

Supporting Information

One-Pot Three-Component Synthesis of Stable Pyrrole-3-Selones Using Propargyl Amines, Acyl Chlorides, and Elemental Selenium

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1. General information

All reactions were carried out under an argon atmosphere. Acyl chlorides **4a-f**, PdCl₂, CuI, Ph₃P, Et₃N, elemental selenium, SnCl₂·2H₂O and KOH·0.5H₂O are commercial reagents (Aldrich). Propargyl amines **3a-j** were prepared from aryl(hetaryl)ketimines and acetylene as previously described.¹

The ¹H, ¹³C, ¹⁵N, and ⁷⁷Se NMR spectra were recorded on a Bruker DPX 400 and Bruker AV-400 spectrometer (400.13, 100.62, 40.56, and 76.31 MHz, respectively) in CDCl₃ solutions and referenced to HMDS (¹H, ¹³C), MeNO₂ (¹⁵N), and Me₂Se (⁷⁷Se). The assignment of signals in ¹H spectra was performed using 2D homonuclear correlation method COSY. Resonance signals of ¹³C were assigned with application of 2D heteronuclear correlation methods HSQC and HMBC. The values of the δ ¹⁵N were measured through the 2D ¹H–¹⁵N HMBC experiment. Since the concentration of the studied selones was, in some cases, moderate, the chemical shifts of ⁷⁷Se were obtained by the inverse correlation method ⁷⁷Se–¹H HMBC, which is much more sensitive. However, to obtain this two-dimensional spectrum, it is necessary to observe the proton signal in the ¹H NMR spectrum in the position 4 of the pyrrole ring. Therefore, for compounds in which this signal is masked by other resonance signals, it was not possible to obtain the ⁷⁷Se chemical shifts.

FT-IR spectra were obtained with a Bruker Vertex 70 spectrometer. UV spectra were recorded on a Lambda 35 UV/vis spectrometer in the spectrometer cuvette. Mass spectra were recorded on an Agilent 6210 HRMS–TOF–ESI Mass spectrometer. Electrostatic sputtering, registration of positive ions. Sample solvent – MeCN with the addition of 0.1% heptafluorobutanoic acid and with the addition of calibration mixture for mass spectrometer.

¹ E. Yu. Schmidt, I. A. Bidusenko, N. I. Protsuk, Y. V. Demyanov, I. A. Ushakov and B. A. Trofimov, Superbase-promoted addition of acetylene gas to the C=N bond, *Eur. J. Org. Chem.*, 2019, 5875–5881.

2. One-pot synthesis of 1,2-dihydro-3*H*-pyrrole-3-selones 2a-x: General procedure and Spectral data

To a solution of propargyl amine **3a-j** (1.0 mmol) and acyl chloride **4a-f** (1.1 mmol) in toluene (3 mL), CuI (0.04 mmol, 0.008 g), PdCl₂ (0.02 mmol, 0.003 g), Ph₃P (0.02 mmol, 0.005 g) and Et₃N (0.6 mL) were added. The mixture was stirred under an argon atmosphere at 40–45 °C for 2–3 h (*i*). Elemental selenium (1.5 mmol, 0.117 g) was mixed with EtOH (3 mL), KOH·0.5H₂O (9 mmol, 0.585 g) and SnCl₂·2H₂O (2.0 mmol, 0.451 g). The reaction mixture was stirred at 70–75 °C for 5 h (*ii*). Then, the mixtures (*i*) and (*ii*) were combined and further stirred at room temperature for 10–11 h (*iii*). The reaction mixture was filtered (eluent: benzene). The solvent was removed under reduced pressure, the residue was purified by column chromatography on SiO₂ (eluent: toluene/Et₂O, 20:1), the solution was dried *in vacuo* to obtain the corresponding pyrroleselone **2a-x**.

The structures of all synthesized compounds **2** were unambiguously proven by IR, NMR (¹H and ¹³C) spectroscopy, including homo- and heteronuclear 2D COSY, HSQC and HMBC NMR. Thus, in the ¹H NMR spectra, the characteristic signal of pyrrole-3-selones is the H-4 proton of the dihydropyrrole ring, located in the region of 6.83–7.21 ppm. For dihydropyrroleselones **2a-g,t-x** with a Me group at the quaternary carbon atom, the characteristic signal of methyl protons is located in the region of 1.40–1.89 ppm. Also in the ¹H NMR spectra of dihydropyrroleselones **2a-d,h-q,u-x**, the signals of the ortho-protons of the NPh fragment appear as a multiplet or broadened doublet with a chemical shift of 6.64–7.23 ppm. The signals of other aromatic protons, in most cases, overlap and are not characteristic. Therefore, the ¹³C NMR spectra are more suitable for describing the structure of the obtained dihydropyrroleselone systems. Thus, the signal of the C-2 carbon atom is in the region of 86.7–91.1 ppm, and the signals of C-4 and C-5 have chemical shift values of 123.2–129.5 and 157.6–181.1 ppm, respectively. The signal of methyl carbon in pyrrole-3-selones **2a-g,t-x** is represented by a singlet with a chemical shift value of 23.1–26.6 ppm. The signal of the double C=Se bond of pyrrole-3-selones is observed in the region of 212.4–224.5 ppm. Noteworthy, such known selones as adamantyl(*tert*-butyl)-, di(1-adamantyl)- and 2,2,6,6-tetramethylcyclohexaneselones have a chemical shift of the C=Se bond carbon of 292.9–294.4 ppm.² The C=Se bond in selones obtained by us earlier from imidazoles, phenylcyanoacetylene and elemental selenium is observed at 157.8–159.5 ppm.³ Only for bis(4-methoxyphenyl)- and bis(4-

² R. Okazaki, A. Ishii and N. Inamoto, A new, convenient synthesis of selenoketones, *J. Chem. Soc., Chem. Commun.*, 1983, 1429–1430.

