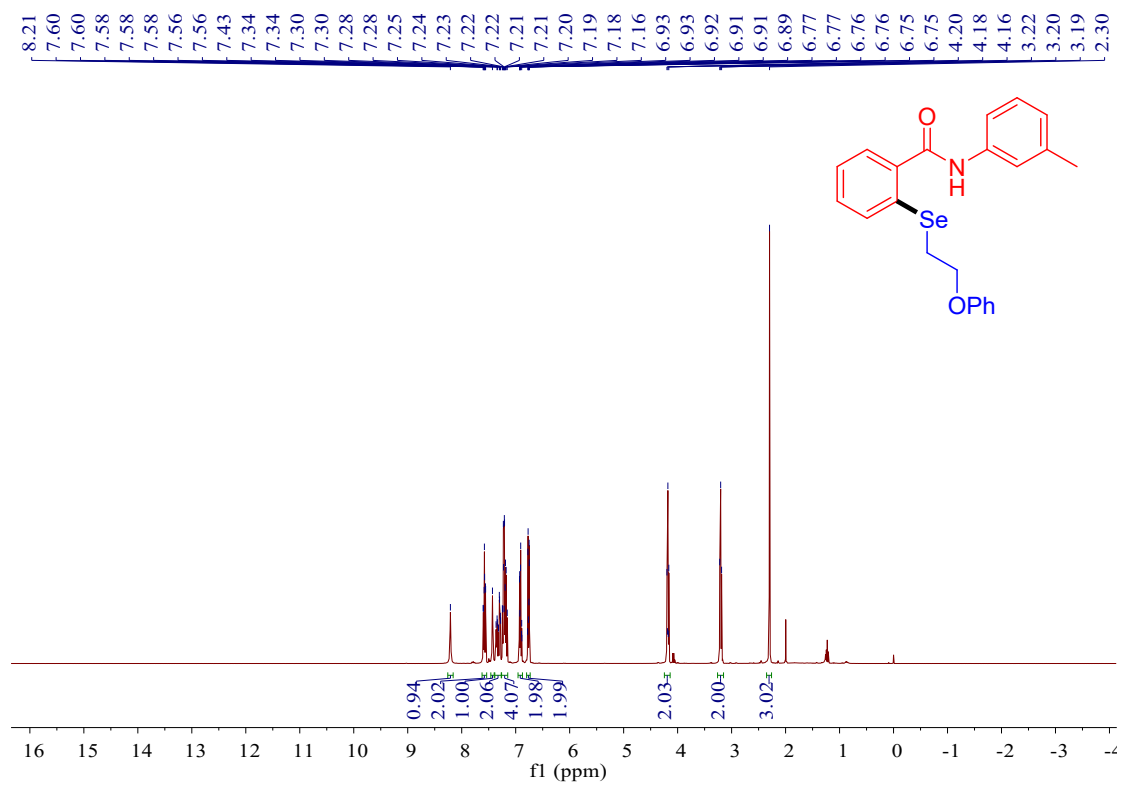


<sup>77</sup>Se NMR Spectra of **3e** (400 MHz, DMSO-*d*<sub>6</sub>)

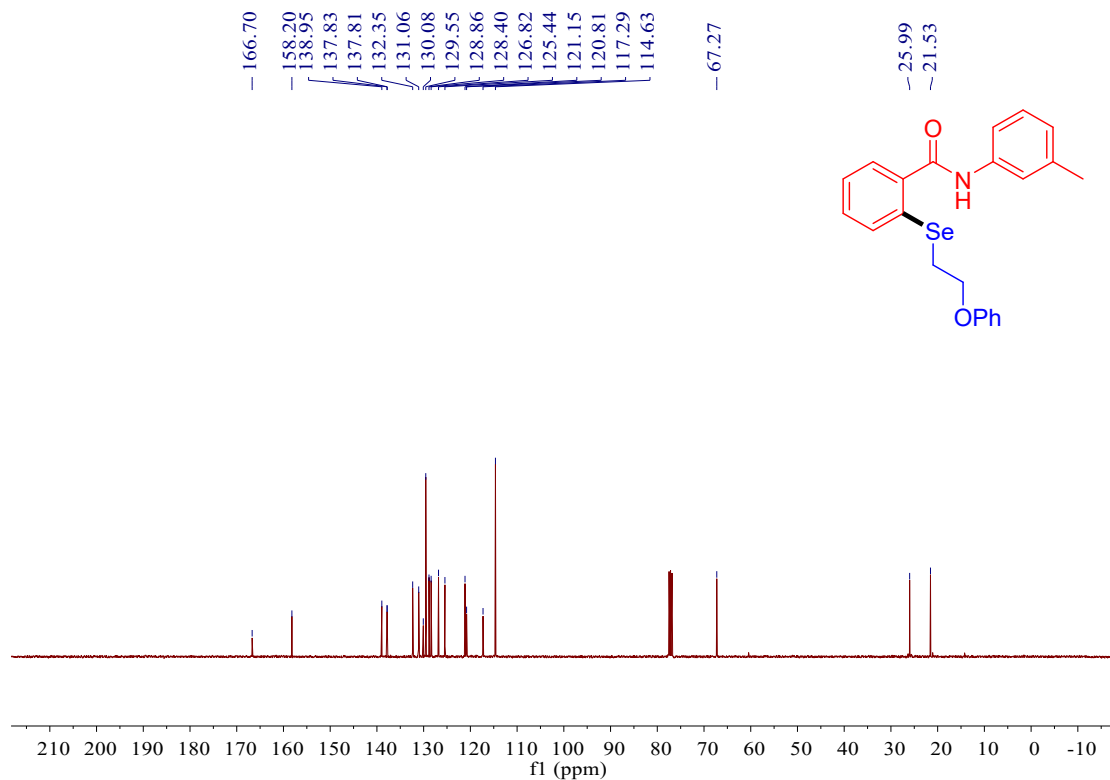




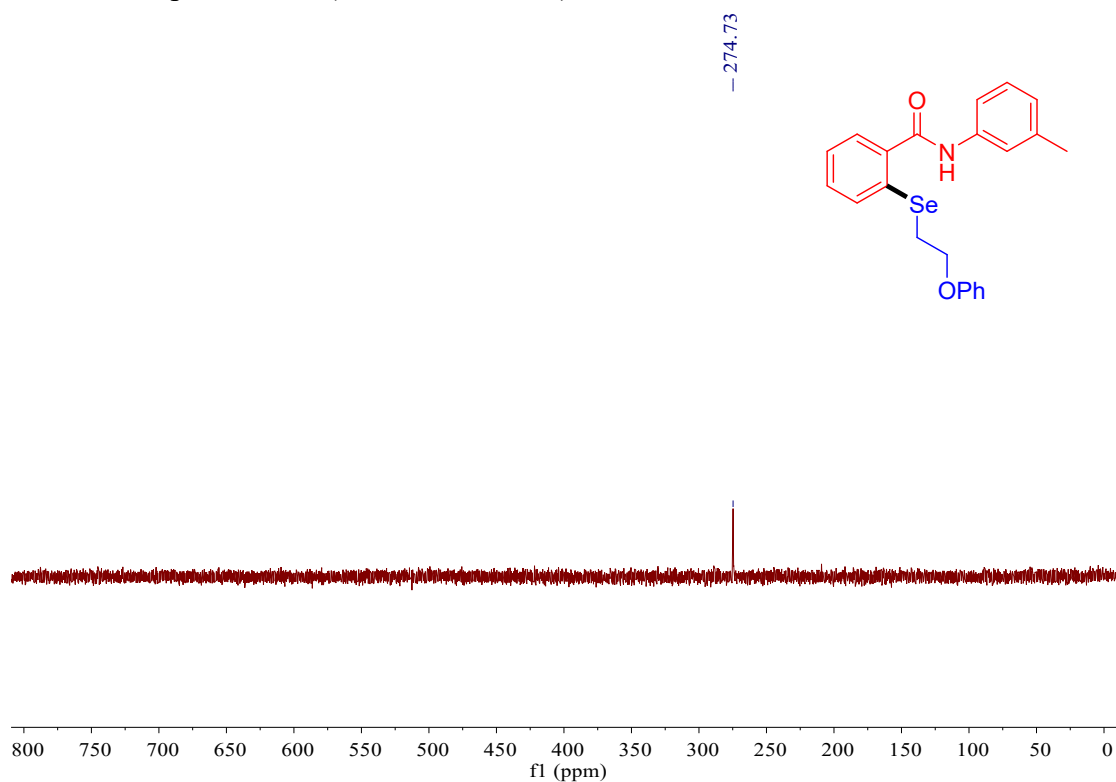
<sup>1</sup>H NMR Spectra of **3f** (400 MHz, CDCl<sub>3</sub>)



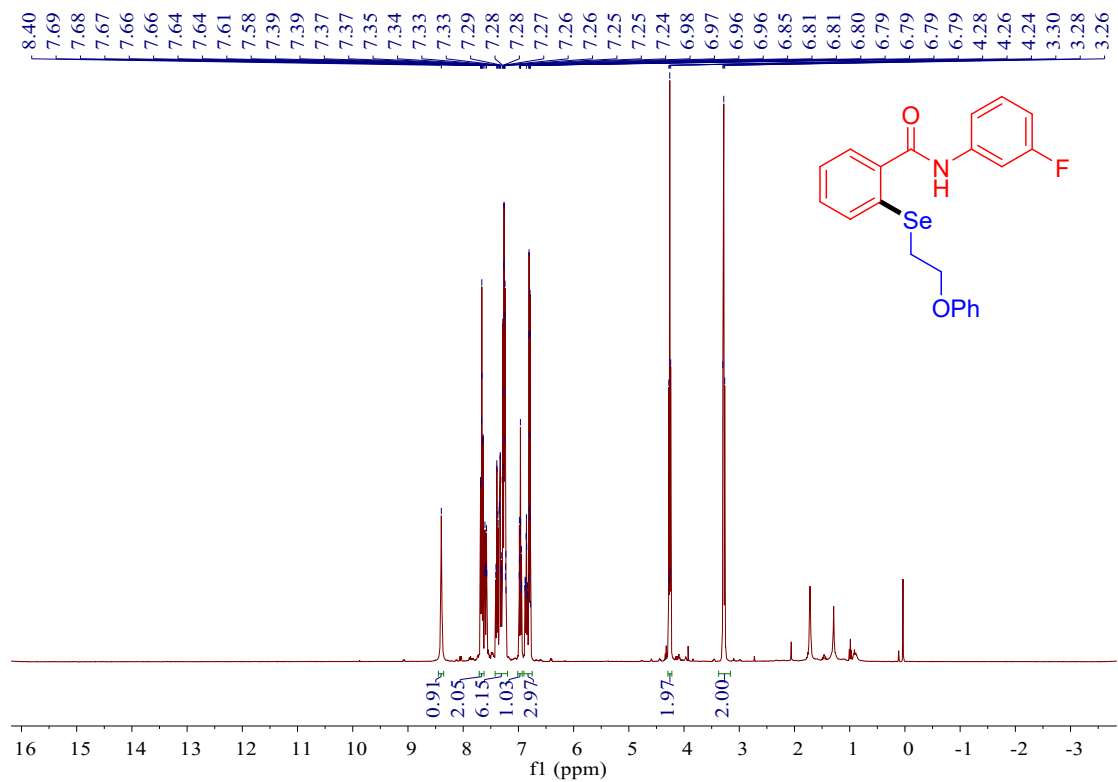
<sup>13</sup>C NMR Spectra of **3f** (400 MHz, CDCl<sub>3</sub>)



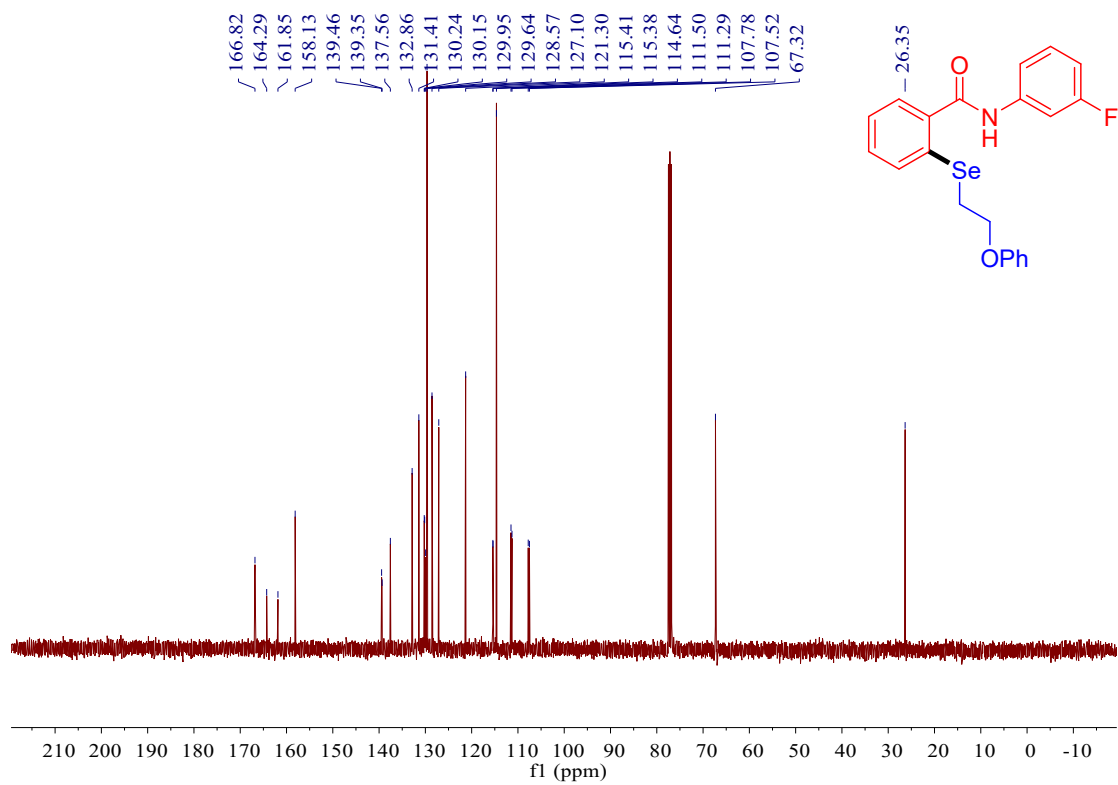
$^{77}\text{Se}$  NMR Spectra of **3f** (400 MHz,  $\text{CDCl}_3$ )



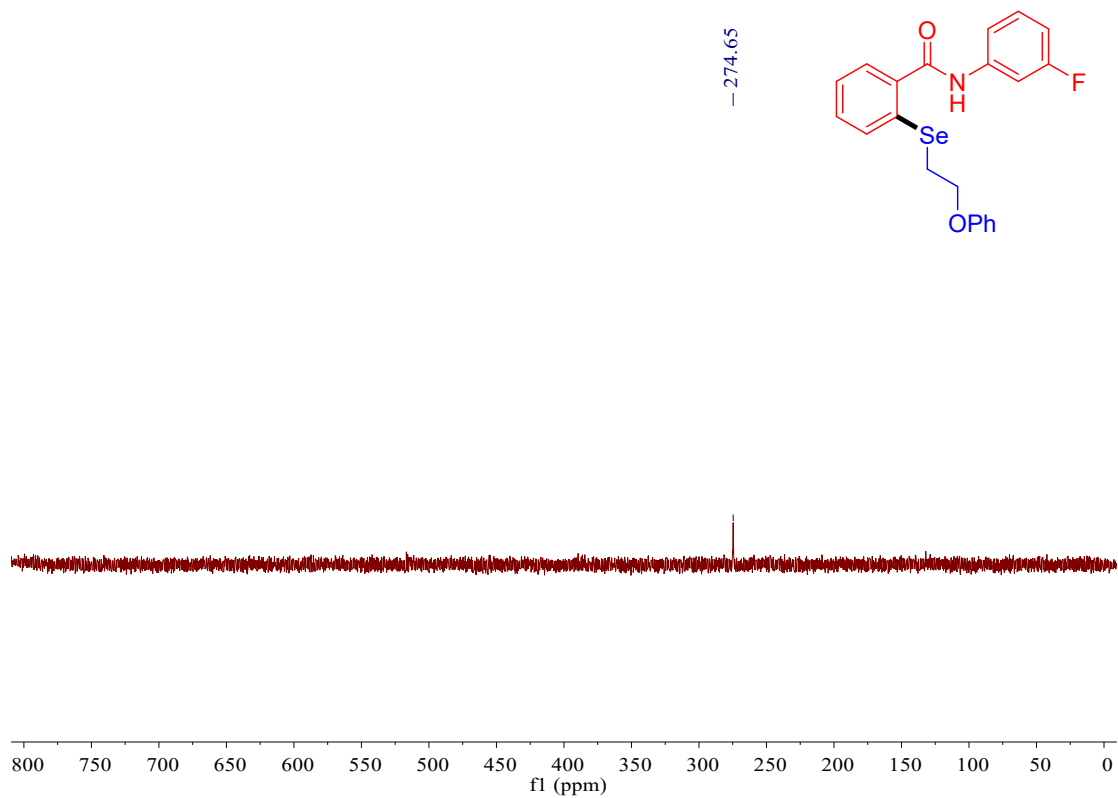
$^1\text{H}$  NMR Spectra of **3g** (400 MHz,  $\text{CDCl}_3$ )



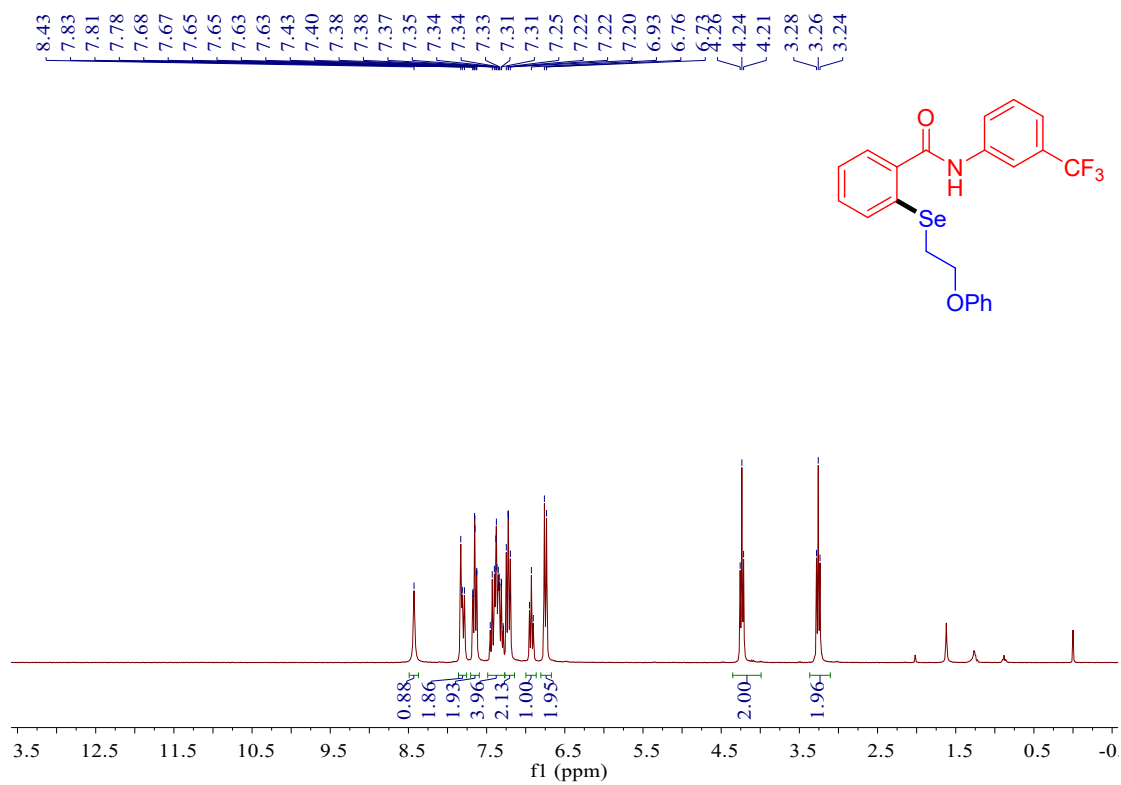
<sup>13</sup>C NMR Spectra of **3g** (400 MHz, CDCl<sub>3</sub>)



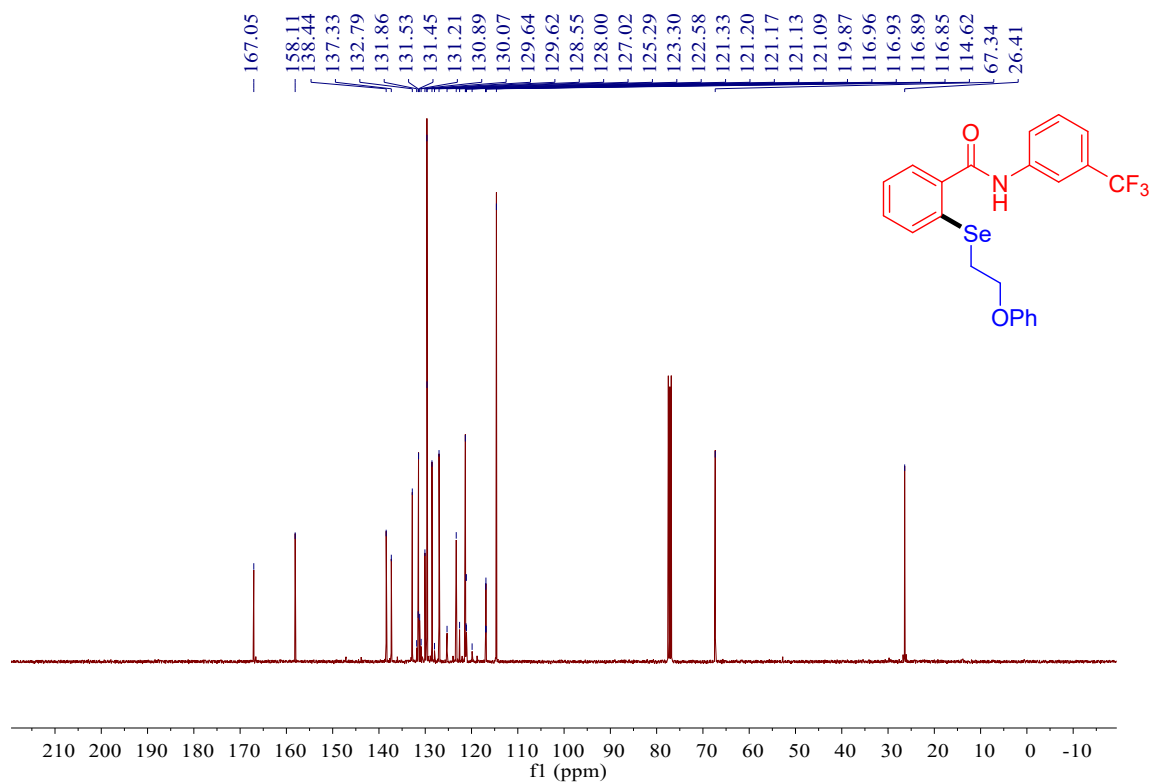
<sup>77</sup>Se NMR Spectra of **3g** (400 MHz, CDCl<sub>3</sub>)



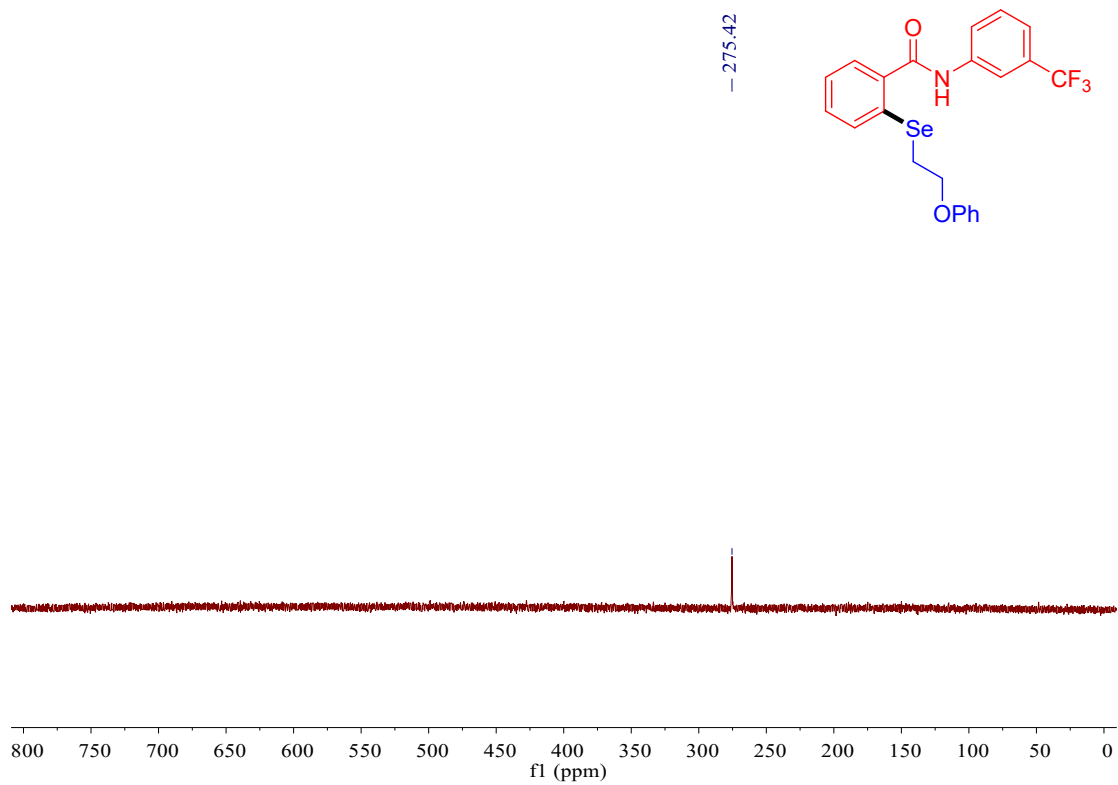
<sup>1</sup>H NMR Spectra of **3h** (300 MHz, CDCl<sub>3</sub>)



