# Seleno-warfare against cancer: Decoding antitumor activity of novel acylselenoureas and *Se*-acylisoselenoureas.

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Table of contents


| | |
|---|---|
| **Biological evaluation** | |
| Cytotoxicity screening | Figure S1 |
| NCI-60 Analysis | |
| Compound 1 (One-Dose Assay) | Figure S2 |
| Compound 4 (One-Dose Assay) | Figure S3 |
| Compound 8 (One-Dose Assay) | Figure S4 |
| Compound 9 (One-Dose Assay) | Figure S5 |
| Compound 10 (One-Dose Assay) | Figure S6 |
| Compound 12 (One-Dose Assay) | Figure S7 |
| Compound 15 (One-Dose Assay) | Figure S8 |
| Compound 16 (One-Dose Assay) | Figure S9 |
| Compound 17 (One-Dose Assay) | Figure S10 |
| Compound 19 (One-Dose Assay) | Figure S11 |
| Compound 1 (Five-Dose Assay) | Figure S12 |
| Compound 4 (Five-Dose Assay) | Figure S13 |
| Compound 9 (Five-Dose Assay) | Figure S14 |
| Compound 10 (Five-Dose Assay) | Figure S15 |
| Compound 15 (Five-Dose Assay) | Figure S16 |
| Compound 16 (Five-Dose Assay) | Figure S17 |
| Compound 17 (Five-Dose Assay) | Figure S18 |
| **Structural characterization** | |
| $^{1}$H-, $^{13}$C- and $^{77}$Se-NMR spectra | Figures S19–S83 |
| Characterization of the compounds synthesized in this work | |

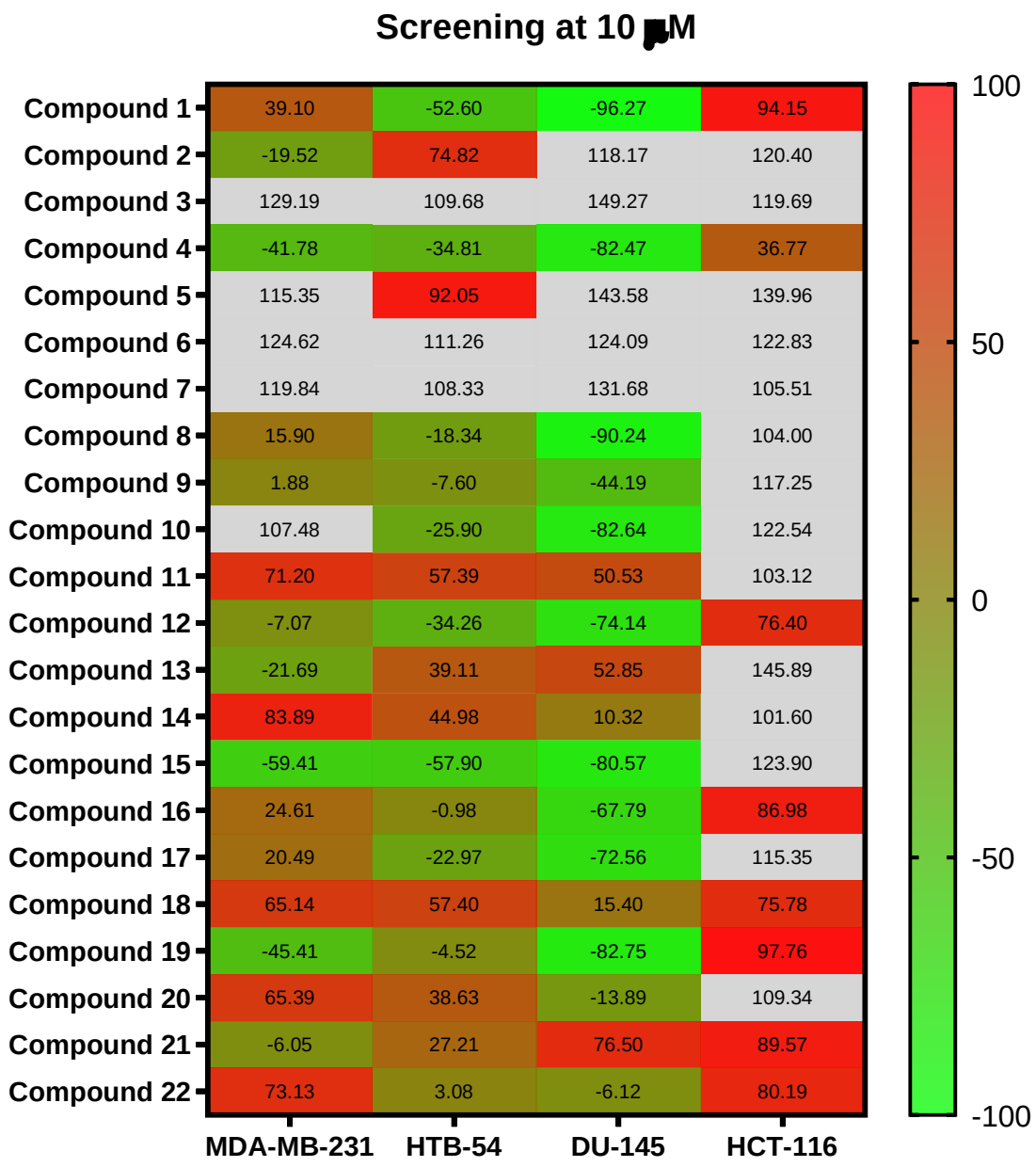


**Figure S1.** Heat map of screening results where the percentage of cell growth is represented at 10 μM for the 22 novel compounds in MDA-MB-231, HTB-54, DU-145 and HCT-116 cells.