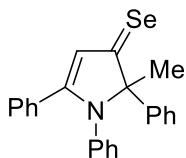
³ K. V. Belyaeva, L. V. Andriyankova, L. P. Nikitina, A. G. Mal'kina, A. V. Afonin, I. A. Ushakov, I. Y. Bagryanskaya and B. A. Trofimov, Three-component reaction of imidazoles, cyanophenylacetylene, and chalcogens: stereoselective synthesis of 3-alkenyl-2-imidazolethiones and –selones, *Tetrahedron*, 2014, **70**, 1091–1098.

methylphenyl)selone, the chemical shift of the C=Se bond carbon is located in the region of 240.1–244.4 ppm,⁴ which is close to the values for synthesized in this work 1,2-dihydro-3*H*-pyrrole-3-selones **2**.

The ⁷⁷Se NMR spectra were recorded using inverse two-dimensional HMBC (¹H-⁷⁷Se) technique, based on spin-spin coupling of the selenium atom with a proton in position 4 of the ring (through 3 bonds). In this case, the characteristic shift of the selenium atom in the obtained 1,2-dihydro-3*H*-pyrrole-3-selones **2** is located in the region of 2249–2425 ppm. At the same time, for known representatives of selones, derivatives of 1,3-diazacarbenes, this value is 77–856 ppm.^{3,5} However, other selones, synthesized by the reaction of hydrazones with diselenium dichloride, have a δ_{Se} value of 2026–2134 ppm.² Additionally, 1,2-dihydro-3*H*-pyrrole-3-selones **2** were characterized using the ¹⁵N NMR. The nitrogen atom chemical shift value of the obtained heterocycles is -193(-213) ppm.

To study the physical and physicochemical characteristics of the obtained 1,2-dihydro-3*H*-pyrrole-3-selones **2**, we also used UV spectroscopy. The absorption spectra were recorded in MeCN. Thus, the spectra of selones **2j,l,u** contain an intense absorption band in the region of 447–473 nm and an absorption band in the region of 248–253 nm. Noteworthy, adamantyl(*tert*-butyl)-, di(1-adamantyl)- and 2,2,6,6-tetramethylcyclohexaneselones have the absorption bands of 686–712 nm.²

2-Methyl-1,2,5-triphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2a).⁶



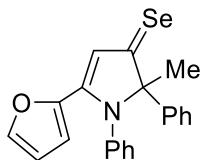
Yield: 0.237 g (70%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.48–7.44 (m, 2H, H_o, PhC-5); 7.33–7.30 (m, 8H, H_{o,m,p}, PhC-2; H_{m,p}, PhC-5); 7.23–7.19 (m, 1H, H_p, NPh); 7.15–7.11 (m, 2H, H_m, NPh); 7.06 (s, 1H, H-4, pyrroleselone); 6.64–6.62 (m, 2H, H_o, NPh); 1.83 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 223.1 (C=Se); 171.2 (C-5, pyrroleselone); 138.8 (C_i, NPh); 137.5 (C_i, PhC-2); 131.5 (C_p, PhC-5); 129.6 (C_i, PhC-5); 129.1 (C_m, NPh); 128.9 (C_m, PhC-2); 128.72 (C_m, PhC-5); 128.68 (C_o, PhC-5); 128.3 (C_p, PhC-2); 128.0 (C_p, NPh); 127.9 (C-4, pyrroleselone); 127.0 (C_o, NPh); 126.3 (C_o, PhC-2); 90.8 (C-2, pyrroleselone); 23.8 (Me). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2459.4. **HRMS** (ESI-TOF) calcd for [C₂₃H₁₉NSe + H]⁺ 390.0761, found 390.0771.

⁴ K. Okuma, K. Kojima, I. Kaneko and H. Ohta, Isolation and reaction of selenobenzophenones, *Chem. Lett.*, 1991, **20**, 1053–1056.

⁵ S. Yadav, R. Deka and H. B. Singh, Recent developments in the chemistry of NHC-based selones: syntheses, applications and reactivity, *Chem. Lett.*, 2019, **48**, 65–79.

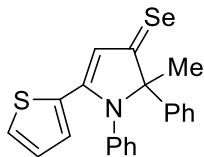
⁶ P. A. Volkov, S. I. Verkhuturova, K. O. Khrapova, S. N. Arbuzova, I. A. Bidusenko, A. I. Albanov and B. A. Trofimov, Selenium transfer from secondary phosphine selenides to aminoacetylenic ketones: access to 1,2-dihydro-3*H*-pyrrole-3-selones with a stable C=Se bond, *Org. Lett.*, 2024, **26**, 7336–7340.

