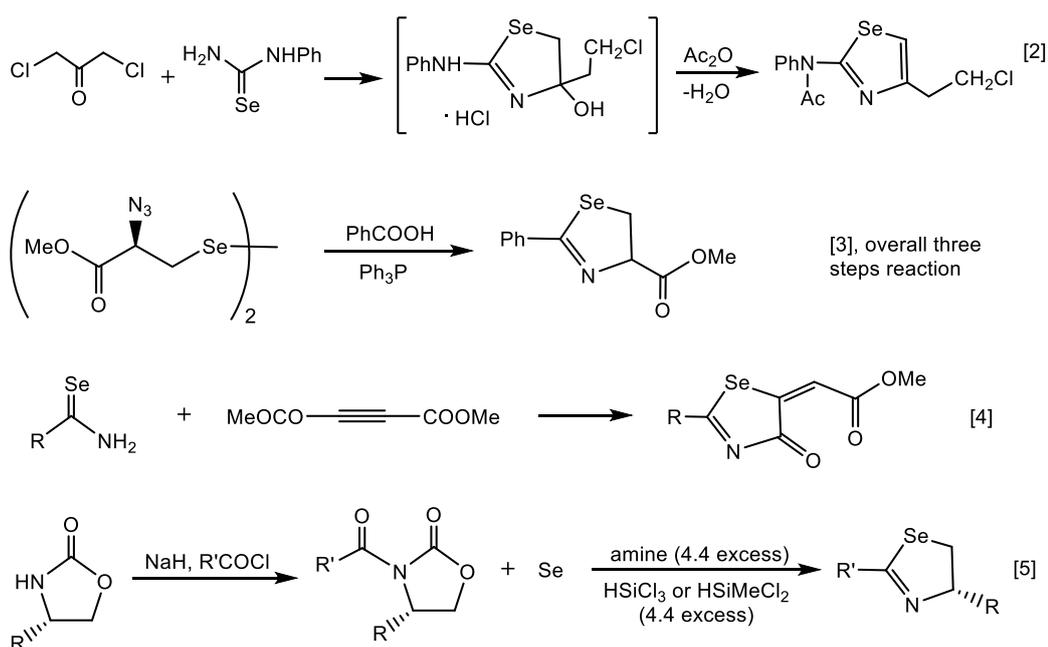


**One-pot assembling of selenazolines from elemental selenium, alkenes and acetonitrile**

Evgeny O. Kurkutov and Bagrat A. Shainyan

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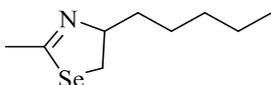


**Scheme S1.** Literature approaches to 1,3-selenazolines (references see in the main text).

### Spectral characteristic of compounds 2a–c

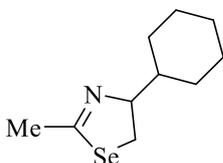
$^1\text{H}$  (400.1 MHz),  $^{13}\text{C}$  (100.6 MHz), and  $^{77}\text{Se}$  (76.2 MHz) NMR spectra were recorded on a Bruker DPX-400 spectrometer, in 5–10% solution in  $\text{CDCl}_3$ .  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts ( $\delta$ ) are reported in parts per million (ppm), relative to the residual solvent peak of  $\text{CDCl}_3$  ( $\delta = 7.27$  ( $^1\text{H}$ ) and 77.00 ( $^{13}\text{C}$ ) ppm, respectively).  $^{77}\text{Se}$  NMR spectra were registered as  $\{^{77}\text{Se}-^1\text{H}\}$  2D NMR spectra, the chemical shifts ( $\delta$ ) are given relative to  $\text{Me}_2\text{Se}$ . High-resolution mass spectra (HRMS) were measured at 70 eV on an Agilent 1200 HPLC chromatograph with Agilent 6210 mass spectrometer (HR-TOF-MS, ESI + ionization in acetonitrile with 0.1% HFBA).

2-Methyl-4-pentyl-4,5-dihydro-1,3-selenazole **2a**.