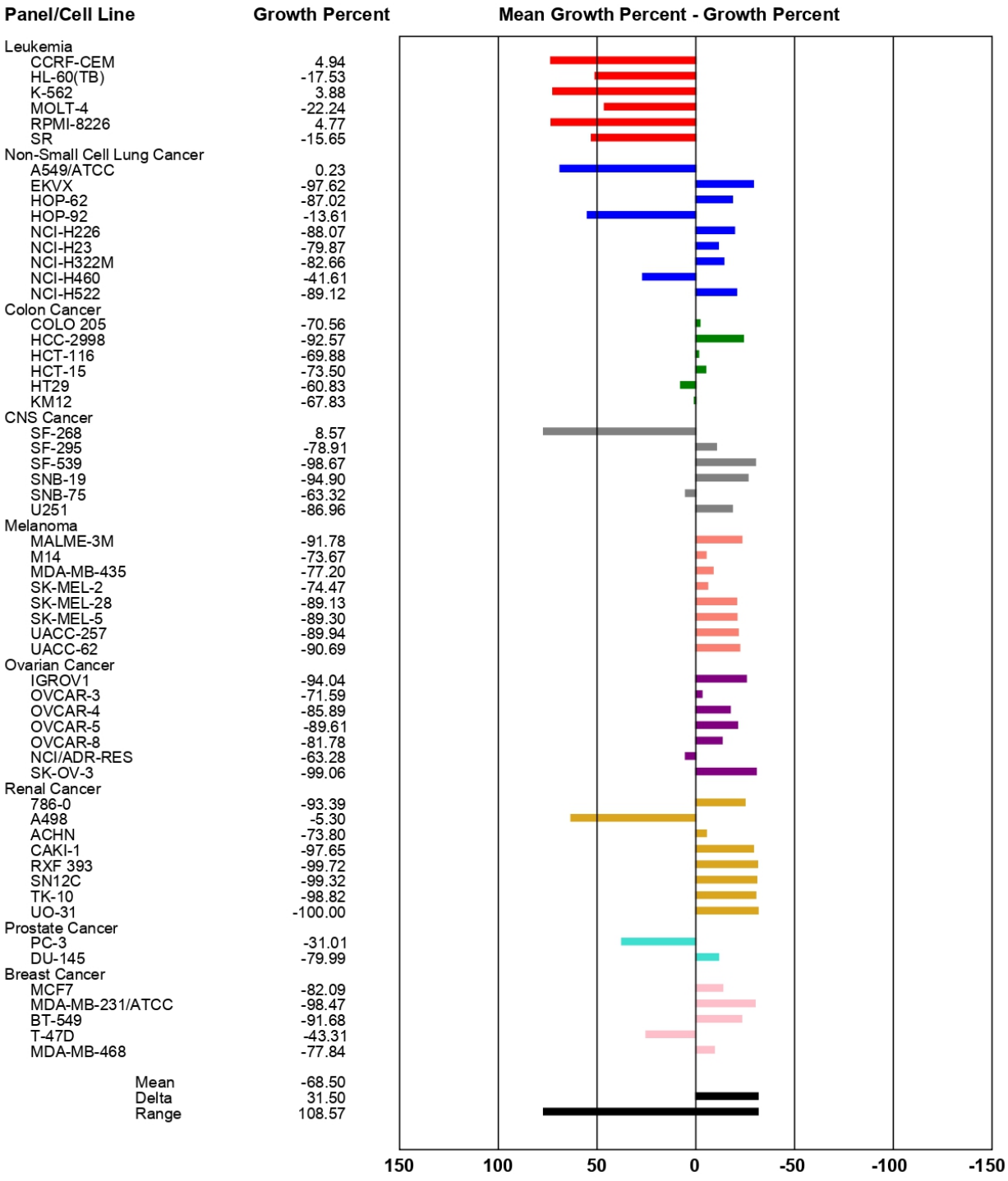


**Figure S2**. One-Dose Assay of compound **1** at 10 μM after 48h of treatment.

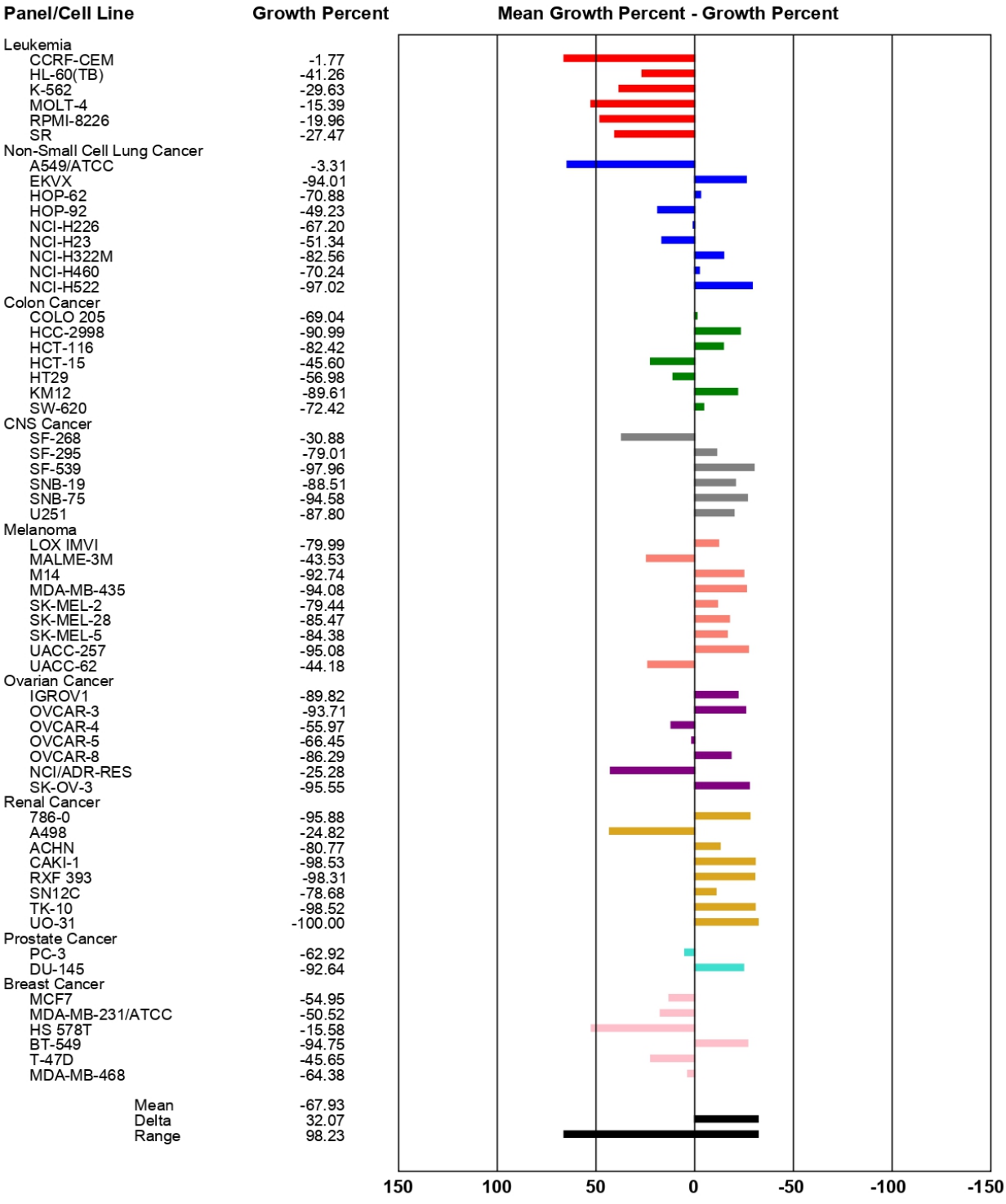


**Figure S3**. One-Dose Assay of compound **4** at 10 μM after 48h of treatment.

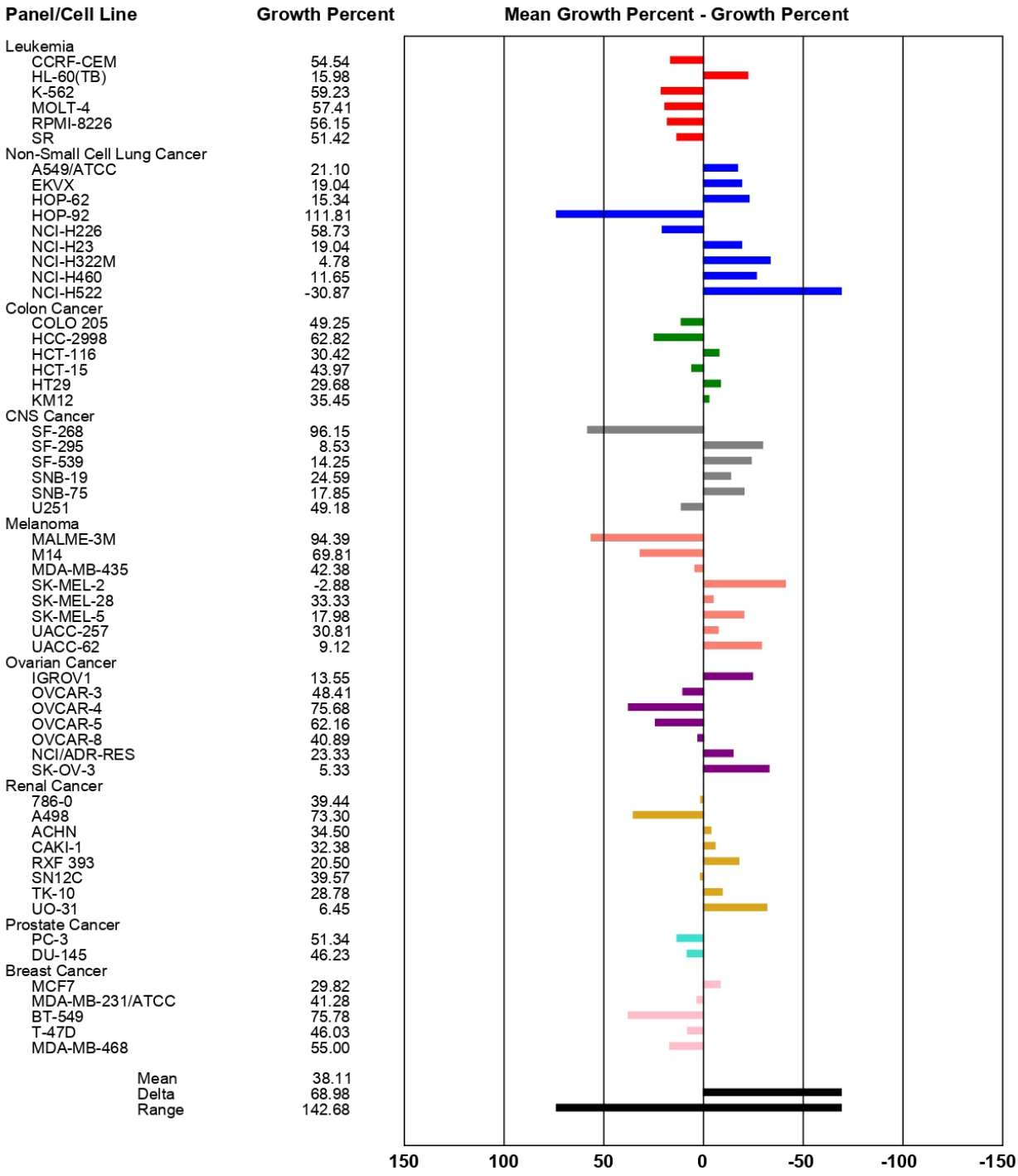


**Figure S4**. One-Dose Assay of compound **8** at 10 μM after 48h of treatment.

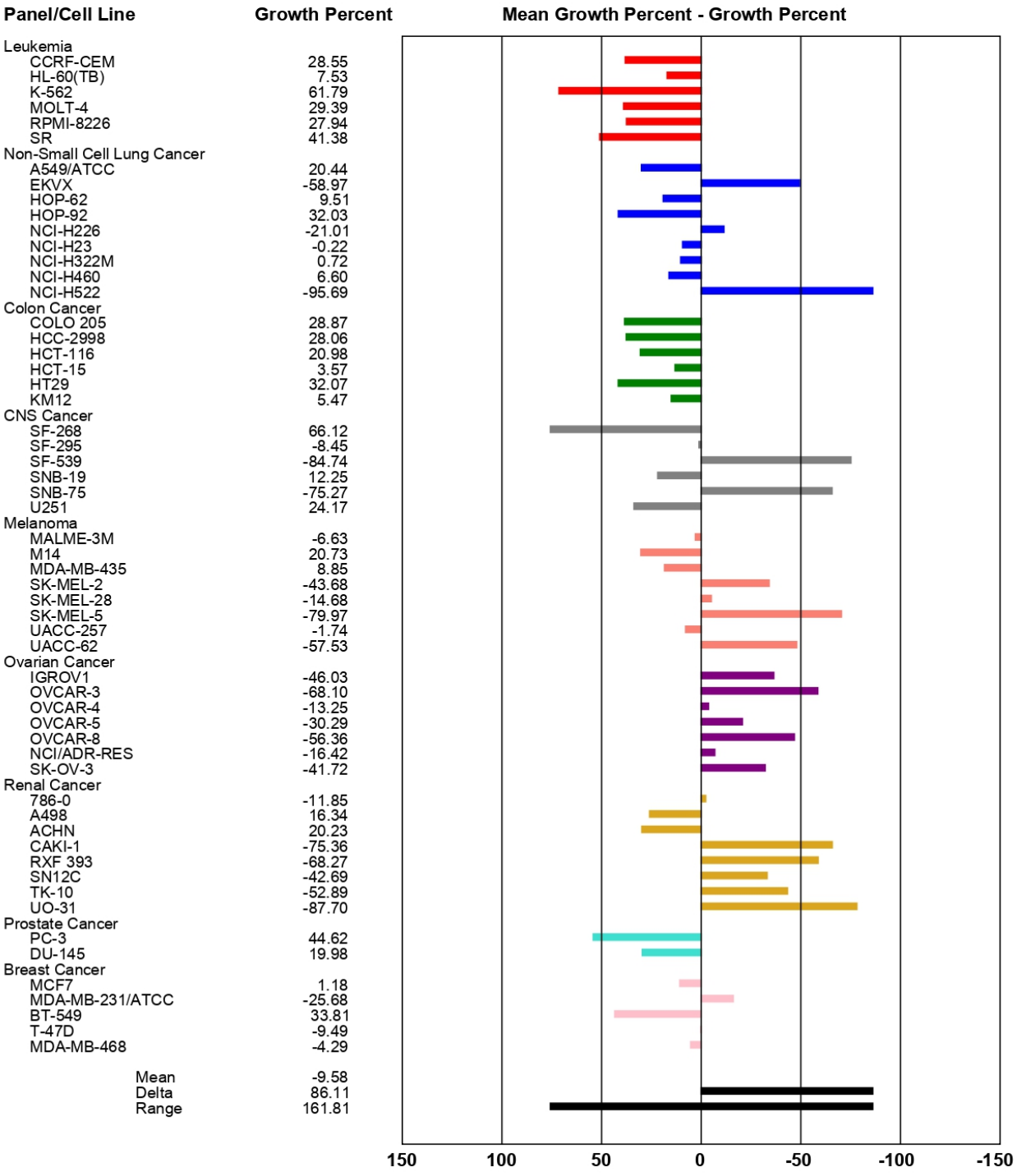


**Figure S5**. One-Dose Assay of compound **9** at 10 μM after 48h of treatment.

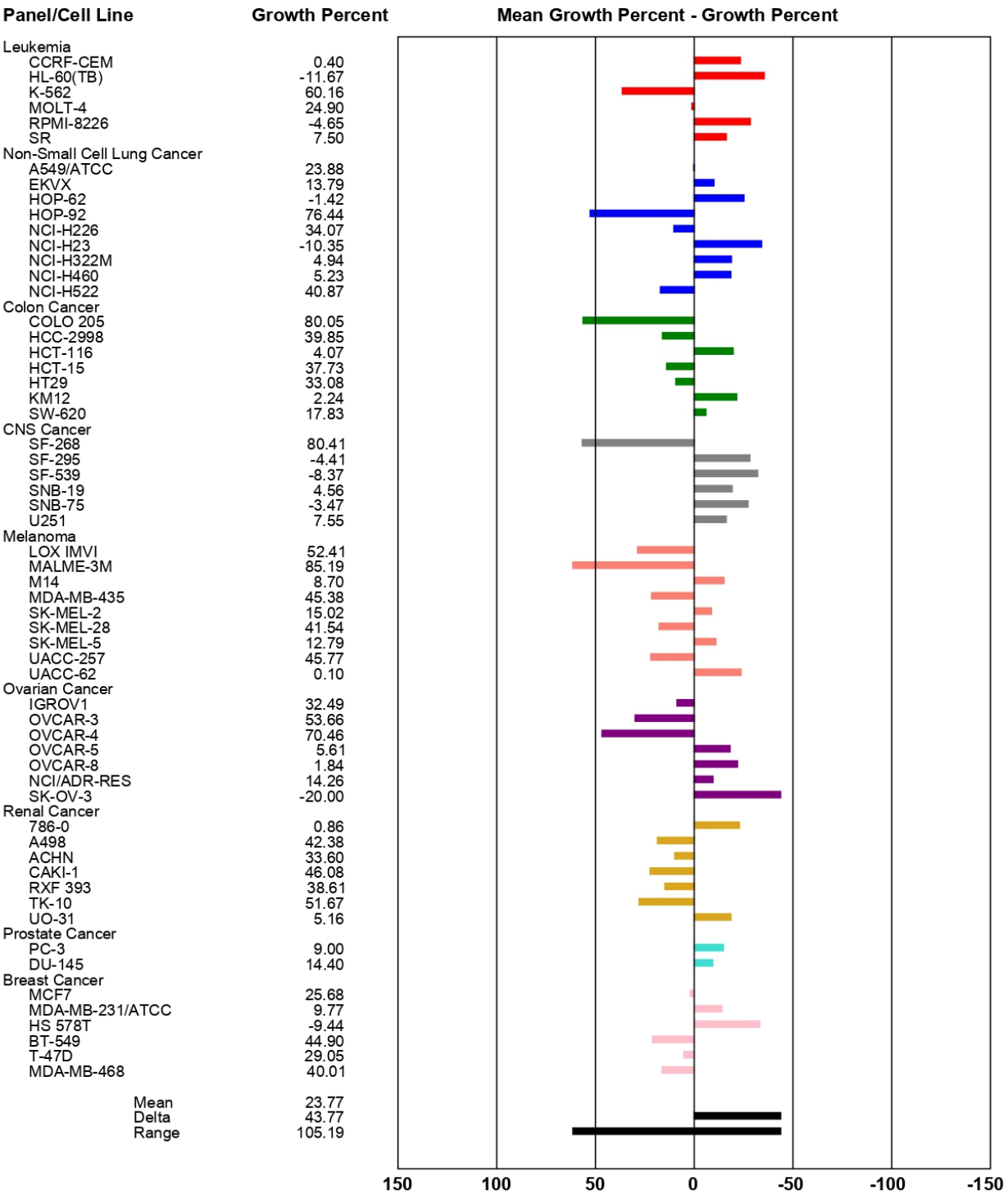


**Figure S6**. One-Dose Assay of compound **10** at 10 μM after 48h of treatment.

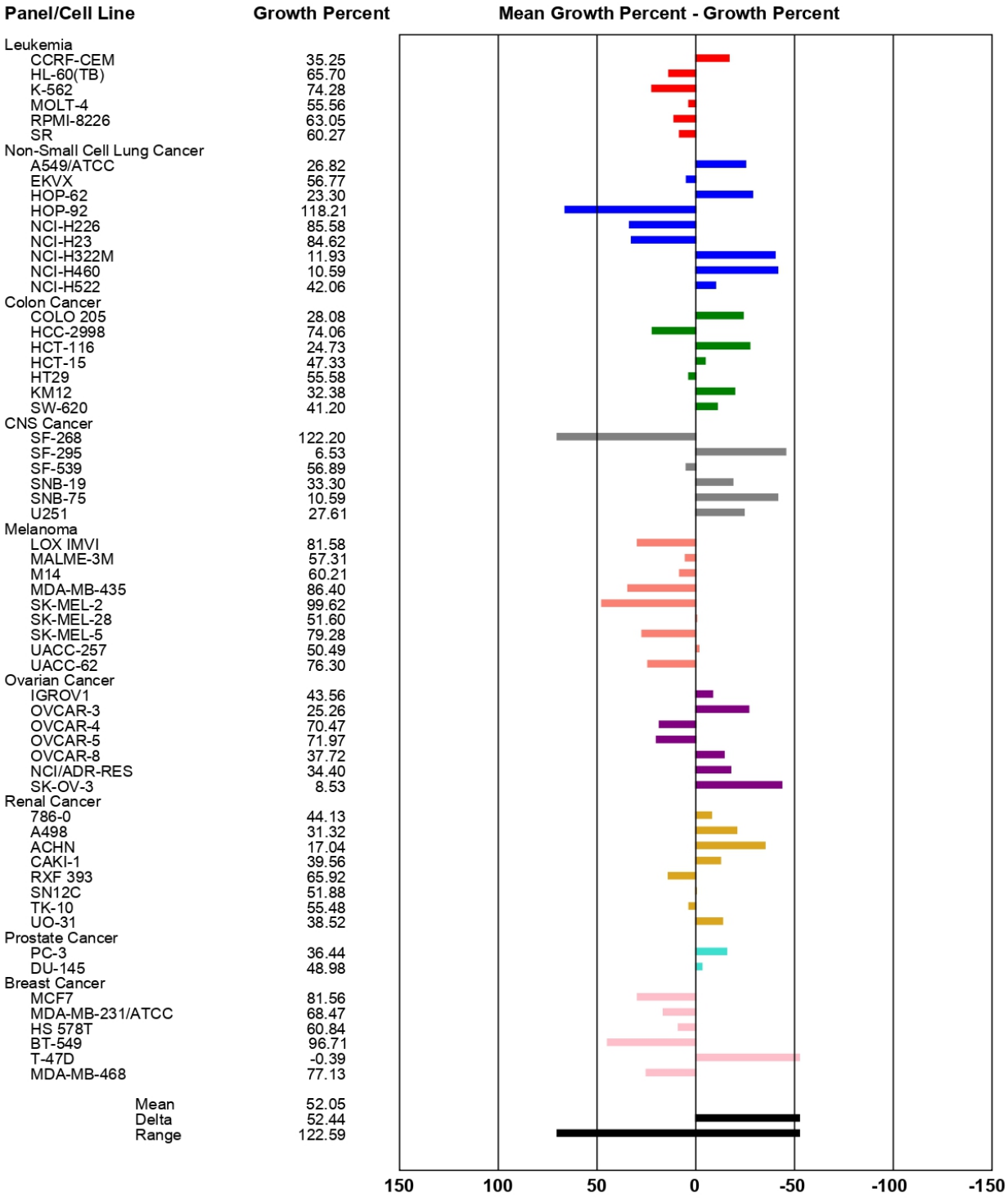


**Figure S7**. One-Dose Assay of compound **12** at 10 μM after 48h of treatment.

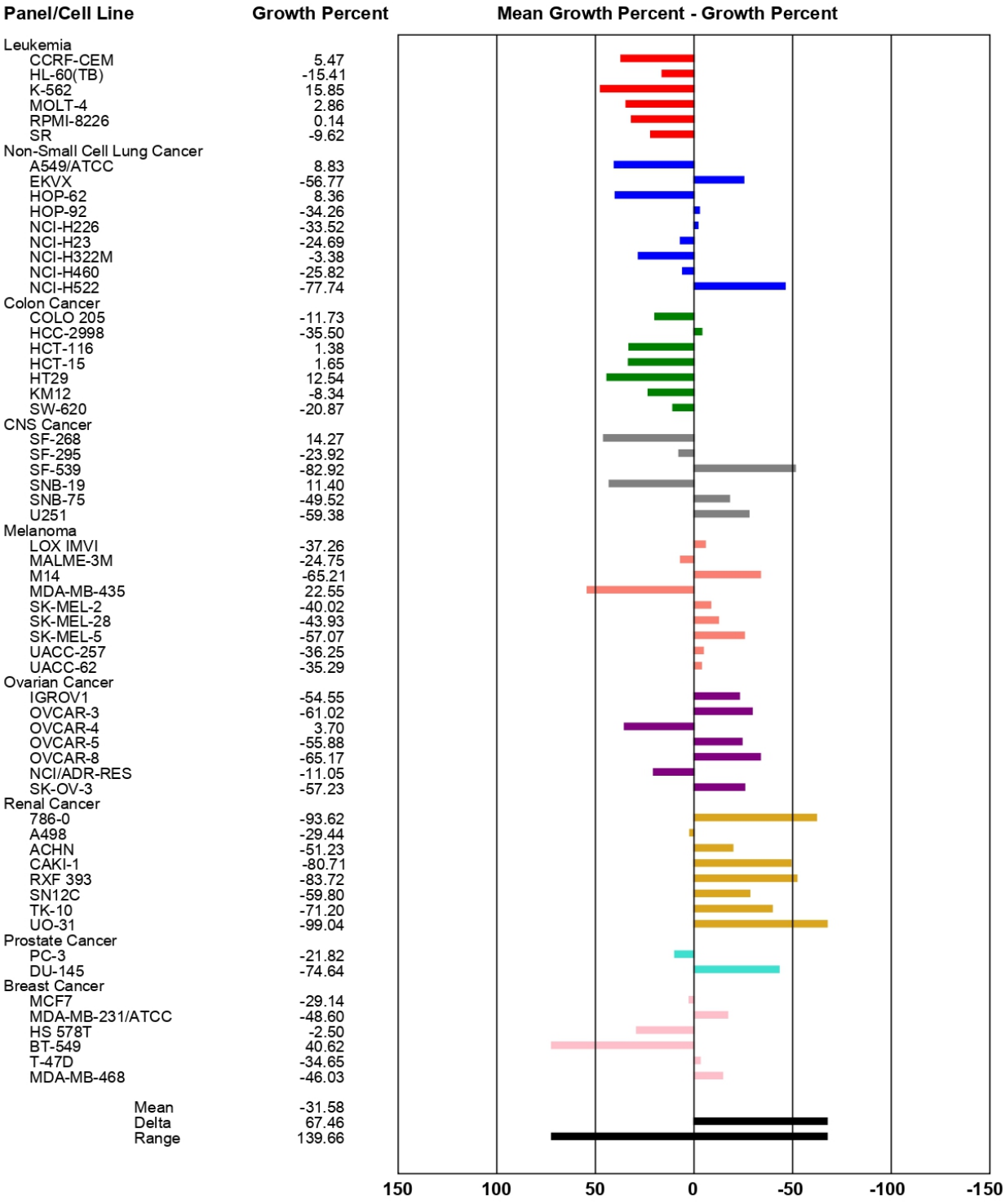


**Figure S8**. One-Dose Assay of compound **15** at 10 μM after 48h of treatment.

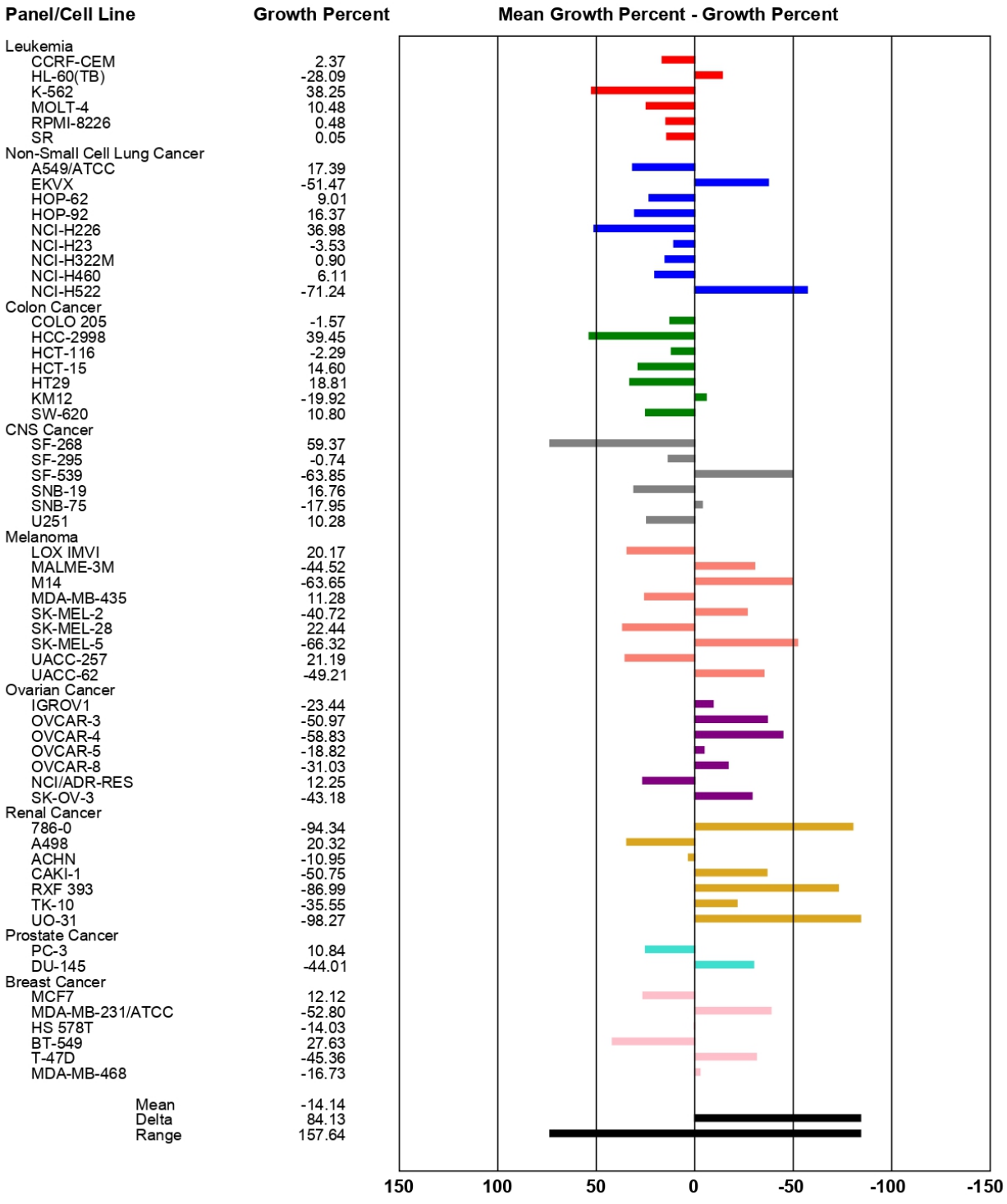


**Figure S9**. One-Dose Assay of compound **16** at 10 μM after 48h of treatment.

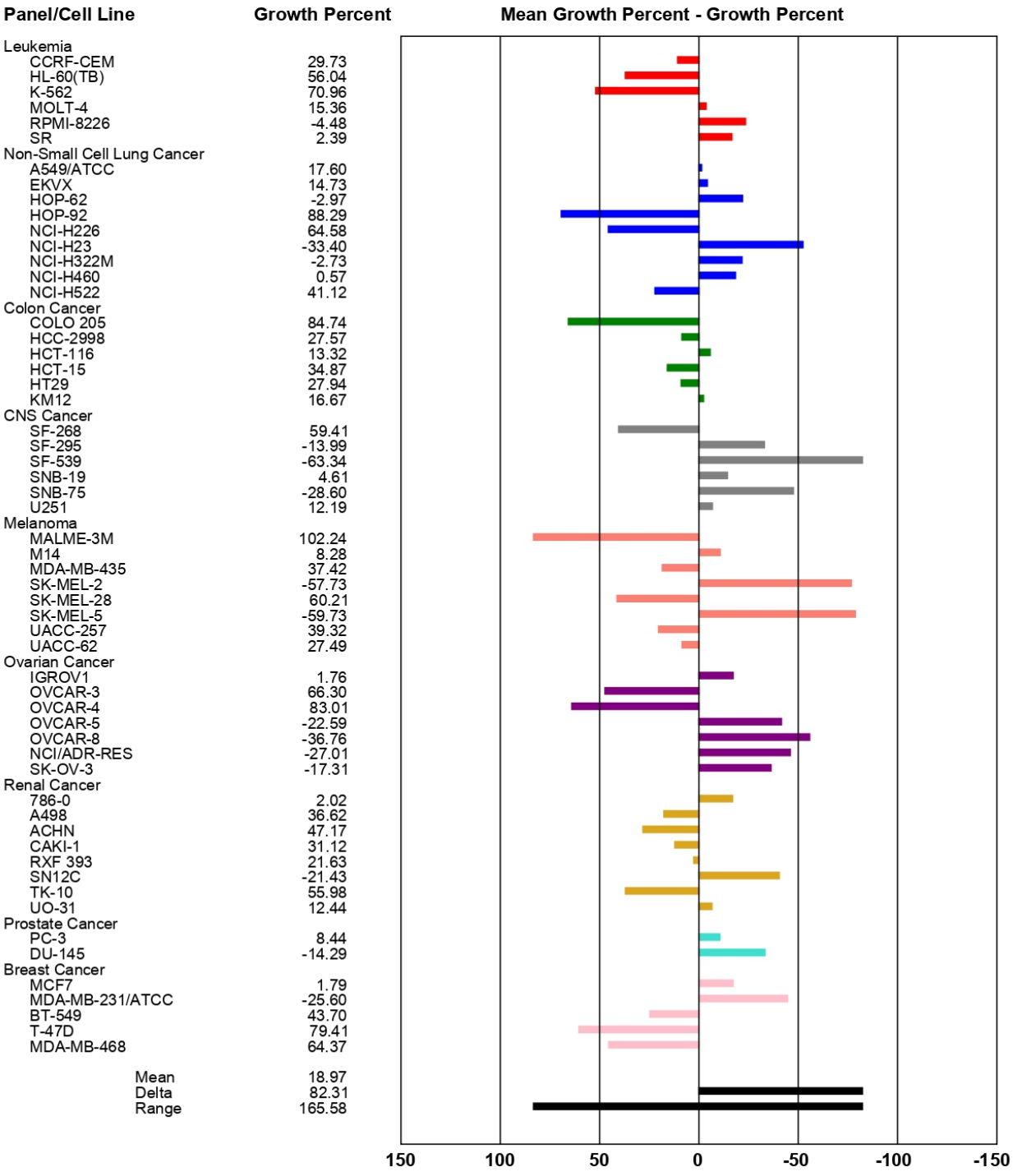


**Figure S10**. One-Dose Assay of compound **17** at 10 μM after 48h of treatment.

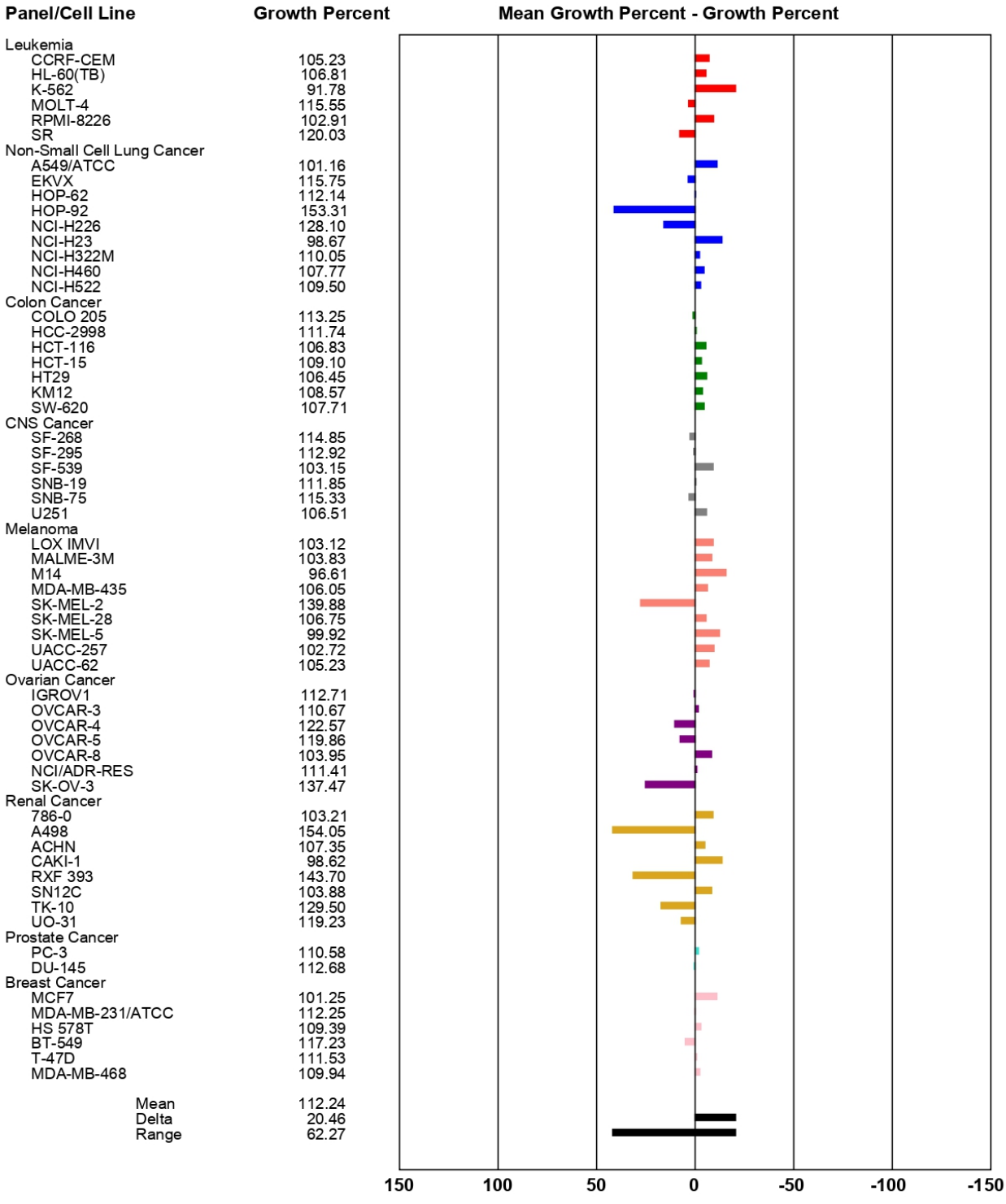


**Figure S11**. One-Dose Assay of compound **19** at 10 μM after 48h of treatment.

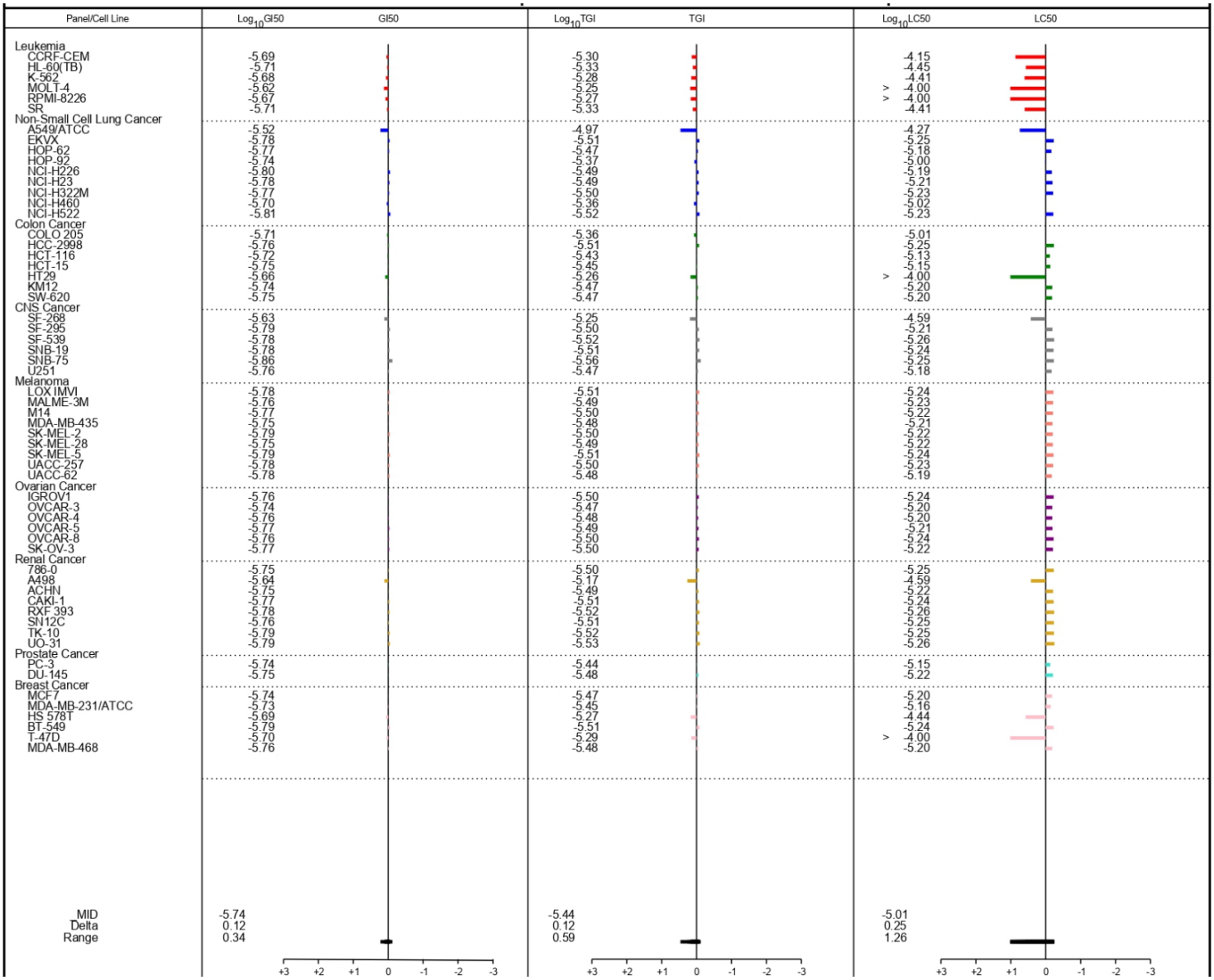


**Figure S12**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **1** after 48h of treatment.

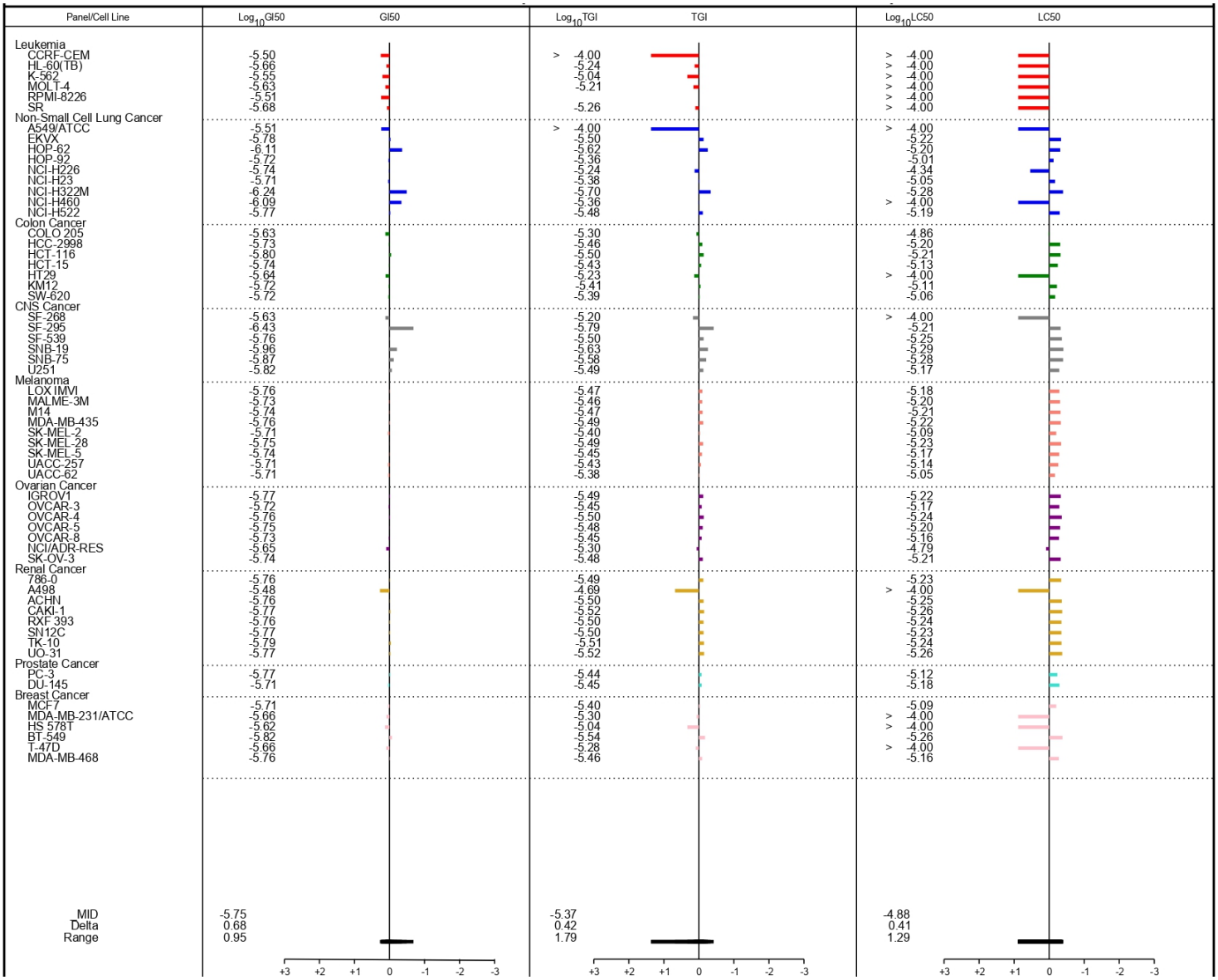


**Figure S13**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **4** after 48h of treatment.

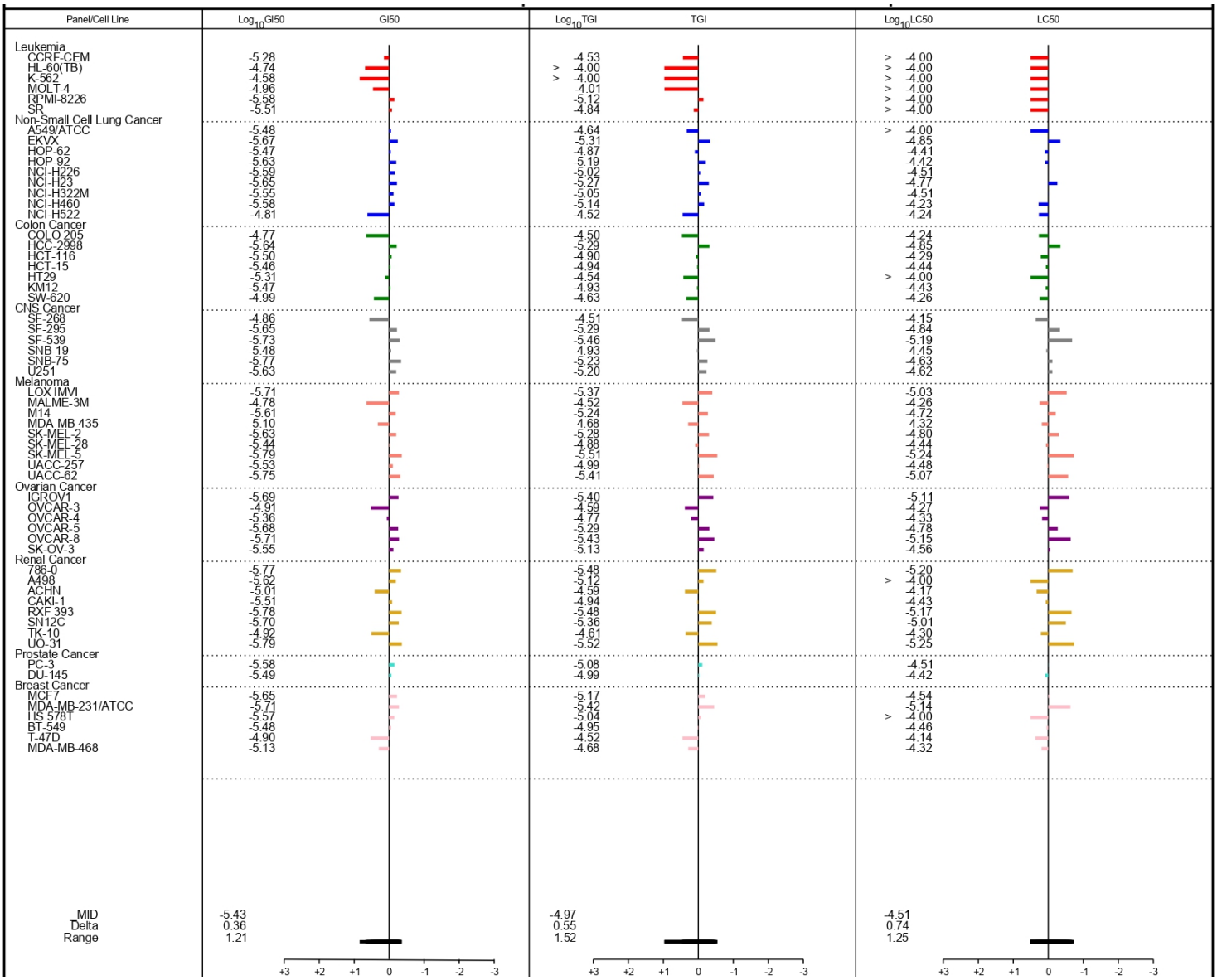


**Figure S14**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **9** after 48h of treatment.

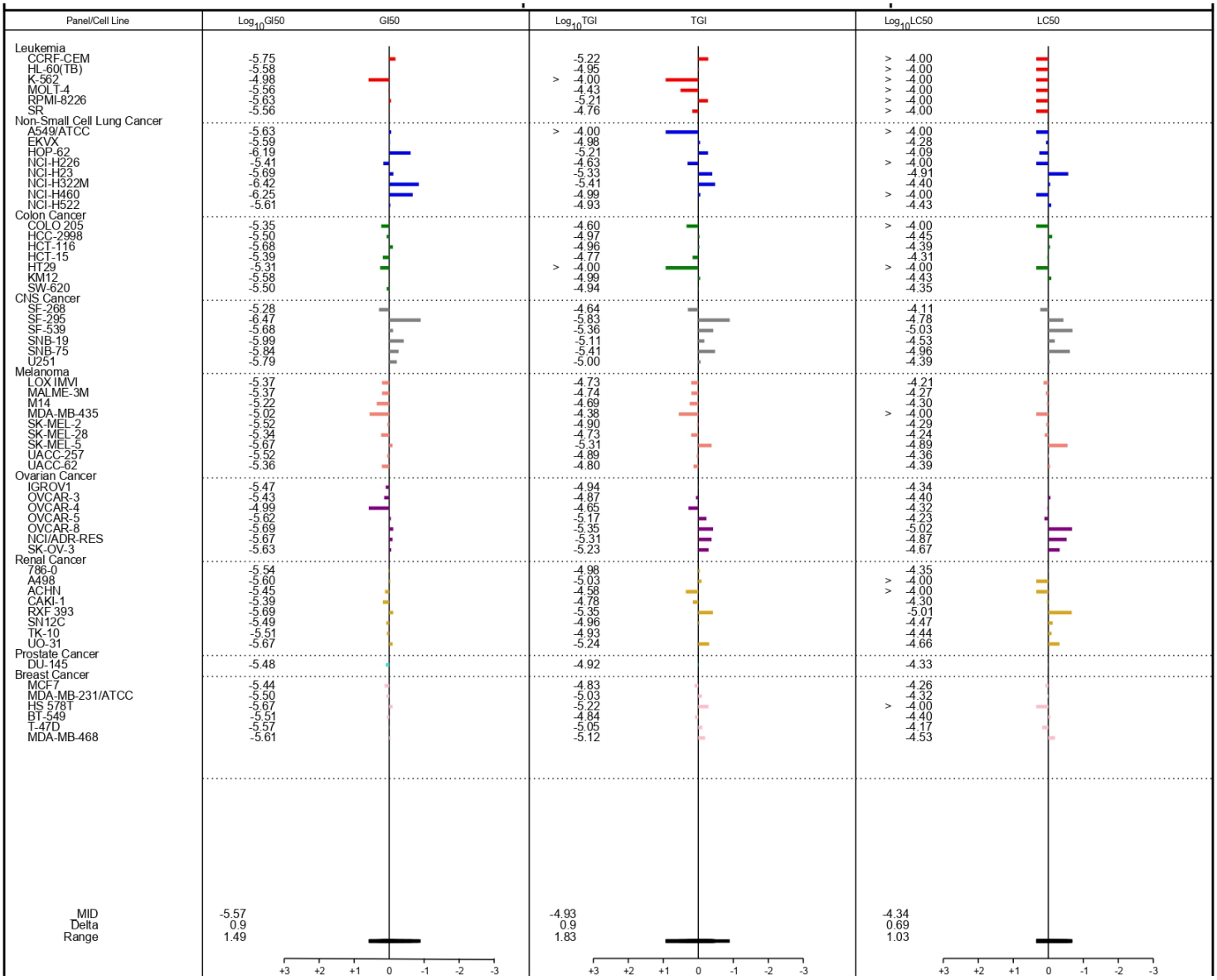


**Figure S15**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **10** after 48h of treatment.

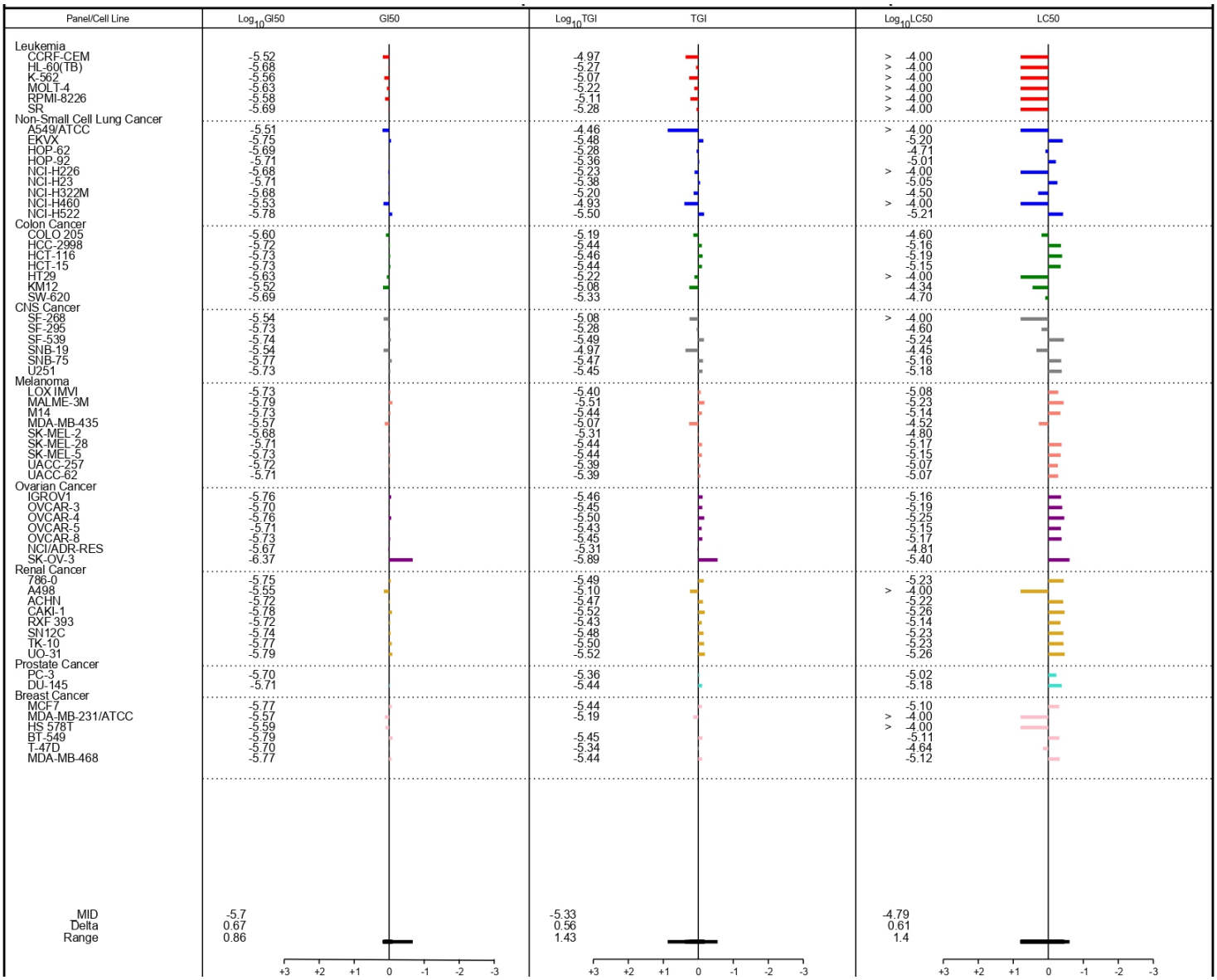


**Figure S16**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **15** after 48h of treatment.

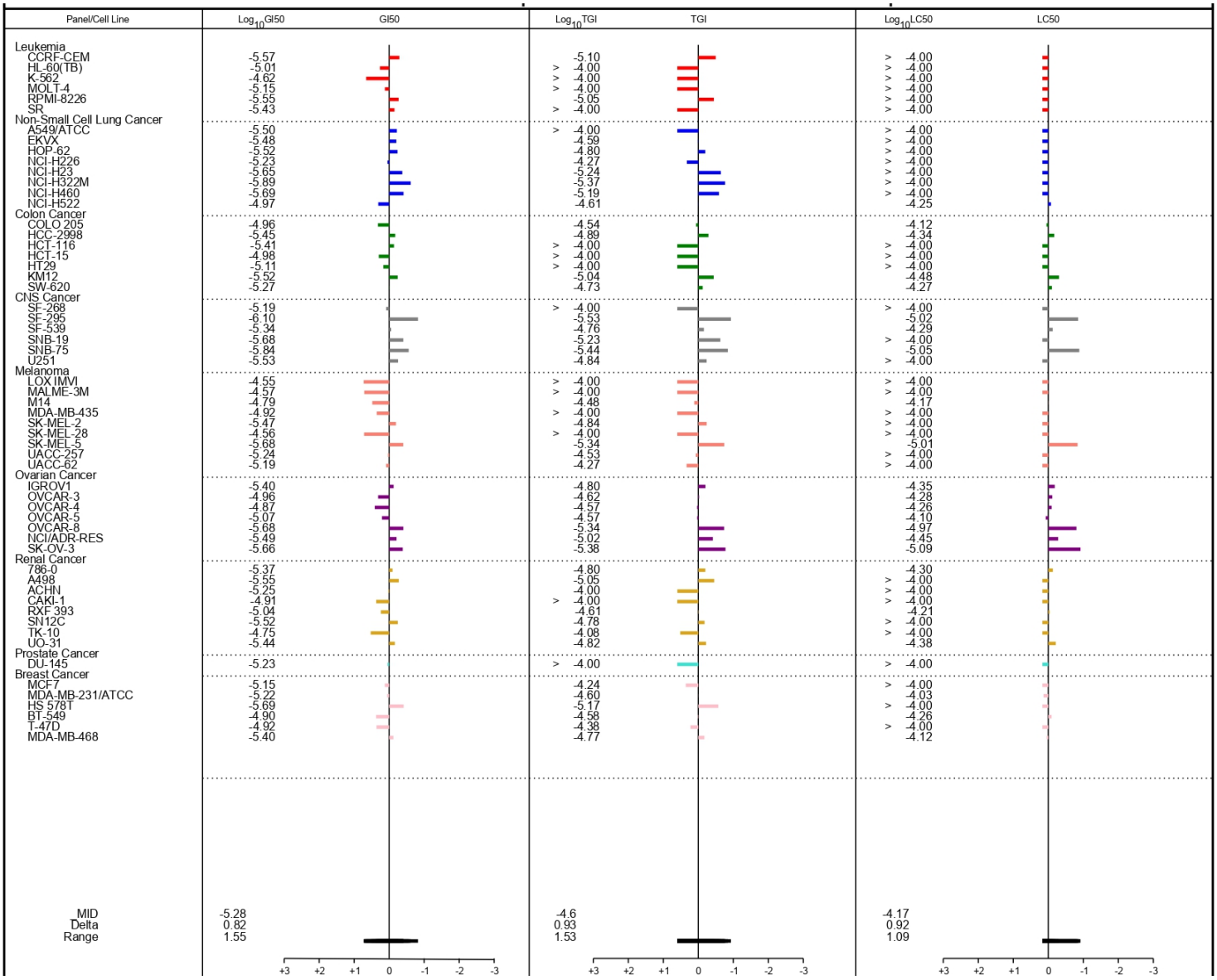


**Figure S17**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **16** after 48h of treatment.

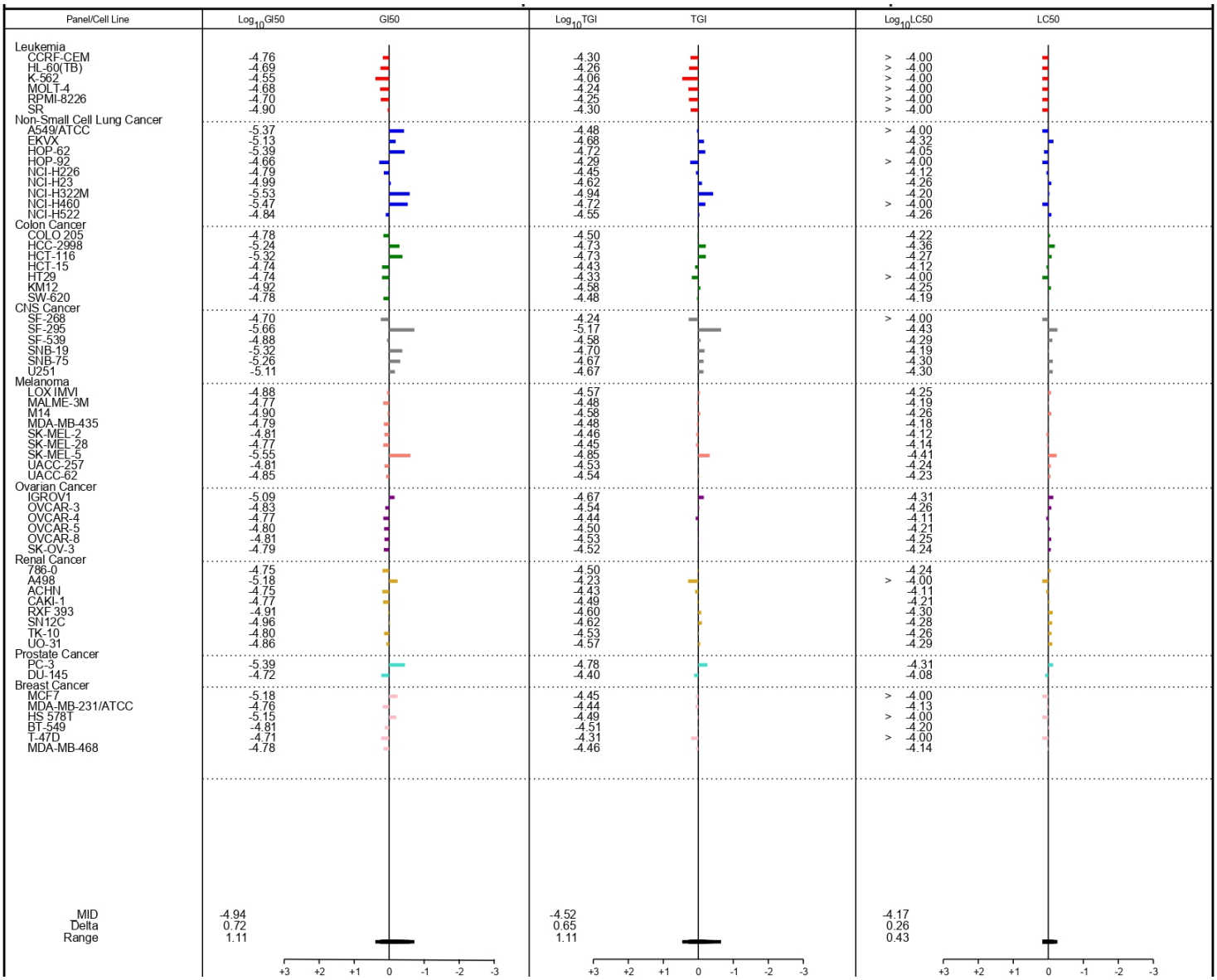


**Figure S18**. Growth inhibition 50, total growth inhibition, and lethal concentration 50 values for compound **17** after 48h of treatment.

