

## Arylseleninic acid derivatives decomposition towards Se(II)-based electrophiles: an elegant approach to construct 3-selanyl-imidazopyridines

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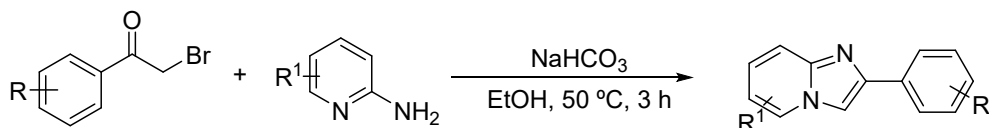
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## 1. General information

The reactions were monitored by TLC carried out on precoated TLC sheets ALUGRAM® Xtra SIL G/UV254 by using UV light as visualization agent. Merck silica gel (particle size 63-200  $\mu\text{m}$ ) was used to flash chromatography, and PTLC Glass Plates L  $\times$  W 20 cm  $\times$  20 cm, silica gel 60 F254, 1 mm, was used in the preparative thin layer chromatography. Hydrogen nuclear magnetic resonance spectra ( $^1\text{H}$  NMR) were obtained at 400 MHz on A Bruker Ascend 400 spectrometer. The spectra were recorded in  $\text{CDCl}_3$  solutions. The chemical shifts are reported in ppm, referenced to tetramethylsilane (TMS) as the external reference. Hydrogen coupling patterns are described as singlet (s), doublet (d), triplet (t), doublet of doublets (dd) and multiplet (m). Coupling constants (J) are reported in Hertz. Carbon-13 nuclear magnetic resonance spectra ( $^{13}\text{C}$  NMR) were obtained at 100 MHz on Bruker Nuclear Ascend 400 spectrometer. The chemical shifts are reported in ppm, referenced to the solvent peak of  $\text{CDCl}_3$ . Selenium-77 nuclear magnetic resonance spectra ( $^{77}\text{Se}$  NMR) were obtained at 76 MHz on Bruker Nuclear Ascend 400 spectrometer. The HRMS analyses were performed in a HESI Quadrupole-Orbitrap (Q extractive focus, Thermo Scientific) spectrometer equipped with an APCI source operating in positive mode. The samples were solubilized in acetonitrile and analyzed by direct infusion at a constant flow rate. The acquisition parameters were: Scan type Full MS; resolution 70000; polarity positive. Ionization conditions HESI: Sheath gas 20; aux gas 10; spray voltage 2.8kV; capillary temperature 300  $^\circ\text{C}$ . The mass-to-charge ratio (m/z) data were processed and analyzed using Bruker Daltonics softwares: Compass Data Analysis and Isotope Pattern.

## 2. General procedures and characterization data for all reaction products

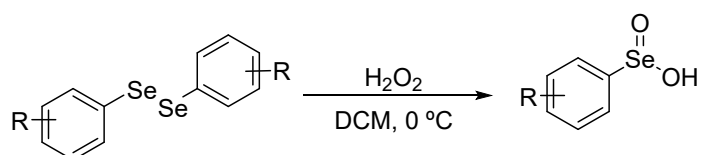
### 2.1 General procedure for the synthesis of 2-phenylimidazo[1,2-*a*]pyridines.<sup>1</sup>



Scheme 1.

The typical experimental procedure for synthesis of 2-phenylimidazo[1,2-*a*]pyridine derivatives: To a 10 mL vial was added a mixture of 2-aminopyridine (5.0 mmol), 2-bromoacetophenone derivative (5.0 mmol) and NaHCO<sub>3</sub> (4.0 mmol) in EtOH at room temperature for 3 hours. Then, the reaction mixture was received in water (10 mL) and extracted with ethyl acetate (3 x 15 mL), dried over MgSO<sub>4</sub> and concentrated under vacuum. After that, the crude was purified by column chromatography using silica gel and a mixture of ethyl acetate/hexane as the eluent.

### 2.2. General procedure for the synthesis of the arylseleninic acids 2a-h.<sup>2</sup>

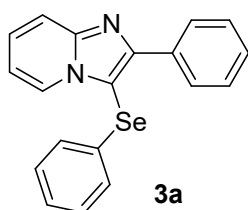


Scheme 2.

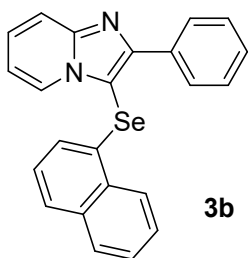
In a round-bottomed flask were added the diphenyl diselenide derivatives (0.6 mmol) and DCM (3.0 mL), being the resulting mixture cooled with an ice bath (0 °C). Then, H<sub>2</sub>O<sub>2</sub> (3.0 equiv) was added dropwise. The resulting mixture was stirred at 0 °C until the formation of a white suspension and the disappearance of the yellowish solution. After, the solvent was evaporated, removing DCM and residual water, being the precipitate washed several times with hexanes and dried using the vacuum pump. The freshly dried white solid was directly employed in the next reaction step.

### 2.3 General procedure for the synthesis of 2-phenyl-3-(phenylselanyl)imidazo[1,2-*a*]pyridines 3a-ah.

In a glass tube were added the 2-phenylimidazo[1,2-*a*]pyridine (0.25 mmol), arylseleninic acids **2** (0.5 mmol) and DMF as solvent (1.0 mL). The resulting mixture was stirred at 110 °C for 3 hours. After that, the reaction was received in water, extracted with ethyl acetate (3x 10 mL), washed with brine (2x 15 mL), dried over MgSO<sub>4</sub>, and concentrated under vacuum. Then, the crude was purified by column chromatography using a mixture of hexane/ethyl acetate as the eluent.

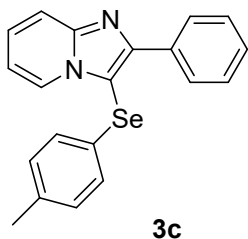


**2-phenyl-3-(phenylselanyl)imidazo[1,2-*a*]pyridine (3a).**<sup>3</sup> Yield: 0.076 g (88%); Yellow solid, mp: 91.2-93.0 °C; Lit.: 91.1-93.1 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.33 (d, *J* = 6.8 Hz, 1H), 8.15 (d, *J* = 7.4 Hz, 2H), 7.71 (d, *J* = 9.0 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.37 (d, *J* = 7.2 Hz, 1H), 7.32 – 7.23 (m, 1H), 7.21 – 7.03 (m, 5H), 6.82 (t, *J* = 6.8 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 151.88, 147.82, 133.83, 130.97, 129.77, 128.85, 128.55, 128.39, 128.30, 126.76, 126.56, 125.69, 117.59, 113.10, 102.94. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 214.97.

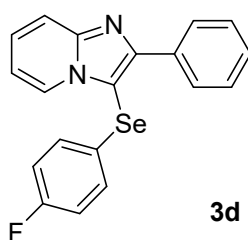


**3-(naphthalen-1-ylselanyl)-2-phenylimidazo[1,2-*a*]pyridine (3b).**<sup>4</sup> Yield: 0.088 g (94%); Colorless plate, mp: 160-162 °C; Lit.: 160-161 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.25 (d, *J* = 6.9 Hz, 1H), 8.14 (dd, *J* = 16.2, 7.6 Hz, 3H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.54 (t, *J* = 8.6 Hz, 2H), 7.46 – 7.31 (m, 3H), 7.31 – 7.21 (m, 1H), 7.11 (t, *J* = 7.7 Hz, 1H), 6.86 (d, *J* = 7.2 Hz, 1H), 6.76 (t, *J* = 6.8 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 152.49, 148.03, 134.25, 133.72, 132.21, 129.18,

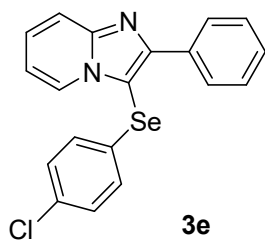
128.75, 128.51, 128.34, 127.16, 126.62, 126.50, 126.44, 126.27, 125.71, 125.52, 125.12, 117.53, 113.02, 101.58.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  188.57.



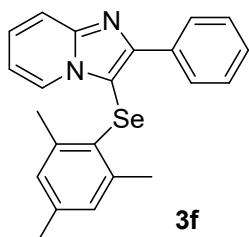
**2-phenyl-3-(p-tolylselanyl)imidazo[1,2-a]pyridine (3c).**<sup>4</sup> Yield: 0.074 g (70%); Colorless plate, mp: 134-135 °C; Lit.: 134-135 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (d,  $J = 6.9$  Hz, 1H), 8.17 8.15 (d,  $J = 7.1$  Hz, 2H), 7.70 (d,  $J = 9.0$  Hz, 1H), 7.44 (t,  $J = 7.4$  Hz, 2H), 7.38 – 4.36 (m, 1H), 7.32 – 7.24 (m, 1H), 7.06 – 6.94 (m, 4H), 6.85 – 6.82 (m, 1H), 2.24 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.58, 147.65, 136.68, 133.83, 130.46, 128.76, 128.49, 128.39, 128.28, 126.94, 126.34, 125.63, 117.48, 112.91, 103.23, 20.93.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  211.46.



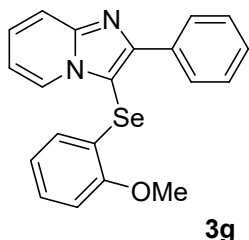
**3-((4-fluorophenyl)selanyl)-2-phenylimidazo[1,2-a]pyridine (3d).**<sup>4</sup> Yield: 0.062 g (69%); Yellow solid, mp: 116-118 °C; Lit.: 116.5-118.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (d,  $J = 6.9$  Hz, 1H), 8.20 – 8.09 (m, 2H), 7.71 (d,  $J = 9.0$  Hz, 1H), 7.50 – 7.28 (m, 4H), 7.17 – 7.03 (m, 2H), 6.94 – 6.78 (m, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) 162.09 (d,  $J = 246.5$  Hz), 151.73, 147.73, 133.69, 130.38 (d,  $J = 7.8$  Hz), 128.76, 128.55, 128.36, 126.54, 125.47, 125.15 (d,  $J = 3.3$  Hz), 117.63, 116.89 (d,  $J = 21.9$  Hz), 113.11, 103.15.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  211.14.



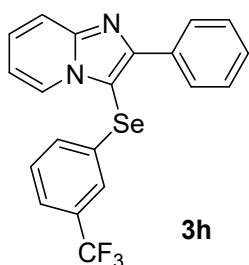
**3-((4-chlorophenyl)selanyl)-2-phenylimidazo[1,2-*a*]pyridine (3e).**<sup>4</sup> Yield: 0.070 g (74%); Colorless plate, mp: 162-163 °C; Lit.: 162-163 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.31 (d, *J* = 6.8 Hz, 1H), 8.12 (d, *J* = 7.2 Hz, 2H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.50 – 7.27 (m, 4H), 7.14 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.87 (t, *J* = 6.8 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 147.85, 133.62, 132.87, 129.82, 129.53, 129.12, 128.73, 128.60, 128.38, 126.64, 125.45, 117.67, 113.20, 102.41. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 218.60.



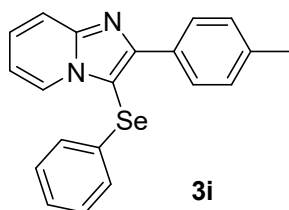
**3-(mesityl)selanyl)-2-phenylimidazo[1,2-*a*]pyridine (3f).**<sup>4</sup> Yield: 0.064 g (70%); Colorless plate, mp: 158-160 °C; Lit.: 159-161 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.05 (d, *J* = 8.6 Hz, 3H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.51 – 7.31 (m, 3H), 7.24 – 7.13 (m, 1H), 6.79 – 6.74 (m, 3H), 2.22 (s, 6H), 2.18 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 150.18, 146.88, 141.38, 138.03, 134.30, 129.40, 129.02, 128.11, 126.31, 125.34, 117.41, 112.56, 104.59, 23.61, 20.79. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 140.95.



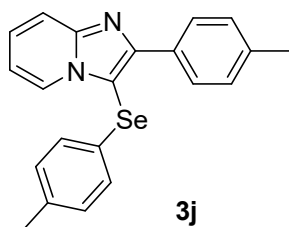
**3-(2-methoxyphenyl)selanyl)-2-phenylimidazo[1,2-*a*]pyridine (3g).** Yield: 0.077 g (80%); Yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.26 (d, *J* = 6.7 Hz, 1H), 8.11 (d, *J* = 7.7 Hz, 2H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.49 – 7.21 (m, 4H), 7.17 (d, *J* = 7.4 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.88 – 6.82 (m, 2H), 6.54 (d, *J* = 7.8 Hz, 1H), 2.46 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 152.49, 148.11, 136.60, 133.90, 131.53, 130.77, 128.86, 128.56, 128.41, 127.29, 126.94, 126.54, 125.80, 117.67, 113.12, 101.92, 21.24. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 192.35. HRMS *m/z*: [M+H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>OSe, 381,0501; found: 381,3012.



**2-Phenyl-3-[3-(trifluoromethyl)phenyl]selanylimidazo[1,2-*a*]pyridine (3h).**<sup>5</sup> Yield: 0.083 g (84%); Yellow solid, mp: 93.5-95.7 °C; Lit.: 93.1 - 95.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.32 (d, *J* = 6.9 Hz, 1H), 8.11 (d, *J* = 7.2 Hz, 2H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.53 – 7.29 (m, 6H), 7.28 – 7.19 (m, 1H), 7.10 (d, *J* = 7.9 Hz, 1H), 6.88 (t, *J* = 6.6 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 152.58, 148.12, 133.65, 132.52, 131.9 (q, *J* = 32.5 Hz), 131.24, 130.18, 128.52, 128.89, 128.3, 126.89, 125.09, 124.9 (q, *J* = 3.8 Hz), 123.5 (q, *J* = 3.6 Hz), 123.0 (q, *J* = 273.4 Hz), 117.88, 113.43, 101.88. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 228.18.

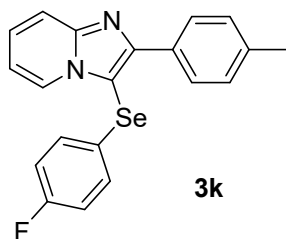


**3-(phenylselanyl)-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (3i).**<sup>3</sup> Yield: 0.079 g (77%); Orange solid, mp: 66-68 °C; Lit.: 77-79 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.33 (d, *J* = 6.9 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 9.0 Hz, 1H), 7.27 (m, 3H), 7.20 – 7.02 (m, 5H), 6.82 (t, *J* = 6.8 Hz, 1H), 2.38 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 151.95, 147.73, 138.38, 131.02, 129.68, 129.08, 128.64, 128.22, 126.64, 126.39, 125.59, 117.44, 112.92, 102.52, 21.37. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 214.93.

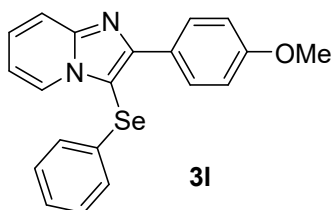


**2-(*p*-Tolyl)-3-(*p*-tolylselanyl)imidazo[1,2-*a*]pyridine (3j).**<sup>3</sup> Yield: 0.087 g (87%); Yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.33 (d, *J* = 6.9 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 3H), 6.99 (q, *J* = 8.3 Hz, 4H), 6.82 (s, 1H), 2.38 (s, 3H), 2.23 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 151.61, 147.57, 138.29,

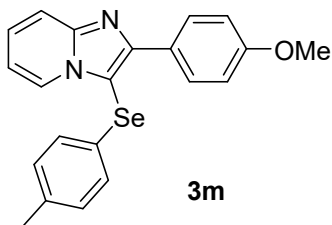
136.62, 130.89, 130.42, 129.02, 128.62, 128.46, 127.00, 126.30, 125.57, 117.31, 112.84, 102.93, 20.91.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  208.88.



**3-((4-fluorophenyl)selanyl)-2-(p-tolyl)imidazo[1,2-a]pyridine (3k).** Yield: 0.072 g (73%); Yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.32 (d,  $J = 6.9$  Hz, 1H), 8.05 (d,  $J = 8.1$  Hz, 2H), 7.70 (d,  $J = 9.0$  Hz, 1H), 7.28 (m, 3H), 7.08 (m, 2H), 6.96 – 6.73 (m, 3H), 2.39 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.05 (d,  $J = 246.4$  Hz), 151.79, 147.67, 138.48, 130.58 (d,  $J = 41.1$  Hz), 129.11, 128.62, 126.48, 125.41, 125.24 (d,  $J = 3.3$  Hz), 117.49, 116.85 (d,  $J = 21.9$  Hz), 113.02, 102.83, 21.36.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  211.05. HRMS  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{15}\text{FN}_2\text{Se}$ , 383,0458; found: 383,0454.



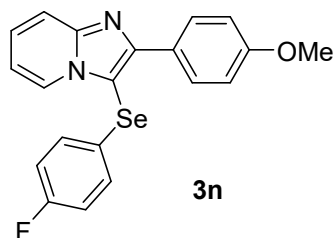
**2-(4-methoxyphenyl)-3-(phenylselanyl)imidazo[1,2-a]pyridine (3l).**<sup>3</sup> Yield: 0.074 g (68%); Yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (d,  $J = 6.8$  Hz, 1H), 8.12 (d,  $J = 8.8$  Hz, 2H), 7.70 (d,  $J = 9.0$  Hz, 1H), 7.26 – 7.21 (m, 1H), 7.23 – 7.04 (m, 5H), 6.97 (d,  $J = 8.8$  Hz, 2H), 6.83 (t,  $J = 6.7$  Hz, 1H), 3.83 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.94, 151.69, 147.71, 131.04, 130.02, 129.69, 128.16, 126.64, 126.39, 125.55, 117.29, 113.78, 112.87, 102.01, 55.30.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  214.23.



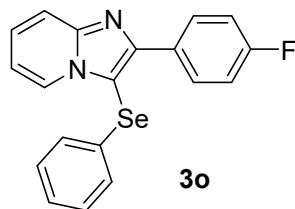
**2-(4-methoxyphenyl)-3-(p-tolylselanyl)imidazo[1,2-a]pyridine (3m).**<sup>6</sup> Yield: 0.070g (74%); Colorless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (d,  $J = 6.8$  Hz, 1H), 8.13 (d,  $J = 8.8$  Hz, 2H), 7.69 (d,  $J = 9.0$  Hz, 1H), 7.34 – 7.21 (m, 1H), 7.06 – 6.92 (m, 6H), 6.82 (t,



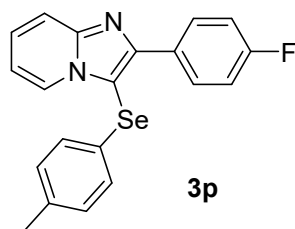
$J = 6.8$  Hz, 1H), 3.84 (s, 3H), 2.24 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.91, 151.40, 147.58, 136.65, 130.47, 130.03, 128.43, 127.08, 126.32, 125.57, 117.24, 113.76, 112.81, 102.43, 55.29, 20.95.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  208.17.



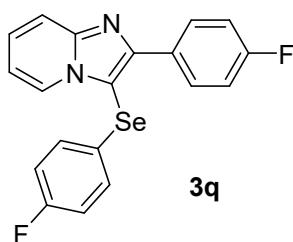
**3-((4-fluorophenyl)selanyl)-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (3n).** Yield: 0.077 g (78%); Yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (d,  $J = 6.8$  Hz, 1H), 8.12 (d,  $J = 8.7$  Hz, 2H), 7.69 (d,  $J = 9.0$  Hz, 1H), 7.28 (t,  $J = 8.1$  Hz, 2H), 7.09 – 7.06 (m, 2H), 6.98 (d,  $J = 8.7$  Hz, 2H), 6.92 – 6.73 (m, 3H), 3.83 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.05 (d,  $J = 246.6$  Hz), 160.82, 159.98, 151.56, 147.67, 130.27 (d,  $J = 7.7$  Hz), 130.00, 126.35 (d,  $J = 19.2$  Hz), 125.37, 117.36, 116.86 (d,  $J = 21.9$  Hz), 113.81, 112.94, 102.29, 55.30.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  210.42. HRMS  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{15}\text{FN}_2\text{OSe}$ , 399,0407; found: 399,0408.



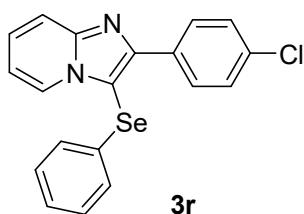
**2-(4-fluorophenyl)-3-(phenylselanyl)imidazo[1,2-*a*]pyridine (3o).**<sup>3</sup> Yield: 0.084 g (84%); Yellow solid, mp: 69-70 °C; Lit.: 70 - 72 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (d,  $J = 6.9$  Hz, 1H), 8.14 (dd,  $J = 8.7, 5.5$  Hz, 2H), 7.70 (d,  $J = 9.0$  Hz, 1H), 7.37 – 7.26 (m, 1H), 7.22 – 7.01 (m, 7H), 6.84 (t,  $J = 6.7$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  163.05 (d,  $J = 248.0$  Hz), 150.91, 147.74, 130.77, 130.52 (d,  $J = 8.2$  Hz), 129.76, 128.19, 126.71 (d,  $J = 17.3$  Hz), 125.63, 117.48, 115.30 (d,  $J = 21.5$  Hz), 113.11, 102.65.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  213.19.



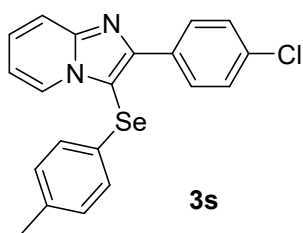
**2-(4-fluorophenyl)-3-(p-tolylselanyl)imidazo[1,2-*a*]pyridine (3p).** Yield: 0.086 g (87%); Yellow solid, mp 89-94 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (d,  $J = 6.8$  Hz, 1H), 8.14 (d,  $J = 8.4$  Hz, 2H), 7.68 (d,  $J = 9.0$  Hz, 1H), 7.39 (d,  $J = 8.4$  Hz, 2H), 7.33 – 7.22 (m, 1H), 6.98 (s, 4H), 6.82 (t,  $J = 6.8$  Hz, 1H), 2.23 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.93 (d,  $J = 248.0$  Hz), 150.50, 147.53, 136.75, 130.49, 130.46, 130.41, 129.92 (d,  $J = 3.2$  Hz), 128.40, 126.60 (d,  $J = 25.5$  Hz), 125.56, 117.31, 115.18 (d,  $J = 21.4$  Hz), 112.97, 103.02, 20.86.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  207.08. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{15}\text{FN}_2\text{Se}$ , 383,0458 found: 383,0457.



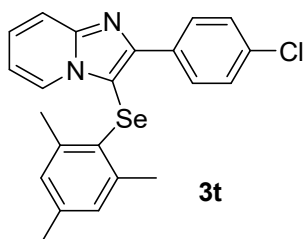
**2-(4-fluorophenyl)-3-((4-fluorophenyl)selanyl)imidazo[1,2-*a*]pyridine (3q).** Yield: 0.056 g (62%); Yellow solid, mp: 114-116 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.32 (d,  $J = 6.7$  Hz, 1H), 8.14 (dd,  $J = 8.2, 6.7$  Hz, 2H), 7.69 (d,  $J = 8.9$  Hz, 1H), 7.31 (d,  $J = 7.7$  Hz, 1H), 7.20 – 6.98 (m, 4H), 6.89 – 6.83 (m, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ ) 163.75 (d,  $J = 97.0$  Hz), 161.29 (d,  $J = 95.5$  Hz), 150.63, 147.60, 130.49, 130.45 (d,  $J = 8.2$  Hz), 130.29 (d,  $J = 7.8$  Hz), 130.25, 129.79, 129.76, 126.02 (d,  $J = 128.0$  Hz), 124.93 (d,  $J = 3.3$  Hz), 116.87 (d,  $J = 21.9$  Hz), 116.76, 115.28 (d,  $J = 21.5$  Hz), 113.15, 102.91.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  209.63. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{12}\text{F}_2\text{N}_2\text{Se}$ , 387,0207; found: 387,0213.



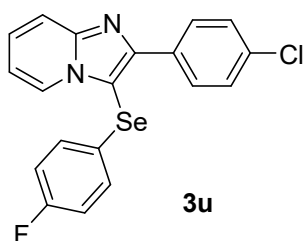
**2-(4-chlorophenyl)-3-(phenylselanyl)imidazo[1,2-*a*]pyridine (3r).**<sup>5</sup> Yield: 0.065 g (69%); Yellow solid, mp: 94-96 °C; Lit.: 96-98 °C.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (d,  $J = 6.8$  Hz, 1H), 8.12 (d,  $J = 8.3$  Hz, 2H), 7.70 (d,  $J = 8.9$  Hz, 1H), 7.39 (d,  $J = 8.3$  Hz, 2H), 7.34 – 7.27 (m, 1H), 7.21 – 7.00 (m, 5H), 6.85 (t,  $J = 6.8$  Hz, 1H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.52, 147.75, 134.47, 132.28, 130.64, 129.96, 129.77, 128.54, 128.25, 126.85, 126.72, 125.63, 117.53, 113.20, 103.04.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  218.90.



**2-(4-chlorophenyl)-3-(p-tolylselanyl)imidazo[1,2-*a*]pyridine (3s).** Yield: 0.063 g (67%); Yellow solid, 102-105 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (d,  $J = 6.8$  Hz, 1H), 8.14 (d,  $J = 8.4$  Hz, 2H), 7.68 (d,  $J = 9.0$  Hz, 1H), 7.39 (d,  $J = 8.4$  Hz, 2H), 7.33 – 7.22 (m, 1H), 6.98 (s, 4H), 6.82 (t,  $J = 6.8$  Hz, 1H), 2.23 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.23, 147.61, 136.85, 134.35, 132.35, 130.50, 129.92, 128.47, 126.68, 126.54, 125.60, 117.45, 113.05, 103.40, 20.92.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  207.66. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{15}\text{ClN}_2\text{Se}$ , 399,0160; found: 399,0161.

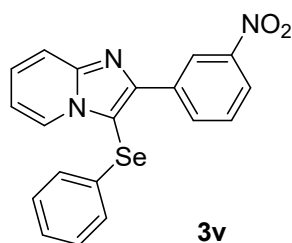


**2-(4-chlorophenyl)-3-(mesityl)imidazo[1,2-*a*]pyridine (3t).** Yield: 0.070 g (75%); Yellow pale oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (dd,  $J = 14.5, 7.7$  Hz, 3H), 7.61 (d,  $J = 9.0$  Hz, 1H), 7.41 (d,  $J = 8.5$  Hz, 2H), 7.24 – 7.16 (m, 1H), 6.79 (d,  $J = 10.4$  Hz, 3H), 2.22 (s, 6H), 2.18 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.91, 146.91, 141.31, 138.19, 134.08, 132.85, 130.14, 129.48, 128.33, 126.21, 125.57, 125.44, 117.44, 112.72, 104.68, 23.61, 20.79.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  141.06. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{19}\text{ClN}_2\text{Se}$ , 427,0473; found: 427,0475.

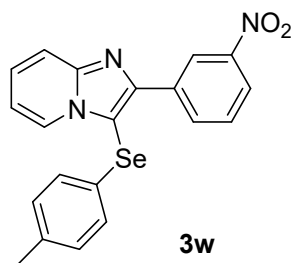


**2-(4-chlorophenyl)-3-((4-fluorophenyl)selanyl)imidazo[1,2-*a*]pyridine (3u).** Yield: 0.070 g (72%); Orange solid, mp: 115-118 °C  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (d,  $J = 6.9$  Hz, 1H), 8.12 (d,  $J = 8.5$  Hz, 2H), 7.69 (d,  $J = 9.0$  Hz, 1H), 7.41 (d,  $J = 8.5$  Hz, 2H), 7.36 – 7.28 (m, 1H), 7.08 (dd,  $J = 8.7, 5.2$  Hz, 2H), 6.96 – 6.81 (m, 3H).  $^{13}\text{C NMR}$  (101

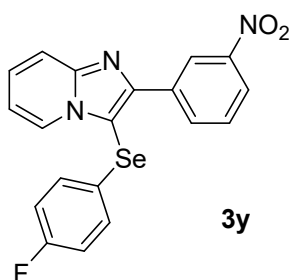
MHz, CDCl<sub>3</sub>)  $\delta$  162.14 (d,  $J$  = 246.9 Hz), 150.41, 147.71, 134.56, 132.20, 130.43 (d,  $J$  = 7.8 Hz), 129.94, 128.58, 126.77, 125.46, 124.90 (d,  $J$  = 3.3 Hz), 117.63, 116.97 (d,  $J$  = 21.9 Hz), 113.28, 103.30. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>)  $\delta$  209.93. HRMS  $m/z$ : [M+H]<sup>+</sup> calcd for C<sub>19</sub>H<sub>12</sub>ClFN<sub>2</sub>Se, 402,9909; found: 402,9914.



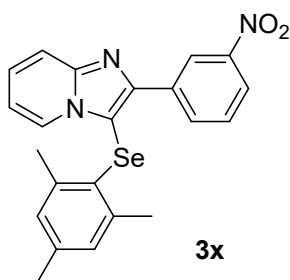
**2-(3-nitrophenyl)-3-(phenylselanyl)imidazo[1,2-*a*]pyridine (3v).**<sup>7</sup> Yield: 0.077 g (78%); Yellow solid, mp: 169-171 °C; Lit.: 169-170 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.11 (s, 1H), 8.54 (d,  $J$  = 7.6 Hz, 1H), 8.42 (d,  $J$  = 6.8 Hz, 1H), 8.21 (d,  $J$  = 8.0 Hz, 1H), 7.74 (d,  $J$  = 9.0 Hz, 1H), 7.59 (t,  $J$  = 8.0 Hz, 1H), 7.45 – 7.30 (m, 1H), 7.23 – 7.07 (m, 5H), 6.92 (t,  $J$  = 6.7 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  148.89, 148.38, 147.82, 135.61, 134.41, 130.24, 129.87, 129.24, 128.65, 127.09, 125.71, 123.60, 122.99, 117.80, 113.59, 104.22. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>)  $\delta$  211.71.



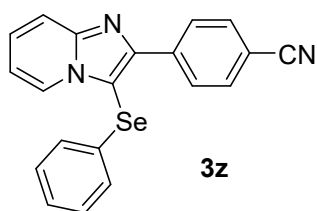
**2-(3-nitrophenyl)-3-(p-tolylselanyl)imidazo[1,2-*a*]pyridine (3w).** Yield: 0.070 g (77%); Yellow solid, mp: 175-177 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.13 (s, 1H), 8.55 (d,  $J$  = 7.8 Hz, 1H), 8.43 (d,  $J$  = 6.9 Hz, 1H), 8.20 (d,  $J$  = 9.1 Hz, 1H), 7.71 (d,  $J$  = 9.0 Hz, 1H), 7.58 (t,  $J$  = 8.0 Hz, 1H), 7.39 – 7.29 (m, 1H), 7.02 (q,  $J$  = 8.2 Hz, 4H), 6.91 (d,  $J$  = 6.8 Hz, 1H), 2.24 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  148.57, 148.35, 147.70, 137.28, 135.71, 134.42, 130.63, 129.21, 129.00, 126.98, 126.33, 125.71, 123.57, 122.91, 117.74, 113.50, 104.67, 20.97. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>)  $\delta$  205.64. HRMS  $m/z$ : [M+H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>Se, 410,0403; found: 410,0404.



**3-(4-fluorobenzyl)-2-(3-nitrophenyl)imidazo[1,2-*a*]pyridine (3y).** Yield: 0.070 g (73%); Yellow solid, mp: 171-173°C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.11 (s, 1H), 8.54 (d,  $J = 7.8$  Hz, 2H), 8.44 (d,  $J = 6.9$  Hz, 2H), 8.27 – 8.17 (m, 2H), 7.73 (d,  $J = 9.0$  Hz, 2H), 7.62 (t,  $J = 8.0$  Hz, 1H), 7.45 – 7.33 (m, 2H), 7.19 – 7.08 (m, 2H), 7.03 – 6.71 (m, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.30 (d,  $J = 247.4$  Hz), 148.74, 148.37, 147.78, 135.53, 134.39, 130.91 (d,  $J = 7.9$  Hz), 129.32, 127.15, 125.53, 123.30 (d,  $J = 46.7$  Hz), 117.90, 117.10 (d,  $J = 22.0$  Hz), 113.68, 104.46.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  208.28. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{12}\text{FN}_3\text{O}_2\text{Se}$ , 414,0152; found: 414,0158.

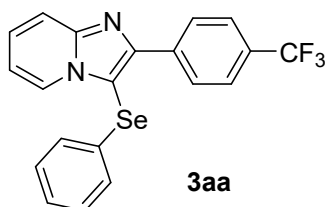


**3-(mesitylselanyl)-2-(3-nitrophenyl)imidazo[1,2-*a*]pyridine (3x).** Yield: 0.073 g (76%); Yellow solid, mp: 178-180 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.98 (s, 1H), 8.44 (d,  $J = 7.8$  Hz, 1H), 8.21 (d,  $J = 9.4$  Hz, 1H), 8.12 (d,  $J = 6.9$  Hz, 2H), 7.78 – 7.45 (m, 2H), 7.48 – 7.09 (m, 1H), 6.86 – 6.80 (m, 3H), 2.21 (s, 6H), 2.18 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.20, 147.00, 141.20, 138.38, 136.08, 129.59, 129.06, 126.06, 125.55, 123.53, 122.72, 117.66, 113.16, 105.63, 23.59, 20.77.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  139.54. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_2\text{Se}$ , 438,0716; found: 438,0713.

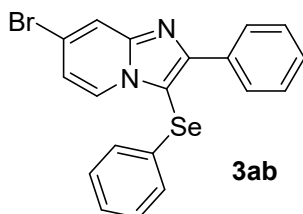


**4-(3-(phenylselanyl)imidazo[1,2-*a*]pyridin-2-yl)benzonitrile (3z).**<sup>3</sup> Yield: 0.053 g (57%); Yellow oil;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (dd,  $J = 15.5, 7.4$  Hz, 3H), 7.71

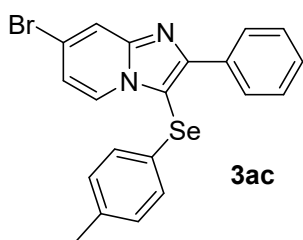
(t,  $J = 7.4$  Hz, 3H), 7.45 – 7.29 (m, 1H), 7.25 – 7.14 (m, 3H), 7.13 – 7.02 (m, 2H), 6.90 (d,  $J = 6.8$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  149.27, 147.88, 138.34, 132.10, 130.22, 129.90, 129.06, 128.31, 127.09, 125.71, 119.00, 117.80, 113.61, 111.70, 104.23.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  214.74.



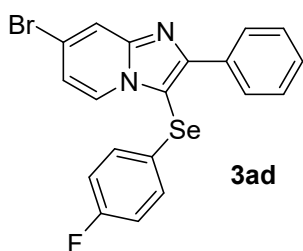
**3-(phenylselanyl)-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridine (3aa).** Yield: 0.072 g (70%); Yellow oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (dd,  $J = 20.2, 7.5$  Hz, 3H), 7.70 (dd,  $J = 14.3, 8.6$  Hz, 3H), 7.39 – 7.26 (m, 1H), 7.21 – 7.00 (m, 5H), 6.86 (t,  $J = 6.8$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.05, 147.84, 137.32, 130.35 (q,  $J = 32$  Hz), 129.83, 128.90, 128.35, 128.33, 128.28, 128.22, 126.96, 126.91, 125.69, 125.24 (q,  $J = 3.8$  Hz), 122.92, 103.80.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  214.03. HRMS  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{13}\text{F}_3\text{N}_2\text{Se}$ , 419,0269; found: 419,0272.



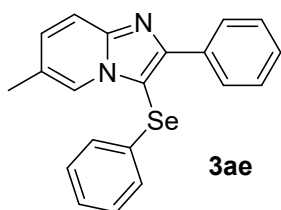
**7-bromo-2-phenyl-3-(phenylselanyl)imidazo[1,2-*a*]pyridine (3ab).** Yield 0.066 g (64%); White solid. m.p 115-117 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.18 (d,  $J = 7.2$  Hz, 1H), 8.13 (d,  $J = 7.6$  Hz, 2H), 7.88 (s, 1H), 7.49 – 7.32 (m, 3H), 7.17 (d,  $J = 5.6$  Hz, 3H), 7.13 – 7.01 (m, 2H), 6.93 (d,  $J = 7.2$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  152.42, 147.70, 133.36, 130.40, 129.81, 128.73, 128.41, 128.36, 126.94, 125.92, 120.52, 103.43.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  216.43. HRMS  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{13}\text{BrN}_2\text{Se}$ , 428,9497; found: 428,9503.



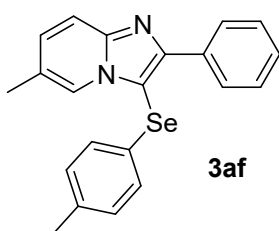
**7-bromo-2-phenyl-3-(p-tolylselanyl)imidazo[1,2-a]pyridine (3ac).** Yield 0.089 g (81%); White solid. m.p 118-121 °C;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 (d,  $J = 7.2$  Hz, 1H), 8.14 (d,  $J = 7.2$  Hz, 2H), 7.87 (d,  $J = 1.6$  Hz, 1H), 7.53 – 7.32 (m, 3H), 7.00 (s, 4H), 6.94 (dd,  $J = 7.2, 1.8$  Hz, 1H), 2.25 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  152.17, 147.60, 137.01, 133.43, 130.58, 128.74, 128.68, 128.38, 126.41, 125.94, 120.39, 119.71, 116.81, 103.86, 20.96.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  210.47. **HRMS** m/z:  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{15}\text{BrN}_2\text{Se}$ , 442,9654; found: 442,9658.



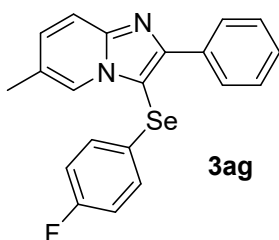
**7-bromo-3-((4-fluorophenyl)selanyl)-2-phenylimidazo[1,2-a]pyridine (3ad).** Yield 0.055 g (50%); White solid. m.p 128-134 °C.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 (d,  $J = 7.2$  Hz, 1H), 8.13 (d,  $J = 7.2$  Hz, 2H), 7.88 (s, 1H), 7.53 – 7.34 (m, 3H), 7.09 (dd,  $J = 8.6, 5.2$  Hz, 2H), 6.96 (dd,  $J = 7.2, 1.6$  Hz, 1H), 6.90 (t,  $J = 8.6$  Hz, 2H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  163.42, 160.96, 152.30, 147.66, 133.25, 130.60, 130.52, 128.81, 128.71, 128.44, 125.74, 124.66, 124.63, 120.61, 119.83, 117.00, 116.91, 103.72.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  214.78. **HRMS** m/z:  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{12}\text{BrFN}_2\text{Se}$ , 446,9403; found: 446,9409.



**6-methyl-2-phenyl-3-(phenylselanyl)imidazo[1,2-a]pyridine (3ae).** Yield 0.062 g (69%); Yellow oil.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.13 (d,  $J = 7.1$  Hz, 3H), 7.61 (d,  $J = 9.1$  Hz, 1H), 7.47 – 7.28 (m, 3H), 7.21 – 7.00 (m, 6H), 2.29 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.64, 146.81, 133.90, 131.29, 129.69, 129.66, 128.69, 128.35, 128.29, 126.58, 123.33, 122.86, 116.86, 102.36, 18.41.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  214.30. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{13}\text{BrN}_2\text{Se}$ , 428,9497; found: 428,9503.

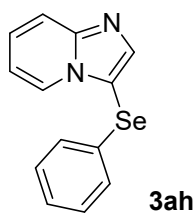


**6-methyl-2-phenyl-3-(p-tolylselanyl)imidazo[1,2-a]pyridine (3af).**<sup>6</sup> Yield 0.069 g (74%); Yellow oil.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.24 – 8.04 (m, 3H), 7.59 (d,  $J = 9.1$  Hz, 1H), 7.41 (t,  $J = 7.5$  Hz, 2H), 7.33 (t,  $J = 7.3$  Hz, 1H), 7.11 (d,  $J = 9.1$  Hz, 1H), 7.05 – 6.86 (m, 4H), 2.27 (s, 3H), 2.22 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.45, 146.73, 136.54, 134.03, 130.48, 129.51, 128.69, 128.27, 127.39, 123.36, 122.72, 116.85, 102.72, 20.97, 18.42.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  208.06.



**3-((4-fluorophenyl)selanyl)-6-methyl-2-phenylimidazo[1,2-a]pyridine (3ag).** Yield 0.076 g (80%); Yellow oil.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.12 (d,  $J = 7.3$  Hz, 3H), 7.61 (d,  $J = 9.0$  Hz, 1H), 7.45 – 7.35 (m, 3H), 7.16 (dd,  $J = 9.0, 1.3$  Hz, 1H), 7.12 – 7.01 (m, 2H), 6.89 (t,  $J = 8.7$  Hz, 2H), 2.32 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.03 (d,  $J = 246.2$  Hz), 151.51, 146.76, 133.80, 130.13 (d,  $J = 7.8$  Hz), 129.72, 128.66, 128.42, 128.32, 125.47 (d,  $J = 3.3$  Hz), 123.06 (d,  $J = 19.7$  Hz), 116.95 (d,  $J = 4.6$  Hz), 116.75, 102.63, 18.42.  $^{77}\text{Se NMR}$  (76 MHz,  $\text{CDCl}_3$ )  $\delta$  210.84. **HRMS**  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{15}\text{FN}_2\text{Se}$ , 383,0458; found: 383,0459.





**3-(phenylselanyl)imidazo[1,2-a]pyridine (3ah).**<sup>8</sup> Yield: 0.049 g (73%); Yellow solid. m.p 76-78 °C.; Lit.: 77-79 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.09 (d, *J* = 6.8 Hz, 1H), 8.00 – 7.90 (m, 2H), 7.84 (s, 1H), 7.63 (d, *J* = 9.1 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.21 – 7.09 (m, 1H), 6.81 – 6.68 (m, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 145.85, 145.71, 133.80, 128.74, 127.98, 126.07, 125.59, 124.63, 117.60, 112.42, 108.13. <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) δ 214.78.