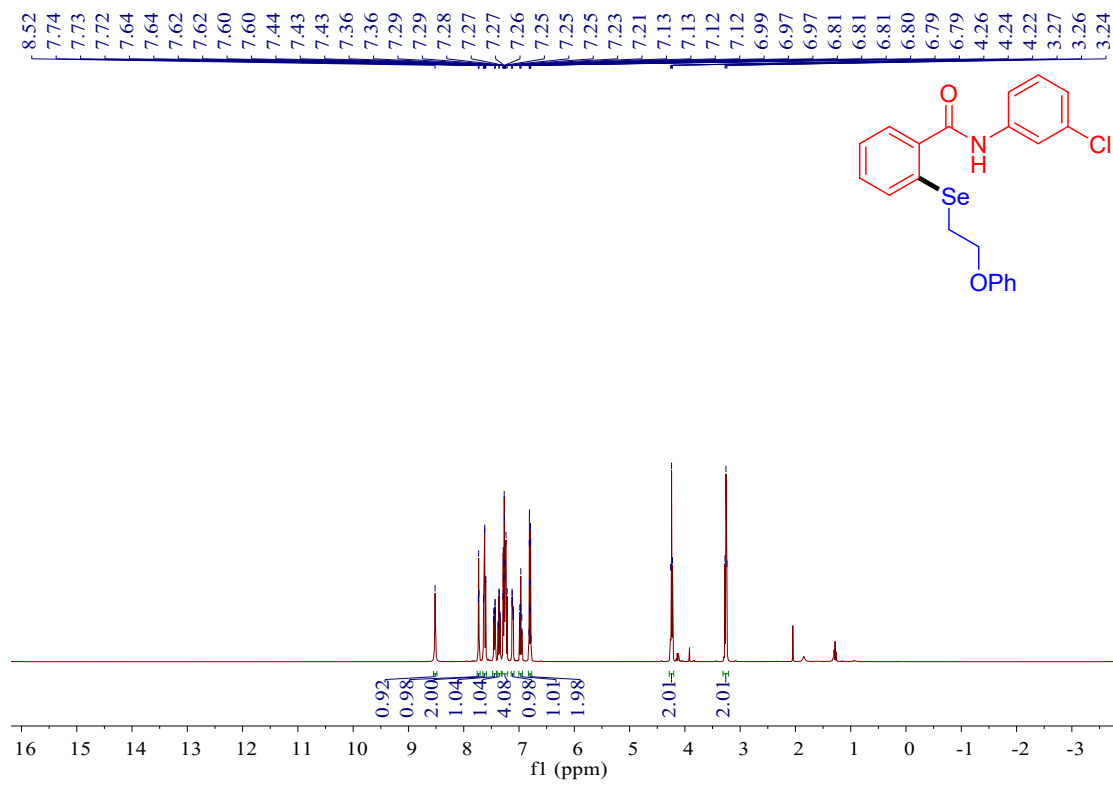
<sup>13</sup>C NMR Spectra of **3h** (400 MHz, CDCl<sub>3</sub>)



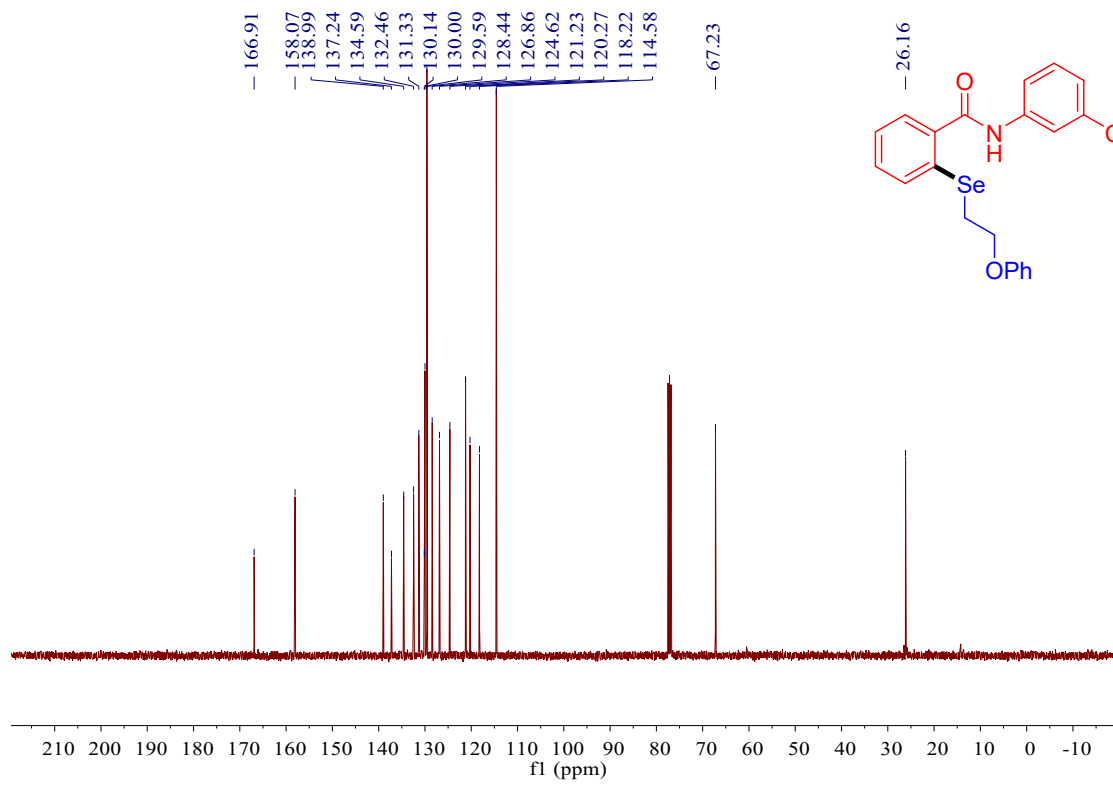
<sup>77</sup>Se NMR Spectra of **3h** (400 MHz, CDCl<sub>3</sub>)



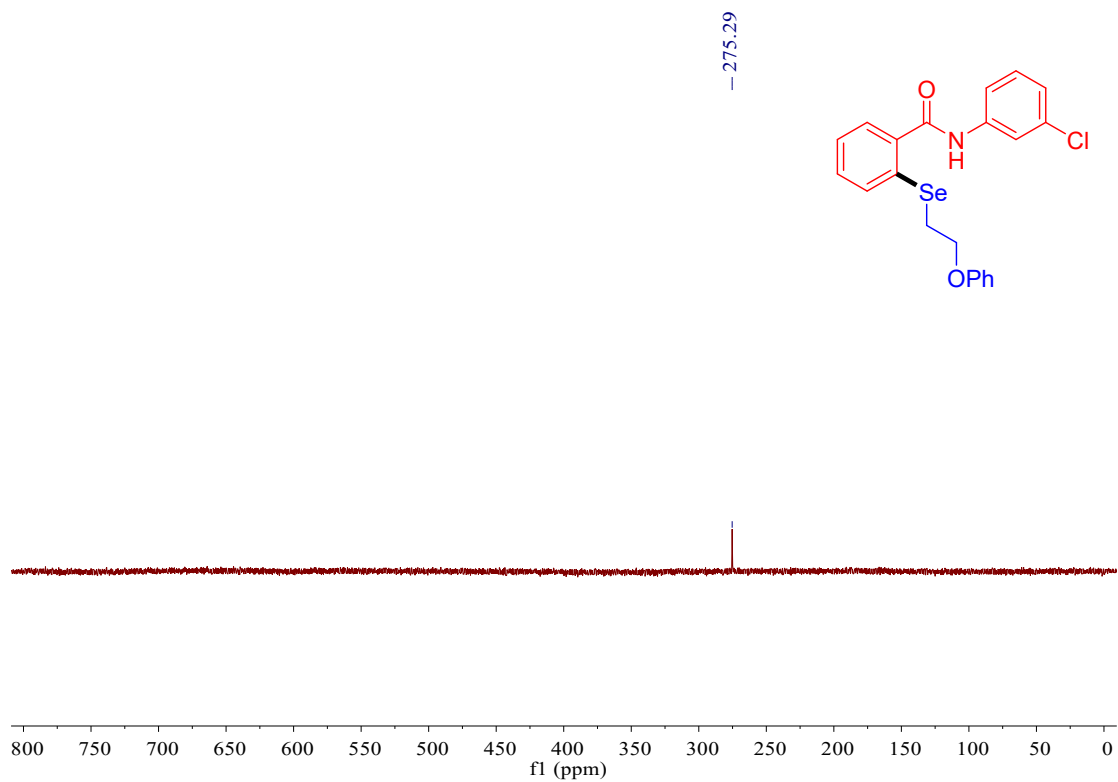
<sup>1</sup>H NMR Spectra of **3i** (400 MHz, CDCl<sub>3</sub>)



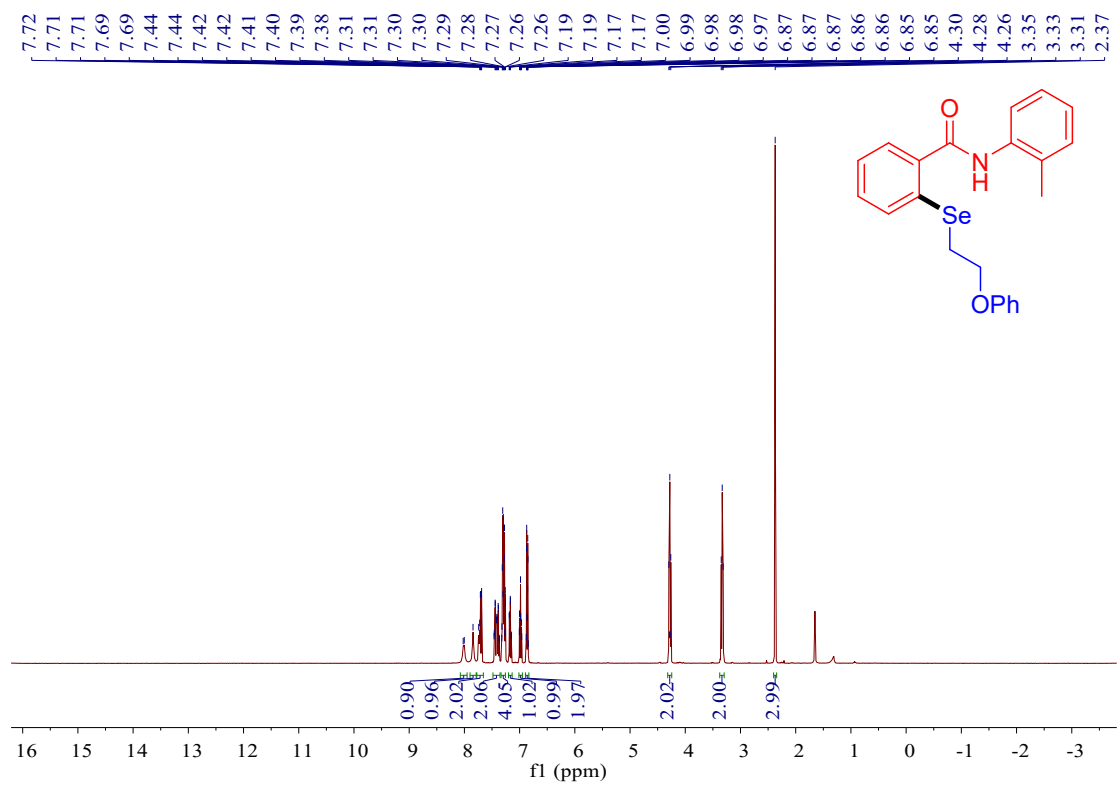
<sup>13</sup>C NMR Spectra of 3i (400 MHz, CDCl<sub>3</sub>)



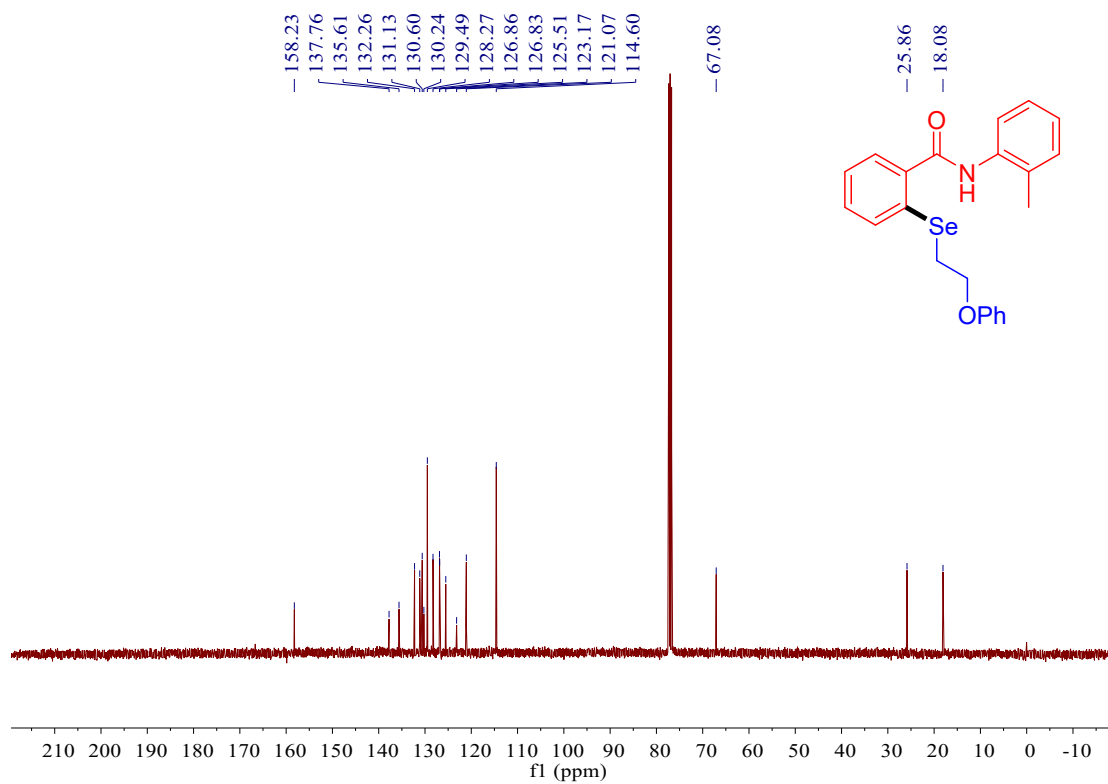
<sup>77</sup>Se NMR Spectra of 3i (400 MHz, CDCl<sub>3</sub>)



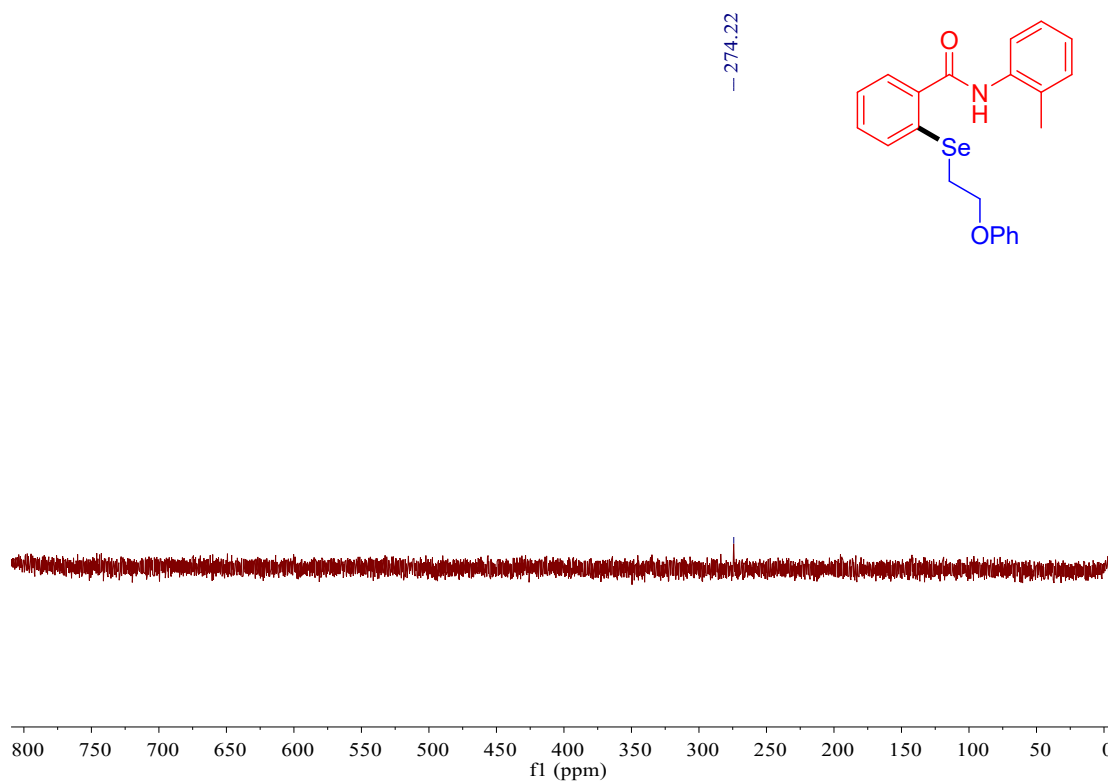
<sup>1</sup>H NMR Spectra of **3j** (400 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR Spectra of **3j** (400 MHz, CDCl<sub>3</sub>)

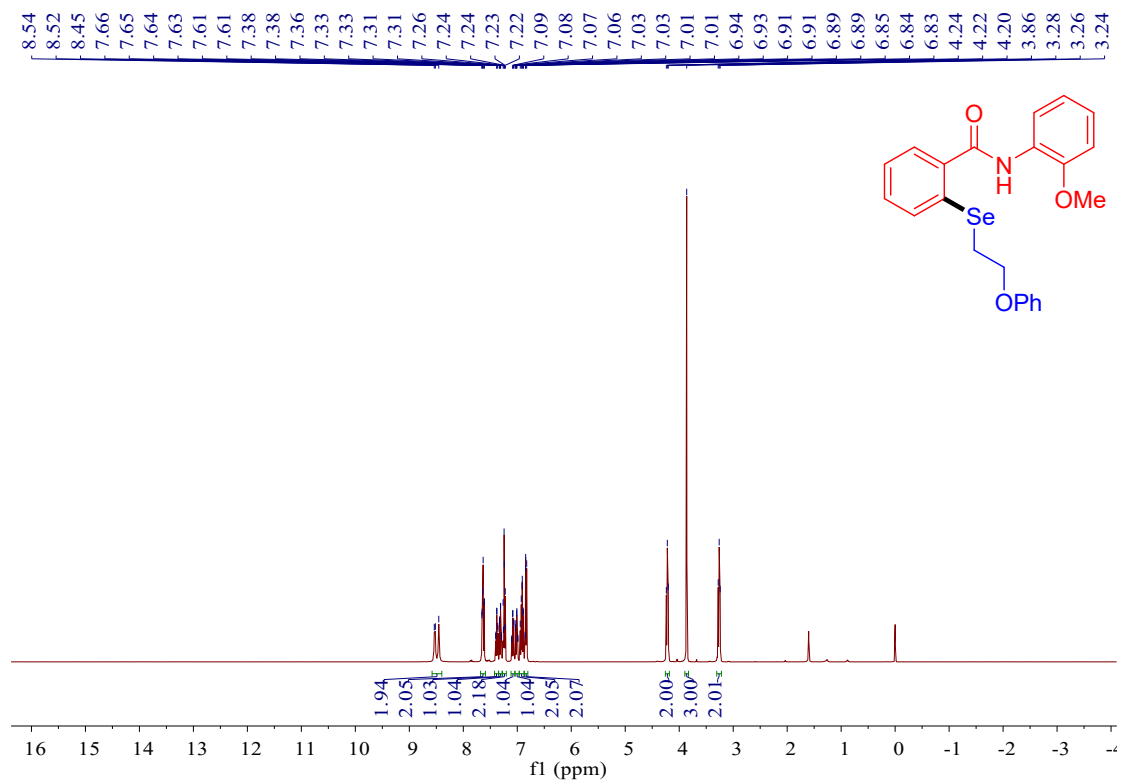


$^{77}\text{Se}$  NMR Spectra of **3j** (400 MHz,  $\text{CDCl}_3$ )

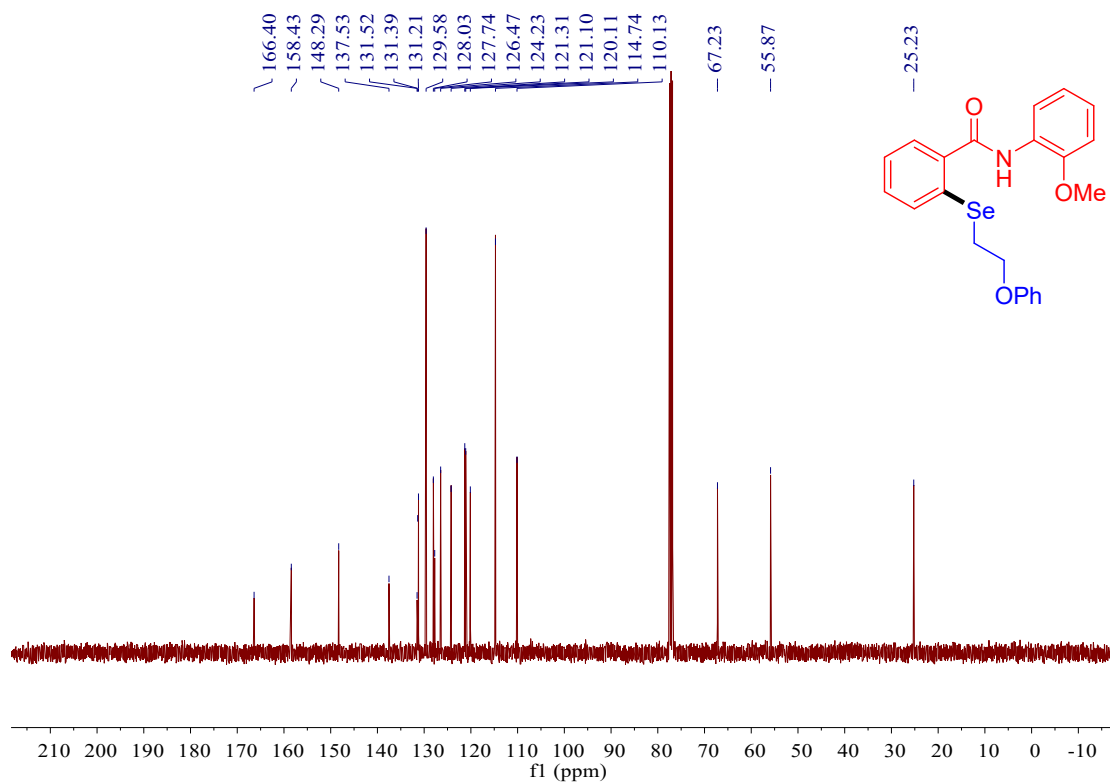


$^1\text{H}$  NMR Spectra of **3k** (400 MHz,  $\text{CDCl}_3$ )