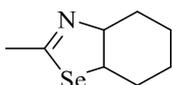
Brown oil. 42% yield (selenium conversion 62%),  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  0.88-0.92 (m, 3H), 1.32-1.38 (m, 4H), 1.51-1.53 (m, 1H), 1.78-1.87 (m, 1H), 2.30 (s, 3H), 3.15 (t,  $J = 9.3$  Hz, 1H), 3.54 (d.d,  $J = 10.1$ ,  $J = 7.5$  Hz, 1H), 4.27-4.31 (m, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  14.12, 22.65, 24.06, 26.80, 31.93, 34.94, 36.22, 79.89, 162.14.  $^{77}\text{Se}$  NMR ( $\text{CDCl}_3$ )  $\delta$  479.67 HRMS (APPI+)  $m/z$ : calculated for  $\text{C}_9\text{H}_{17}\text{NSe}$   $[\text{M}+\text{H}]^+$ : 220.0599; found: 220.0608.

4-Cyclohexyl-2-methyl-4,5-dihydro-1,3-selenazole **2b**.



Brown oil. 46% yield (selenium conversion 62%),  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.13-1.30 (m, 5H), 1.67-1.75 (m, 5H), 1.95-1.99 (m, 1H), 2.30 (s, 3H), 3.25 (t, 1H,  $J = 10.1$  Hz), 3.44 (d.d  $J = 10.1$ ,  $J = 7.8$  Hz, 1H), 4.05-4.11 (m, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ) 24.08, 26.32, 26.39, 26.55, 29.73, 30.84, 33.74, 42.82, 85.38, 161.68.  $^{77}\text{Se}$  NMR ( $\text{CDCl}_3$ )  $\delta$  490.64. HRMS (APPI+)  $m/z$ : calculated for  $\text{C}_{10}\text{H}_{17}\text{NSe}$   $[\text{M}+\text{H}]^+$ : 232.0599; found: 232.0605.

2-Methyl-3a,4,5,6,7,7a-hexahydro-1,3-benzoselenazole **2c**.



Brown oil.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.25-1.92 (m, 8H), 2.33 (s, 3H), 3.29-3.7 (m, 1H), 3.71-3.78 (m, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ) 25.21, 25.24, 26.70, 30.40, 32.18, 58.53, 83.21, 166.37.  $^{77}\text{Se}$  NMR ( $\text{CDCl}_3$ )  $\delta$  558.03. HRMS (APPI+)  $m/z$ : calculated for  $\text{C}_8\text{H}_{13}\text{NSe}$   $[\text{M}+\text{H}]^+$ : 204.0286; found: 204.0293.

Copies of  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of all new compounds