## References

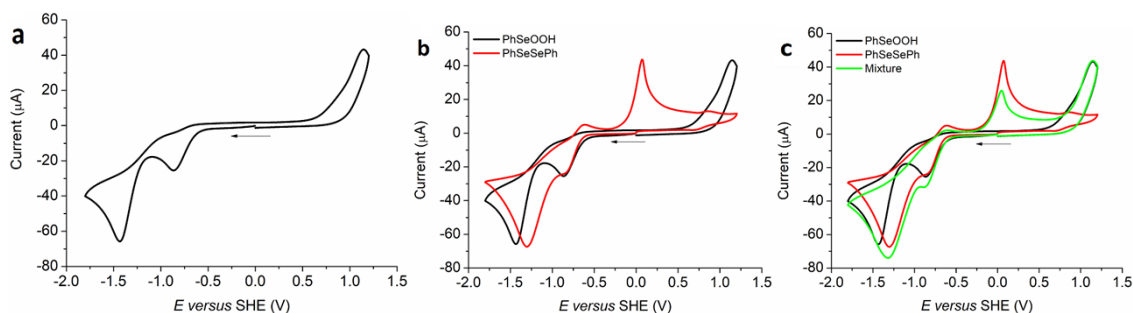
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2. L. Syper and J. Mlochowski, *Synthesis*, 1984, 747-752
3. K. Kondo, M. Mio, K. Keiko, M. Yuki, K. Naoki and Y. Shuji, *Synthesis*, 2018, **50**, 2200-2210.
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### 3. Electrochemical Analysis

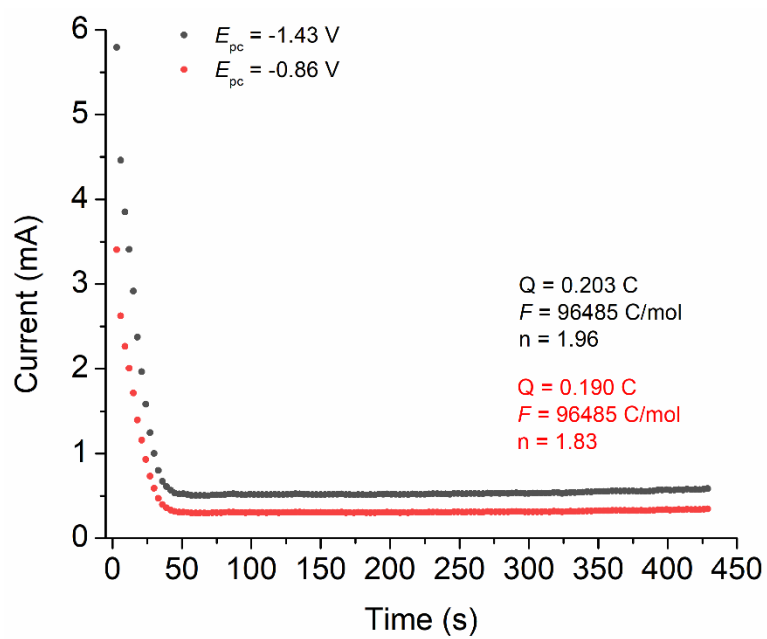
Electrochemical analysis by cyclic voltammetry (CV) and coulometry were recorded with a potentiostat/galvanostat AutoLab Eco Chemie PGSTAT 128N system at room temperature and under an argon atmosphere in dry *N,N*-dimethylformamide (DMF) solution. Electrochemical grade tetrabutylammonium hexafluorophosphate (0.1 M TBAPF<sub>6</sub>) was used as a supporting electrolyte. The redox experiments were carried out by employing a standard three-component system: a glassy carbon working electrode, a platinum-wired auxiliary electrode, and a platinum-wire pseudo-reference electrode. To monitor the reference electrode, the Fc/Fc<sup>+</sup> redox couple pair was used as an internal reference and the redox potentials are plotted *versus* SHE.<sup>1</sup> For coulometry analysis, a Fischer Pt work electrode was used.

Table S1. Redox potentials of PhSeO<sub>2</sub>H and PhSeSePh in DMF solution, at scan rate of 100 mV/s (*E* *versus* SHE).

Compound	Redox potentials				Energy parameters		
	$E_{red1}$ (V)	$E_{red2}$ (V)	$E_{ox1}$ (V)	$E_{ox2}$ (V)	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	$\Delta E$ (eV)
PhSeOOH	-0.86	-1.43	+1.15	-----	-5.95	-3.94	2.01
PhSeSePh	-0.82	-1.31	-0.62	+0.07	-4.18	-3.98	0.20



**Figure S1.** Cyclic voltammetry of a) PhSeO<sub>2</sub>H ; b) PhSeO<sub>2</sub>H and PhSeSePh; c) PhSeO<sub>2</sub>H, PhSeSePh, and a 1:1 mixture of PhSeO<sub>2</sub>H and PhSeSePh.



**Figures S2.** Coulometry analysis of PhSeO<sub>2</sub>H

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## NMR SPECTRA COPIES

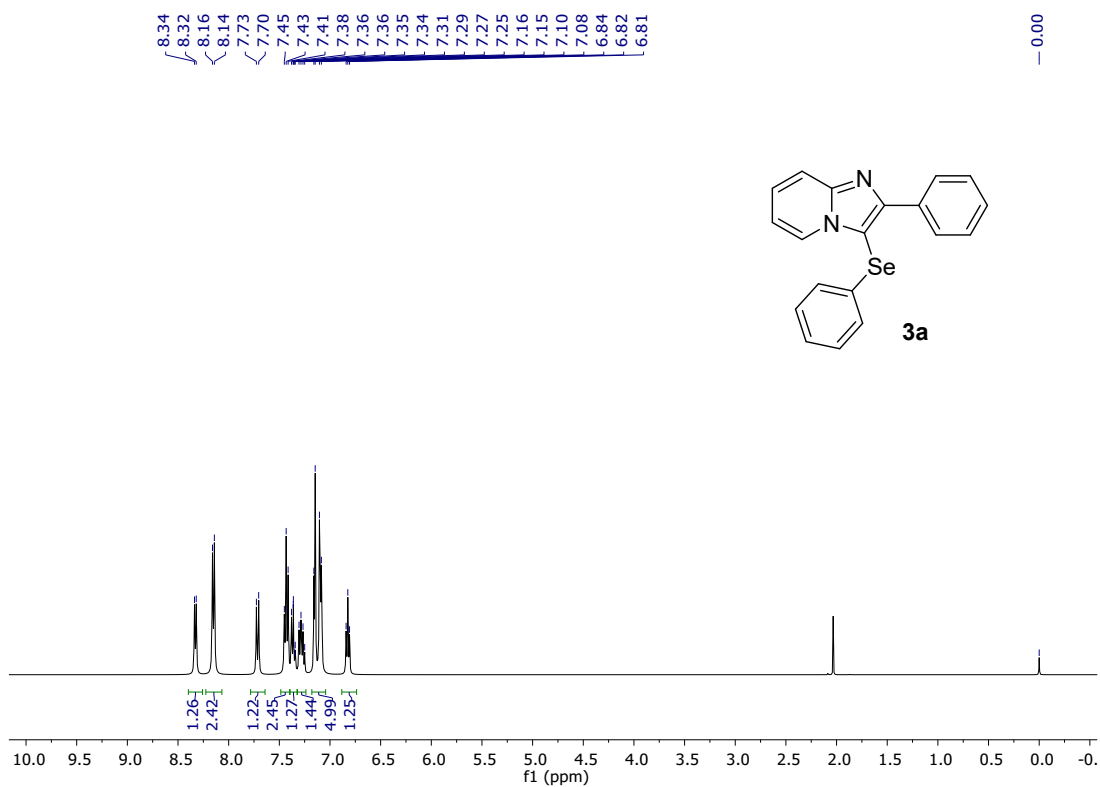


Figure S3. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3a**.

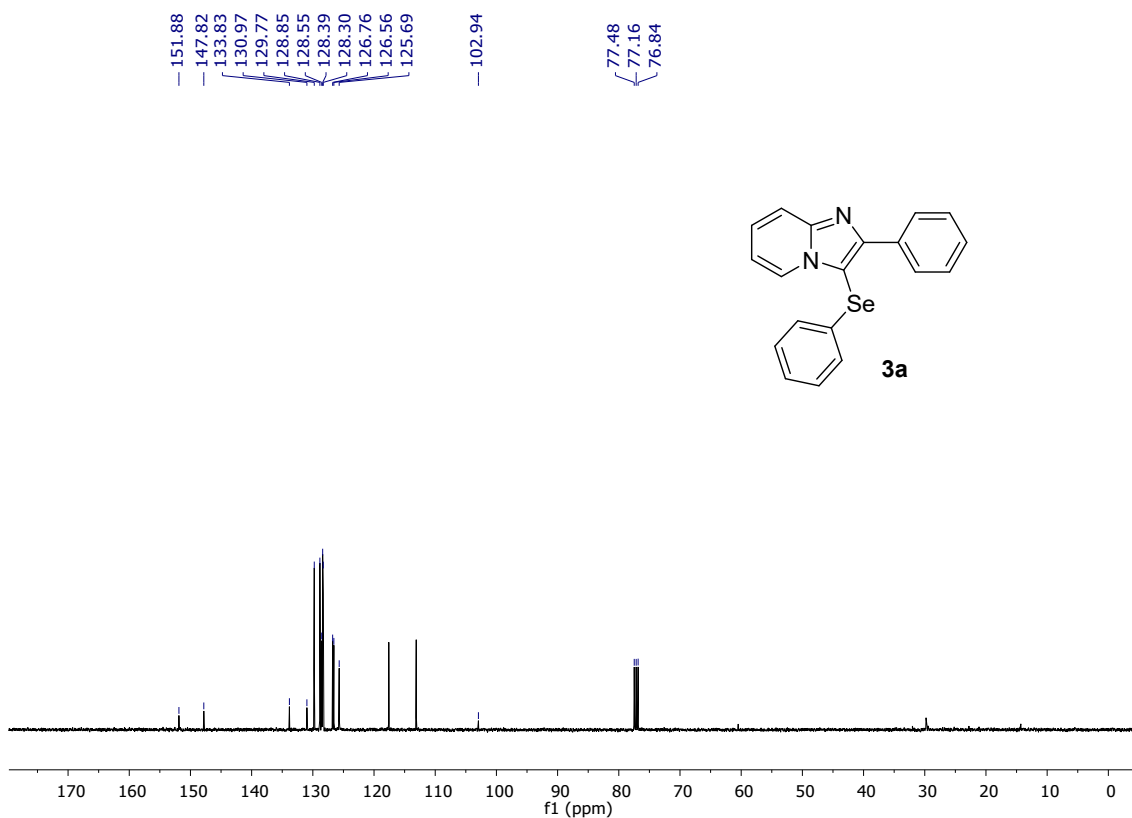
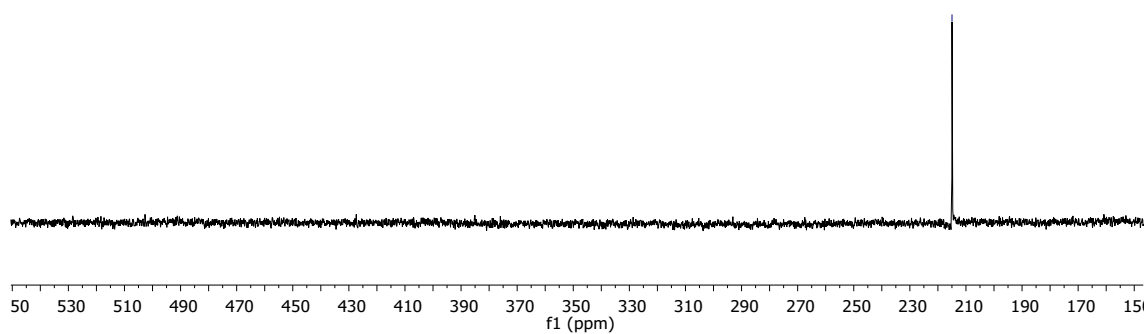
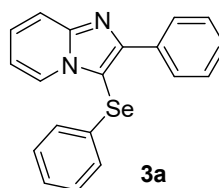
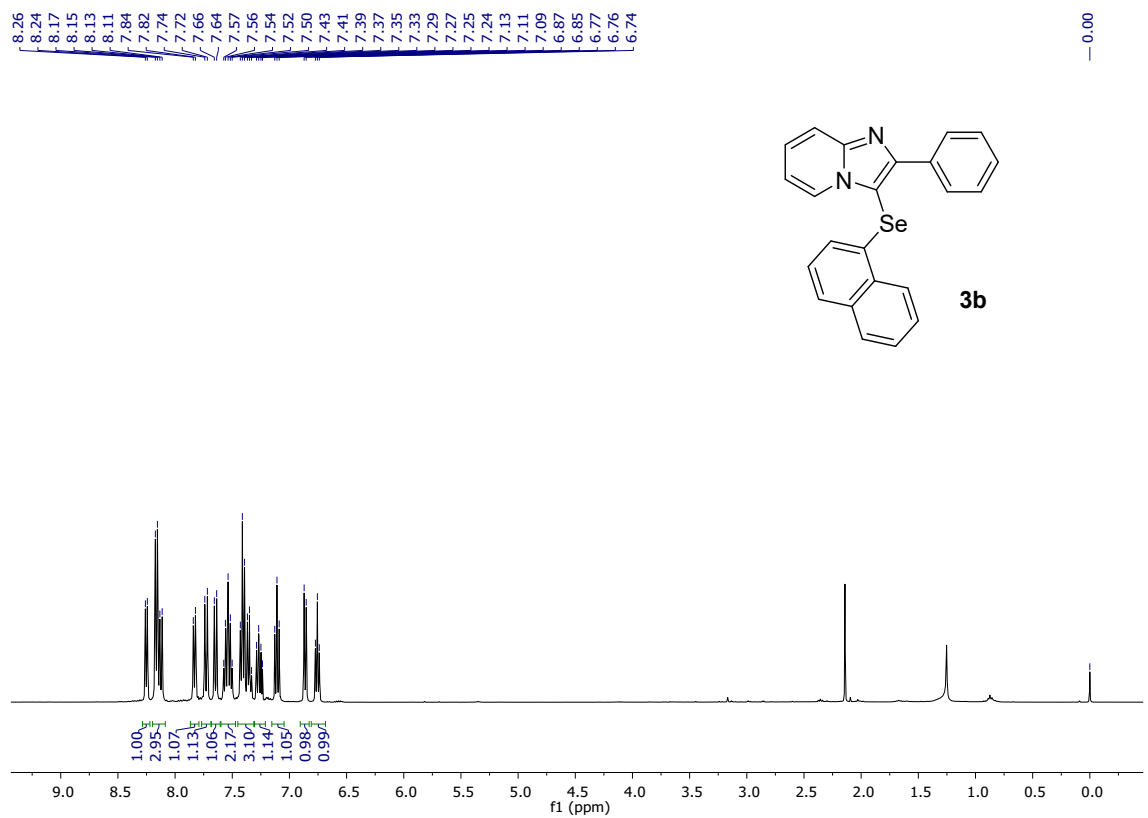


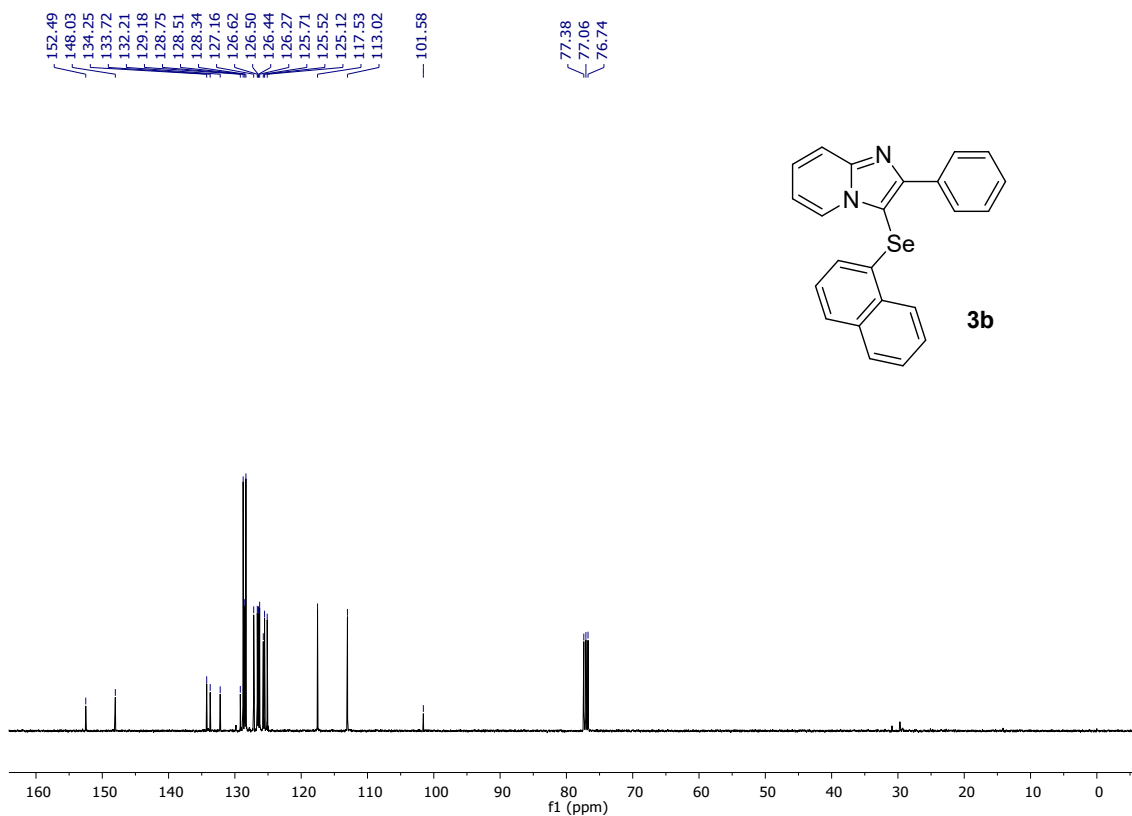
Figure S4. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3a**.



**Figure S5.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3a**.



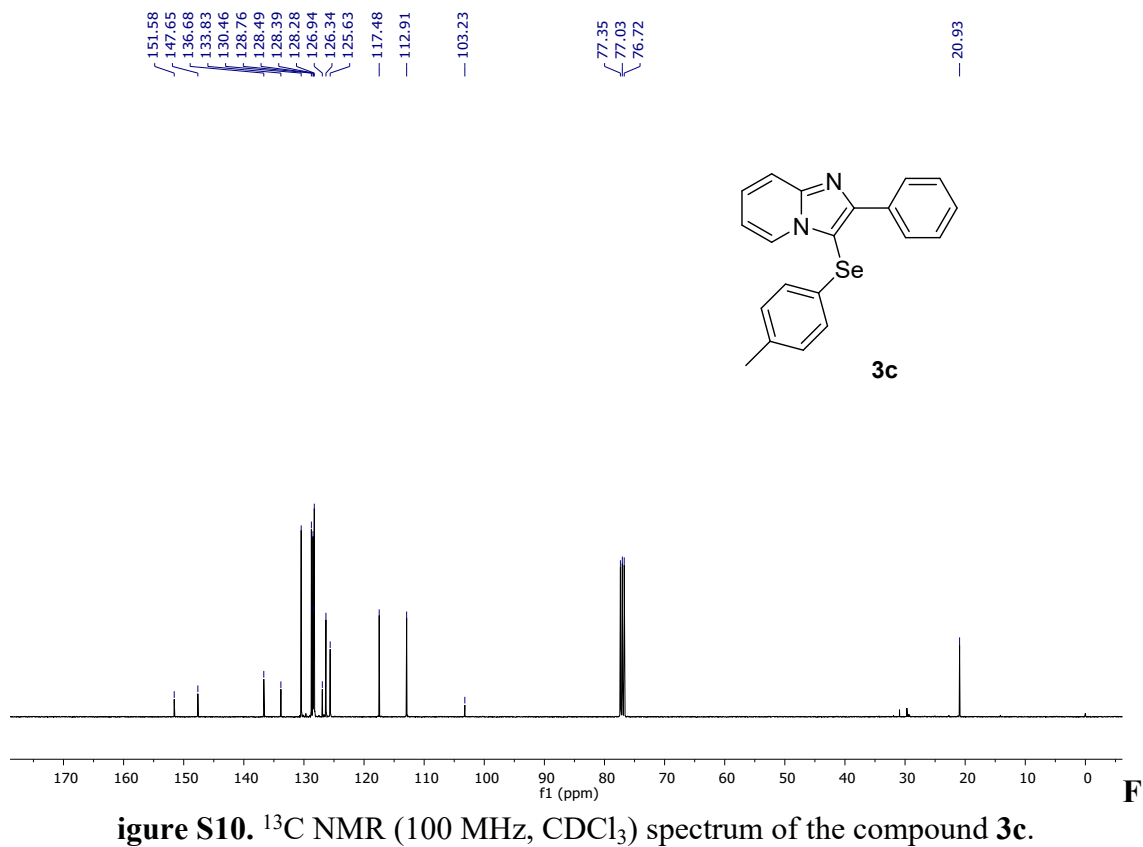
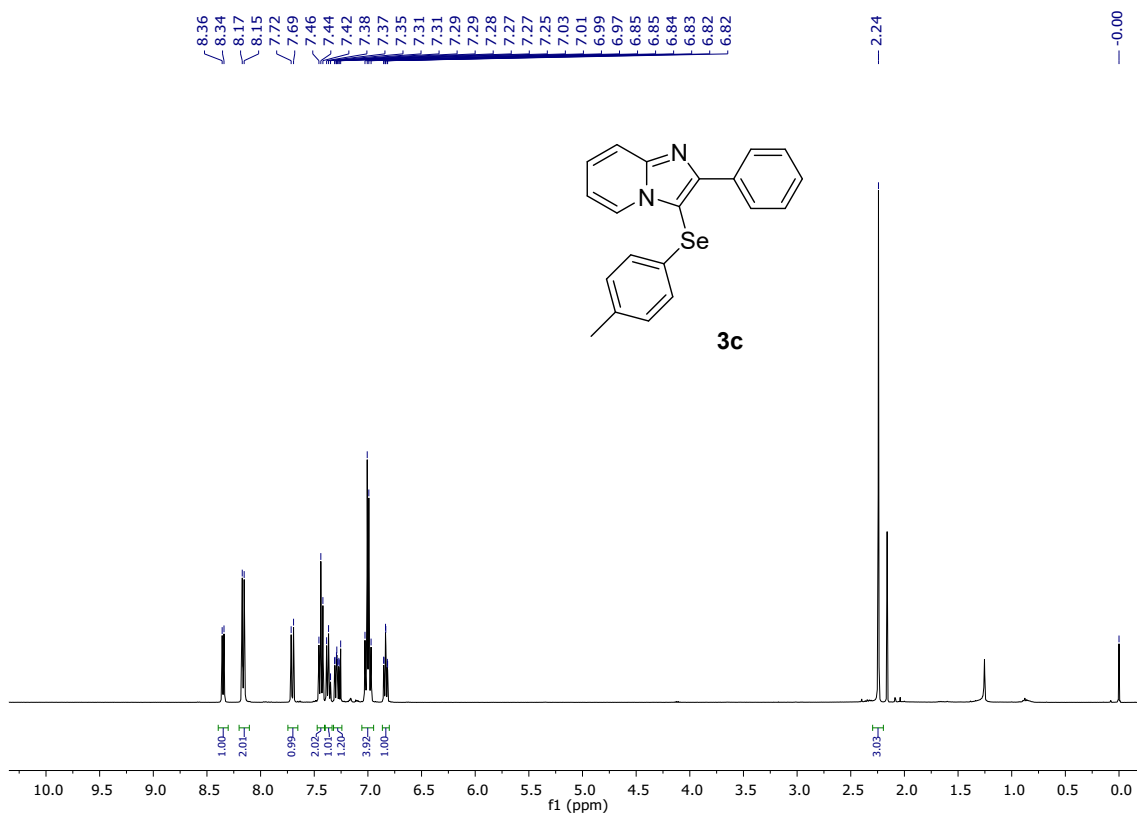
**Figure S6.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3b**.

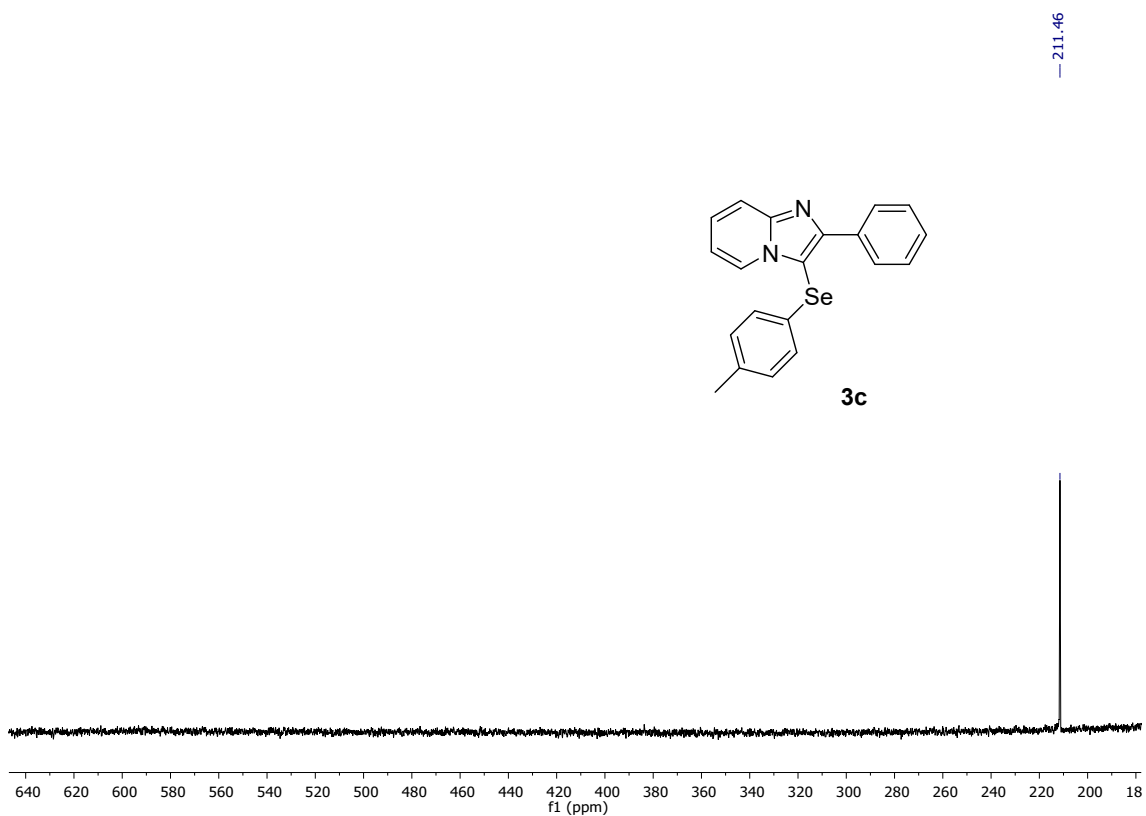


**Figure S7.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3b**.

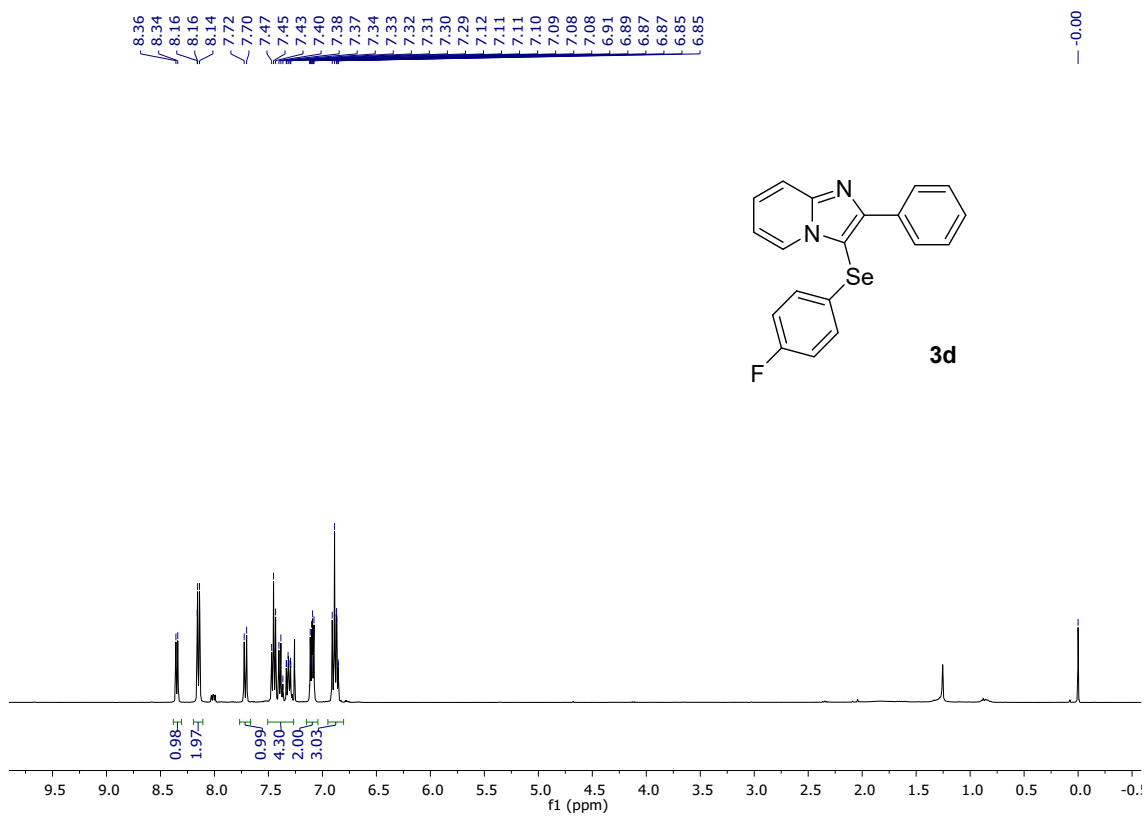


**Figure S8.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3b**.



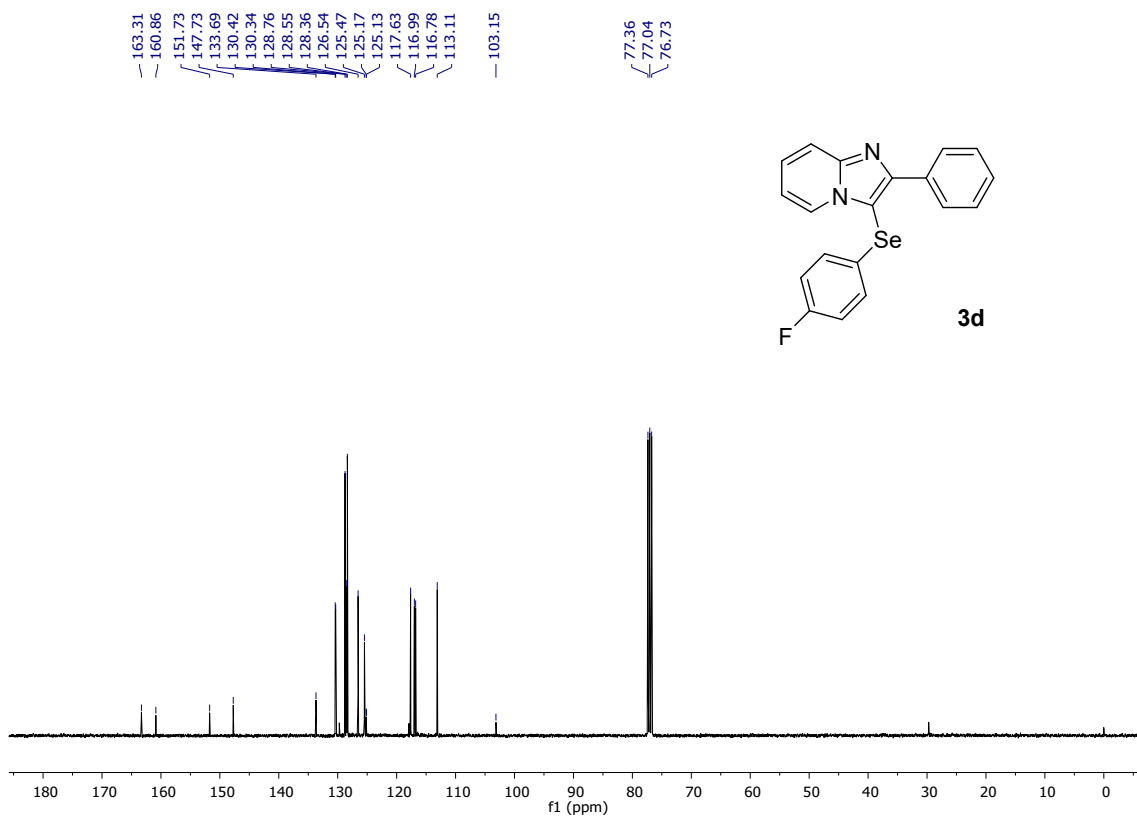


**Figure S11.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3c**.

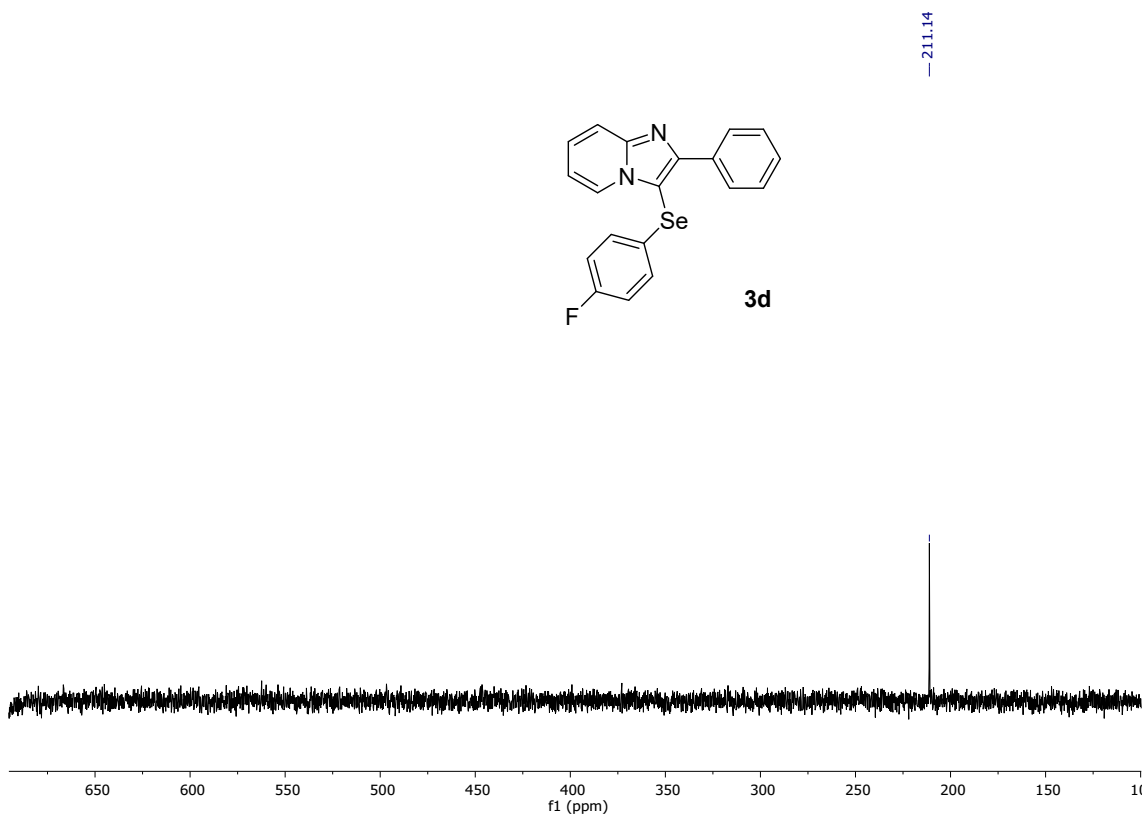


**Figure S12.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3d**.

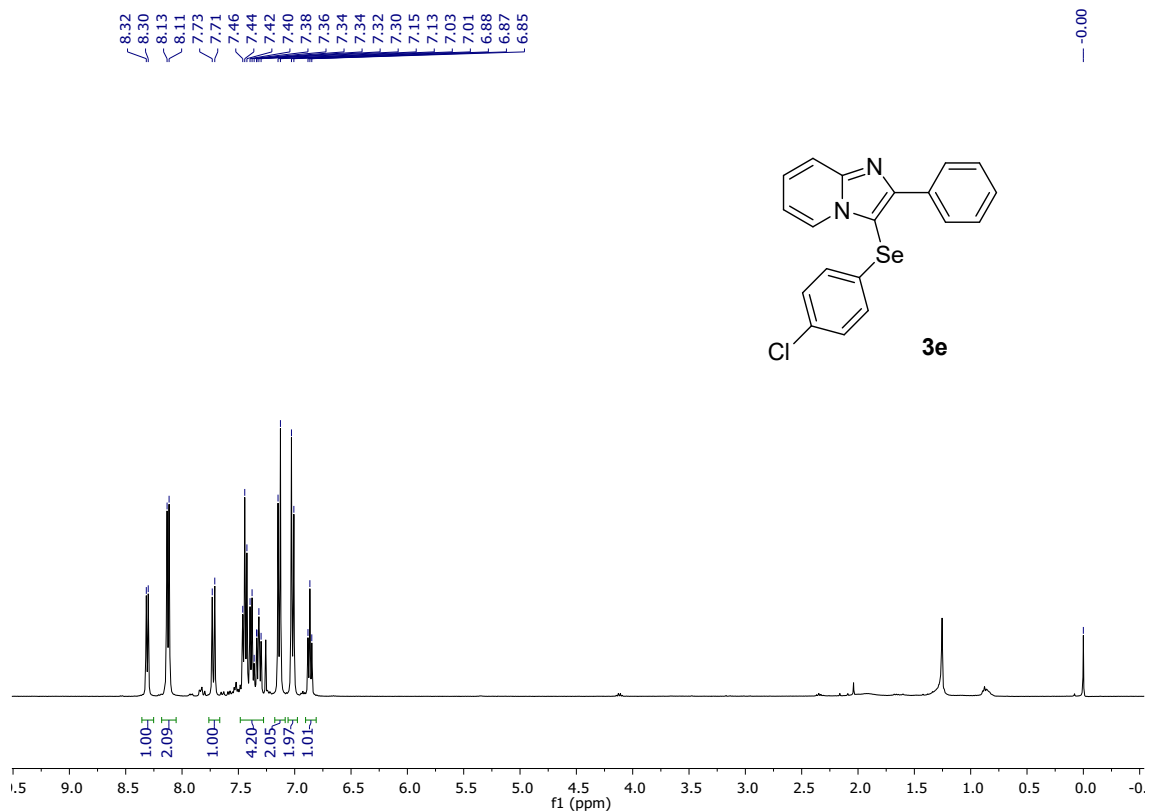




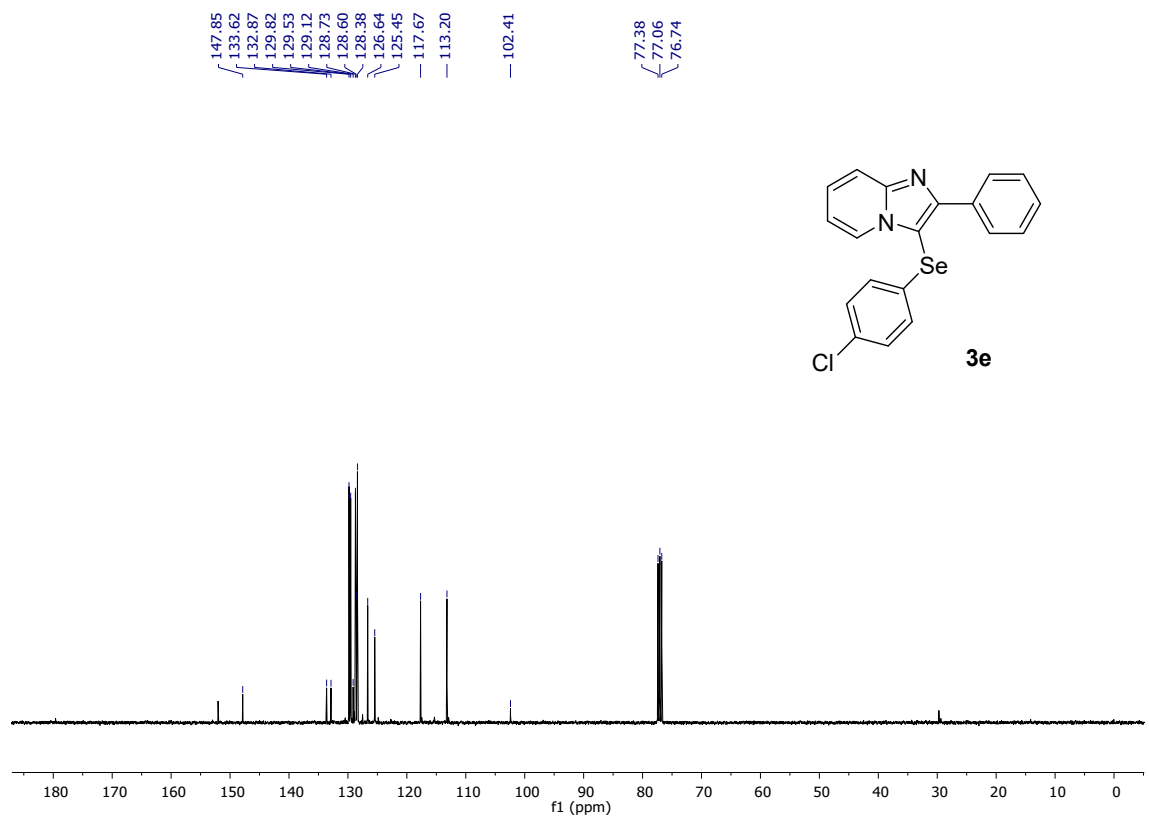
**Figure S13.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3d**.



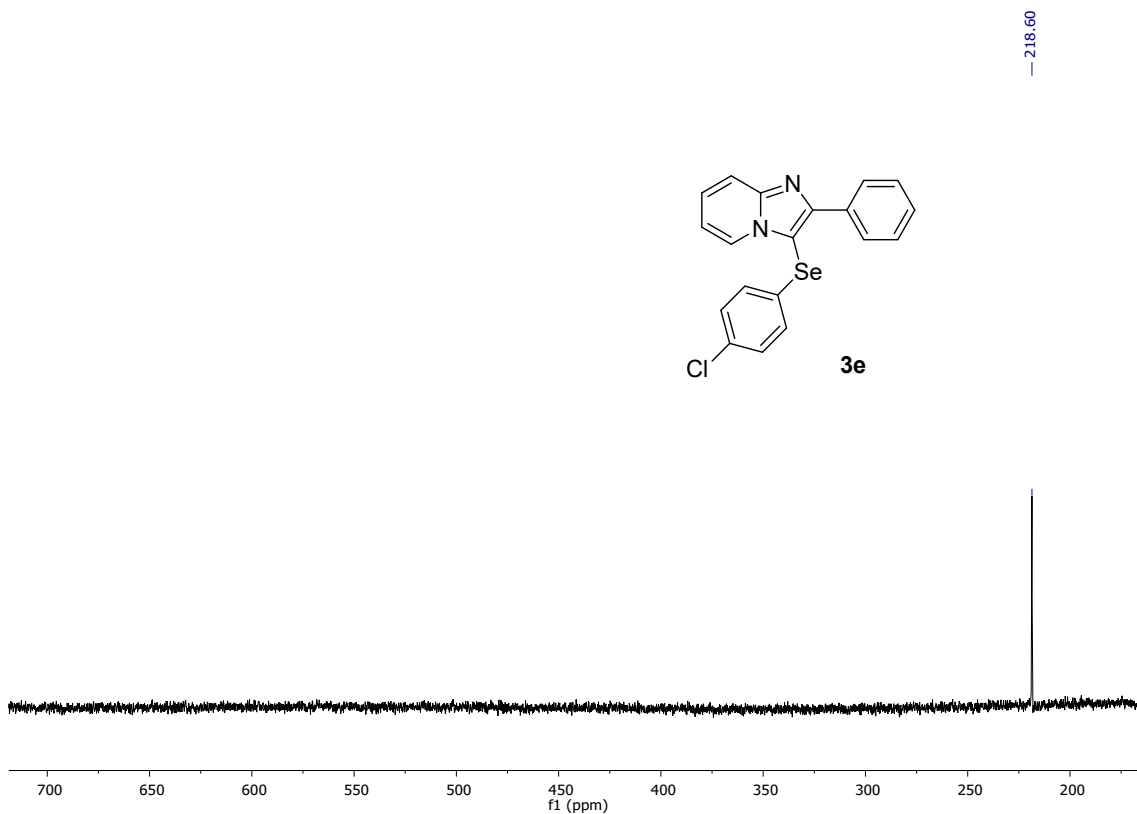
**Figure S14.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3d**.