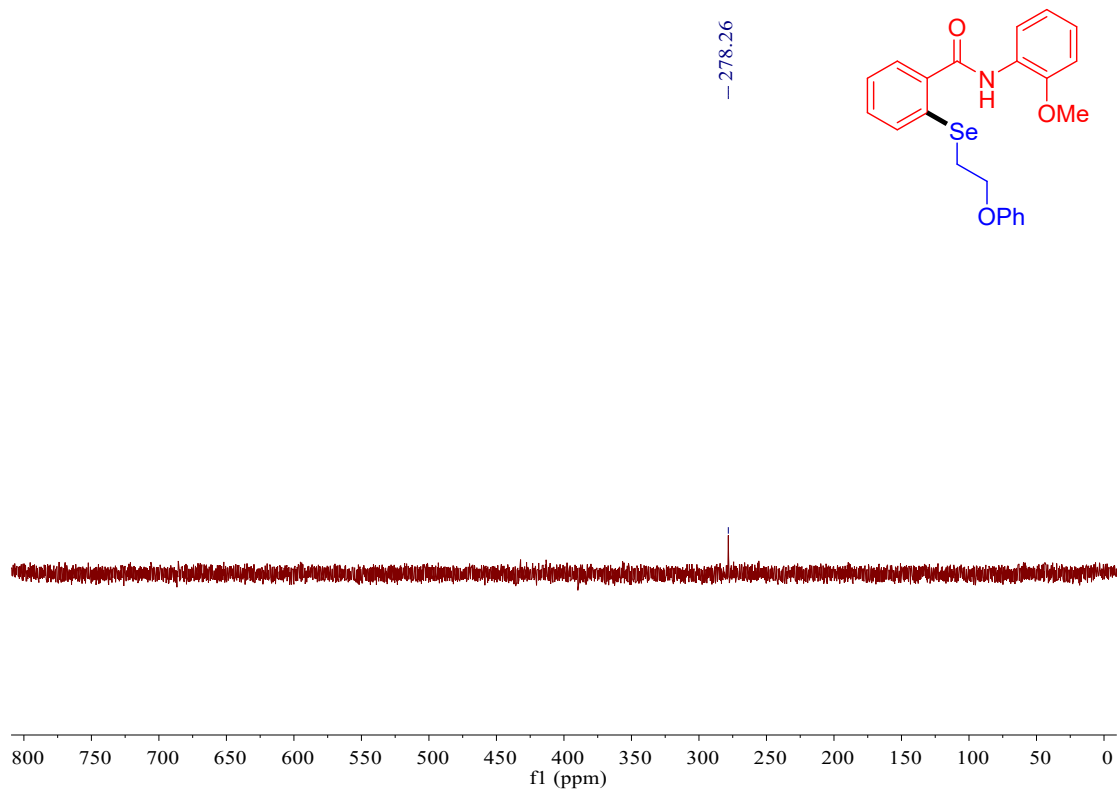




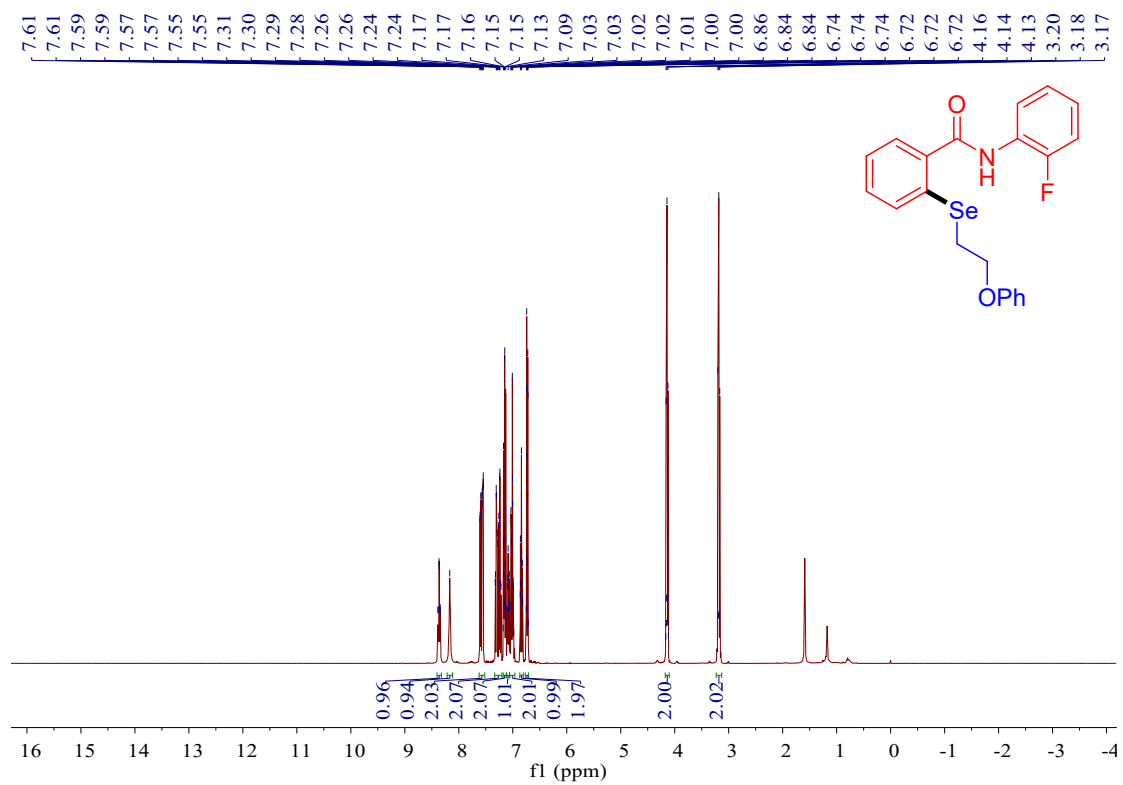
<sup>13</sup>C NMR Spectra of 3k (400 MHz, CDCl<sub>3</sub>)



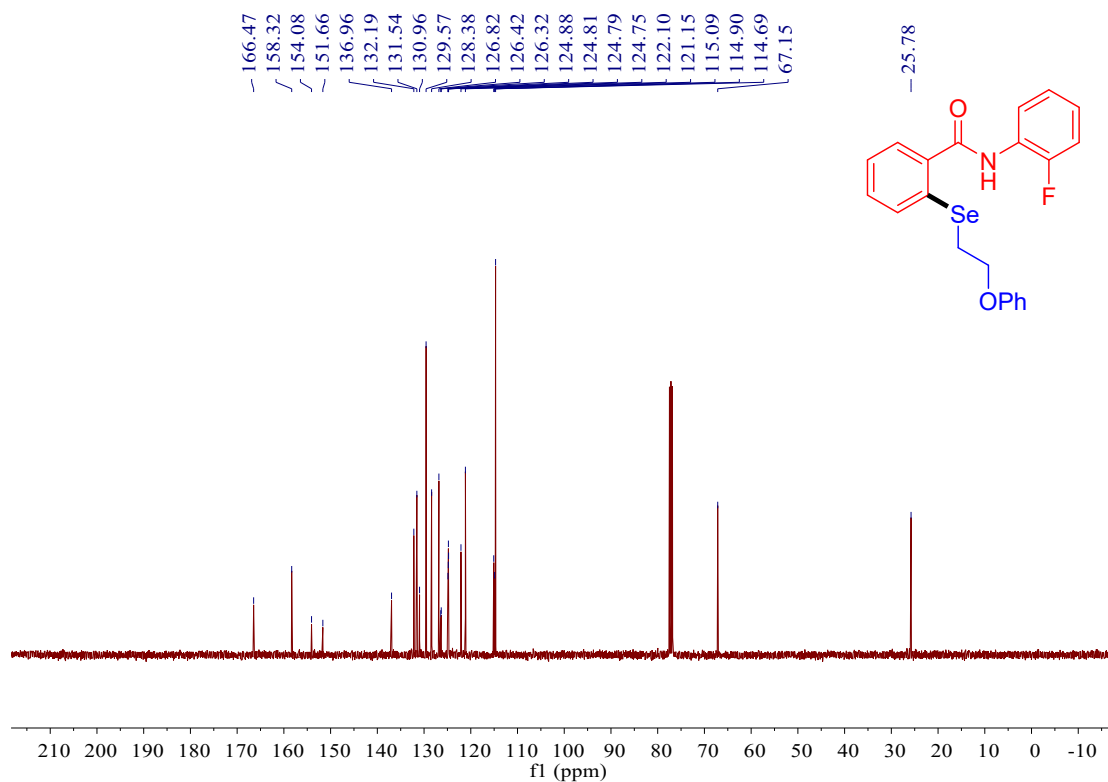
<sup>77</sup>Se NMR Spectra of 3k (400 MHz, CDCl<sub>3</sub>)



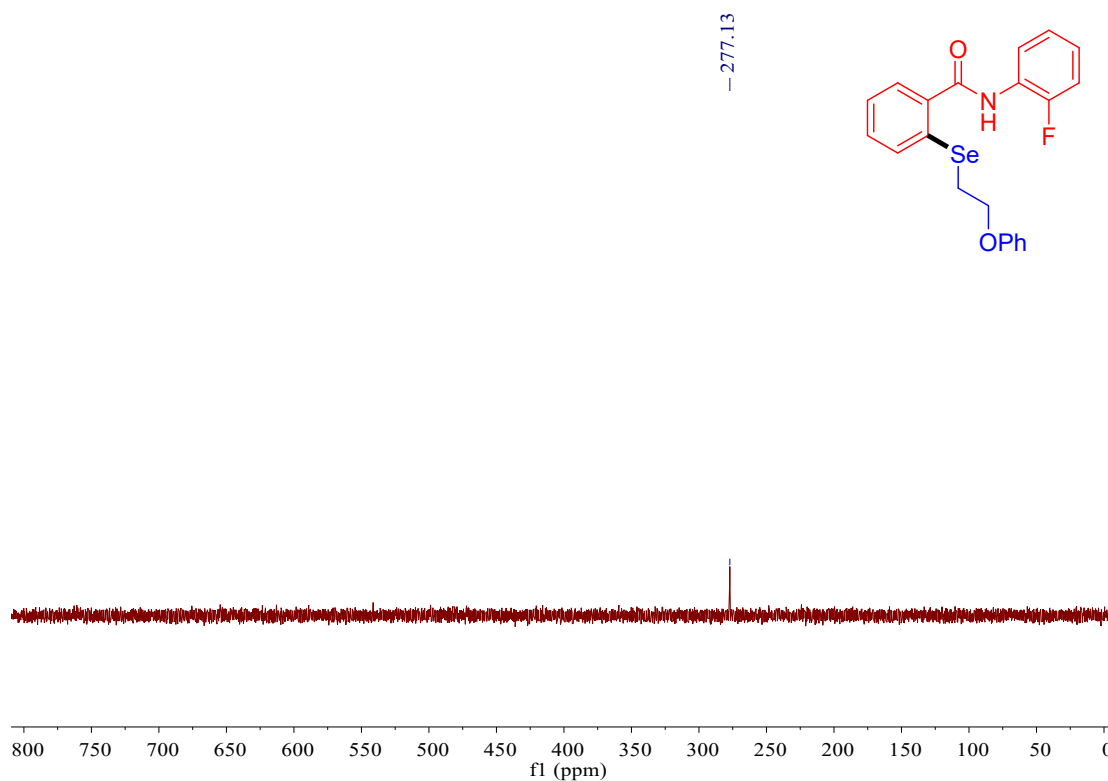
<sup>1</sup>H NMR Spectra of **31** (400 MHz, CDCl<sub>3</sub>)



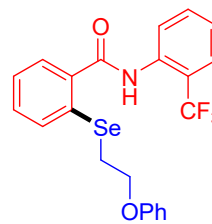
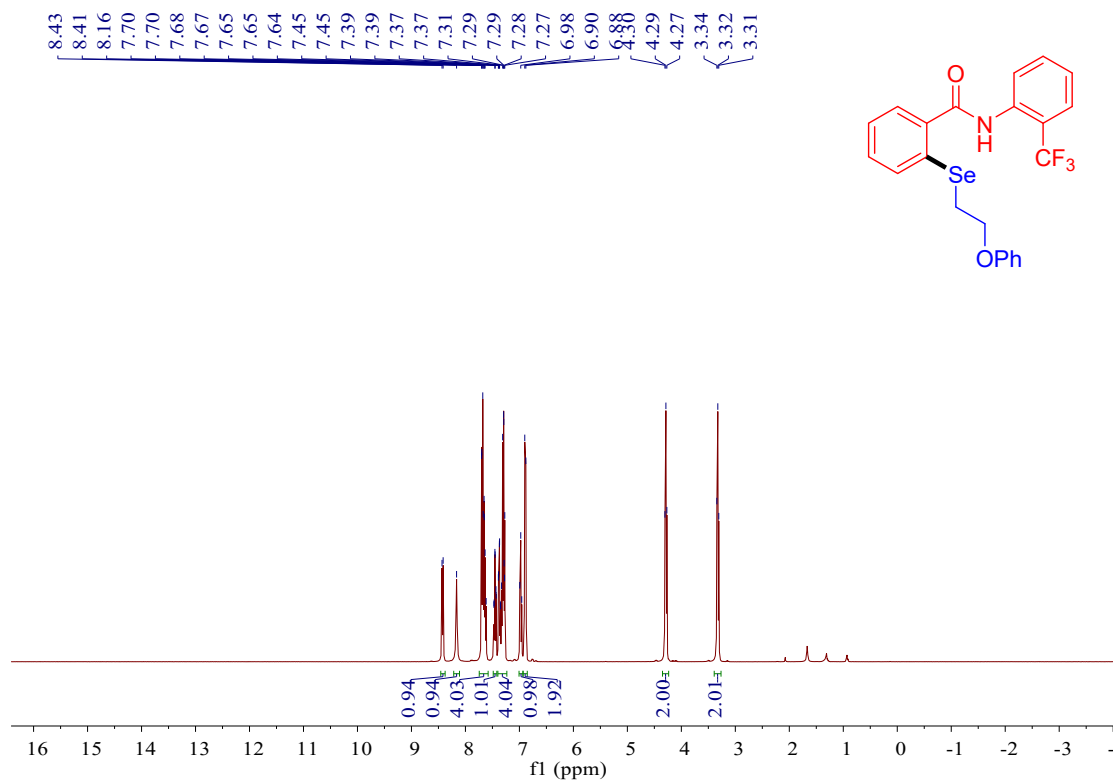
<sup>13</sup>C NMR Spectra of **31** (400 MHz, CDCl<sub>3</sub>)



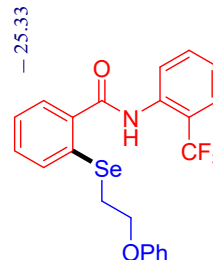
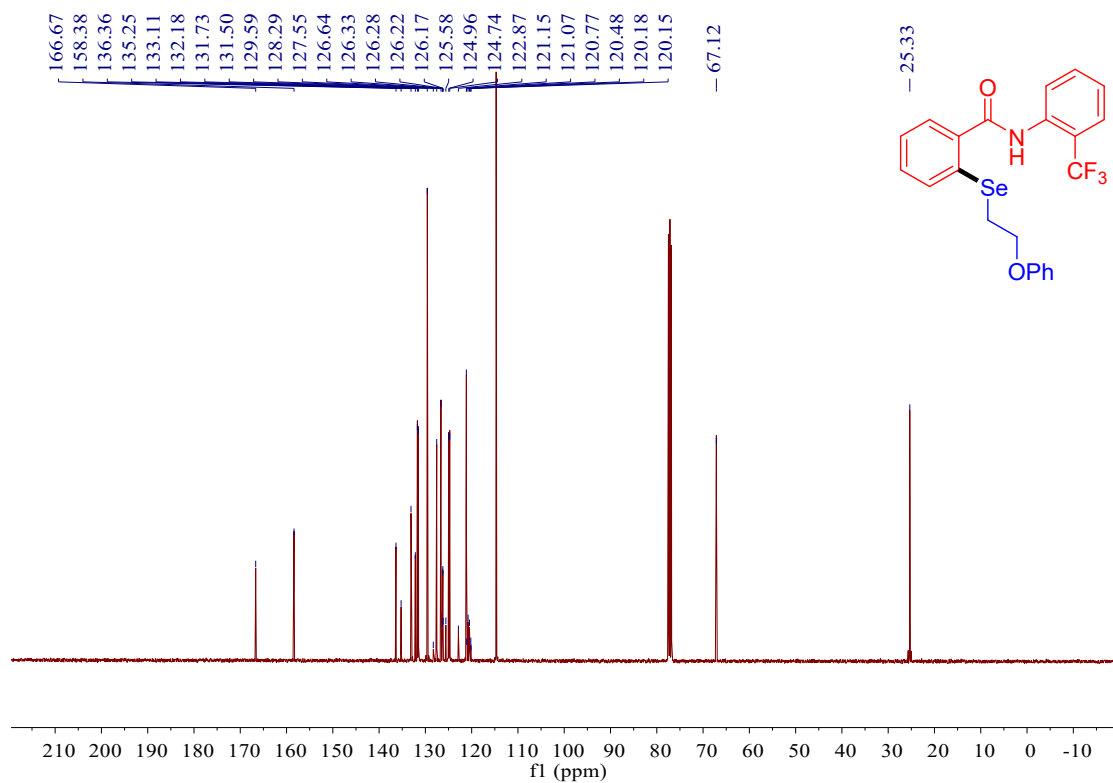
$^{77}\text{Se}$  NMR Spectra of **3l** (400 MHz,  $\text{CDCl}_3$ )



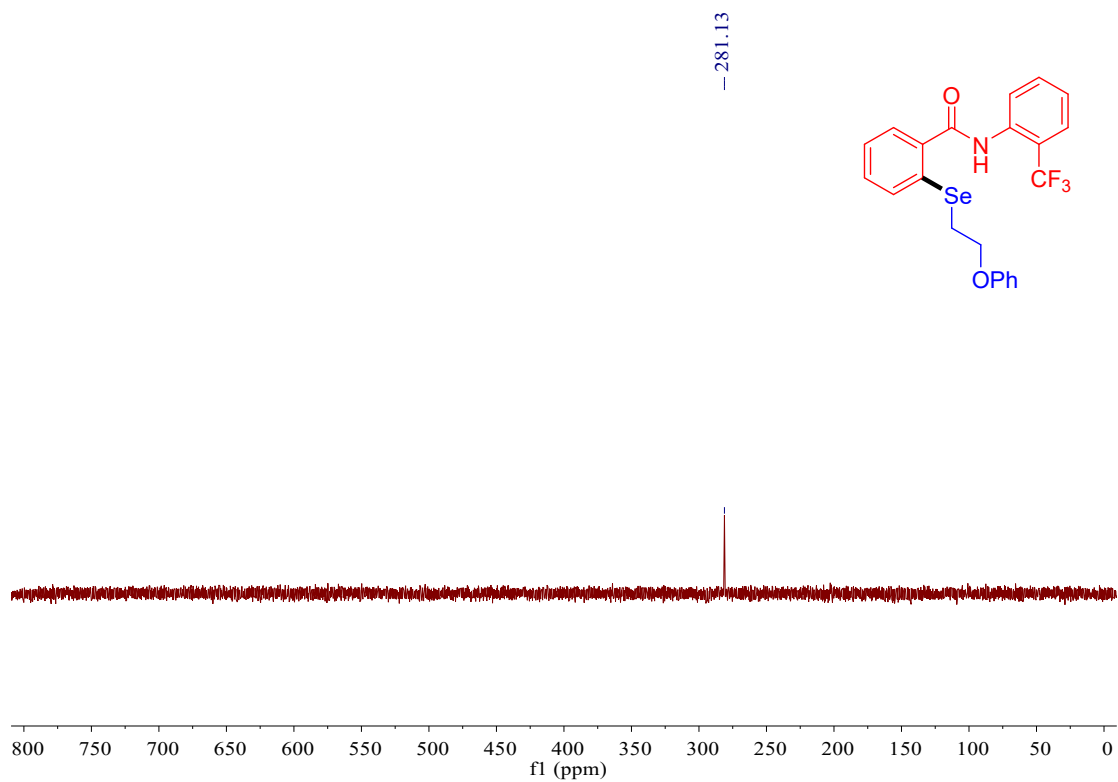
$^1\text{H}$  NMR Spectra of **3m** (400 MHz,  $\text{CDCl}_3$ )



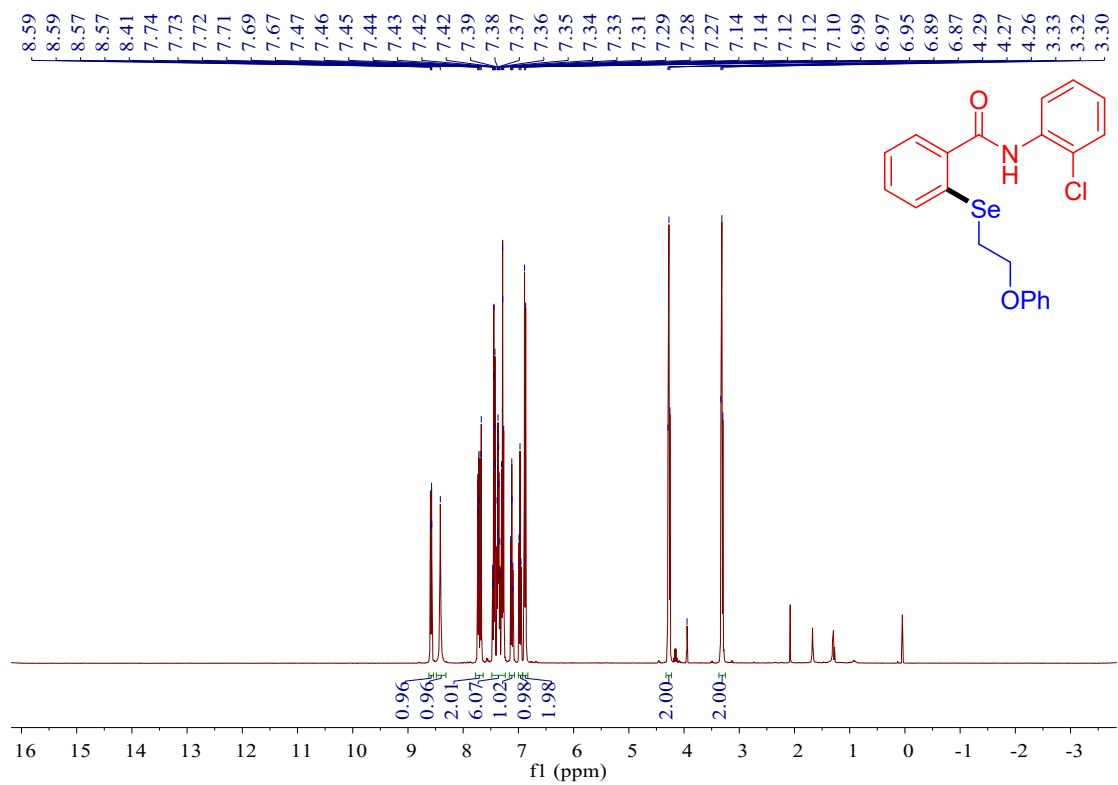
**<sup>13</sup>C NMR Spectra of 3m (400 MHz, CDCl<sub>3</sub>)**



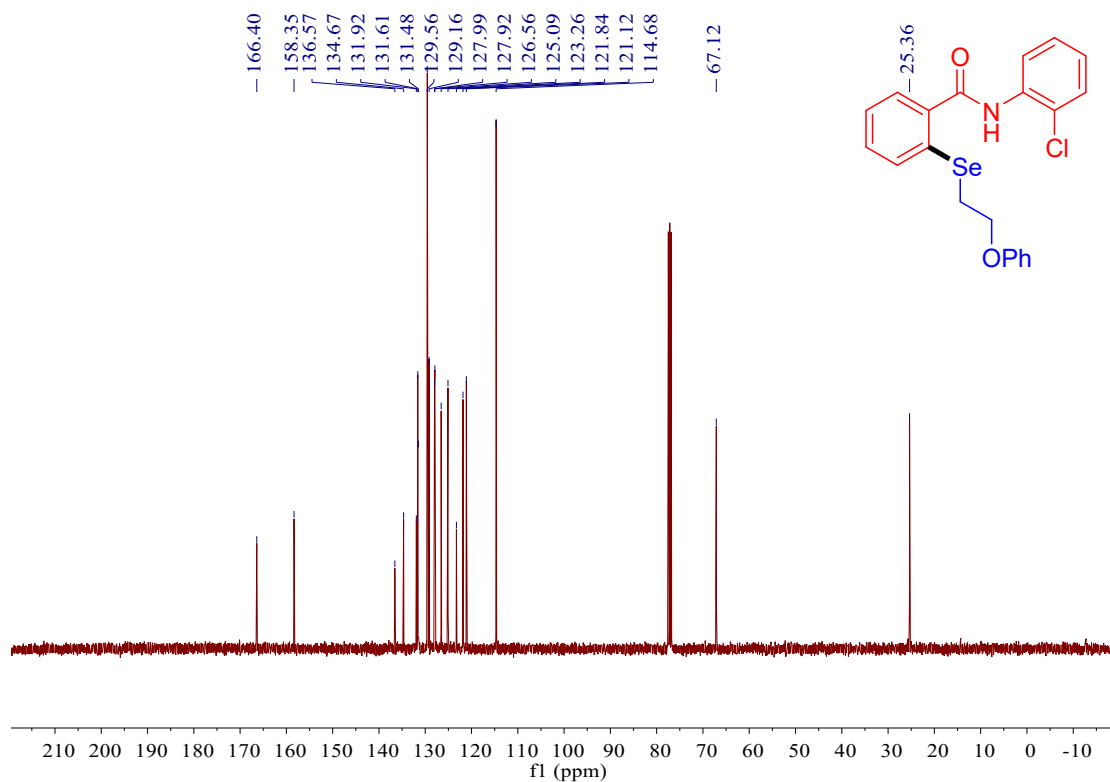
**<sup>77</sup>Se NMR Spectra of 3m (400 MHz, CDCl<sub>3</sub>)**