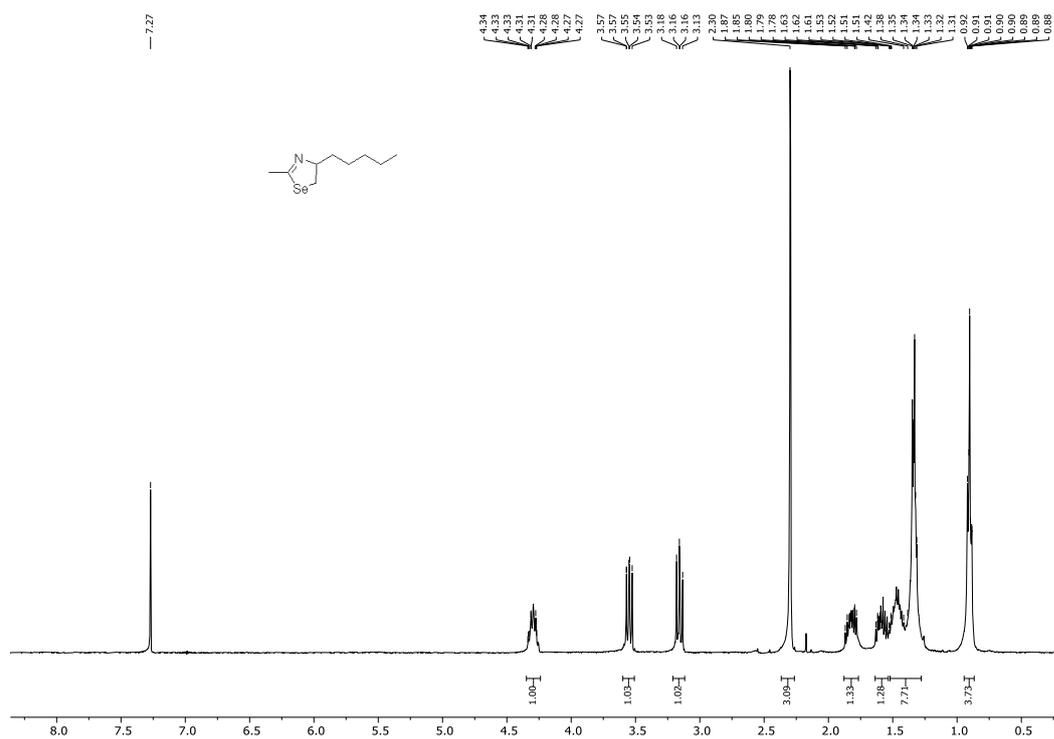


Figure S1.  $^1\text{H}$  NMR spectrum of compound **2a**

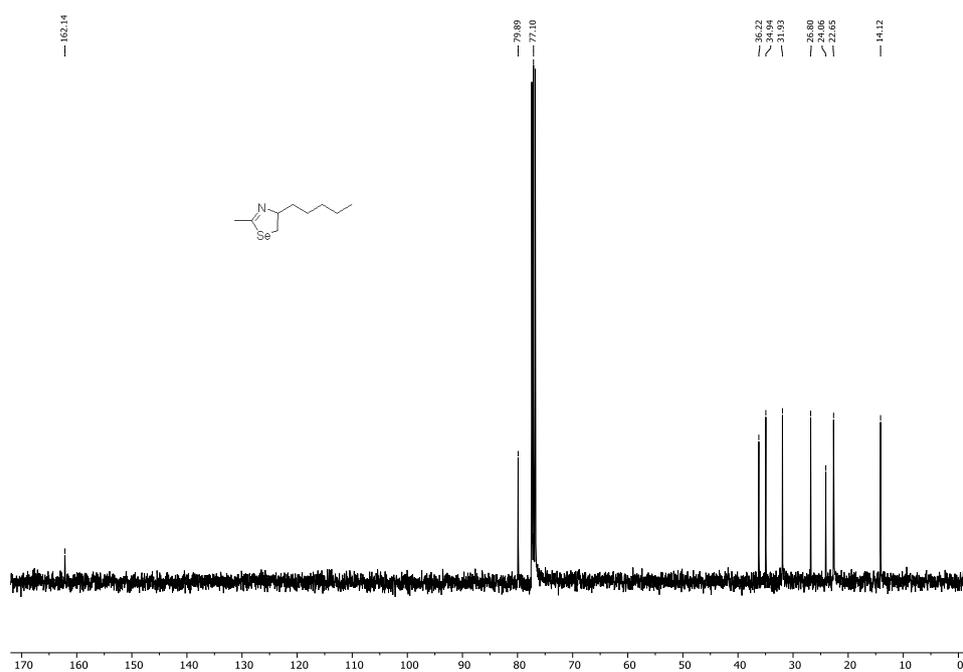


Figure S2.  $^{13}\text{C}$  NMR spectrum of compound **2a**