5-(Furan-2-yl)-2-methyl-1,2-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2b).⁶



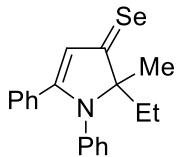
Yield: 0.276 g (73%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.70 (d, 1H, H-5, furyl, ³J₅₋₄ = 1.8 Hz); 7.42–7.38 (m, 1H, H_p, NPh); 7.31–7.28 (m, 6H, H_{o,m,p}, PhC-2; H-4, pyrroleselone); 7.23–7.21 (m, 2H, H_m, NPh); 6.80–6.78 (m, 2H, H_o, NPh); 6.39 (dd, 1H, H-4, furyl, ³J₄₋₃ = 3.7 Hz, ³J₄₋₅ = 1.8 Hz); 6.03 (d, 1H, H-3, furyl, ³J₃₋₄ = 3.7 Hz); 1.89 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 219.0 (C=Se); 158.8 (C-5, pyrroleselone); 147.3 (C-5, furyl); 144.3 (C-2, furyl); 138.5 (C_i, PhC-2); 137.3 (C_i, NPh); 129.51, 129.47 (C_{m,p}, NPh); 128.61, 128.58 (C_{m,p}, PhC-2); 128.4 (C_o, NPh); 127.0 (C_o, PhC-2); 124.2 (C-4, pyrroleselone); 119.3 (C-3, furyl); 113.5 (C-4, furyl); 90.6 (C-2, pyrroleselone); 23.6 (Me). **⁷⁷Se NMR** could not be recorded (see General information for details). **HRMS** (ESI-TOF) calcd for [C₂₁H₁₇NOSe + H]⁺ 380.0554, found 380.0554.

2-Methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2c).⁶



Yield: 0.296 g (75%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.61 (d, 1H, H-5, thienyl, ³J₅₋₄ = 5.0 Hz); 7.43–7.39 (m, 2H, H_p, NPh; H-3, thienyl); 7.31–7.21 (m, 8H, H_{o,m,p}, PhC-2; H_m, NPh; H-4, pyrroleselone); 7.03 (dd, 1H, H-4, thienyl, ³J₄₋₅ = 5.0 Hz, ³J₄₋₃ = 4.0 Hz,); 6.79 (br d, 2H, H_o, NPh, ³J = 7.6 Hz); 1.89 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 217.6 (C=Se); 163.4 (C-5, pyrroleselone); 137.8 (C_i, NPh); 137.3 (C_i, PhC-2); 134.3 (C-3, thienyl); 134.1 (C-5, thienyl); 130.9 (C-2, thienyl); 129.8 (C_p, NPh); 129.6 (C_m, NPh); 129.2 (C_o, NPh); 128.7 (C_m, PhC-2); 128.64 (C_p, PhC-2); 128.60 (C-4, thienyl); 127.0 (C_o, PhC-2); 125.6 (C-4, pyrroleselone); 90.8 (C-2, pyrroleselone); 23.6 (Me). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2340.6. **HRMS** (ESI-TOF) calcd for [C₂₁H₁₇NSSe + H]⁺ 396.0325, found 396.0324.

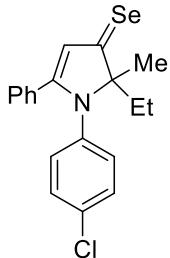
2-Ethyl-2-methyl-1,5-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2d).⁶



Yield: 0.197 g (58%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.36–7.21 (m, 8H, H_{o,m,p}, PhC-5; H_{m,p}, NPh); 6.96–6.94 (m, 2H, H_o, NPh); 6.83 (s, 1H, H-4, pyrroleselone); 2.26, 1.91 (AB-dq, 2H, MeCH₂, ²J = 13.9 Hz, ³J = 7.4 Hz); 1.56 (s, 3H, Me); 1.08 (t, 3H, MeCH₂, ³J = 7.4 Hz). **¹³C{¹H} NMR**

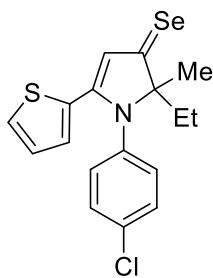
(100.62 MHz, CDCl₃): δ 219.9 (C=Se); 171.7 (C-5, pyrroleselone); 138.7 (C_i, PhC-5); 131.1 (C_p, NPh); 129.6 (C_i, NPh); 129.4 (C_m, NPh); 128.8 (C_p, PhC-5); 128.62 (C_o, PhC-5); 128.56 (C_m, PhC-5); 128.2 (C-4, pyrroleselone); 127.5 (C_o, NPh); 90.3 (C-2, pyrroleselone); 31.7 (MeCH₂); 26.3 (Me); 7.2 (MeCH₂). ⁷⁷Se NMR could not be recorded (see General information for details). HRMS (ESI-TOF) calcd for [C₁₉H₁₉NSe + H]⁺ 342.0761, found 342.0763.

1-(4-Chlorophenyl)-2-ethyl-2-methyl-5-phenyl-1,2-dihydro-3H-pyrrole-3-selone (2f).



Yield: 0.217 g (58%); waxy product. ¹H NMR (400.13 MHz, CDCl₃): δ 7.45–7.42 (m, 1H, H_p, PhC-5); 7.35–7.31 (m, 4H, H_{o,m}, PhC-5); 7.30 (d, 2H, H-3,5, C₆H₄Cl, ³J = 8.2 Hz); 7.00 (d, 2H, H-2,6, C₆H₄Cl, ³J = 8.2 Hz); 6.96 (s, 1H, H-4, pyrroleselone); 2.22, 1.93 (AB-dq, 2H, MeCH₂, ²J = 14.4 Hz, ³J = 7.2 Hz); 1.40 (s, 3H, Me); 0.77 (t, 3H, MeCH₂, ³J = 7.2 Hz). ¹³C{¹H} NMR (100.62 MHz, CDCl₃): δ 221.5 (C=Se); 171.7 (C-5, pyrroleselone); 137.6 (C-4, C₆H₄Cl); 134.2 (C-1, C₆H₄Cl); 131.5 (C_p, PhC-5); 129.7 (C_i, PhC-5); 129.5 (C-4, pyrroleselone); 129.1 (C-2,6, C₆H₄Cl); 128.9 (C-3,5, C₆H₄Cl); 128.8 (C_o, PhC-5); 128.7 (C_m, PhC-5); 90.7 (C-2, pyrroleselone); 32.0 (MeCH₂); 26.6 (Me); 7.4 (MeCH₂). ⁷⁷Se NMR could not be recorded (see General information for details). IR (neat): ν_{max} = 2927, 2851, 1643, 1599, 1580, 1518, 1494, 1463, 1417, 1404, 1359, 1315, 1288, 1262, 1180, 1147, 1125, 1095, 1075, 1064, 1050, 1028, 1015, 1008, 973, 911, 874, 831, 819, 794, 768, 735, 702, 648, 625, 616, 584, 562, 505 cm⁻¹. HRMS (ESI-TOF) calcd for [C₁₉H₁₈ClNSe + H]⁺ 376.0371, found 376.0373.