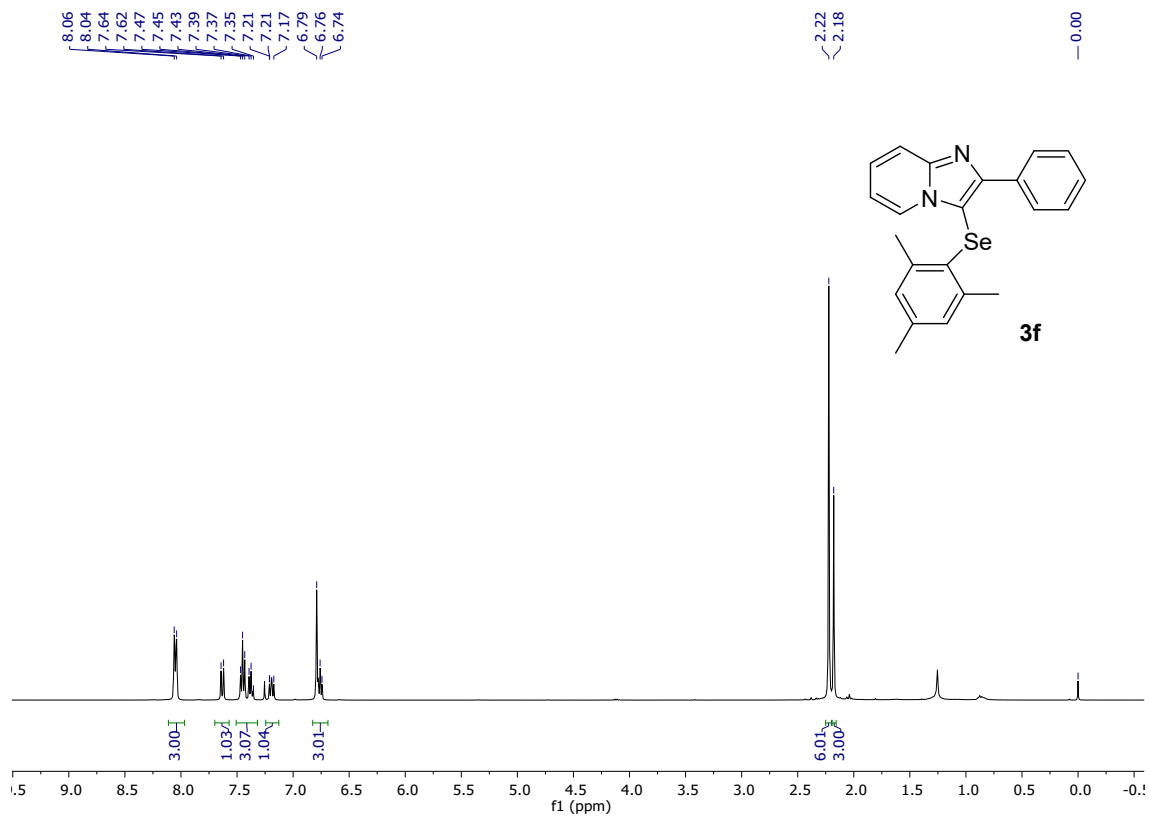
**Figure S15.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3e**.



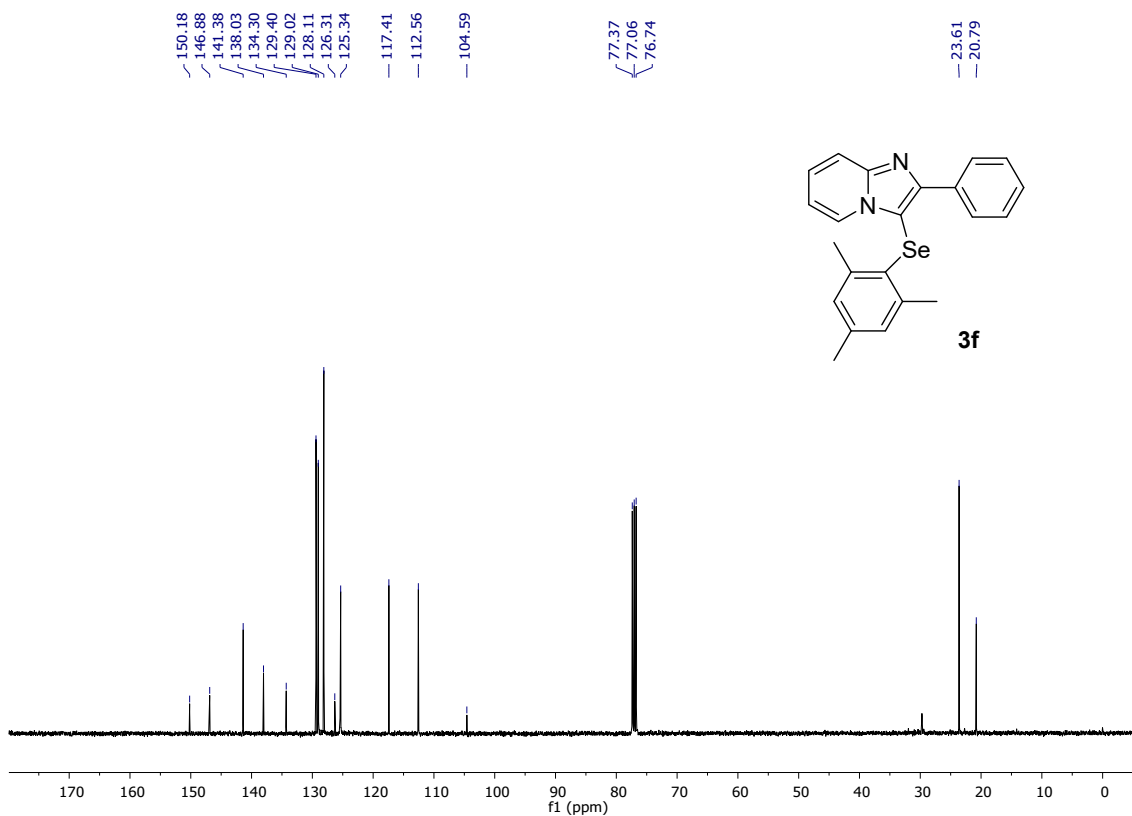
**Figure S16.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3e**.



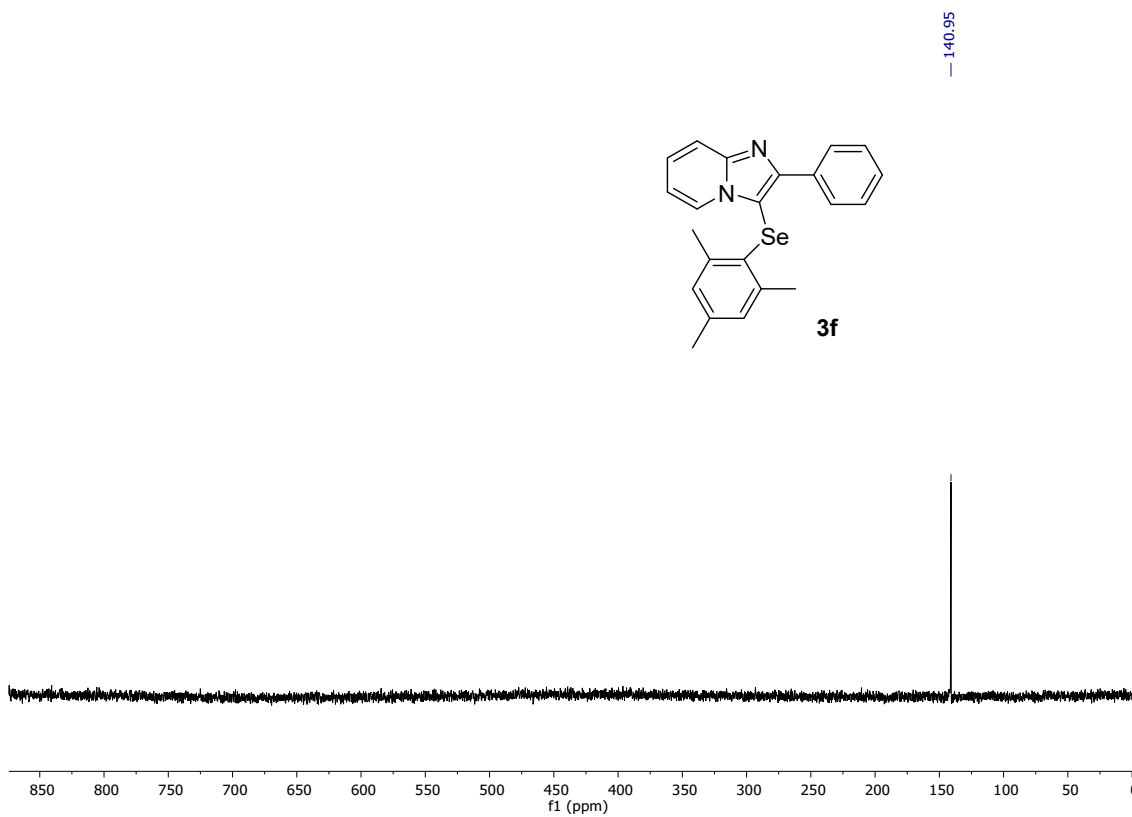
**Figure S17.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3e**.



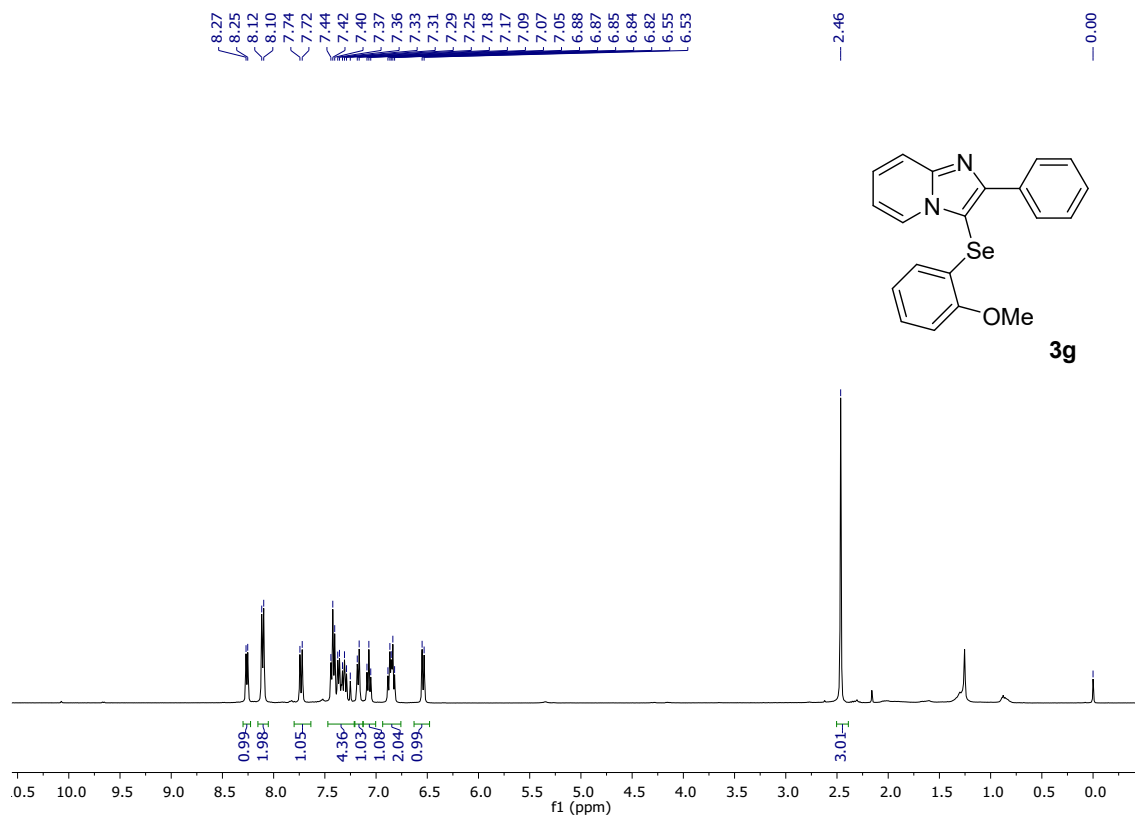
**Figure S18.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3f**.



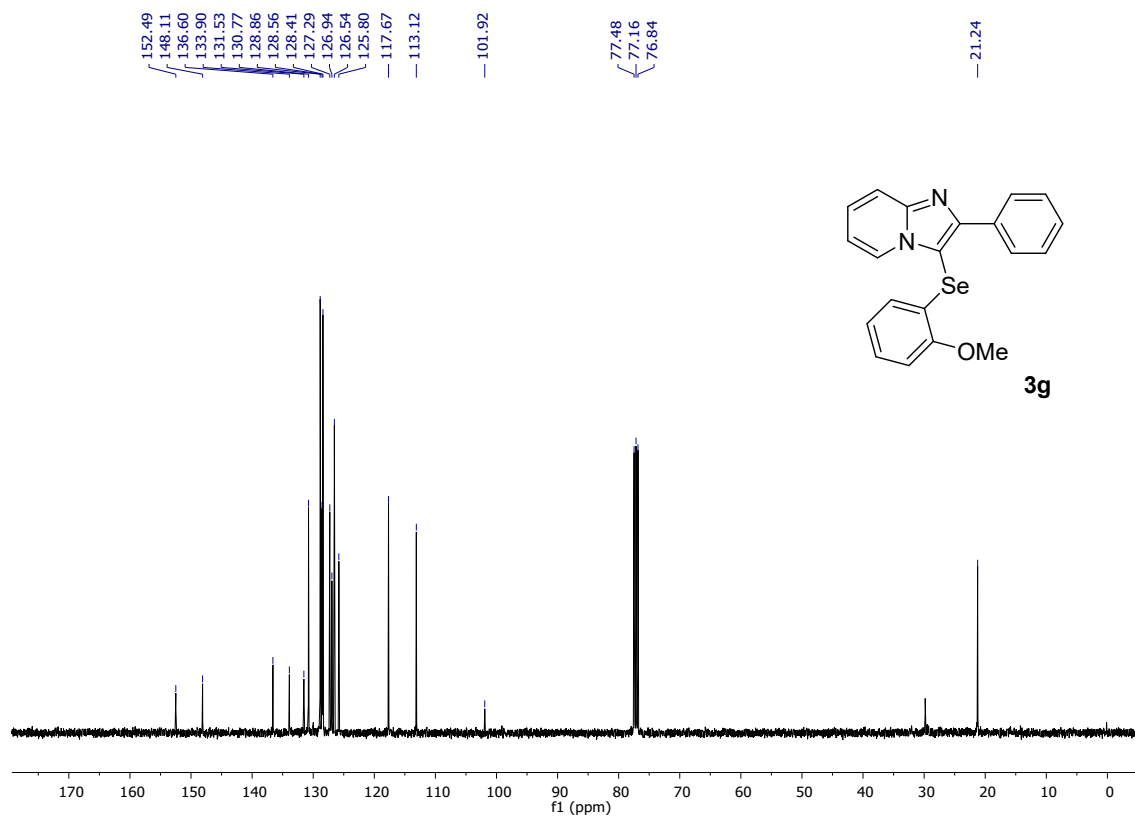
**Figure S19.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3f**.



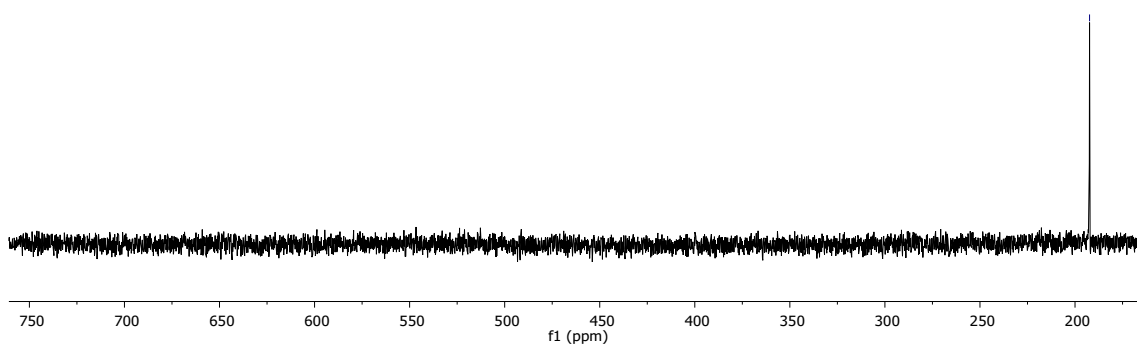
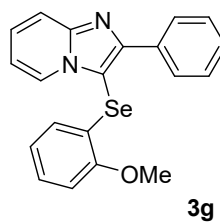
**Figure S20.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3f**.



**Figure S21.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3g**.



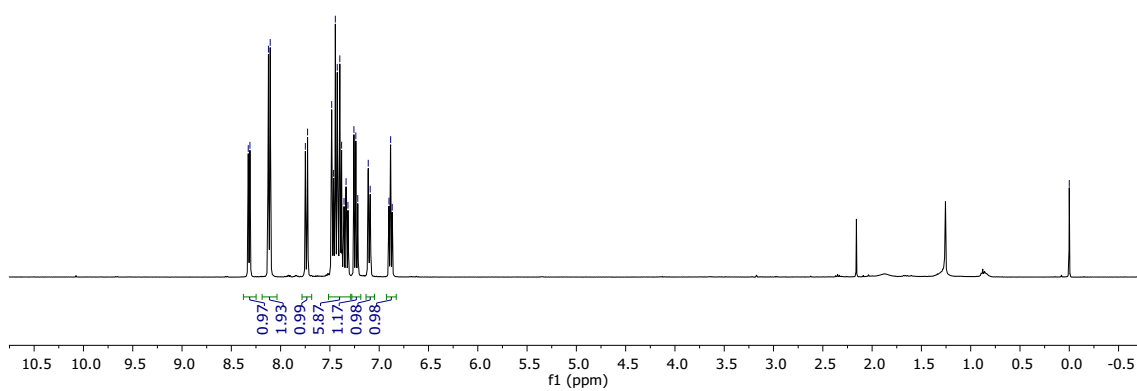
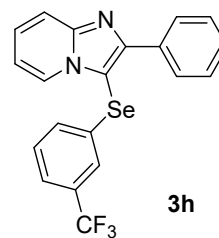
**Figure S22.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3g**.



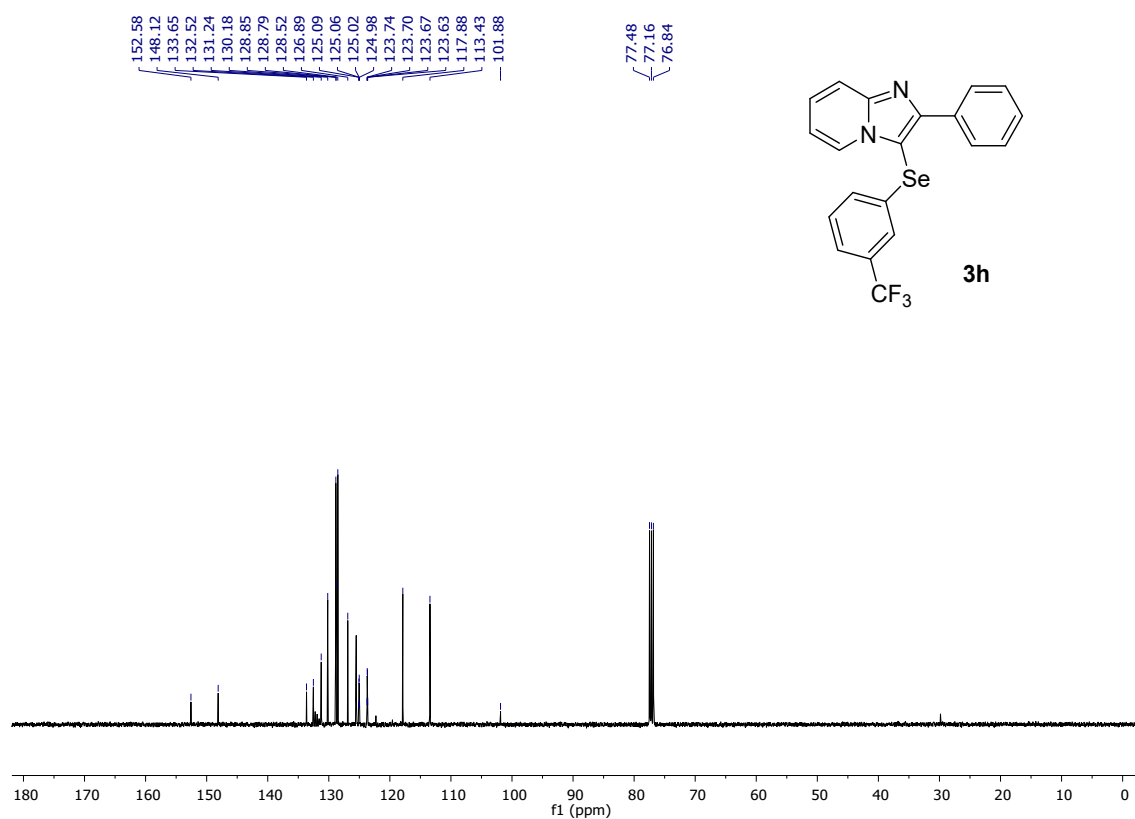
**Figure S23.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3g**.

8.33  
8.31  
8.12  
8.11  
7.75  
7.73  
7.48  
7.46  
7.45  
7.43  
7.40  
7.38  
7.36  
7.34  
7.32  
7.26  
7.24  
7.22  
7.11  
7.09  
6.90  
6.88  
6.87

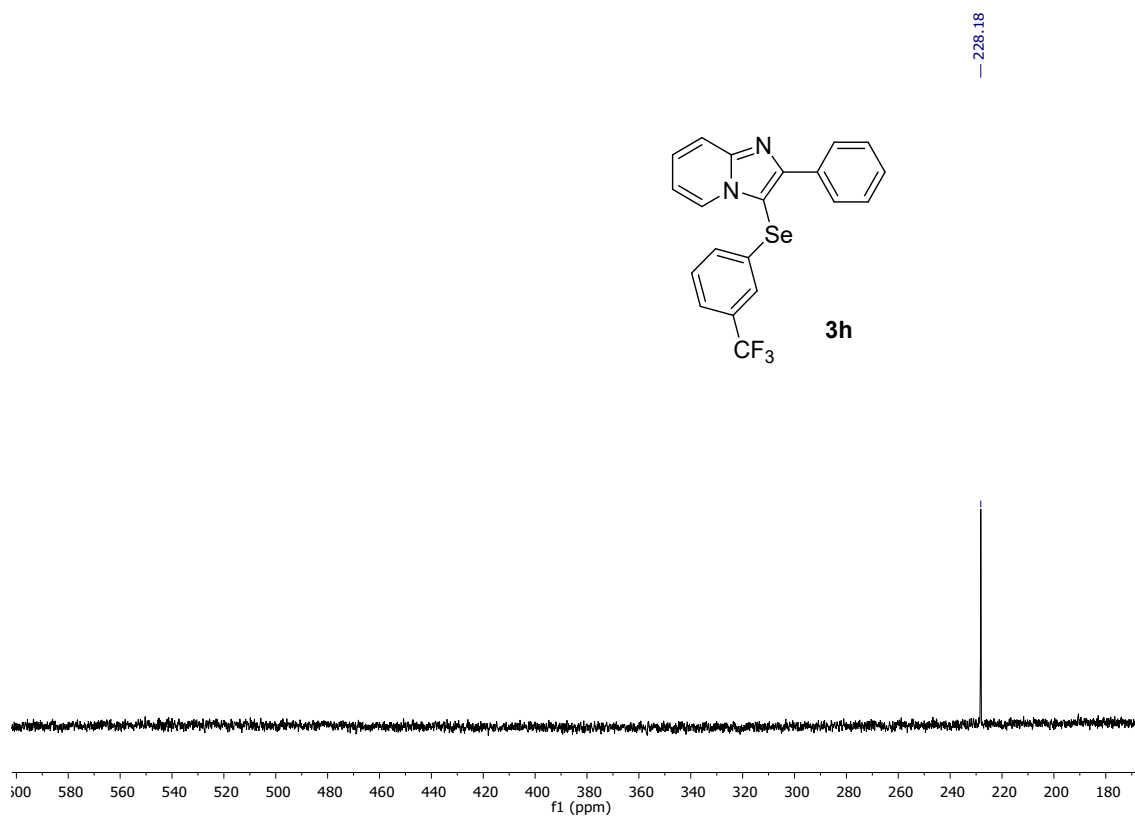
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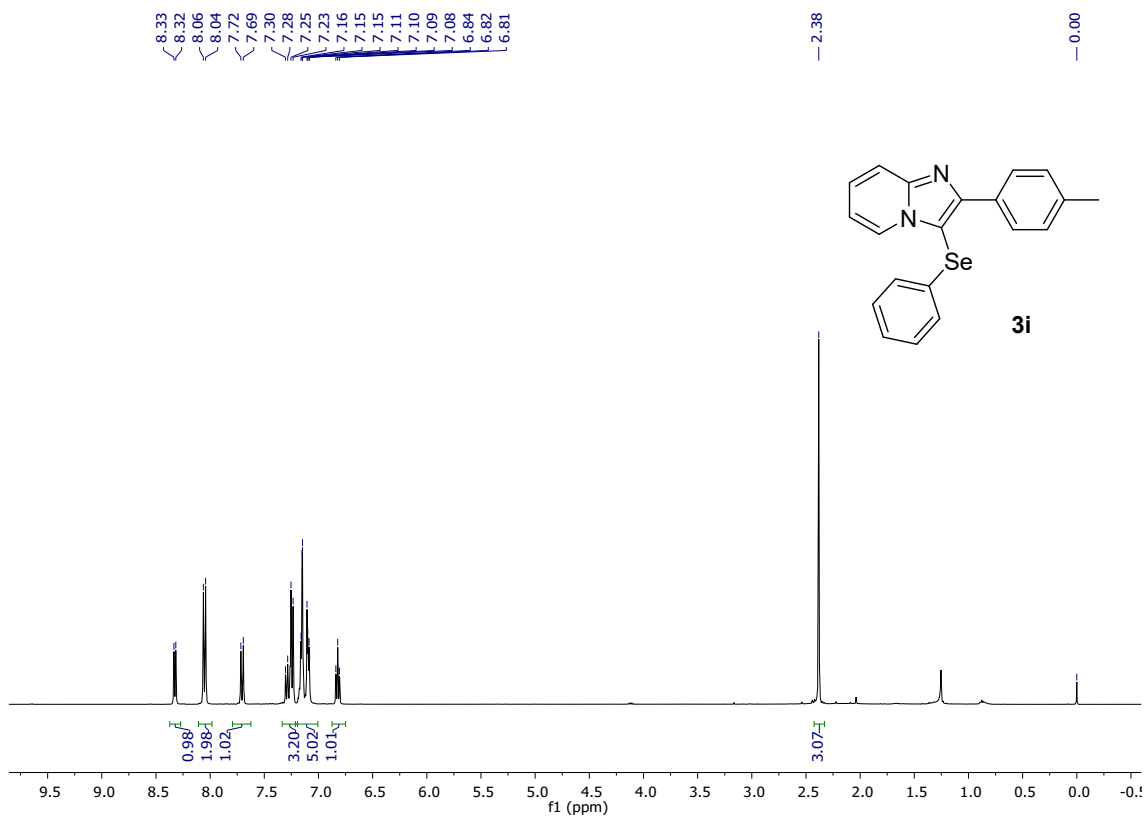
**Figure S24.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3h**.



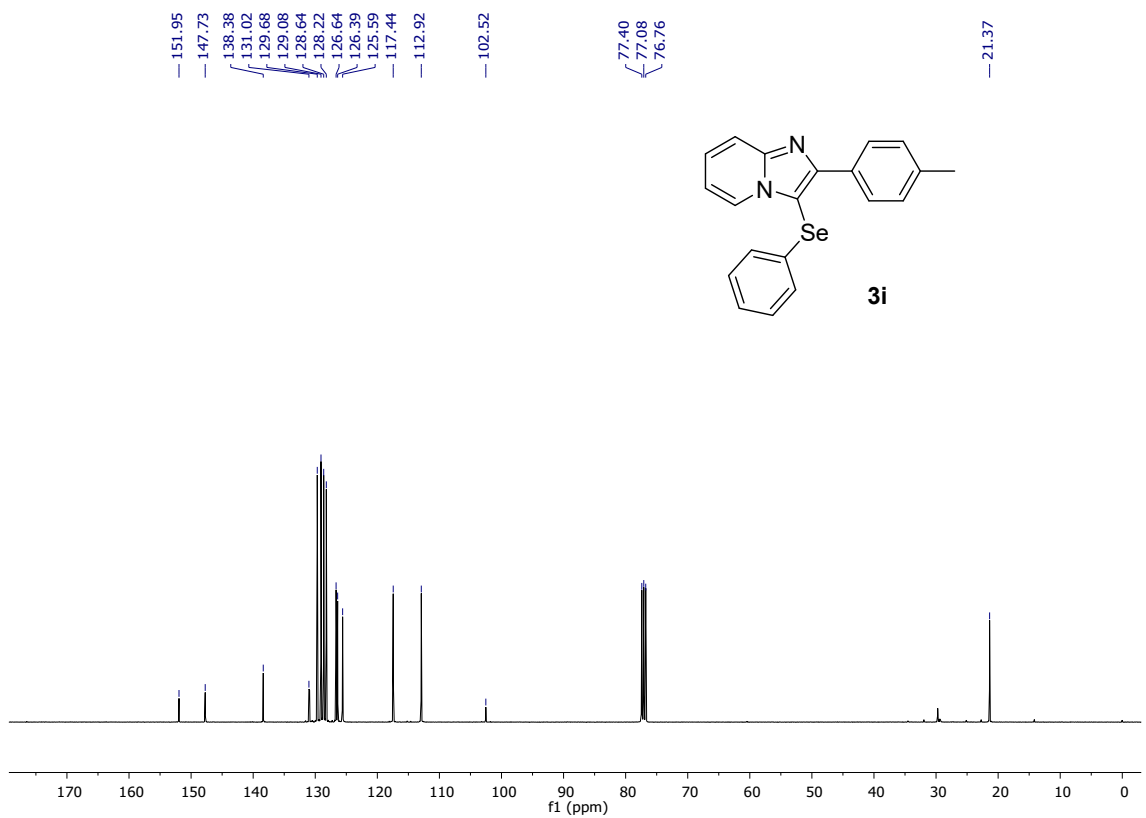
**Figure S25.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3h**.



**Figure S26.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3h**.

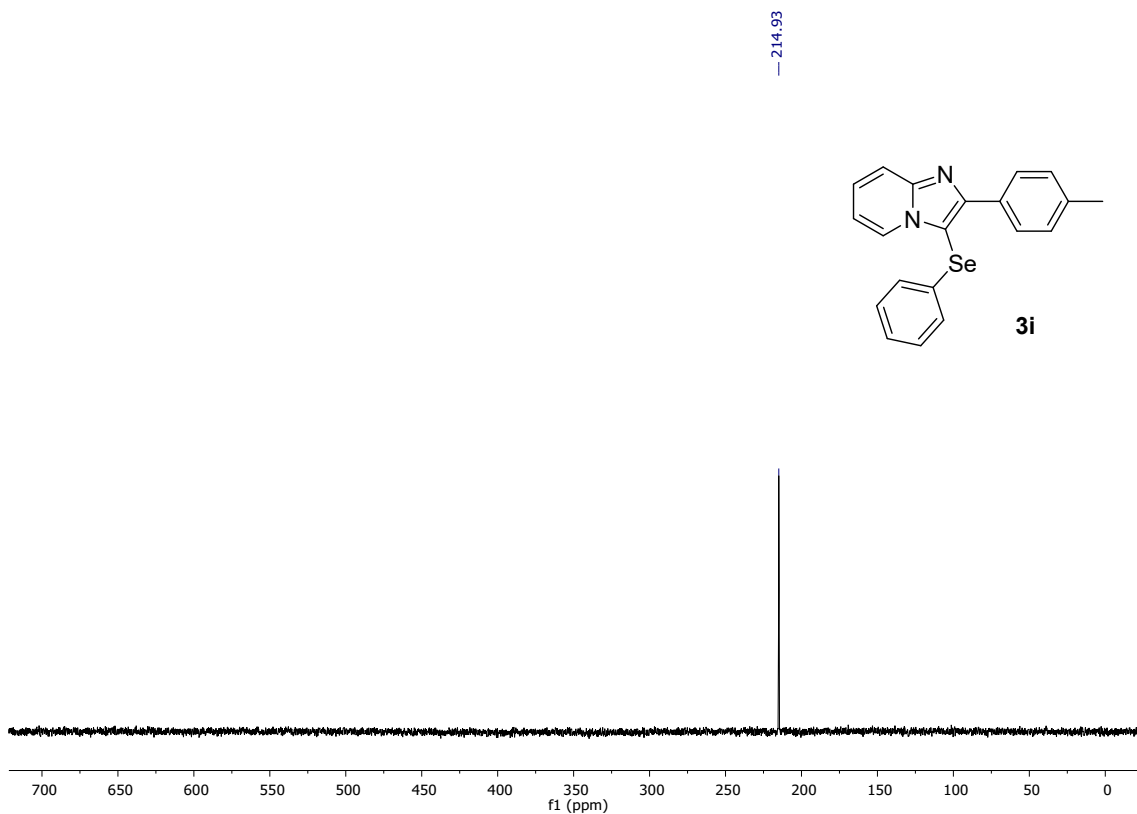


**Figure S27.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3i**.

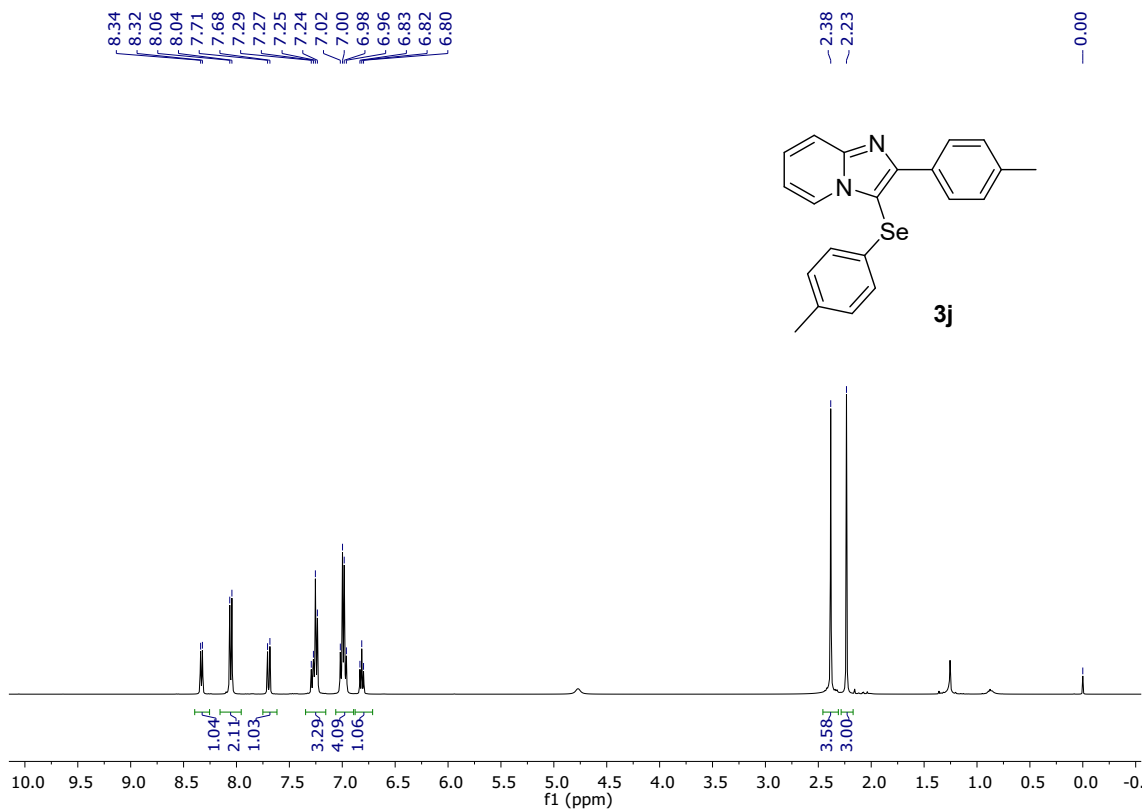


**Figure S28.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3i**.

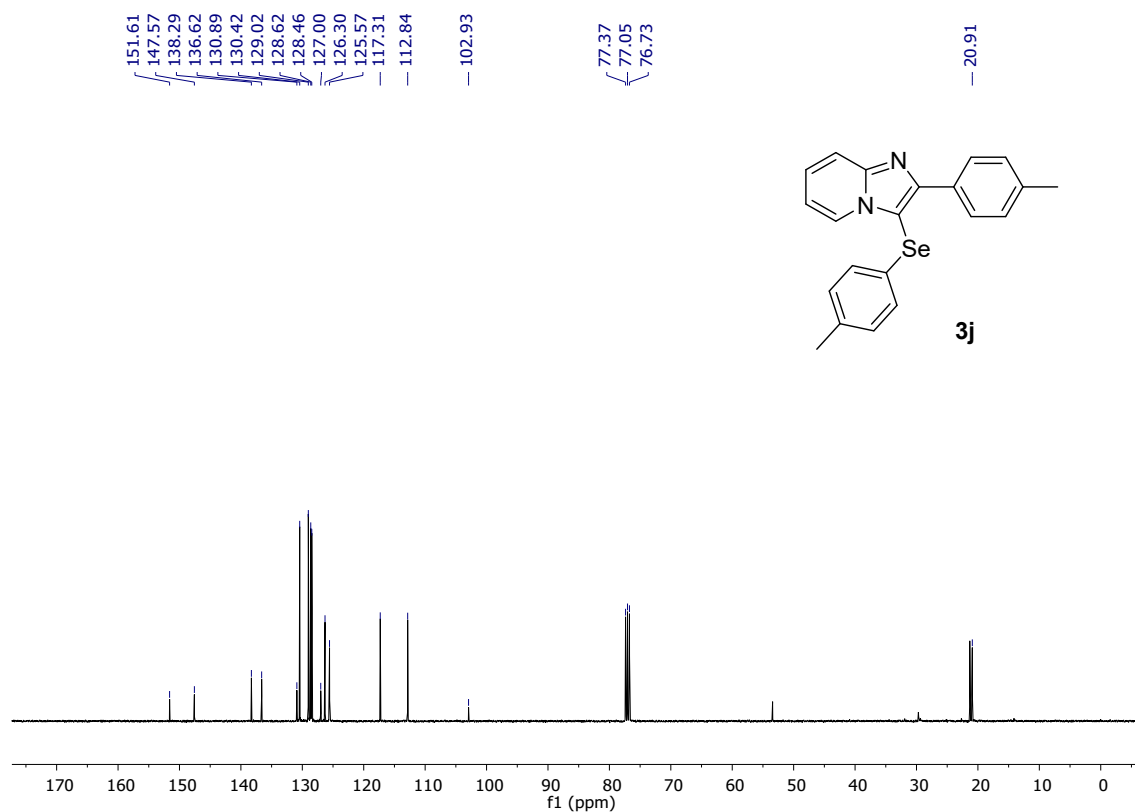




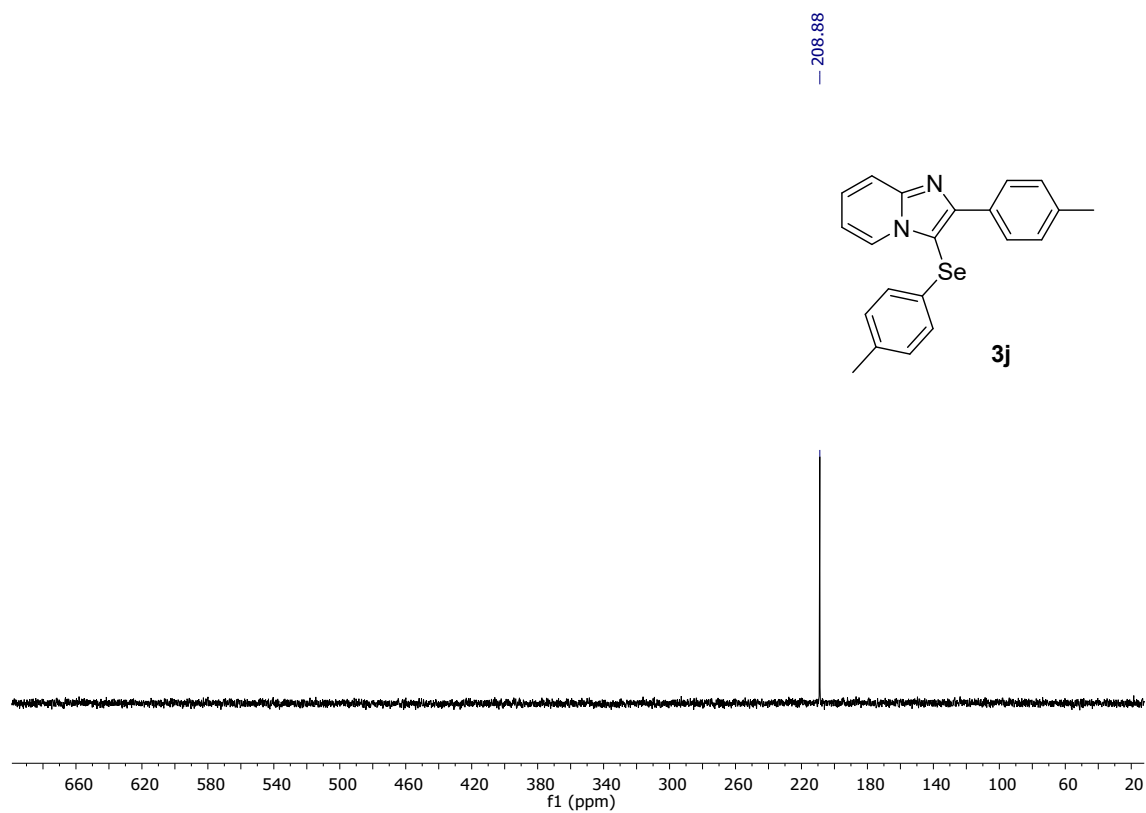
**Figure S29.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3i**.