Figure S3.  $\{^{77}\text{Se}-^1\text{H}\}$  2D NMR spectrum of compound **2a**

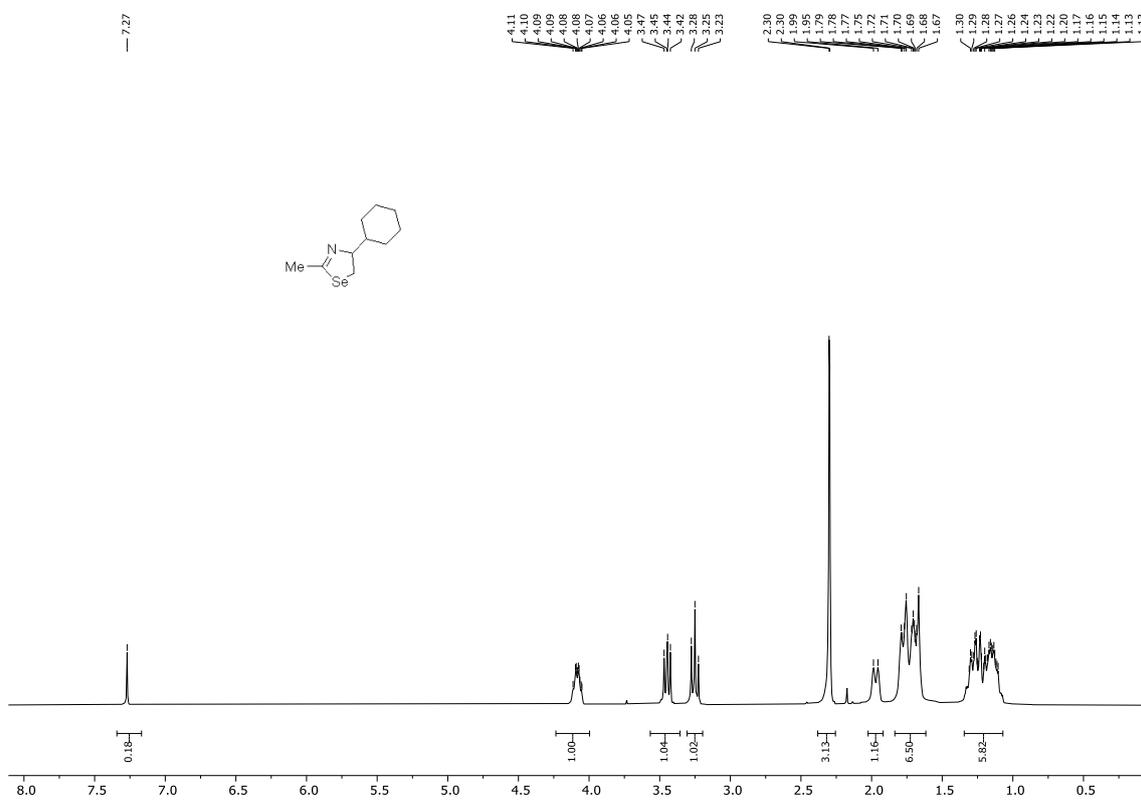


Figure S4.  $^1\text{H}$  NMR spectrum of compound **2b**

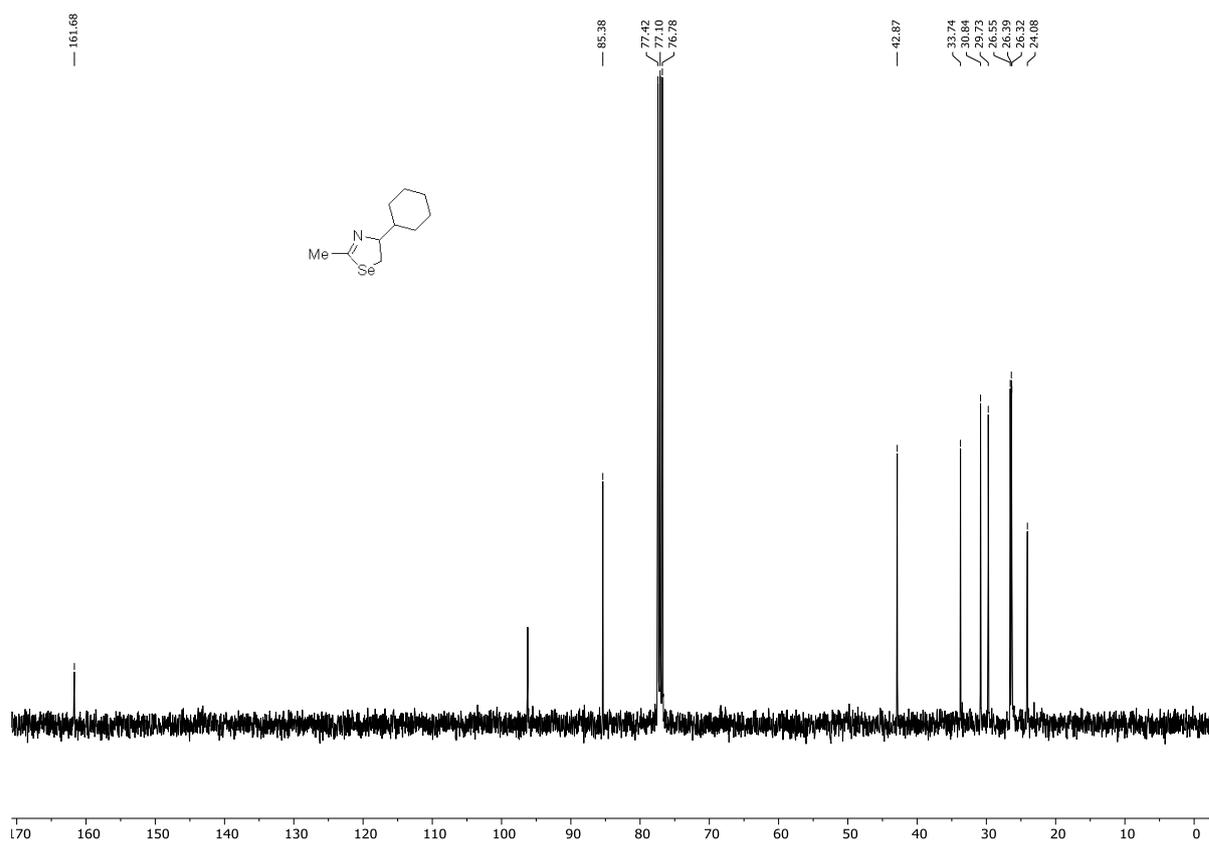