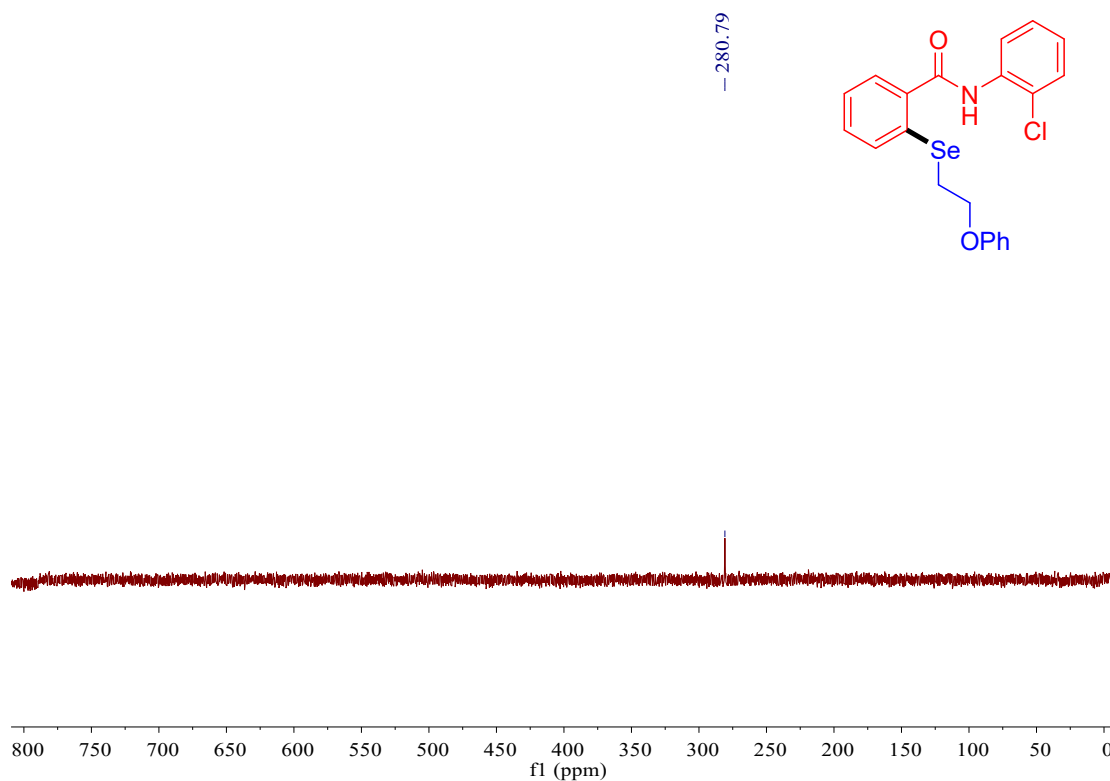
$^1\text{H}$  NMR Spectra of **3n** (400 MHz,  $\text{CDCl}_3$ )



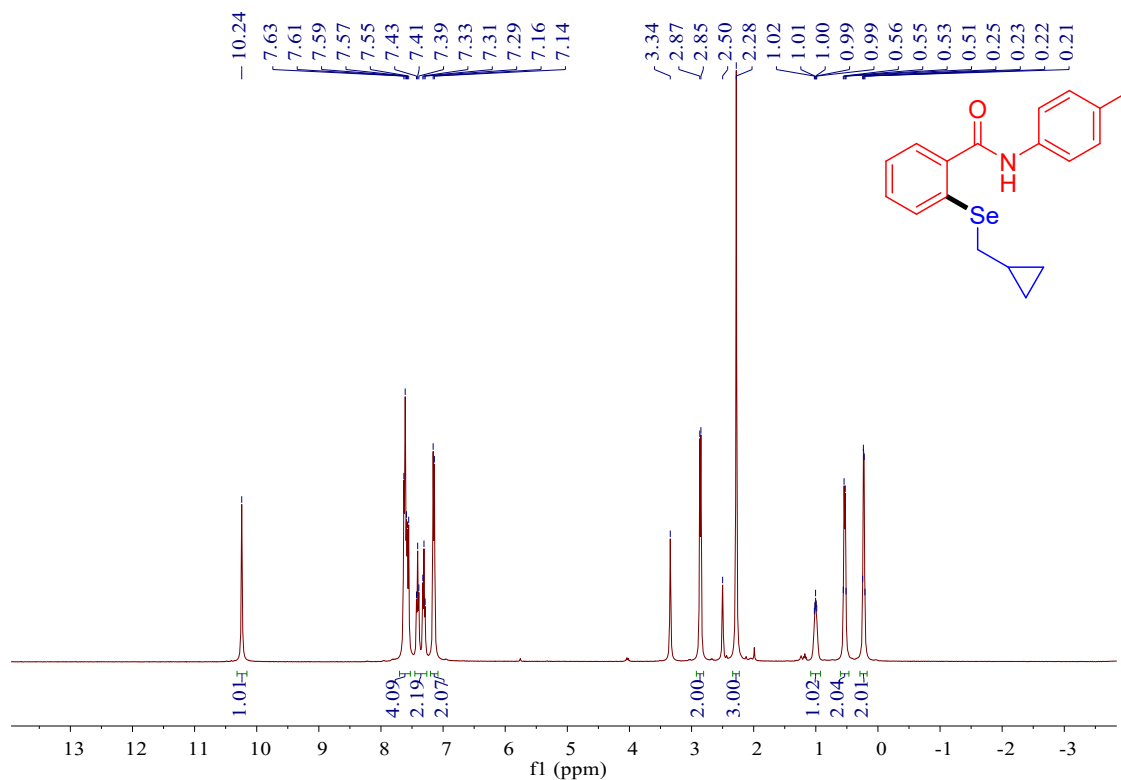
$^{13}\text{C}$  NMR Spectra of **3n** (400 MHz,  $\text{CDCl}_3$ )



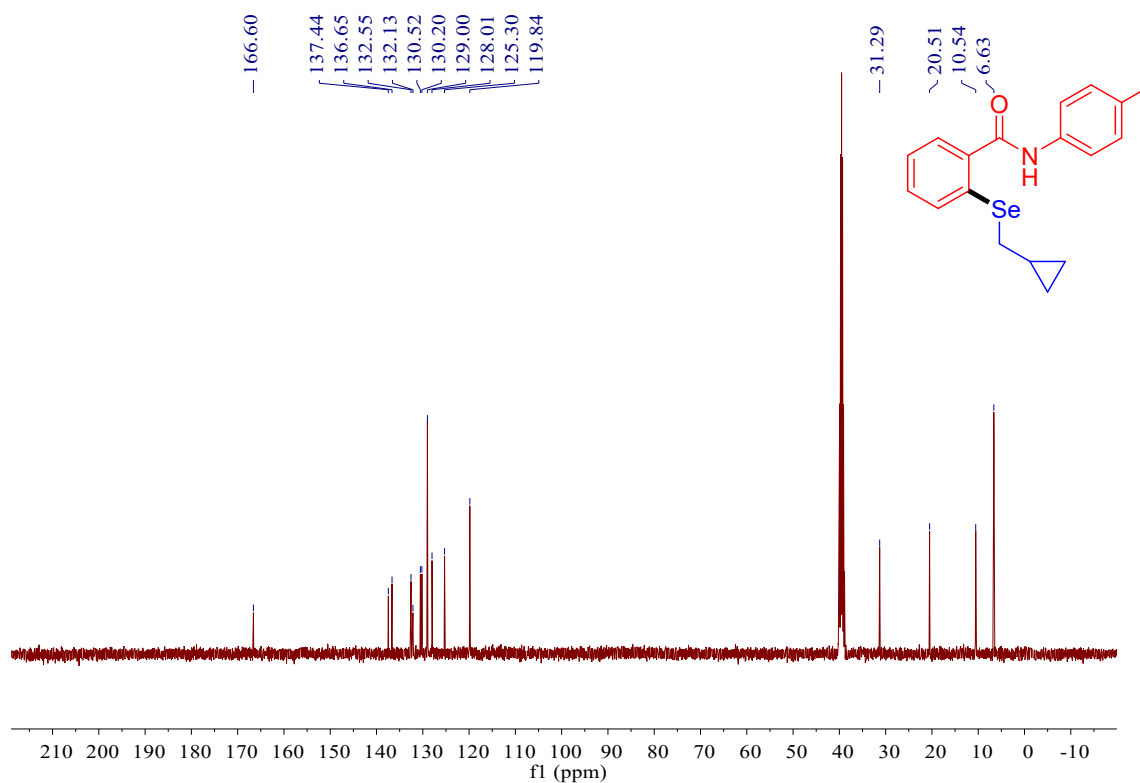
$^{77}\text{Se}$  NMR Spectra of **3n** (400 MHz,  $\text{CDCl}_3$ )



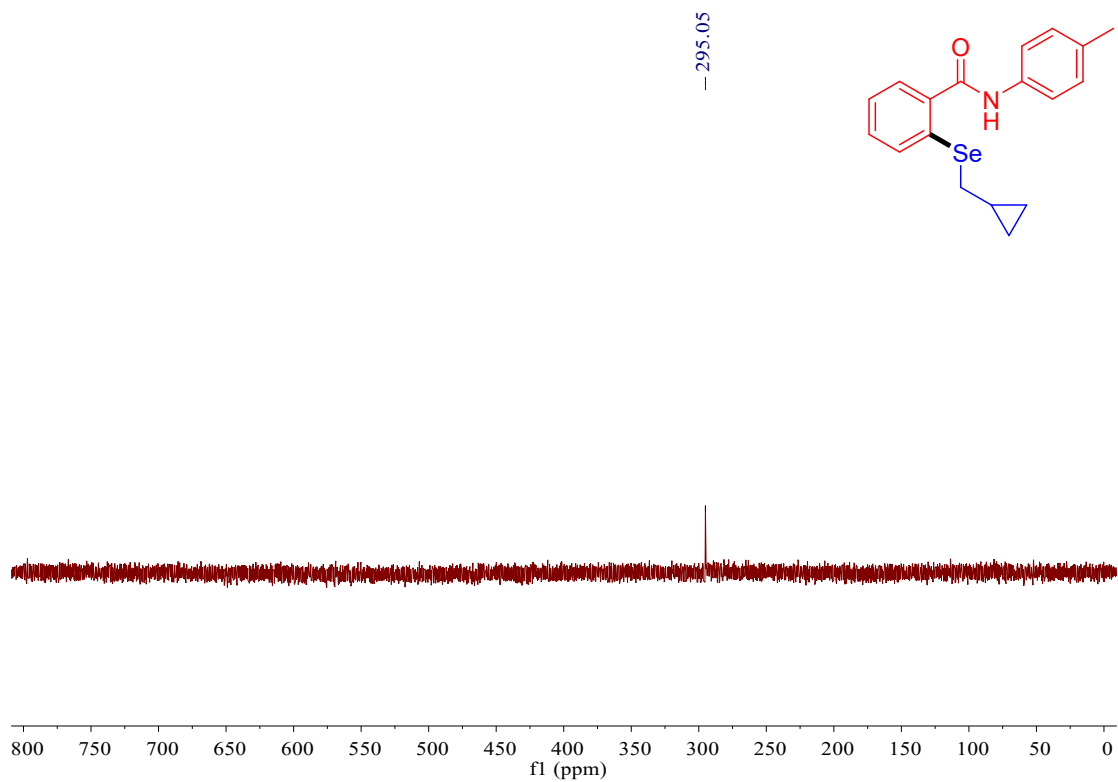
$^1\text{H}$  NMR Spectra of **3q** (400 MHz,  $\text{DMSO}-d_6$ )



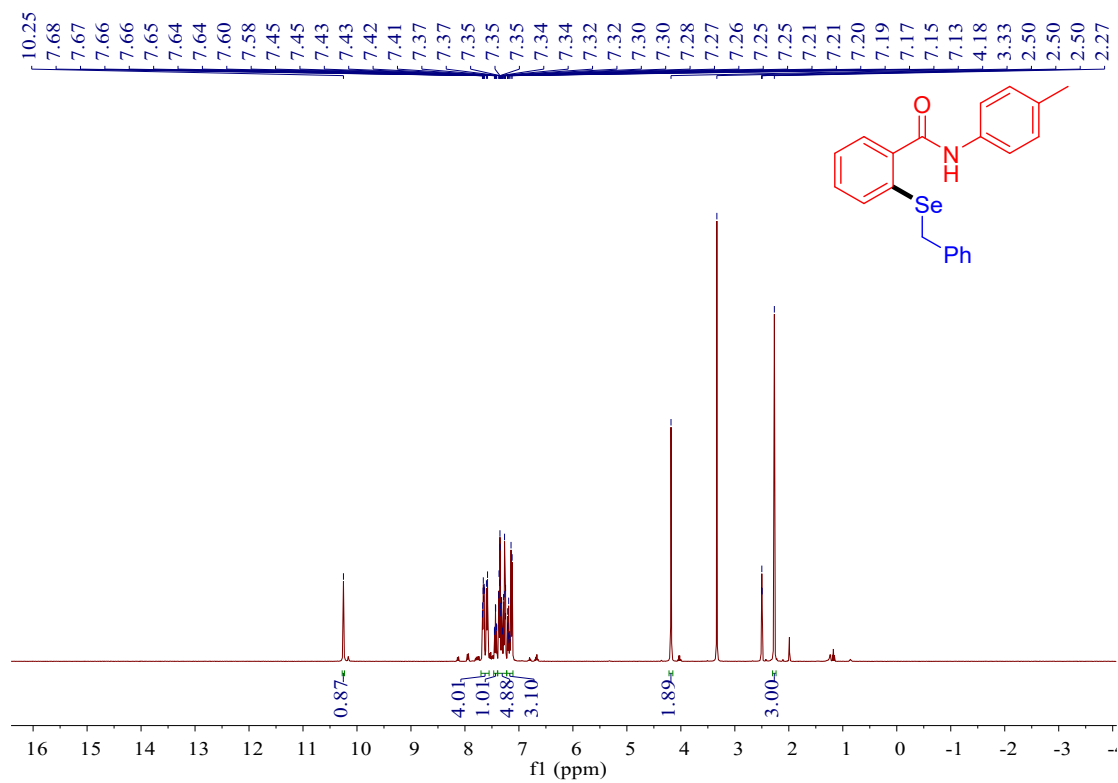
$^{13}\text{C}$  NMR Spectra of **3q** (400 MHz,  $\text{DMSO-}d_6$ )



$^{77}\text{Se}$  NMR Spectra of **3q** (400 MHz,  $\text{DMSO-}d_6$ )

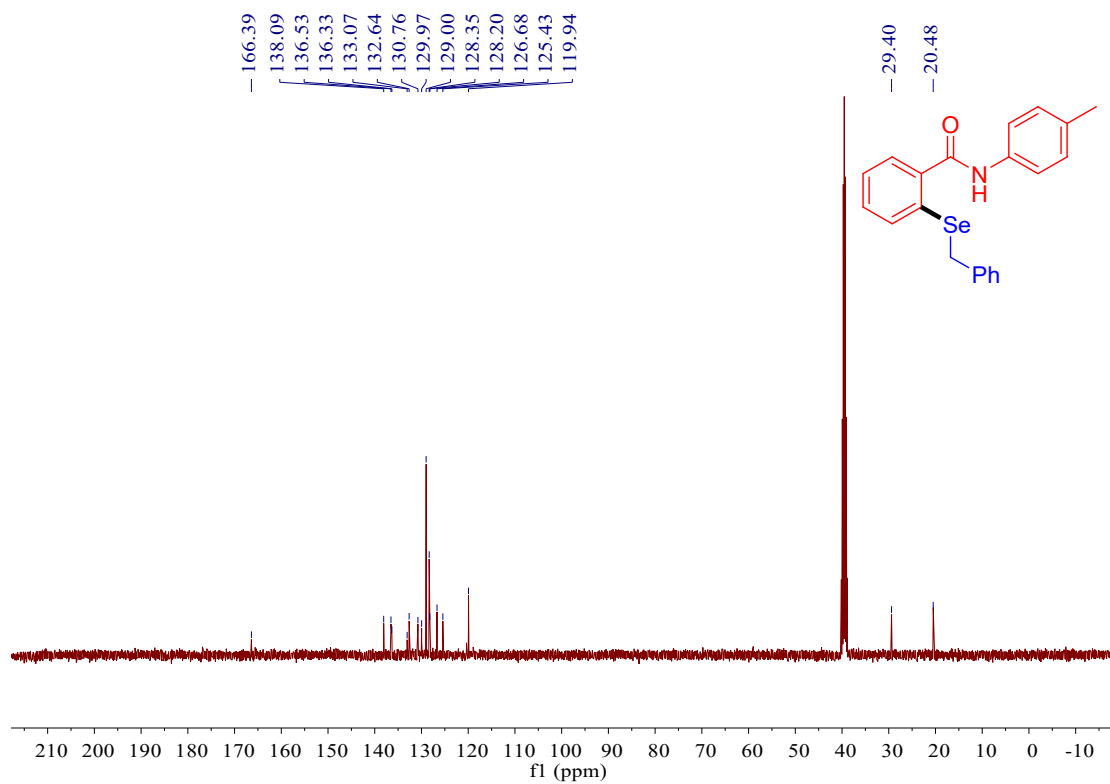


$^1\text{H}$  NMR Spectra of **3r** (400 MHz,  $\text{DMSO-}d_6$ )

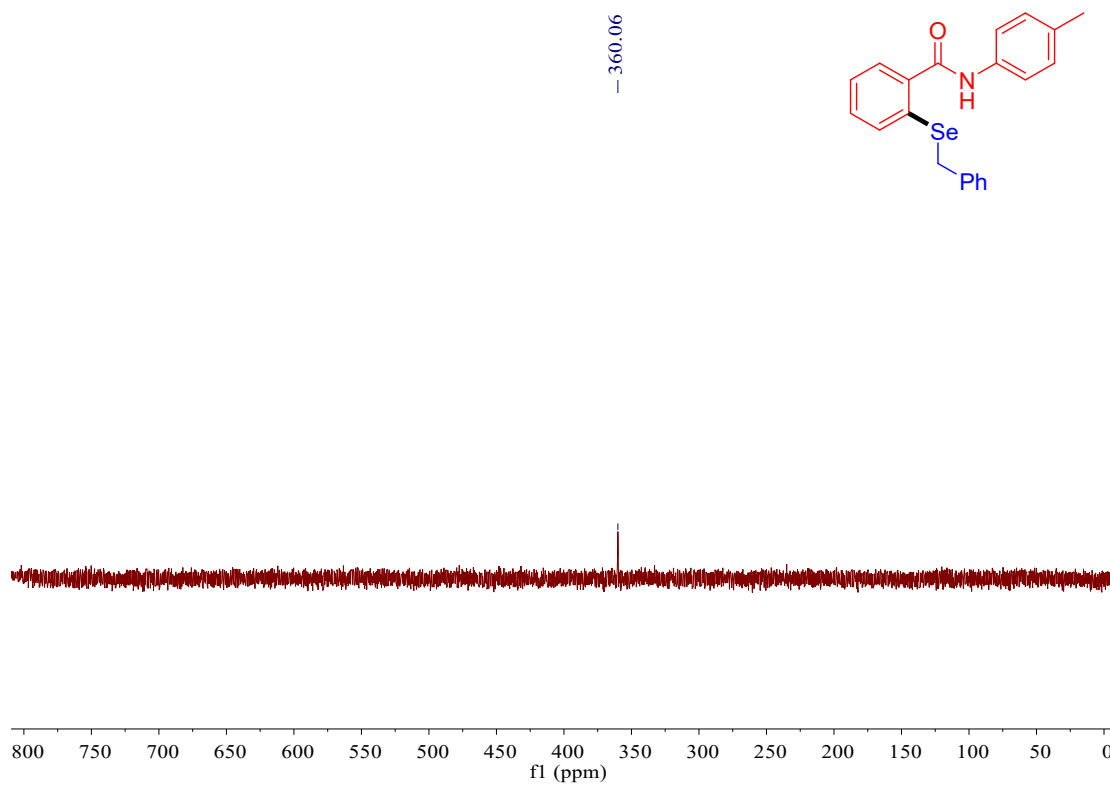


$^{13}\text{C}$  NMR Spectra of **3r** (400 MHz,  $\text{DMSO-}d_6$ )

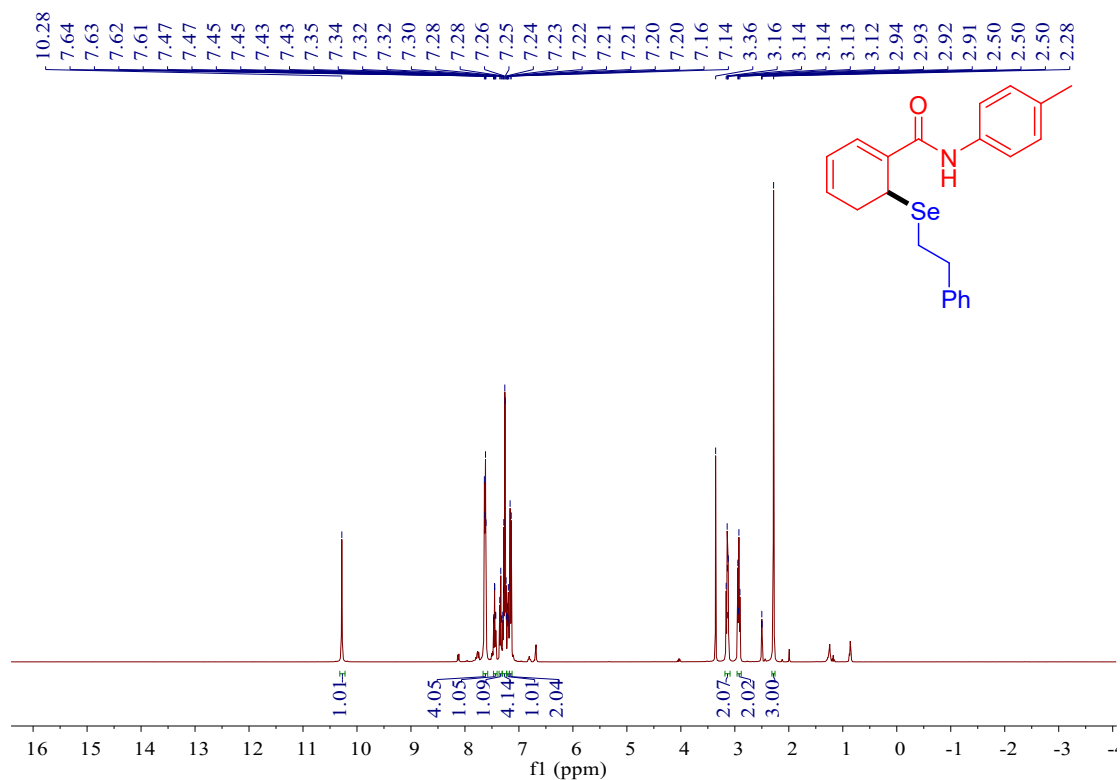




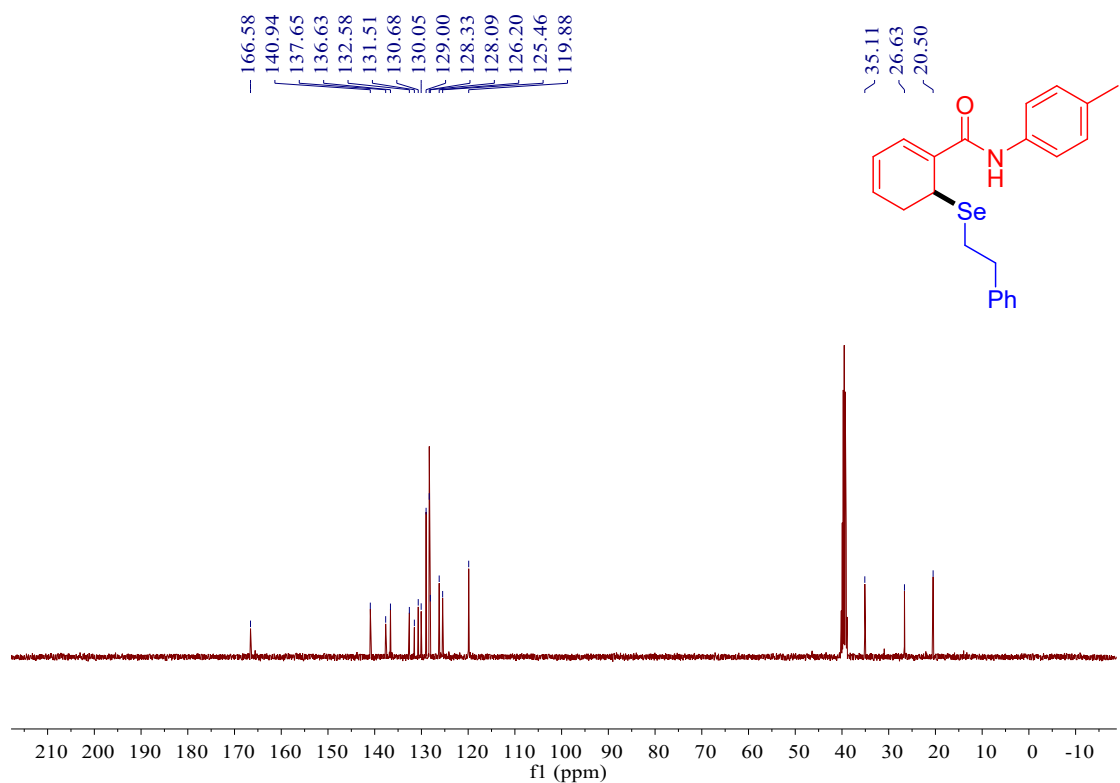
$^{77}\text{Se}$  NMR Spectra of **3r** (400 MHz,  $\text{DMSO-}d_6$ )