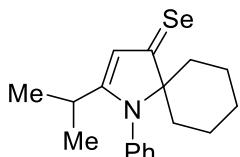
1-(4-Chlorophenyl)-2-ethyl-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-selone (2g).



Yield: 0.228 g (60%); waxy product. ¹H NMR (400.13 MHz, CDCl₃): δ 7.62 (dd, 1H, H-5, thiienyl, ³J_{5,4} = 5.0 Hz, ⁴J_{5,3} = 1.2 Hz); 7.48 (d, 2H, H-3,5, C₆H₄Cl, ³J = 8.1 Hz); 7.38 (dd, 1H, H-3, thiienyl, ³J_{3,4} = 3.9 Hz, ⁴J_{3,5} = 1.2 Hz); 7.19 (d, 2H, H-2,6, C₆H₄Cl, ³J = 8.1 Hz); 7.13 (s, 1H, H-4, pyrroleselone); 7.05 (dd, 1H, H-4, thiienyl, ³J_{4,3} = 3.9 Hz, ³J_{4,5} = 5.0 Hz); 2.14, 1.78 (AB-dq, 2H, MeCH₂, ²J = 14.4 Hz, ³J = 7.2 Hz); 1.41 (s, 3H, Me); 0.76 (t, 3H, MeCH₂, ³J = 7.2 Hz). ¹³C{¹H} NMR (100.62 MHz, CDCl₃): δ 216.3 (C=Se); 164.0 (C-5, pyrroleselone); 136.5 (C-4, C₆H₄Cl); 136.2 (C-1, C₆H₄Cl); 134.0 (C-3, thiienyl);

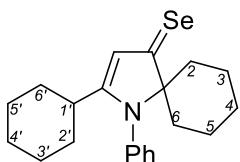
133.8 (C-5, thienyl); 130.7 (C-2, thienyl); 130.5 (C-2,6, C₆H₄Cl); 130.4 (C-3,5, C₆H₄Cl); 128.6 (C-4, thienyl); 126.5 (C-4, pyrroleselone); 90.4 (C-2, pyrroleselone); 31.3 (MeCH₂); 26.4 (Me); 7.7 (MeCH₂). ⁷⁷**Se NMR** could not be recorded (see General information for details). **IR** (neat): $\nu_{\text{max}} = 2926, 2851, 1614, 1537, 1493, 1480, 1435, 1411, 1378, 1342, 1330, 1321, 1286, 1223, 1181, 1141, 1093, 1048, 1015, 1005, 973, 909, 865, 845, 831, 802, 784, 731, 694, 668, 647, 627, 565, 509 \text{ cm}^{-1}$. **HRMS** (ESI-TOF) calcd for [C₁₇H₁₆ClNSSe + H]⁺ 381.9935, found 381.9933.

1-Phenyl-2-(propan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2h).



Yield: 0.123 g (37%); waxy product. ¹**H NMR** (400.13 MHz, CDCl₃): δ 7.52–7.50 (m, 3H, H_{m,p}, NPh); 7.23–7.21 (m, 2H, H_o, NPh); 6.83 (s, 1H, H-4, pyrroleselone); 2.27 (sept, 1H, Me₂CH, ³J = 6.7 Hz); 2.35–2.30, 1.78–1.74 (m, 4H, H-2,6, cyclohexyl); 1.88–1.82, 1.19–1.15 (m, 4H, H-3,5 cyclohexyl); 1.42–1.36 (m, 2H, H-4, cyclohexyl); 1.12 (d, 6H, Me₂CH, ³J = 6.7 Hz). ¹³C{¹H} NMR (100.62 MHz, CDCl₃): δ 219.3 (C=Se); 181.1 (C-5, pyrroleselone); 138.6 (C_i, NPh); 130.0 (C_p, NPh); 129.8 (C_m, NPh); 129.4 (C_o, NPh); 123.3 (C-4, pyrroleselone); 86.9 (C-2, pyrroleselone); 35.5 (C-2,6, cyclohexyl); 27.8 (Me₂CH); 24.0 (C-4, cyclohexyl); 21.1 (Me₂CH); 20.5 (C-3,5, cyclohexyl). ¹⁵N NMR (40.56 MHz, CDCl₃): δ -193.2. ⁷⁷**Se NMR** (76.31 MHz, CDCl₃): δ 2218.7. **IR** (neat): $\nu_{\text{max}} = 2927, 2853, 1642, 1595, 1522, 1493, 1468, 1450, 1389, 1373, 1341, 1300, 1283, 1261, 1216, 1183, 1136, 1099, 1065, 1029, 1005, 986, 963, 926, 904, 874, 818, 755, 705, 664, 622, 605, 560, 515, 502 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₁₈H₂₃NSe + H]⁺ 334.1074, found 334.1075.$

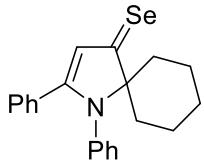
2-Cyclohexyl-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2i).