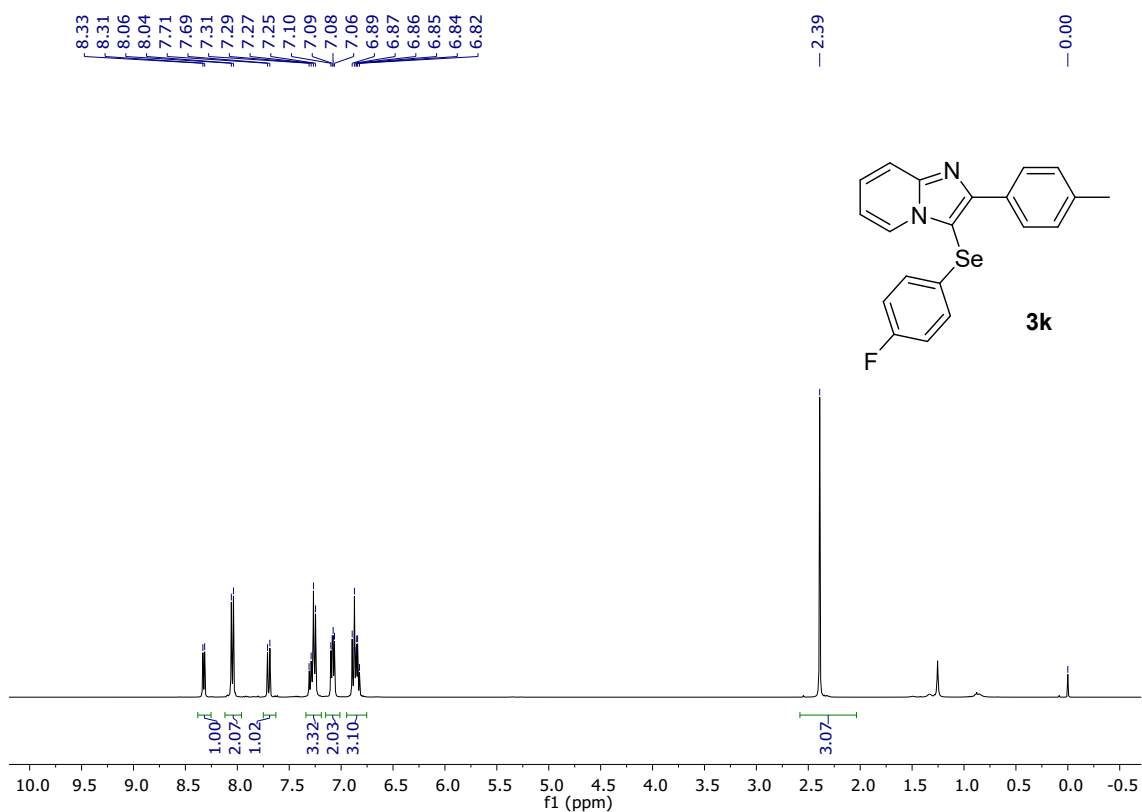
**Figure S30.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3j**.



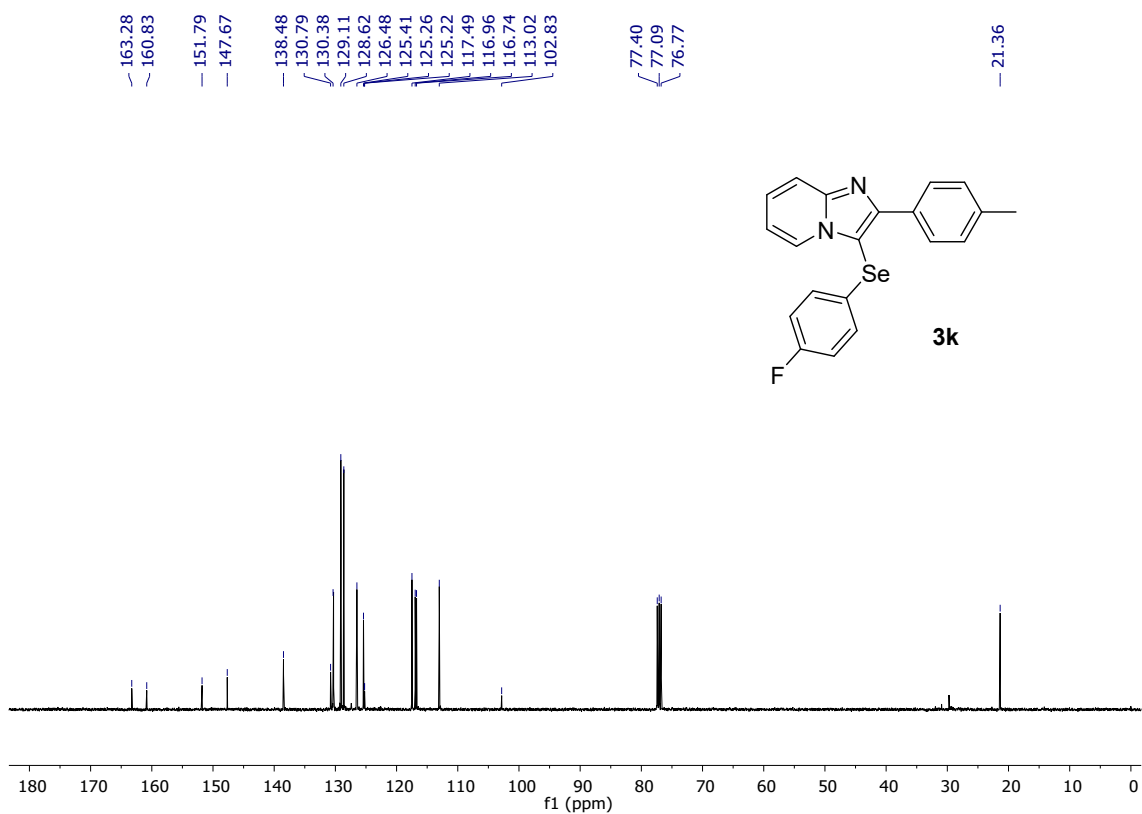
**Figure S31.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3j**.



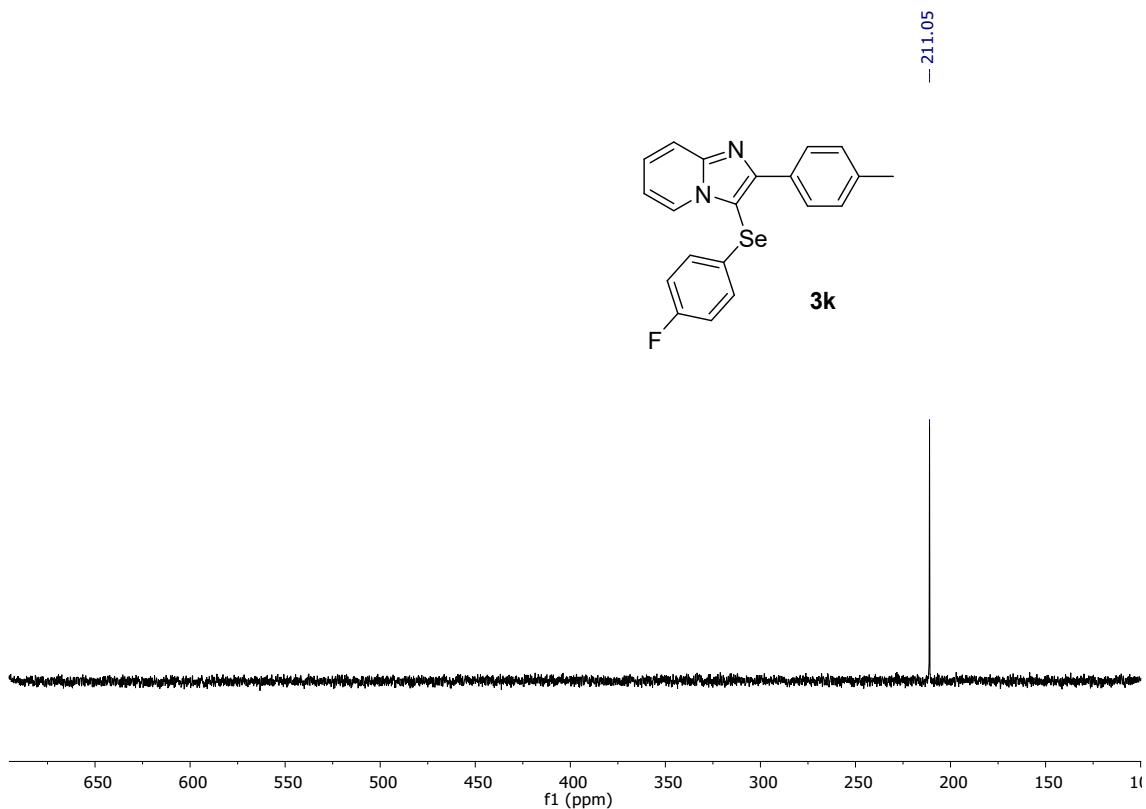
**Figure S32.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3j**.



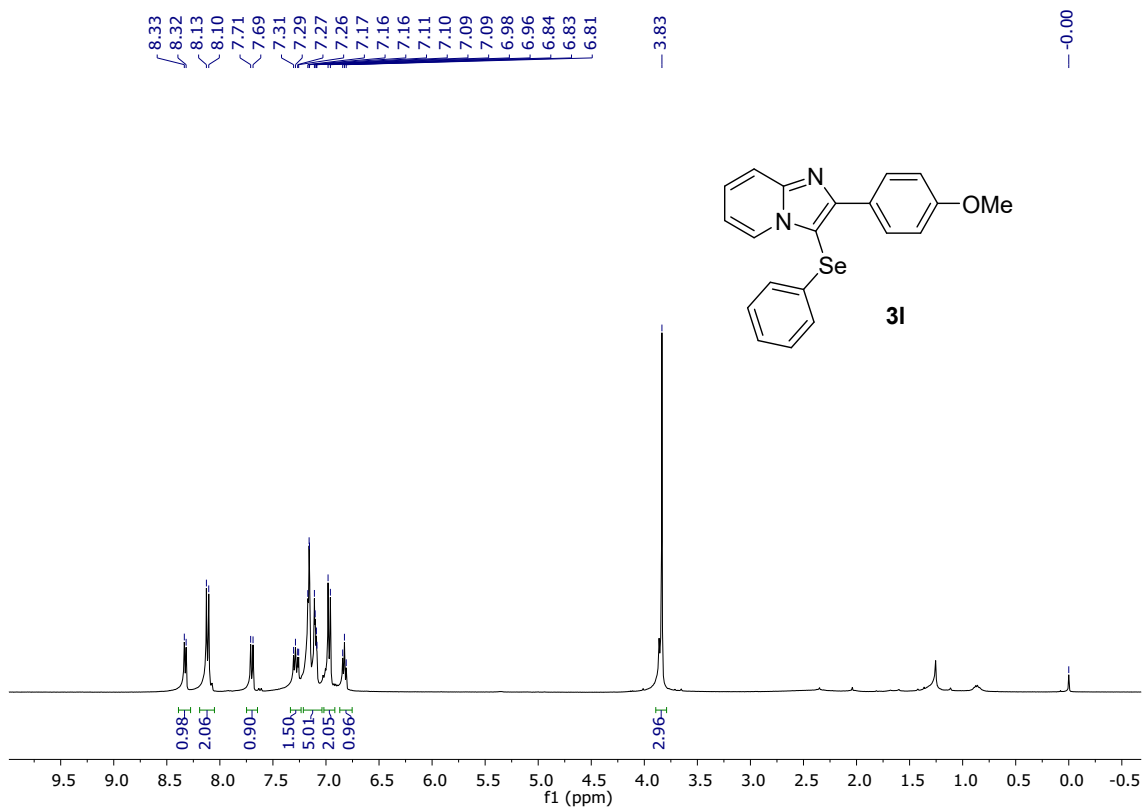
**Figure S33.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3k**.



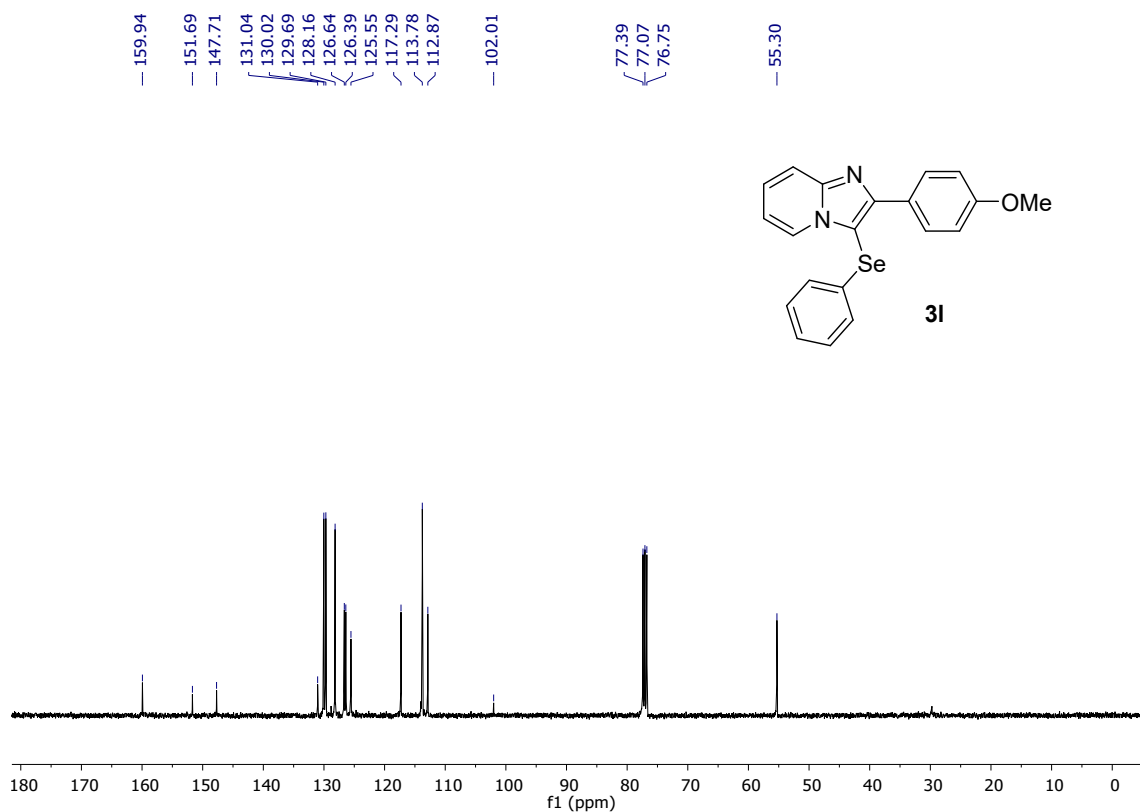
**Figure S34.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3k**.



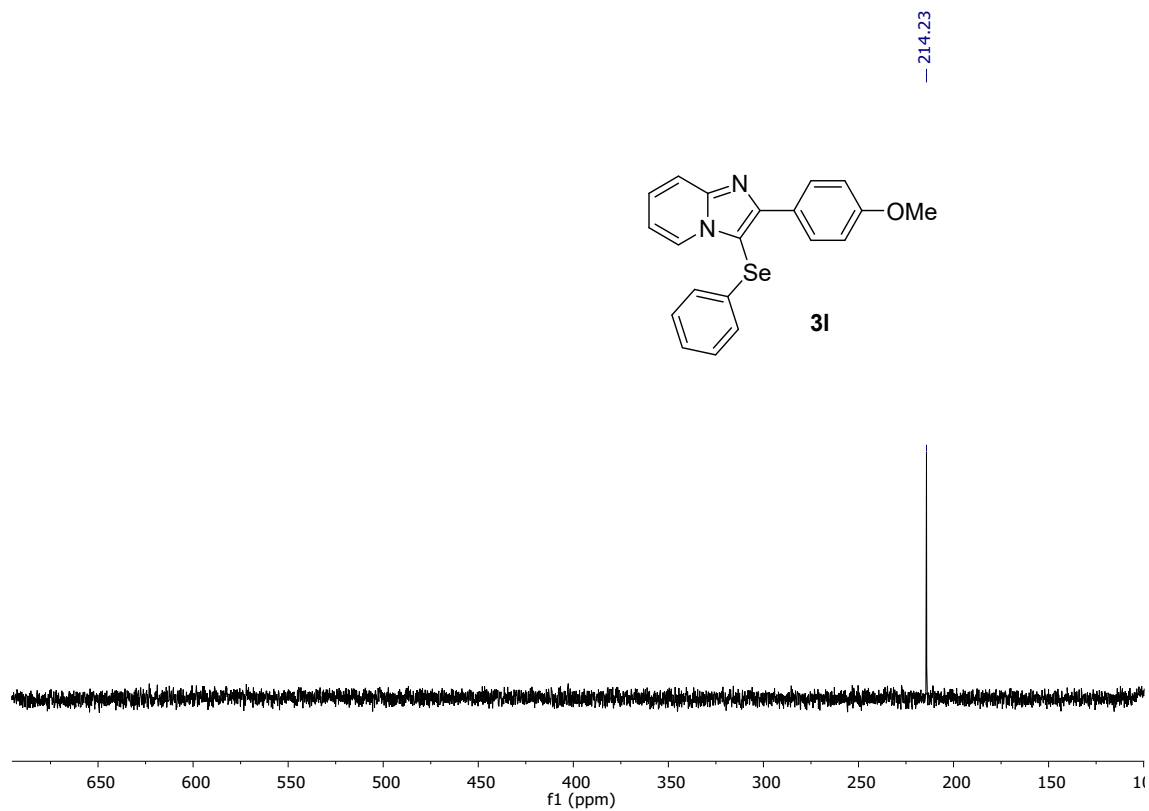
**Figure S35.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3k**.



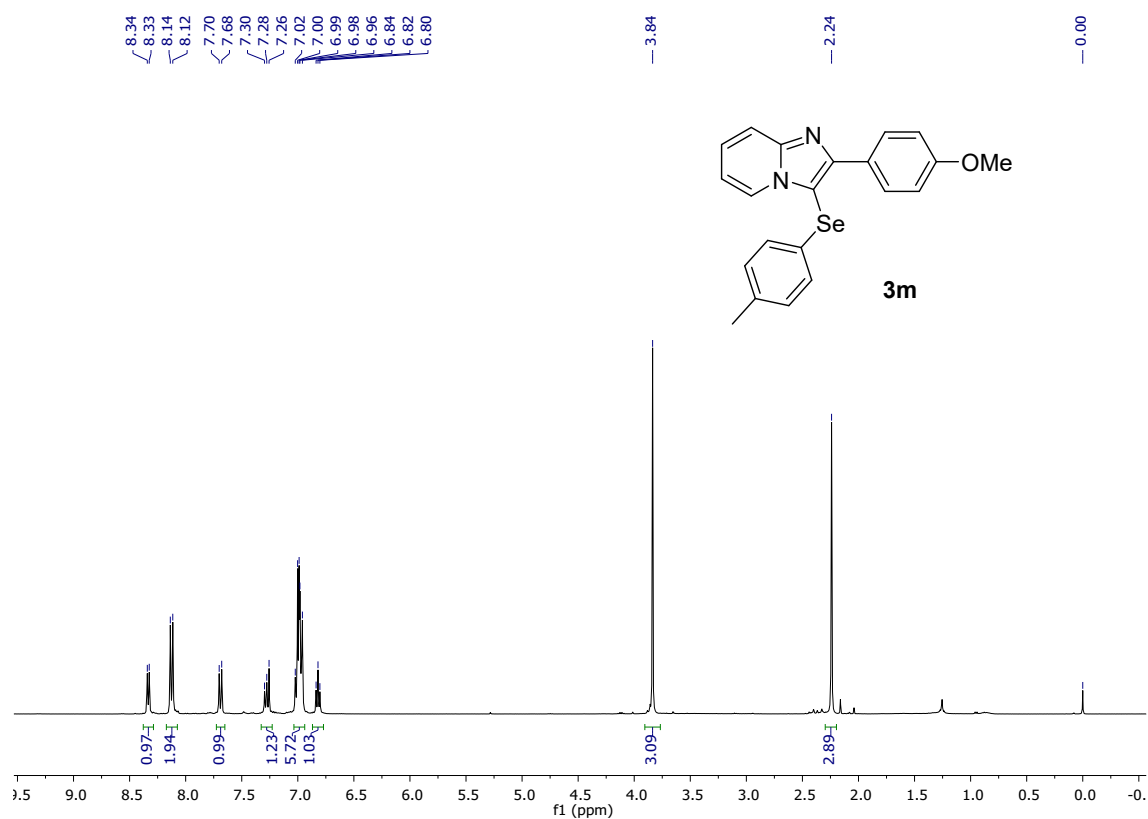
**Figure S36.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3l**.



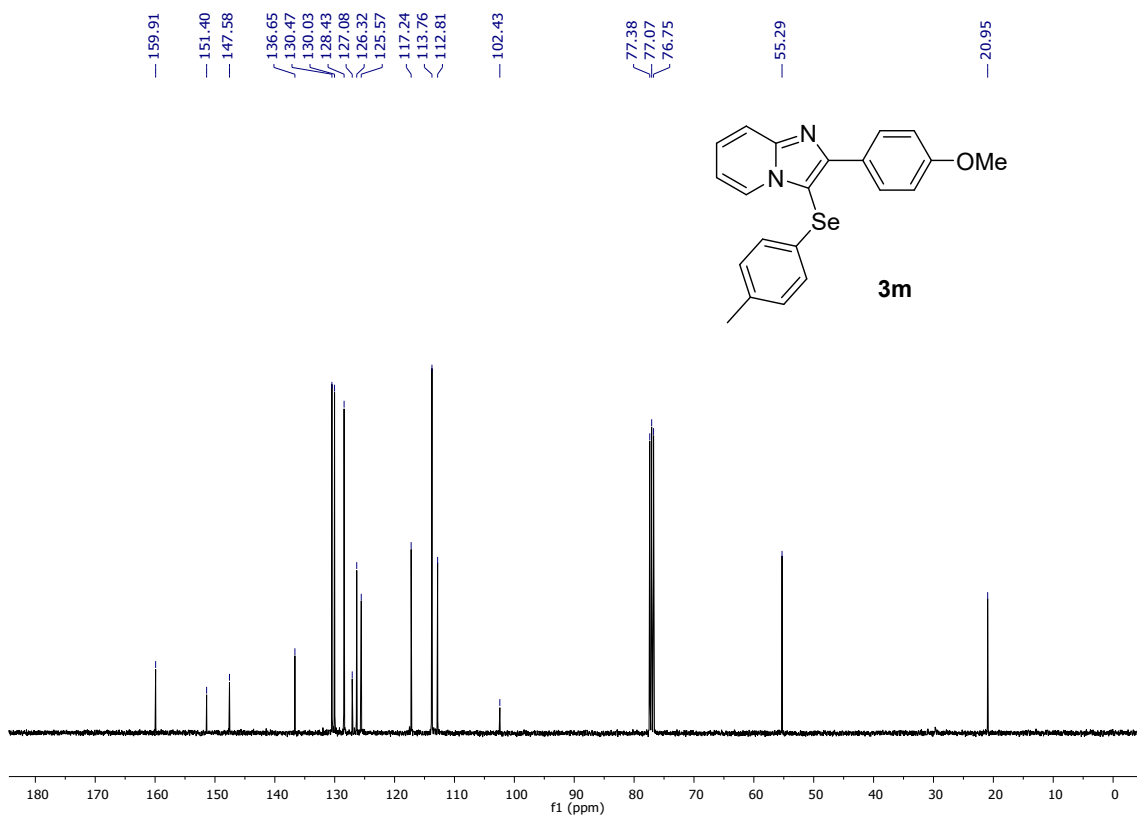
**Figure S37.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **31**.



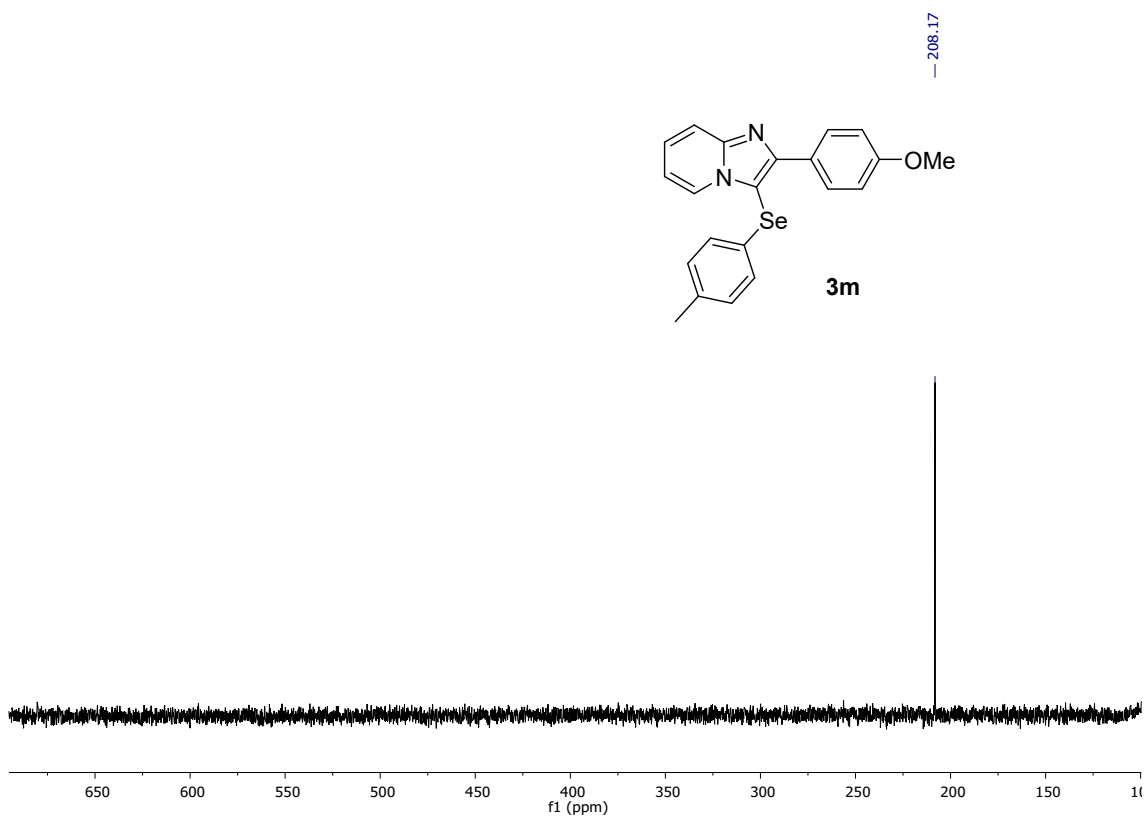
**Figure S38.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **31**.



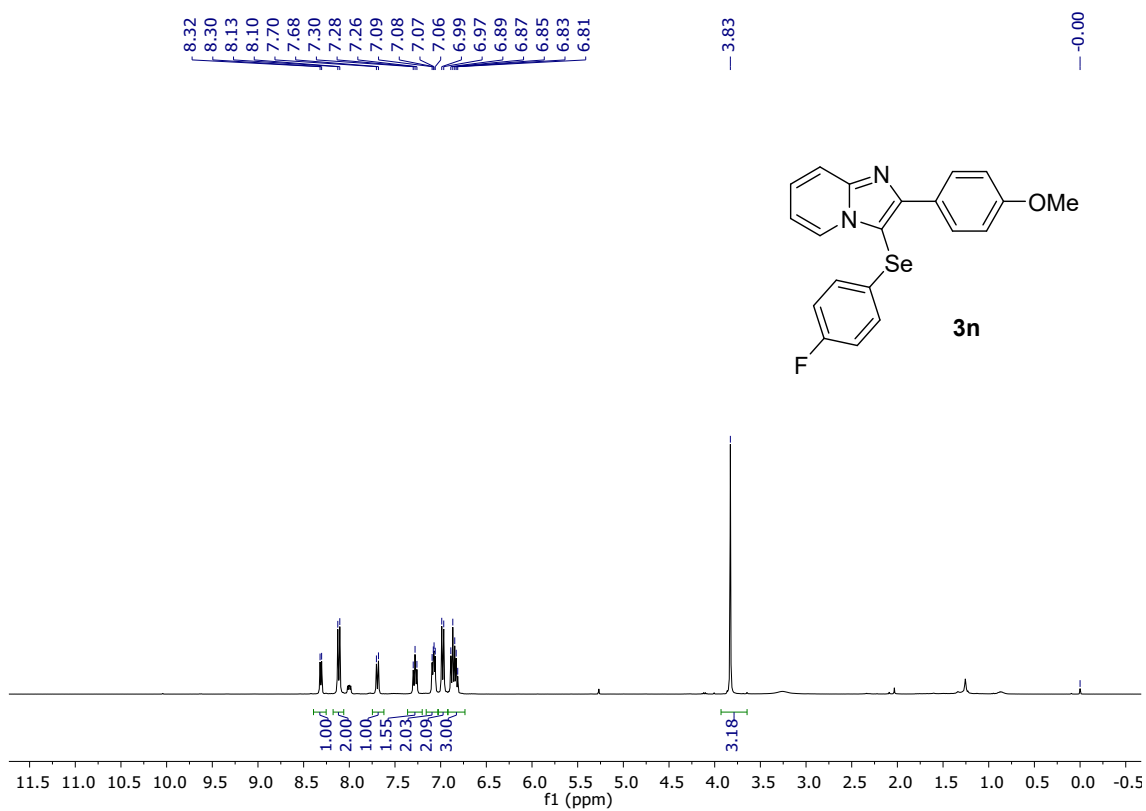
**Figure S39.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3m**.



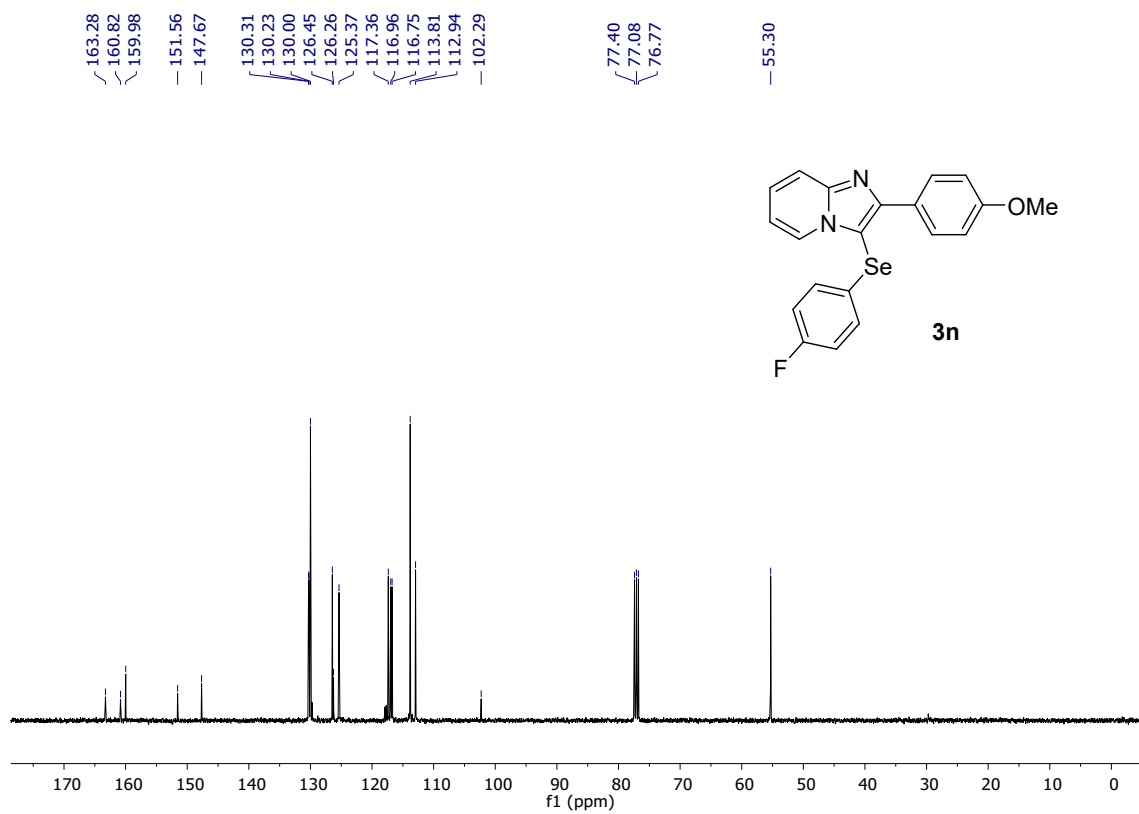
**Figure S40.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3m**.



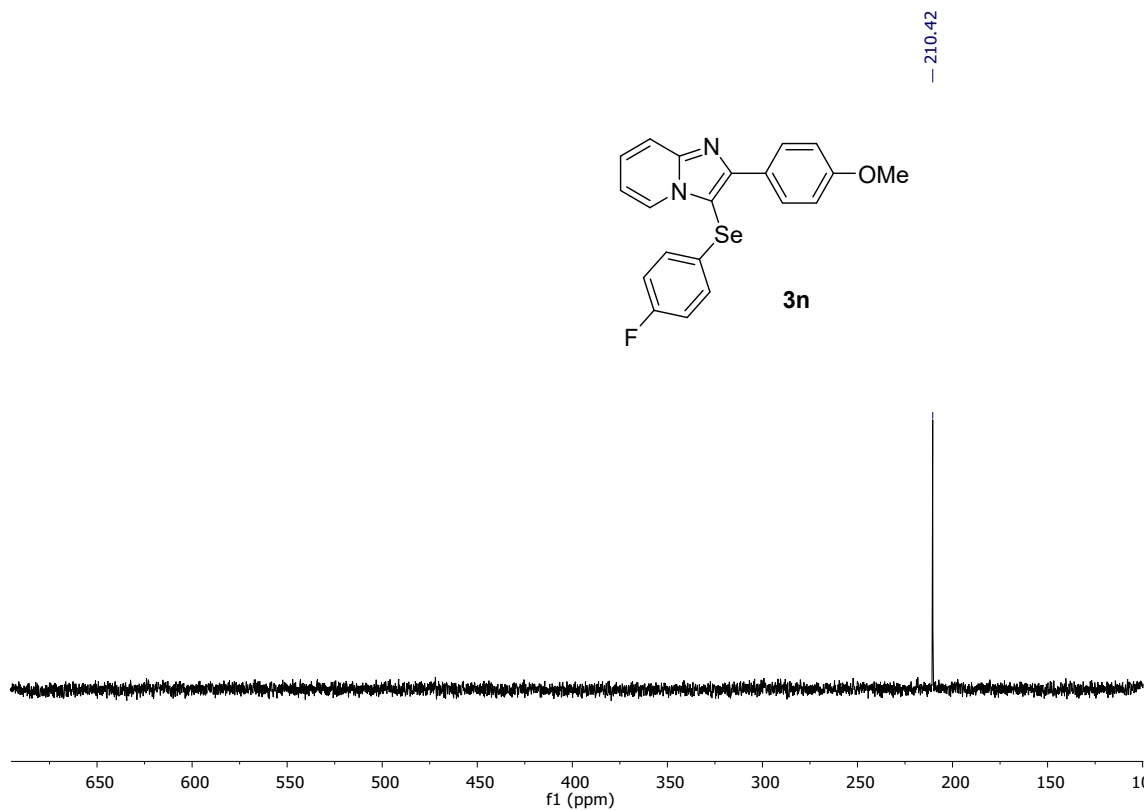
**Figure S41.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3m**.



**Figure S42.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3n**.

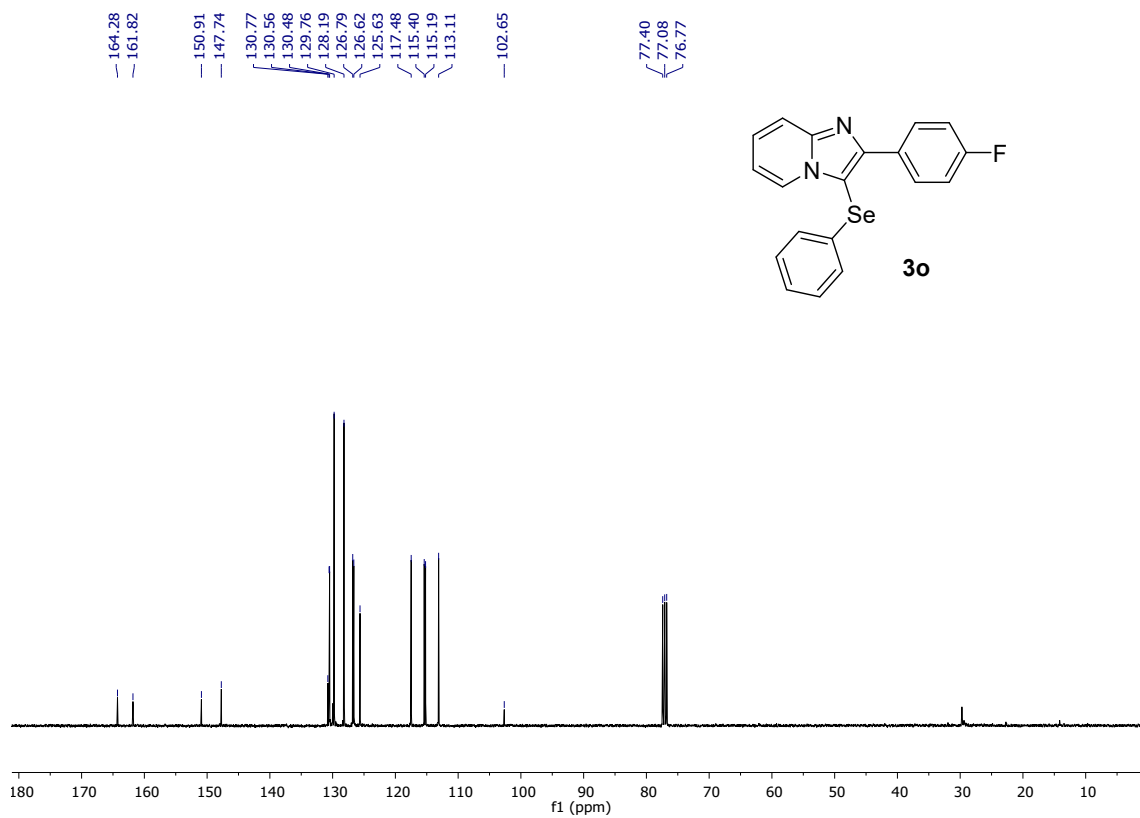
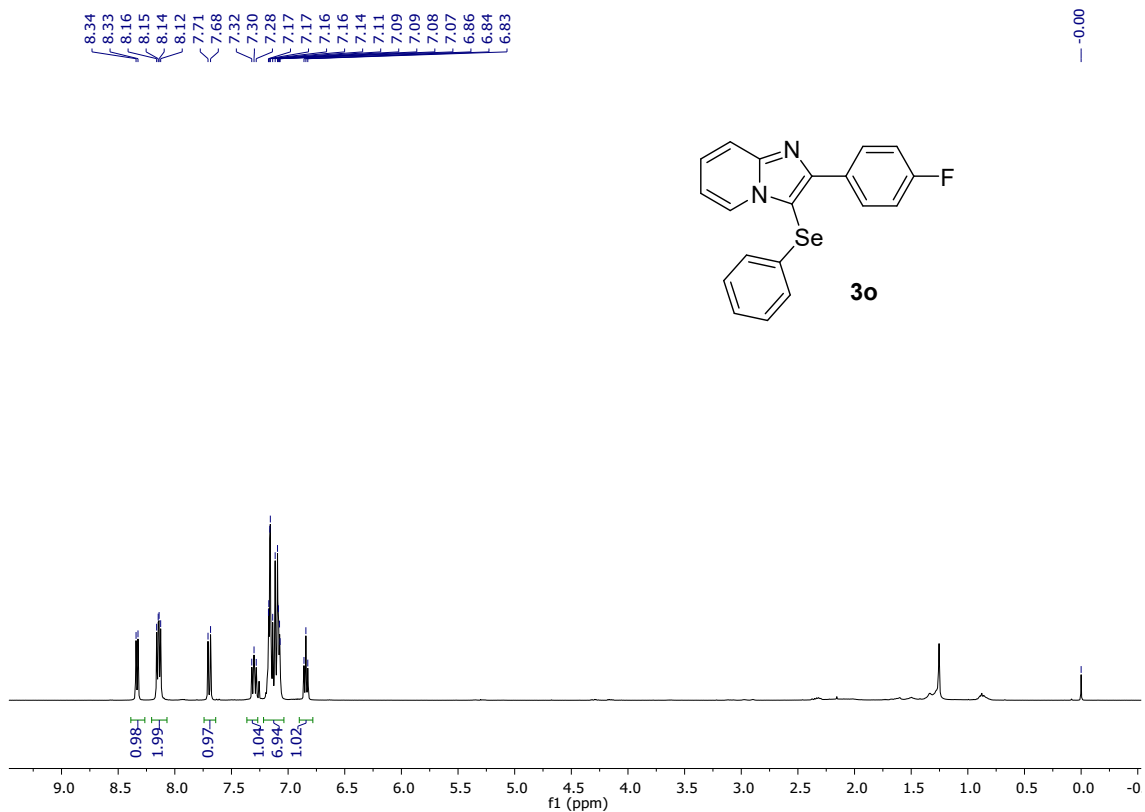


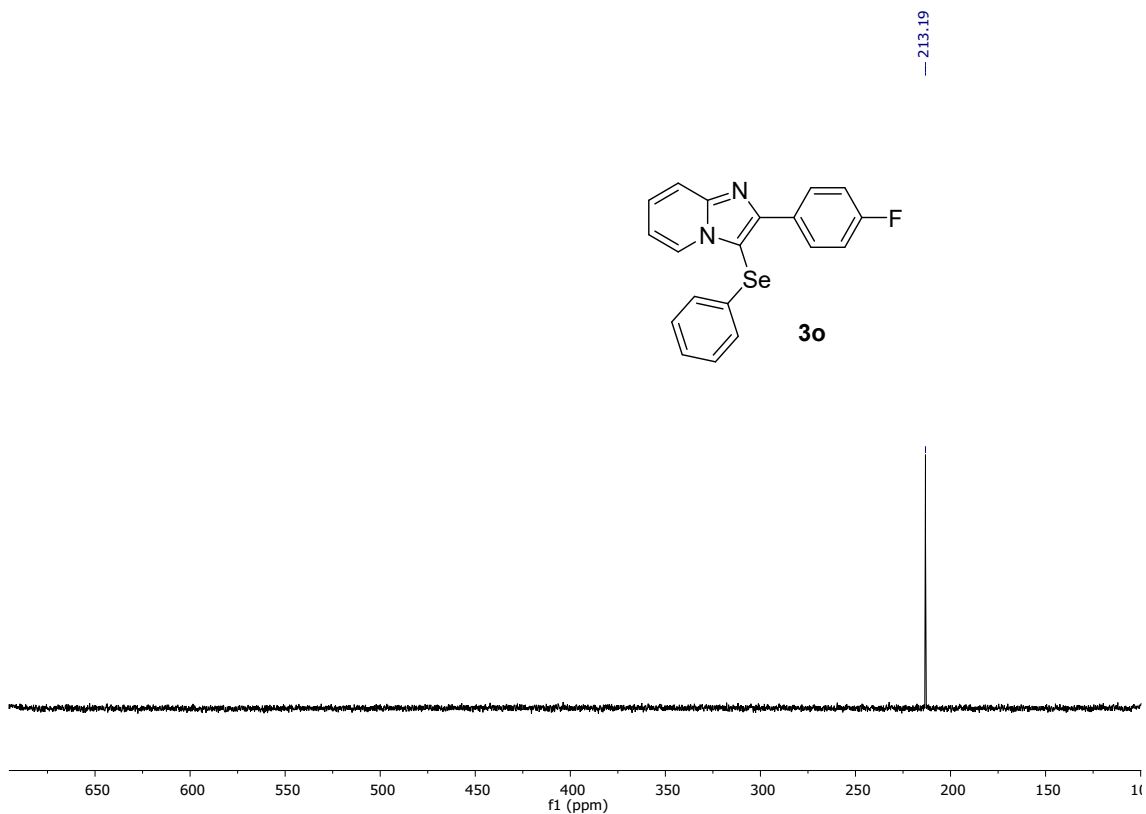
**Figure S43.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3n**.