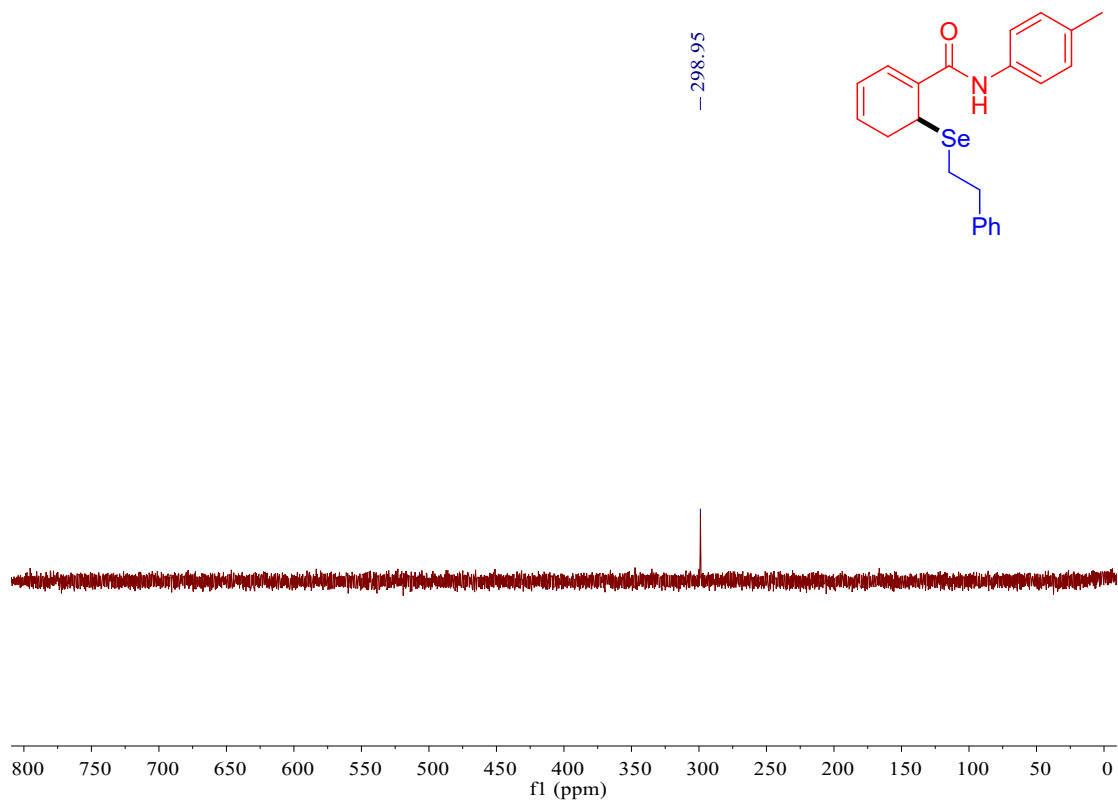
$^1\text{H}$  NMR Spectra of **3s** (400 MHz,  $\text{DMSO-}d_6$ )



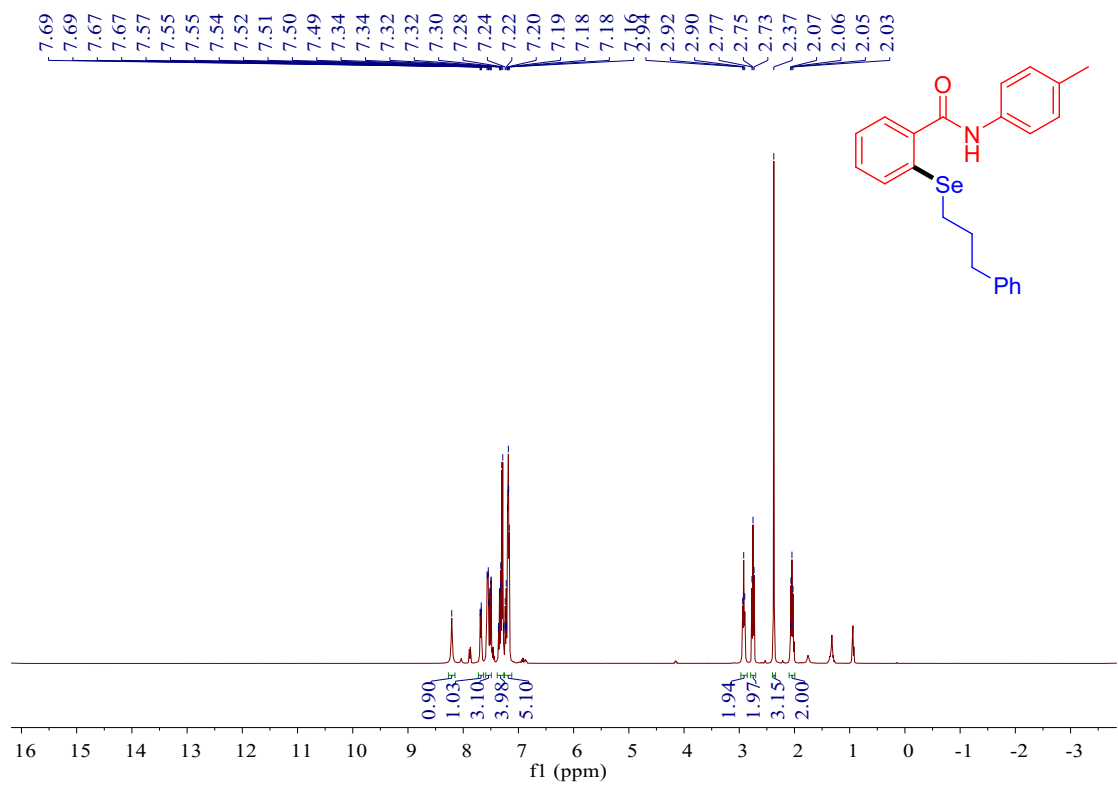
$^{13}\text{C}$  NMR Spectra of **3s** (400 MHz,  $\text{DMSO-}d_6$ )



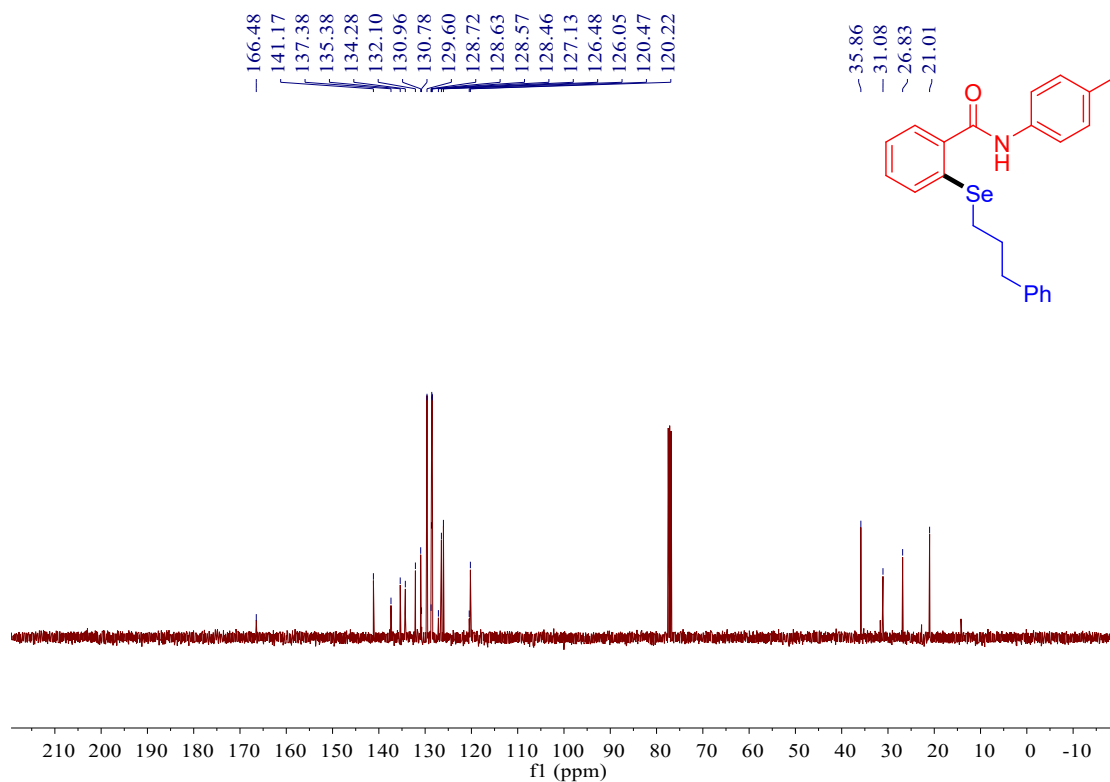
$^{77}\text{Se}$  NMR Spectra of **3s** (400 MHz,  $\text{DMSO-}d_6$ )



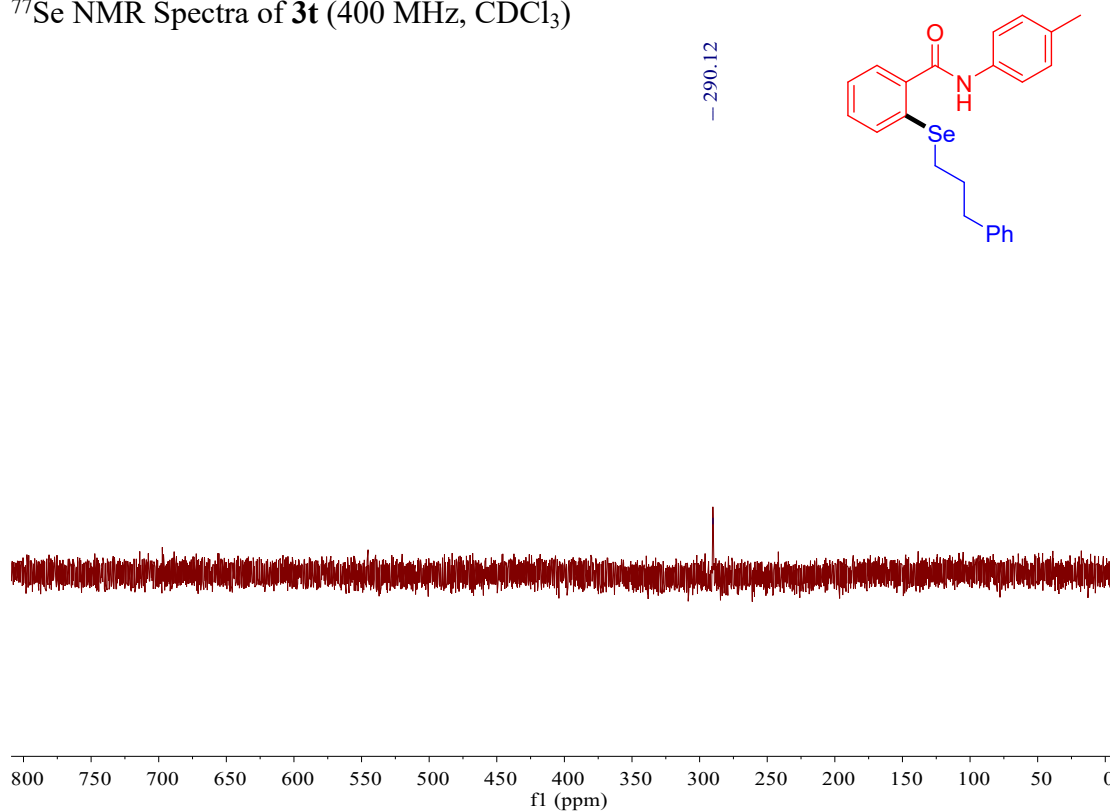
$^1\text{H}$  NMR Spectra of **3t** (400 MHz,  $\text{CDCl}_3$ )



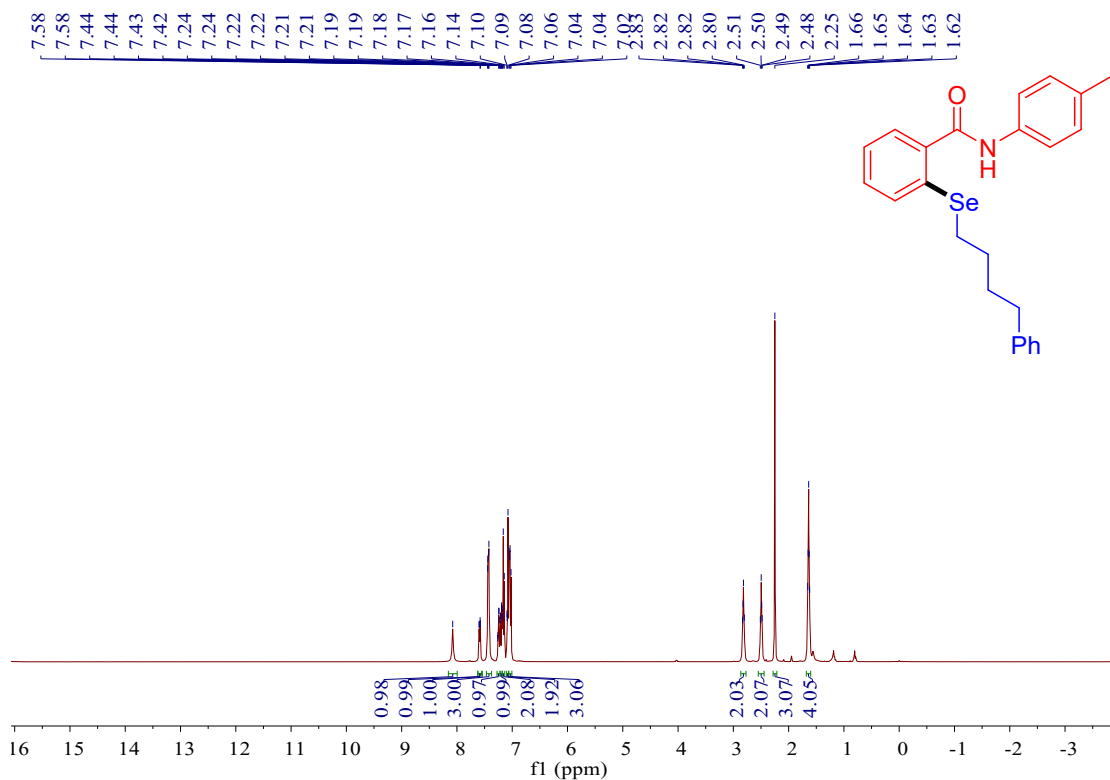
$^{13}\text{C}$  NMR Spectra of **3t** (400 MHz,  $\text{CDCl}_3$ )



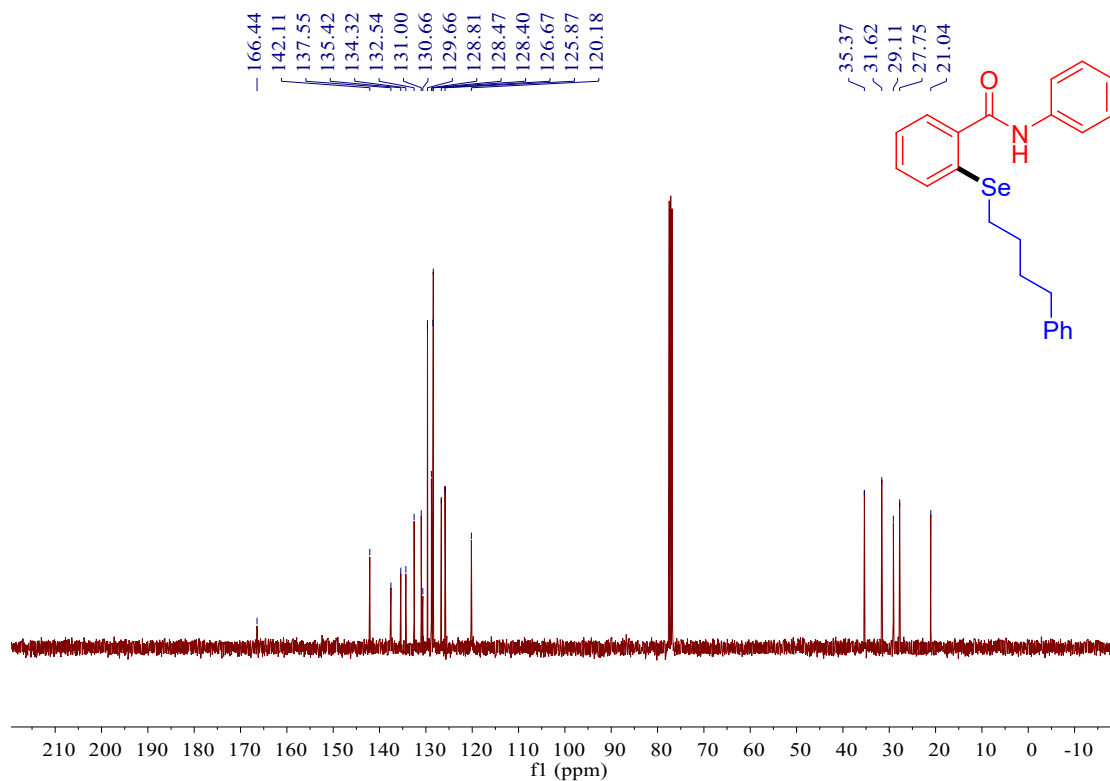
<sup>77</sup>Se NMR Spectra of **3t** (400 MHz, CDCl<sub>3</sub>)



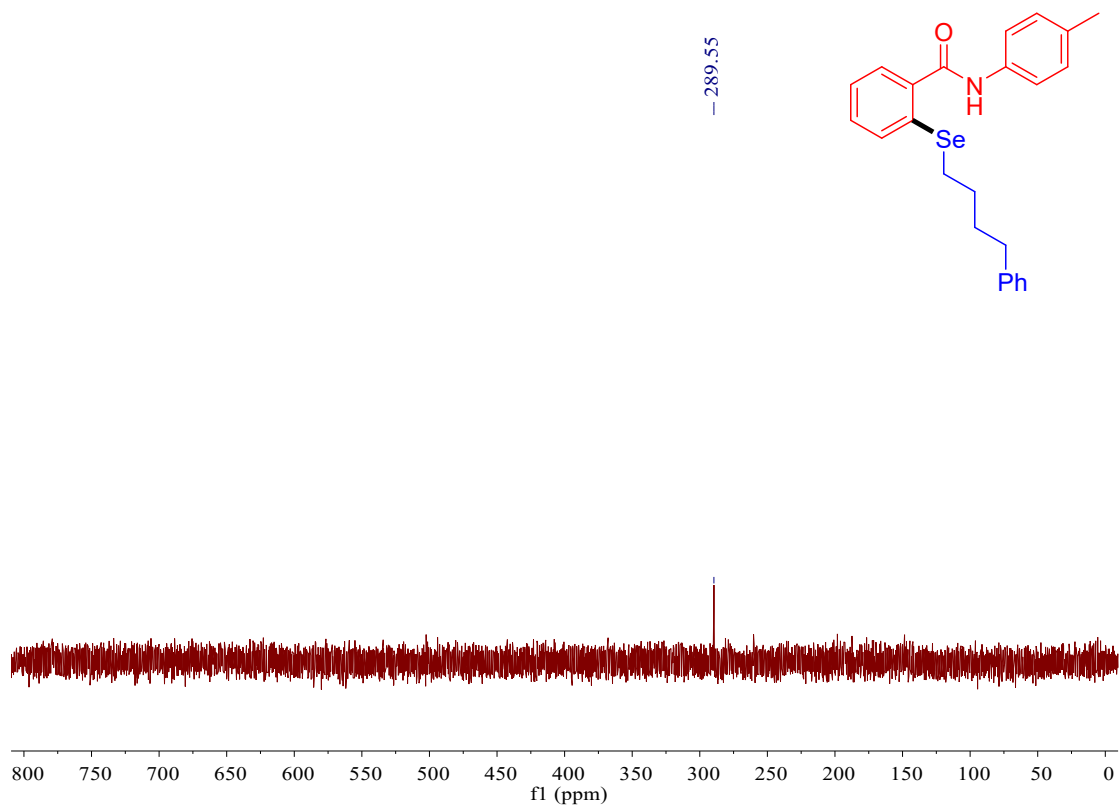
<sup>1</sup>H NMR Spectra of **3u** (400 MHz, CDCl<sub>3</sub>)



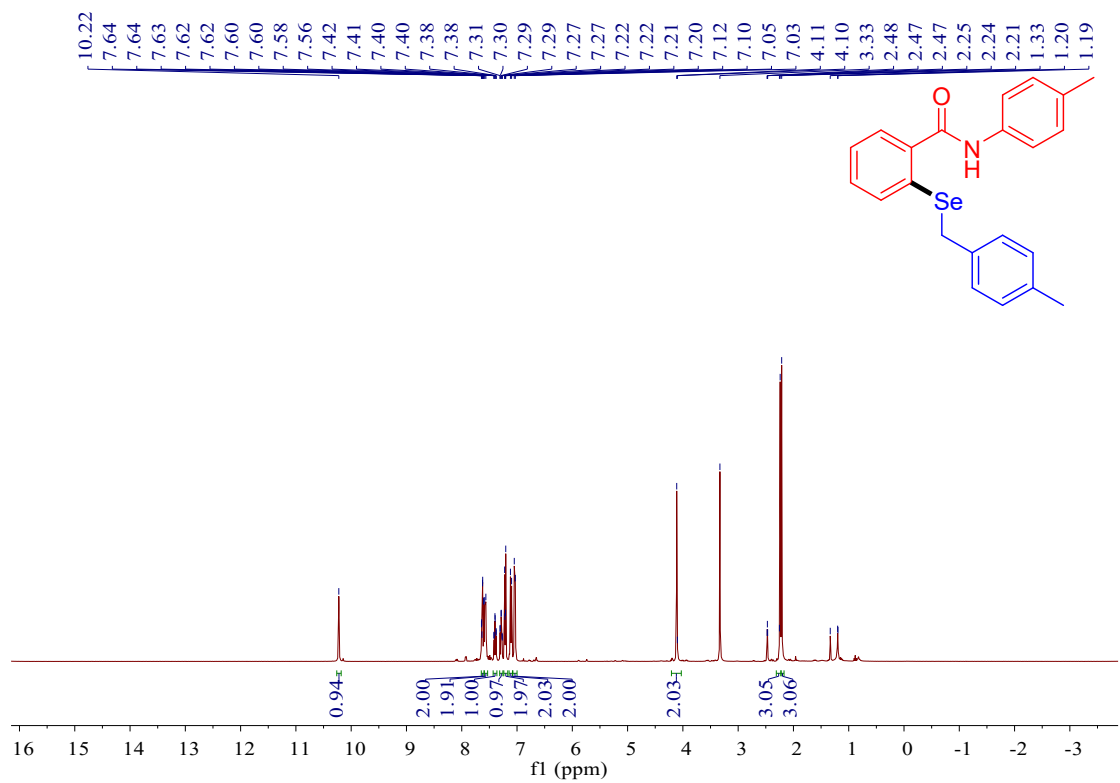
**<sup>13</sup>C NMR Spectra of **3u** (400 MHz, CDCl<sub>3</sub>)**



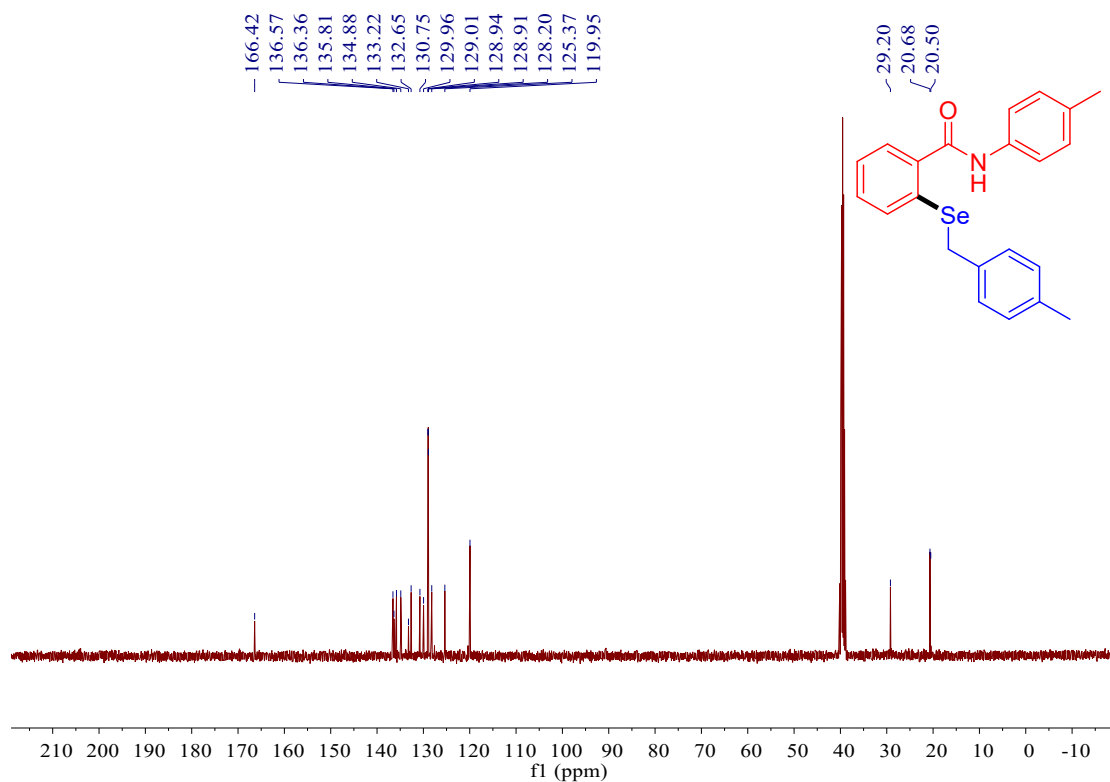
**<sup>77</sup>Se NMR Spectra of **3u** (400 MHz, CDCl<sub>3</sub>)**