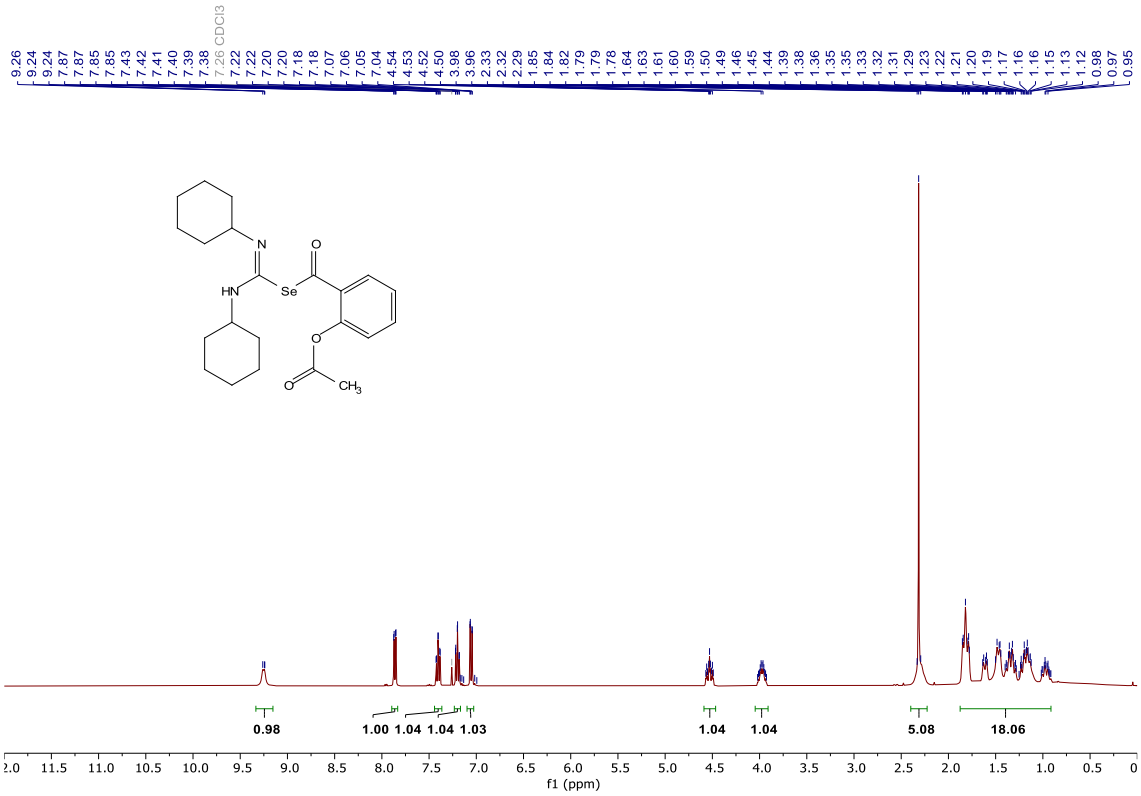


**Figure S19.** [1]H-NMR spectrum of compound **1**.

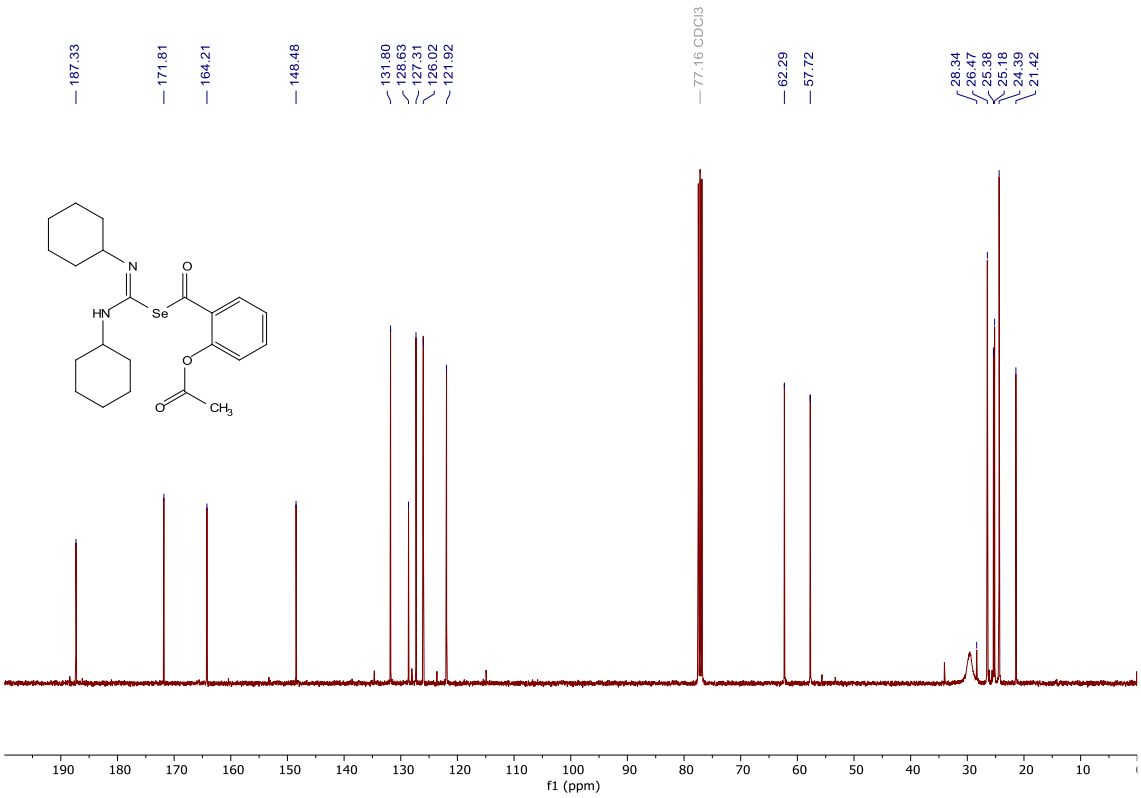


**Figure S20.** [13]C-NMR spectrum of compound **1**.

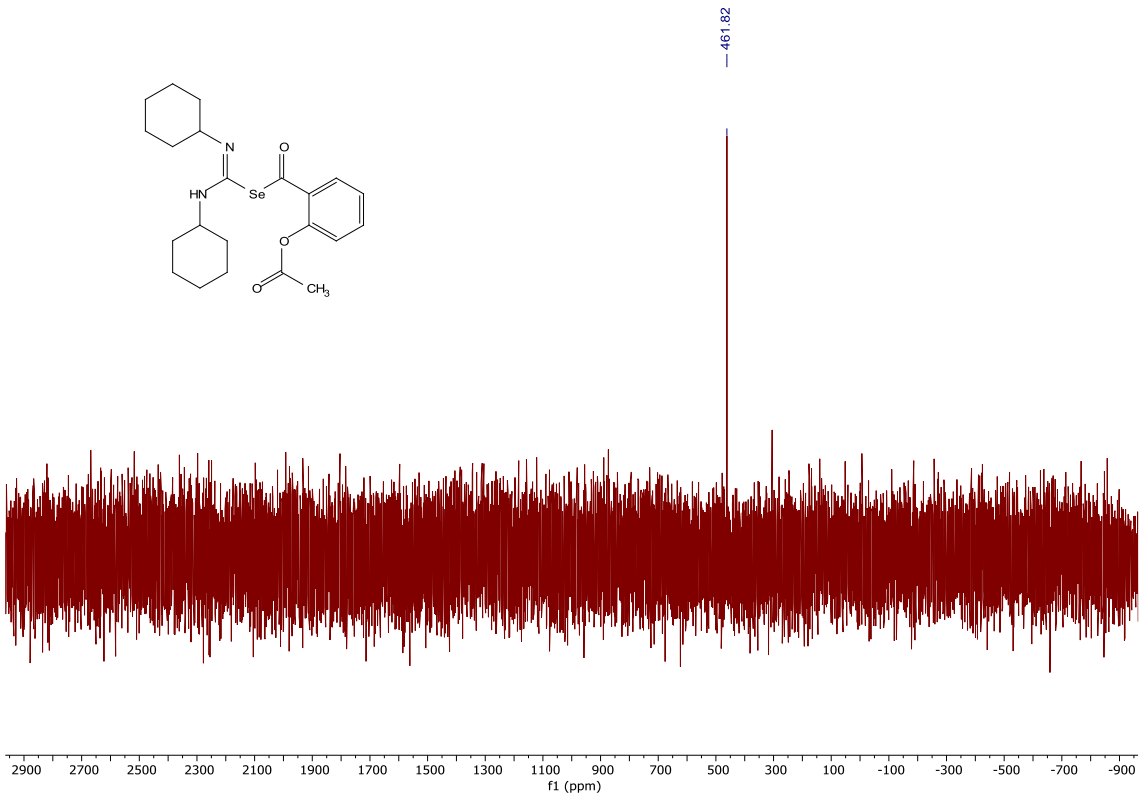


**Figure S21.** $^{77}$Se-NMR spectrum of compound **1**.

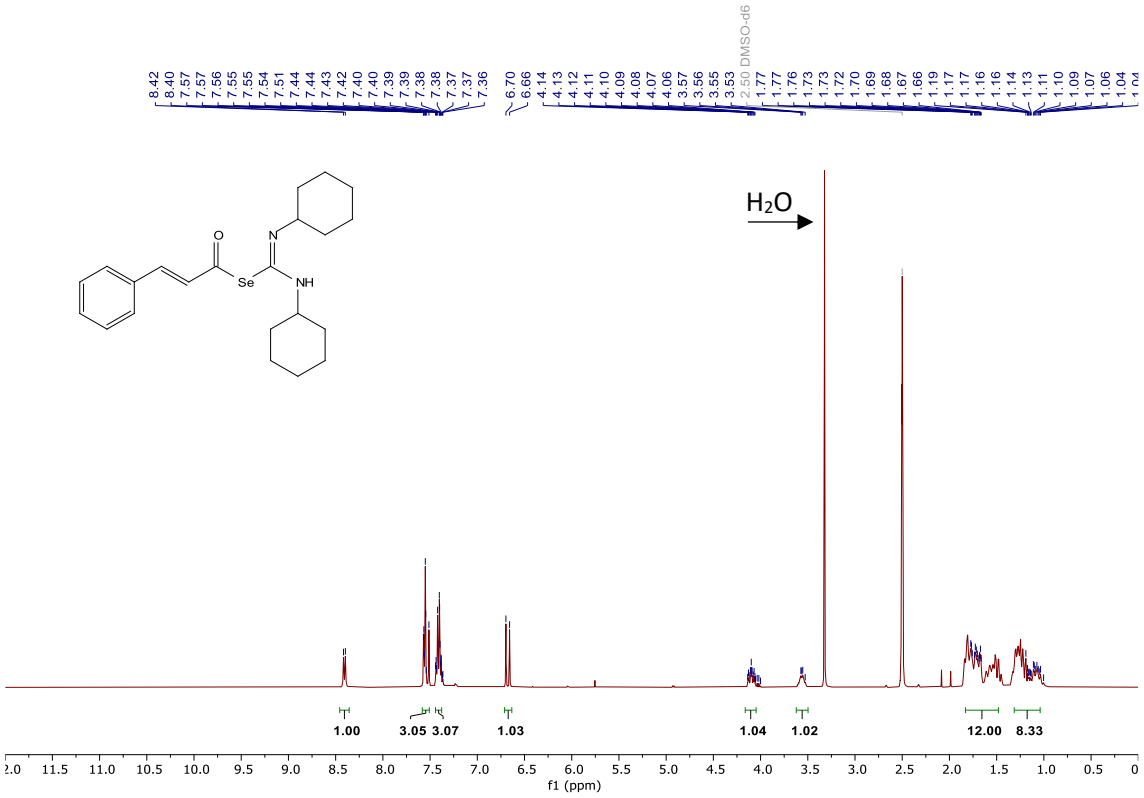


**Figure S22.** $^{1}$H-NMR spectrum of compound **2**.

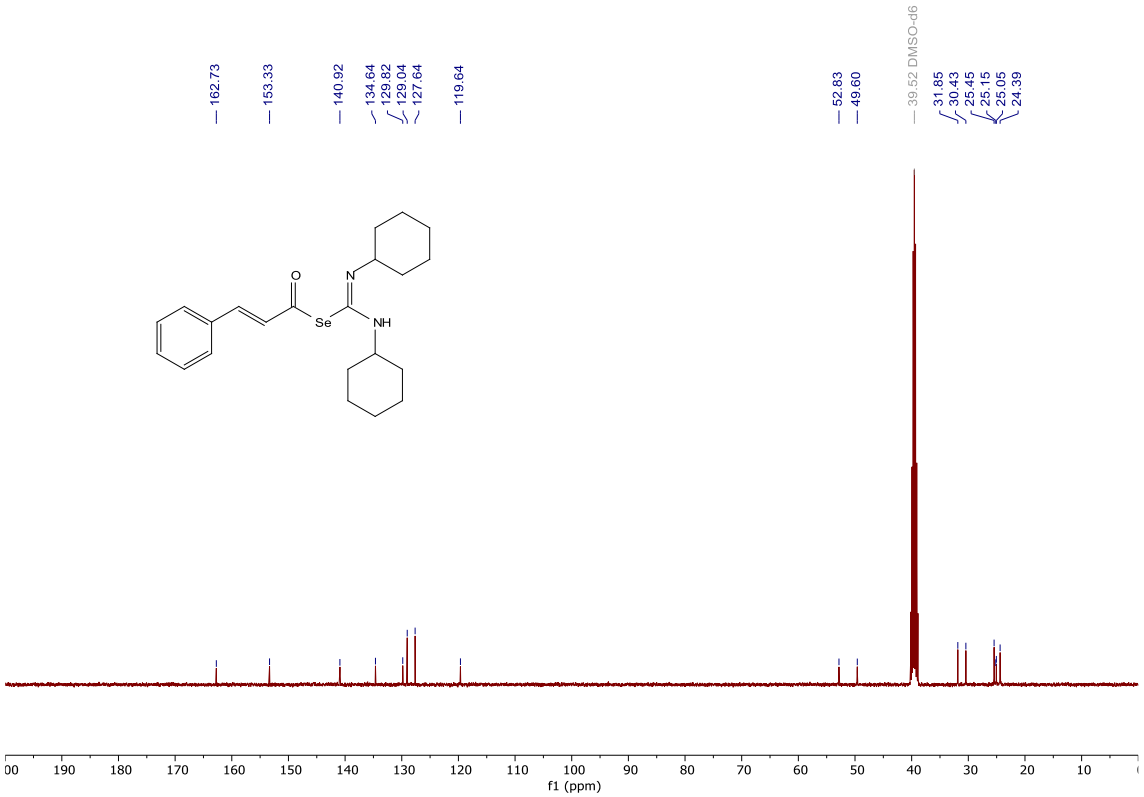


**Figure S23.** $^{13}$C-NMR spectrum of compound **2**.

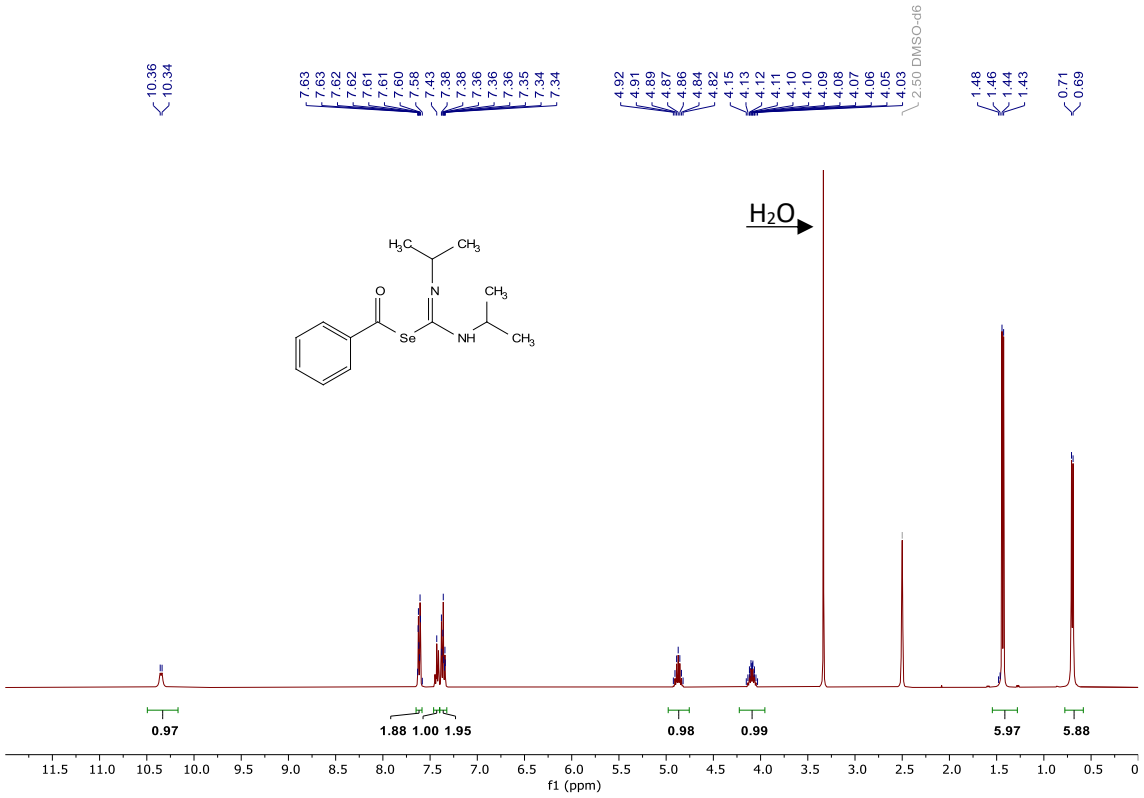


**Figure S24.** $^{1}$H-NMR spectrum of compound **3**.

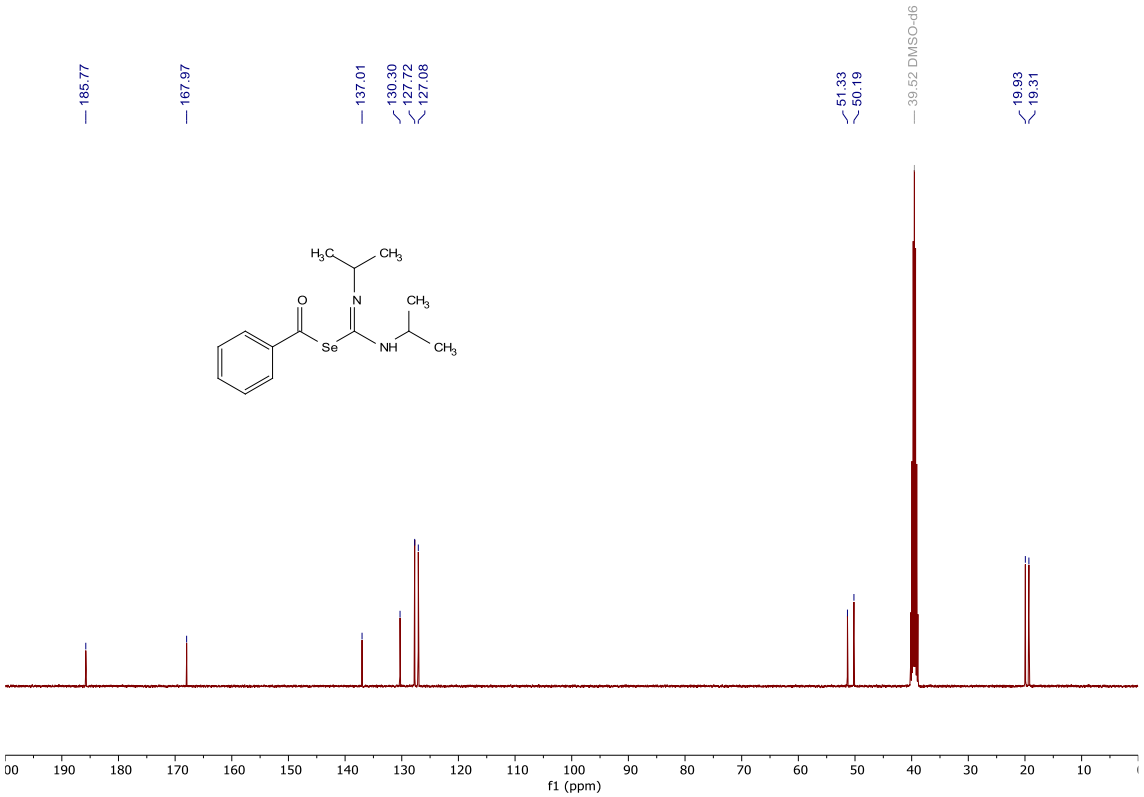


**Figure S25.** $^{13}$C-NMR spectrum of compound **3**.

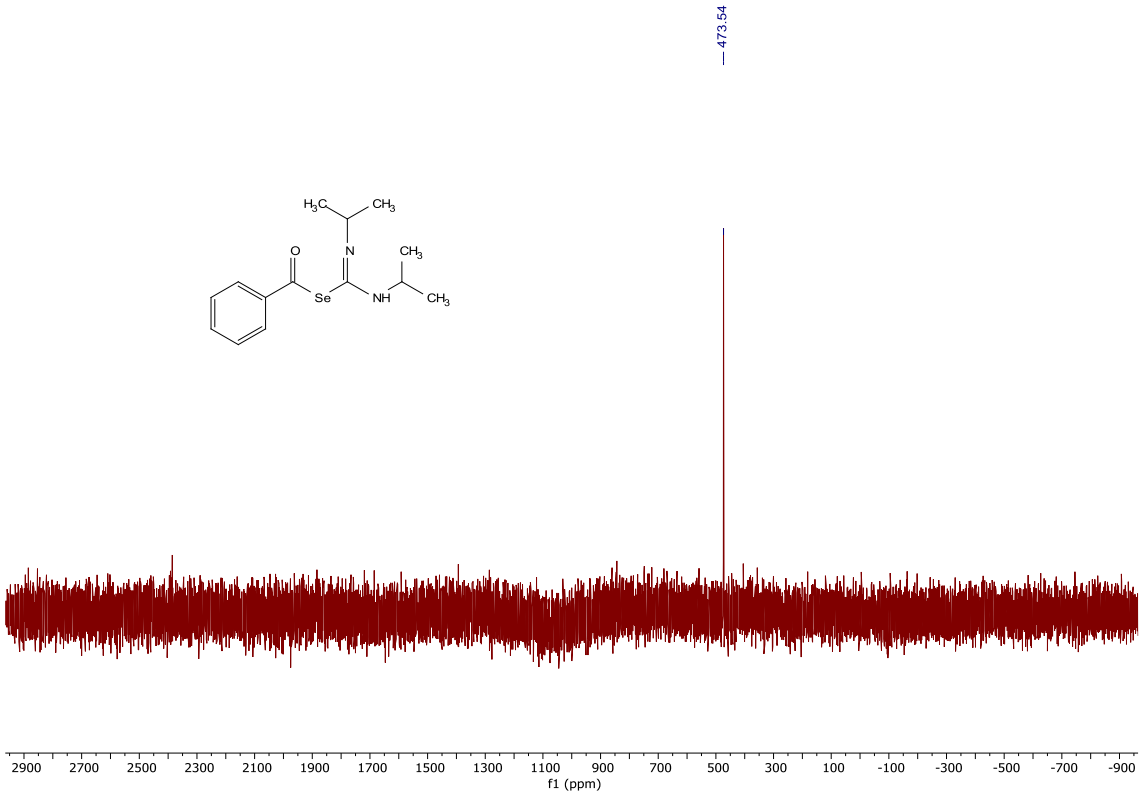


**Figure S26.** $^{77}$Se-NMR spectrum of compound **3**.

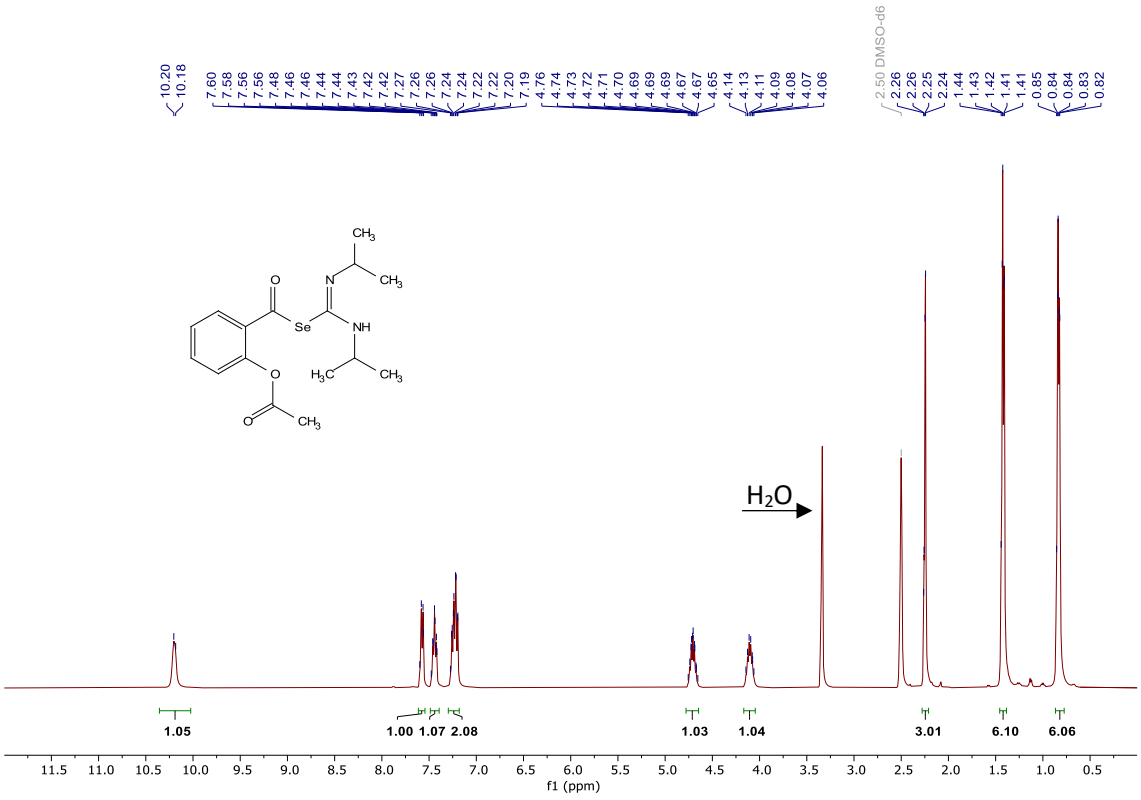


**Figure S27.** [1]H-NMR spectrum of compound **4**.

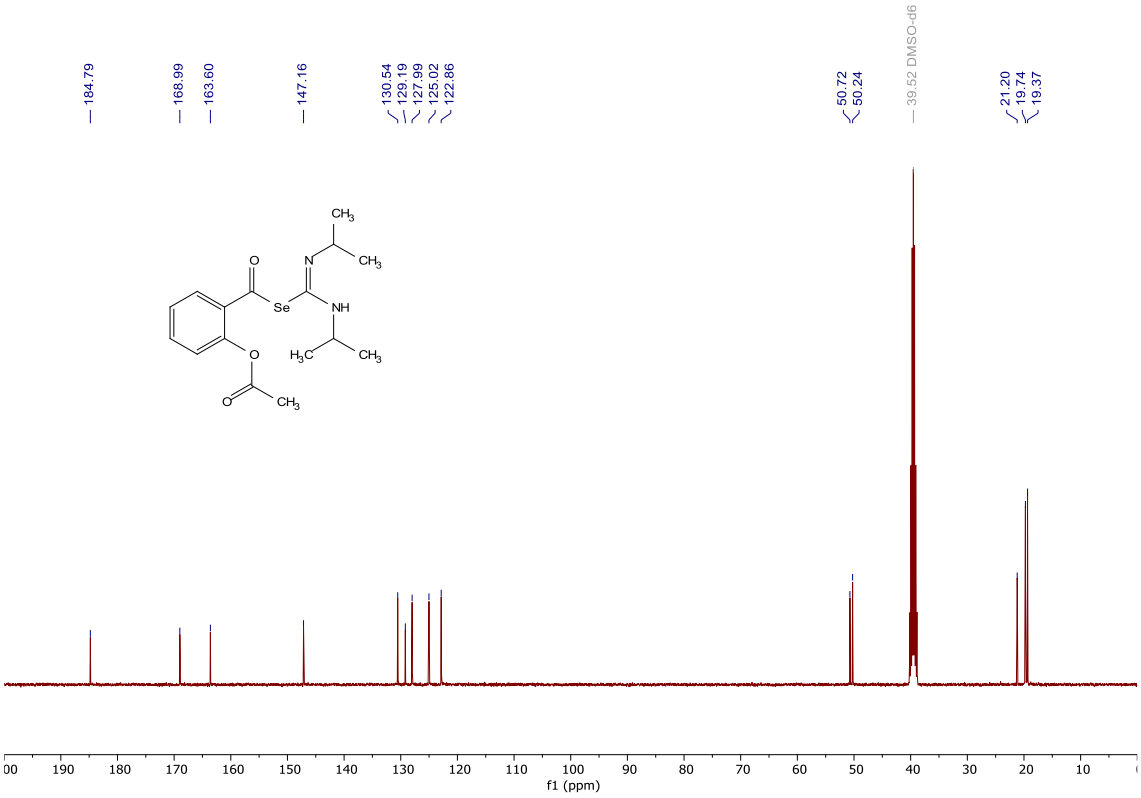


**Figure S28.** [13]C-NMR spectrum of compound **4**.

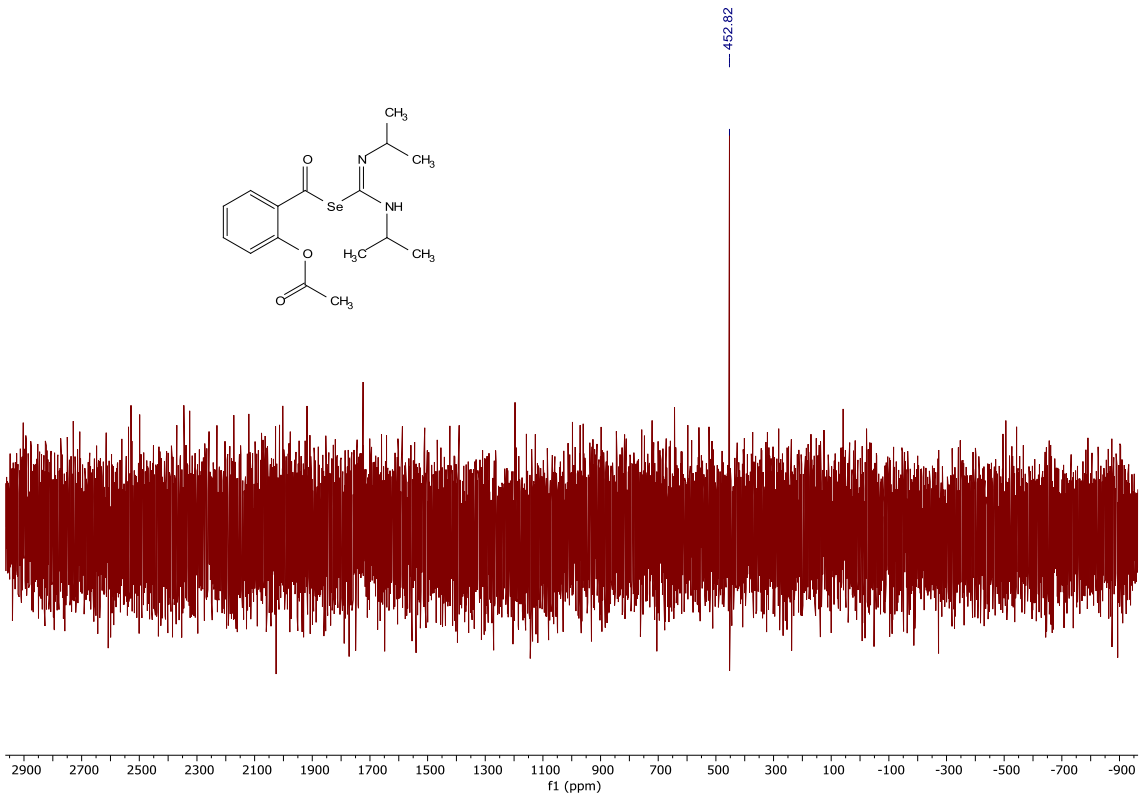


**Figure S29.** $^{77}$Se-NMR spectrum of compound **4**.

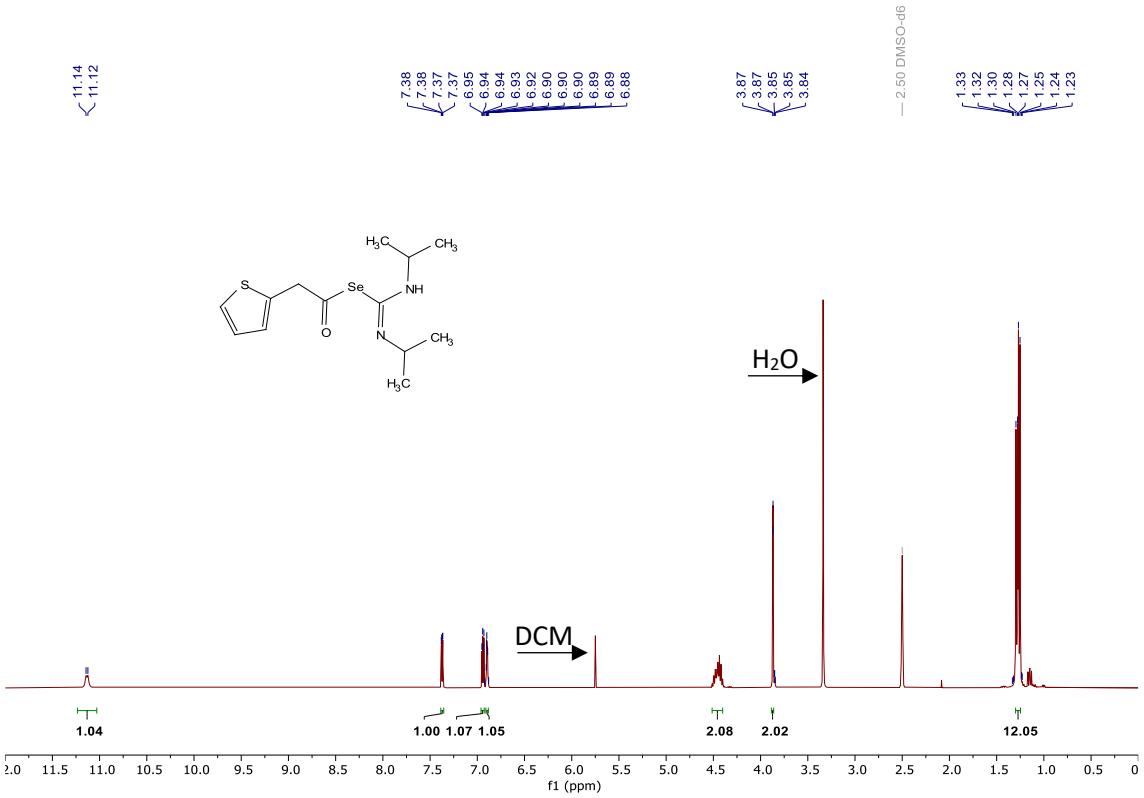


**Figure S30.** $^{1}$H-NMR spectrum of compound **5**.

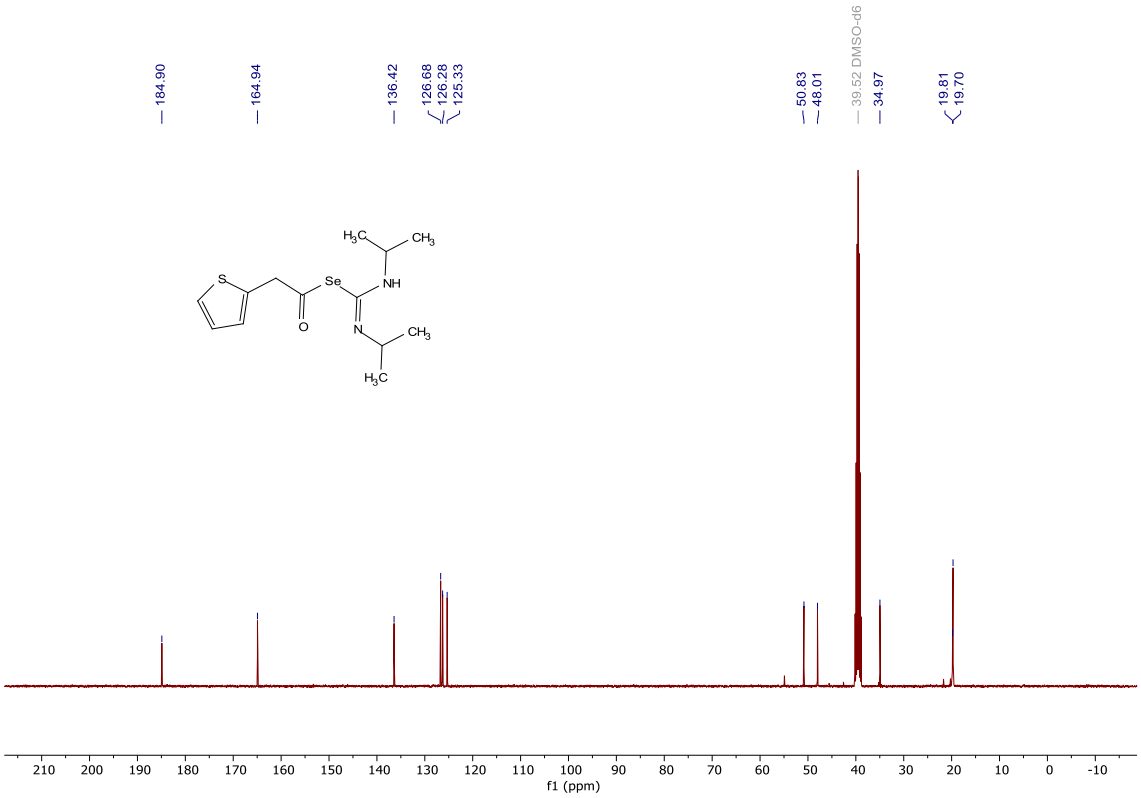


**Figure S31.** $^{13}$C-NMR spectrum of compound **5**.

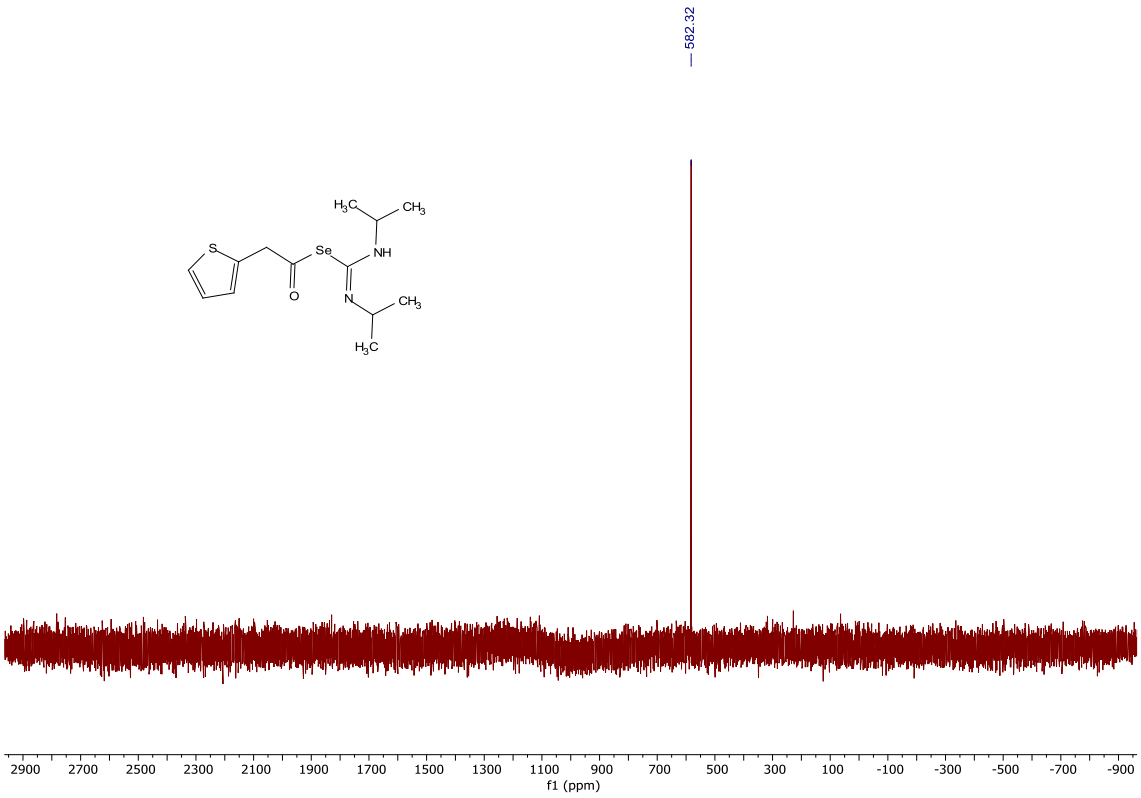


**Figure S32.** $^{77}$Se-NMR spectrum of compound **5**.

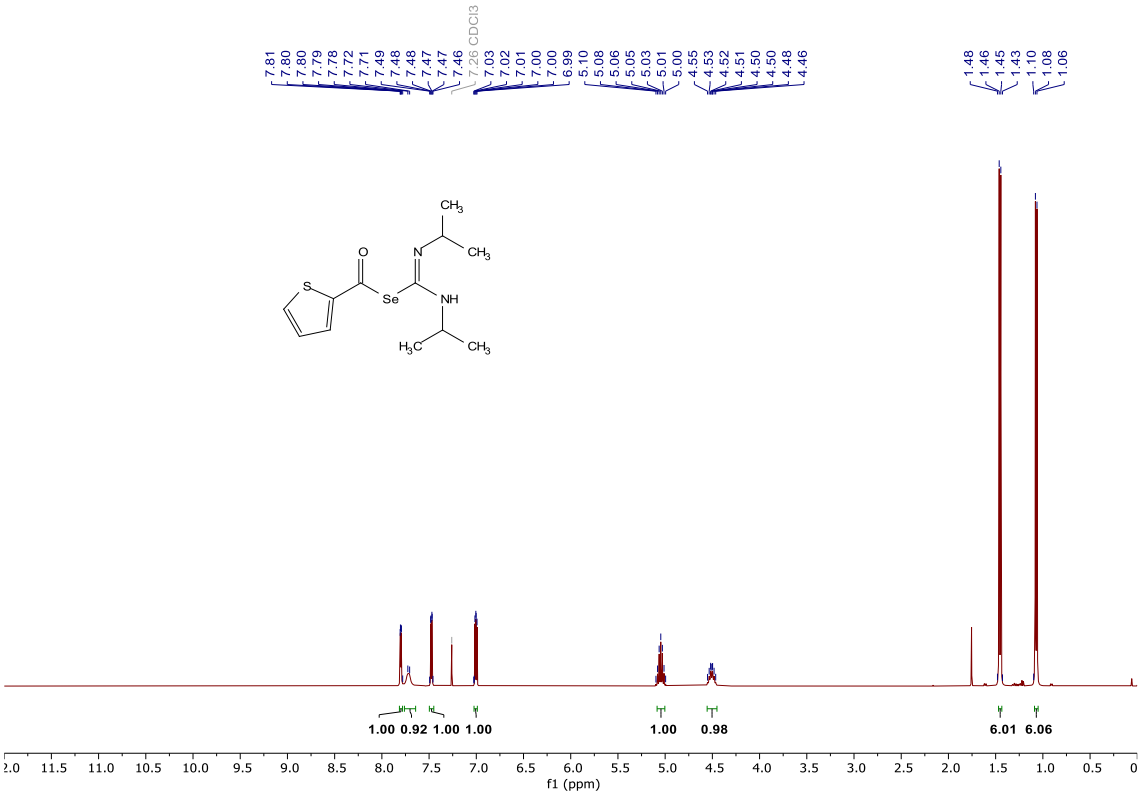


**Figure S33.** [1]H-NMR spectrum of compound **6**.

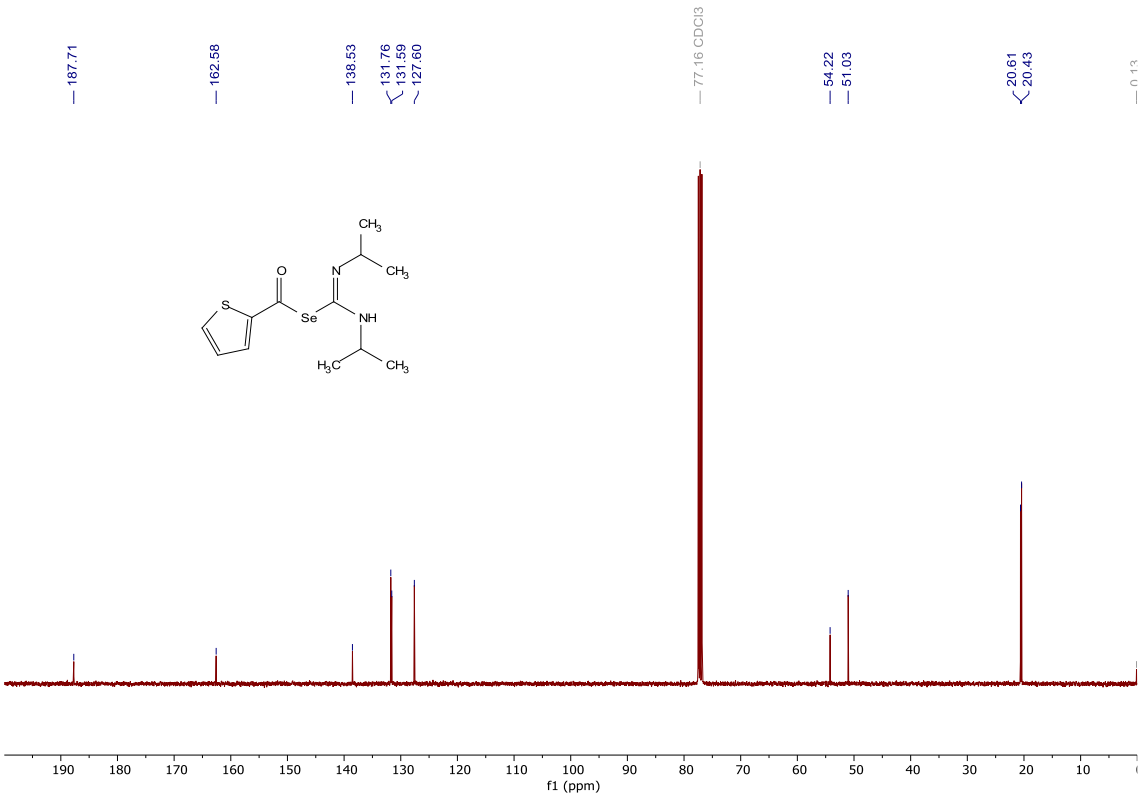