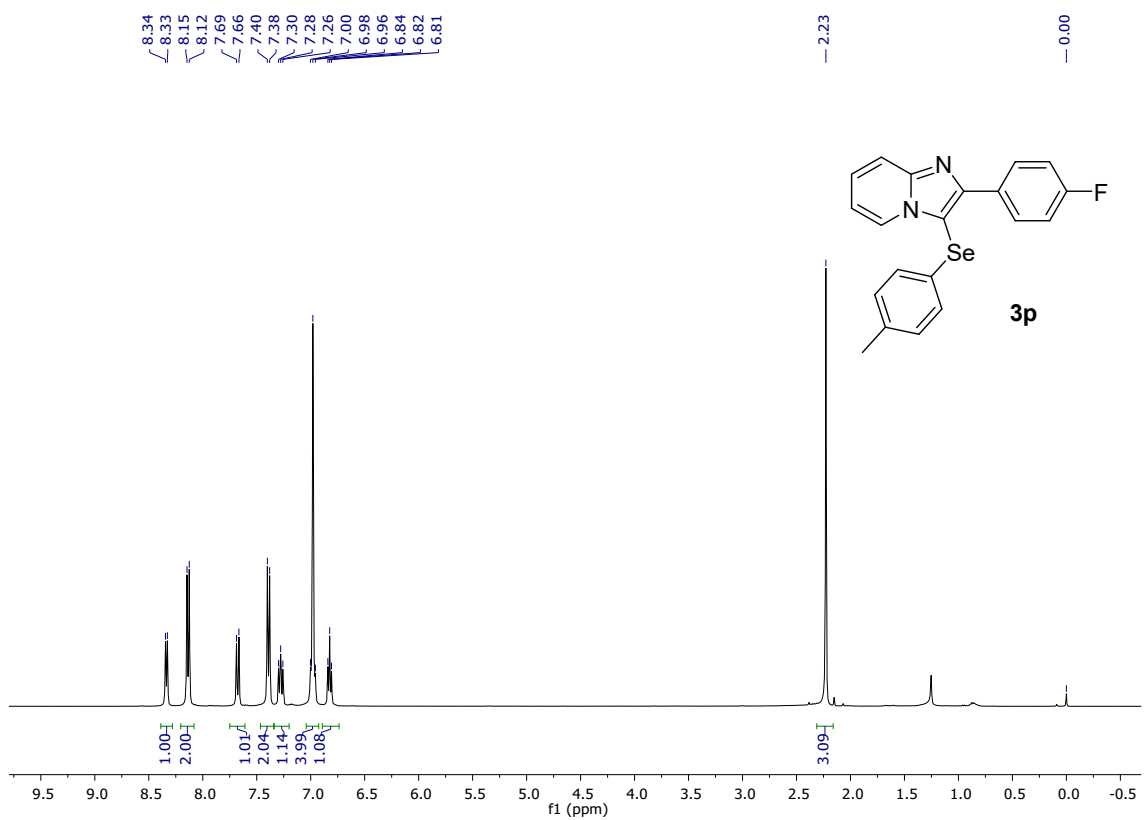
**Figure S44.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3n**.



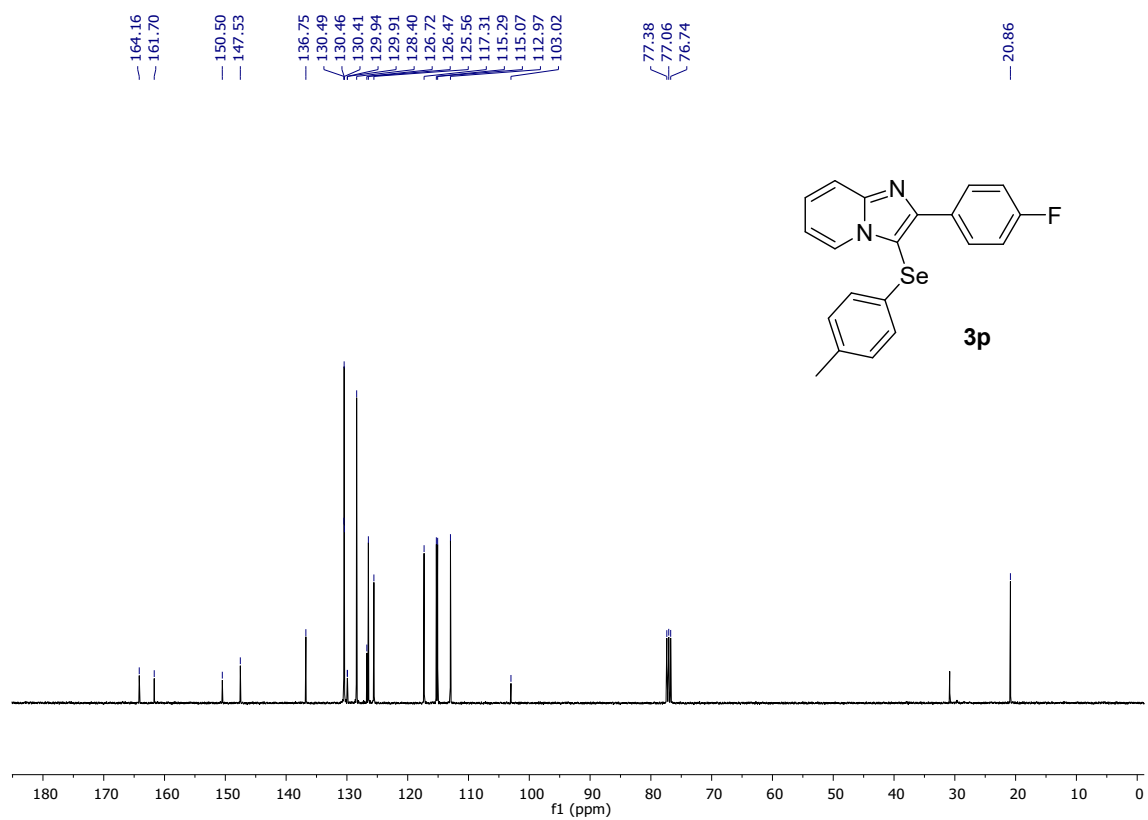




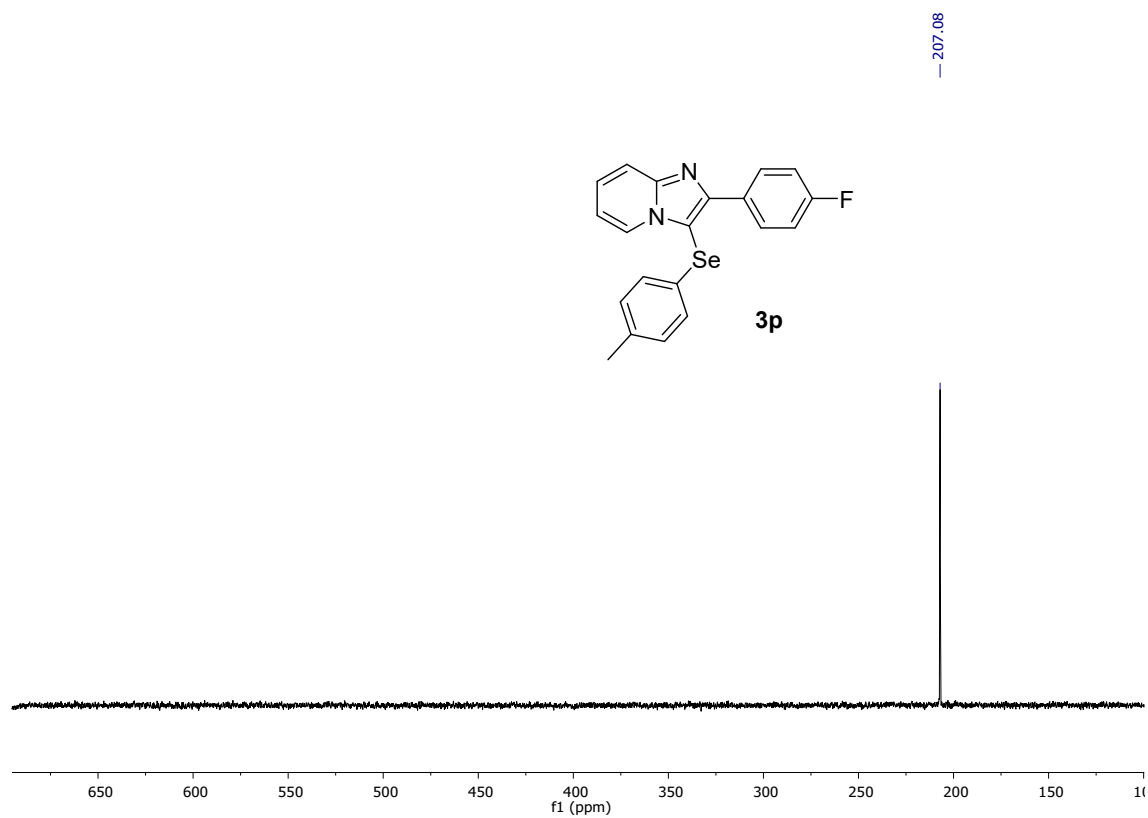
**Figure S47.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3o**.



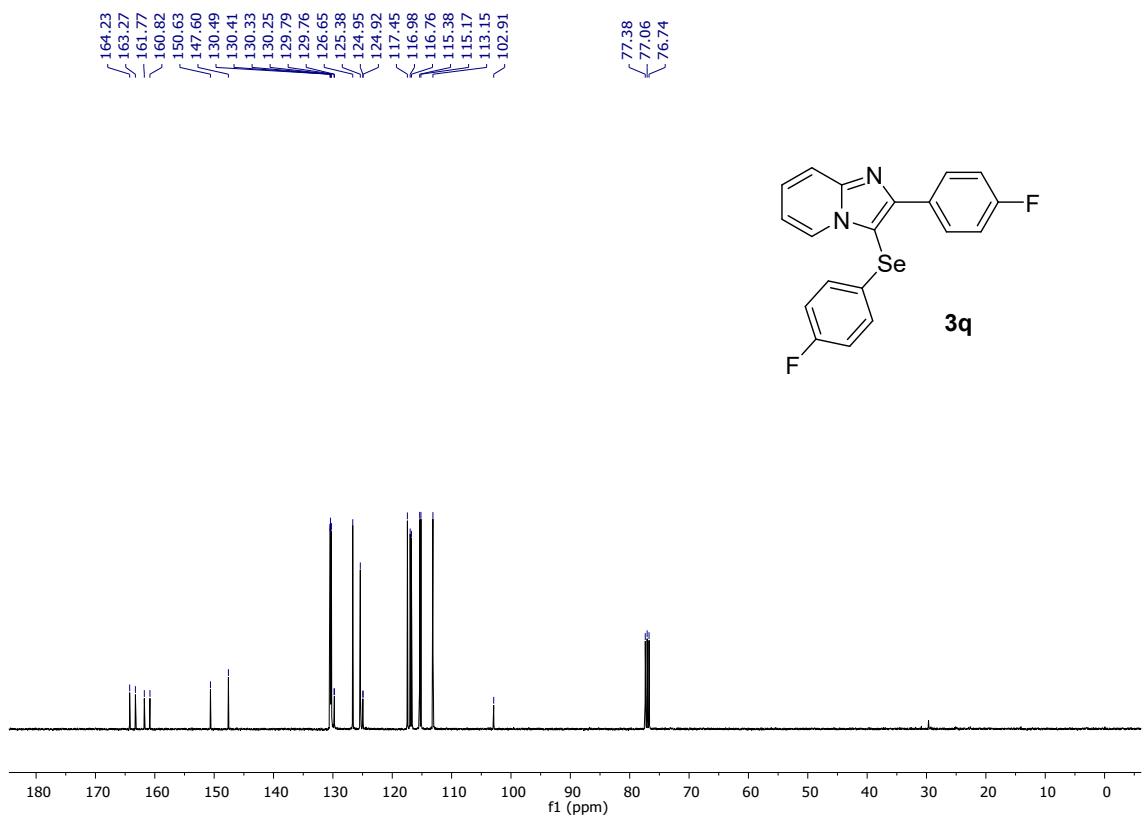
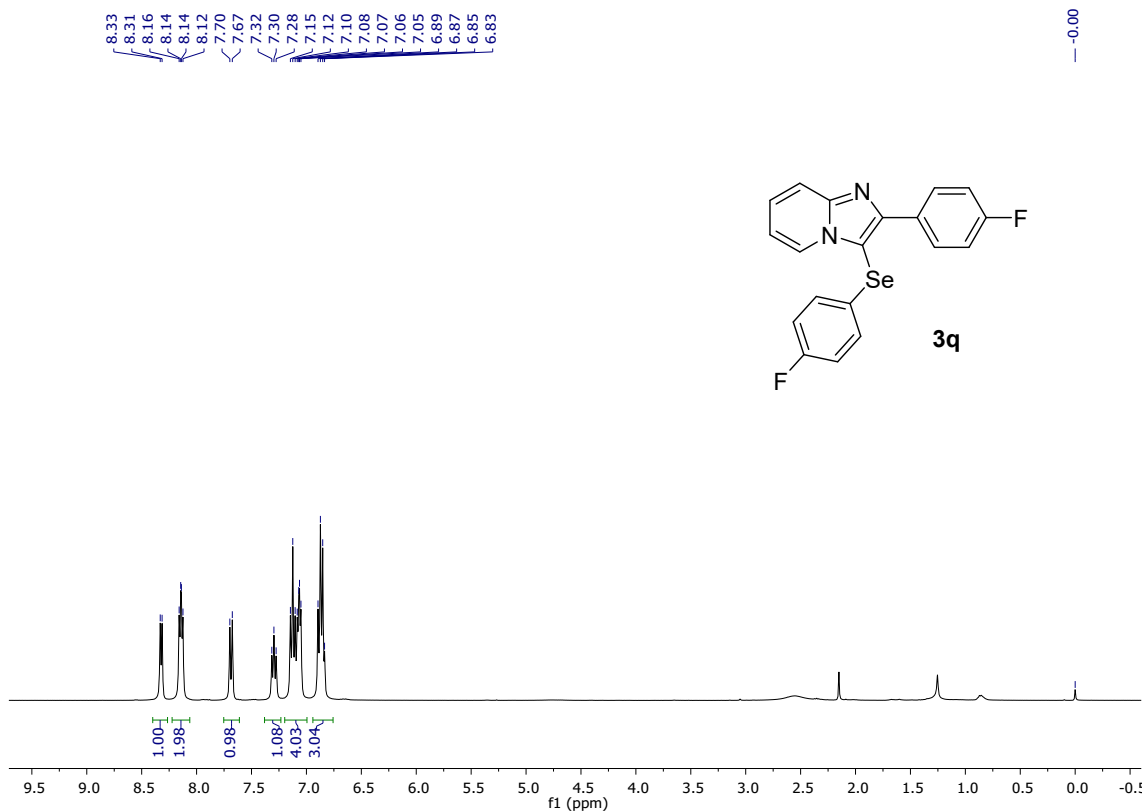
**Figure S48.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3p**.

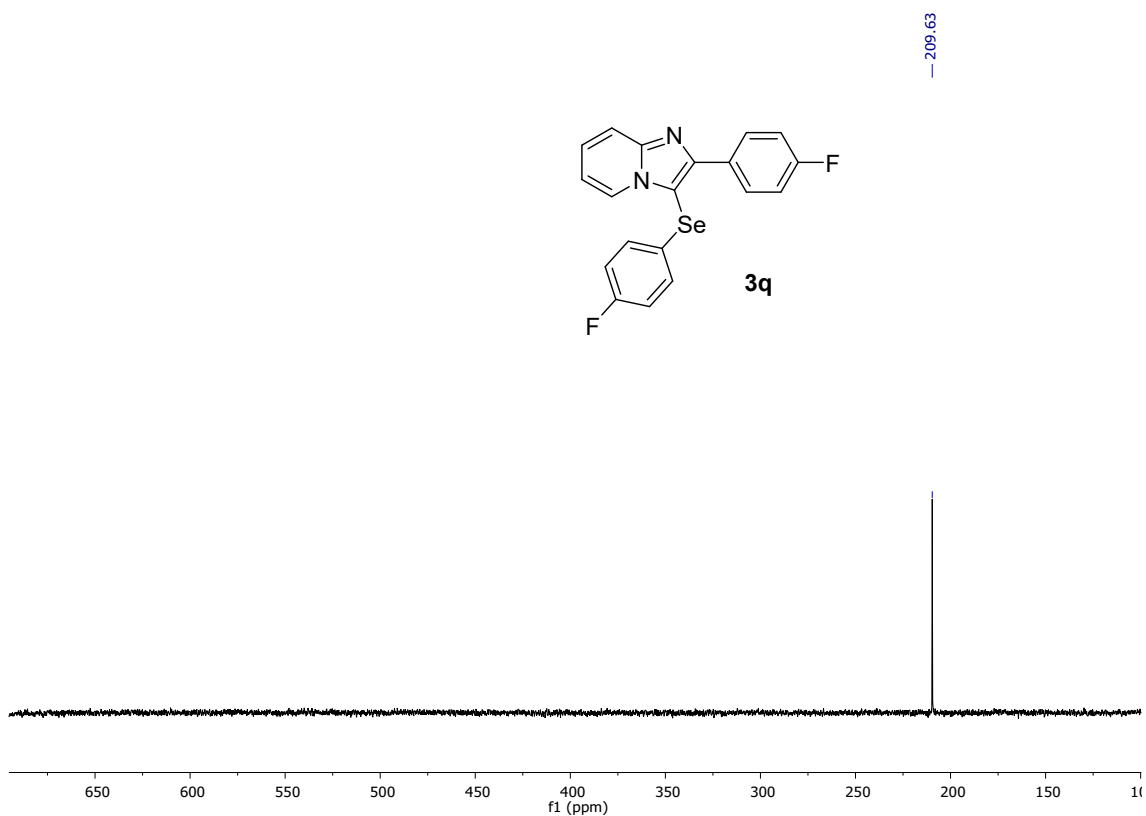


**Figure S49.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3p**.

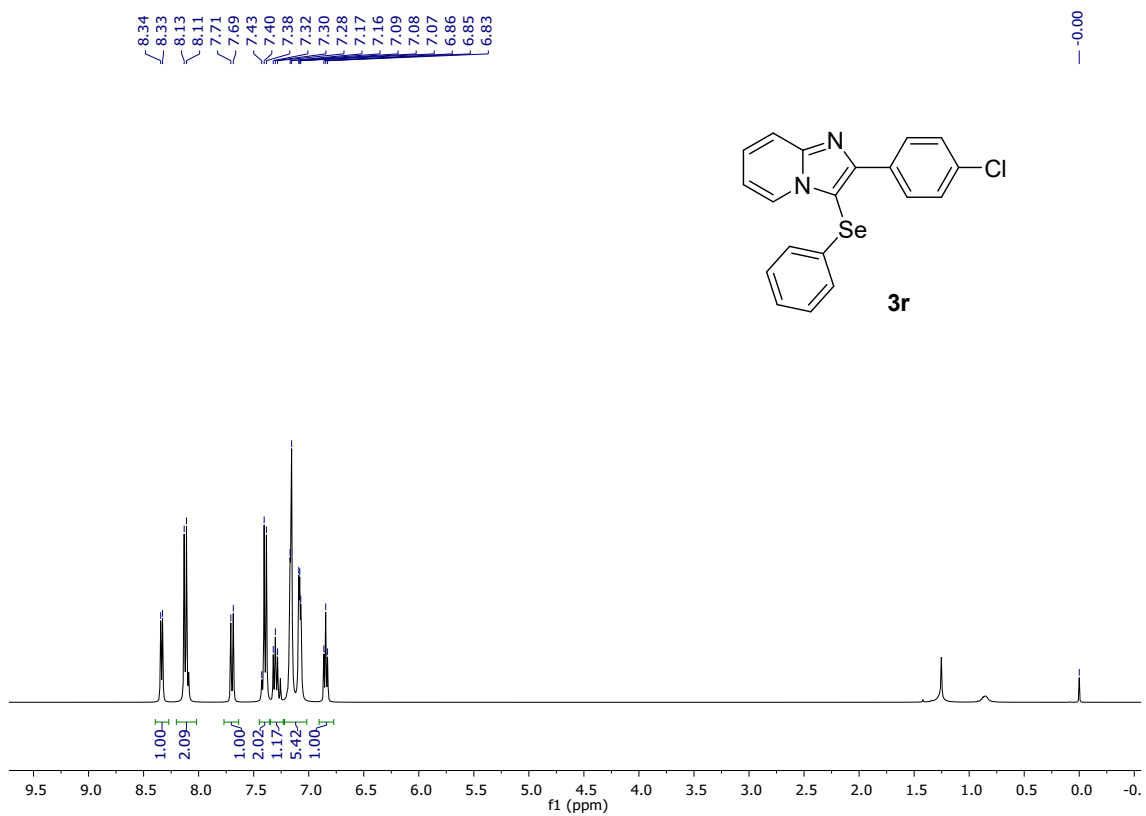


**Figure S50.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3p**.

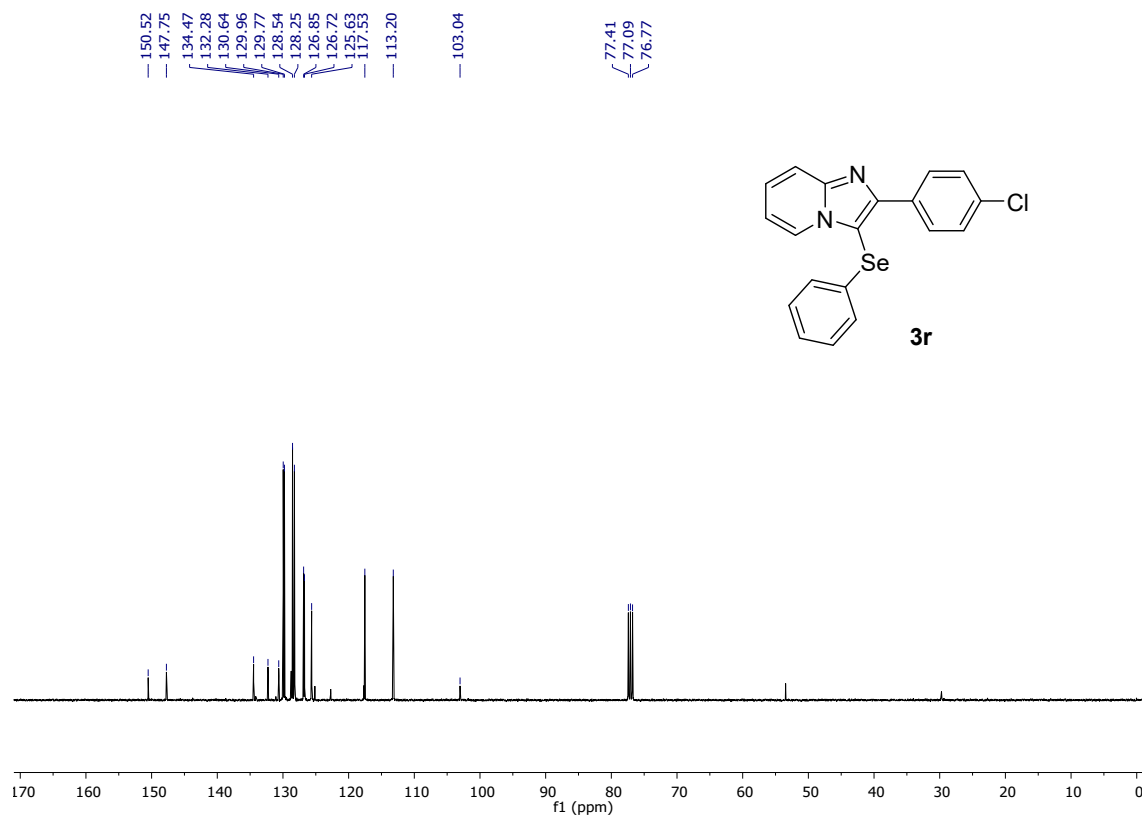




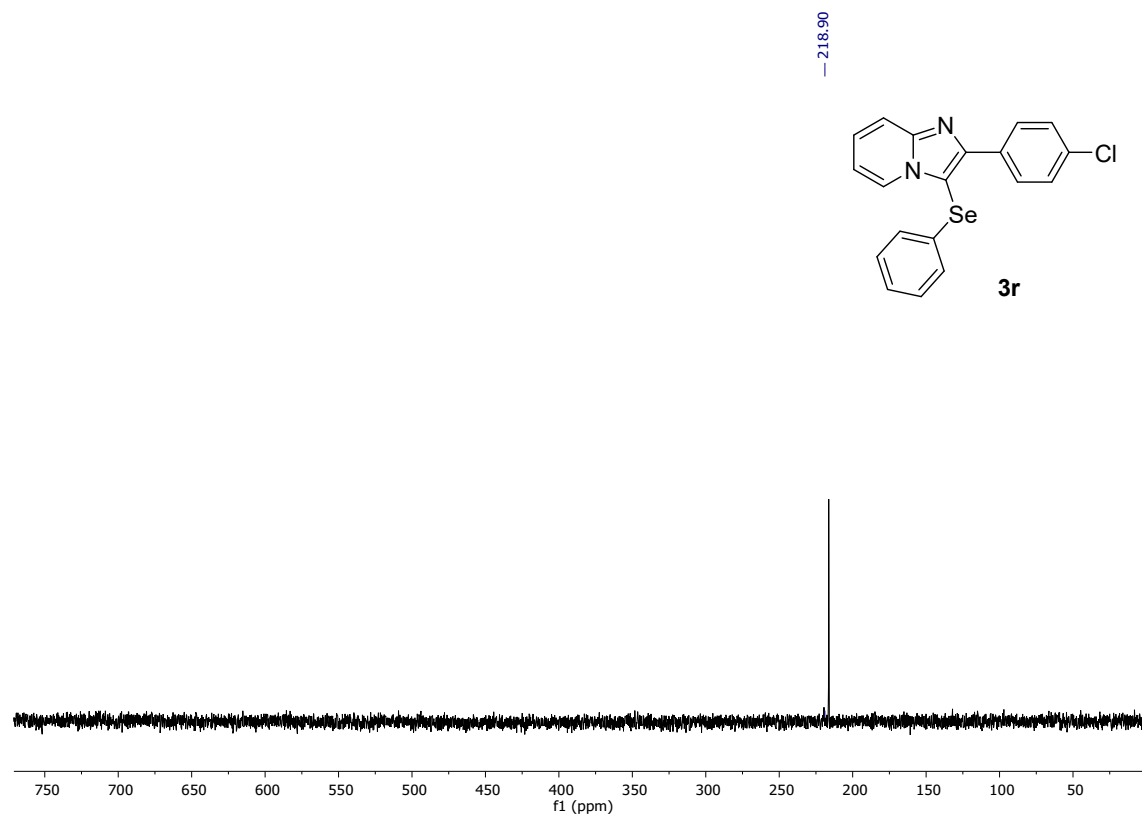
**Figure S53.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3q**.



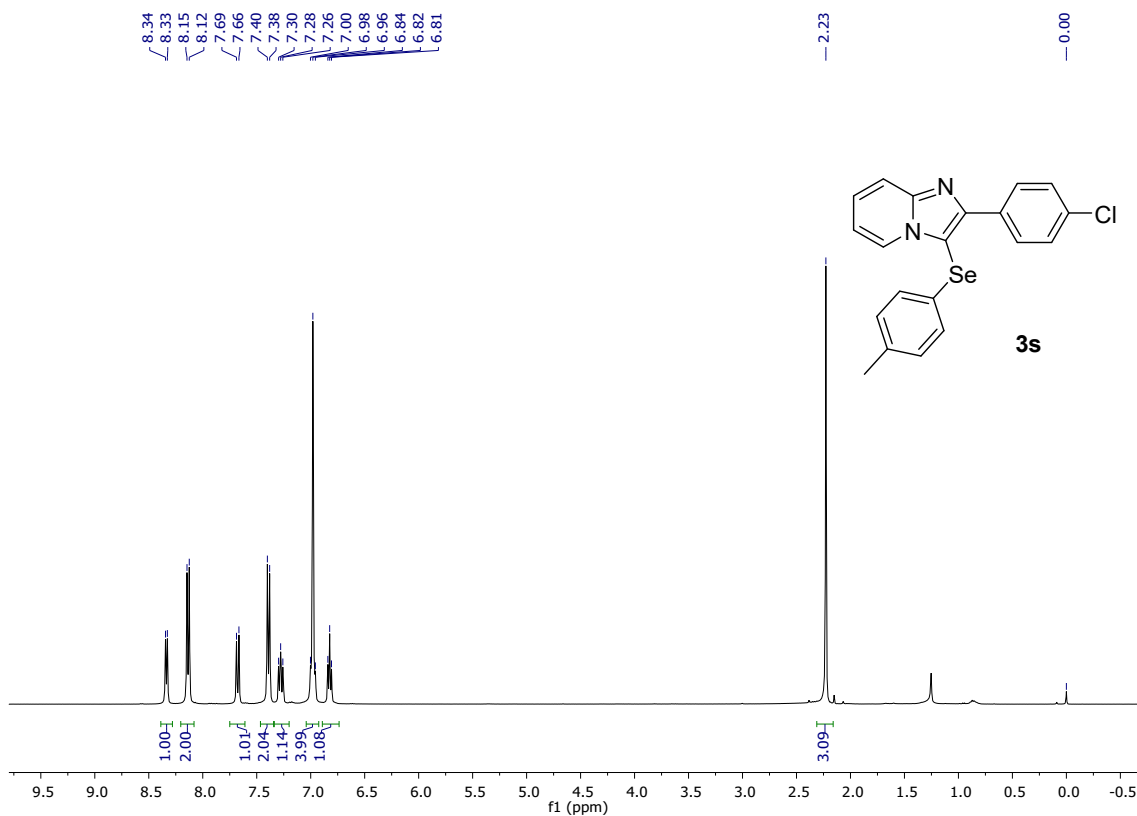
**Figure S54.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3r**.



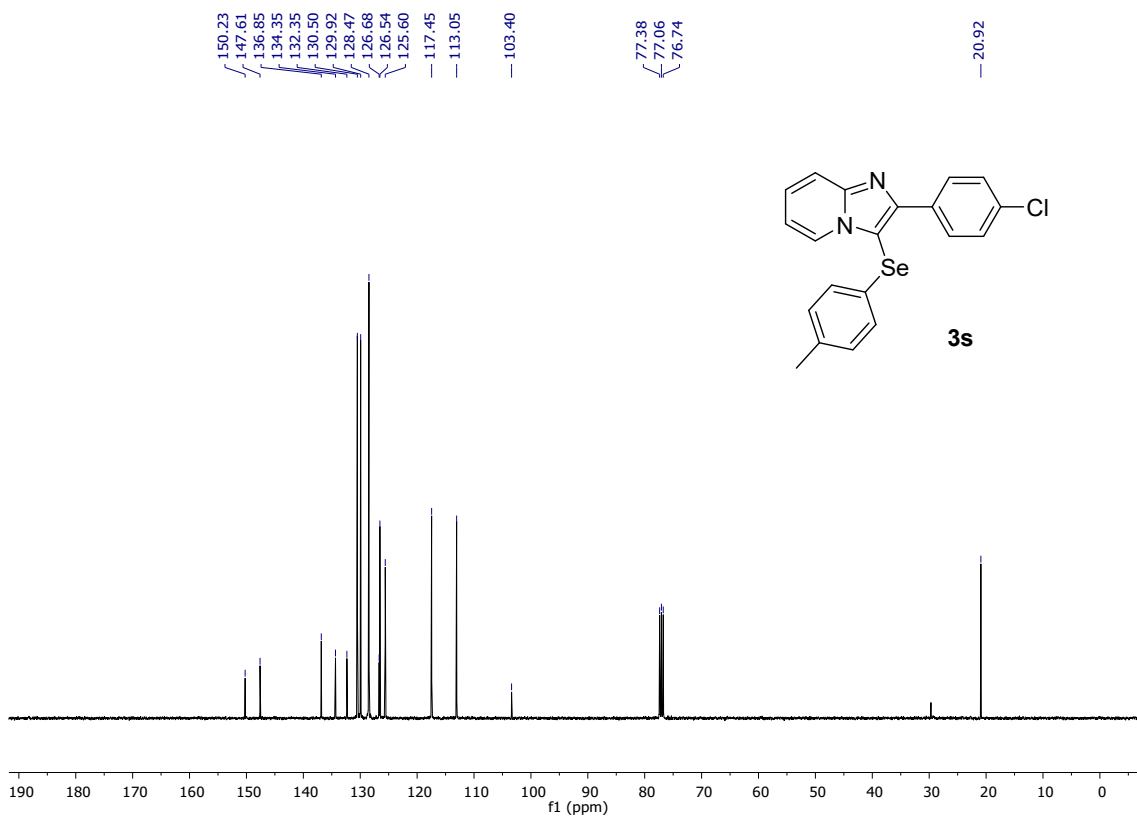
**Figure S55.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3r**.



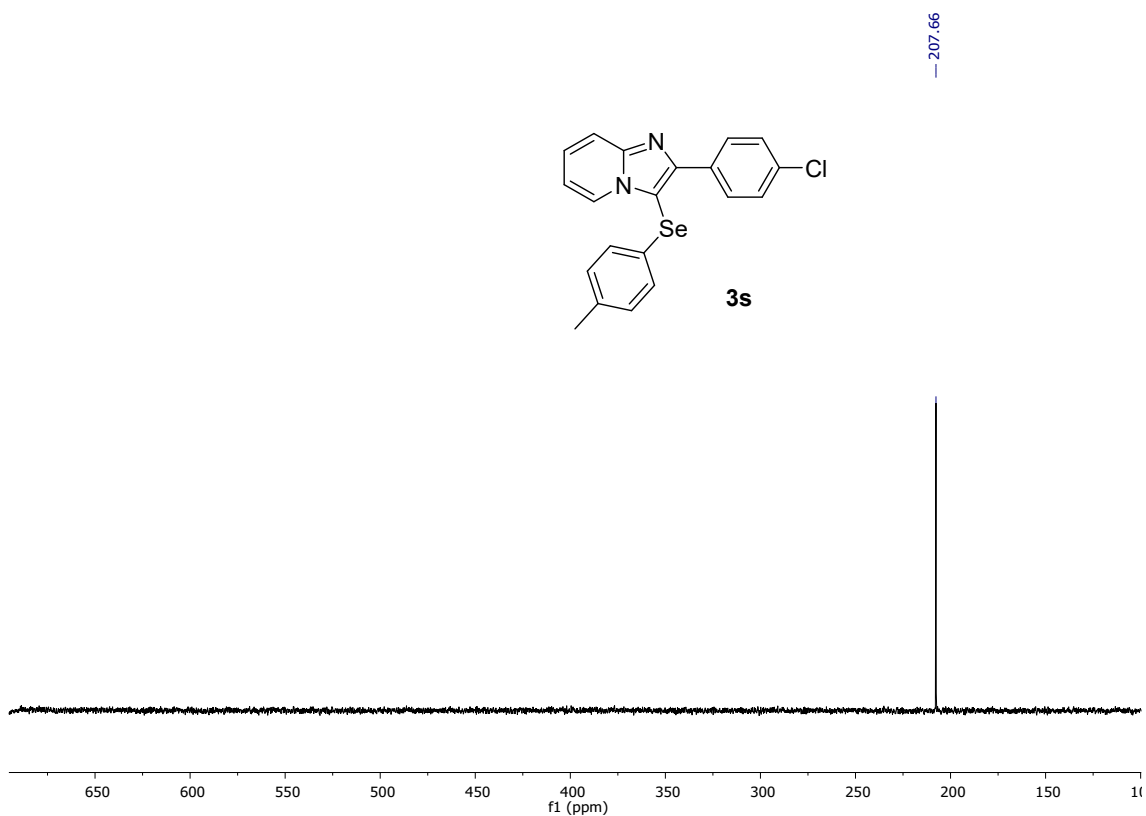
**Figure S56.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3r**.



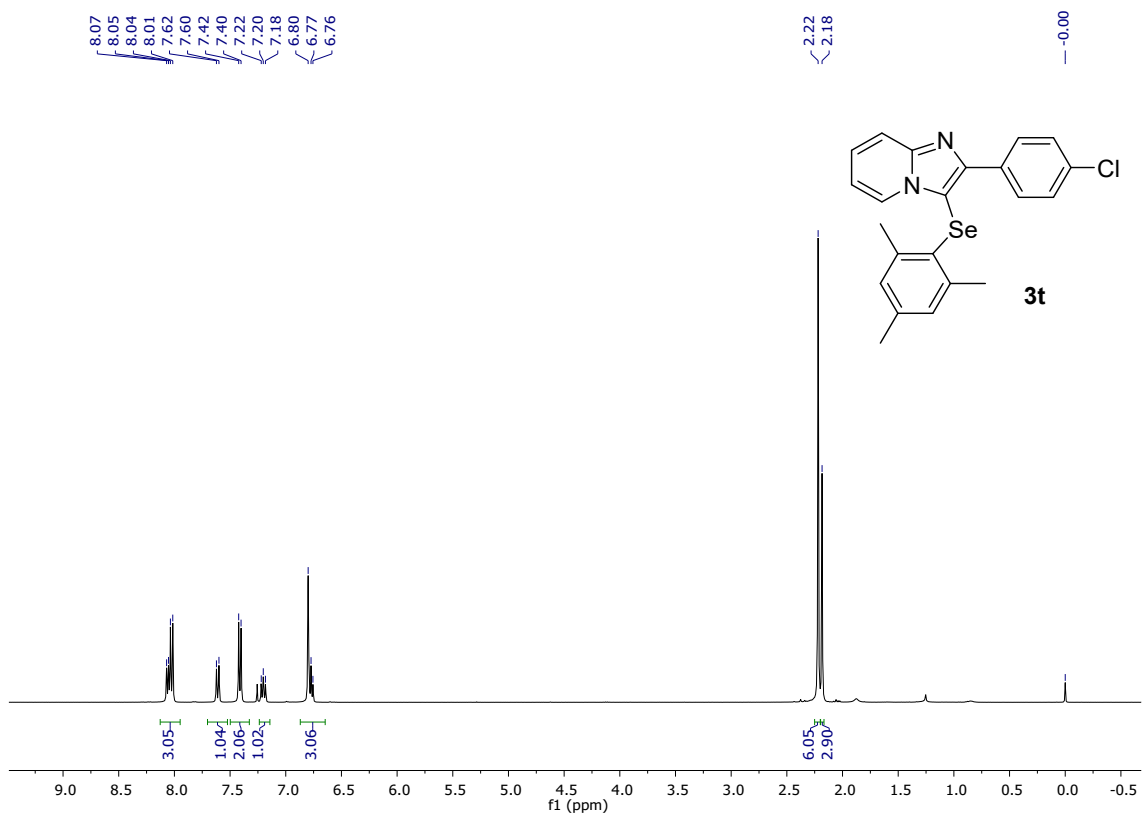
**Figure S57.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3s**.