Yield: 0.223 g (60%); waxy product. ¹**H NMR** (400.13 MHz, CDCl₃): δ 7.55–7.48 (m, 3H, H_{m,p}, NPh); 7.21–7.20 (m, 2H, H_o, NPh); 6.83 (s, 1H, H-4, pyrroleselone); 2.34–2.26, 1.76–1.70 (m, 4H, H-2,6, cyclohexyl); 1.90–1.82 (m, 2H, H-1', cyclohexyl); 1.88–1.82, 1.24–1.13 (m, 4H, H-3,5, cyclohexyl); 1.76–1.70, 1.43–1.35 (m, 4H, H-2',6', cyclohexyl); 1.76–1.70, 1.24–1.13 (m, 4H, H-3',5', cyclohexyl); 1.63–1.60, 1.04–0.95 (m, 2H, H-4', cyclohexyl); 1.43–1.35 (m, 2H, H-4, cyclohexyl). ¹³C{¹H} NMR (100.62 MHz, CDCl₃): δ 218.8 (C=Se); 179.7 (C-5, pyrroleselone); 138.6 (C_i, NPh); 129.9 (C_p, NPh); 129.7 (C_m, NPh); 129.3 (C_o, NPh); 124.1 (C-4, pyrroleselone); 86.7 (C-2, pyrroleselone); 37.9 (C-1', cyclohexyl); 35.5 (C-2,6, cyclohexyl); 30.5 (C-2',6', cyclohexyl); 25.4 (C-4', cyclohexyl); 23.9 (C-4, cyclohexyl); 21.1 (C-3,5, cyclohexyl). ¹⁵N NMR (40.56 MHz, CDCl₃): δ -193.2.

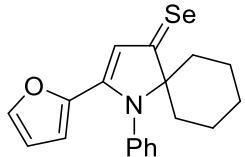
⁷⁷Se NMR (76.31 MHz, CDCl₃): δ 2215.6. **IR** (neat): ν_{max} = 2930, 2854, 1651, 1593, 1492, 1455, 1373, 1338, 1296, 1283, 1260, 1225, 1204, 1188, 1170, 1150, 1142, 1127, 1093, 1074, 1027, 1010, 990, 974, 965, 928, 903, 886, 864, 848, 801, 753, 706, 662, 622, 603, 591, 566, 515 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₁H₂₇NSe + H]⁺ 374.1387, found 374.1386.

1,2-Diphenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2j).⁶



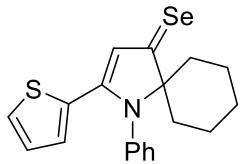
Yield: 0.236 g (64%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.36–7.17 (m, 10H, H_{o,m,p}, PhC-5; H_{o,m,p}, NPh); 7.00 (s, 1H, H-4, pyrroleselone); 2.40–2.32, 2.05–1.92 (m, 4H, H-2,6, cyclohexyl); 2.05–1.92, 1.30–1.22 (m, 4H, H-3,5, cyclohexyl); 1.50–1.41 (m, 2H, H-4, cyclohexyl). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 223.1 (C=Se); 170.9 (C-5, pyrroleselone); 140.1 (C_i, PhC-5); 130.9 (C_p, NPh); 130.2 (C_m, NPh); 129.4 (C_o, NPh); 129.2 (C_p, PhC-5); 128.71 (C_o, PhC-5); 128.69 (C_m, PhC-5); 128.4 (C_i, NPh); 128.2 (C-4, pyrroleselone); 88.5 (C-2, pyrroleselone); 35.6 (C-2,6, cyclohexyl); 24.1 (C-4, cyclohexyl); 20.9 (C-3,5, cyclohexyl). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2376.5. **HRMS** (ESI-TOF) calcd for [C₂₁H₂₁NSe + H]⁺ 368.0917, found 368.0915.

2-(Furan-2-yl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2k).



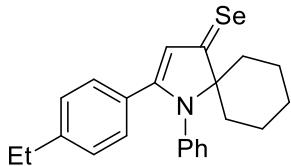
Yield: 0.232 g (65%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.60 (d, 1H, H-5, furyl, ³J_{5,4} = 1.7 Hz); 7.58–7.51 (m, 3H, H_{m,p}, NPh); 7.34–7.32 (m, 2H, H_o, NPh); 7.21 (s, 1H, H-4, pyrroleselone); 6.31 (dd, 1H, H-4, furyl, ³J_{4,3} = 3.7 Hz, ³J_{4,5} = 1.7 Hz); 5.62 (d, 1H, H-3, furyl, ³J_{3,4} = 3.7 Hz); 2.39–2.32, 1.92–1.89 (m, 4H, H-2,6, cyclohexyl); 1.92–1.89, 1.28–1.19 (m, 4H, H-3,5, cyclohexyl); 1.44–1.38 (m, 2H, H-4, cyclohexyl). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 218.7 (C=Se); 158.1 (C-5, pyrroleselone); 146.7 (C-5, furyl); 144.3 (C-2, furyl); 140.2 (C_i, NPh); 130.1 (C_p, NPh); 130.0 (C_m, NPh); 129.6 (C_o, NPh); 123.8 (C-4, pyrroleselone); 118.8 (C-3, furyl); 113.3 (C-4, furyl); 87.7 (C-2, pyrroleselone); 35.9 (C-2,6, cyclohexyl); 24.0 (C-4, cyclohexyl); 21.1 (C-3,5, cyclohexyl). **⁷⁷Se NMR** could not be recorded (see General information for details). **IR** (neat): ν_{max} = 2928, 2853, 1651, 1588, 1493, 1451, 1423, 1382, 1337, 1305, 1275, 1258, 1227, 1204, 1169, 1144, 1121, 1094, 1029, 973, 952, 912, 885, 810, 755, 731, 708, 643, 591, 514 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₁₉H₁₉NOSe + H]⁺ 358.0710, found 358.0710.