Figure S5.  $^{13}\text{C}$  NMR spectrum of compound **2b**

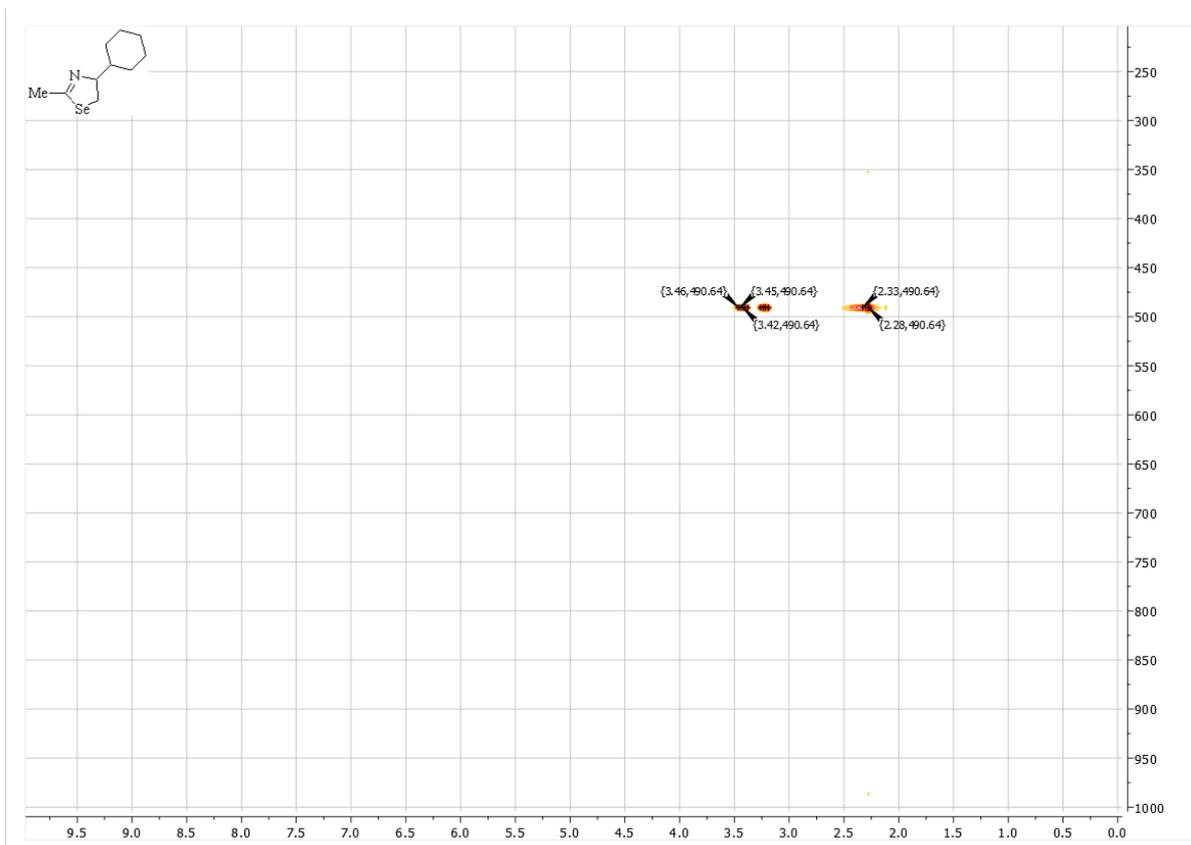


Figure S6.  $\{^{77}\text{Se}-^1\text{H}\}$  2D NMR spectrum of compound **2b**