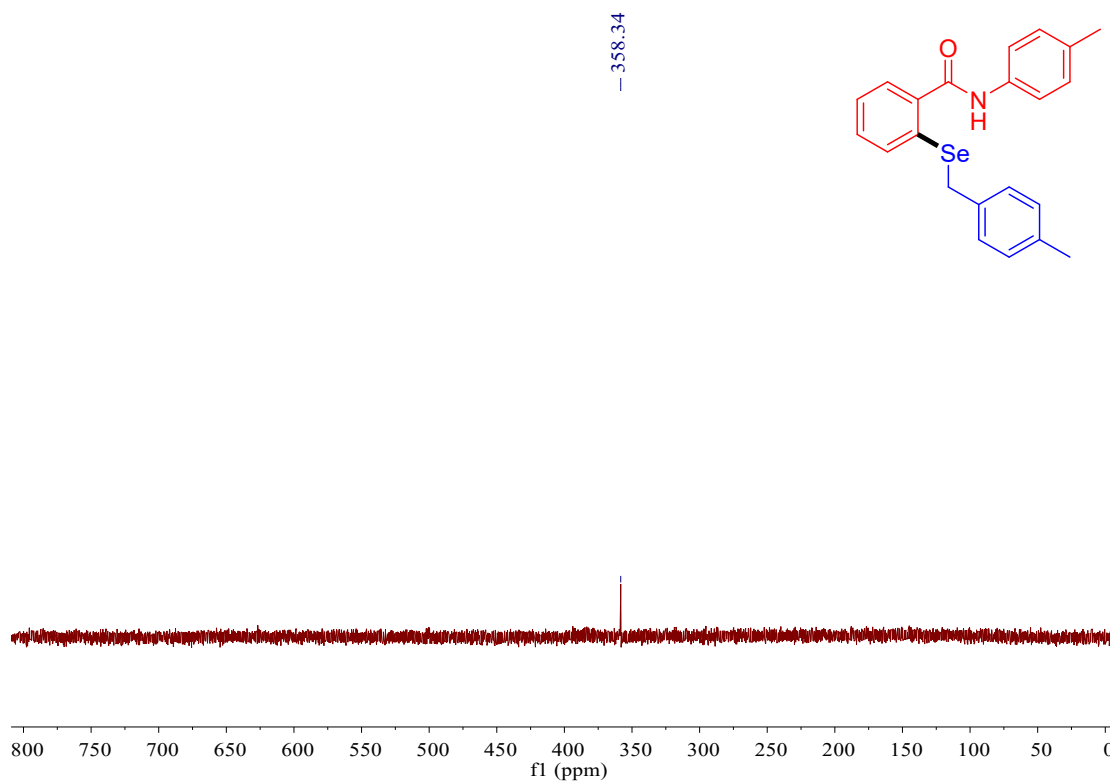
$^1\text{H}$  NMR Spectra of **3v** (400 MHz,  $\text{DMSO-}d_6$ )



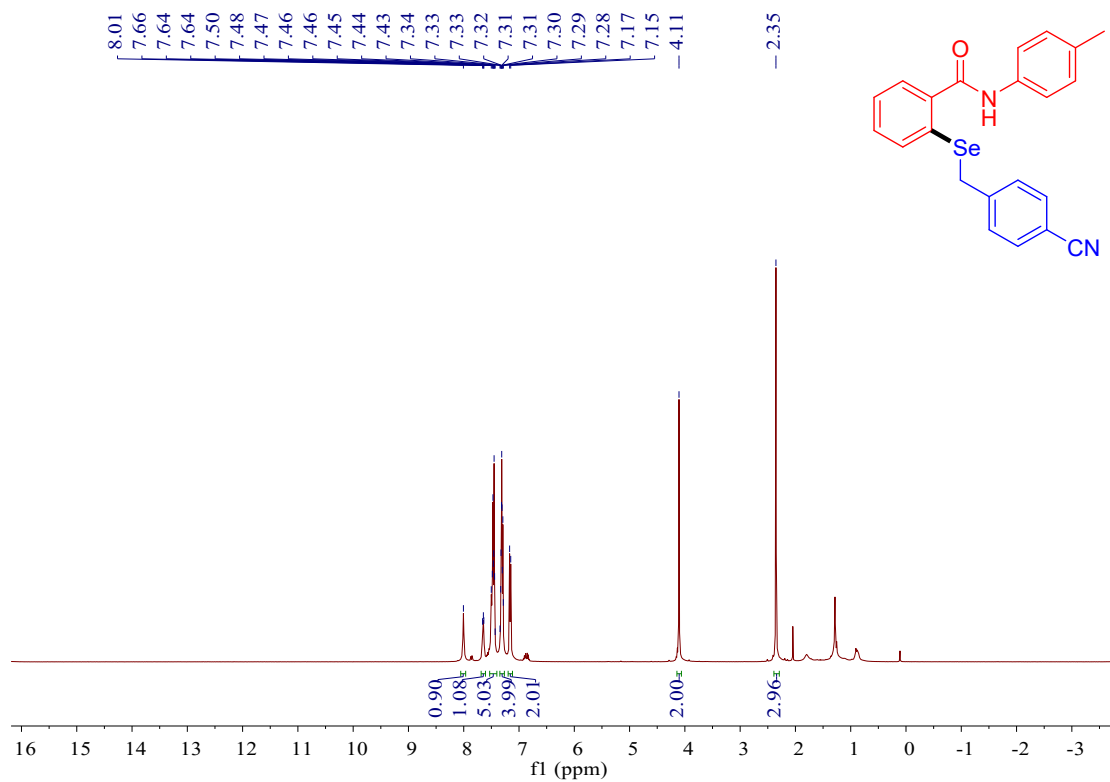
$^{13}\text{C}$  NMR Spectra of **3v** (400 MHz,  $\text{DMSO-}d_6$ )



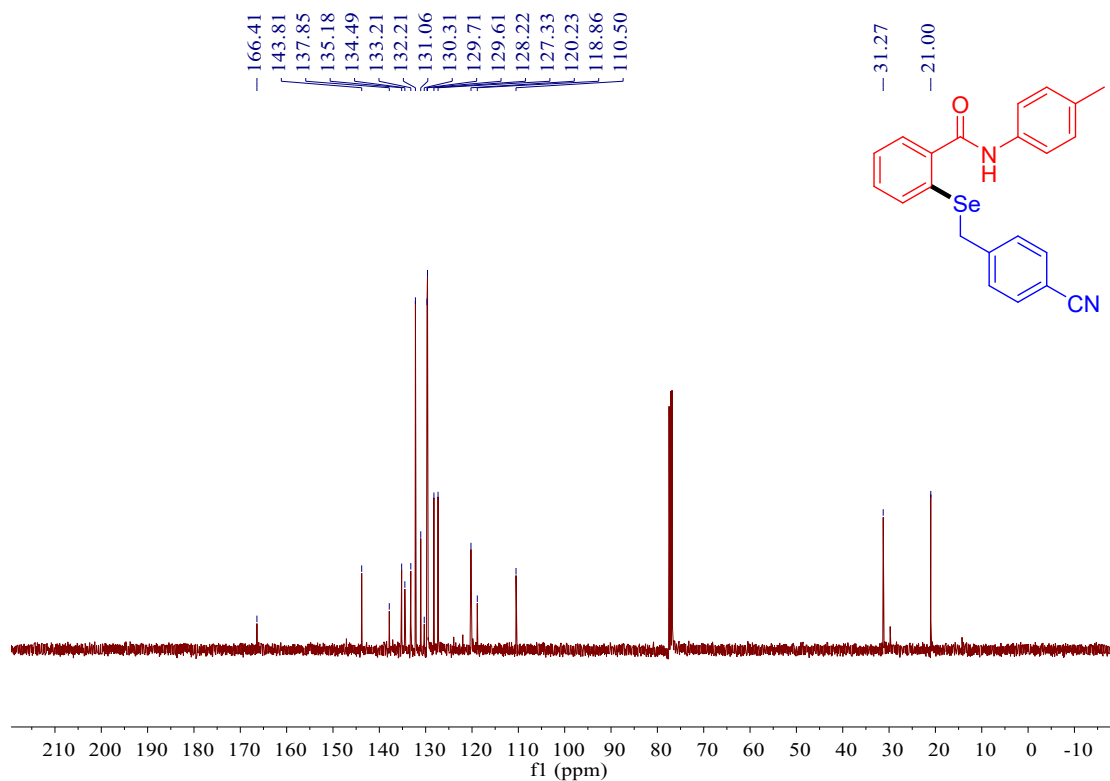
$^{77}\text{Se}$  NMR Spectra of **3v** (400 MHz,  $\text{DMSO-}d_6$ )



$^1\text{H}$  NMR Spectra of **3w** (400 MHz,  $\text{CDCl}_3$ )

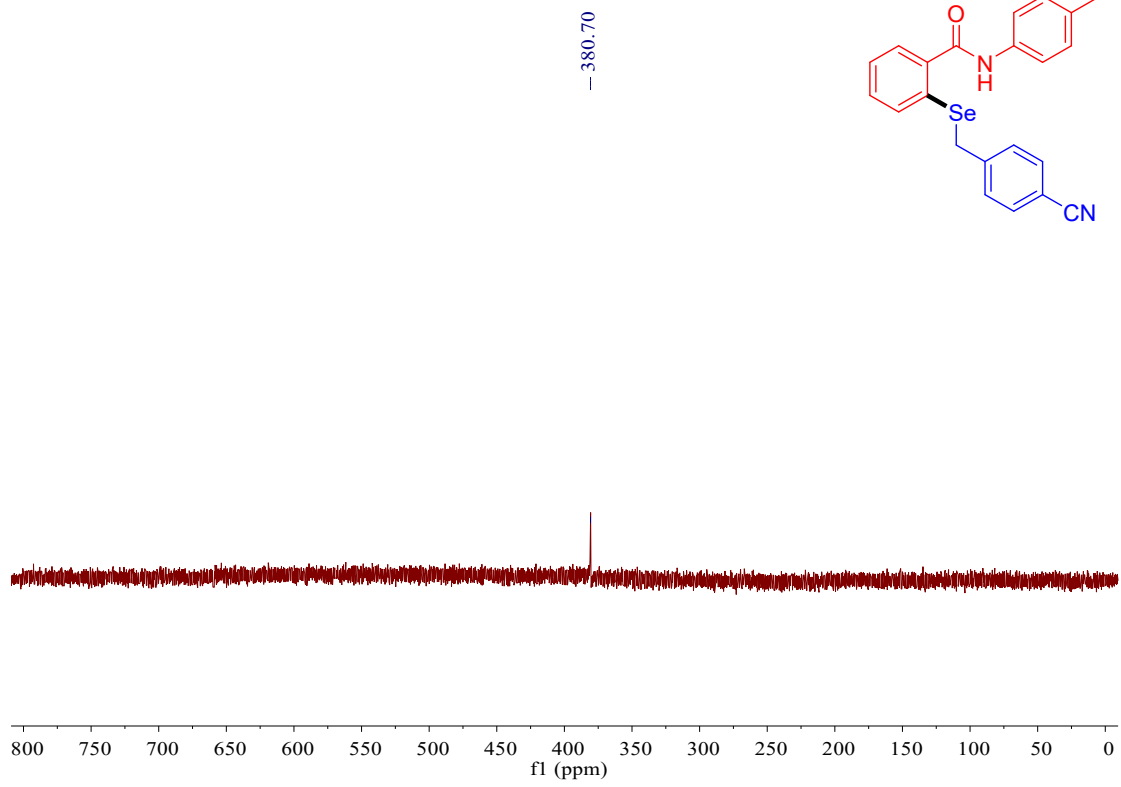


<sup>13</sup>C NMR Spectra of **3w** (400 MHz, CDCl<sub>3</sub>)

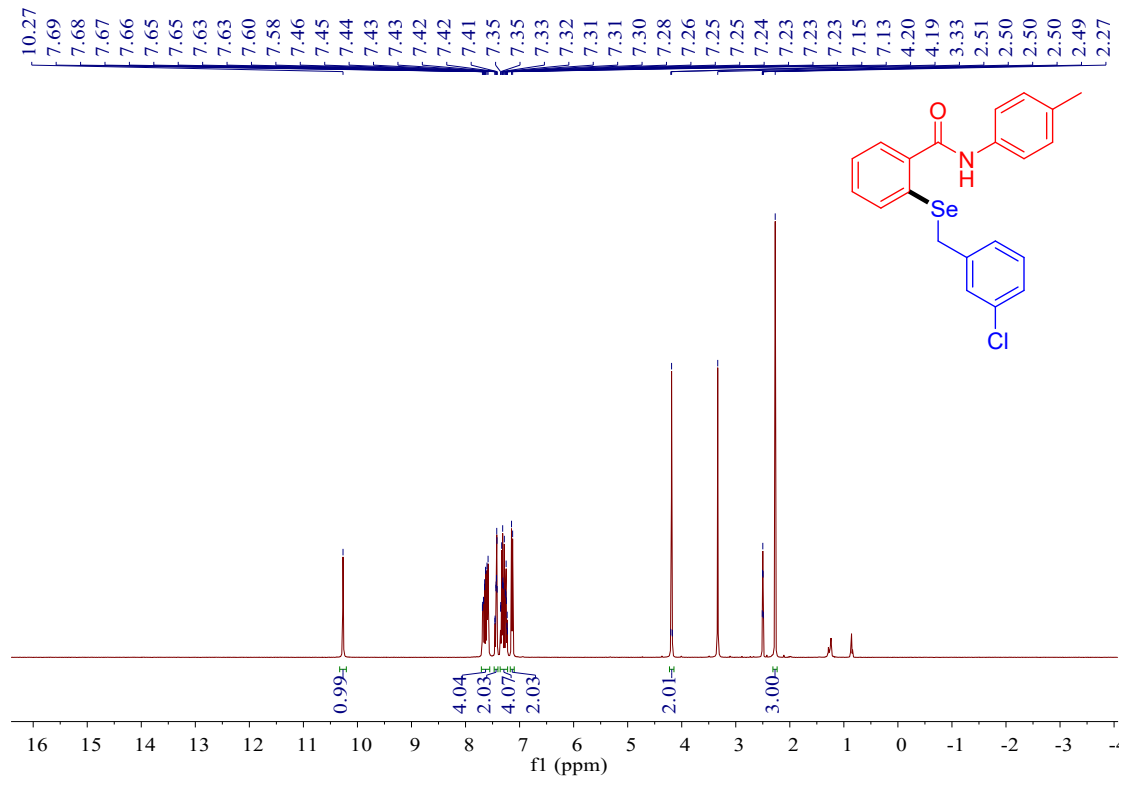


<sup>77</sup>Se NMR Spectra of **3w** (400 MHz, CDCl<sub>3</sub>)

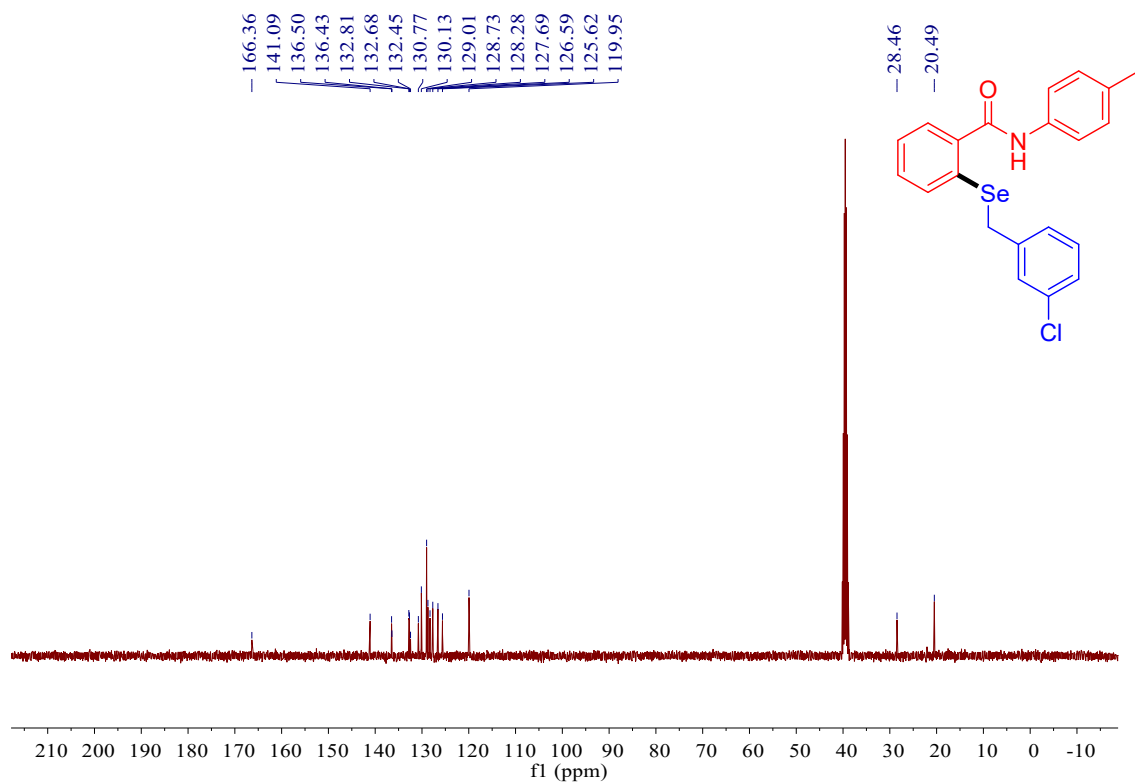




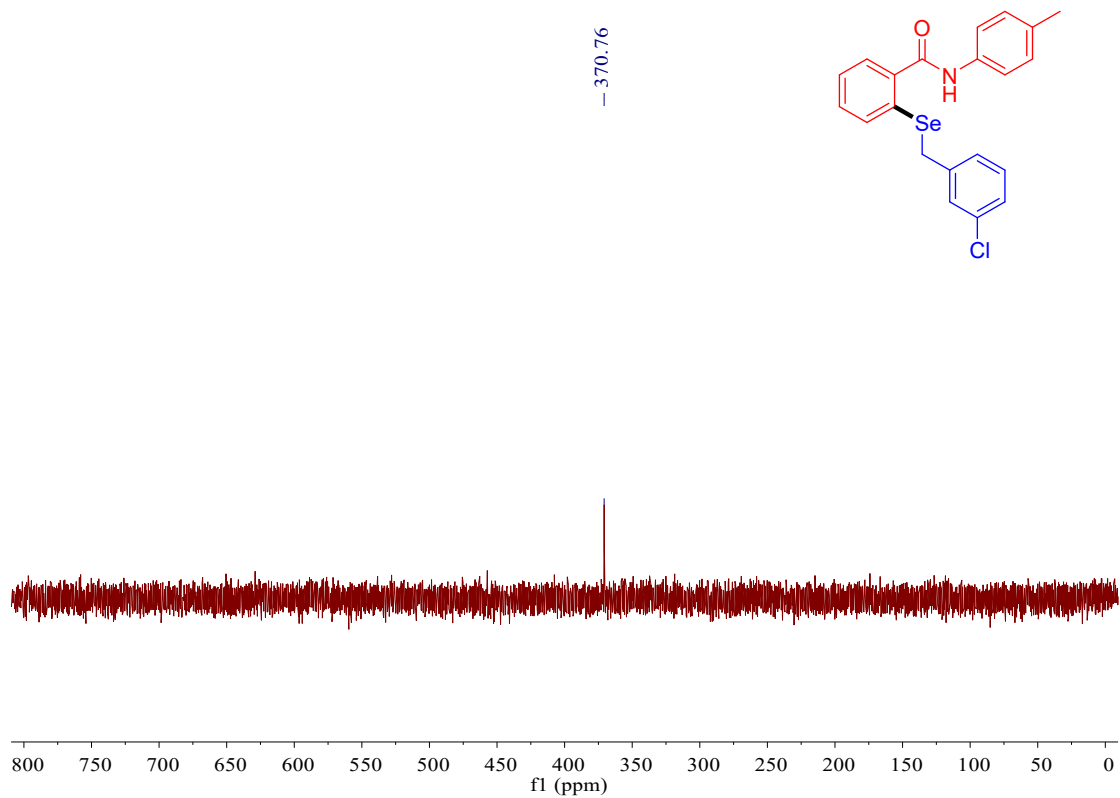
$^1\text{H}$  NMR Spectra of **3x** (400 MHz,  $\text{DMSO-}d_6$ )



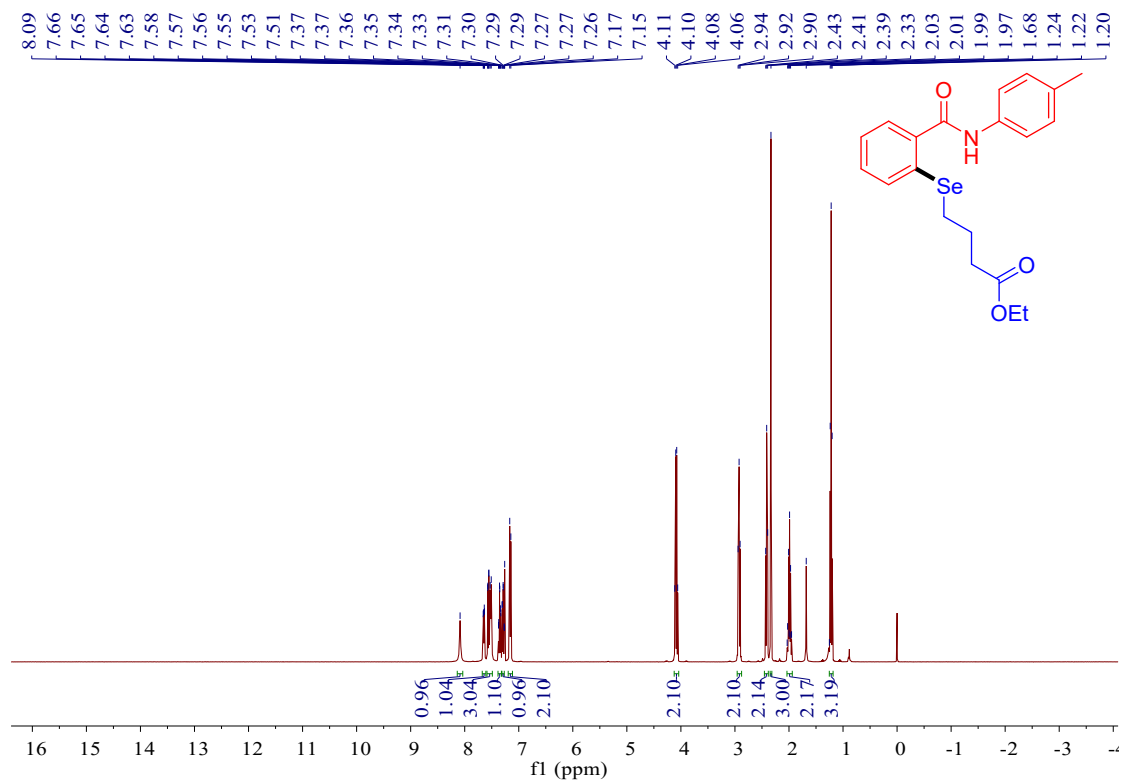
$^{13}\text{C}$  NMR Spectra of **3x** (400 MHz,  $\text{DMSO-}d_6$ )



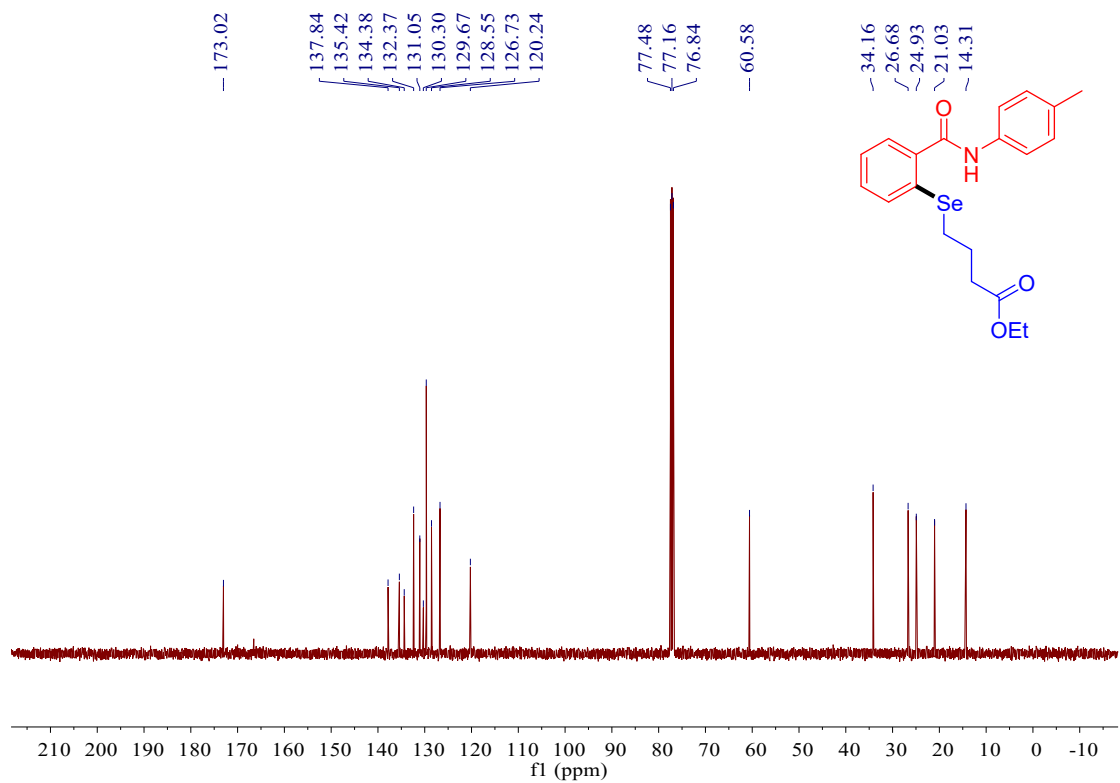
$^{77}\text{Se}$  NMR Spectra of **3x** (400 MHz,  $\text{DMSO-}d_6$ )