1-Phenyl-2-(thiophen-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2l).⁶



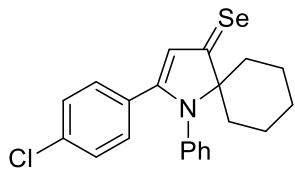
Yield: 0.253 g (68%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.62–7.51 (m, 4H, H-5, furyl; H_{m,p}, NPh); 7.37–7.34 (m, 2H, H_o, NPh); 7.31 (dd, 1H, H-3, thienyl, ³J₃₋₄ = 3.9 Hz, ⁴J₃₋₅ = 1.2 Hz); 7.20 (s, 1H, H-4, pyrroleselone); 6.99 (dd, 1H, H-4, thienyl, ³J₄₋₅ = 5.1 Hz, ³J₄₋₃ = 3.9 Hz); 2.42–2.33, 2.04–1.92 (m, 4H, H-2,6, cyclohexyl); 2.04–1.92, 1.28–1.21 (m, 4H, H-3,5, cyclohexyl); 1.47–1.38 (m, 2H, H-4, cyclohexyl). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 217.7 (C=Se); 162.6 (C-5, pyrroleselone); 139.4 (C_i, NPh); 134.2 (C-3, thienyl); 133.9 (C-5, thienyl); 130.7 (C_o, NPh); 130.6 (C_p, NPh); 130.1 (C_m, NPh); 128.5 (C-2, thienyl); 128.2 (C-4, thienyl); 125.4 (C-4, pyrroleselone); 88.0 (C-2, pyrroleselone); 35.9 (C-2,6, cyclohexyl); 24.1 (C-4, cyclohexyl); 21.2 (C-3,5, cyclohexyl). **⁷⁷Se NMR** could not be recorded (see General information for details). **HRMS** (ESI-TOF) calcd for [C₁₉H₁₉NSSe + H]⁺ 374.0482, found 374.0480.

2-(4-Ethylphenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2m).



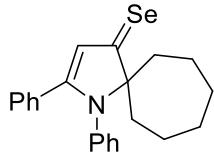
Yield: 0.276 g (70%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.38–7.35 (m, 3H, H_{m,p}, NPh); 7.21–7.19 (m, 4H, H-2,6, C₆H₄Et; H_o, NPh); 7.03 (d, 2H, H-3,5, C₆H₄Et, ³J = 8.2 Hz); 7.00 (s, 1H, H-4, pyrroleselone); 2.55 (q, 2H, MeCH₂, ³J = 7.5 Hz); 2.39–2.30, 1.95–1.90 (m, 4H, H-2,6, cyclohexyl); 2.02–1.98, 1.30–1.22 (m, 4H, H-3,5, cyclohexyl); 1.49–1.39 (m, 2H, H-4, cyclohexyl); 1.17 (t, 3H, MeCH₂, ³J = 7.5 Hz). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 221.5 (C=Se); 170.7 (C-5, pyrroleselone); 147.8 (C-4, C₆H₄Et); 140.1 (C_i, NPh); 130.1 (C_o, NPh); 129.4 (C-2,6, C₆H₄Et); 129.1 (C_p, NPh); 128.9 (C_m, NPh); 128.2 (C-3,5, C₆H₄Et); 127.9 (C-4, pyrroleselone); 127.1 (C-1, C₆H₄Et); 88.2 (C-2, pyrroleselone); 35.5 (C-2,6, cyclohexyl); 28.7 (MeCH₂); 24.0 (C-4, cyclohexyl); 20.8 (C-3,5, cyclohexyl); 14.8 (MeCH₂). **¹⁵N NMR** (40.56 MHz, CDCl₃): δ -202.6. **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2345.8. **IR** (neat): ν_{max} = 2930, 2868, 2855, 1610, 1569, 1530, 1479, 1445, 1400, 1375, 1337, 1306, 1285, 1273, 1202, 1188, 1170, 1144, 1125, 1110, 1089, 1075, 1061, 1051, 1025, 1010, 971, 939, 911, 850, 840, 813, 769, 732, 705, 684, 644, 622, 615, 604, 578, 542 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₃H₂₅NSe + H]⁺ 396.1230, found 396.1228.

2-(4-Chlorophenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2n).