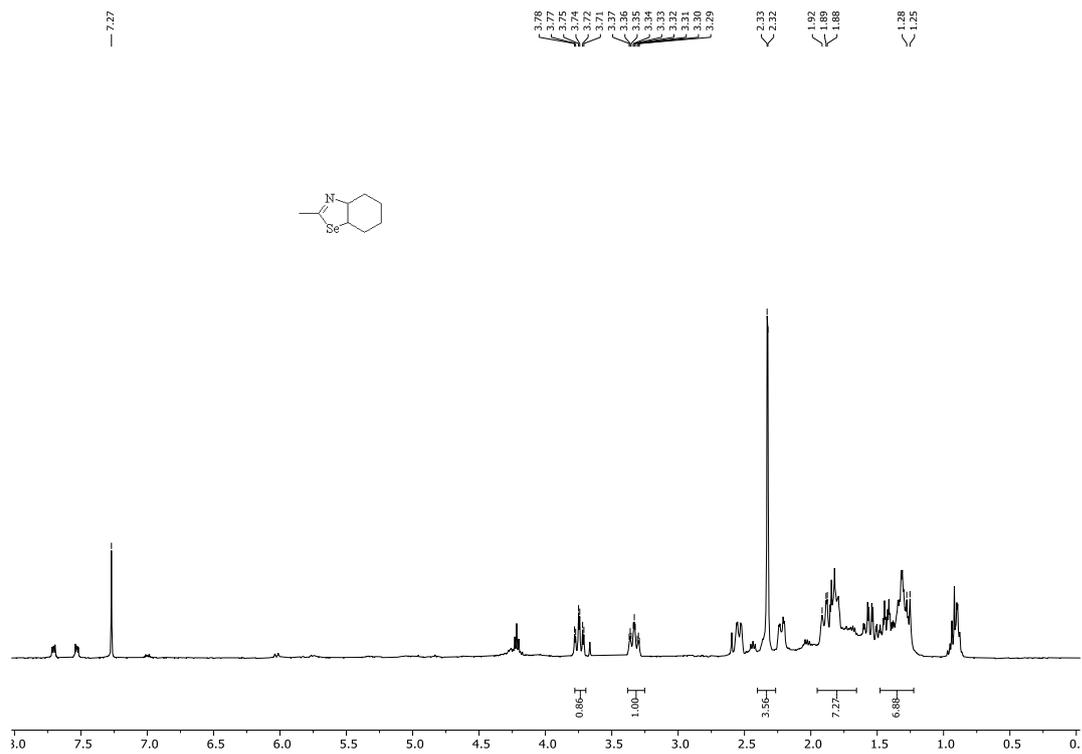


Figure S7.  $^1\text{H}$  NMR spectrum of compound **2c**

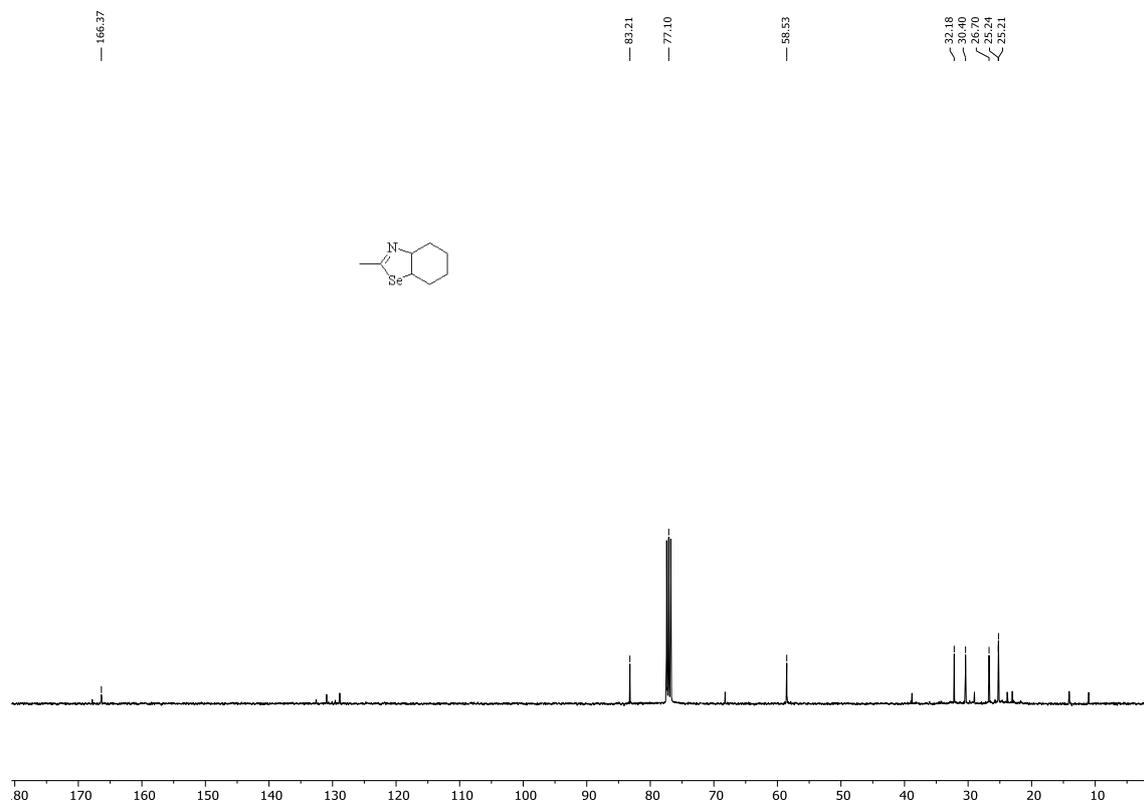


Figure S8.  $^{13}\text{C}$  NMR spectrum of compound **2c**