**Figure S34.** [13]C-NMR spectrum of compound **6**.

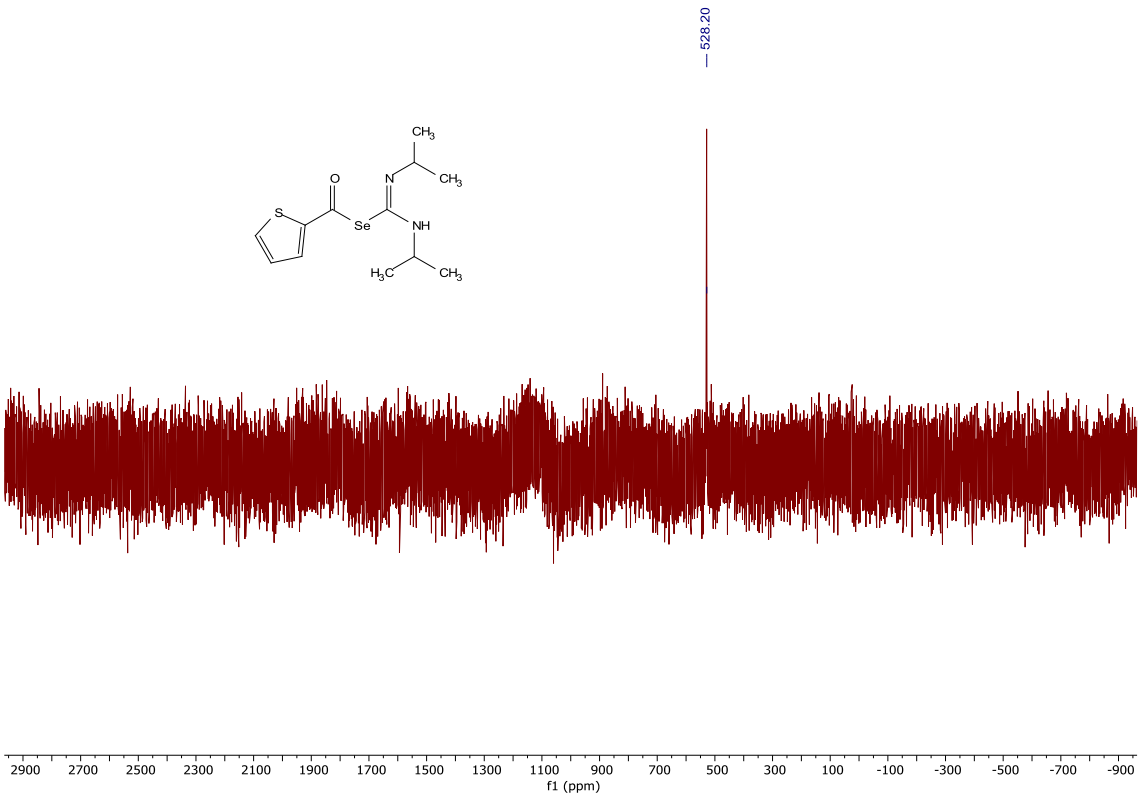


**Figure S35.** $^{77}$Se-NMR spectrum of compound **6**.

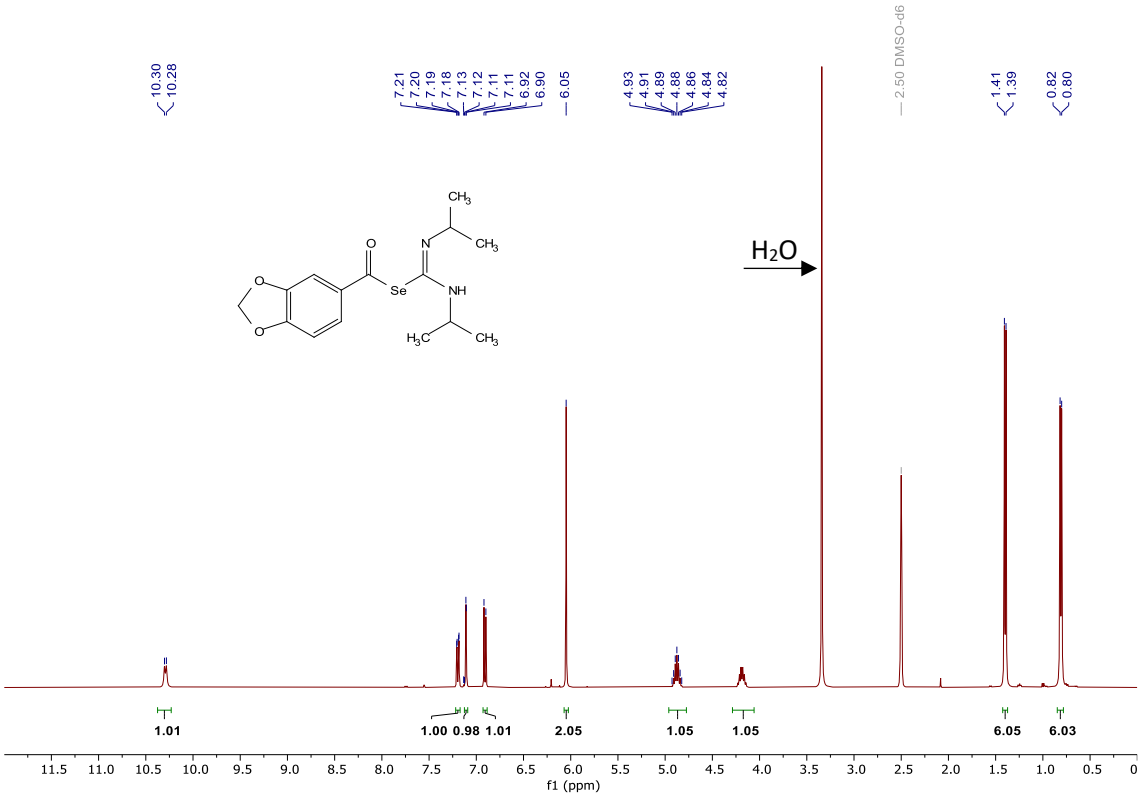


**Figure S36.** $^{1}$H-NMR spectrum of compound **7**.

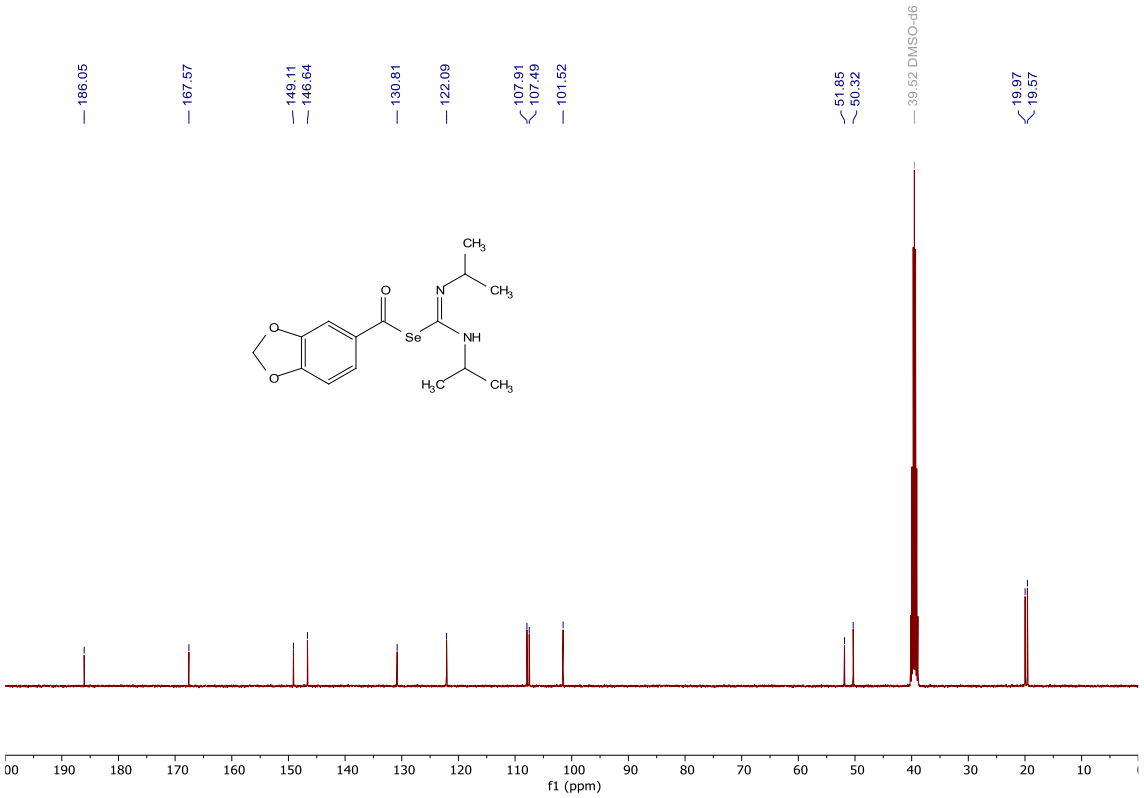


**Figure S37.** $^{13}$C-NMR spectrum of compound **7**.

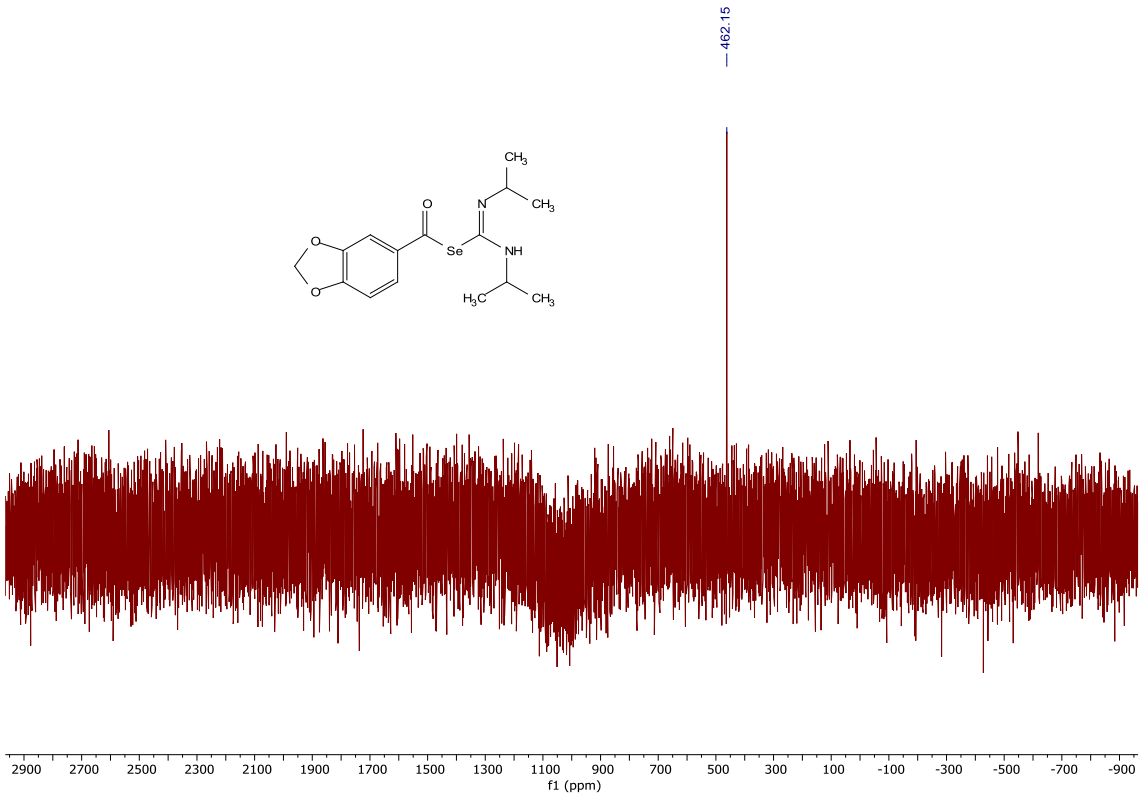


**Figure S38.** $^{77}$Se-NMR spectrum of compound **7**.

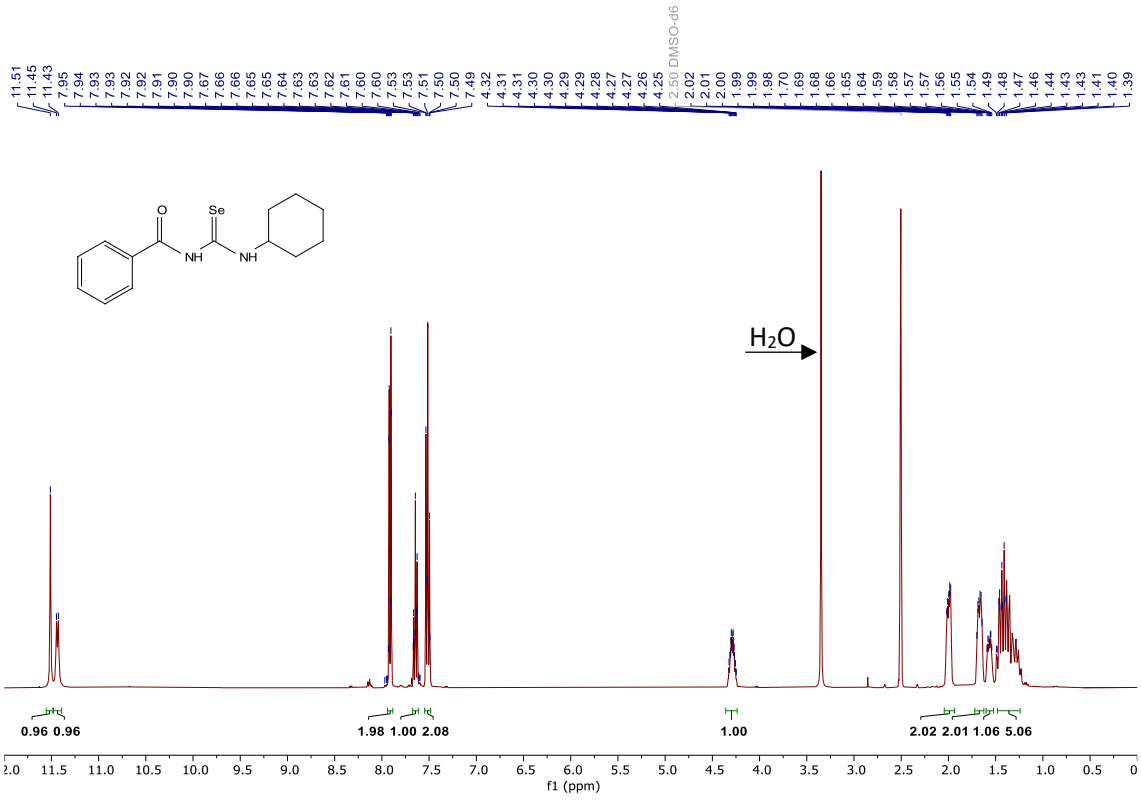


**Figure S39.** [1]H-NMR spectrum of compound **8**.

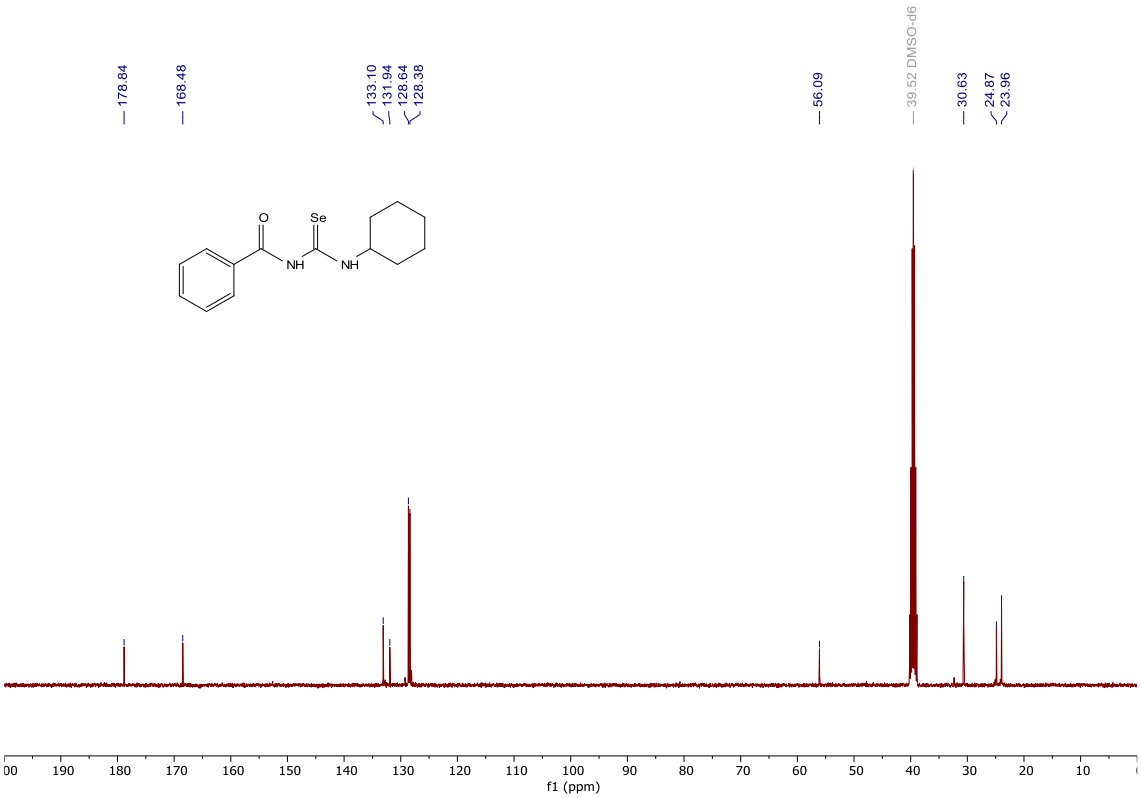


**Figure S40.** [13]C-NMR spectrum of compound **8**.

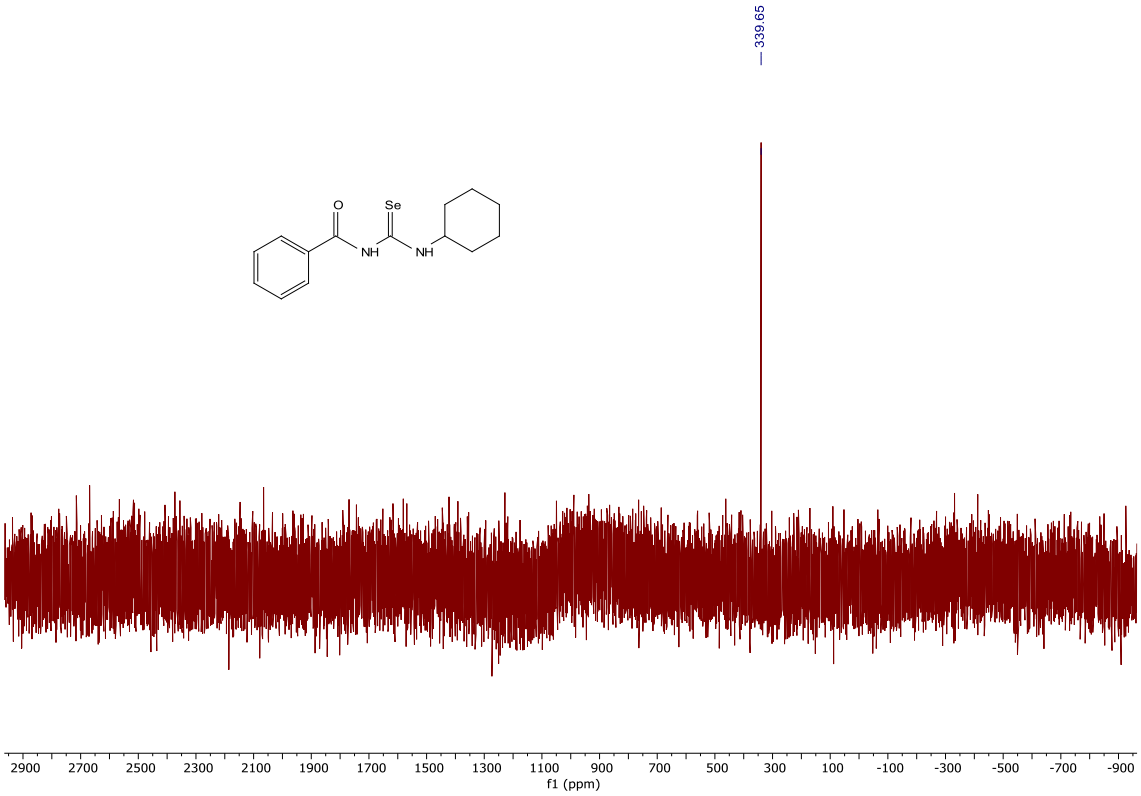


**Figure S41.** $^{77}$Se-NMR spectrum of compound **8**.

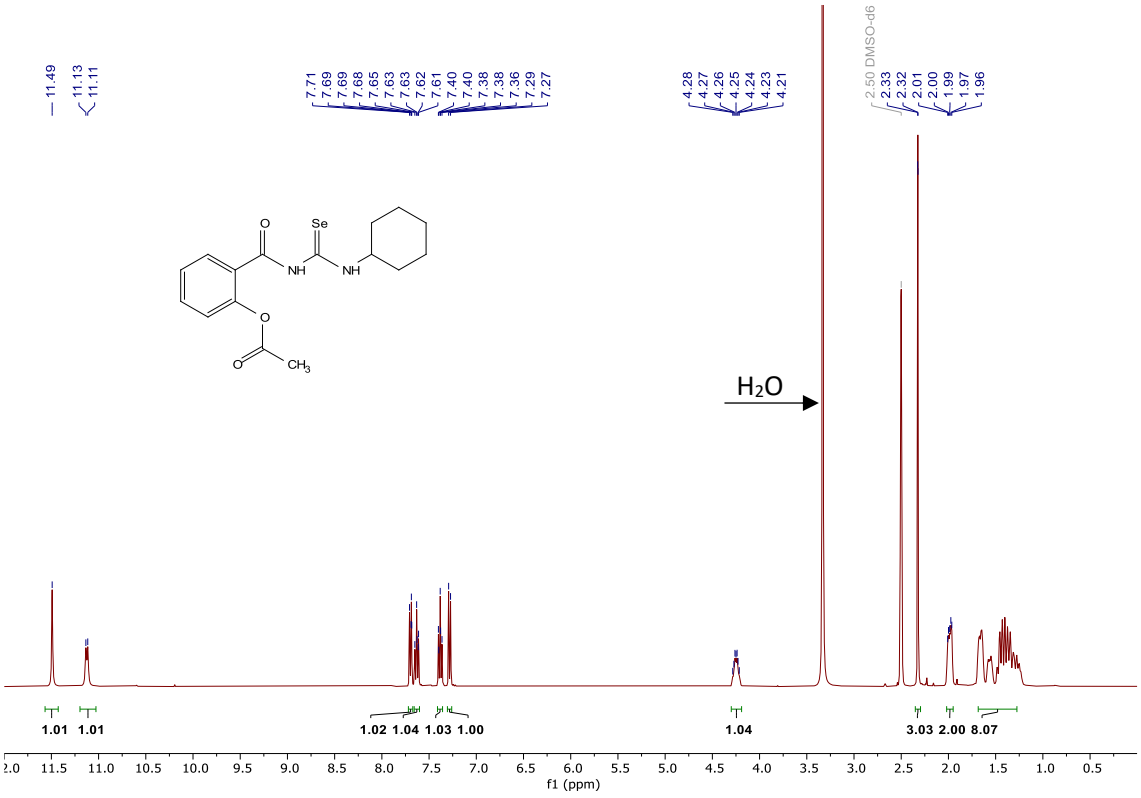


**Figure S42.** $^{1}$H-NMR spectrum of compound **9**.

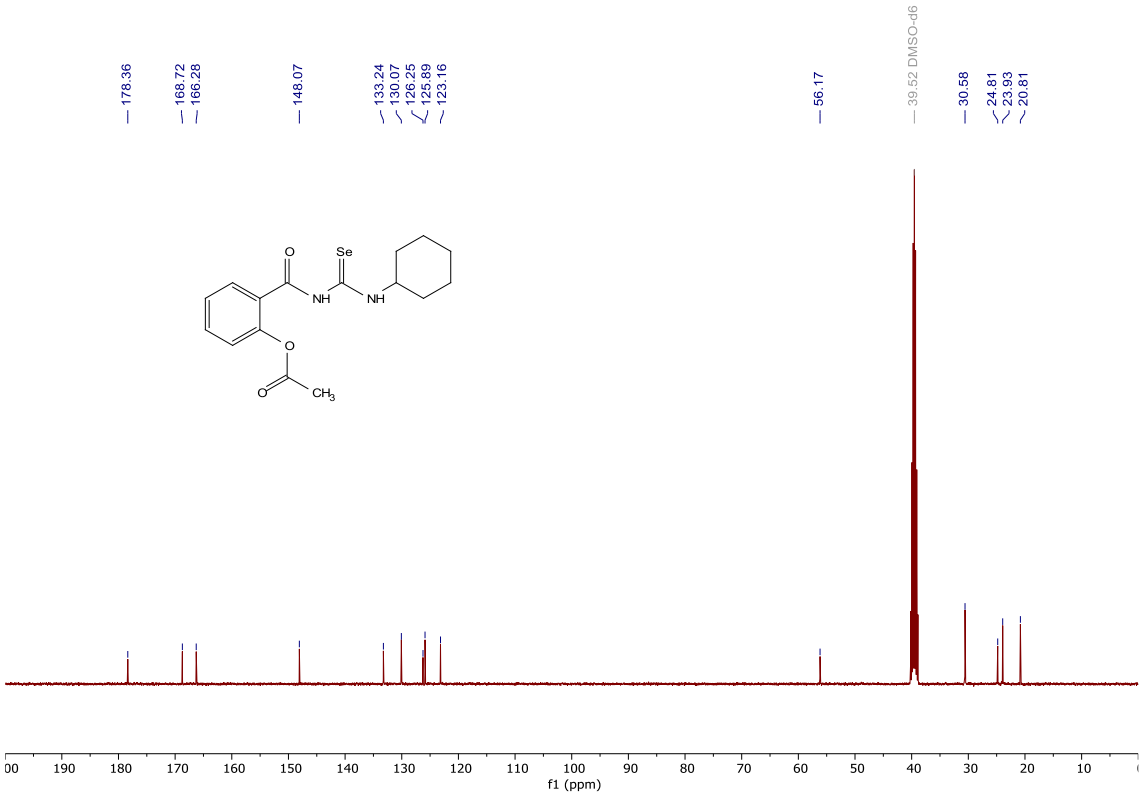


**Figure S43.** $^{13}$C-NMR spectrum of compound **9**.

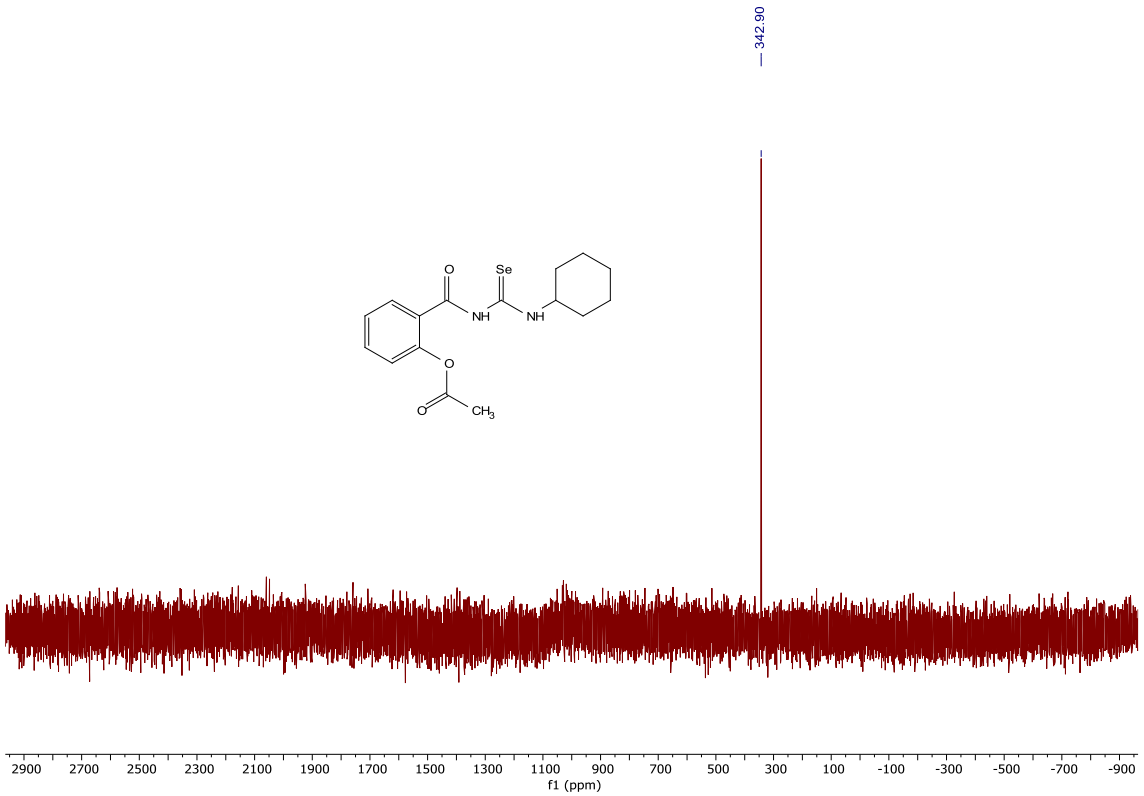


**Figure S44.** $^{77}$Se-NMR spectrum of compound **9**.

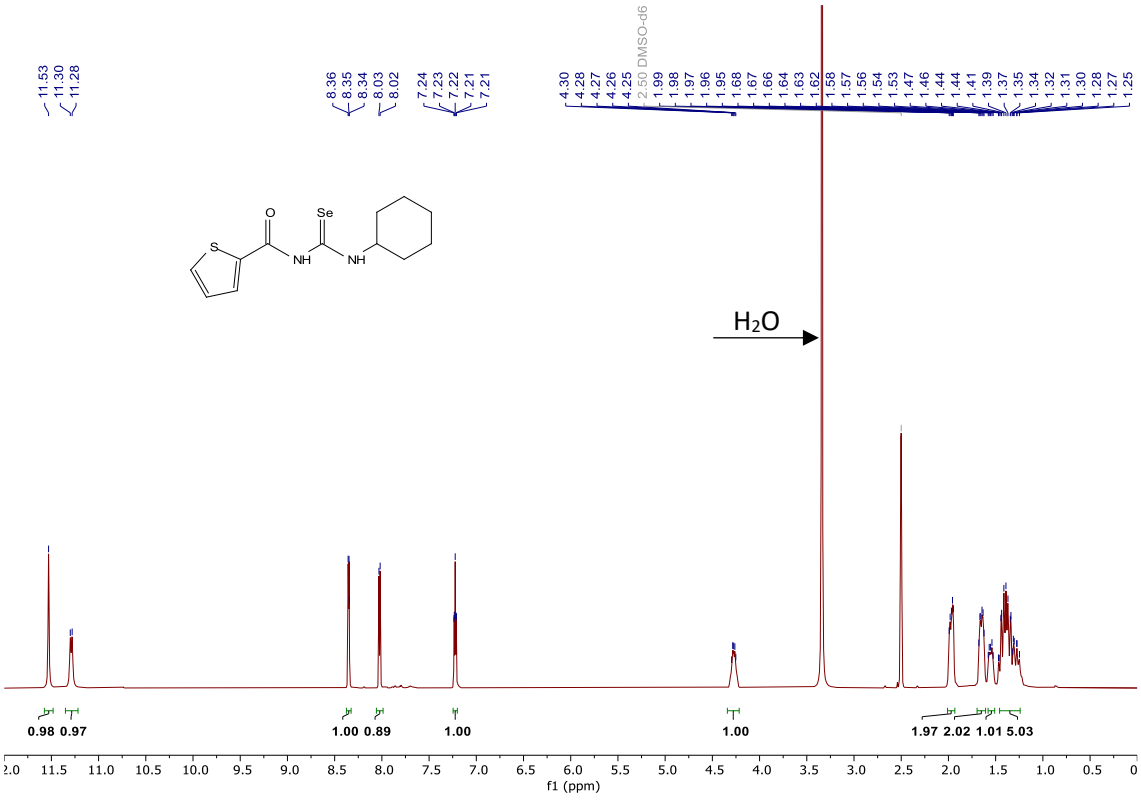


**Figure S45.** [1]H-NMR spectrum of compound **10**.

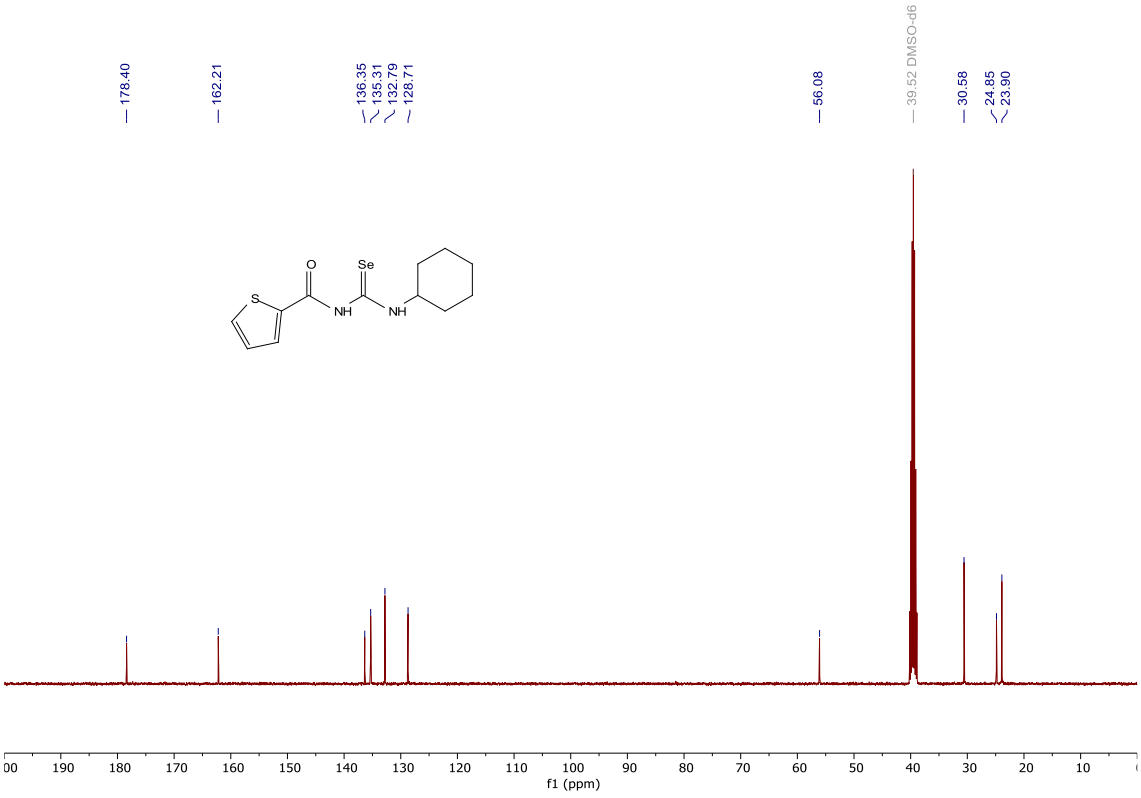


**Figure S46.** [13]C-NMR spectrum of compound **10**.

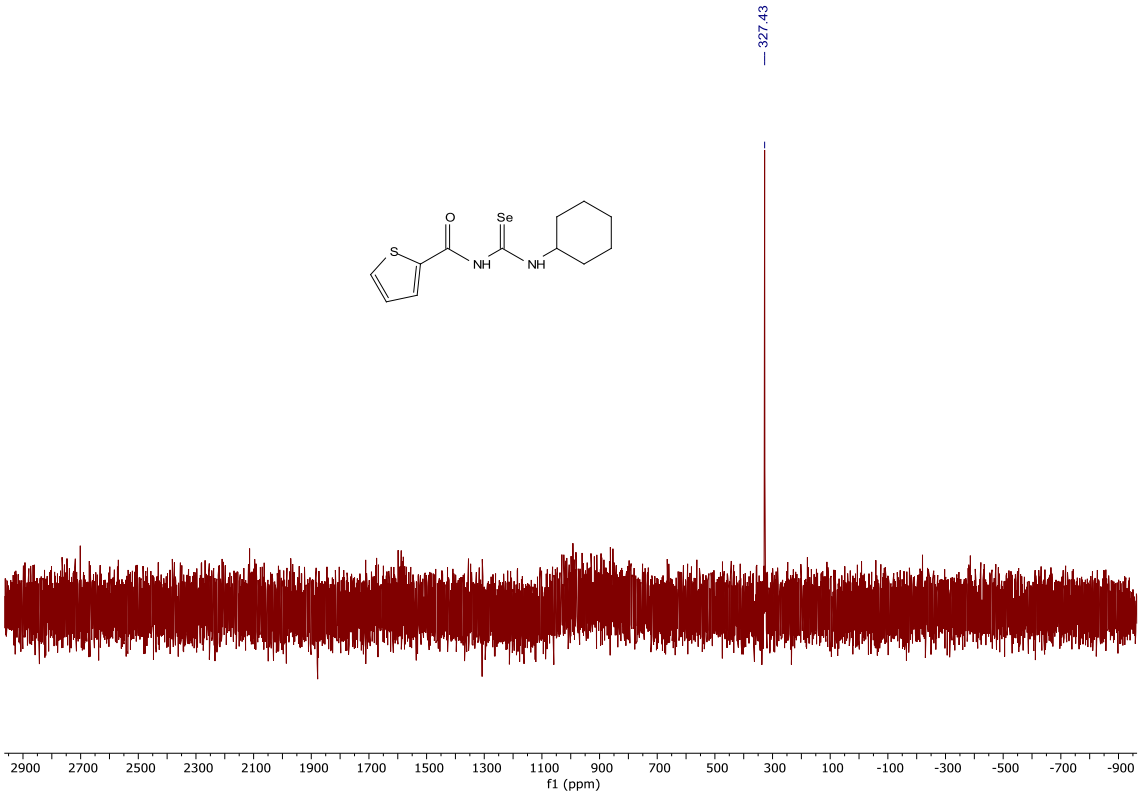


**Figure S47.** $^{77}$Se-NMR spectrum of compound **10**.

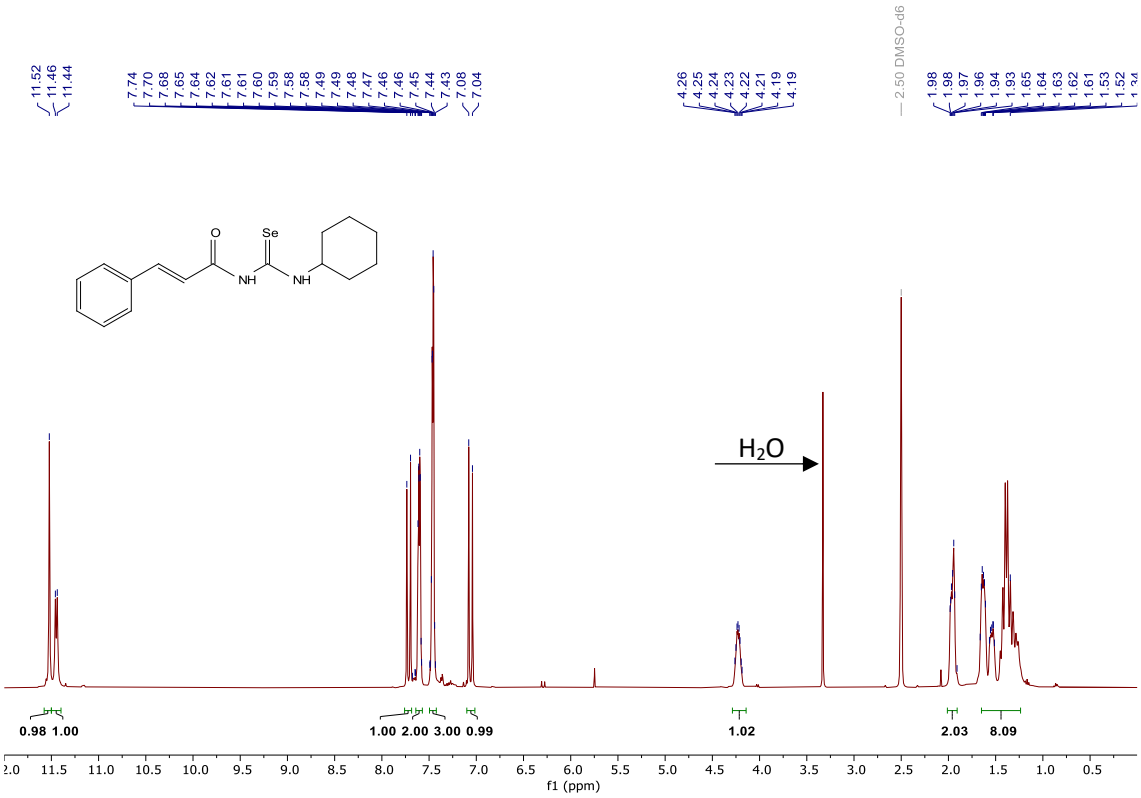


**Figure S48.** $^{1}$H-NMR spectrum of compound **11**.

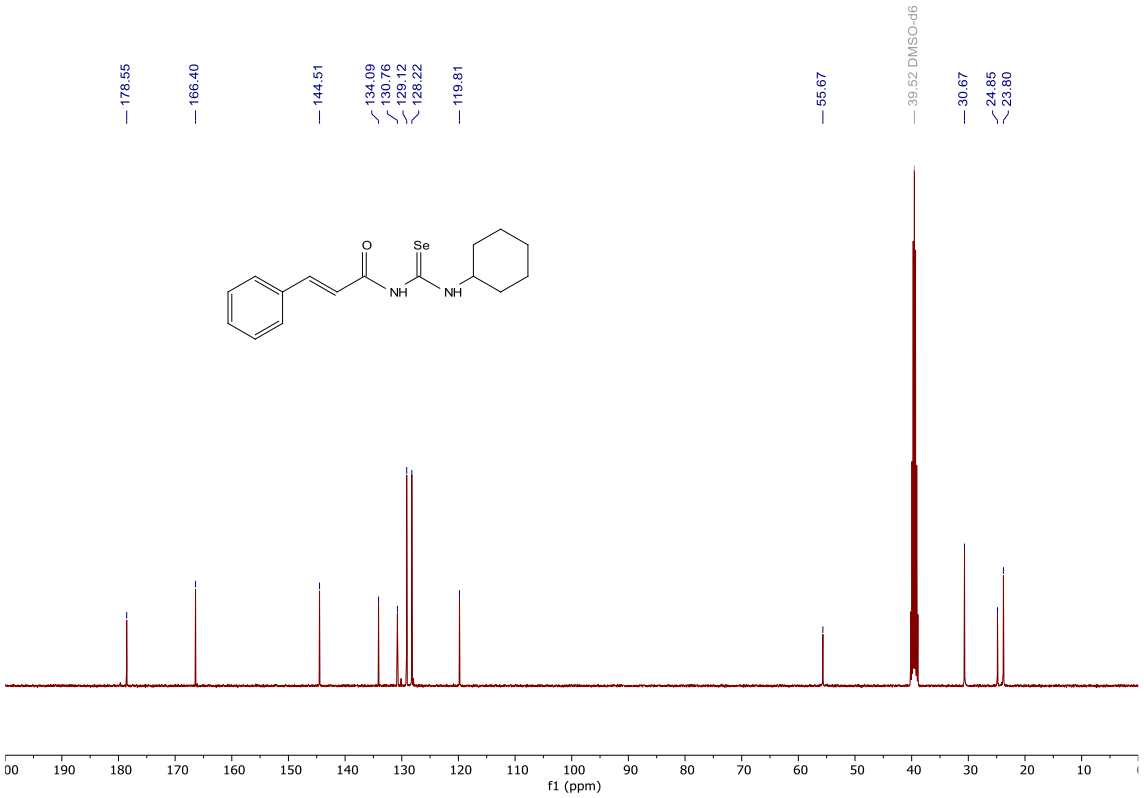


**Figure S49.** $^{13}$C-NMR spectrum of compound **11**.

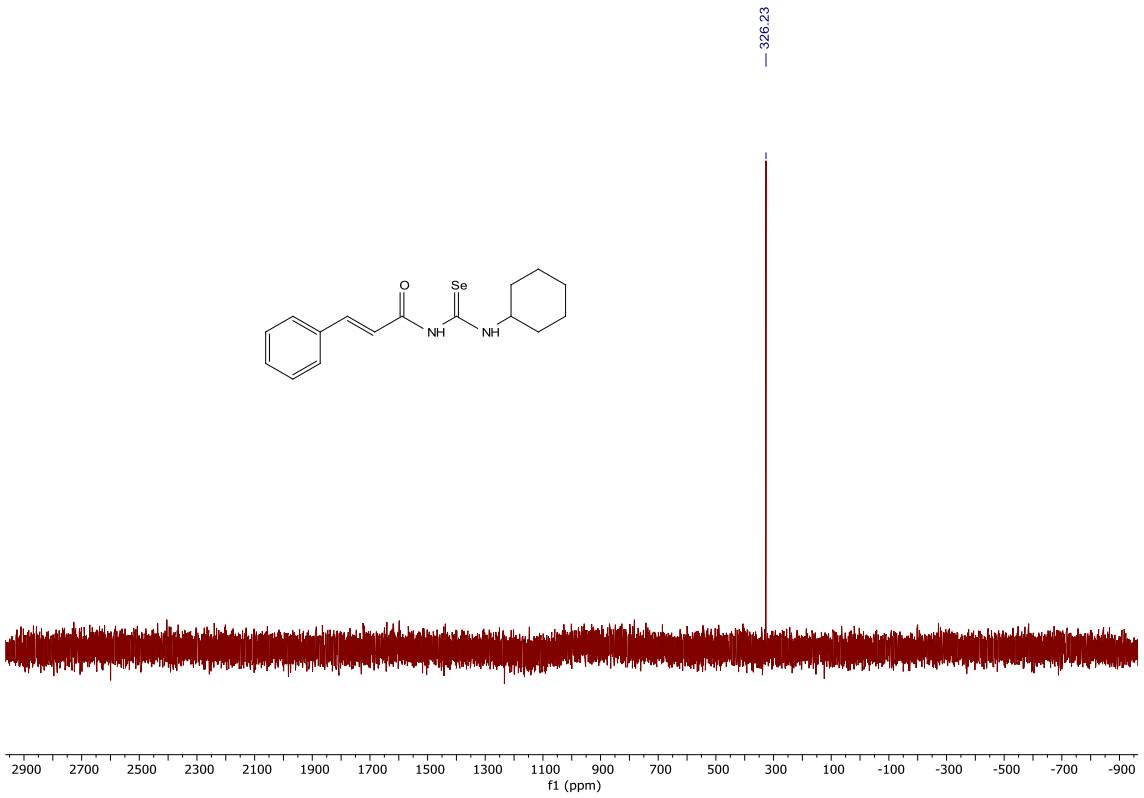