**Figure S58.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3s**.

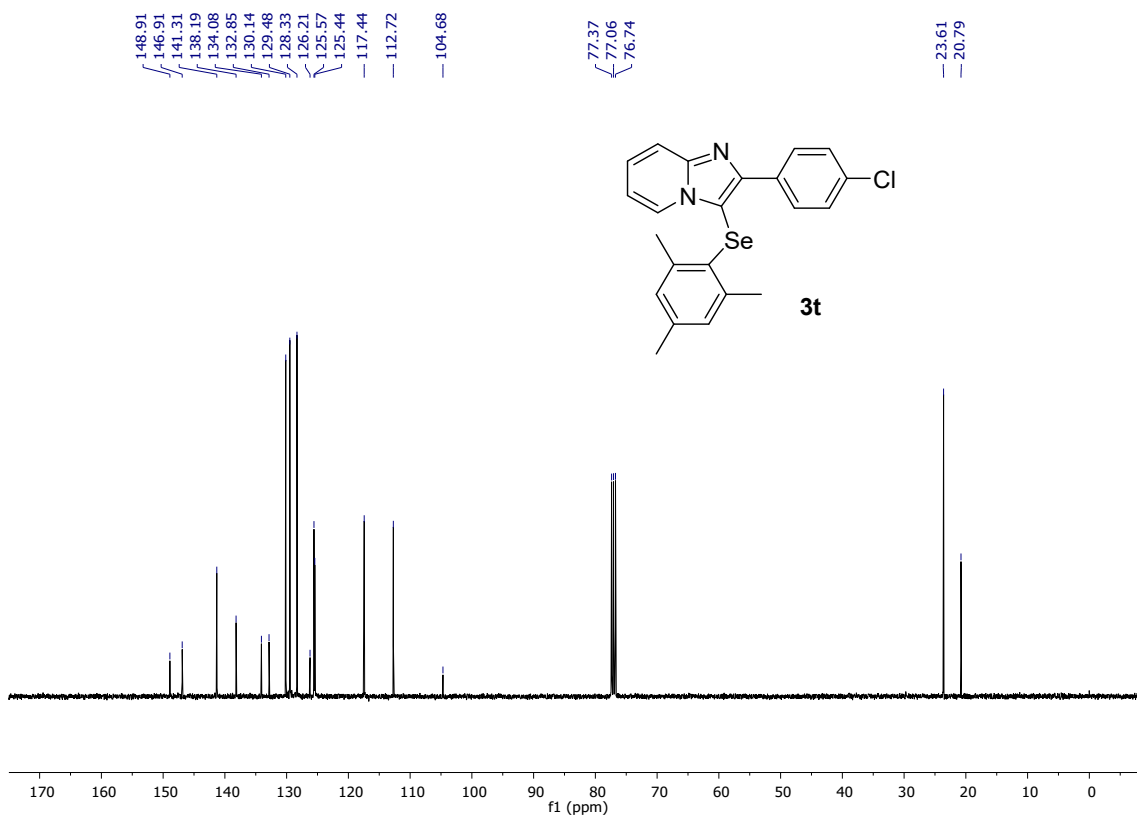


**Figure S59.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3s**.

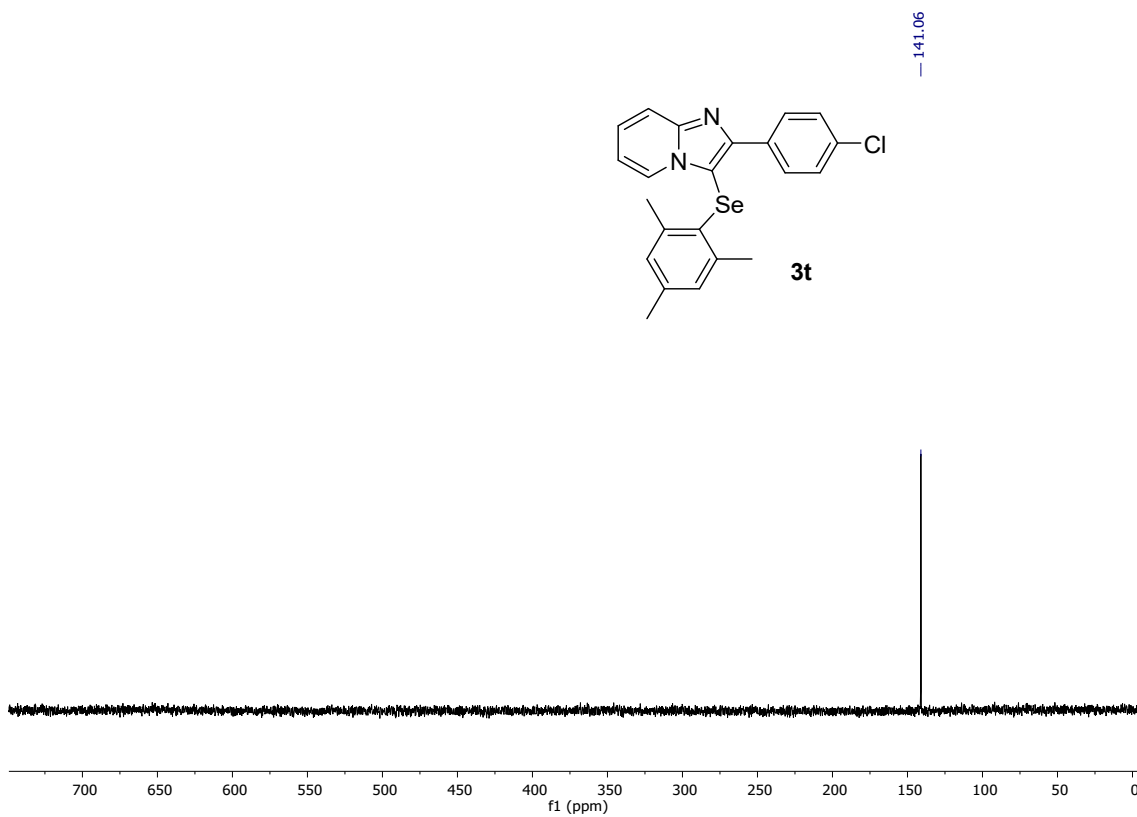


**Figure S60.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3t**.

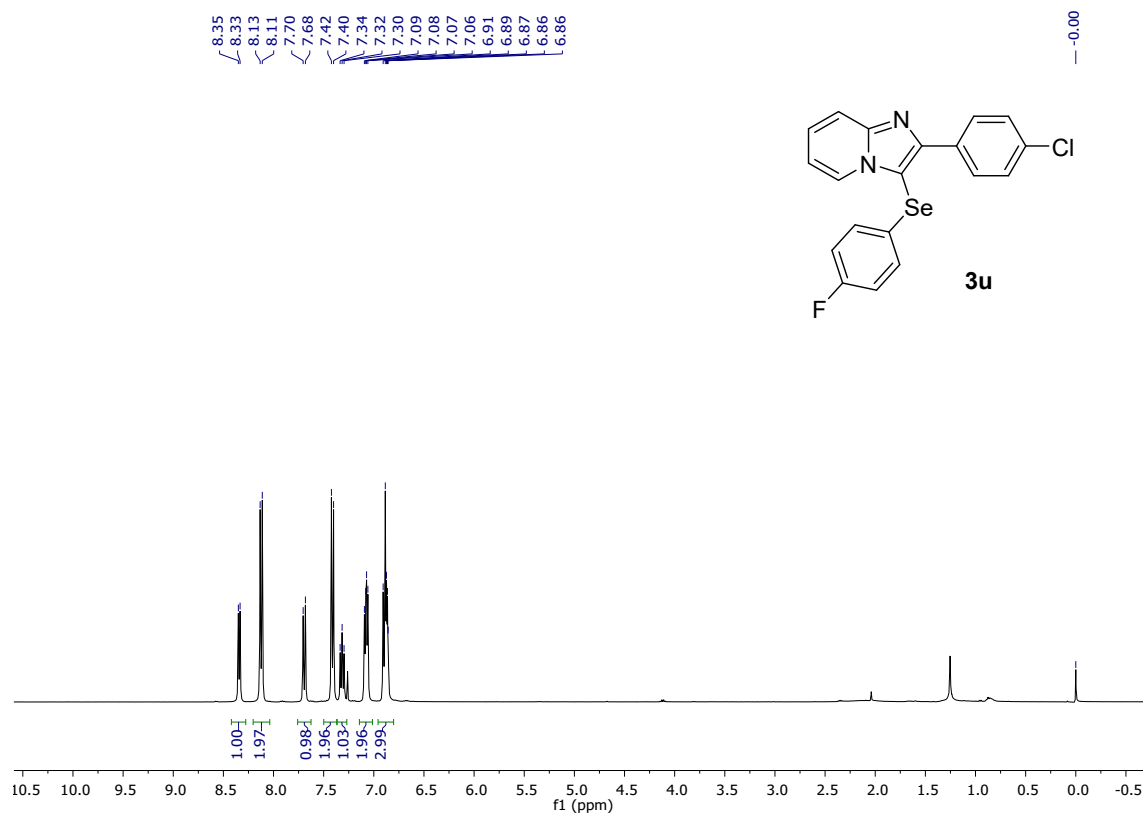




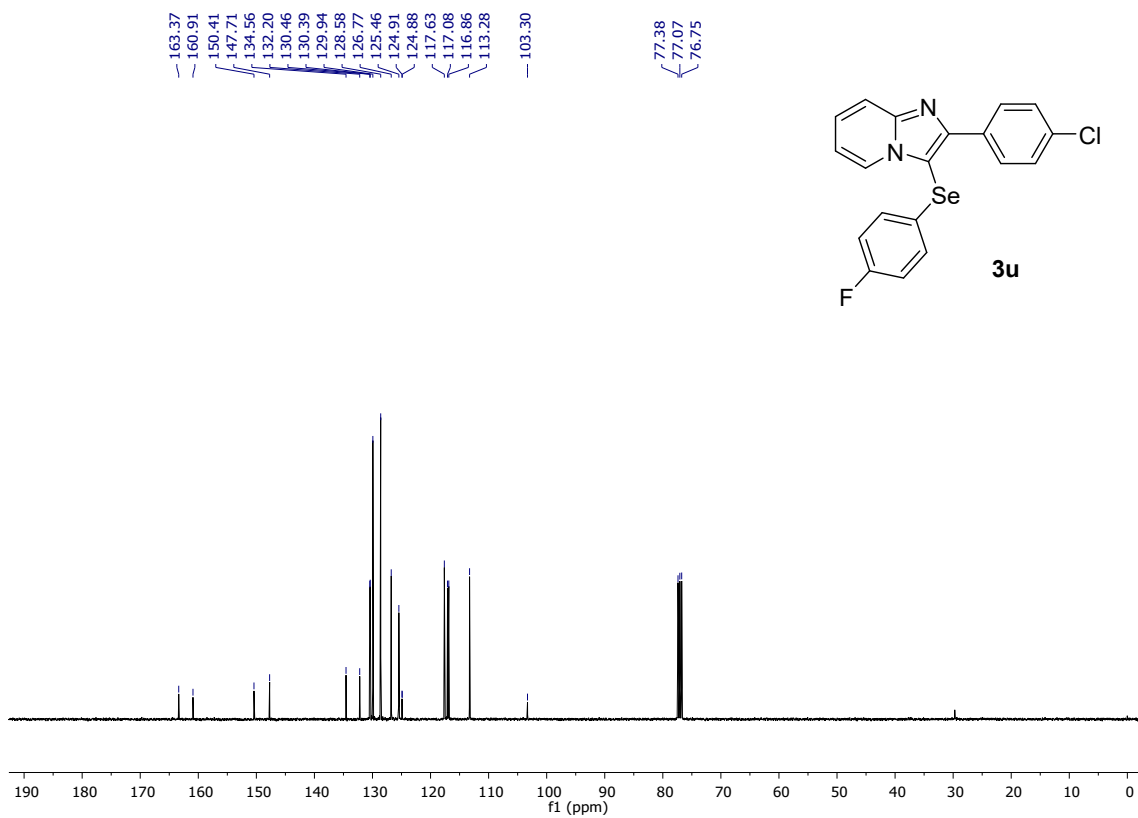
**Figure S61.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3t**.



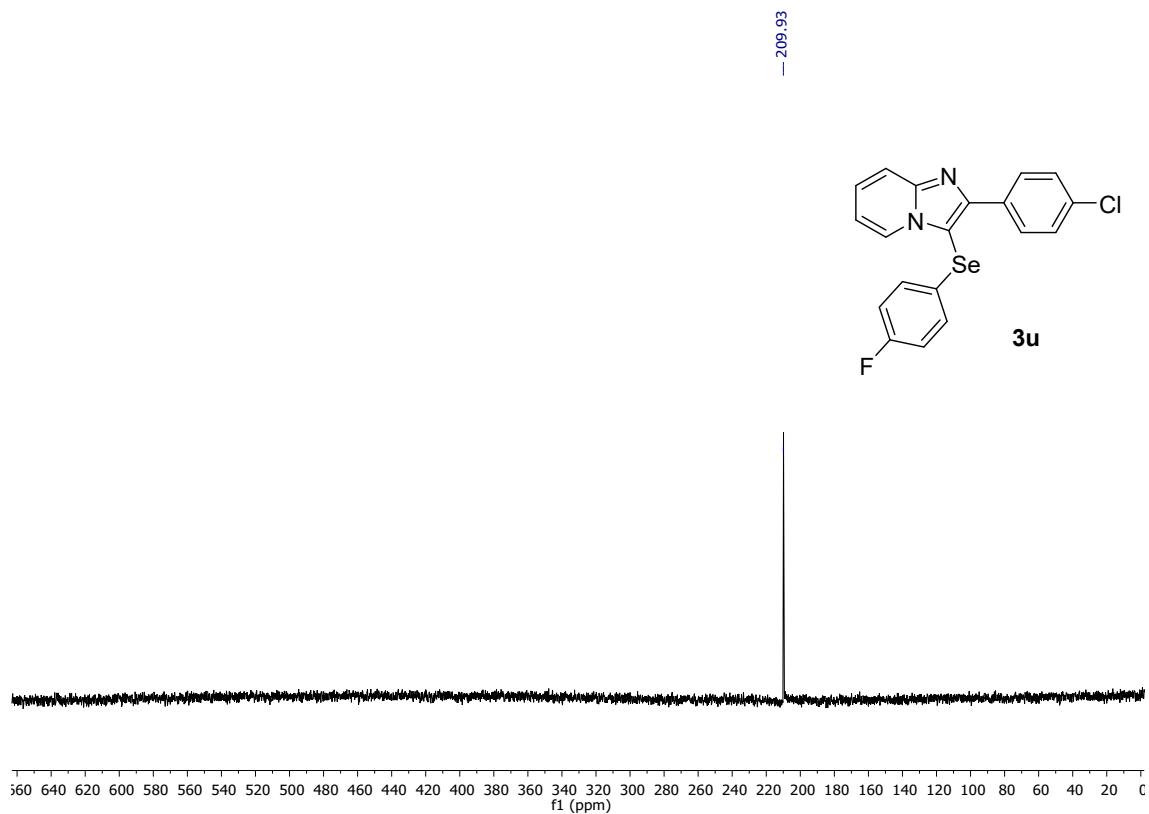
**Figure S62.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3t**.



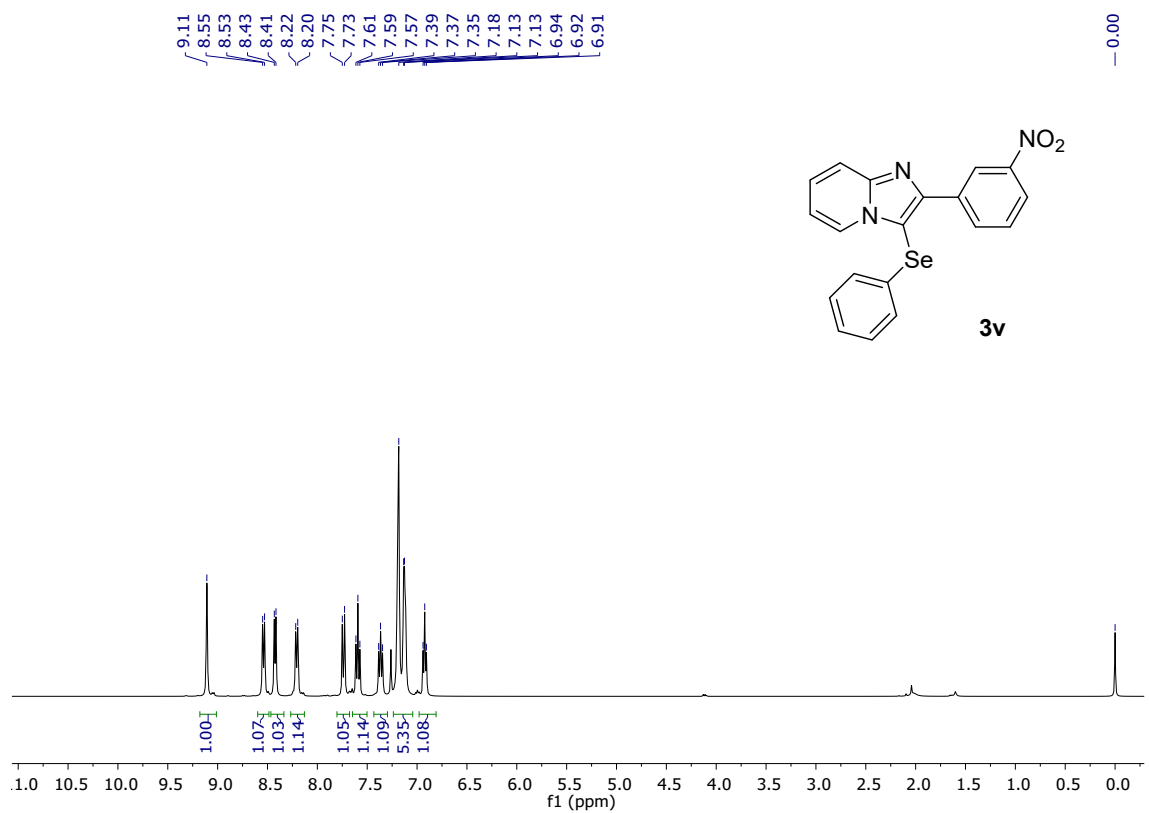
**Figure S63.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3u**.



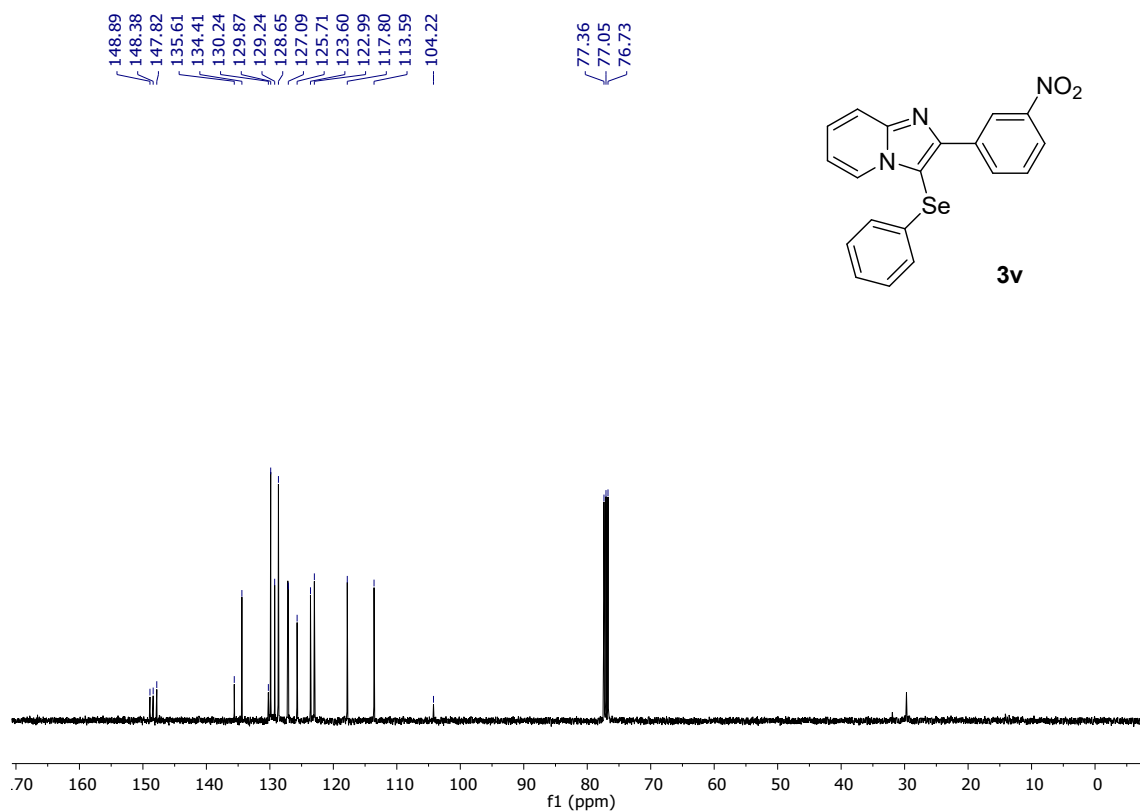
**Figure S64.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3u**.



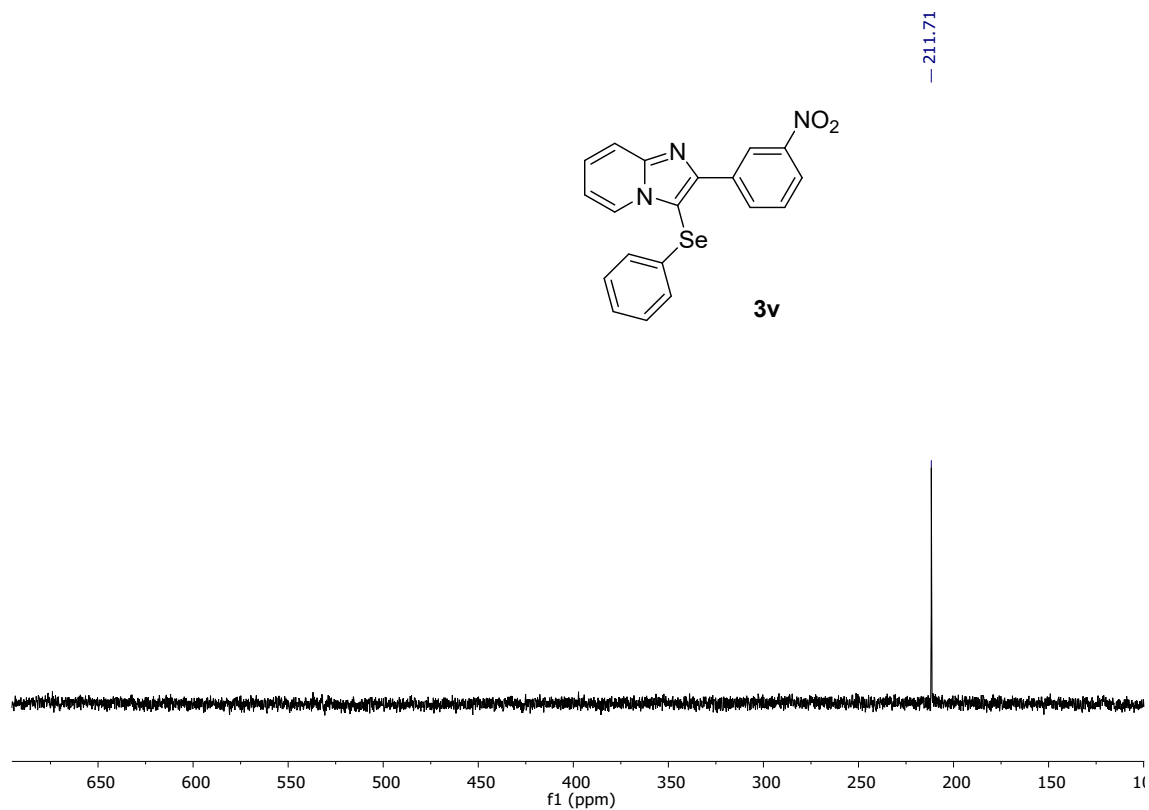
**Figure S65.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3u**.



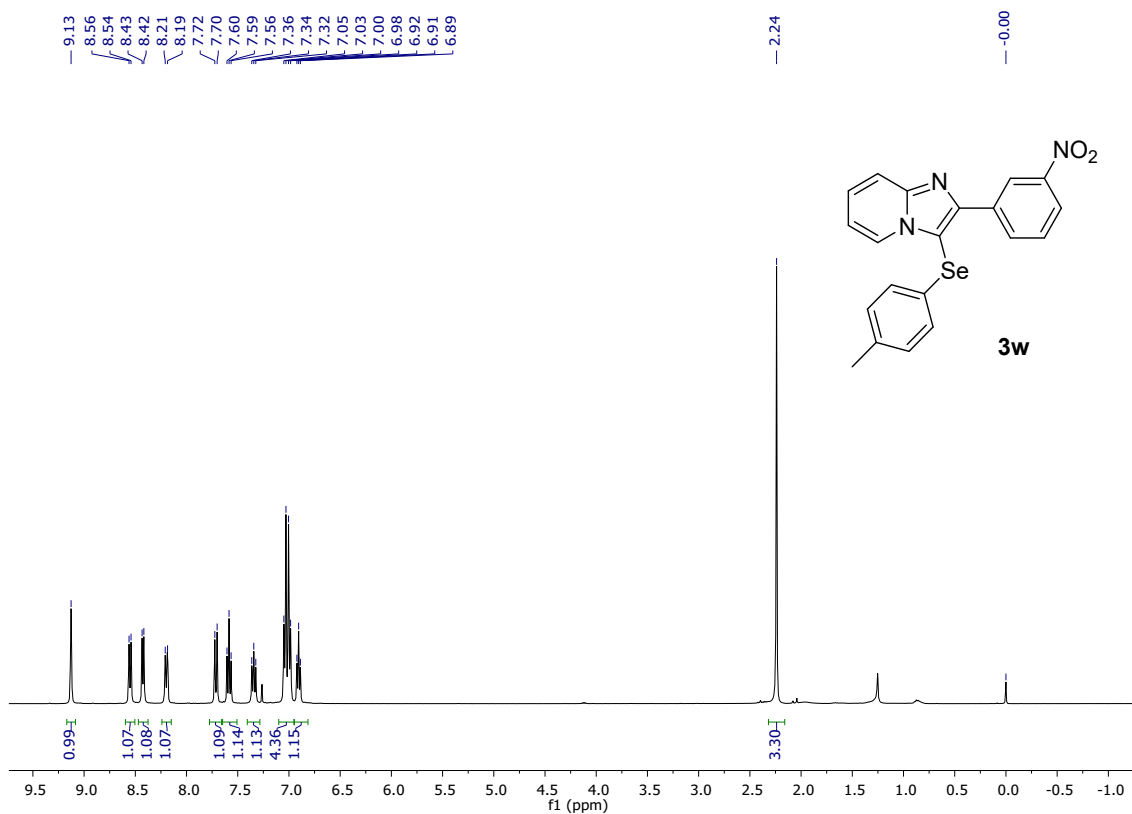
**Figure S66.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3v**.



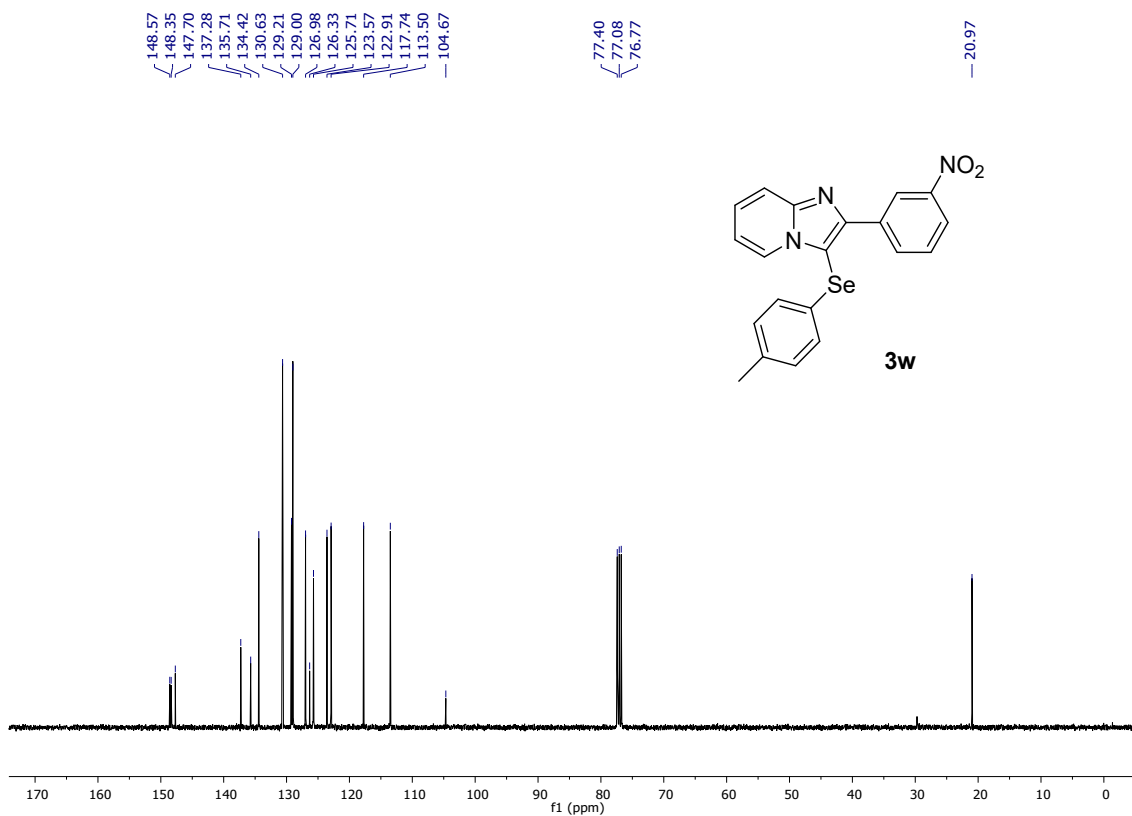
**Figure S67.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3v**.



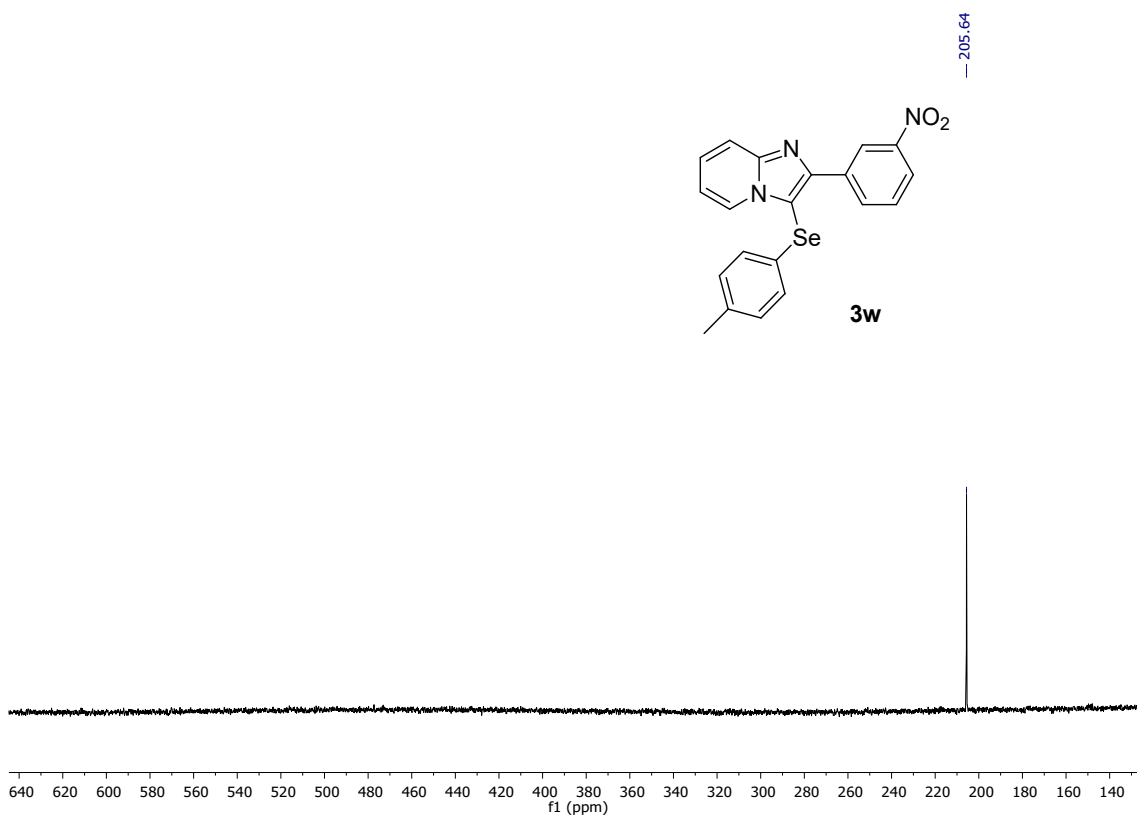
**Figure S68.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3v**.



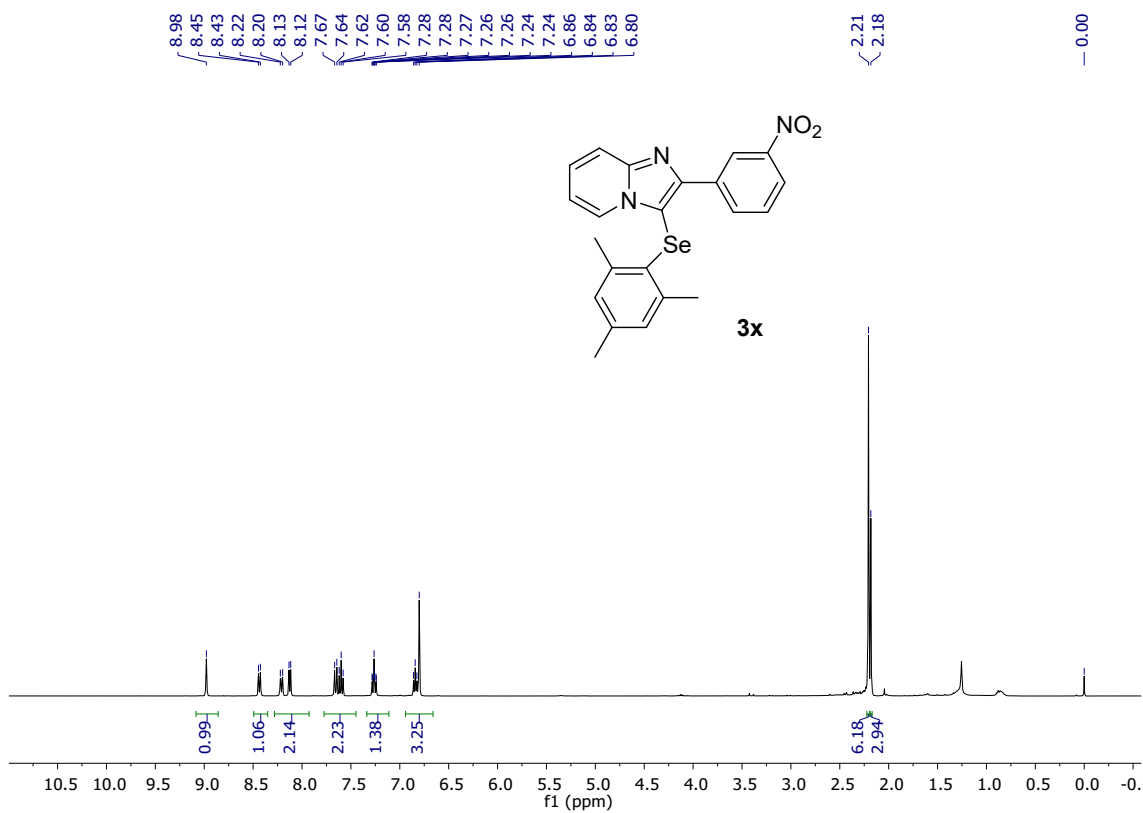
**Figure S69.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3w**.



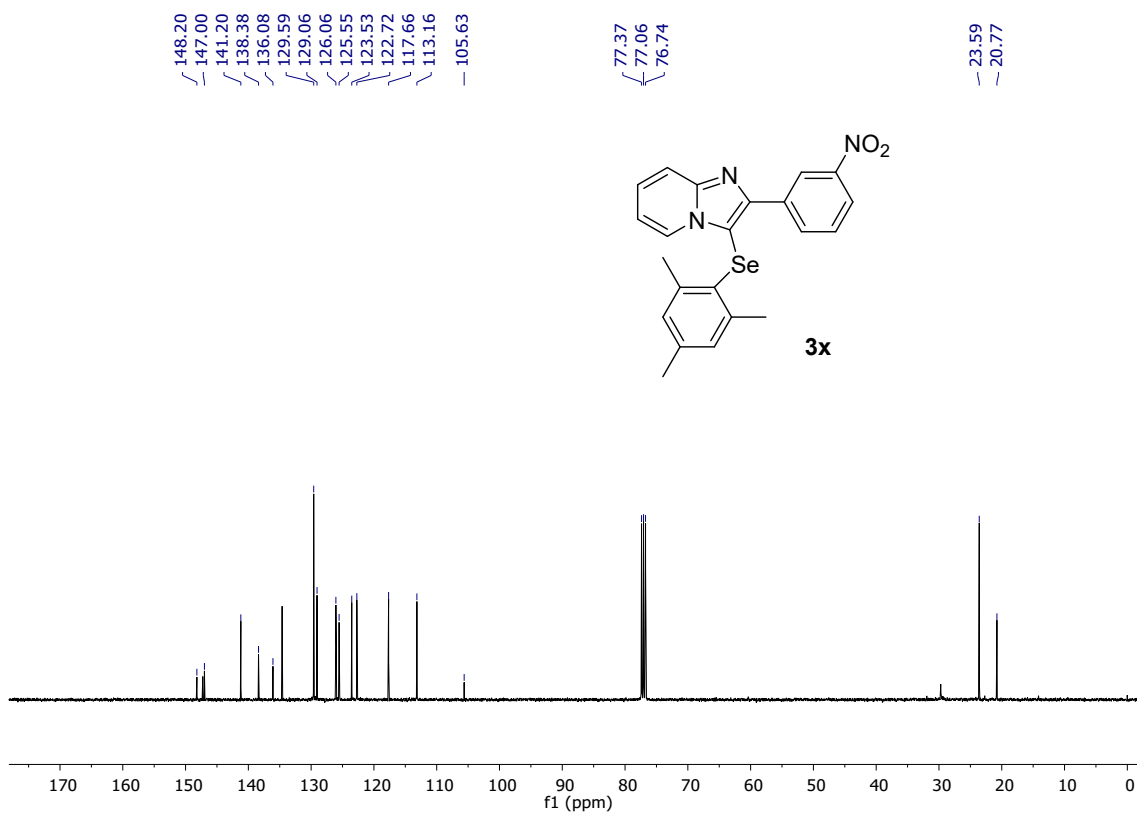
**Figure S70.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3w**.



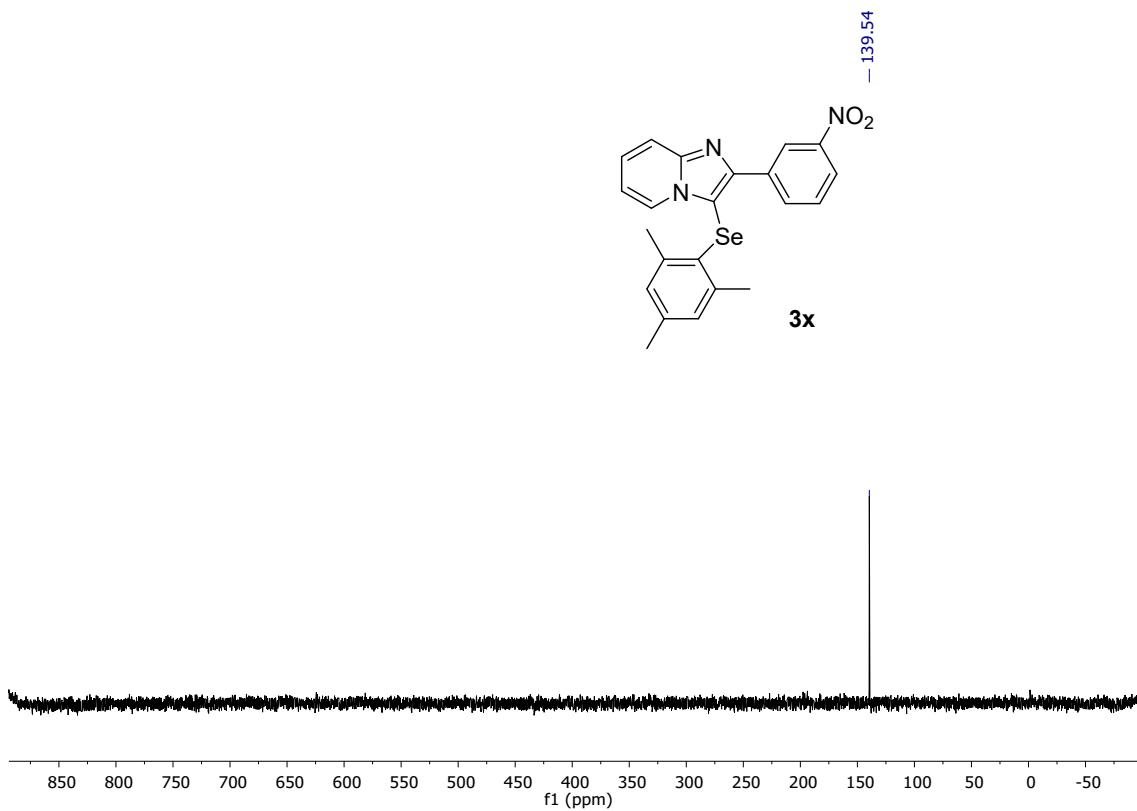
**Figure S71.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3w**.



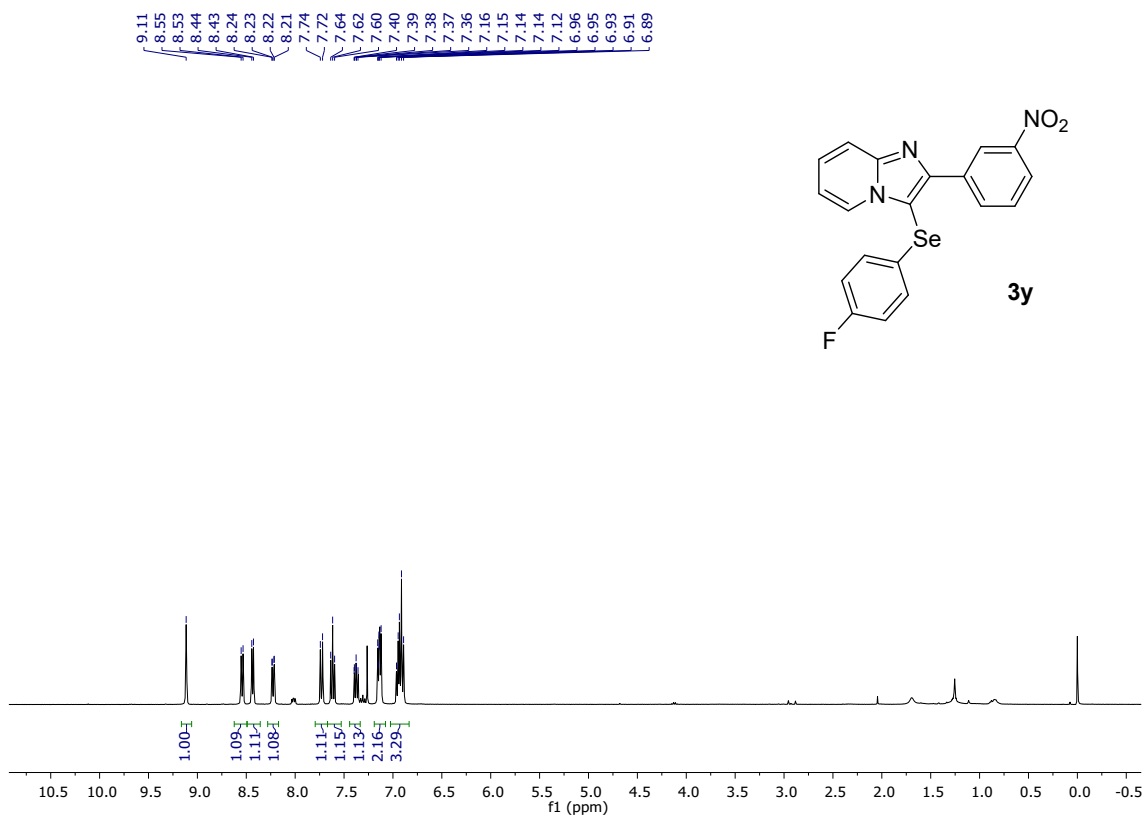
**Figure S72.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3x**.