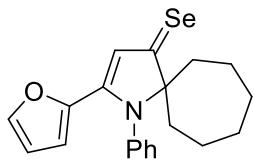
Yield: 0.272 g (68%); waxy product. **$^1\text{H NMR}$** (400.13 MHz, CDCl_3): δ 7.38–7.35 (m, 4H, H-3,5, $\text{C}_6\text{H}_4\text{Cl}$; H_m , NPh); 7.26–7.17 (m, 5H, H-2,6, $\text{C}_6\text{H}_4\text{Cl}$; $\text{H}_{o,p}$, NPh); 6.95 (s, 1H, H-4, pyrroleselone); 2.35–2.28, 1.96–1.91 (m, 4H, H-2,6, cyclohexyl); 2.04–1.99, 1.29–1.20 (m, 4H, H-3,5, cyclohexyl); 1.49–1.43 (m, 2H, H-4, cyclohexyl). **$^{13}\text{C}\{\text{H}\} \text{NMR}$** (100.62 MHz, CDCl_3): δ 223.8 (C=Se); 169.4 (C-5, pyrroleselone); 139.8 (C_i, NPh); 137.1 (C-4, $\text{C}_6\text{H}_4\text{Cl}$); 130.9 (C-3,5, $\text{C}_6\text{H}_4\text{Cl}$); 129.9 (C_o, NPh); 129.5 (C-2,6, $\text{C}_6\text{H}_4\text{Cl}$); 129.3 (C_p, NPh); 128.6 (C-1, $\text{C}_6\text{H}_4\text{Cl}$); 128.1 (C_m, NPh); 128.0 (C-4, pyrroleselone); 88.7 (C-2, pyrroleselone); 35.5 (C-2,6, cyclohexyl); 24.0 (C-4, cyclohexyl); 20.7 (C-3,5, cyclohexyl). **$^{15}\text{N NMR}$** (40.56 MHz, CDCl_3): δ -202.6. **$^{77}\text{Se NMR}$** (76.31 MHz, CDCl_3): δ 2425.5. **IR** (neat): $\nu_{\text{max}} = 2925, 2851, 1656, 1595, 1570, 1518, 1492, 1468, 1444, 1390, 1372, 1335, 1305, 1272, 1202, 1178, 1143, 1109, 1090, 1026, 1014, 972, 940, 909, 892, 848, 836, 809, 772, 746, 731, 725, 702, 664, 644, 619, 603, 576, 551, 536 cm^{-1} . **HRMS** (ESI-TOF) calcd for $[\text{C}_{21}\text{H}_{20}\text{ClNSe} + \text{H}]^+$ 402.0528, found 402.0532.$

1,2-Diphenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2o).



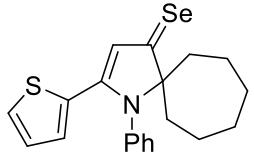
Yield: 0.251 g (66%); waxy product. The NMR spectra contain double signals. This is probably due to the presence of two conformers, the exchange between which is very slow (on the NMR time scale) due to steric hindrance. **$^1\text{H NMR}$** (400.13 MHz, CDCl_3): δ 7.58–7.55 (m, 2H, H_o , PhC-2); 7.24–6.99 (m, 9H, $\text{H}_{m,p}$, PhC-2; $\text{H}_{o,m,p}$, NPh; H-4, pyrroleselone); 2.34–2.28, 2.09–2.03, 2.02–1.96, 1.90–1.84 (m, 4H, H-2,7, cycloheptyl); 2.24–2.16, 1.82–1.74, 1.22–1.14, 1.12–1.03 (m, 4H, H-4,5, cycloheptyl); 1.58–1.50, 1.34–1.31 (m, 4H, H-3,6, cycloheptyl). **$^{13}\text{C}\{\text{H}\} \text{NMR}$** (100.62 MHz, CDCl_3): δ 223.4, 201.9 (C=Se); 174.8, 173.1 (C-5, pyrroleselone); 139.9, 138.9 (C_i, PhC-2); 132.0, 131.2 (C_i, NPh); 130.1, 130.0 (C_o, NPh); 129.7 (C_p, NPh); 129.3, 129.0 (C_m, PhC-2); 128.7, 128.4 (C_o, PhC-2); 128.6 (C_p, PhC-2); 127.8, 127.5 (C_m, NPh); 127.2 (C-4, pyrroleselone); 91.1, 74.7 (C-2, pyrroleselone); 38.2, 36.3 (C-2,7, cycloheptyl); 31.9, 31.6 (C-3,6, cycloheptyl); 23.1, 22.4 (C-4,5, cycloheptyl). **$^{77}\text{Se NMR}$** (76.31 MHz, CDCl_3): δ 2387.5. **IR** (neat): $\nu_{\text{max}} = 2926, 2853, 1662, 1601, 1582, 1517, 1492, 1472, 1445, 1412, 1358, 1313, 1282, 1256, 1232, 1216, 1200, 1170, 1156, 1112, 1090, 1075, 1053, 1027, 1003, 994, 955, 918, 906, 872, 850, 830, 807, 788, 752, 701, 665, 649, 615, 551, 510, 488, 453 cm^{-1} . **HRMS** (ESI-TOF) calcd for $[\text{C}_{22}\text{H}_{23}\text{NSe} + \text{H}]^+$ 382.1074, found 382.1075.$

2-(Furan-2-yl)-1-phenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2p).