**Figure S50.** $^{77}$Se-NMR spectrum of compound **11**.

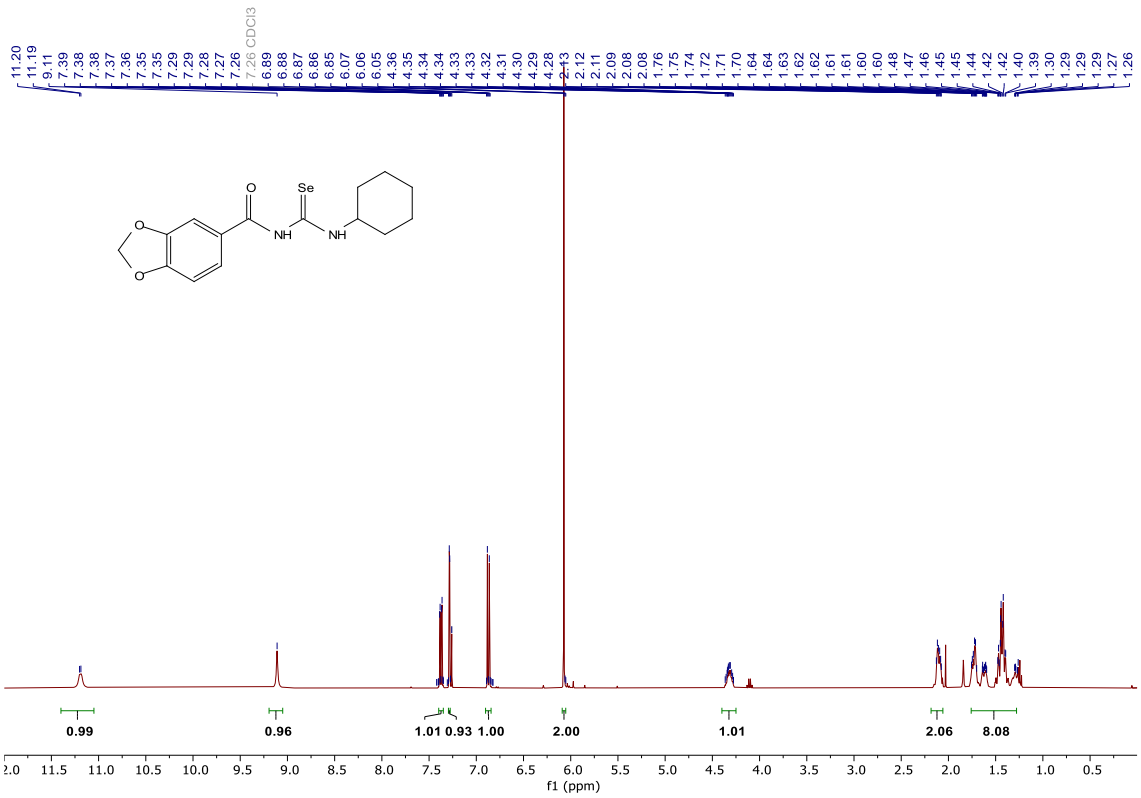


**Figure S51.** [1]H-NMR spectrum of compound **12**.

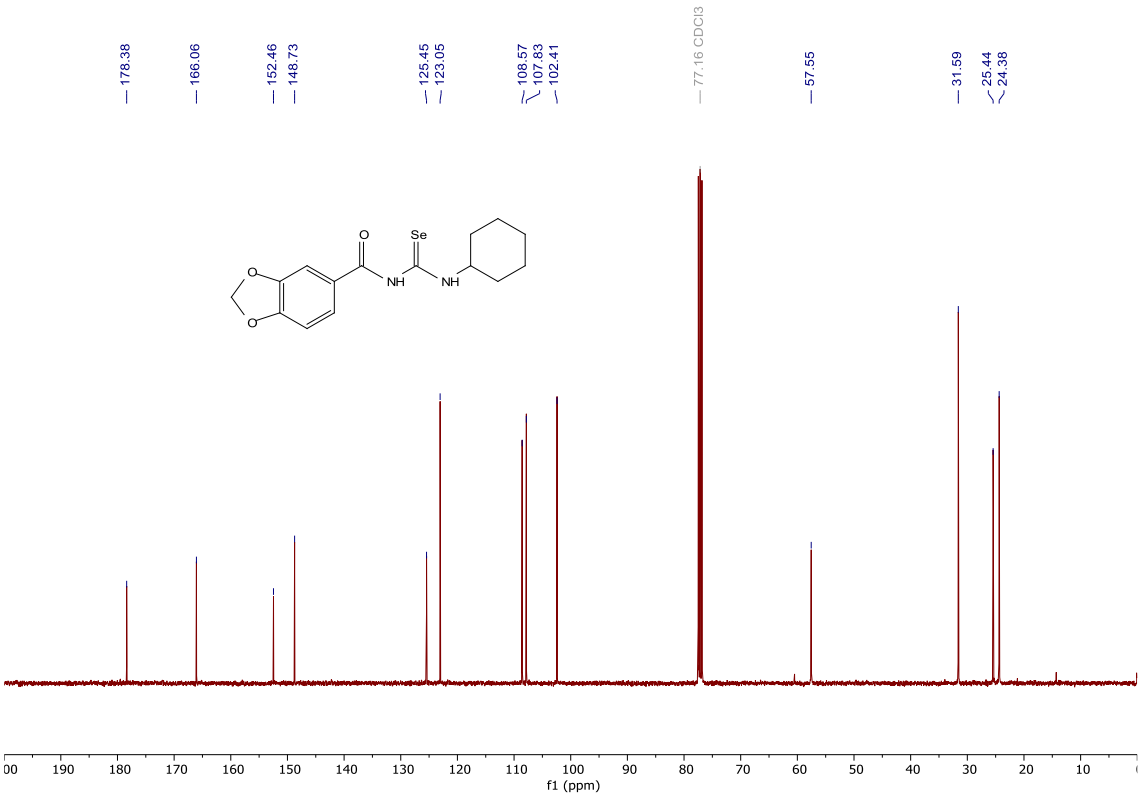


**Figure S52.** [13]C-NMR spectrum of compound **12**.

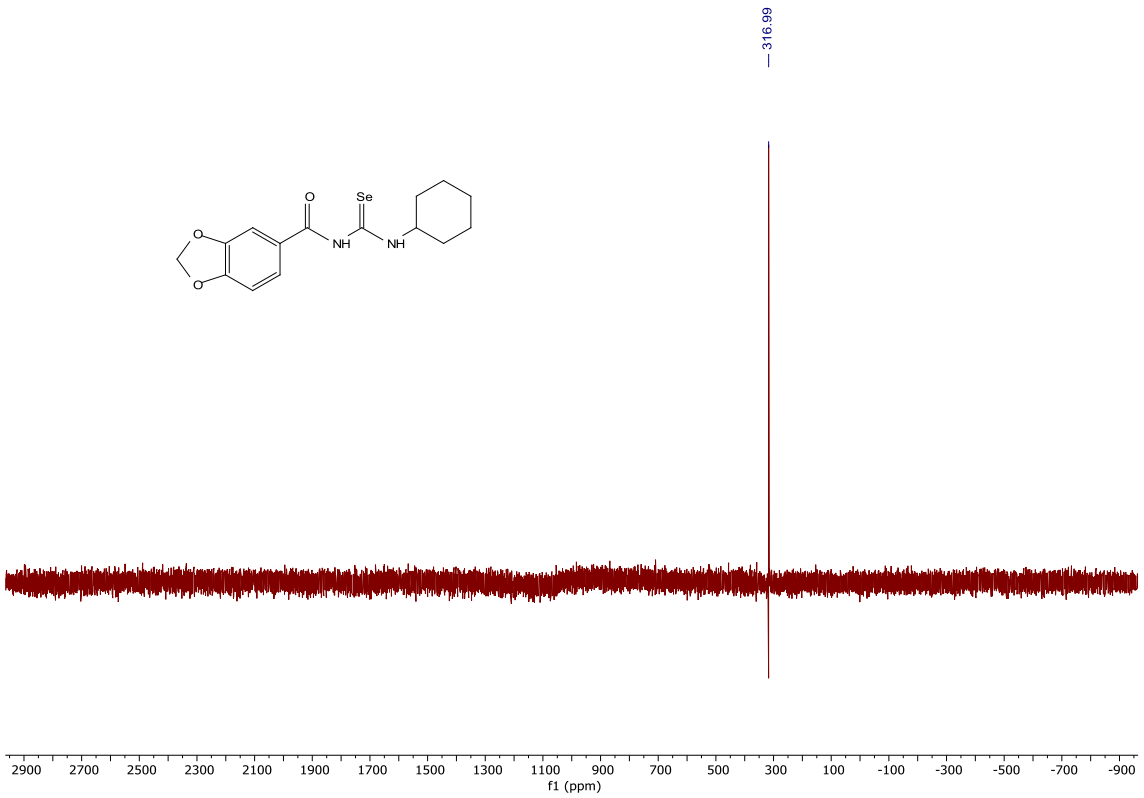


**Figure S53.** $^{77}$Se-NMR spectrum of compound **12**.

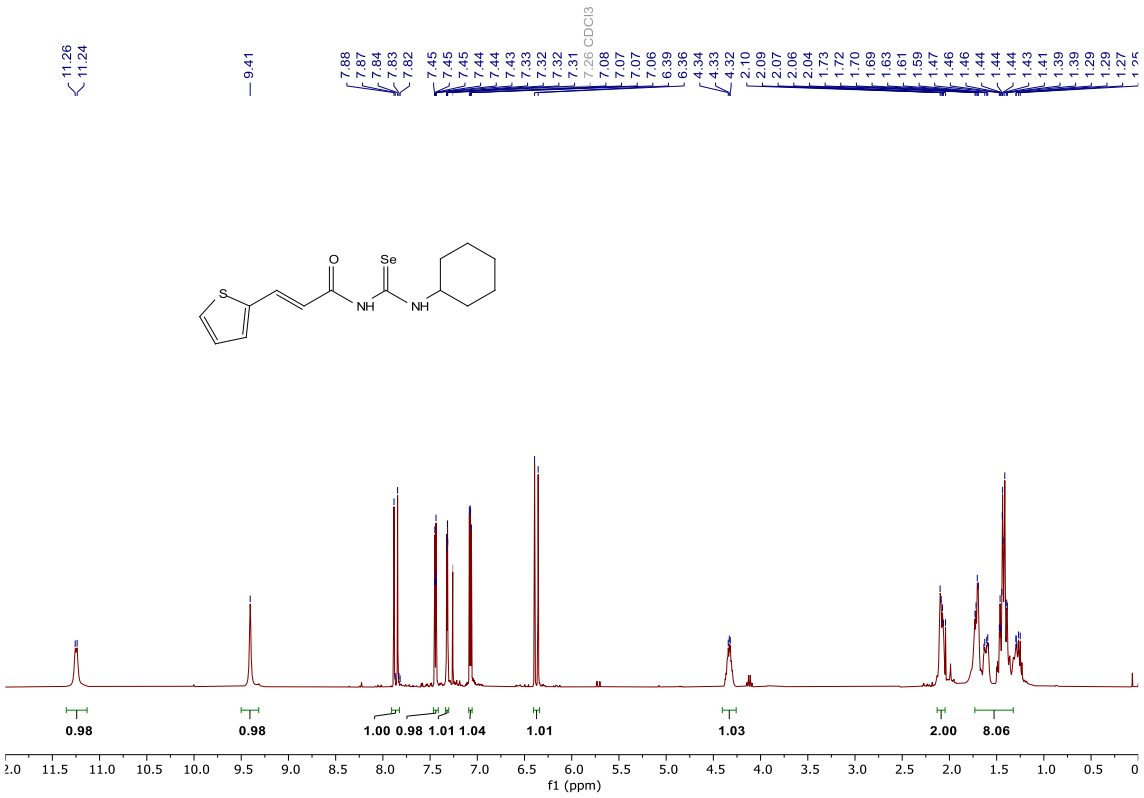


**Figure S54.** $^{1}$H-NMR spectrum of compound **13**.

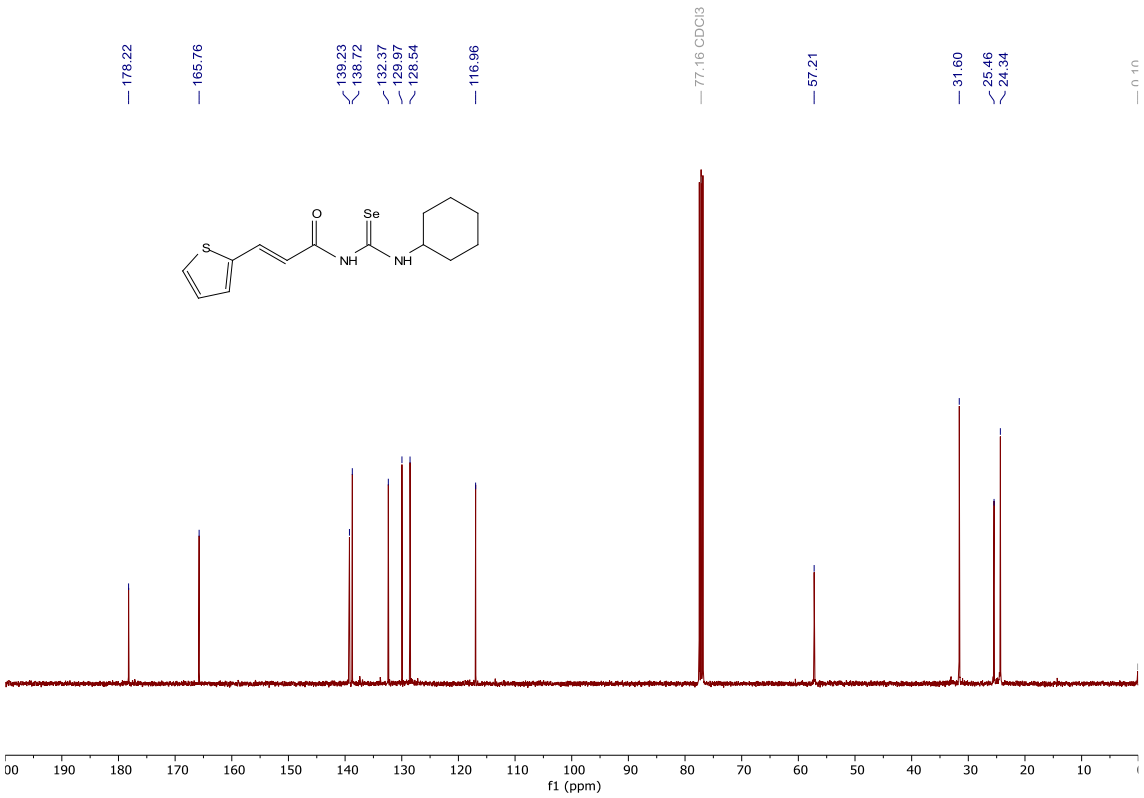


**Figure S55.** $^{13}$C-NMR spectrum of compound **13**.

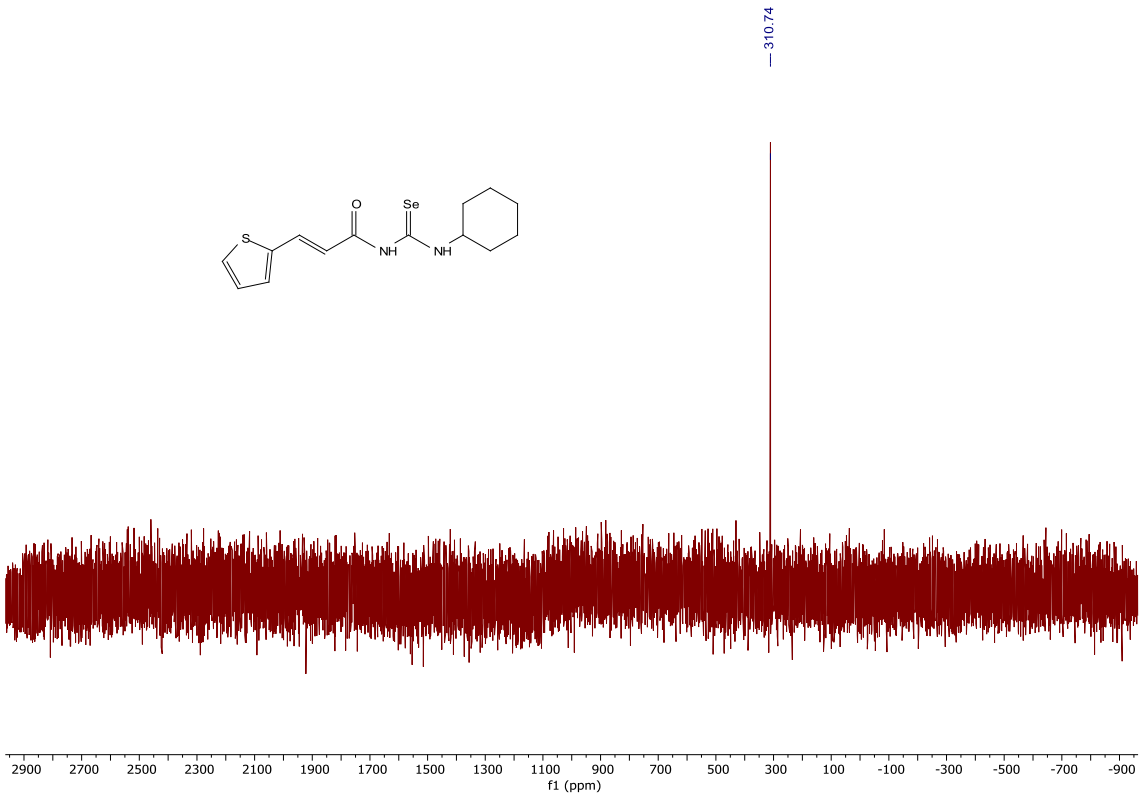


**Figure S56.** $^{7}$Se-NMR spectrum of compound **13**.

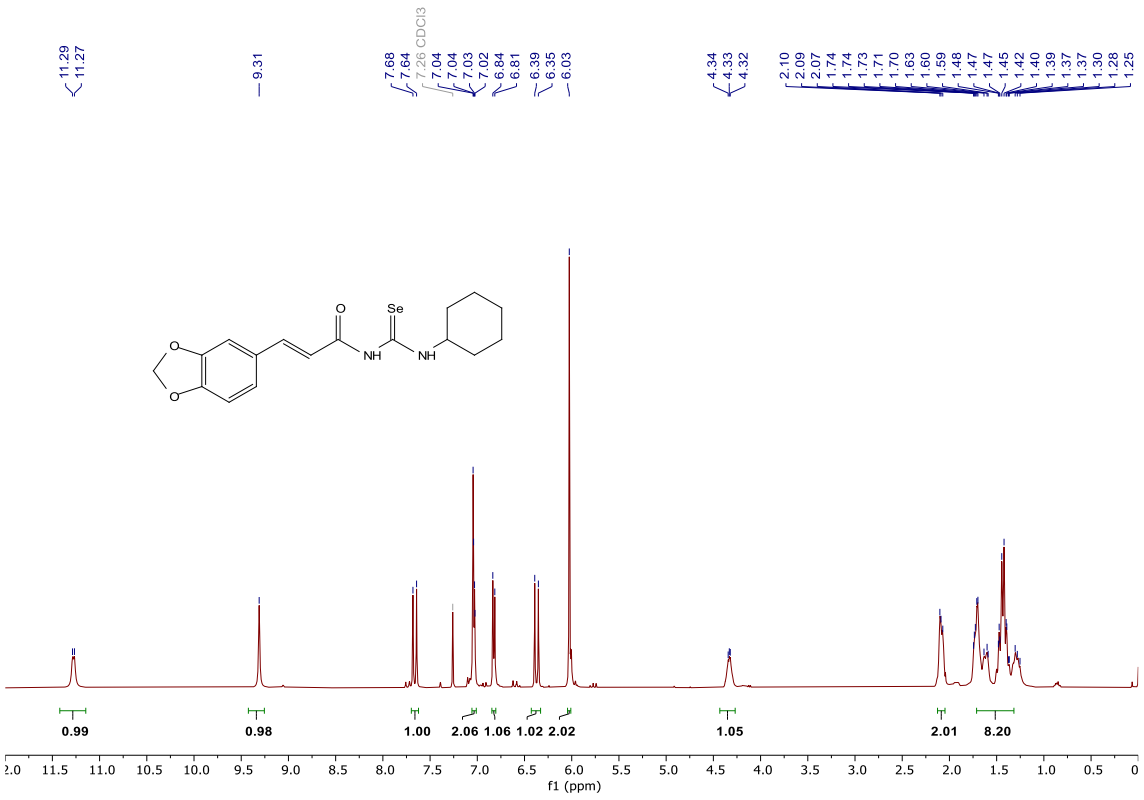


**Figure S57.** [1]H-NMR spectrum of compound **14**.

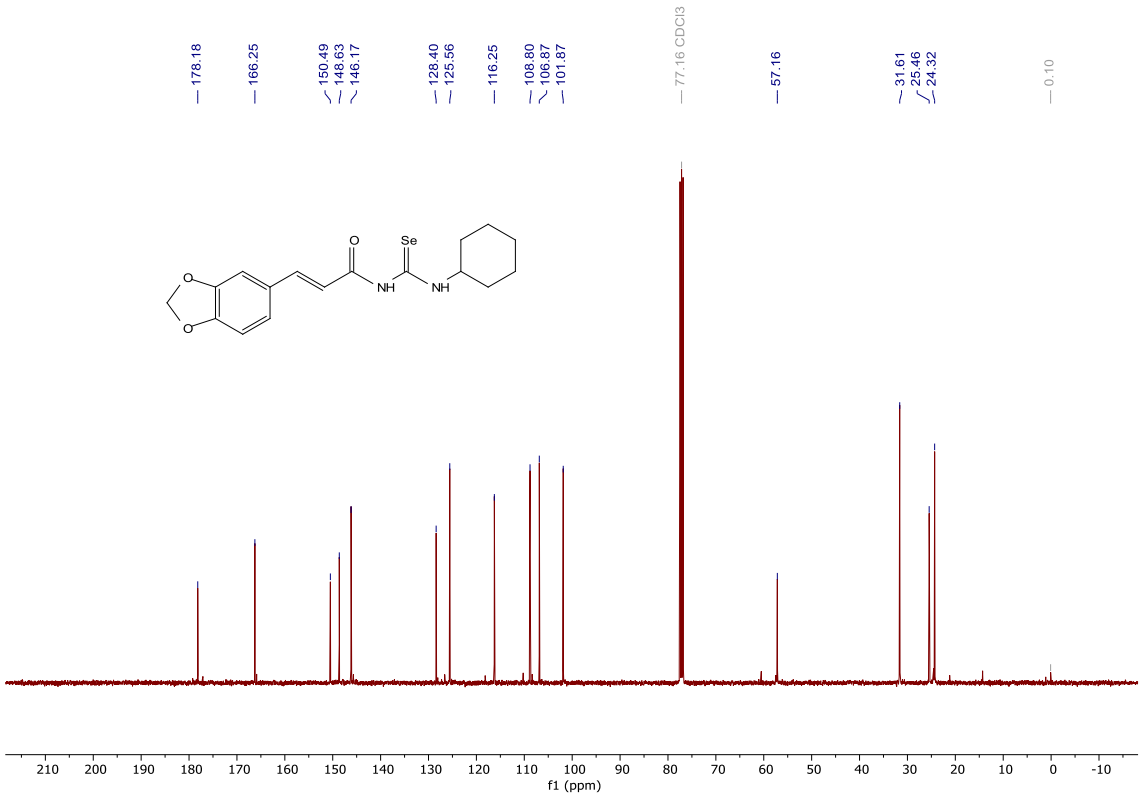


**Figure S58.** [13]C-NMR spectrum of compound **14**.

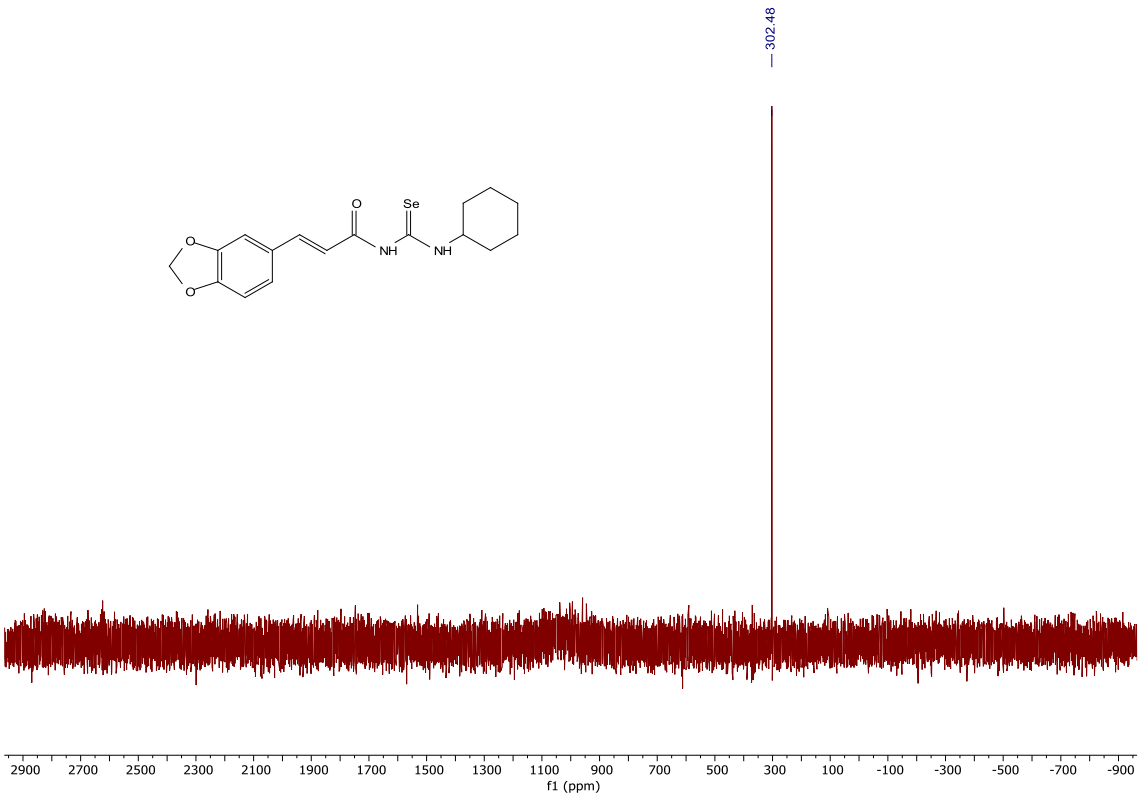


**Figure S59.** $^{77}$Se-NMR spectrum of compound **14**.

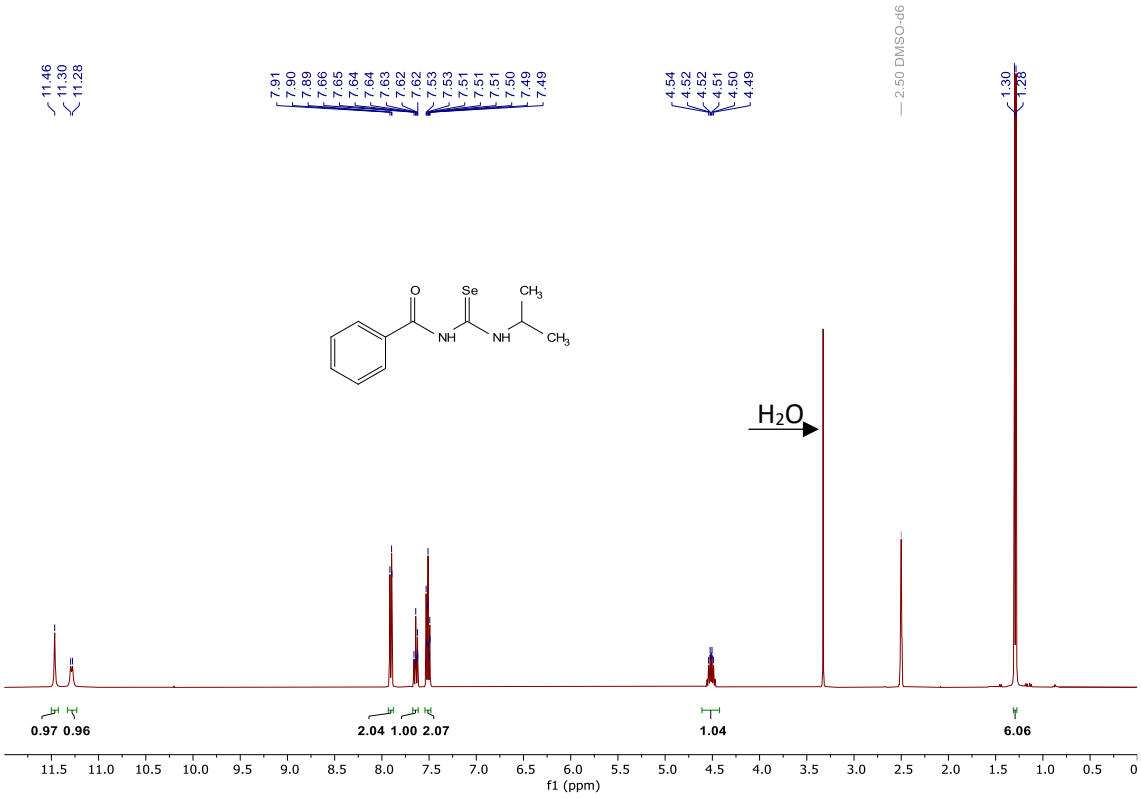


**Figure S60.** $^{1}$H-NMR spectrum of compound **15**.

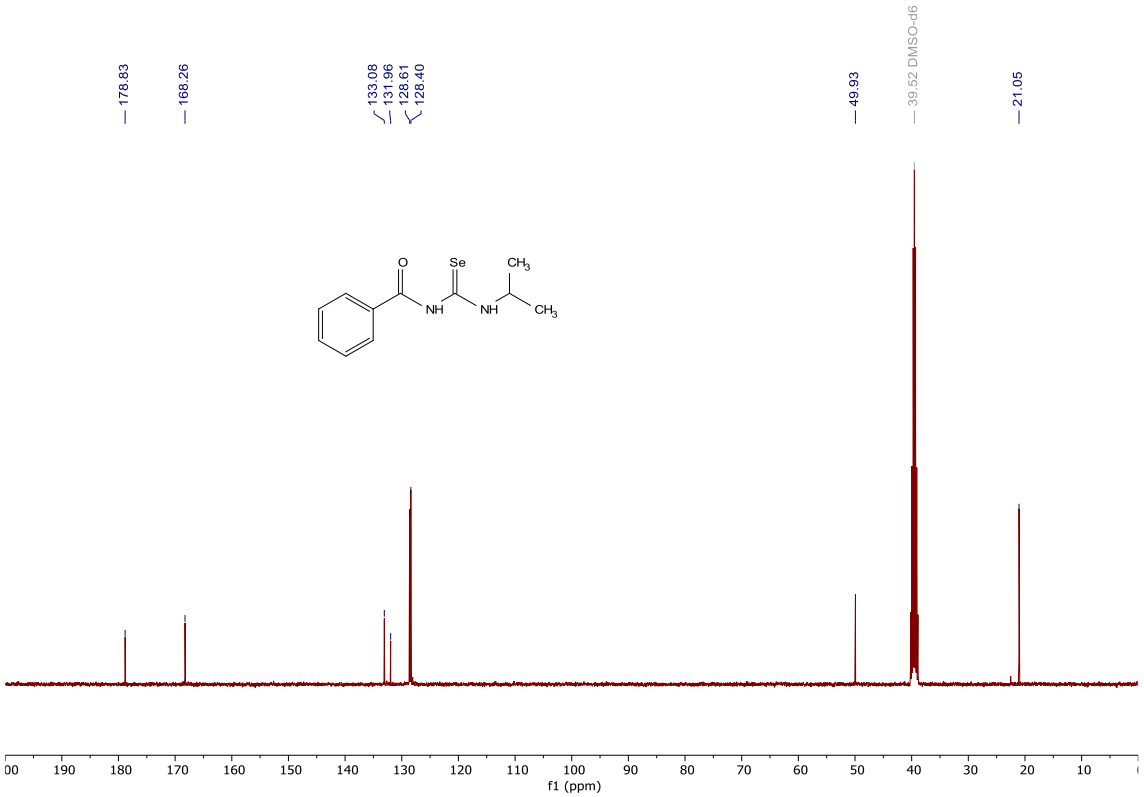


**Figure S61.** $^{13}$C-NMR spectrum of compound **15**.

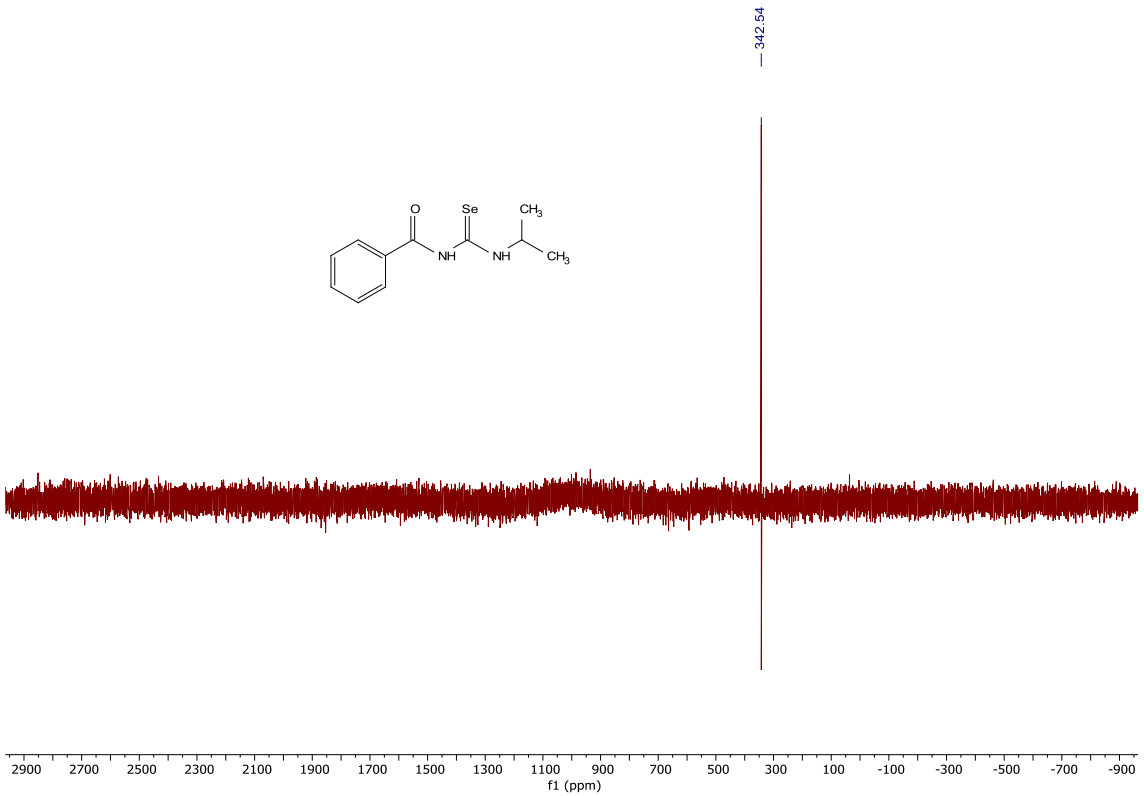


**Figure S62.** $^{77}$Se-NMR spectrum of compound **15**.

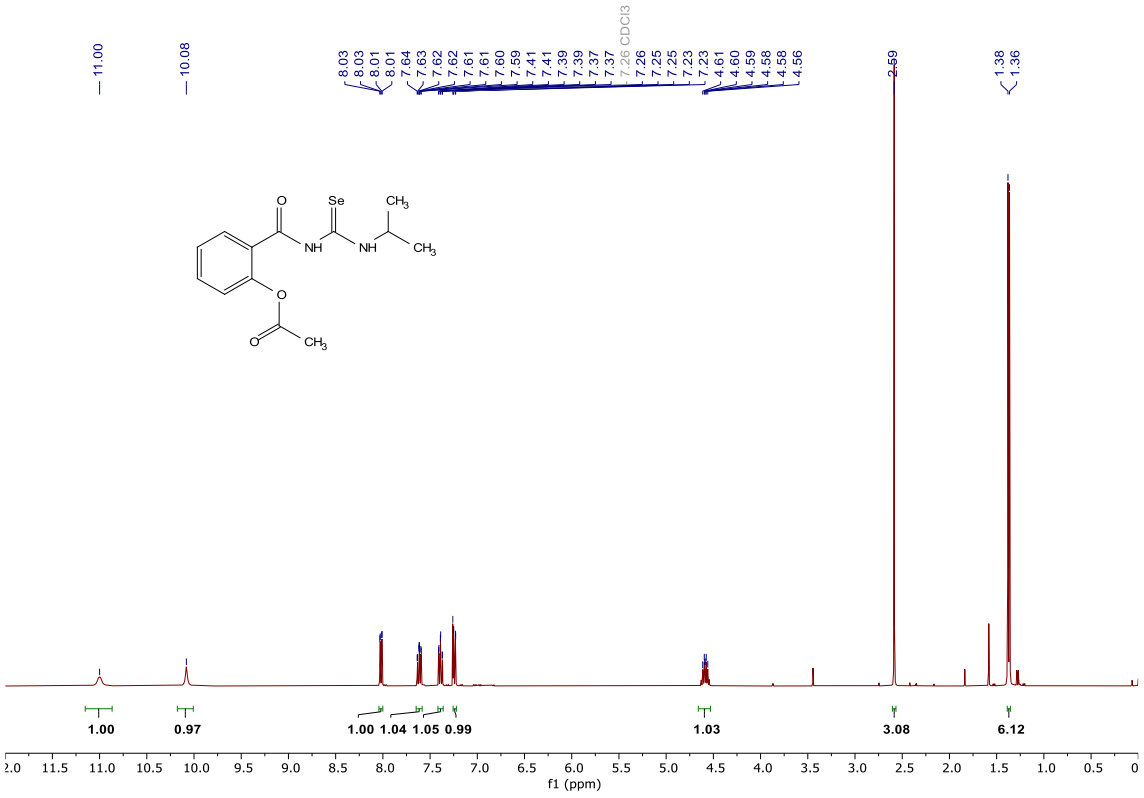


**Figure S63.** [1]H-NMR spectrum of compound **16**.

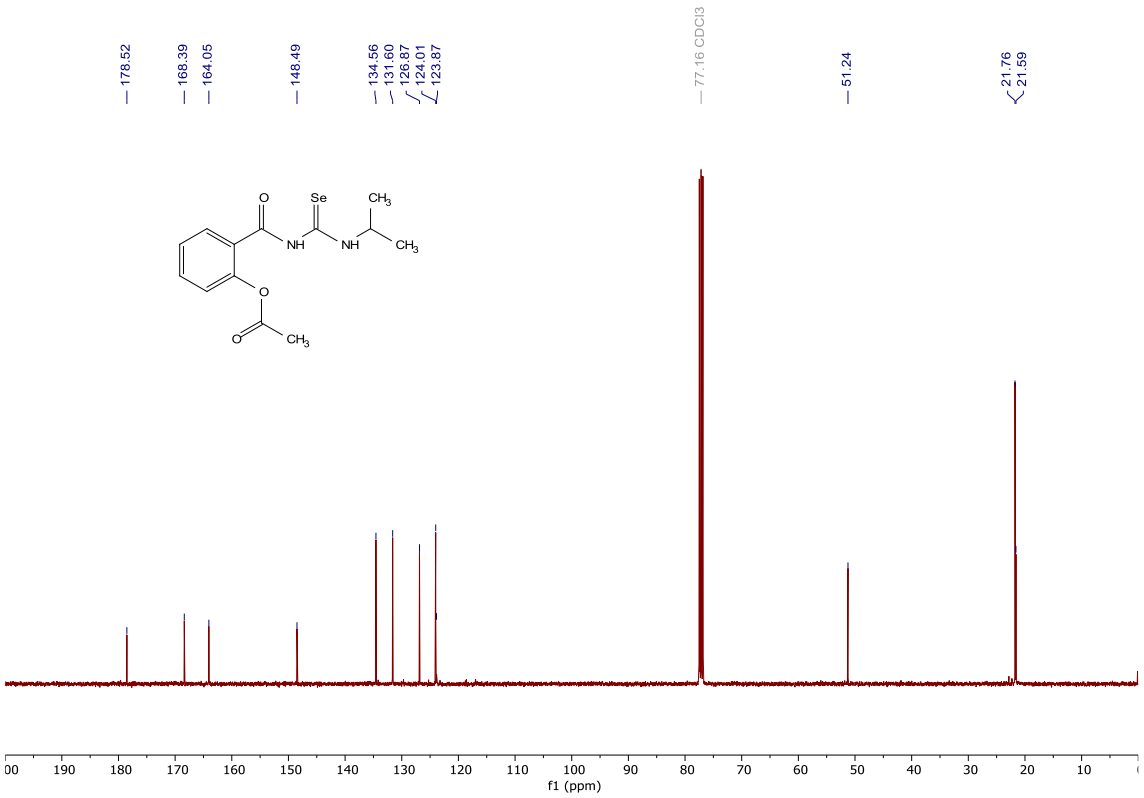


**Figure S64.** [13]C-NMR spectrum of compound **16**.

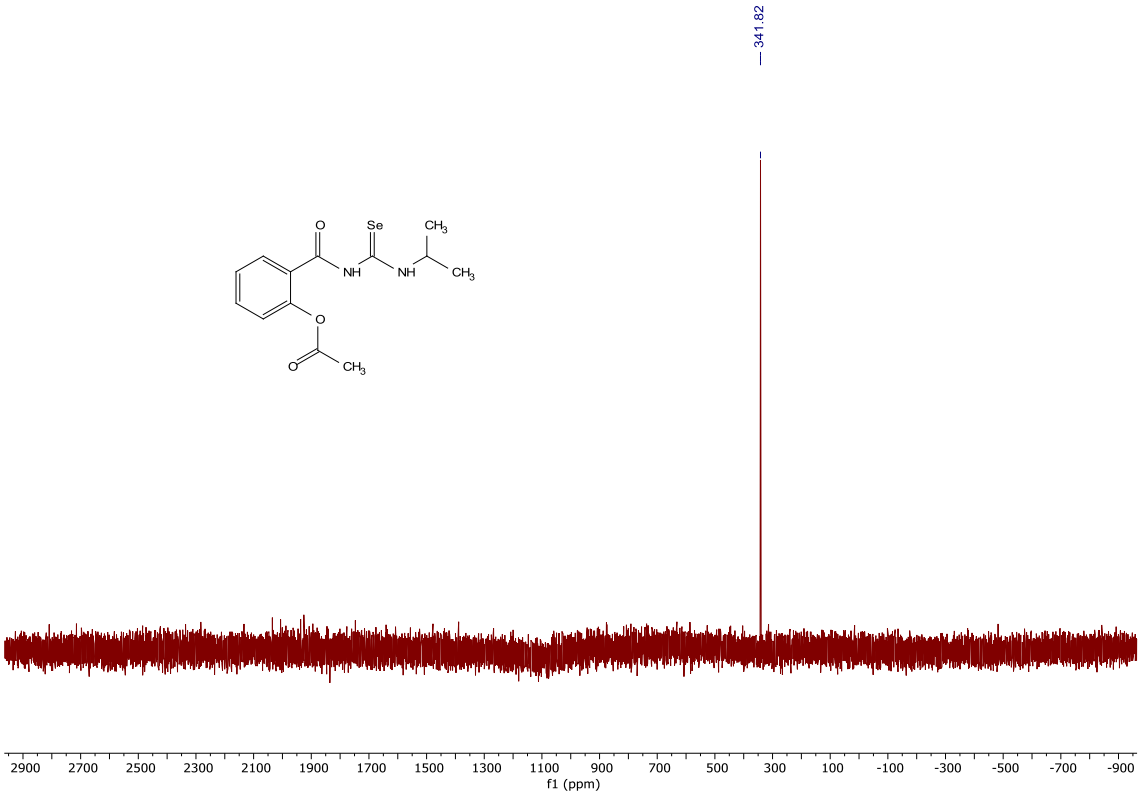


**Figure S65.** $^{77}$Se-NMR spectrum of compound **16**.

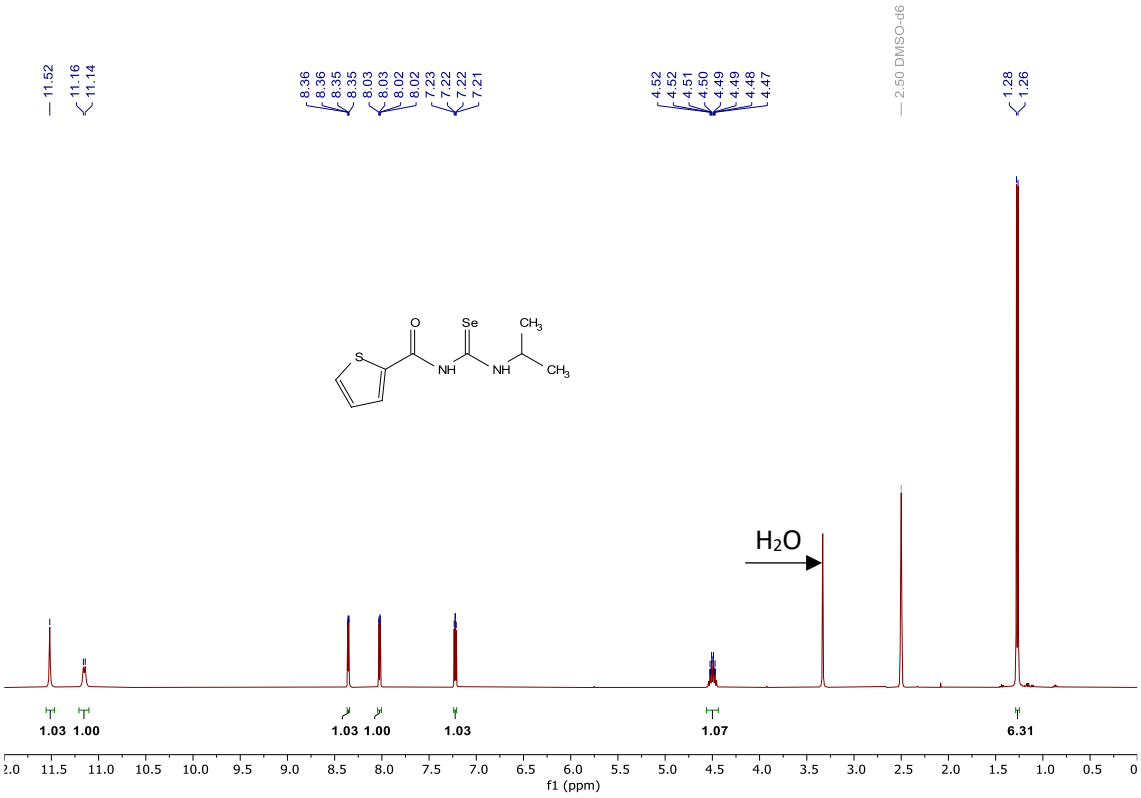