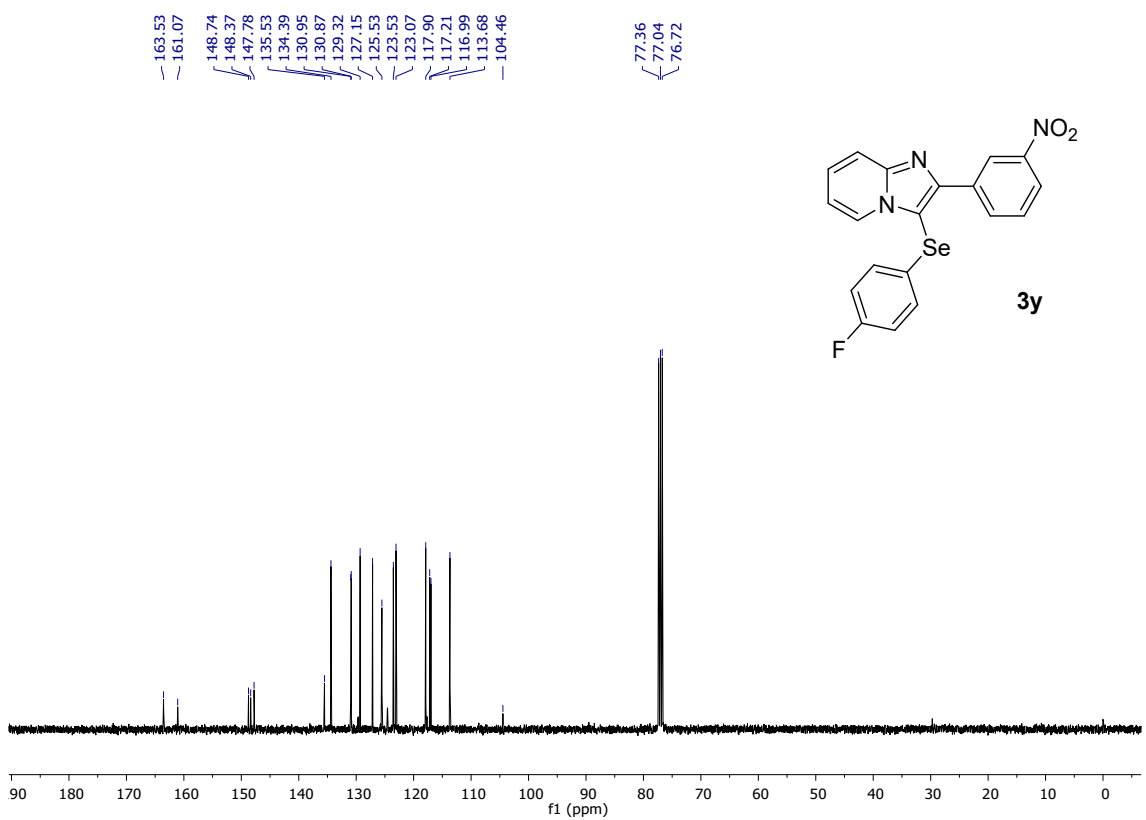
**Figure S73.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3x**.



**Figure S74.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3x**.

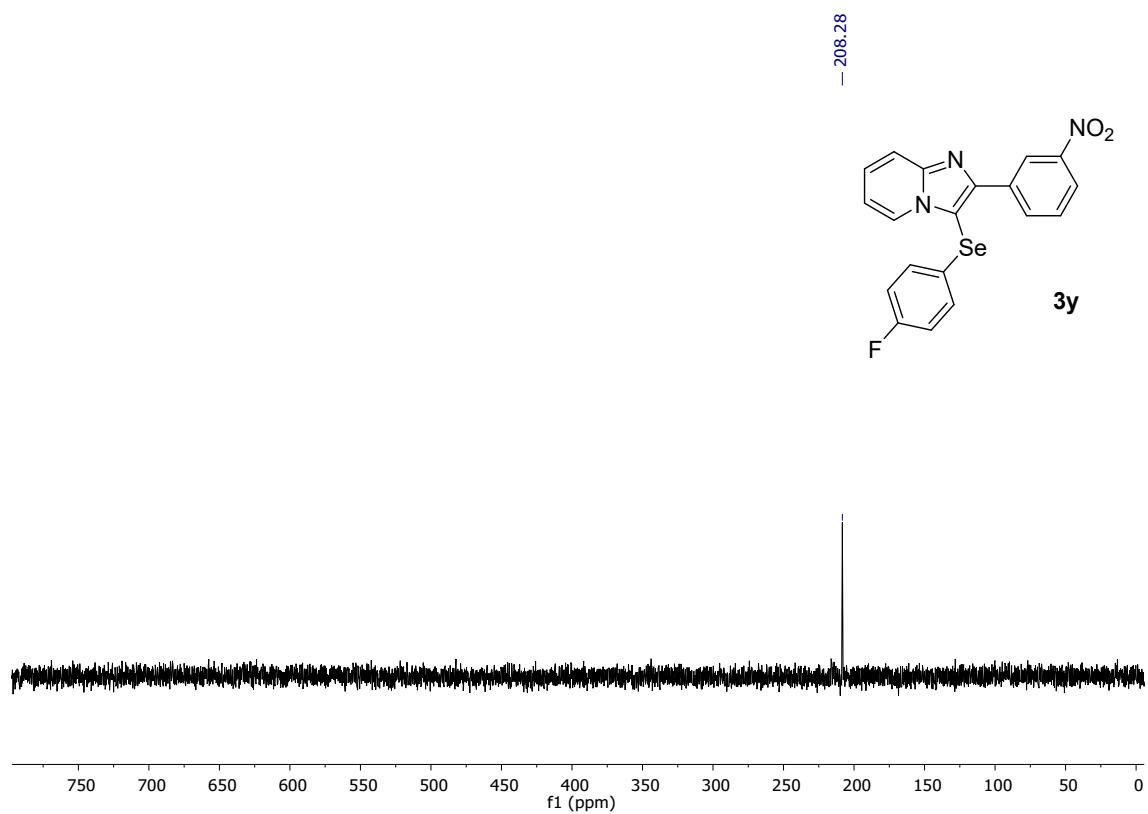


**Figure S75.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3y**.

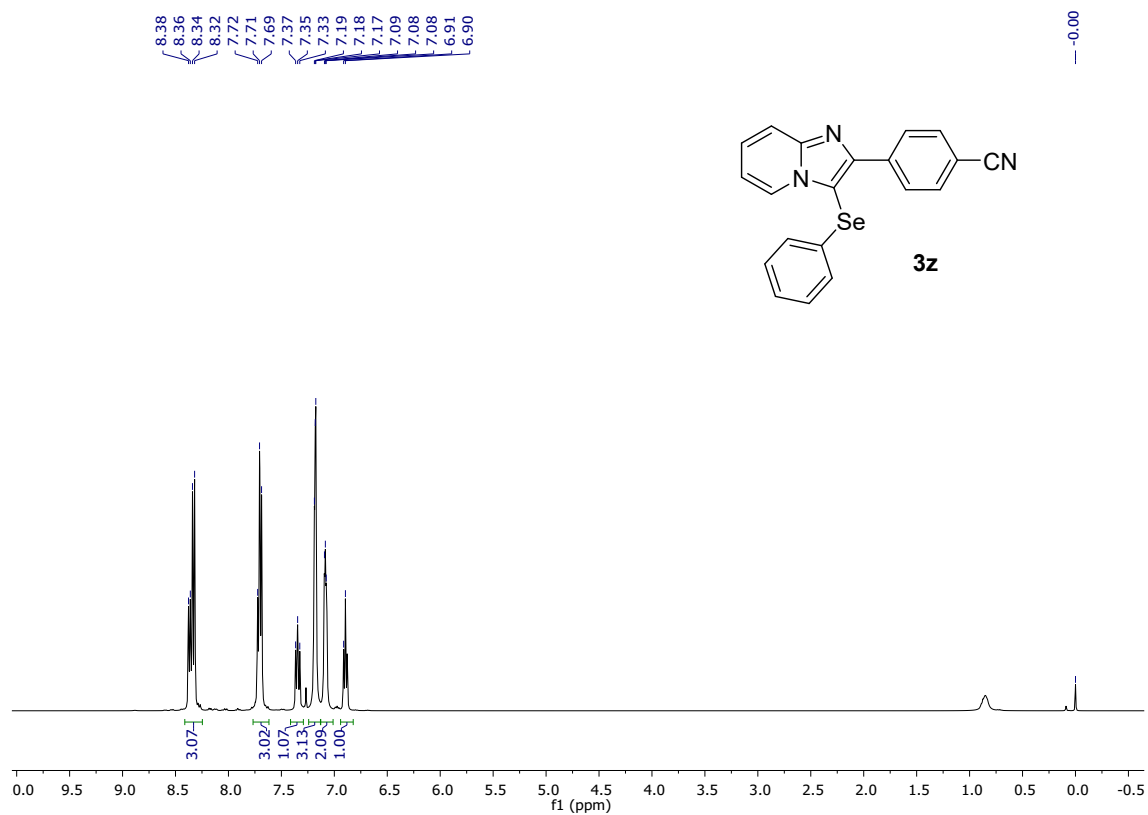


**Figure S76.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3y**.

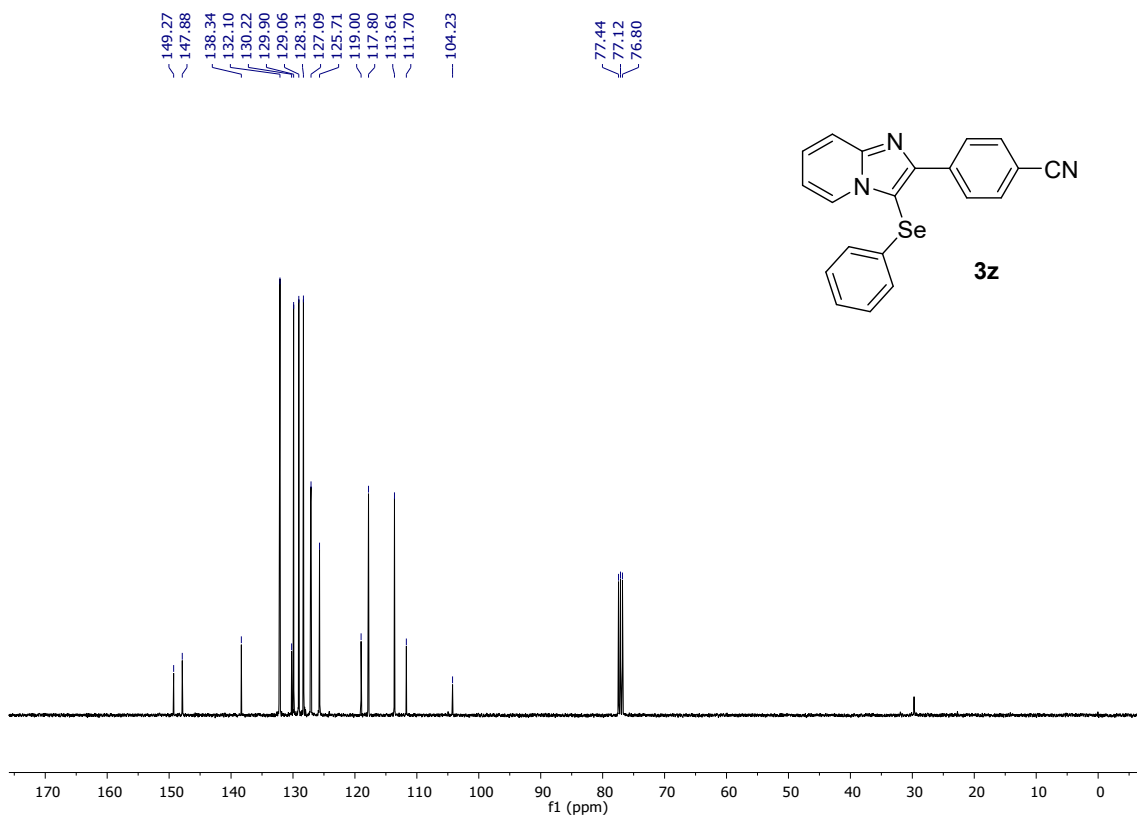




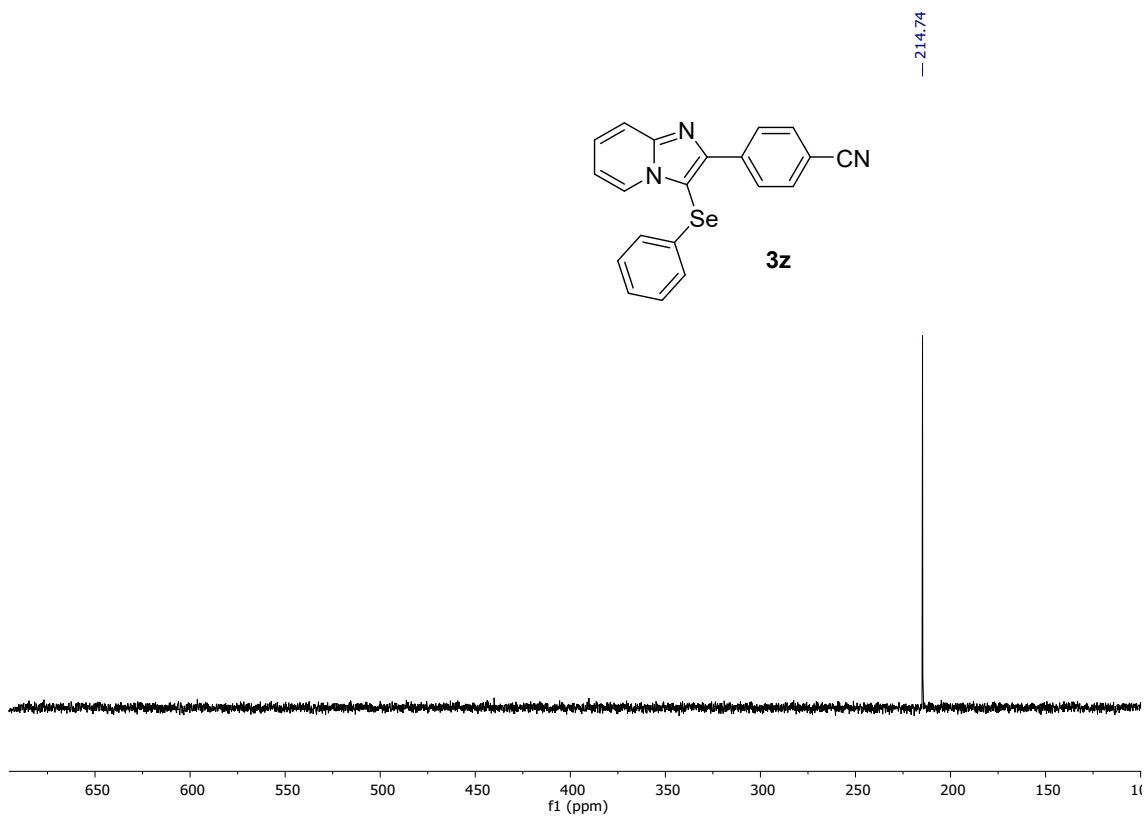
**Figure S77.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3y**.



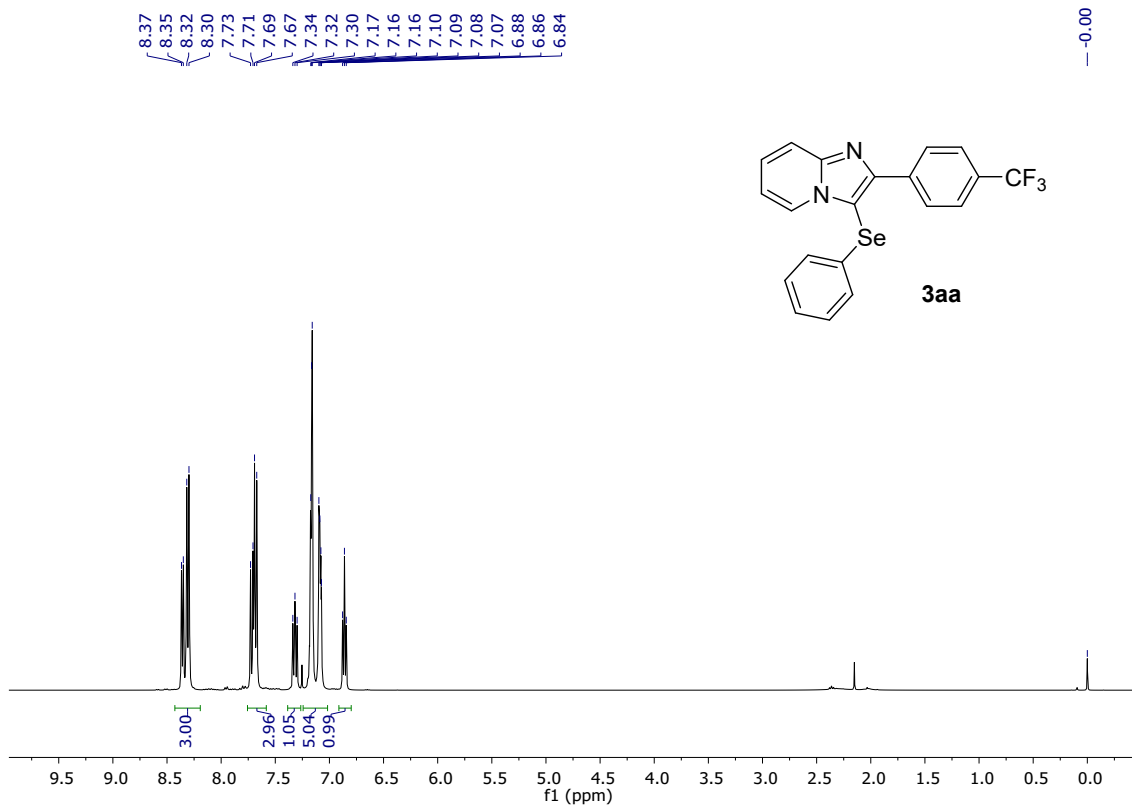
**Figure S78.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3z**.



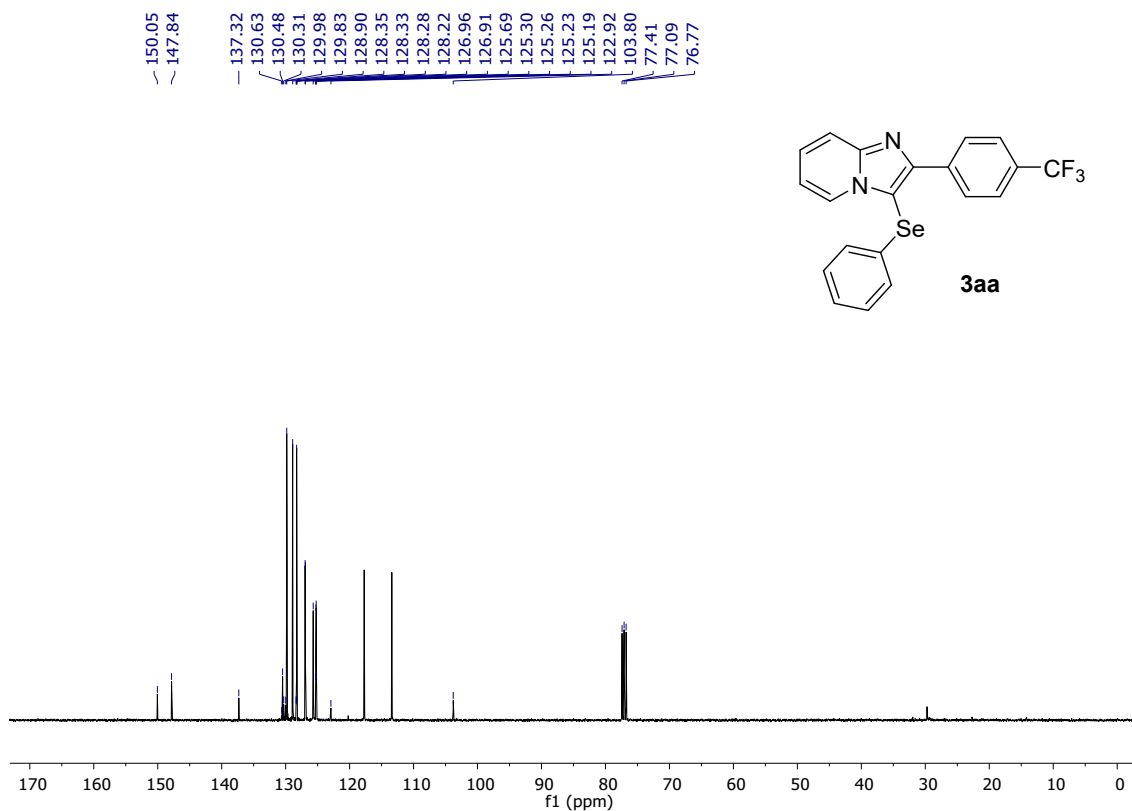
**Figure S79.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3z**.



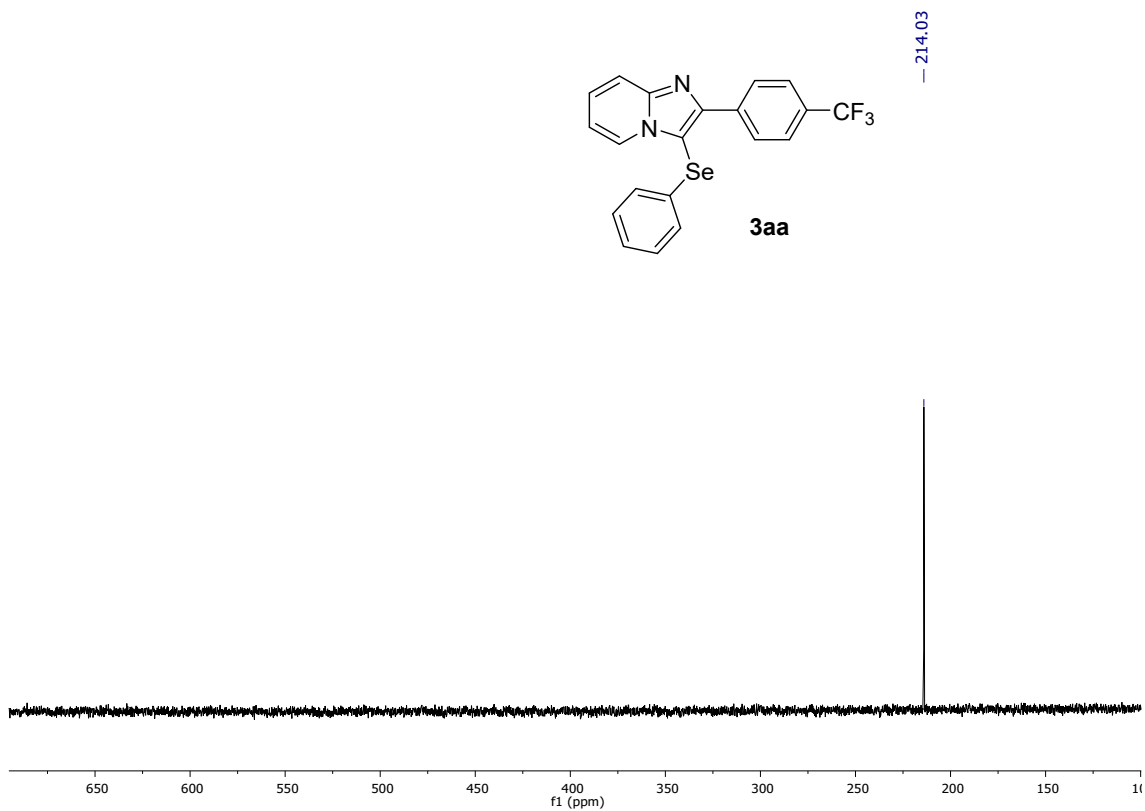
**Figure S80.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3z**.



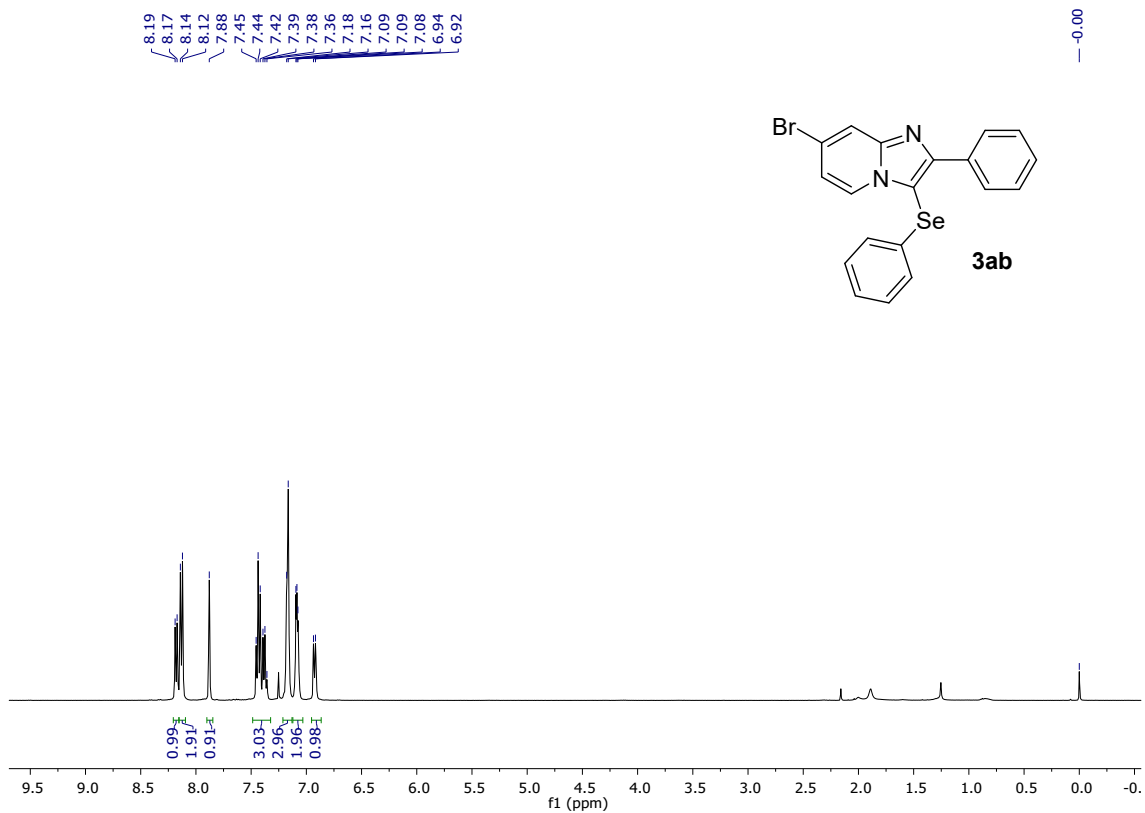
**Figure S81.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3aa**.



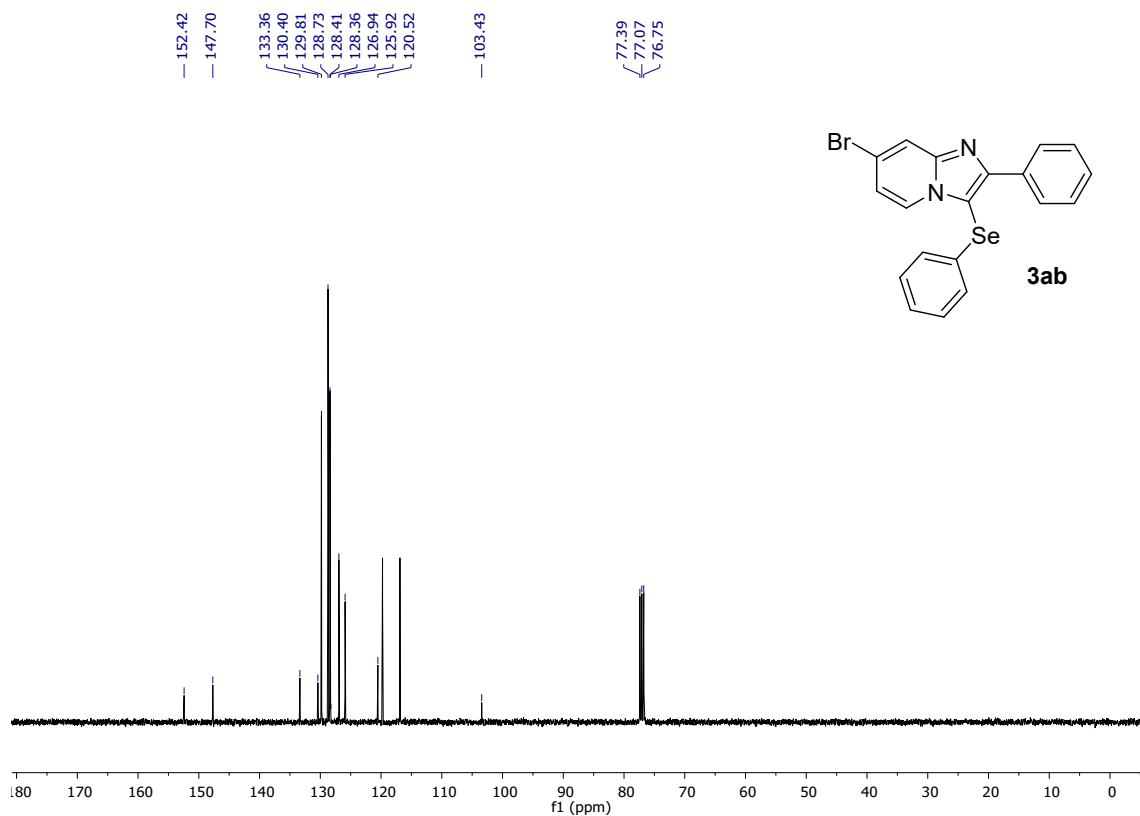
**Figure S82.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3aa**.



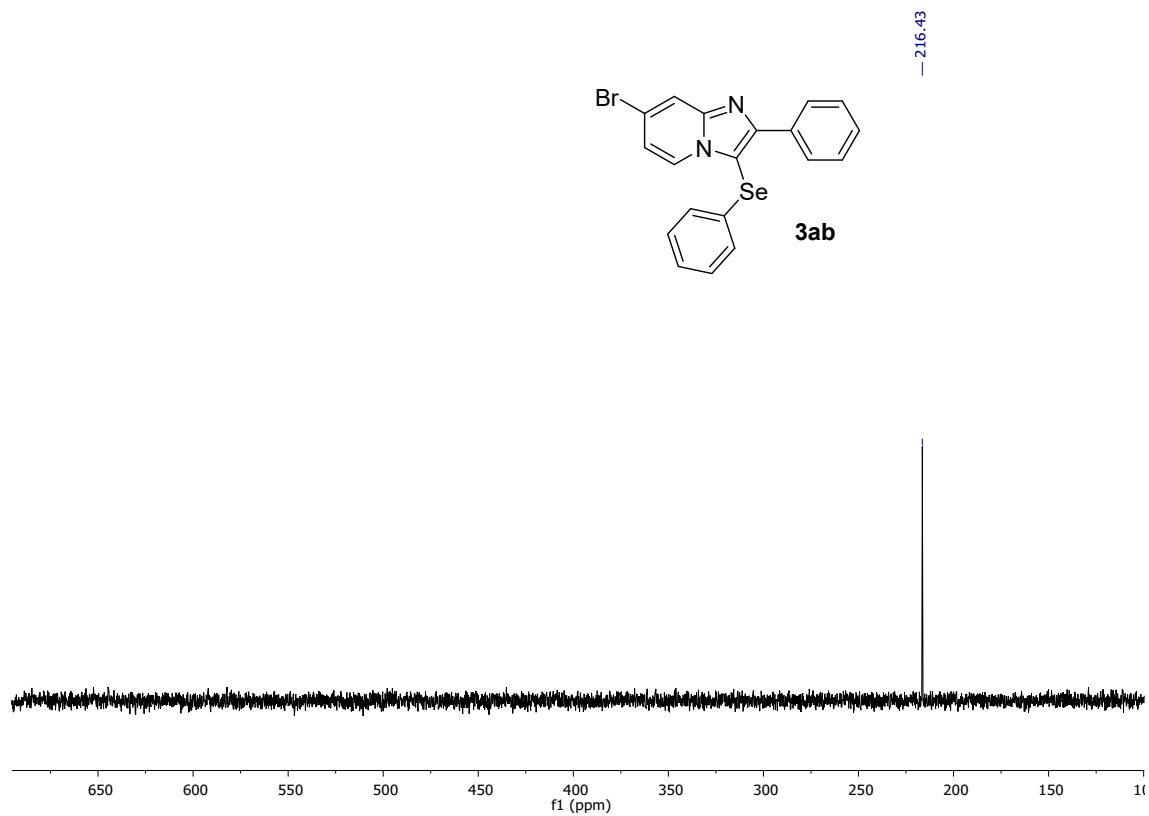
**Figure S83.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3aa**.



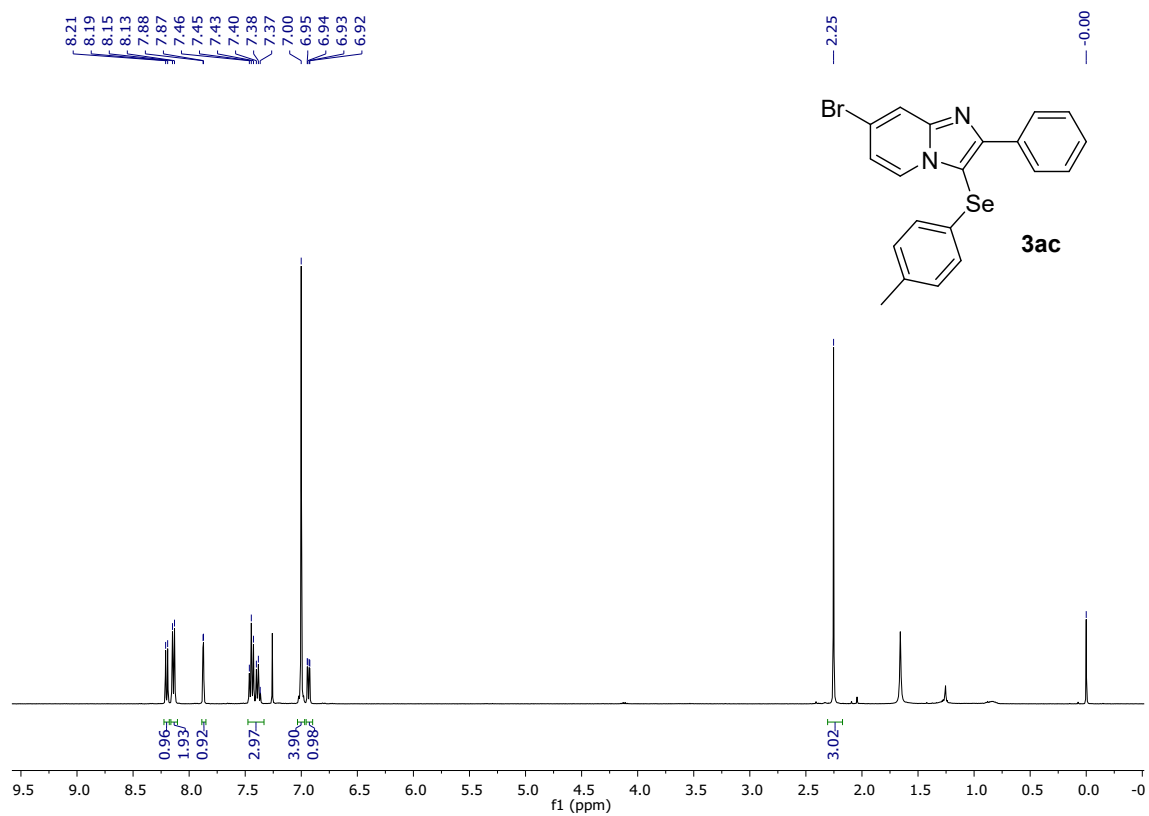
**Figure S84.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3ab**.



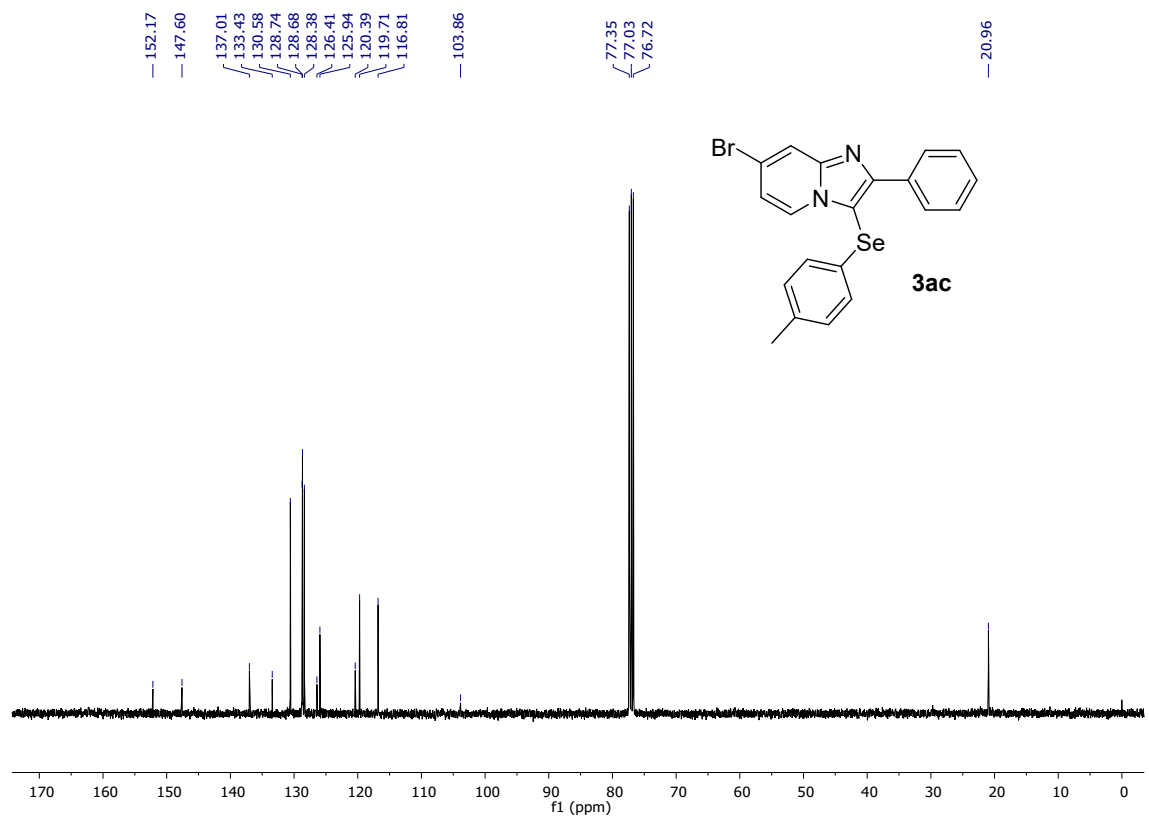
**Figure S85.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ab**.



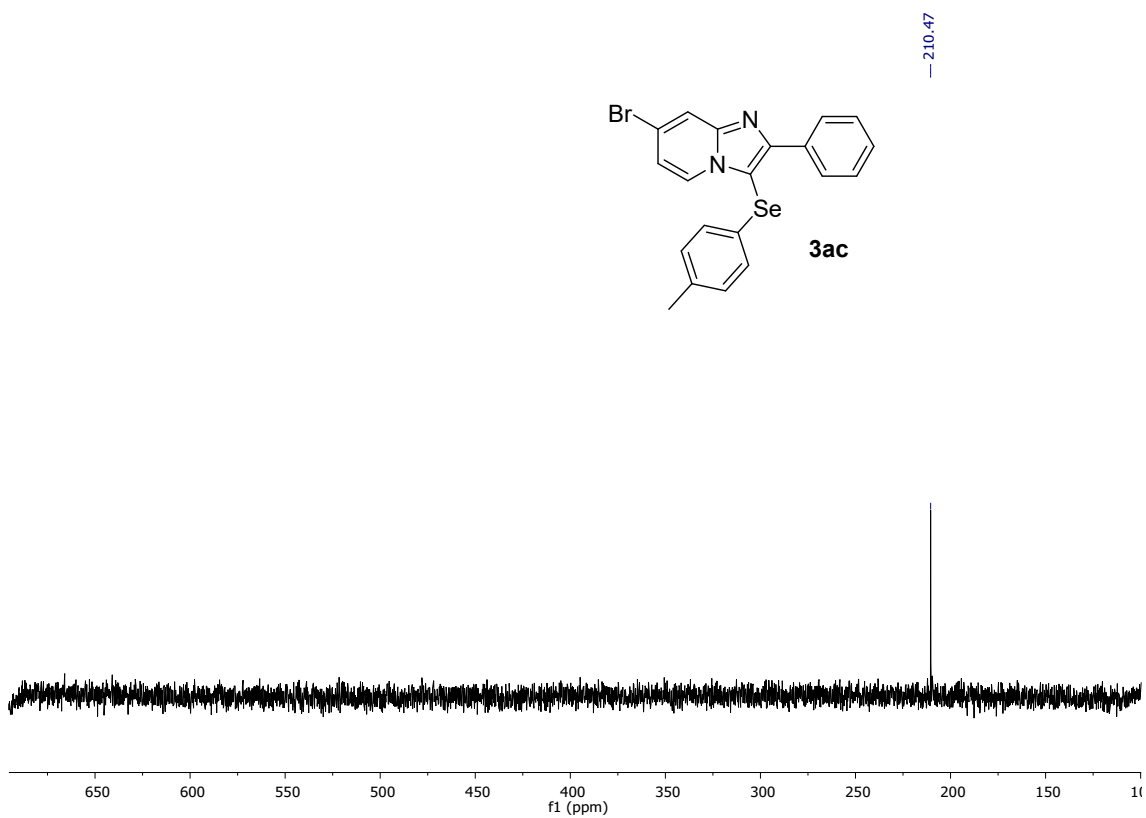
**Figure S86.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ab**.