Figure S9.  $\{^{77}\text{Se}-^1\text{H}\}$  2D NMR spectrum of compound 2c

## Copies of high-resolution mass spectra of new compounds

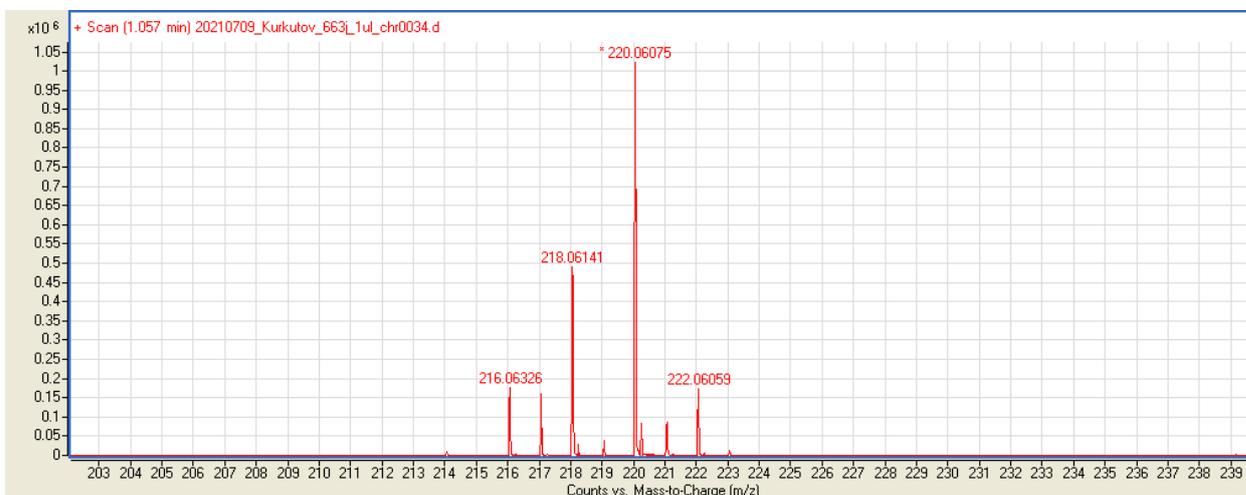
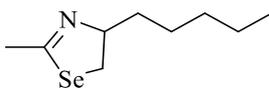