**Figure S66.** $^{1}$H-NMR spectrum of compound **17**.

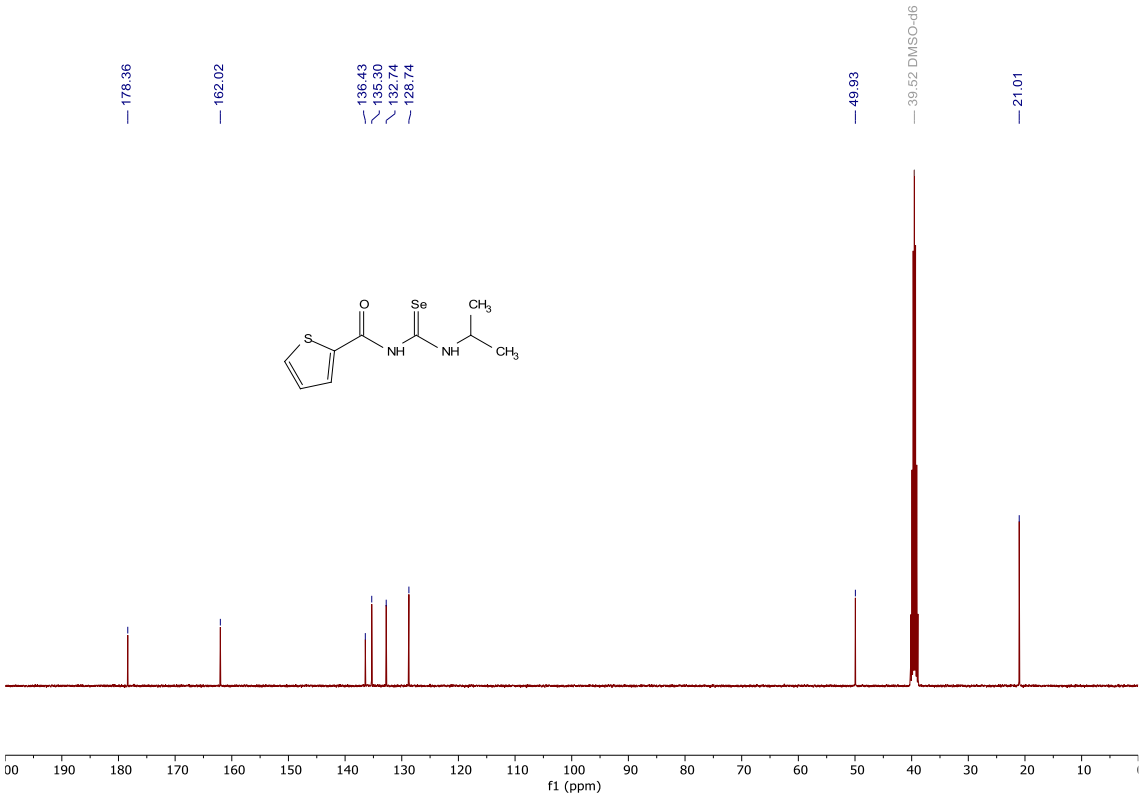


**Figure S67.** $^{13}$C-NMR spectrum of compound **17**.

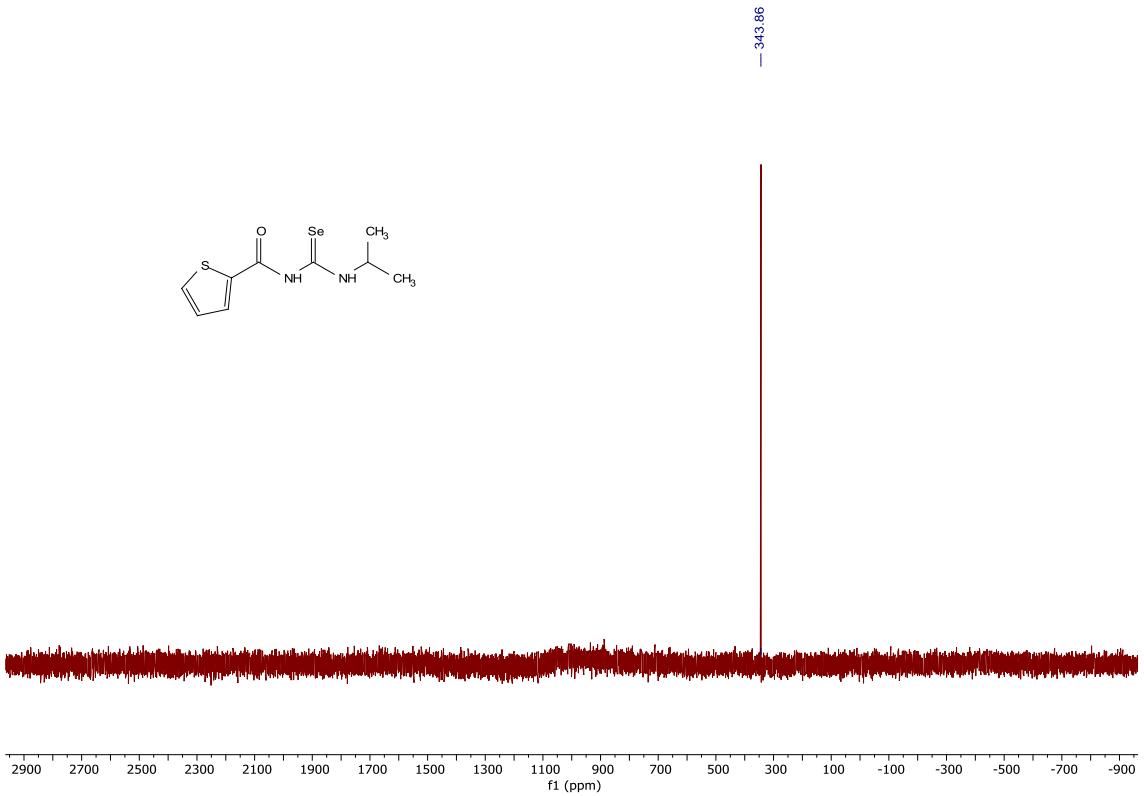


**Figure S68.** $^{77}$Se-NMR spectrum of compound **17**.

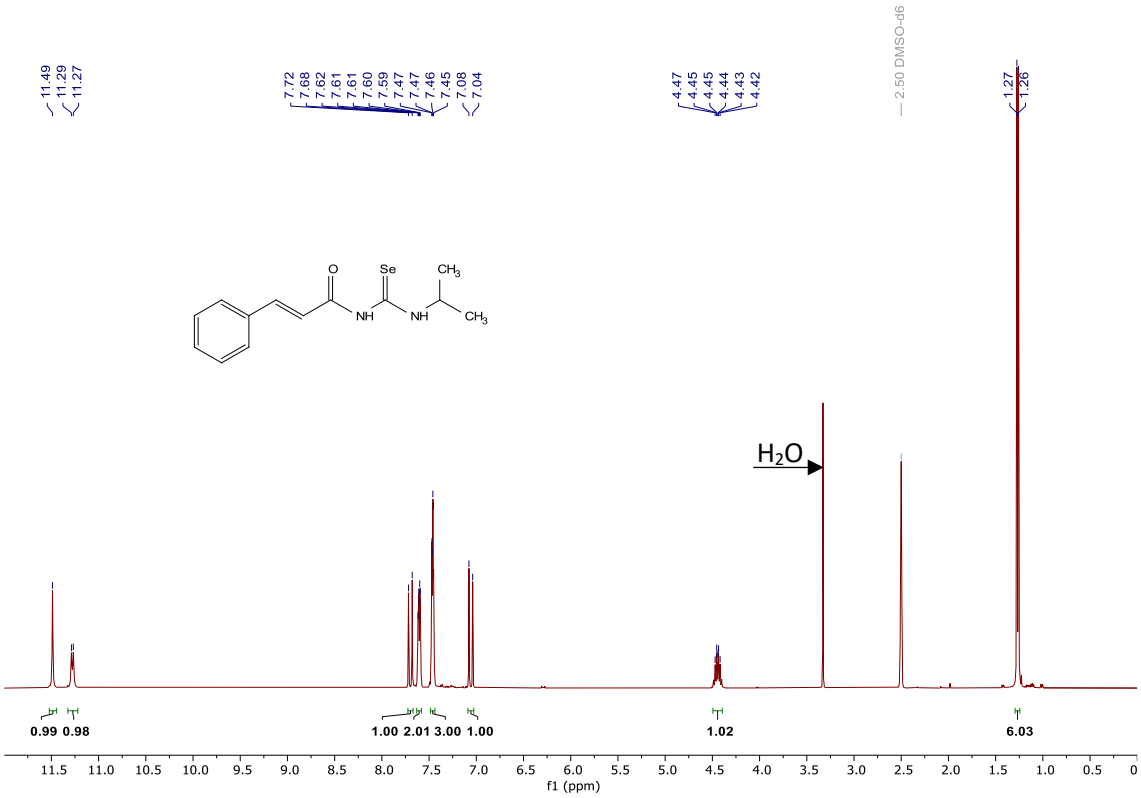


**Figure S69.** [1]H-NMR spectrum of compound **18**.

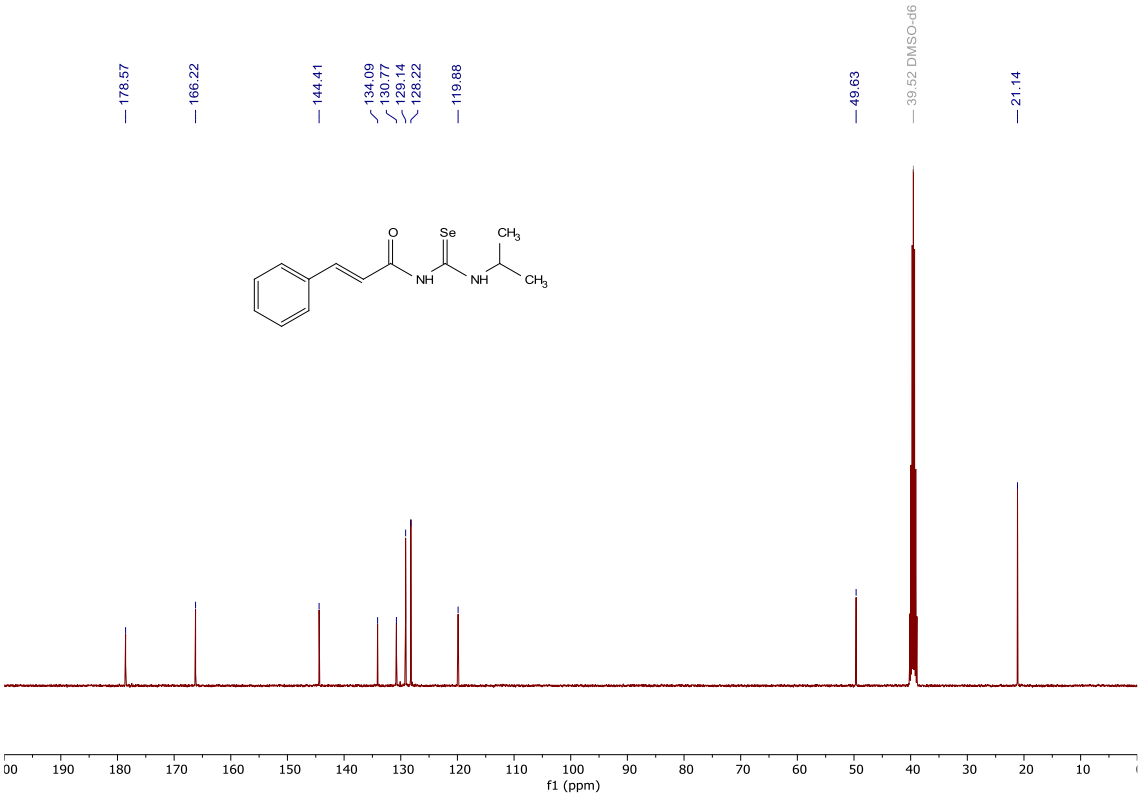


**Figure S70.** [13]C-NMR spectrum of compound **18**.

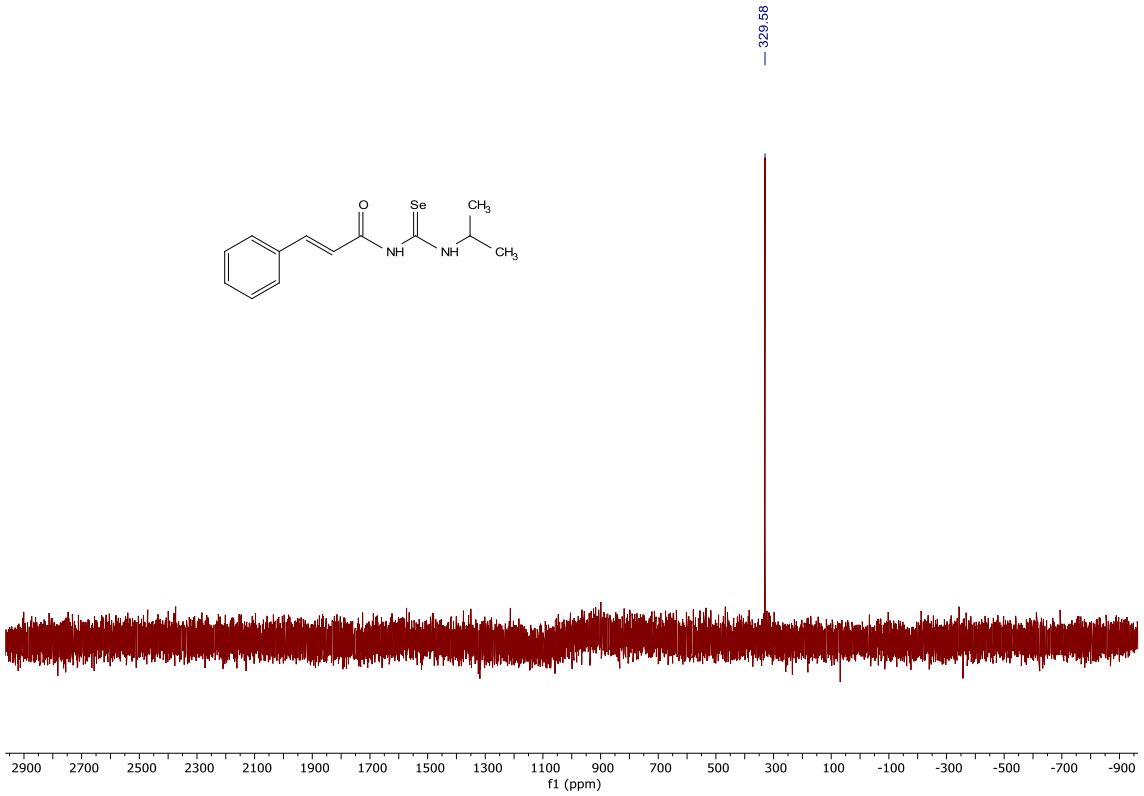


**Figure S71.** $^{77}$Se-NMR spectrum of compound **18**.

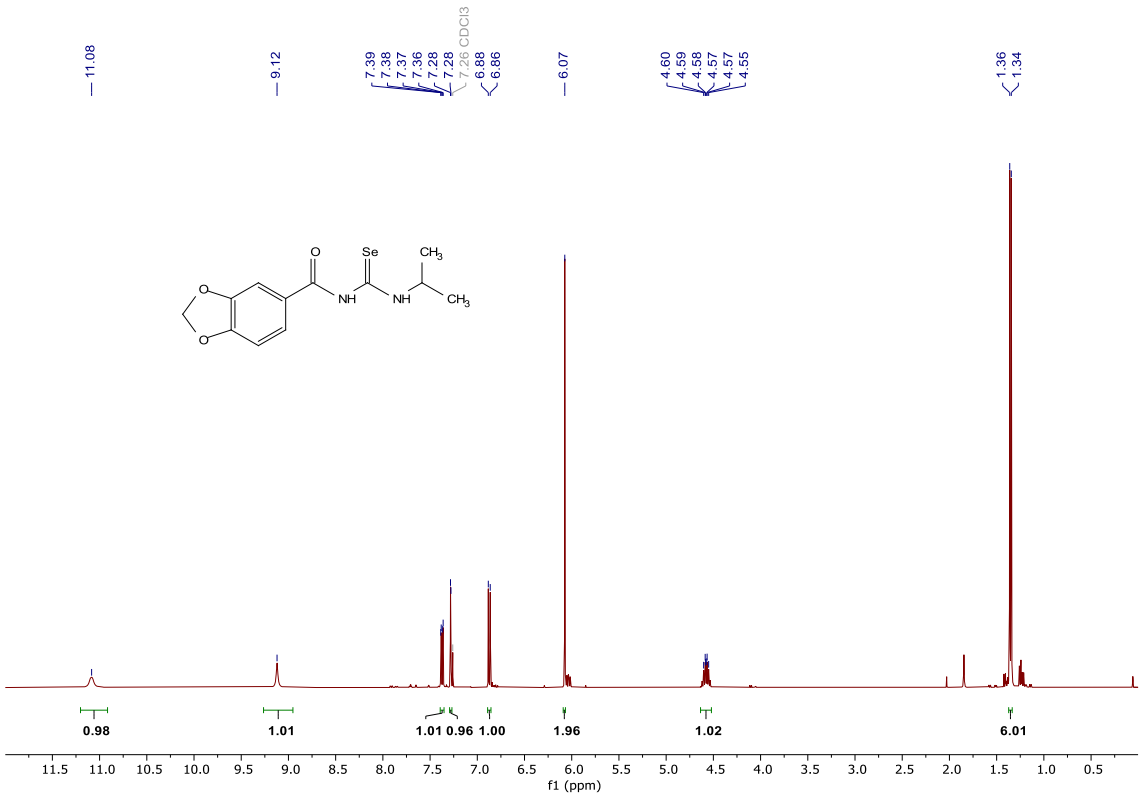


**Figure S72.** $^{1}$H-NMR spectrum of compound **19**.

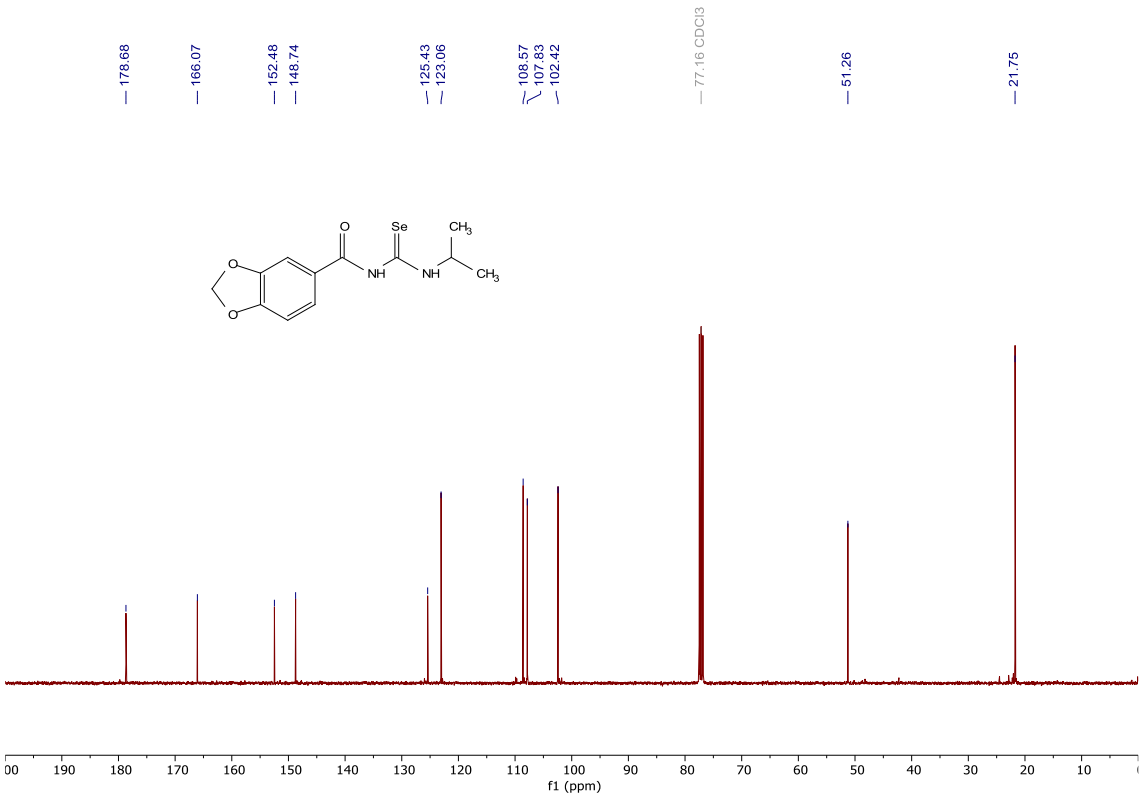


**Figure S73.** $^{13}$C-NMR spectrum of compound **19**.

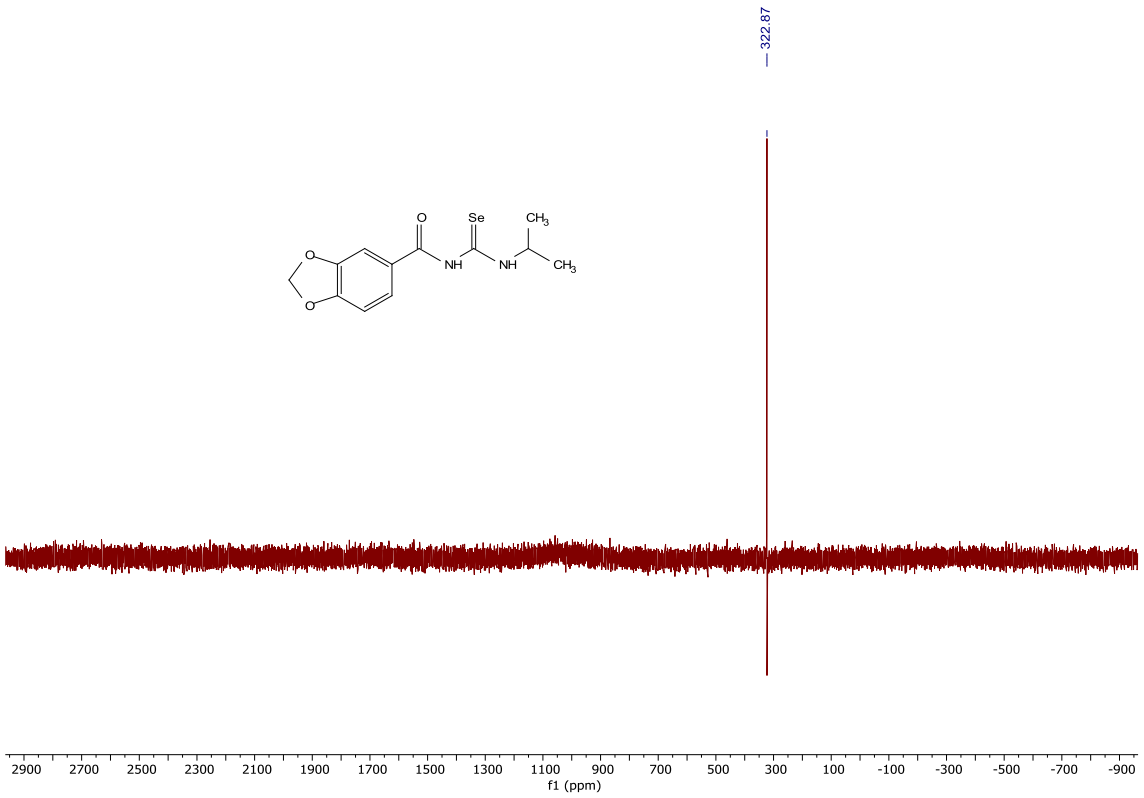


**Figure S74.** $^{77}$Se-NMR spectrum of compound **19**.

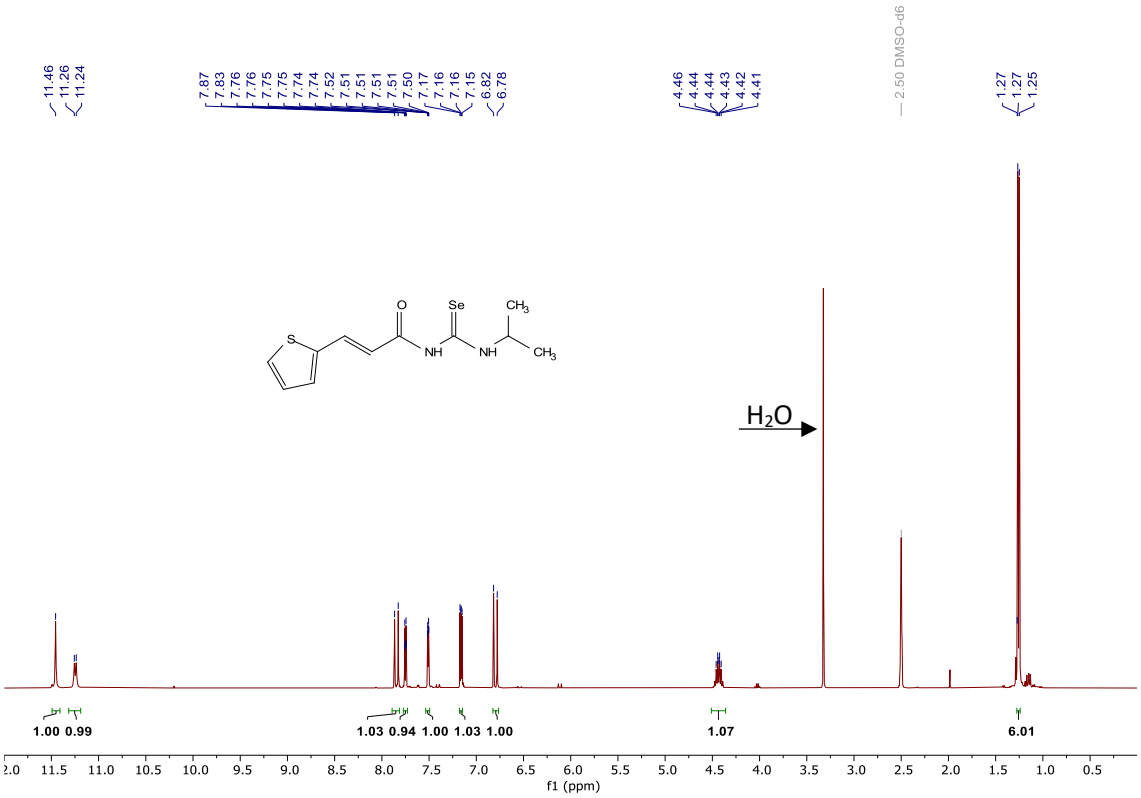


**Figure S75.** [1]H-NMR spectrum of compound **20**.

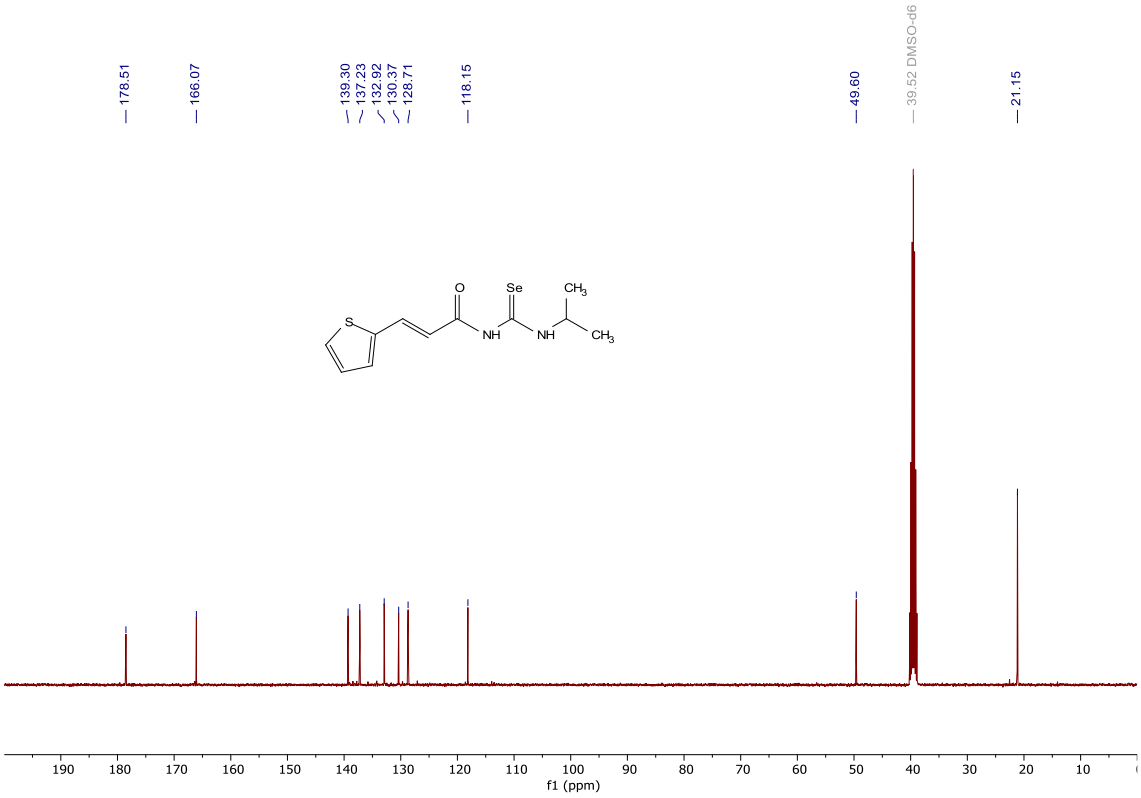


**Figure S76.** [13]C-NMR spectrum of compound **20**.

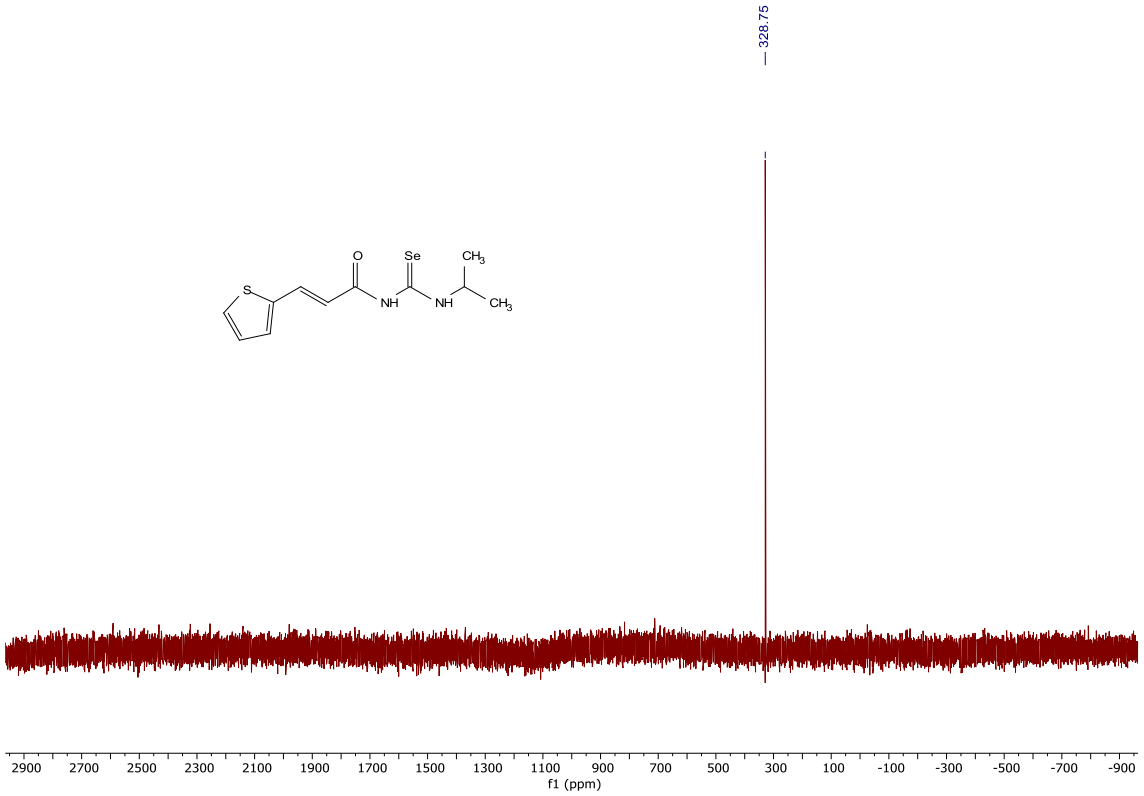


**Figure S77.** $^{77}$Se-NMR spectrum of compound **20**.

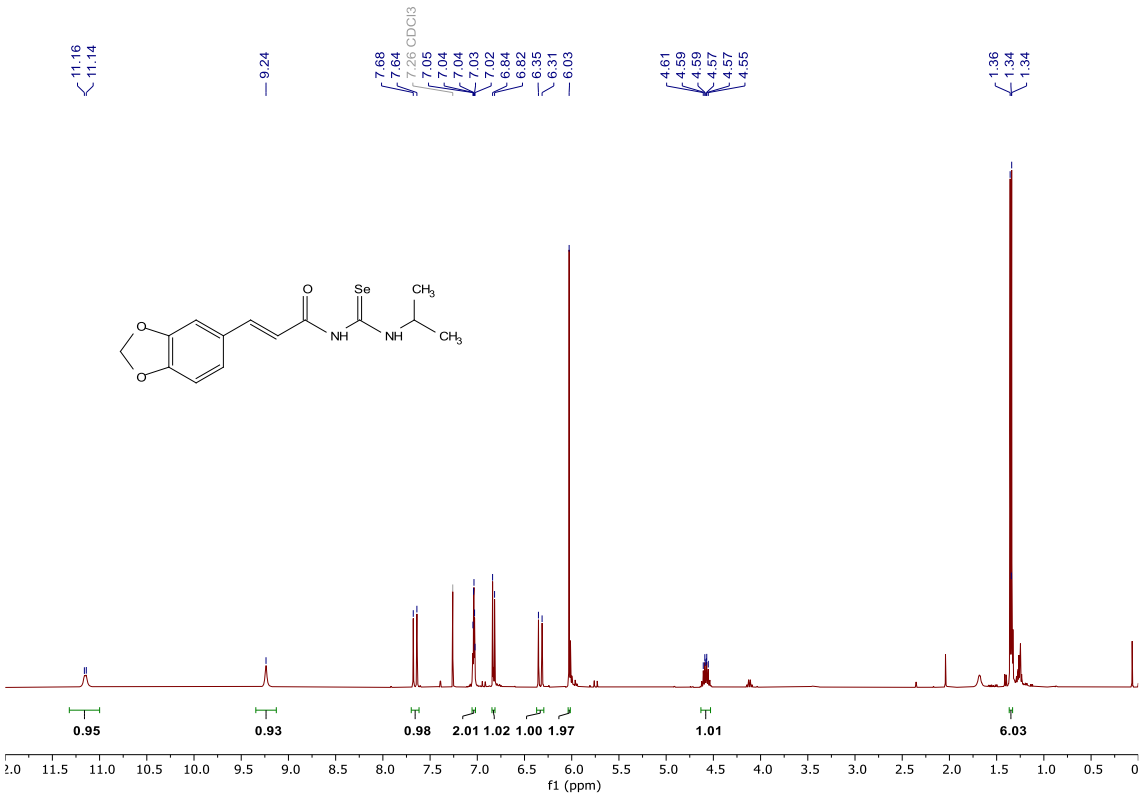


**Figure S78.** $^{1}$H-NMR spectrum of compound **21**.

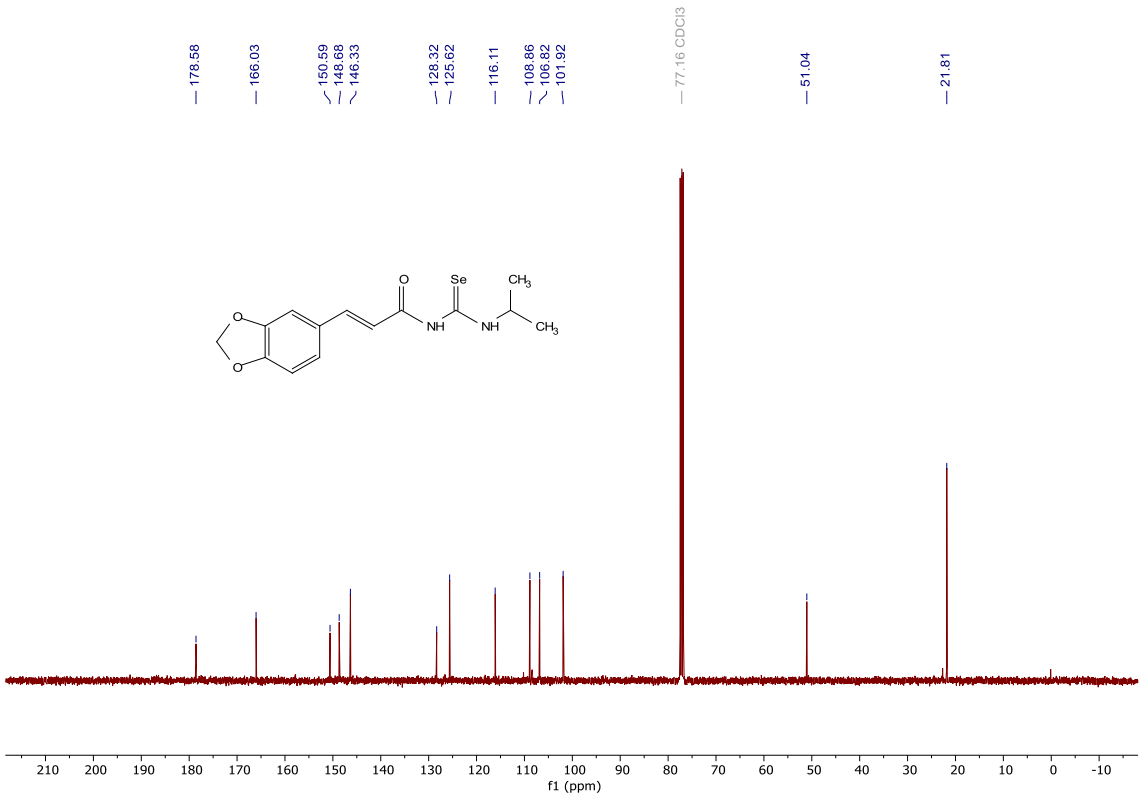


**Figure S79.** $^{13}$C-NMR spectrum of compound **21**.

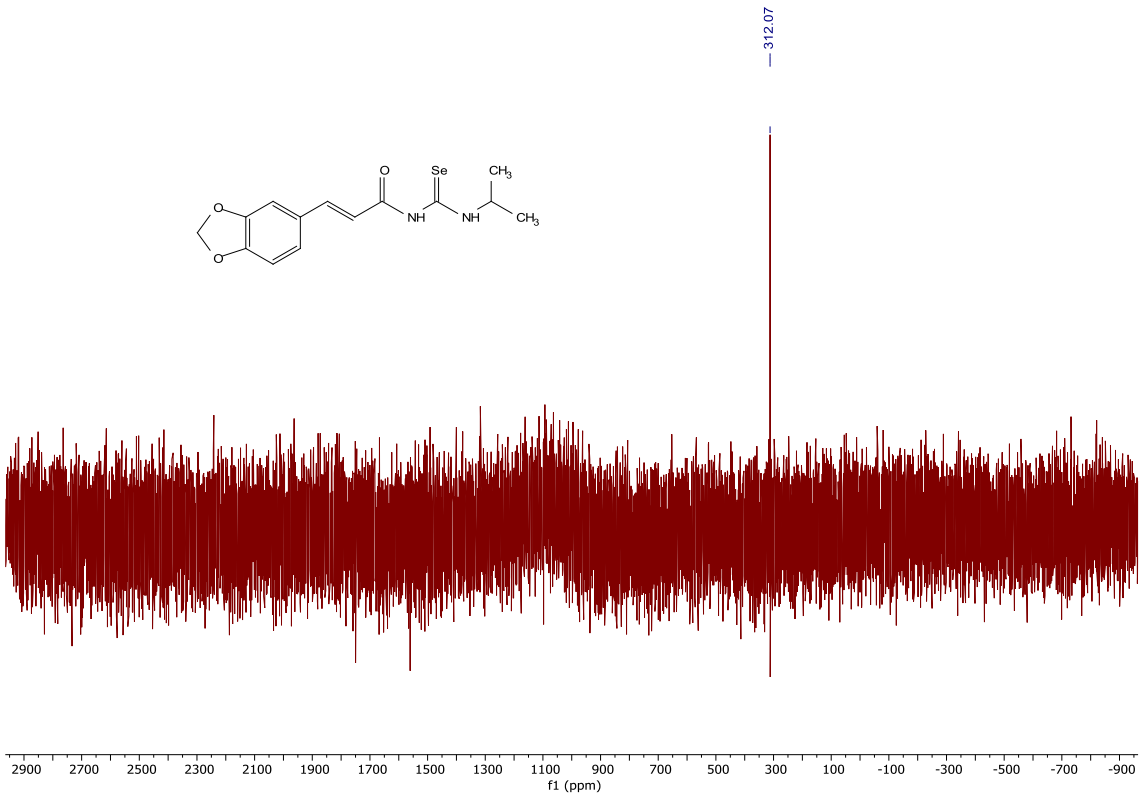


**Figure S80.** $^{77}$Se-NMR spectrum of compound **21**.

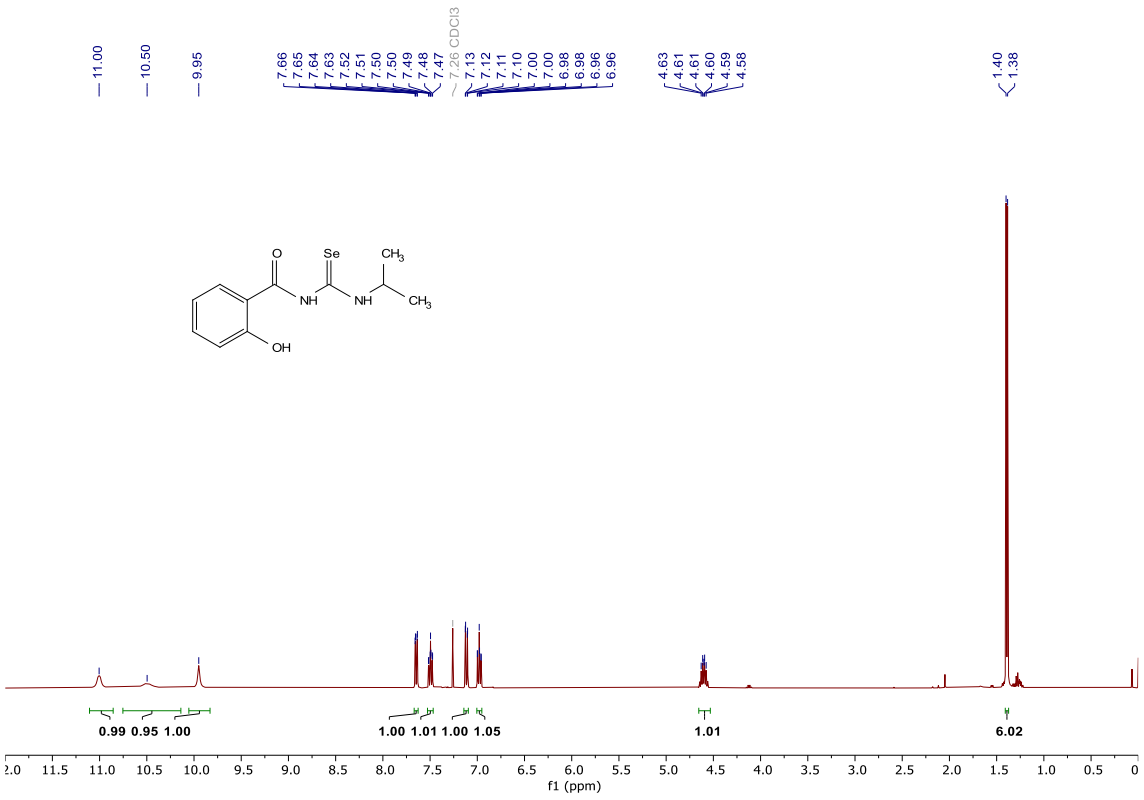