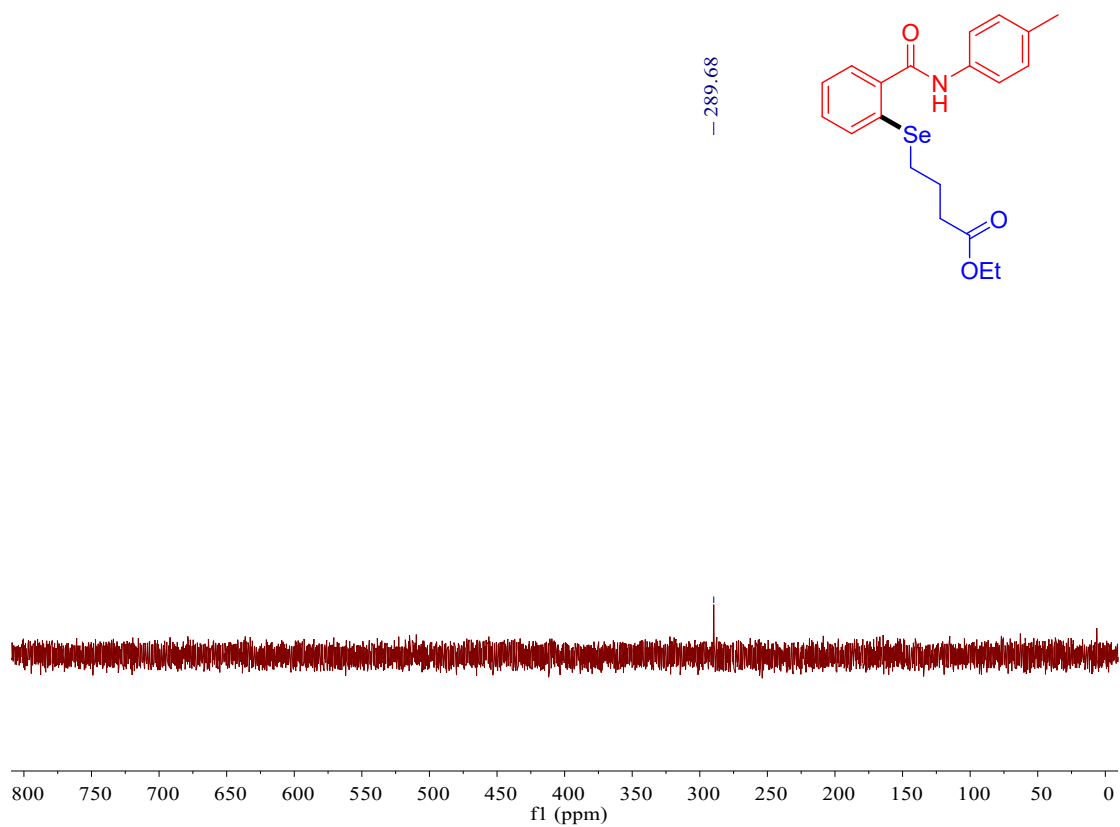
$^1\text{H}$  NMR Spectra of **3y** (400 MHz,  $\text{CDCl}_3$ )



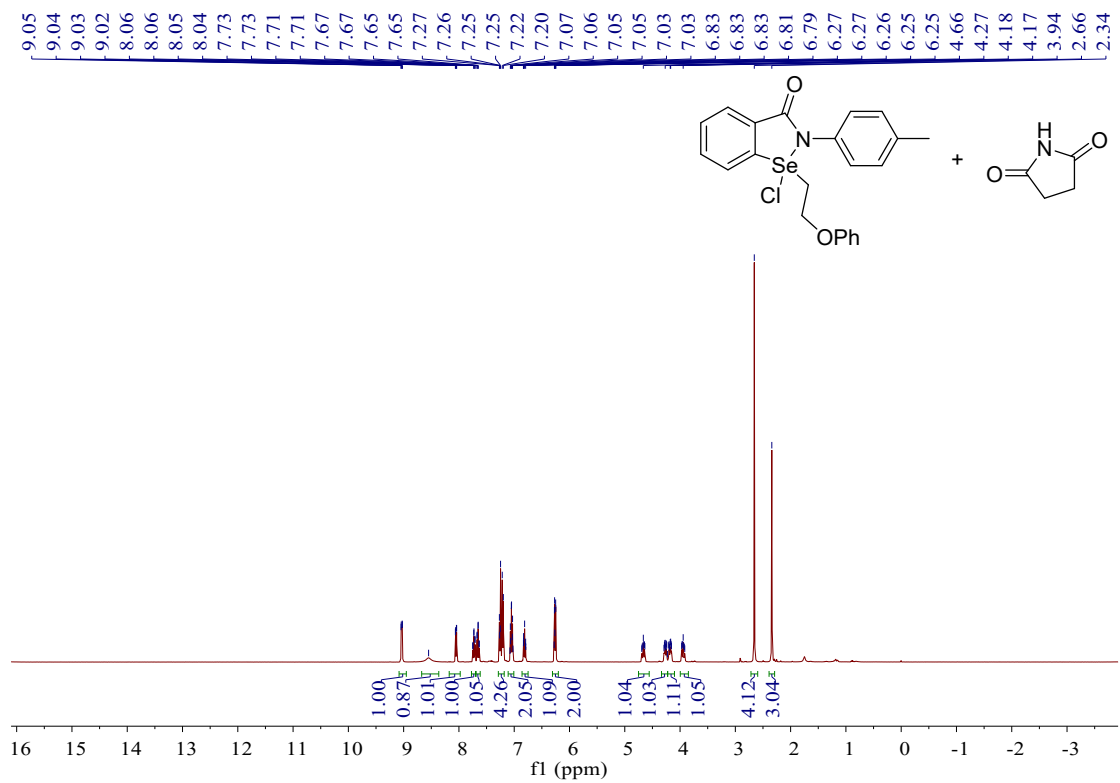
**<sup>13</sup>C NMR Spectra of 3y (400 MHz, CDCl<sub>3</sub>)**



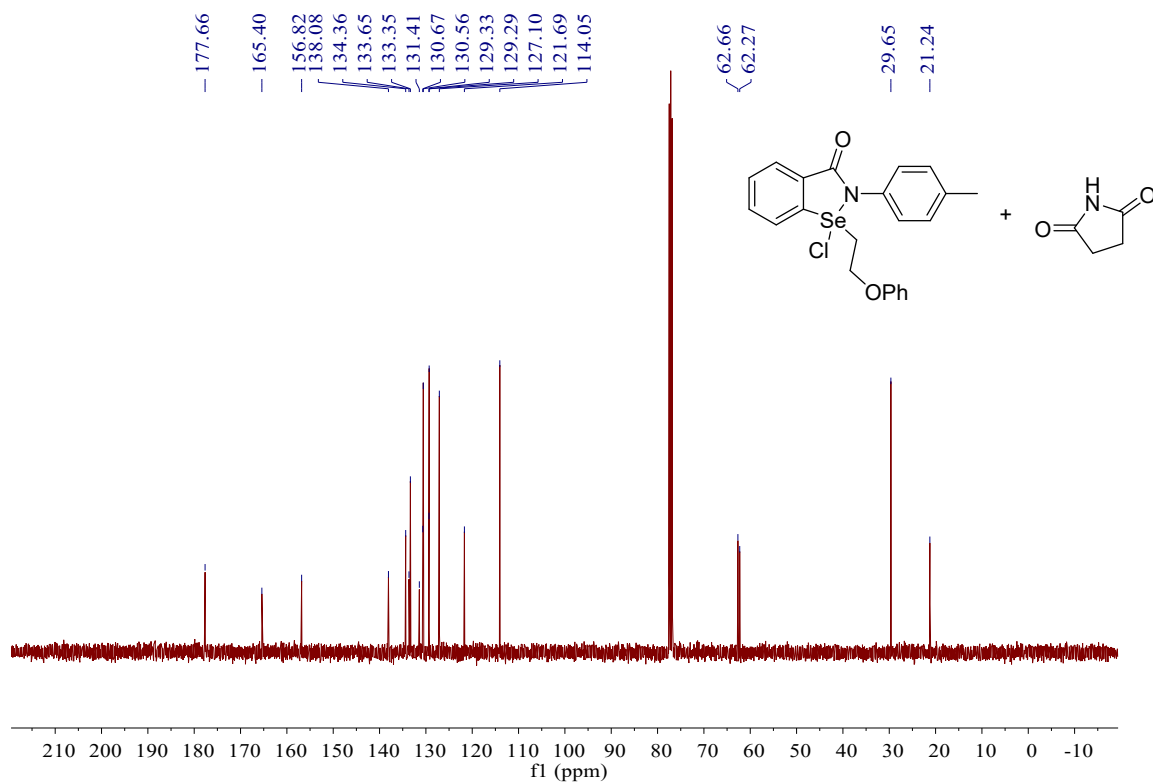
**<sup>77</sup>Se NMR Spectra of 3y (400 MHz, CDCl<sub>3</sub>)**



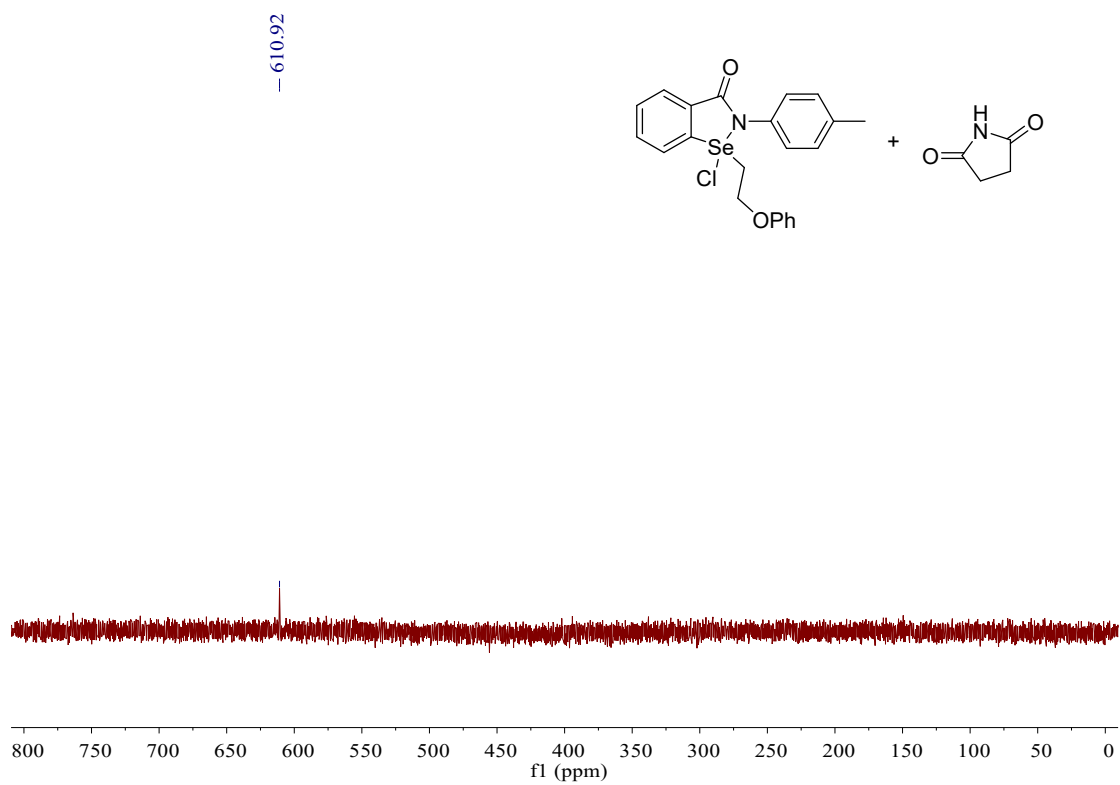
<sup>1</sup>H NMR Spectra of **4a** (400 MHz, CDCl<sub>3</sub>)



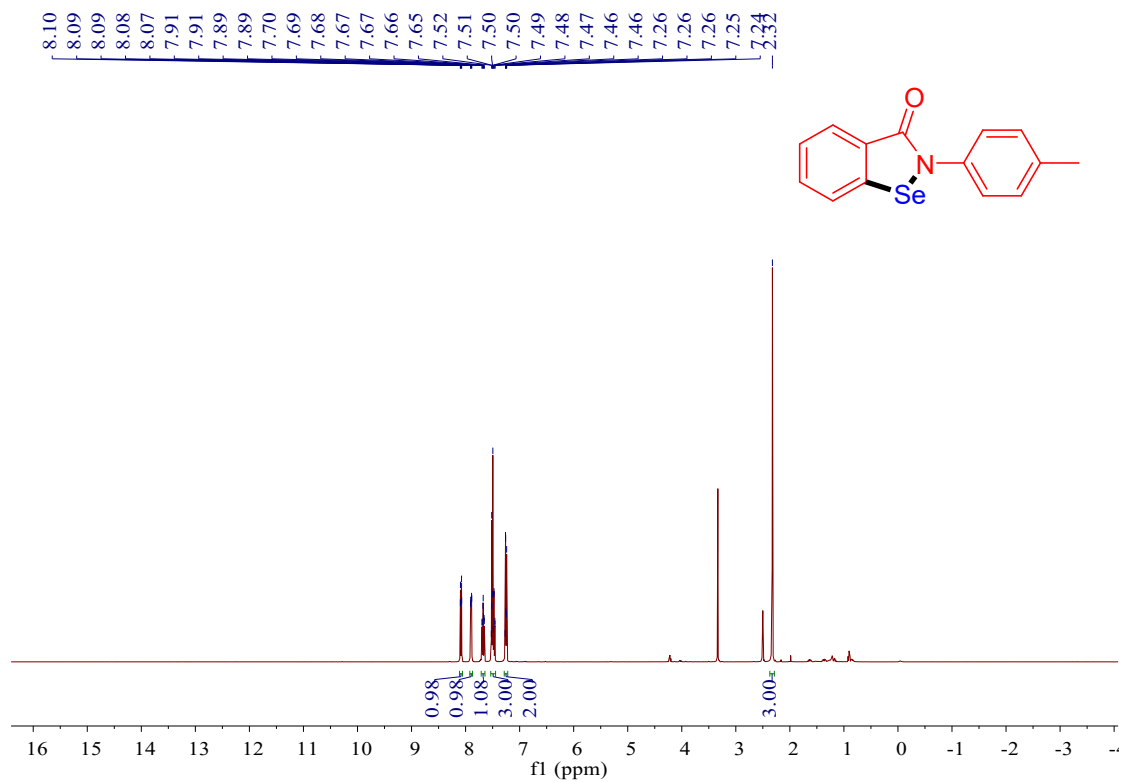
<sup>13</sup>C NMR Spectra of **4a** (400 MHz, CDCl<sub>3</sub>)



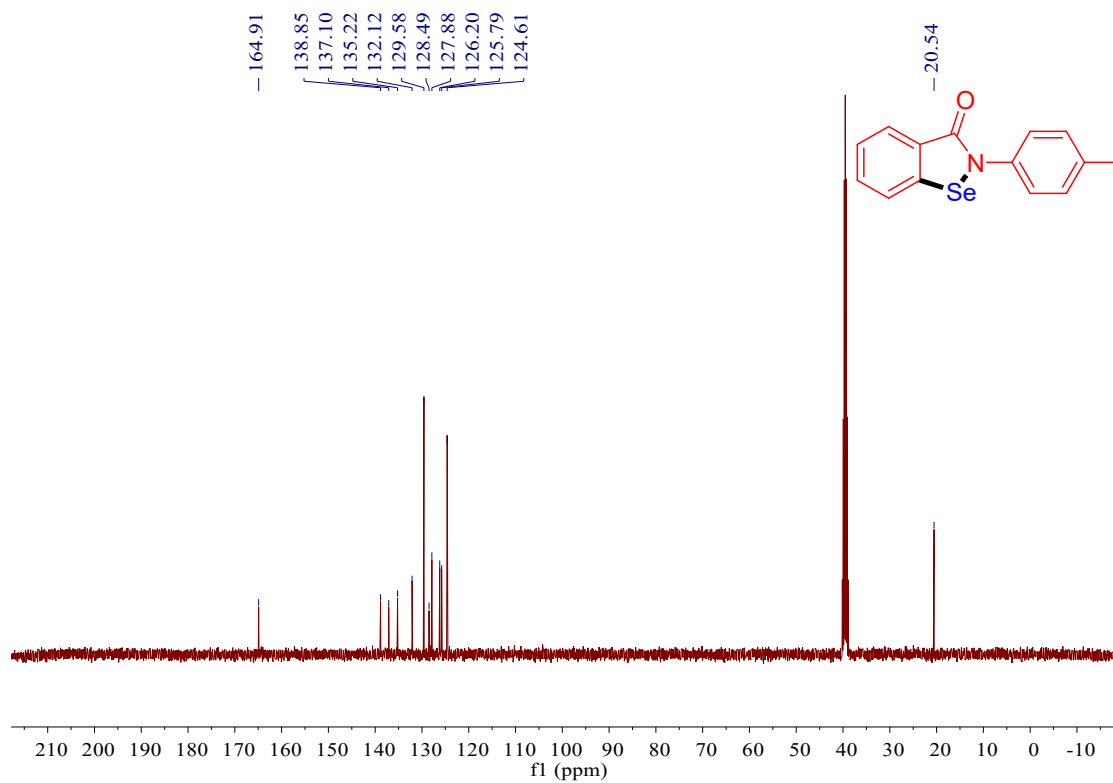
$^{77}\text{Se}$  NMR Spectra of **4a** (400 MHz,  $\text{CDCl}_3$ )



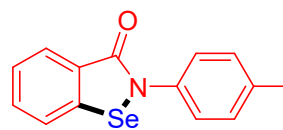
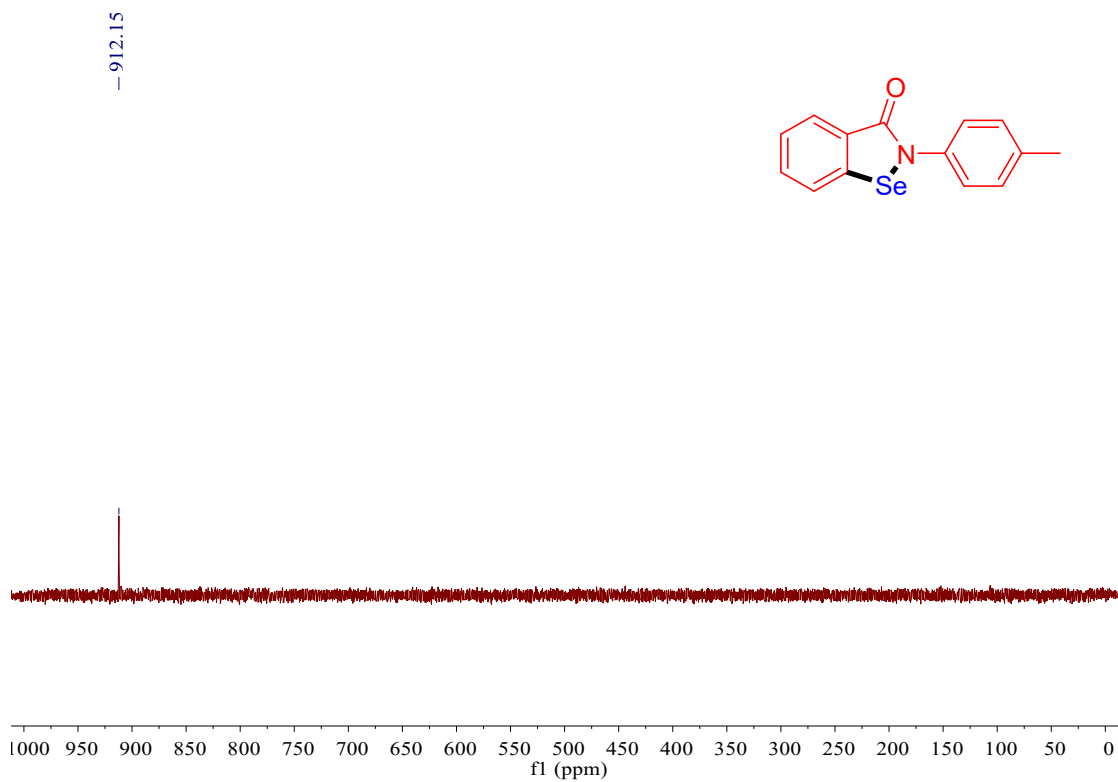
$^1\text{H}$  NMR Spectra of **5a** (400 MHz,  $\text{DMSO-}d_6$ )



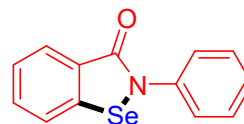
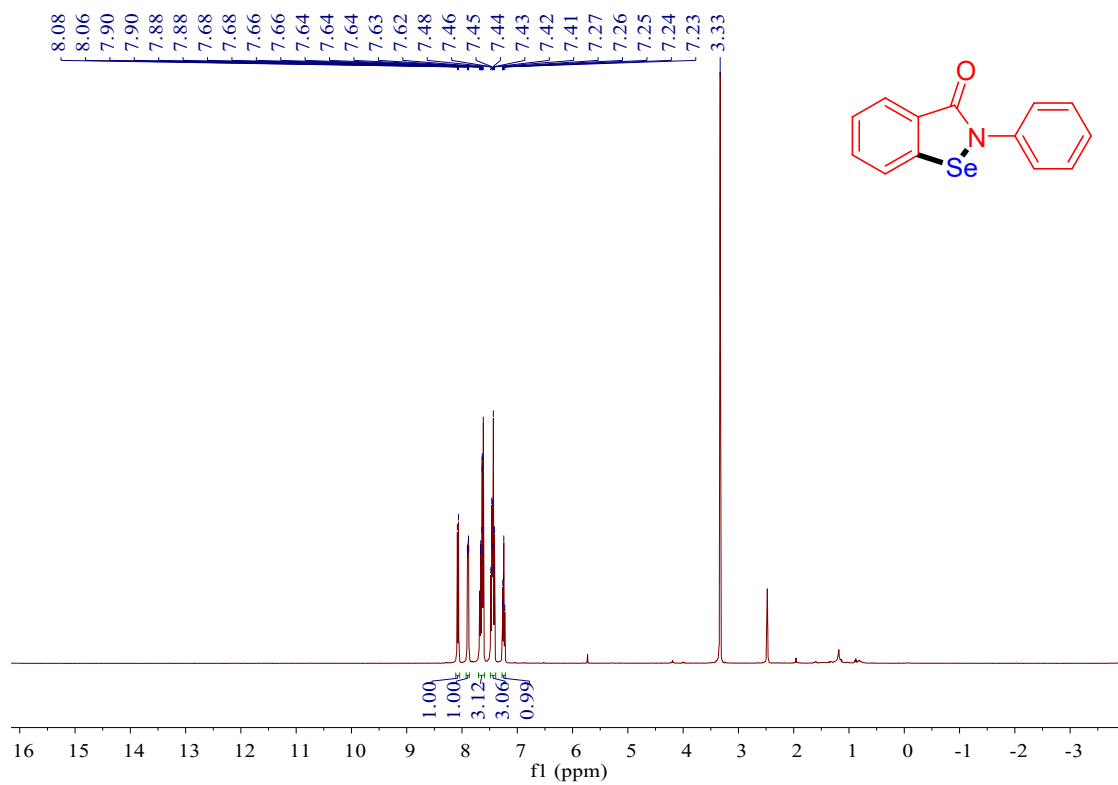
<sup>13</sup>C NMR Spectra of **5a** (400 MHz, DMSO-*d*<sub>6</sub>)



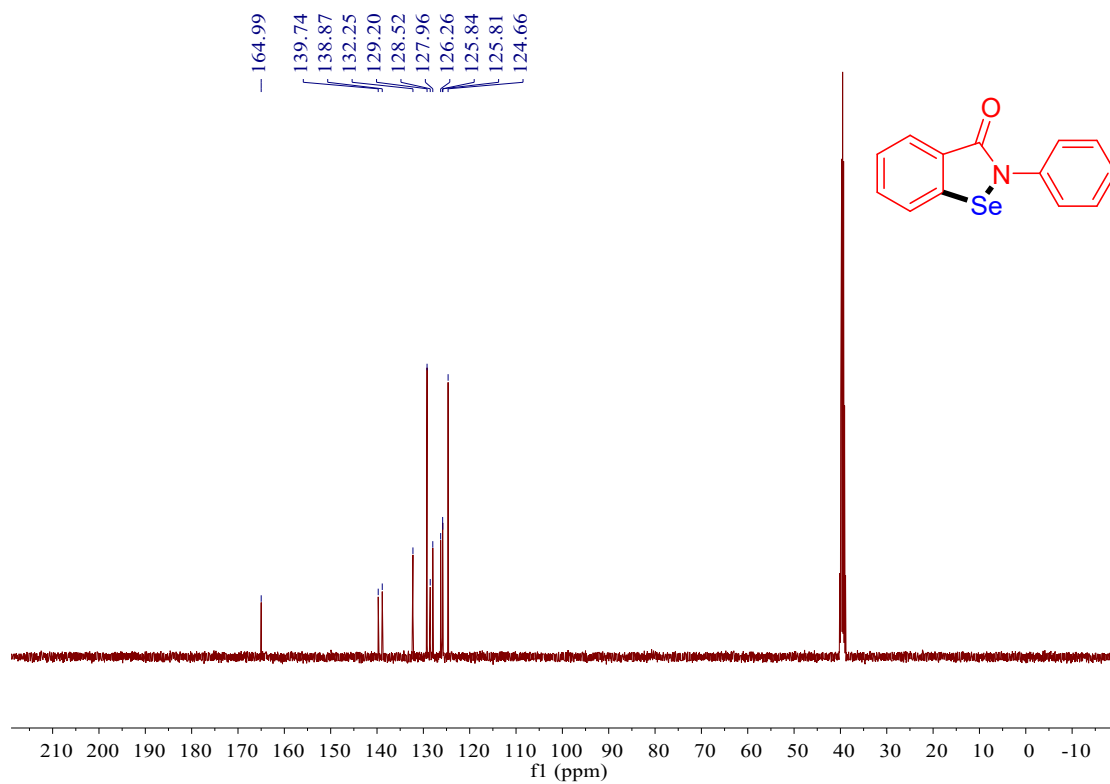
<sup>77</sup>Se NMR Spectra of **5a** (400 MHz, DMSO-*d*<sub>6</sub>)