Figure S10. HRMS of compound **2a**

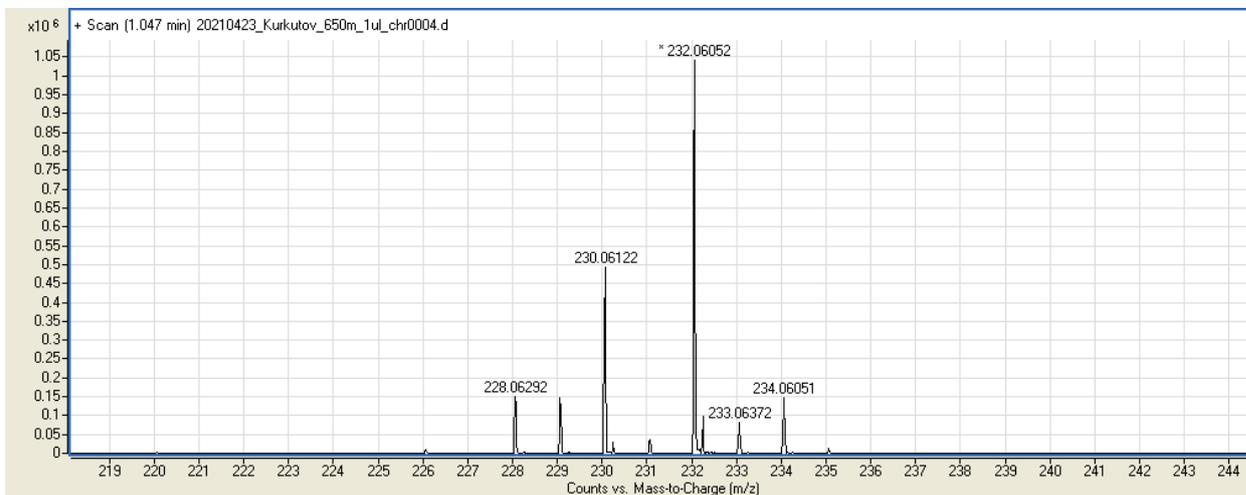
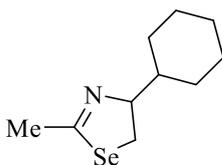


Figure S11. HRMS of compound **2b**

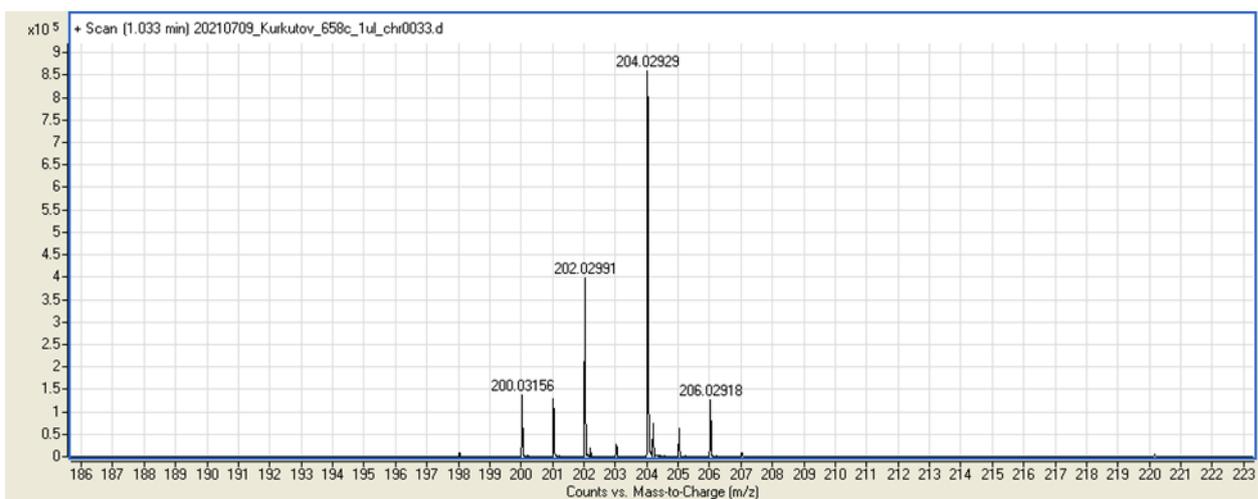
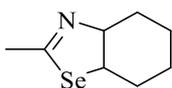


Figure S12. HRMS of compound 2c