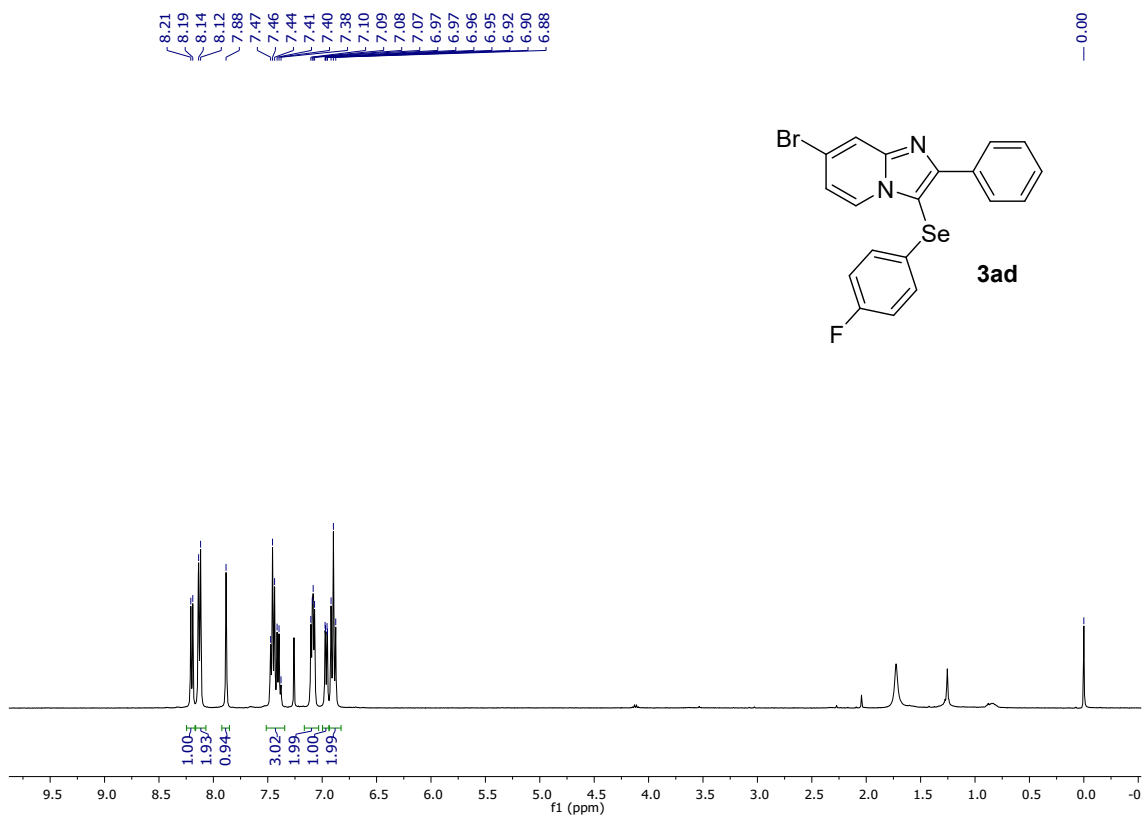
**Figure S87.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ac**.



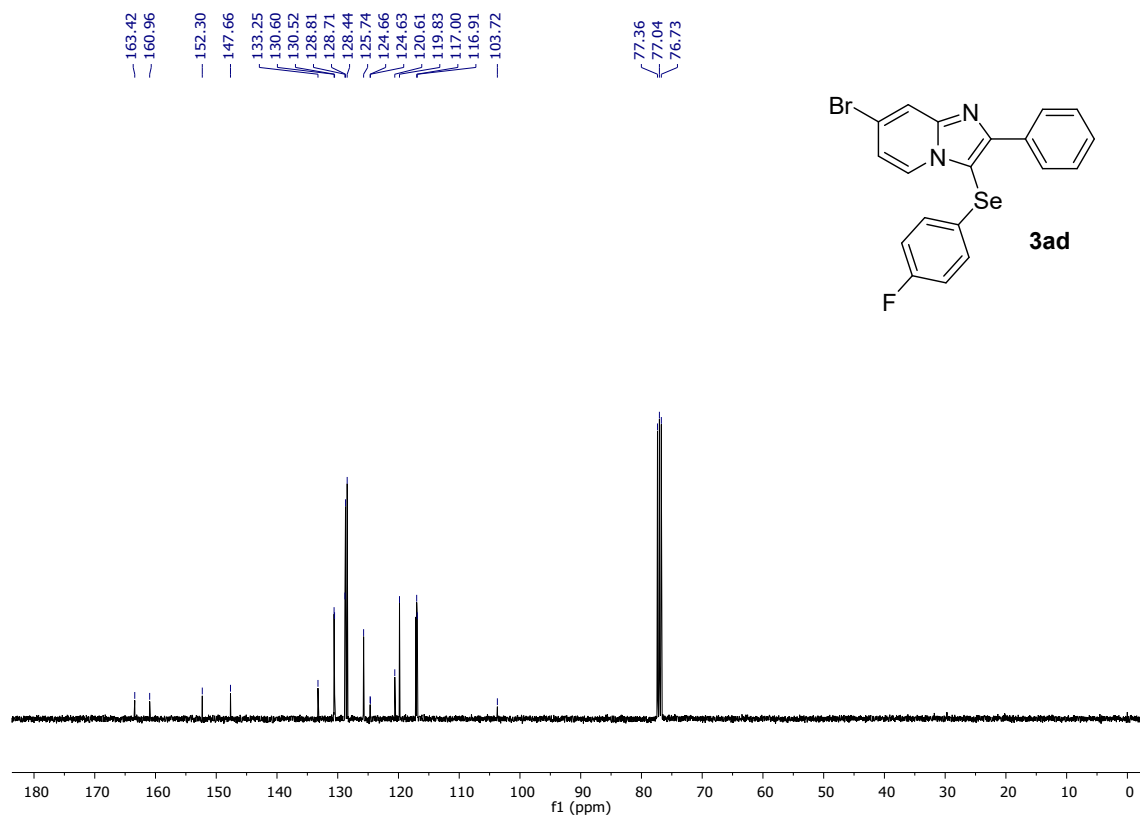
**Figure S88.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ac**



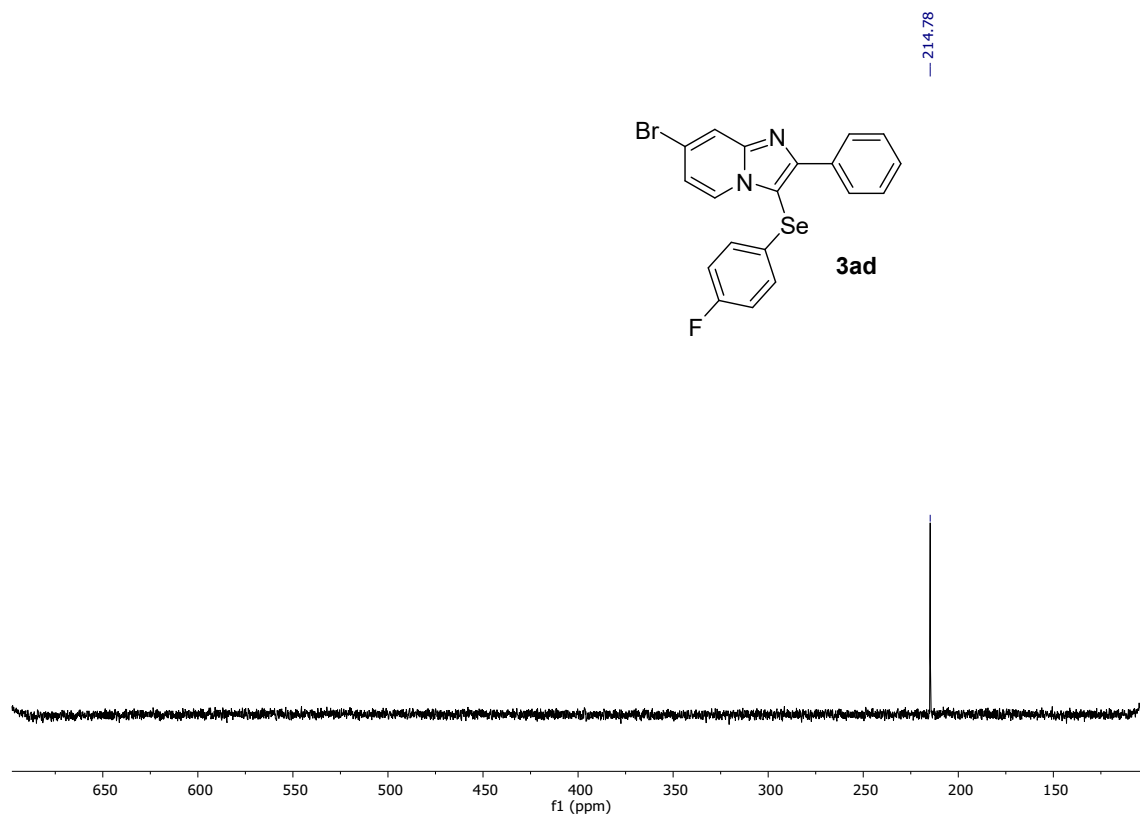
**Figure S89.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3ac**.



**Figure S90.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3ad**.

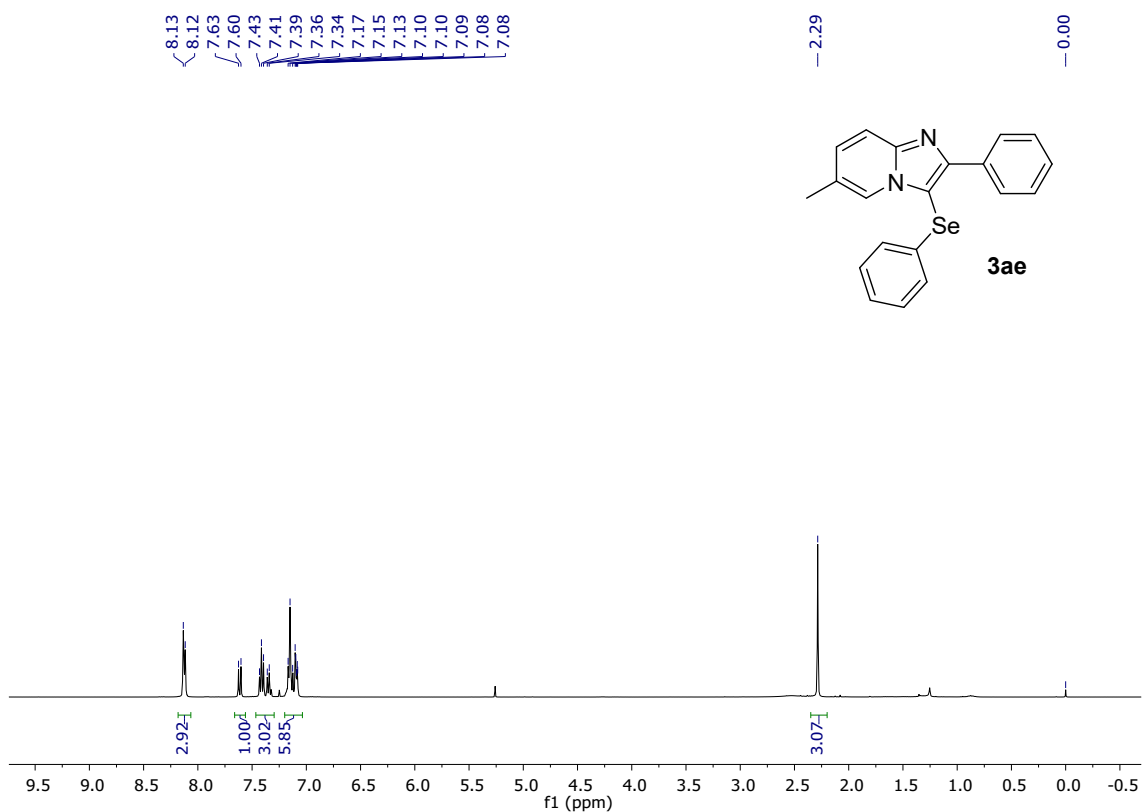


**Figure S91.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ad**.

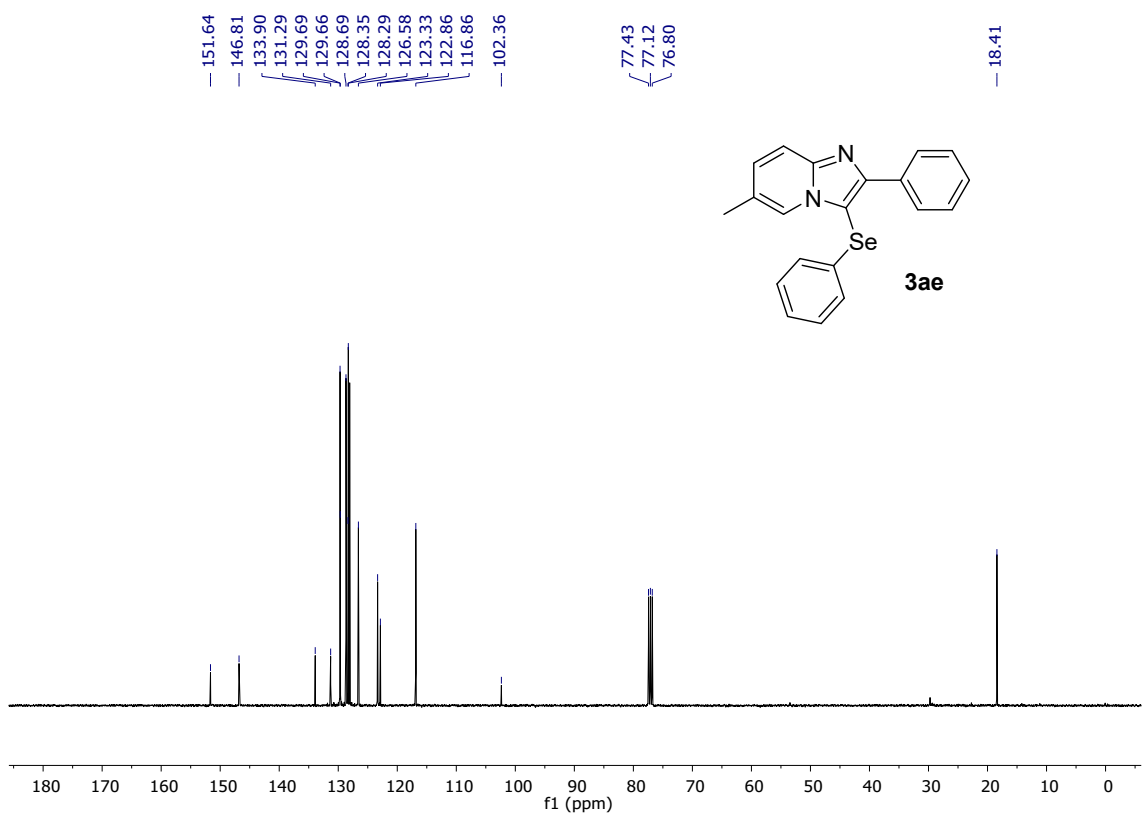


**Figure S92.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ad**.

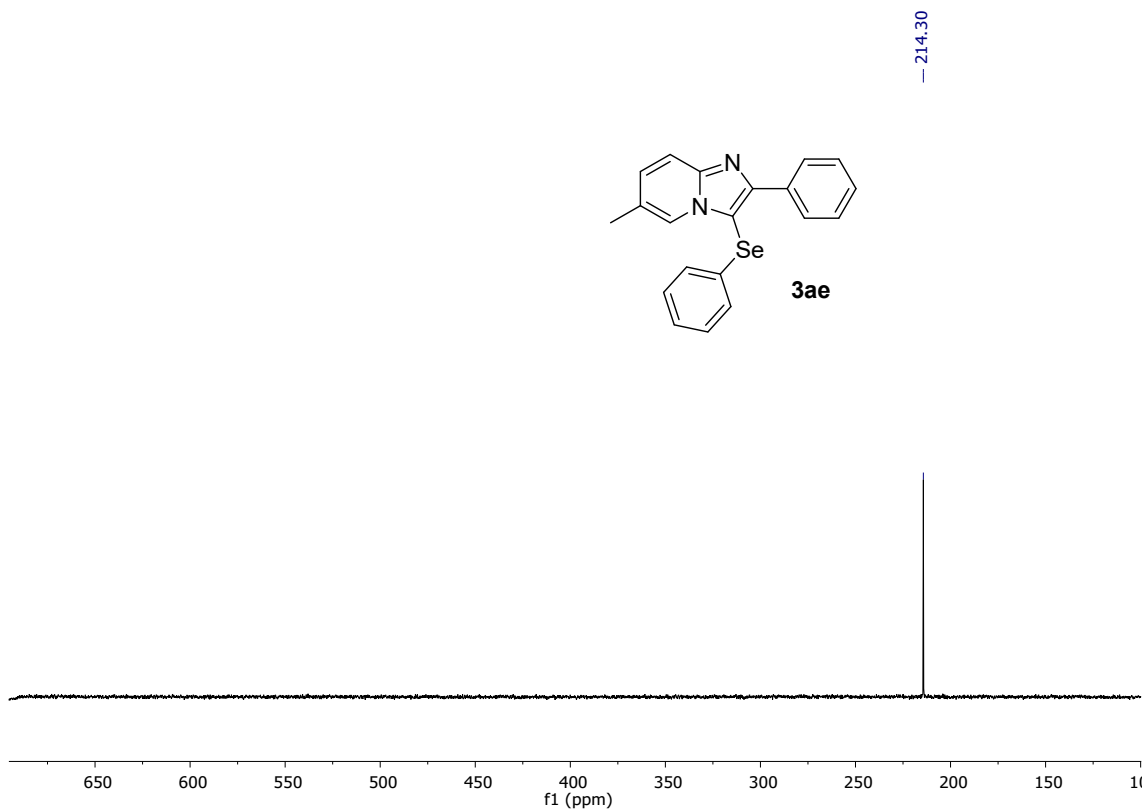




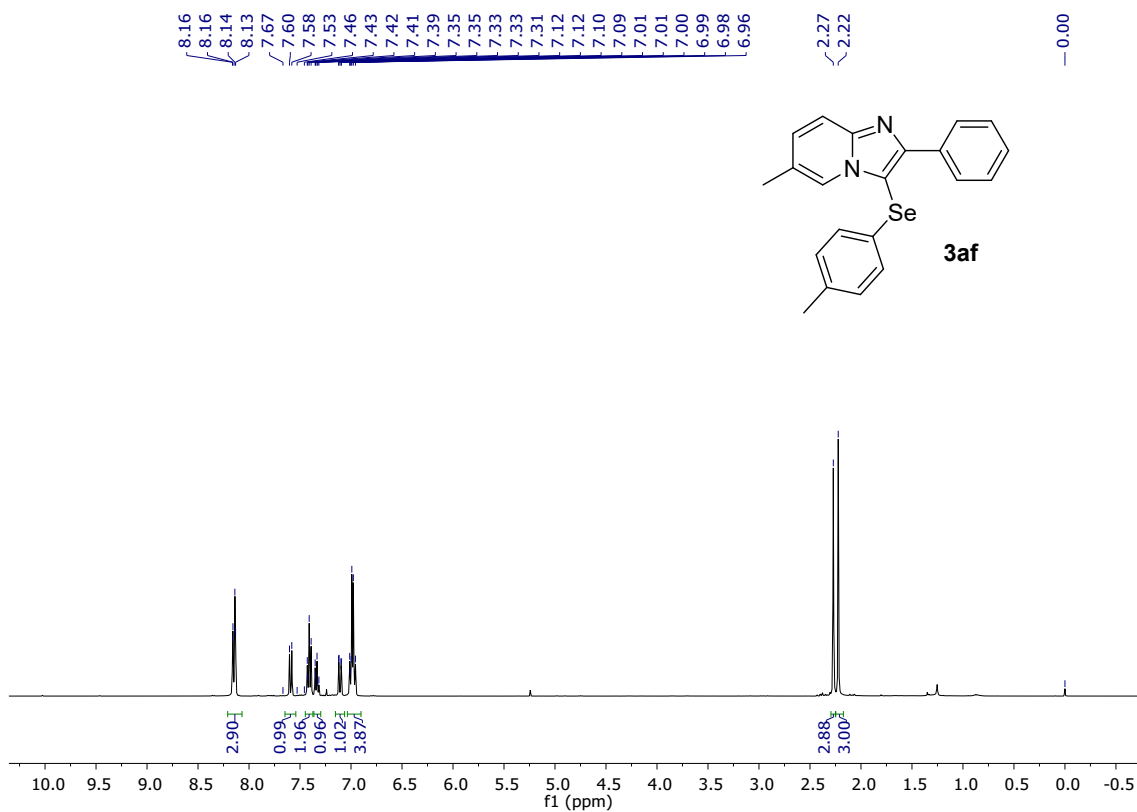
**Figure S93.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ae**.



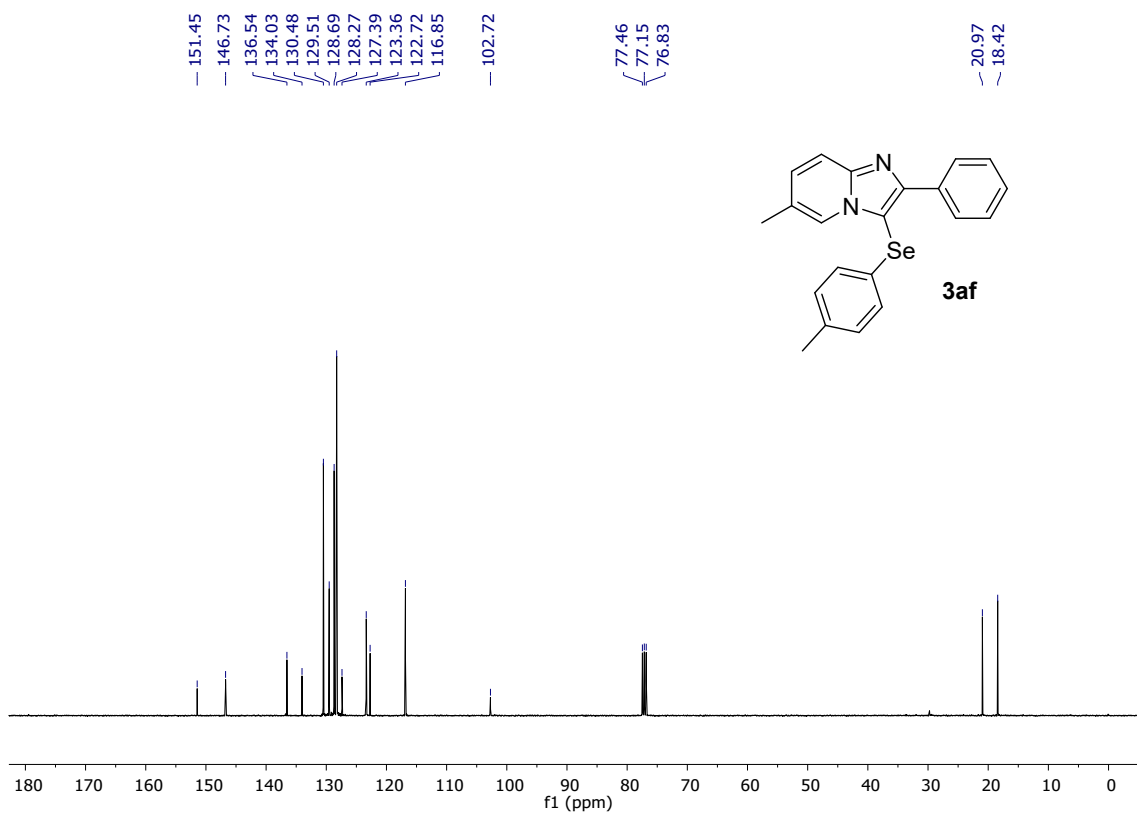
**Figure S94.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ae**.



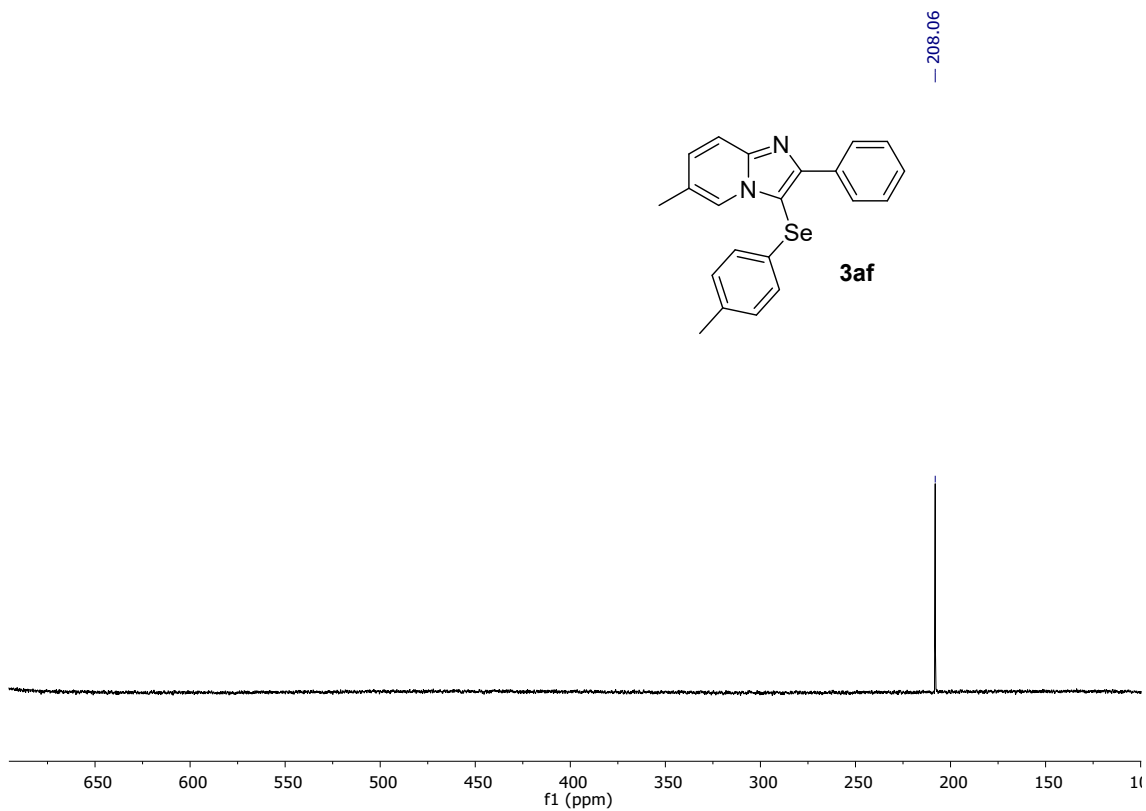
**Figure S95.**  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3ae**.



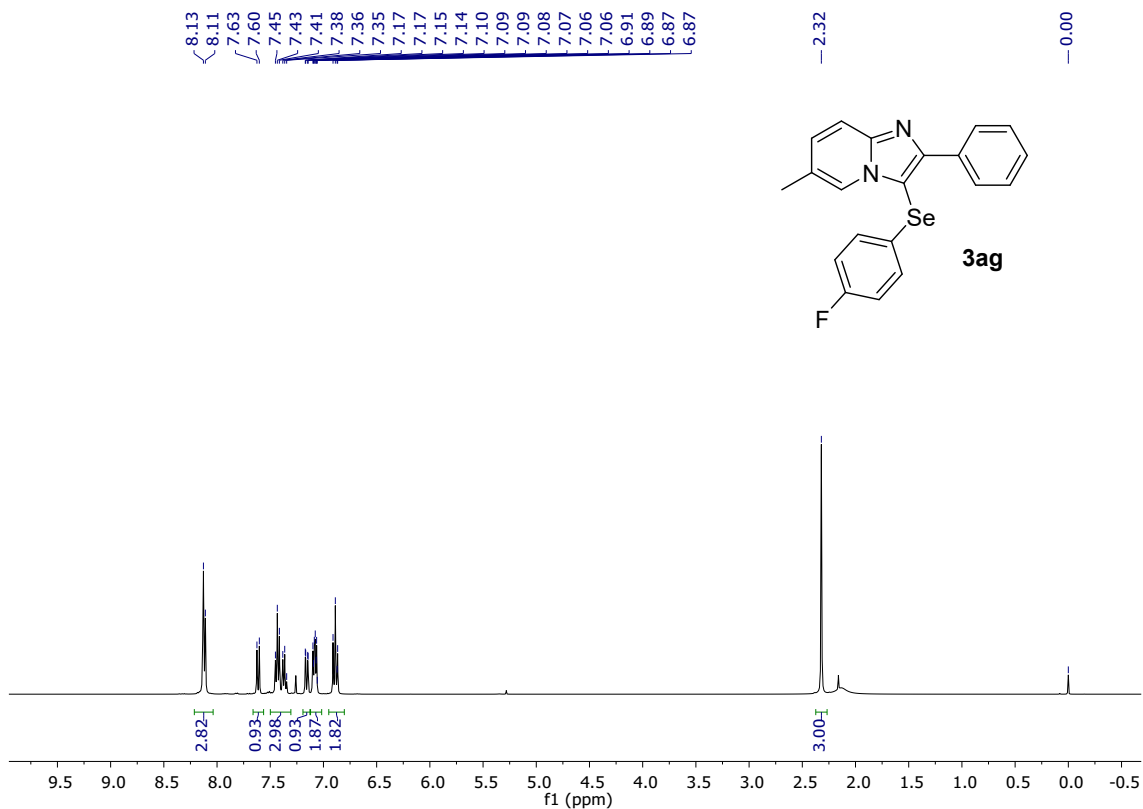
**Figure S96.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3af**.



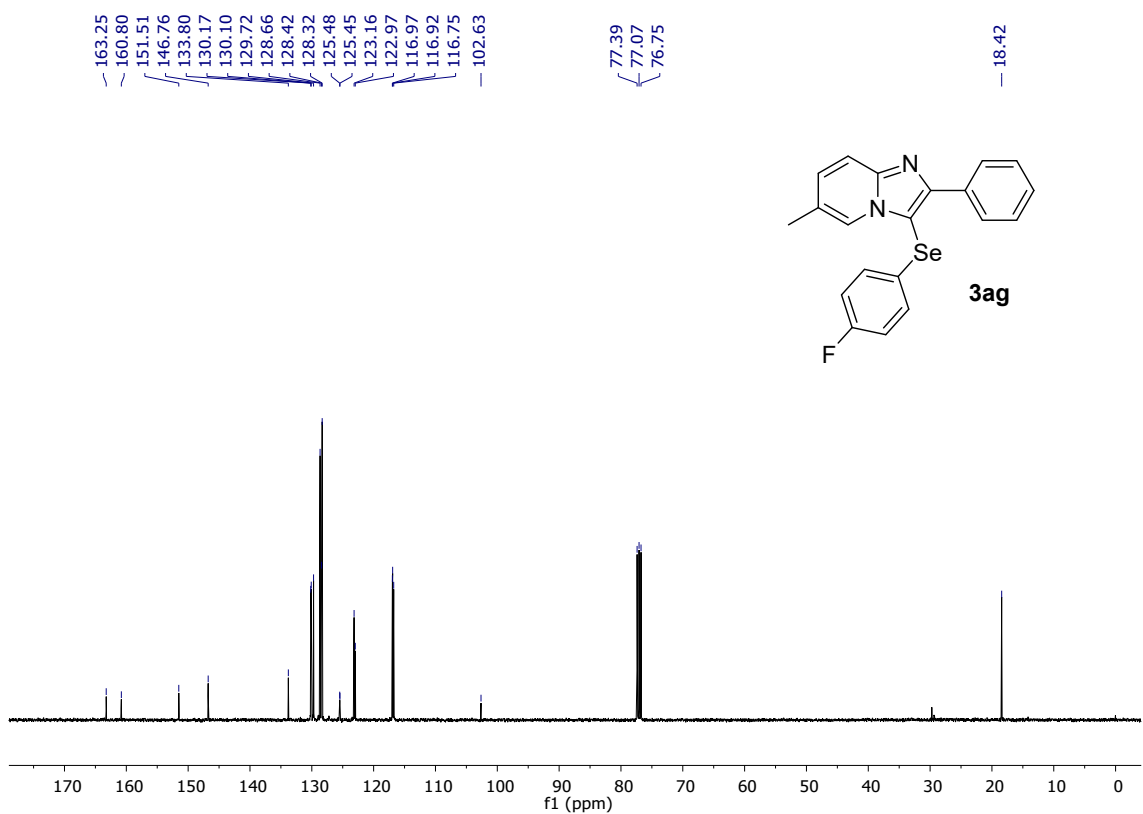
**Figure S97.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3af**.



**Figure S98.** <sup>77</sup>Se NMR (76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3af**.



**Figure S99.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ag**.



**Figure S100.** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ag**.

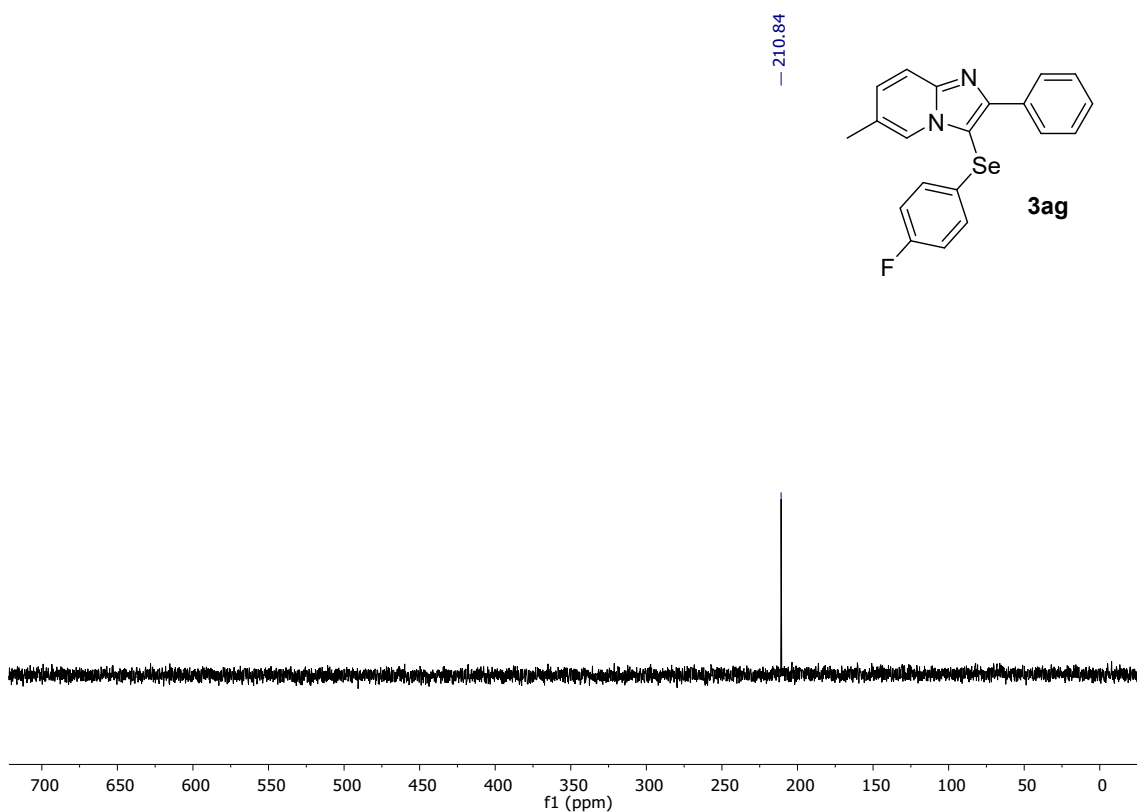


Figure S101  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3ag**.

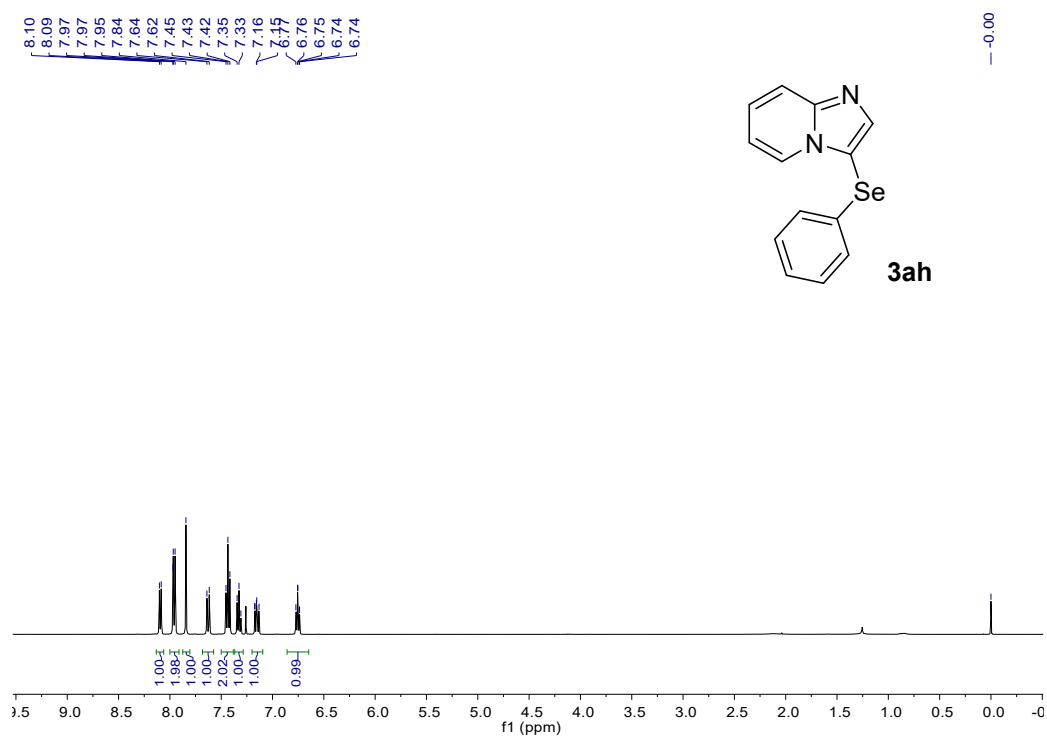
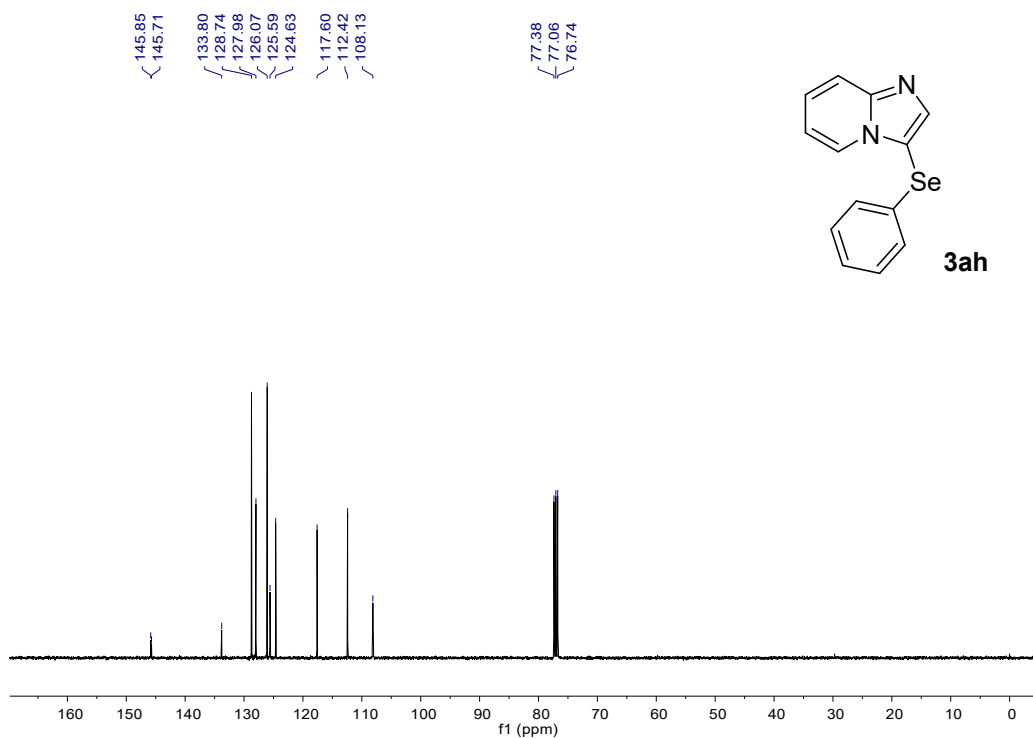
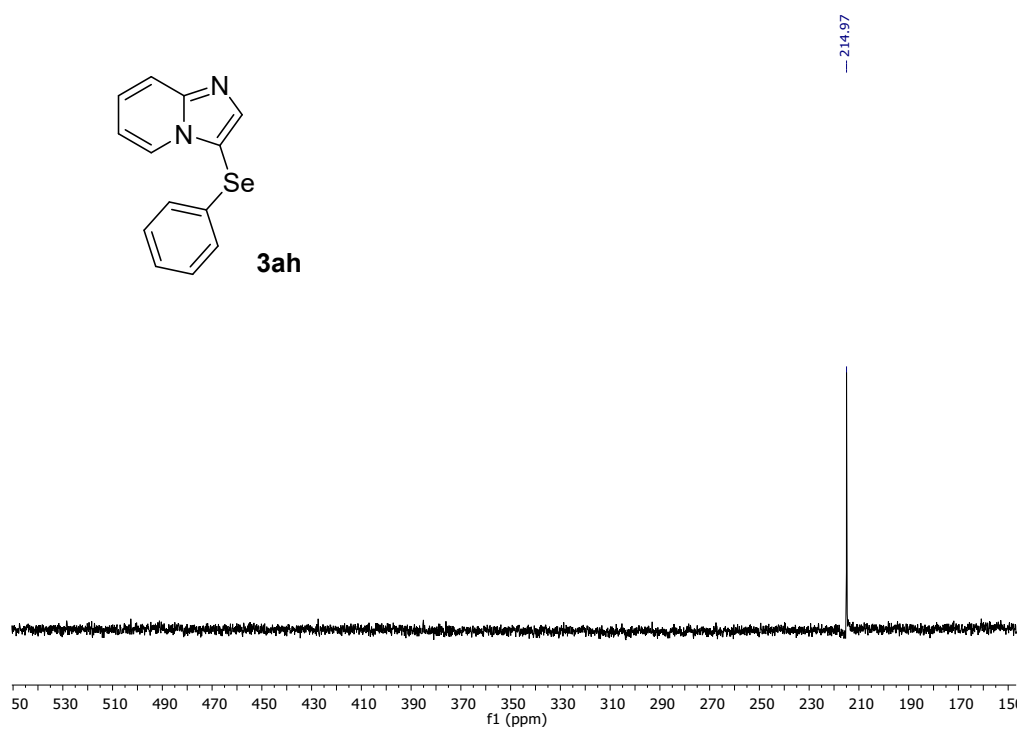


Figure 102  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **3ah**.



**Figure 103** <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ah**.



**Figure 104** <sup>77</sup>Se NMR 76 MHz, CDCl<sub>3</sub>) spectrum of the compound **3ah**.