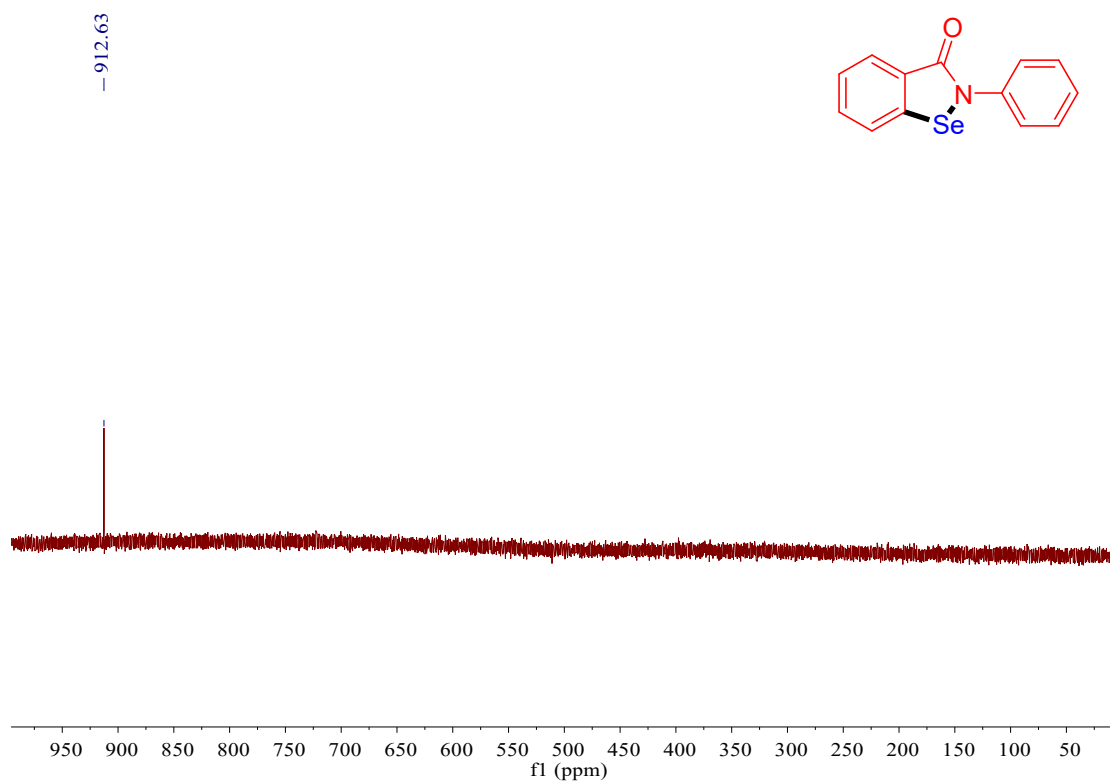
$^1\text{H}$  NMR Spectra of **5b** (400 MHz,  $\text{DMSO-}d_6$ )



$^{13}\text{C}$  NMR Spectra of **5b** (400 MHz,  $\text{DMSO-}d_6$ )

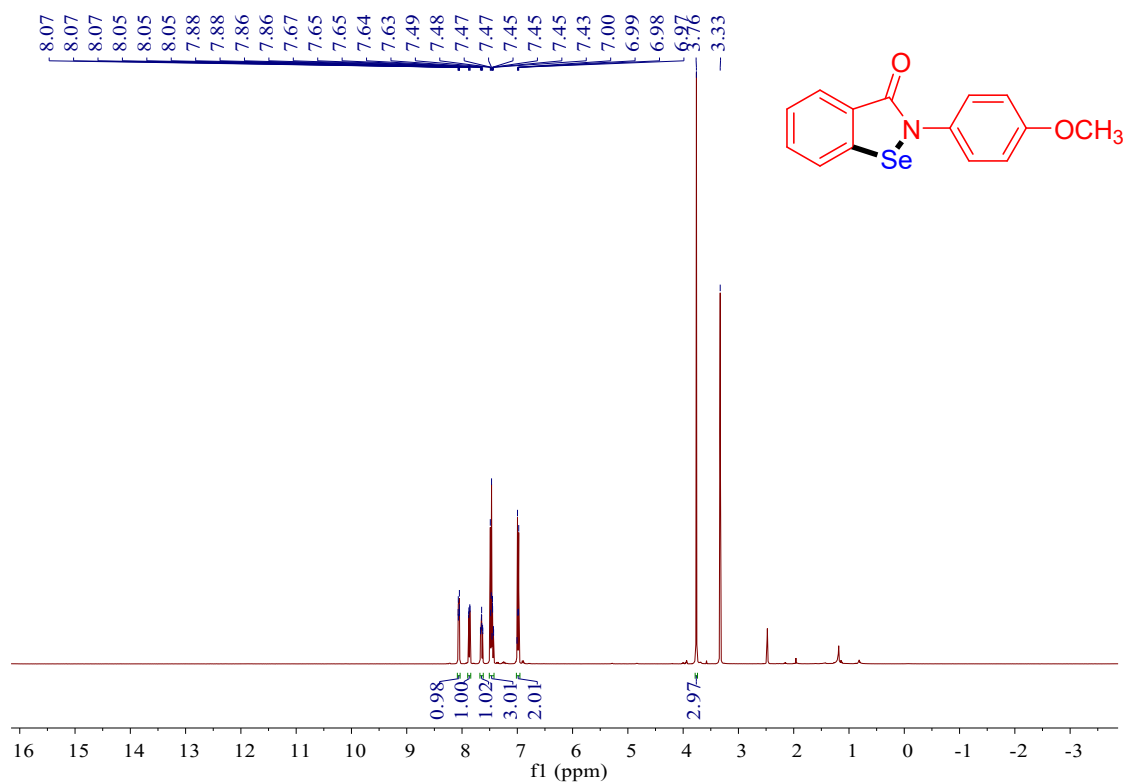


$^{77}\text{Se}$  NMR Spectra of **5b** (400 MHz,  $\text{DMSO-}d_6$ )

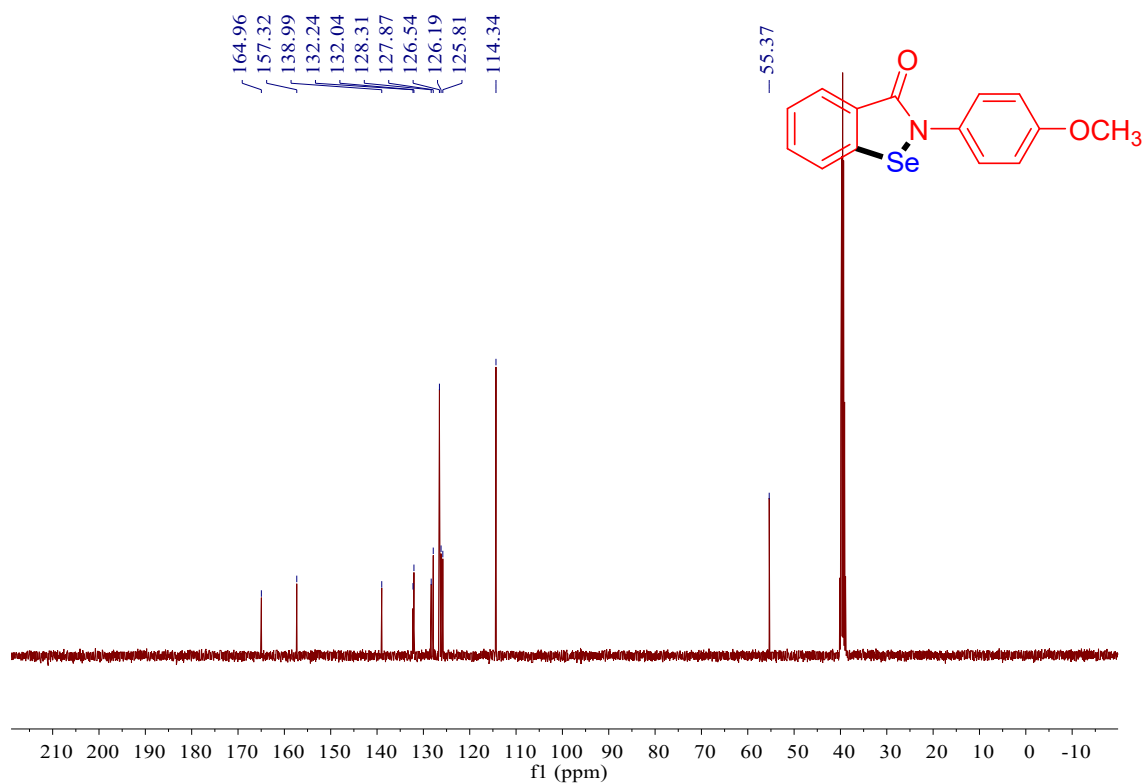


$^1\text{H}$  NMR Spectra of **5c** (400 MHz,  $\text{DMSO-}d_6$ )

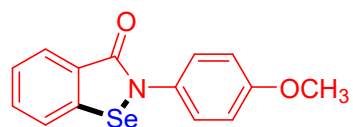




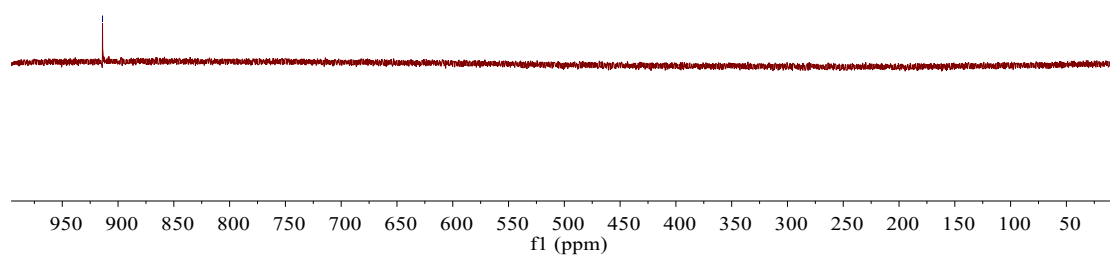
**<sup>13</sup>C NMR Spectra of 5c (400 MHz, DMSO-*d*<sub>6</sub>)**



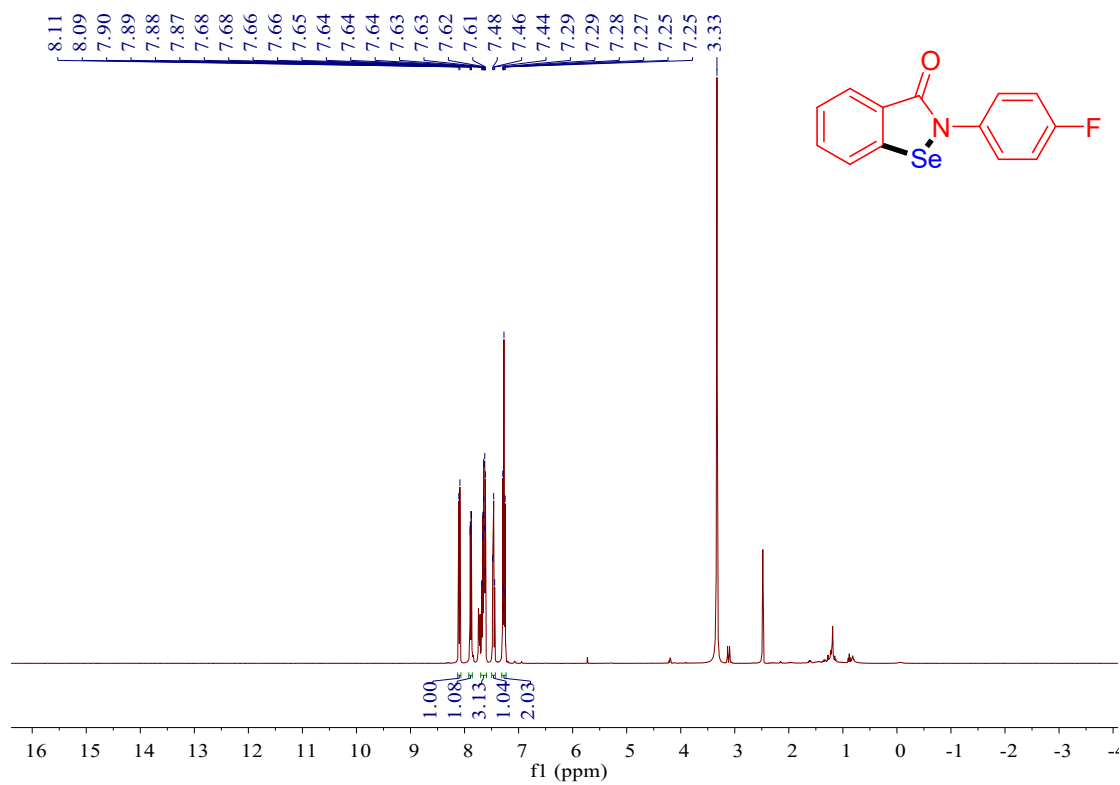
**<sup>77</sup>Se NMR Spectra of 5c (400 MHz, DMSO-*d*<sub>6</sub>)**



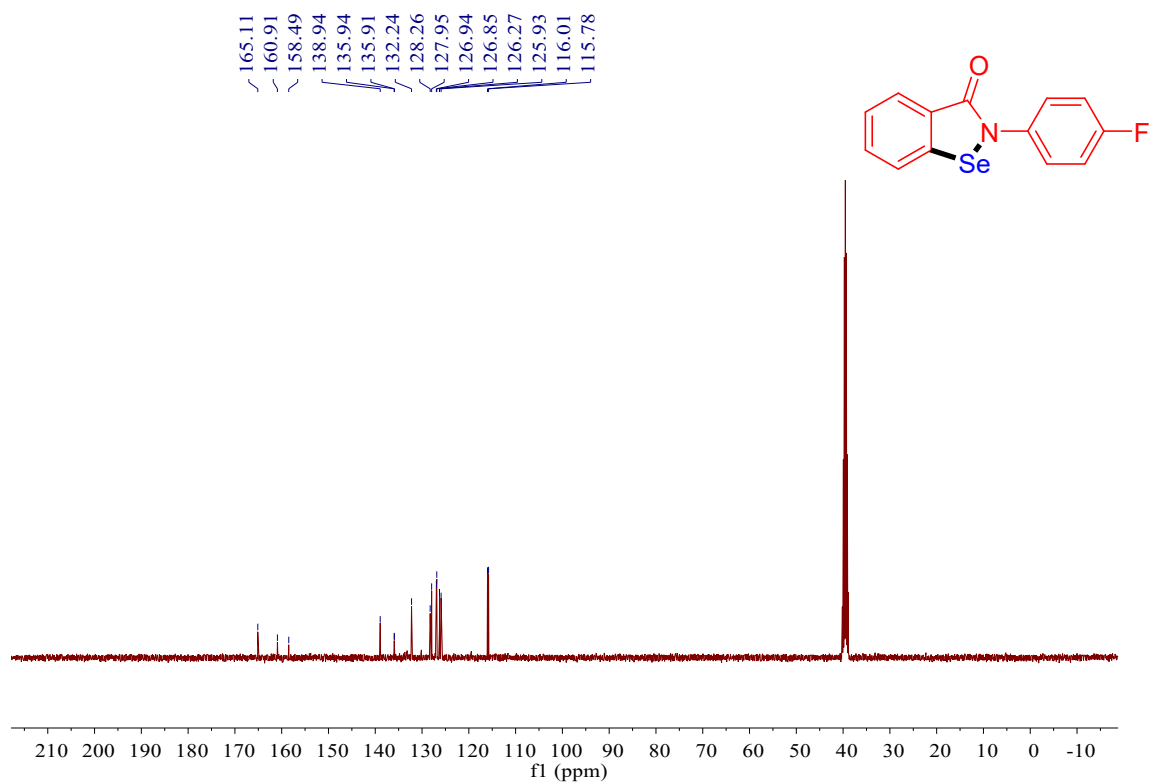
-913.91



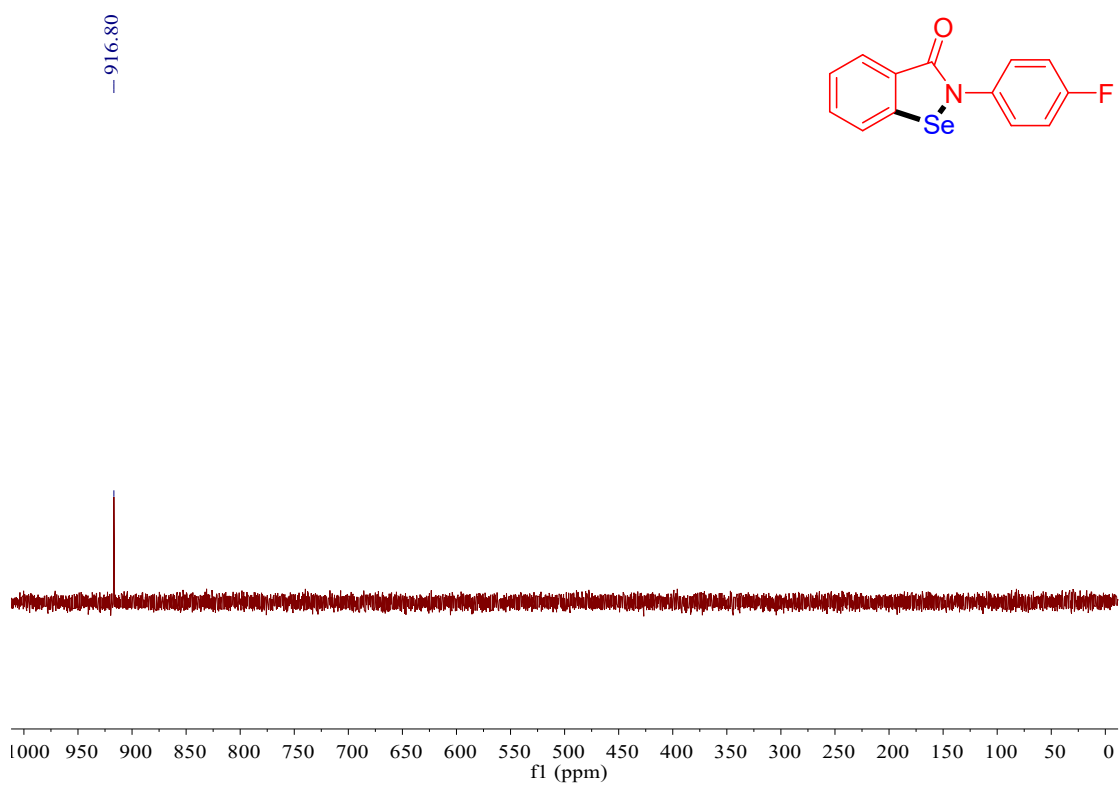
### $^1\text{H}$ NMR Spectra of **5d** (400 MHz, $\text{DMSO-}d_6$ )



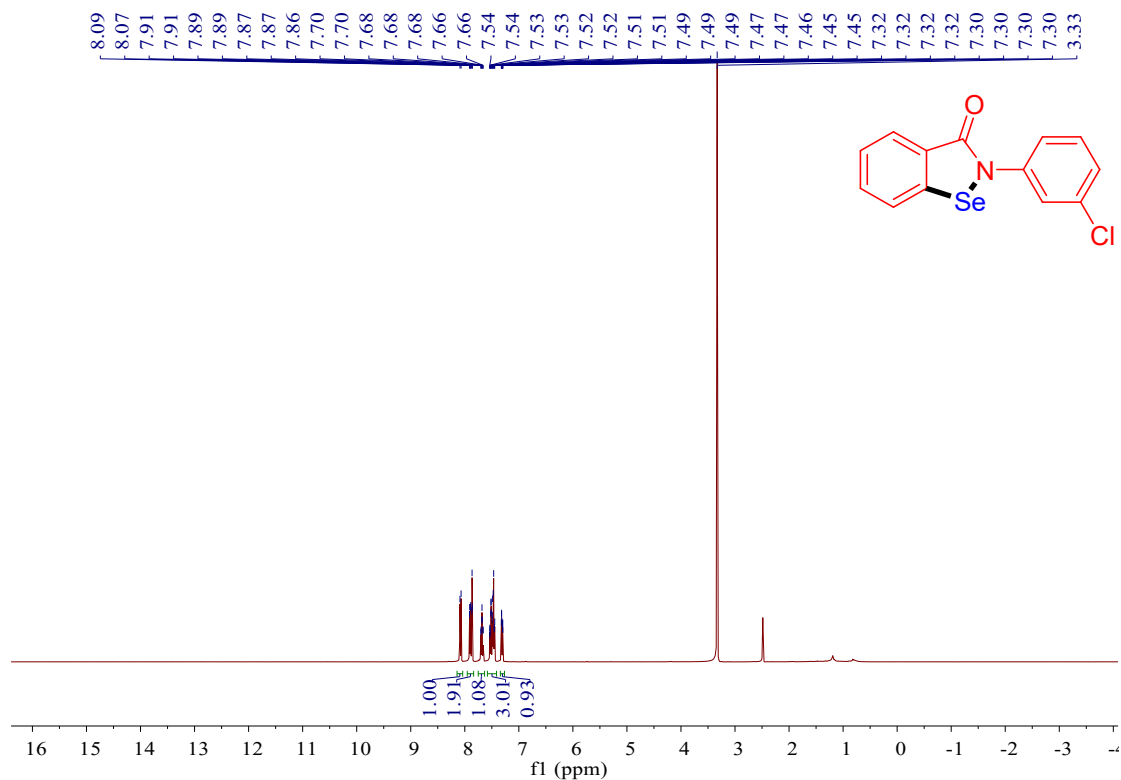
### $^{13}\text{C}$ NMR Spectra of **5d** (400 MHz, $\text{DMSO-}d_6$ )



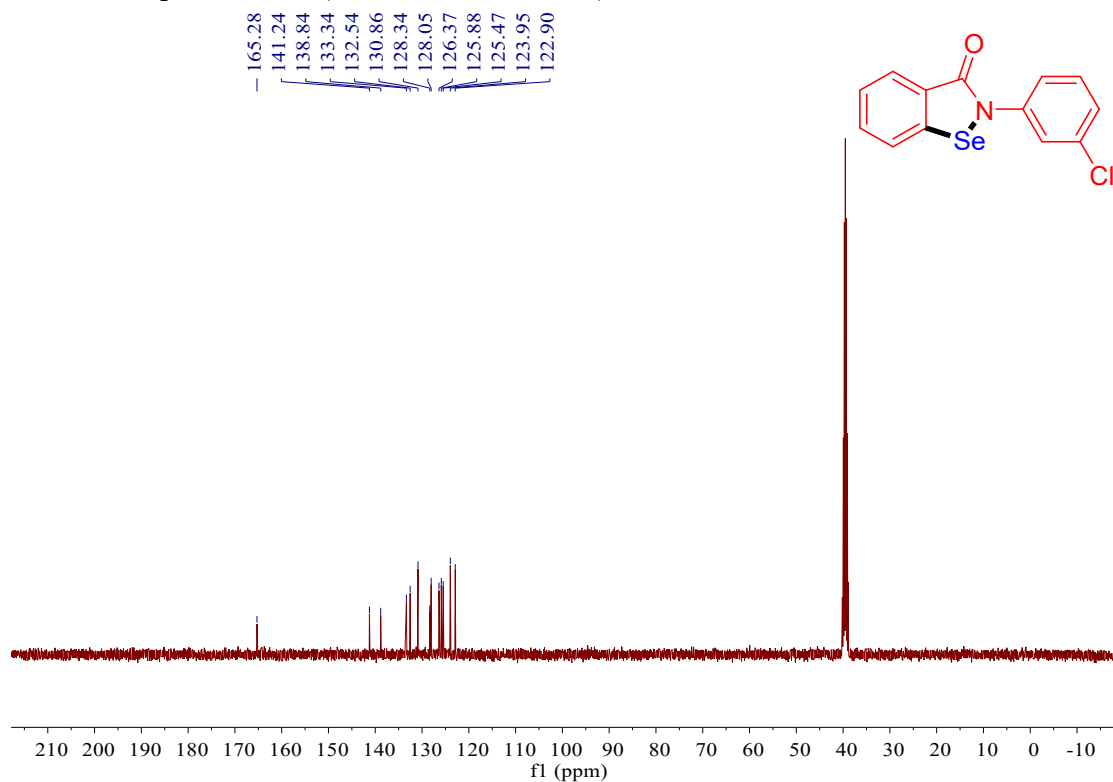
<sup>77</sup>Se NMR Spectra of **5d** (400 MHz, DMSO-*d*<sub>6</sub>)



<sup>1</sup>H NMR Spectra of **5e** (400 MHz, DMSO-*d*<sub>6</sub>)



<sup>13</sup>C NMR Spectra of **5e** (400 MHz, DMSO-*d*<sub>6</sub>)



<sup>77</sup>Se NMR Spectra of **5e** (400 MHz, DMSO-*d*<sub>6</sub>)