**Figure S81.** [1]H-NMR spectrum of compound **22**.

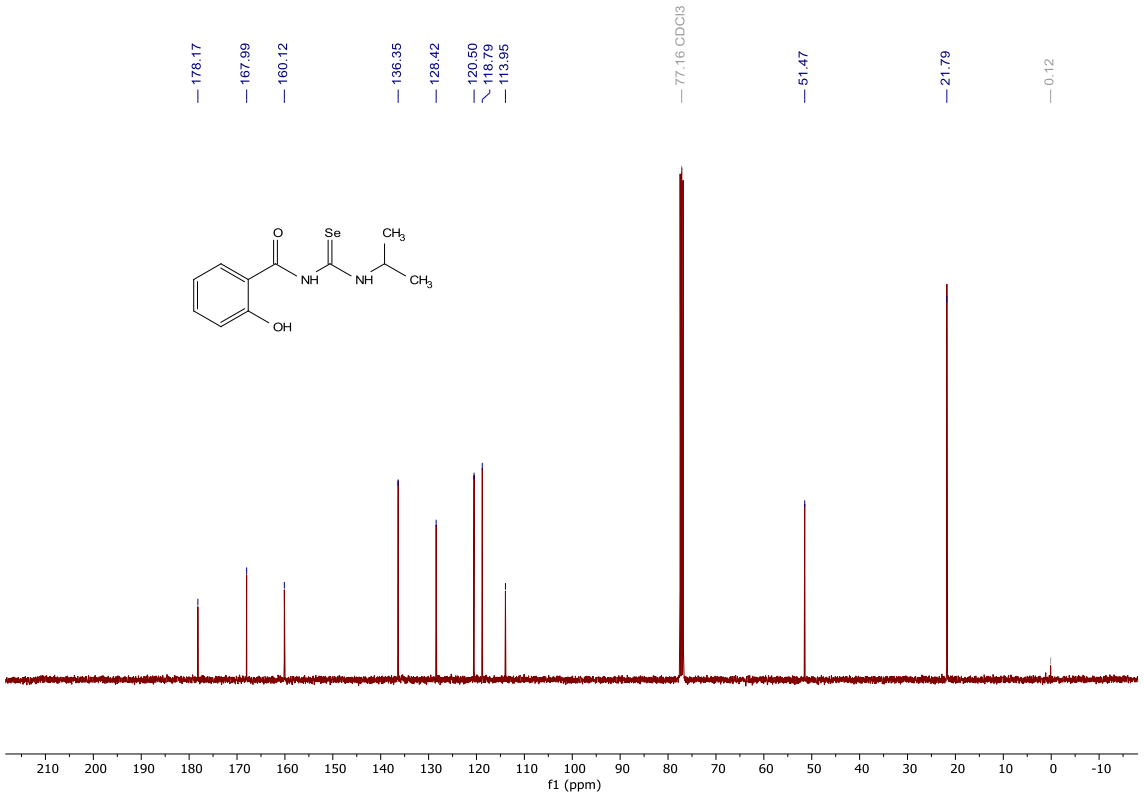


**Figure S82.** [13]C-NMR spectrum of compound **22**.

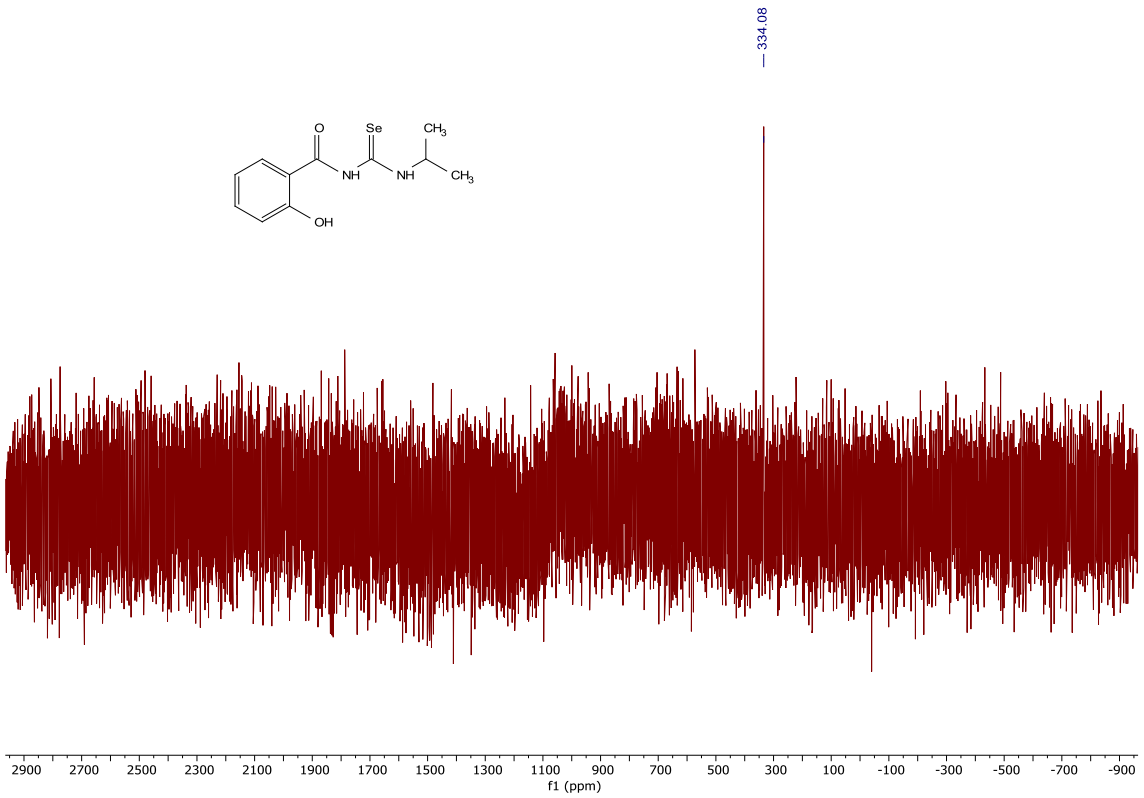


**Figure S83.** $^{77}$Se-NMR spectrum of compound **22**.

# Characterization of the compounds synthetized in this work.

**(*E*)-2-Acetoxybenzoic (*E*)-*N,N'*-dicyclohexylcarbamimidic selenoanhydride (1).** From *O*-acetylsalicyloyl chloride and *N,N´*-dicyclohexylcarbodiimide. Appearance: yellow solid. Melting point: 96-97 ºC. Yield: 21%. $^{1}$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 9.25 (d, *J* = 8.1, 1H, NH), 7.86 (dd, *J* = 7.7, 1.6, 1H, $H_{aryl}$), 7.40 (td, *J* = 7.8, 1.7, 1H, $H_{aryl}$), 7.20 (td, *J* = 7.6, 1.1, 1H, $H_{aryl}$), 7.05 (dd, *J* = 8.2, 1.2, 1H, $H_{aryl}$), 4.53 (tt, *J* = 12.2, 3.6, 1H, $H_{cyclohexyl}$), 3.97 (dtd, *J* = 10.9, 7.4, 4.0, 1H, $H_{cyclohexyl}$), 2.31 (s, 5H, $CH_3$ and $2H_{cyclohexyl}$), 1.93 – 0.79 (m, $18H_{cyclohexyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 187.33 (C=N), 171.81 ($C{=}O_{acetoxy}$), 164.21 (C=O), 148.48 ($C_{aryl}$), 131.80 ($C_{aryl}$), 128.63 ($C_{aryl}$), 127.31 ($C_{aryl}$), 126.02 ($C_{aryl}$), 121.92 ($C_{aryl}$), 62.29 ($C_{cyclohexyl}$), 57.72 ($C_{cyclohexyl}$), 29.58 ($C_{cyclohexyl}$), 26.47 ($C_{cyclohexyl}$), 25.38 ($C_{cyclohexyl}$), 25.18 ($C_{cyclohexyl}$), 24.39 ($C_{cyclohexyl}$), 21.42 ($CH_3$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 462.28. Elemental analysis for $C_{22}H_{30}N_2O_3Se$ calculated/found (percent): C, 58.79/58.83; H, 6.73/6.92; N, 6.23/6.14.

**Cinnamic (*E*)-*N,N'*-dicyclohexylcarbamimidic selenoanhydride (2).** From cinnamoyl chloride and *N,N´*-dicyclohexylcarbodiimide. Appearance: brown solid. Melting point: 156-158 ºC. Yield: 8%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 8.41 (d, *J* = 7.9, 1H, NH), 7.59 – 7.48 (m, 3H, $H_2$, $H_{aryl}$ y $H_{alkene}$ ), 7.47 – 7.36 (m, 3H, $H_{aryl}$), 6.68 (d, *J* = 15.5, 1H, $H_{alkene}$), 4.09 (ddt, *J* = 12.0, 7.3, 3.5, 1H, $H_{cyclohexyl}$), 3.64 – 3.49 (m, 1H, $H_{cyclohexyl}$), 1.86 – 1.42 (m, 12H, $H_{cyclohexyl}$), 1.33 – 0.97 (m, 8H, $H_{cyclohexyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 162.74 (C=O), 153.34 (C=N), 140.93 ($C_{alkene}$), 134.65 ($C_{aryl}$), 129.83 ($C_{aryl}$), 129.04 ($C_{aryl}$), 127.65($C_{aryl}$), 119.65 ($C_{alkene}$), 52.83 ($C_{alkene}$), 49.60 ($C_{alkene}$), 31.85 ($C_{cyclohexyl}$), 30.43 ($C_{cyclohexyl}$), 25.45 ($C_{cyclohexyl}$), 25.15 ($C_{cyclohexyl}$), 25.05

($C_{cyclohexyl}$), 24.38 ($C_{cyclohexyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): peak not found. Elemental analysis for $C_{22}H_{30}N_2OSe$ calculated/found (percent): C, 63.30/63.59; H, 7.24/7.19; N, 6.71/6.74.

**Benzoic *N,N′*-diisopropylcarbamimidic selenoanhydride (3).** From benzoyl chloride and *N,N´*-diisopropylcarbodiimide. Appearance: yellow solid. Melting point: 163-165 ºC. Yield: 58%. $^1$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 10.35 (d, *J* = 7.9, 1H, NH), 7.63 – 7.60 (m, 2H, $H_{aryl}$) , 7.46 – 7.40 (m, 1H, $H_{aryl}$), 7.39 – 7.33 (m, 2H, $H_{aryl}$), 4.87 (p, *J* = 6.8, 1H, $H_{isopropyl}$), 4.09 (dt, *J* = 8.0, 6.5, 1H, $H_{isopropyl}$), 1.43 (d, *J* = 6.9, 6H, $H_{isopropyl}$), 0.70 (d, *J* = 6.6, 6H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 185.77 (C=N), 167.97 (C=O), 137.01 ($C_{aryl}$), 130.30 ($C_{aryl}$), 127.72 ($C_{aryl}$), 127.08 (s, 2C, $C_{aryl}$), 51.33 ($C_{isopropyl}$), 50.19 ($C_{isopropyl}$), 19.93 ($C_{isopropyl}$), 19.31 ($C_{isoporpyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 474.01. Elemental analysis for $C_{14}H_{20}N_2OSe$ calculated/found (percent): C, 54.02/54.37; H, 6.48/6.23; N, 9.00/8.98.

**(*E*)-2-Acetoxybenzoic (*E*)-*N,N′*-diisopropylcarbamimidic selenoanhydride (4).** From *O*-acetylsalicyloyl chloride and *N,N´*-diisopropylcarbodiimide. Appearance: yellow solid. Melting point: 79-81 ºC. Yield: 40%. $^1$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 10.19 (d, *J* = 8.0, 1H, NH), 7.57 (d, *J* = 7.5, 1H, $H_{aryl}$), 7.44 (td, *J* = 10.0, 8.0, 2.0, 1H, $H_{aryl}$), 7.28 – 7.18 (m, 2H, $H_{aryl}$), 4.77 – 4.65 (m, 1H, $H_{isopropyl}$), 4.10 (h, *J* = 6.7, 1H, $H_{isopropyl}$), 2.24 (s, 3H, $CH_3$), 1.42 (dd, *J* = 6.8, 2.3, 6H, $H_{isopropyl}$), 0.83 (dd, *J* = 6.7, 2.3, 6H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 184.80 (C=N), 169.00 ($C{=}O_{acetoxy}$), 163.61 (C=O), 147.17 ($C_{aryl}$), 130.54 ($C_{aryl}$), 129.20 ($C_{aryl}$), 128.00 ($C_{aryl}$), 125.03 ($C_{aryl}$), 122.87 ($C_{aryl}$), 50.72 ($C_{isopropyl}$), 50.24 ($C_{isopropyl}$), 21.19 ($CH_3$), 19.74 ($C_{isopropyl}$), 19.36 ($C_{isopropyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 458.28. Elemental analysis for $C_{16}H_{22}N_2O_3Se$ calculated/found (percent): C, 52.03/51.95; H, 6.00/6.32; N, 7.58/7.48.

**(*E*)-(*E*)-*N,N′*-Diisopropylcarbamimidic 2-(thiophen-2-yl)acetic selenoanhydride (5).** From thiophene-2-acetyl chloride and *N,N´*-diisopropylcarbodiimide. Appearance: yellow solid. Melting point: 108-110 ºC. Yield: 15%. $^1$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.13 (d, *J* = 7.9, 1H, NH), 7.37 (dd, *J* = 5.1, 1.3, 1H, $H_{aryl}$), 6.94 (dd, *J* = 5.1, 3.5, 1H, $H_{aryl}$), 6.90 (dd, *J* = 3.5, 1.2, 1H, $H_{arryl}$), 4.45 (m, 2H, $H_{isopropyl}$), 3.87 (d, *J* = 0.9, 2H, $CH_2$), 1.27 (dd, *J* = 10.4, 6.7, 12H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 184.92 (C=N), 164.95 (C=O), 136.43 ($C_{aryl}$), 126.69 ($C_{aryl}$), 126.29 ($C_{aryl}$), 125.34 ($C_{aryl}$), 50.84 ($C_{isopropyl}$), 48.01 ($C_{isopropyl}$), 34.97 ($CH_2$), 19.80 ($C_{isopropyl}$), 19.70 ($C_{isopropyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 582.90. Elemental analysis for $C_{13}H_{20}N_2OSSe$ calculated/found (percent): C, 47.12/47.37; H, 6.08/6.25; N, 8.45/8.43.

**(*E*)-(*E*)-*N,N′*-Diisopropylcarbamimidic thiophene-2-carboxylic selenoanhydride (6).** From 2-thiophenecarbonyl chloride and *N,N´*-diisopropylcarbodiimide. Appearance: yellow solid. Melting point: 120-122 ºC. Yield: 46%. $^1$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 7.80 (dd, *J* = 3.9, 1.2, 1H, $H_{aryl}$), 7.72 (d, *J* = 7.1, 1H, NH), 7.48 (dd, *J* = 5.0, 1.2, 1H, $H_{aryl}$), 7.00 (dd, *J* = 5.0, 3.8, 1H, $H_{aryl}$), 5.05 (p, *J* = 6.8, 1H, $H_{isopropyl}$), 4.56 – 4.46 (m, 1H, $H_{isopropyl}$), 1.45 (d, *J* = 6.8, 6H, $H_{isopropyl}$), 1.07 (d, *J* = 6.6, 6H, $H_{isopropyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 187.72 (C=N), 162.59 (C=O), 138.53 ($C_{aryl}$), 131.76 ($C_{aryl}$), 131.59 ($C_{aryl}$), 127.61 ($C_{aryl}$), 54.22($C_{isopropyl}$), 51.02 ($C_{isopropyl}$), 20.61 ($C_{isopropyl}$), 20.42 ($C_{isopropyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 529.29. Elemental analysis for $C_{12}H_{18}N_2OSSe$ calculated/found (percent): C, 45.42/45.22; H, 5.72/5.81; N, 8.83/8.90.

**(*E*)-Benzo[*d*][1,3]dioxole-5-carboxylic (*E*)-*N,N′*-diisopropylcarbamimidic selenoanhydride (7).** From piperonylic acid and *N,N´*-diisopropylcarbodiimide. Appearance: yellow solid. Melting point: 138-140 ºC. Yield: 14%. $^1$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 10.29 (d, *J* = 8.1, 1H, NH), 7.20 (dd, *J* = 8.1, 1.7, 1H, $H_{aryl}$), 7.11 (d, *J* = 1.7, 1H, $H_{aryl}$), 6.91 (d, *J* = 8.1, 1H, $H_{aryl}$), 6.05 (s, 2H, $H_{aryl}$), 4.88 (p, *J* = 6.8, 1H, $H_{isopropyl}$), 4.26 – 4.12 (m, 1H, $H_{isopropyl}$), 1.40 (d, *J* = 6.8, 6H, $H_{isopropyl}$), 0.81 (d, *J* = 6.7, 6H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 186.07 (C=N), 167.58 (C=O), 149.13 ($C_{aryl}$), 146.65 ($C_{aryl}$), 130.82 ($C_{aryl}$), 122.10 ($C_{aryl}$), 107.91 ($C_{aryl}$), 107.50 ($C_{aryl}$), 101.53 ($CH_2$), 51.85 ($C_{isopropyl}$), 50.32 ($C_{isopropyl}$), 19.97 ($C_{isopropyl}$), 19.57 ($C_{isopropyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 462.62. Elemental analysis for $C_{15}H_{20}N_2O_3Se$ calculated/found (percent): C, 50.71/51.02; H, 5.67/5.59; N, 7.88/8.00.

***N*-(Cyclohexylcarbamoselenoyl) benzamide (8).** From benzoyl chloride and cyclohexylamine. Appearance: Yellow solid. Melting point: 71-73 ºC. Yield: 11%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.51 (s, 1H, NH), 11.43 (d, *J* = 8.0, 1H, NH), 7.93 – 7.89 (m, 2H, $H_{aryl}$), 7.67 – 7.61 (m, 1H, $H_{aryl}$), 7.51 (t, *J* = 7.8, 2H, $H_{aryl}$), 4.34 – 4.23 (m, 1H, $H_{cyclohexyl}$), 2.03 – 1.96 (m, 2H, $H_{cyclohexyl}$), 1.66 (dt, *J* = 12.8, 4.5, 2H, $H_{cyclohexyl}$), 1.60 – 1.52 (m, 1H, $H_{cyclohexyl}$), 1.50 – 1.25 (m, 5H, $H_{cyclohexyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.85 (C=Se), 168.49 (C=O), 133.11 ($C_{aryl}$), 131.94 ($C_{aryl}$), 128.65 ($C_{aryl}$), 128.39 ($C_{aryl}$), 56.10 ($C_{aryl}$), 30.63($C_{cyclohexyl}$), 24.87 ($C_{cyclohexyl}$), 23.96 ($C_{cyclohexyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 339.64. Elemental analysis for $C_{14}H_{18}N_2OSe$ calculated/found (percent): C, 54.37/54.56; H, 5.87/5.64; N, 9.06/9.13.

**2-((Cyclohexylcarbamoselenoyl)carbamoyl)phenyl acetate (9).** From *O*-acetylsalicyloyl chloride and cyclohexylamine. Appearance: brown solid. Melting point: 79-81 ºC. Yield: 10%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.52 (s, 1H, NH), 11.13 (d, *J* = 8.0, 1H, NH), 7.70 (dd, *J* = 7.7, 1.7, 1H, $H_{aryl}$), 7.63 (ddd, *J* = 8.2, 7.5, 1.7, 1H, $H_{aryl}$), 7.38 (td, *J* = 7.6, 1.1, 1H, $H_{aryl}$), 7.28 (dd, *J* = 8.1, 1.1, 1H, $H_{aryl}$), 4.25 (m, 1H, $H_{cyclohexyl}$), 2.32 (s, 3H, $CH_3$), 1.99 (s, 2H, $H_{cyclohehyl}$), 1.72 – 1.21 (m, 8H, $H_{cyclohexyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.39 (C=Se), 168.75 ($C{=}O_{acetoxy}$), 166.33 (C=O), 148.10 ($C_{aryl}$), 133.25 ($C_{aryl}$), 130.10 ($C_{aryl}$), 126.28 ($C_{aryl}$), 125.90 ($C_{aryl}$), 123.17 ($C_{aryl}$), 56.18 ($C_{cyclohexyl}$), 30.59 ($C_{cyclohexyl}$), 24.82 ($C_{cyclohexyl}$), 23.95 ($C_{ciclohexilo}$), 20.82 ($CH_3$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 343.24. Elemental analysis for $C_{16}H_{20}N_2O_3Se$ calculated/found (percent): C, 52.32/52.01; H, 5.49/5.58; N, 7.63/7.70.

***N*-(Cyclohexylcarbamoselenoyl) tiophene-2-carboxamide (10).** From 2-thiophenecarbonyl chloride and cyclohexylamine. Appearance: yellow solid. Melting point: 64-66 ºC. Yield: 12%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.57 (s, 1H, NH), 11.31 (d, *J* = 8.0, 1H, NH), 8.37 (dd, *J* = 4.0, 1.1, 1H, $H_{aryl}$), 8.04 (dd, *J* = 5.0, 1.1, 1H, $H_{aryl}$), 7.23 (dd, *J* = 5.0, 3.9, 1H, $H_{aryl}$), 4.28 (tq, *J* = 9.3, 5.4, 4.7, 1H, $H_{cyclohexyl}$), 2.00 – 1.94 (m, 2H, $H_{cyclohexyl}$), 1.64 (dt, *J* = 8.8, 4.2, 2H, $H_{cyclohexyl}$), 1.58 – 1.51 (m, 1H, $H_{cyclohexyl}$), 1.47 – 1.20 (m, 5H, $H_{cyclohexyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.41 (C=Se), 162.25 (C=O), 136.39 ($C_{aryl}$), 135.36 ($C_{aryl}$), 132.83 ($C_{aryl}$), 128.75 ($C_{aryl}$), 56.09 ($C_{cyclohexyl}$), 30.59 ($C_{cyclohexyl}$), 24.87 ($C_{cyclohexyl}$), 23.92 ($C_{cyclohexyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 327.75. Elemental analysis for $C_{12}H_{16}N_2OSSe$ calculated/found (percent): C, 45.71/45.91; H, 5.12/5.14; N, 8.88/8.73.

***N*-(Cyclohexylcarbamoselenoyl)cinnamamide (11).** From cinnamoyl chloride and cyclohexylamine. Appearance: yellow solid. Melting point: 140-142 ºC. Yield: 38%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.52 (s, 1H, NH), 11.45 (d, *J* = 8.1, 1H, NH), 7.72 (d, *J* = 15.7, 1H, $H_{alkene}$), 7.60 (m, 2H, $H_{aryl}$), 7.48 – 7.44 (m, 3H, $H_{aryl}$), 7.06 (d, *J* = 15.7, 1H, $H_{alkene}$), 4.23 (dt, *J* = 8.6, 4.3, 1H, $H_{cyclohexyl}$), 1.96 (dt, *J* = 8.7, 4.4, 2H, $H_{cyclohexyl}$), 1.67 – 1.21 (m, 8H, $H_{cyclohexyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.56 (C=Se), 166.41 (C=O), 144.52 ($C_{alkene}$), 134.10 ($C_{aryl}$), 130.77 ($C_{aryl}$), 129.13 ($C_{aryl}$), 128.23 ($C_{aryl}$), 119.82 ($C_{alkene}$), 55.67 ($C_{cyclohexyl}$), 30.67 ($C_{cyclohexyl}$), 24.85 ($C_{cyclohexyl}$), 23.80 ($C_{cyclohexyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 326.55. Elemental analysis for $C_{16}H_{20}N_2OSe$ calculated/found (percent): C, 57.31/57.28; H, 6.01/5.94; N, 8.35/8.53.

***N*-(Cyclohexylcarbamoselenoyl)benzo[d][1,3]dioxole-5-carboxamide (12).** From piperonylic acid and cyclohexylamine. Appearance: brown solid. Melting point: 117-119 ºC. Yield: 51%. $^{1}$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.19 (d, 1H, NH), 9.11 (s, 1H, NH), 7.38 (dd, *J* = 8.2, 1.9, 1H, $H_{aryl}$), 7.28 (d, *J* = 1.9, 1H, $H_{aryl}$), 6.87 (d, *J* = 8.2, 1H, $H_{aryl}$), 6.07 (s, 2H, $CH_2$), 4.37 – 4.27 (m, 1H, $H_{cyclohexyl}$), 2.14 – 2.06 (m, 2H, $H_{cyclohexyl}$), 1.76 – 1.26 (m, 8H, $H_{cyclohexyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.39, (C=Se) 166.07 (C=O), 152.47 ($C_{aryl}$), 148.74 ($C_{aryl}$) 125.45 ($C_{aryl}$), 123.06 ($C_{aryl}$), 108.58 ($C_{aryl}$), 107.83 ($C_{aryl}$), 102.42 ($CH_2$), 57.55 ($C_{cyclohexyl}$), 31.58 ($C_{cyclohexyl}$), 25.44 ($C_{cyclohexyl}$), 24.37 ($C_{cyclohexyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 317.31. Elemental analysis for $C_{15}H_{18}N_2O_3Se$ calculated/found (percent): C, 51.00/50.89; H, 5.14/5.03; N, 7.93/8.06.

**(*E*)-*N*-(Cyclohexylcarbamoselenoyl)-3-(thiophen-2-yl)acrylamide (13).** From 3-(2-thienyl)acrylic acid and cyclohexylamine. Appearance: brown solid. Melting point: 113-115 ºC.

Yield: 33%. $^{1}$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.25 (d, *J* = 8.2, 1H, NH), 9.40 (s, 1H, NH), 7.86 (d, *J* = 15.2, 1H, $H_{alkene}$), 7.44 (d, *J* = 5.3, 1H, $H_{aryl}$), 7.32 (dd, *J* = 3.8, 1.1, 1H, $H_{aryl}$), 7.07 (dd, *J* = 5.1, 3.6, 1H, $H_{aryl}$), 6.37 (d, *J* = 15.2, 1H, $H_{alkene}$), 4.33 (m, 1H, $H_{cyclohexyl}$), 2.12 – 2.05 (m, 2H, $H_{cyclohexyl}$), 1.75 – 1.23 (m, 8H, $H_{cyclohexyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.23 (C=Se), 165.77 (C=O), 139.24 ($C_{aryl}$), 138.73 ($C_{alkene}$), 132.37 ($C_{aryl}$), 129.97 ($C_{aryl}$), 128.54 ($C_{aryl}$), 116.97 ($C_{alkene}$), 57.21 ($C_{cyclohexyl}$), 31.59 ($C_{cyclohexyl}$), 25.45 ($C_{cyclohexyl}$), 24.34 ($C_{cyclohexyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 311.05. Elemental analysis for $C_{14}H_{18}N_2OSSe$ calculated/found (percent): C, 49.26/49.36; H, 5.32/5.48; N, 8.21/8.15.

**(*E*)-3-(Benzo[*d*][1,3]dioxol-5-yl)-*N*-(cyclohexylcarbamoselenoyl)acrylamide (14).** From 3,4-(methylenedioxy)cinnamic acid and cyclohexylamine. Appearance: orange solid. Melting point: 149-151 ºC. Yield: 30%. $^{1}$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.28 (d, *J* = 8.3, 1H, NH), 9.32 (s, 1H, NH), 7.66 (d, *J* = 15.4, 1H, $H_{alkene}$), 7.05 – 7.01 (m, 2H, $H_{aryl}$), 6.83 (d, *J* = 8.5, 1H, $H_{aryl}$), 6.37 (d, *J* = 15.4, 1H, $H_{alkene}$), 6.03 (s, 2H, $CH_2$), 4.33 (dt, *J* = 9.3, 4.6, 1H, $H_{cyclohexyl}$), 2.11 – 2.05 (m, 2H, $H_{cyclohexyl}$), 1.75 – 1.23 (m, 8H, $H_{cyclohexyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.19 (C=Se), 166.26 (C=O), 150.50 ($C_{aryl}$), 148.64 ($C_{aryl}$), 146.18 ($C_{alkene}$), 128.41 ($C_{aryl}$), 125.56 ($C_{aryl}$), 116.26 ($C_{alkene}$), 108.80 ($C_{aryl}$), 106.87 ($C_{aryl}$), 101.87 ($CH_2$), 57.16 ($C_{cyclohexyl}$), 31.61 ($C_{cyclohexyl}$), 25.46 ($C_{cyclohexyl}$), 24.31 ($C_{cyclohexyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 302.79. Elemental analysis for $C_{17}H_{20}N_2O_3Se$ calculated/found (percent): C, 53.83/54.02; H, 5.31/5.69; N, 7.39/7.35.

***N*-(Isopropylcarbamoselenoyl) benzamide (15).** From benzoyl chloride and isopropylamine. Appearance: brown solid. Melting point: 125-127 ºC. Yield: 10%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.46 (s, 1H, NH), 11.29 (d, *J* = 8.0, 1H, NH), 7.91 (dd, *J* = 8.4, 1.3, 2H, $H_{aryl}$), 7.64 (m, 1H, $H_{aryl}$), 7.51 (ddd, *J* = 8.1, 6.7, 1.2, 2H, $H_{aryl}$), 4.51 (dt, *J* = 8.0, 6.6, 1H, $H_{isopropyl}$), 1.29 (d, *J* = 6.6, 6H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.84 (C=Se), 168.27 (C=O), 133.09 ($C_{aryl}$), 131.97 ($C_{aryl}$), 128.62 ($C_{aryl}$), 128.41 ($C_{aryl}$), 49.93 ($C_{isopropyl}$), 21.05 ($C_{isopropyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 342.44. Elemental analysis for $C_{11}H_{14}N_2OSe$ calculated/found (percent): C, 49.08/48.94; H, 5.24/5.13; N, 10.41/10.56.

**2-((Isopropylcarbamoselenoyl)carbamoyl)phenyl acetate (16).** From *O*-acetylsalicyloyl chloride and isopropylamine. Appearance: red solid. Melting point: 75-77 ºC. Yield: 9%. $^{1}$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.00 (s, 1H, NH), 10.08 (s, 1H, NH), 8.02 (dd, *J* = 7.9, 1.7, 1H, $H_{aryl}$), 7.61 (ddd, *J* = 8.2, 7.4, 1.8, 1H, $H_{aryl}$), 7.39 (td, *J* = 7.6, 1.1, 1H, $H_{aryl}$), 7.25 (dd, *J* = 8.3, 1.1, 1H, $H_{aryl}$), 4.58 (m, 1H, $H_{isopropyl}$), 2.59 (s, 3H, $CH_3$), 1.37 (d, *J* = 6.5, 6H, $H_{isopropyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.53 (C=Se), 168.39 ($C{=}O_{acetoxi}$), 164.06 (C=O), 148.50 ($C_{aryl}$), 134.56 ($C_{aryl}$), 131.61 ($C_{aryl}$), 126.87 ($C_{aryl}$), 124.01 ($C_{aryl}$), 123.88 ($C_{aryl}$), 51.24 ($C_{isopropyl}$), 21.75 ($C_{isopropyl}$), 21.59 ($CH_3$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 341.81. Elemental analysis for $C_{13}H_{16}N_2O_3Se$ calculated/found (percent): C, 47.71/47.83; H, 4.93/5.06; N, 8.56/8.68.

***N*-(Isopropylcarbamoselenoyl)thiophene-2-carboxamide (17).** From 2-thiophenecarbonyl chloride and isopropylamine. Appearance: brown solid. Melting point: 120-122 ºC. Yield: 16%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.52 (s, 1H, NH), 11.15 (d, *J* = 7.9, 1H, NH), 8.35 (dd, *J* = 3.9, 1.1, 1H, $H_{aryl}$), 8.02 (dd, *J* = 5.0, 1.1, 1H, $H_{aryl}$), 7.22 (dd, *J* = 5.0, 3.9, 1H, $H_{aryl}$), 4.78 – 4.22 (m, 1H, $H_{isopropyl}$), 1.27 (d, *J* = 6.5, 6H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.37 (C=Se), 162.03 (C=O), 136.44 ($C_{aryl}$), 135.31 ($C_{aryl}$), 132.75 ($C_{aryl}$), 128.75 ($C_{aryl}$), 49.94 (s, 1C, $C_{isopropyl}$), 21.01 (s, 2C, $C_{isopropyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 343.84. Elemental analysis for $C_9H_{12}N_2OSSe$ calculated/found (percent): C, 39.27/39.33; H, 4.39/4.56; N, 10.18/10.09.

***N*-(Isopropylcarbamoselenoyl)cinnamamide (18).** From cinnamoyl chloride and isopropylamine. Appearance: yellow solid. Melting point: 147-149 ºC. Yield: 38%. $^{1}$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.49 (s, 1H, NH), 11.28 (d, *J* = 7.9, 1H, NH), 7.70 (d, *J* = 15.7, 1H, $H_{alkene}$), 7.60 (dd, *J* = 6.8, 2.9, 2H, $H_{aryl}$), 7.46 (dd, *J* = 4.8, 1.9, 3H, $H_{aryl}$), 7.06 (d, *J* = 15.8, 1H, $H_{alkene}$), 4.44 (dt, *J* = 8.0, 6.6, 1H, $H_{isopropylamine}$), 1.27 (d, *J* = 6.5, 6H, $H_{isopropylamine}$). $^{13}$C-NMR in DMSO-$d_6$ (100

MHz) δ (ppm): 178.58 (C=Se), 166.23 (C=O), 144.42 ($C_{alkene}$), 134.10 ($C_{alkene}$), 130.78 ($C_{aryl}$), 129.15 ($C_{aryl}$), 128.23 ($C_{aryl}$), 119.89 ($C_{alkene}$), 49.63 ($C_{isopropyl}$), 21.14 ($C_{isopropyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 329.91. Elemental analysis for $C_{13}H_{16}N_2OSe$ calculated/found (percent): C, 52.88/52.73; H, 5.46/5.51; N, 9.49/9.37.

***N*-(Isopropylcarbamoselenoyl)benzo[*d*][1,3]dioxole-5-carboxamide (19).** From piperonylic acid and isopropylamine. Appearance: brown solid. Melting point: 128-130 ºC. Yield: 22%. $^1$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.08 (s, 1H, NH), 9.12 (s, 1H, NH), 7.37 (dd, *J* = 8.2, 1.9, 1H, $H_{aryl}$), 7.28 (d, *J* = 1.9, 1H, $H_{aryl}$), 6.87 (d, *J* = 8.2, 1H, $H_{aryl}$), 6.07 (s, 2H, $CH_2$), 4.58 (dt, *J* = 8.2, 6.6, 1H, $H_{isopropyl}$), 1.35 (d, *J* = 6.6, 6H, $H_{isopropyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.69 (C=Se), 166.08 (C=O), 152.48 ($C_{aryl}$), 148.74 ($C_{aryl}$), 125.43 ($C_{aryl}$), 123.06 ($C_{aryl}$), 108.58 ($C_{aryl}$), 107.83 ($C_{aryl}$), 102.42 ($CH_2$), 51.26 ($C_{isopropyl}$), 21.74 ($C_{isopropyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 322.77. Elemental analysis for $C_{12}H_{14}N_2O_3Se$ calculated/found (percent): C, 46.02/45.90; H, 4.51/4.58; N, 8.94/9.10.

**(E)-*N*-(Isopropylcarbamoselenoyl)-3-(thiophen-2-yl)acrylamide (20).** From 3-(2-thienyl)acrylic acid and isopropylamine. Appearance: yellow solid. Melting point: 148-149 ºC. Yield: 15%. $^1$H-NMR in DMSO-$d_6$ (400 MHz) δ (ppm): 11.46 (s, 1H, NH), 11.25 (d, *J* = 8.0, 1H, NH), 7.85 (d, *J* = 15.5, 1H, $H_{alkene}$), 7.75 (d, *J* = 5.1, 1H, $H_{aryl}$), 7.51 (d, *J* = 3.51, 1H, $H_{aryl}$), 7.16 (dd, *J* = 5.0, 3.6, 1H, $H_{aryl}$), 6.80 (d, *J* = 15.4, 1H, $H_{alkene}$), 4.43 (dt, *J* = 8.0, 6.6, 1H, $H_{isopropyl}$), 1.26 (d, *J* = 6.6, 6H, $H_{isopropyl}$). $^{13}$C-NMR in DMSO-$d_6$ (100 MHz) δ (ppm): 178.52 (C=Se), 166.08 (C=O), 139.31 ($C_{aryl}$), 137.24 ($C_{alkene}$), 132.93 ($C_{alkene}$), 130.37 ($C_{aryl}$), 128.72 ($C_{aryl}$), 118.16 ($C_{alkene}$), 49.60 ($C_{isopropyl}$), 21.15 ($C_{isopropyl}$). $^{77}$Se-NMR in DMSO-$d_6$ (76 MHz) δ (ppm): 329.07. Elemental analysis for $C_{11}H_{14}N_2OSSe$ calculated/found (percent): C, 43.85/43.80; H, 4.68/4.44; N, 9.30/9.62.

**(*E*)-3-(Benzo[*d*][1,3]dioxol-5-yl)-*N*-(isopropylcarbamoselenoyl)acrylamide (21).** From 3,4-(methylenedioxy)cinnamic acid and isopropylamine. Appearance: orange solid. Melting point: 172-174 ºC. Yield: 10%. $^1$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.15 (d, *J* = 8.0, 1H, NH), 9.24 (s, 1H, NH), 7.66 (d, *J* = 15.4, 1H, $H_{alkene}$), 7.07 – 7.00 (m, 2H, $H_{aryl}$), 6.83 (d, *J* = 8.4, 1H, $H_{aryl}$), 6.33 (d, *J* = 15.4, 1H, $H_{alkene}$), 6.03 (s, 2H, $CH_2$), 4.83 – 4.37 (m, 1H, $H_{isopropyl}$), 1.35 (d, *J* = 6.6, 6H, $H_{isopropyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.59 (C=Se), 166.04 (C=O), 150.59 ($C_{aryl}$), 148.69 ($C_{aryl}$), 146.34 ($C_{alkene}$), 128.33 ($C_{aryl}$), 125.62 ($C_{aryl}$), 116.11 ($C_{alkene}$), 108.86 ($C_{aryl}$), 106.83 ($C_{aryl}$), 101.92 ($CH_2$), 51.03 ($C_{isopropyl}$), 21.81 ($C_{isopropyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 312.38. Elemental analysis for $C_{14}H_{16}N_2O_3Se$ calculated/found (percent): C, 49.56/49.67; H, 4.75/4.59; N, 8.26/8.48.

**2-Hydroxy-*N*-(isopropylcarbamoselenoyl)benzamide (22).** From *O*-acetylsalicyloyl chloride and isopropylamine. Appearance: yellow solid. Melting point: 162-164 º C. Yield: 9%. $^1$H-NMR in $CDCl_3$ (400 MHz) δ (ppm): 11.00 (s, 1H, OH), 10.50 (s, 1H, NH), 9.95 (s, 1H, NH), 7.65 (dd, *J* = 8.1, 1.6, 1H, $H_{aryl}$), 7.50 (ddd, *J* = 8.7, 7.2, 1.6, 1H, $H_{aryl}$), 7.12 (dd, *J* = 8.5, 1.1, 1H, $H_{aryl}$), 6.98 (ddd, *J* = 7.6, 7.0, 1.1, 1H, $H_{aryl}$), 4.60 (dt, *J* = 8.2, 6.6, 1H, $H_{isopropyl}$), 1.39 (d, *J* = 6.5, 6H, $H_{isopropyl}$). $^{13}$C-NMR in $CDCl_3$ (100 MHz) δ (ppm): 178.17 (C=Se), 167.99 (C=O), 160.12 ($C_{aryl}$), 136.35 ($C_{aryl}$), 128.42 ($C_{aryl}$), 120.50 ($C_{aryl}$), 118.79 ($C_{aryl}$), 113.95 ($C_{aryl}$), 51.47 ($C_{isopropyl}$), 21.79 ($C_{isopropyl}$). $^{77}$Se-NMR in $CDCl_3$ (76 MHz) δ (ppm): 334.36. Elemental analysis for $C_{11}H_{14}N_2O_2Se$ calculated/found (percent): C, 46.32/46.56; H, 4.95/4.88; N, 9.82/9.71.