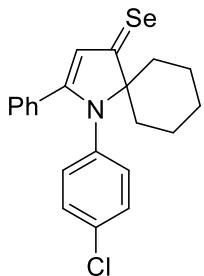
Yield: 0.244 g (66%); waxy product. **$^1\text{H NMR}$** (400.13 MHz, CDCl_3): δ 7.60 (dd, 1H, H-5, furyl, $^3J_{5-4} = 1.7$ Hz, $^4J_{5-3} = 0.7$ Hz); 7.58–7.51 (m, 3H, $\text{H}_{m,p}$, NPh); 7.27–7.25 (m, 2H, H_o , NPh); 7.11 (s, 1H, H-4, pyrroleselone); 6.31 (dd, 1H, H-4, furyl, $^3J_{4-3} = 3.7$ Hz, $^3J_{4-5} = 1.7$ Hz); 5.68 (dd, 1H, H-3, furyl, $^3J_{3-4} = 3.7$ Hz, $^4J_{3-5} = 0.7$ Hz); 2.34–2.27, 2.13–2.07 (m, 4H, H-2,7, cycloheptyl); 2.24–2.18, 1.17–1.09 (m, 4H, H-3,6, cycloheptyl); 1.63–1.54, 1.36–1.23 (m, 4H, H-4,5, cycloheptyl). **$^{13}\text{C}\{^1\text{H}\} \text{NMR}$** (100.62 MHz, CDCl_3): δ 219.8 (C=Se); 157.6 (C-5, pyrroleselone); 146.8 (C-5, furyl); 144.3 (C-2, furyl); 138.9 (C_i , NPh); 130.0 ($\text{C}_{m,p}$, NPh); 129.5 (C_o , NPh); 123.2 (C-4, pyrroleselone); 118.7 (C-3, furyl); 113.2 (C-4, furyl); 90.7 (C-2, pyrroleselone); 38.0 (C-2,7, cycloheptyl); 31.9 (C-4,5, cycloheptyl); 23.1 (C-3,6, cycloheptyl). **$^{15}\text{N NMR}$** (40.56 MHz, CDCl_3): δ -211.9. **$^{77}\text{Se NMR}$** (76.31 MHz, CDCl_3): δ 2340.8. **IR** (neat): $\nu_{\text{max}} = 2926, 2850, 1588, 1520, 1492, 1449, 1428, 1381, 1353, 1342, 1282, 1227, 1201, 1181, 1154, 1127, 1112, 1083, 1063, 1027, 1004, 993, 972, 957, 939, 906, 884, 852, 834, 811, 760, 731, 708, 699, 658, 646, 618, 608, 594, 588 cm^{-1} . **HRMS** (ESI-TOF) calcd for $[\text{C}_{20}\text{H}_{21}\text{NOSe} + \text{H}]^+$ 372.0867, found 372.0869.$

1-Phenyl-2-(thiophen-2-yl)-1-azaspiro[4.6]undec-2-ene-4-selone (2q).⁶



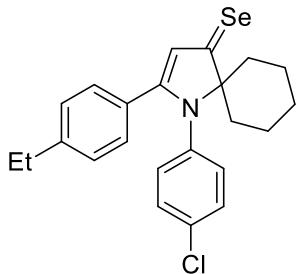
Yield: 0.255 g (66%); waxy product. **$^1\text{H NMR}$** (400.13 MHz, CDCl_3): δ 7.61–7.57 (m, 1H, H_p , NPh); 7.55–7.51 (m, 3H, H-5, thienyl; H_m , NPh); 7.31–7.28 (m, 3H, H-3, thienyl; H_o , NPh); 7.10 (s, 1H, H-4, pyrroleselone); 6.98 (dd, 1H, H-4, thienyl, $^3J_{4-5} = 5.1$ Hz, $^3J_{4-3} = 3.9$ Hz); 2.38–2.32, 2.17–2.11 (m, 4H, H-2,7, cycloheptyl); 2.27–2.21, 1.19–1.10 (m, 4H, H-3,6, cycloheptyl); 1.62–1.57, 1.38–1.32 (m, 4H, H-4,5, cycloheptyl). **$^{13}\text{C}\{^1\text{H}\} \text{NMR}$** (100.62 MHz, CDCl_3): δ 218.4 (C=Se); 162.0 (C-5, pyrroleselone); 138.1 (C_i , NPh); 134.0 (C-3, thienyl); 133.8 (C-5, thienyl); 130.4 ($\text{C}_{m,p}$, NPh); 130.1 (C_o , NPh); 128.4 (C-2, thienyl); 128.2 (C-4, thienyl); 124.6 (C-4, pyrroleselone); 90.9 (C-2, pyrroleselone); 38.1 (C-2,7, cycloheptyl); 31.9 (C-4,5, cycloheptyl); 23.1 (C-3,6, cycloheptyl). **$^{77}\text{Se NMR}$** (76.31 MHz, CDCl_3): δ 2306.2. **HRMS** (ESI-TOF) calcd for $[\text{C}_{20}\text{H}_{21}\text{NSSe} + \text{H}]^+$ 388.0638, found 388.0642.

1-(4-Chlorophenyl)-2-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2r).



Yield: 0.272 g (68%); waxy product. **$^1\text{H NMR}$** (400.13 MHz, CDCl_3): δ 7.39–7.38 (m, 1H, H_p , $\text{PhC}-2$); 7.33–7.31 (m, 2H, H-3,5, $\text{C}_6\text{H}_4\text{Cl}$); 7.28–7.24 (m, 4H, $\text{H}_{o,m}$, $\text{PhC}-2$); 7.14–7.11 (m, 2H, H-2,6, $\text{C}_6\text{H}_4\text{Cl}$); 6.96 (s, 1H, H-4, pyrroleselone); 2.36–2.28, 1.92–1.88 (m, 4H, H-2,6, cyclohexyl); 2.07–2.03, 1.28–1.22 (m, 4H, H-3,5, cyclohexyl); 1.48–1.46 (m, 2H, H-4, cyclohexyl). **$^{13}\text{C}\{\text{H}\} \text{NMR}$** (100.62 MHz, CDCl_3): δ 224.5 ($\text{C}=\text{Se}$); 170.8 (C-5, pyrroleselone); 138.7 (C-4, $\text{C}_6\text{H}_4\text{Cl}$); 135.1 (C-1, $\text{C}_6\text{H}_4\text{Cl}$); 131.5 (C-2,6, $\text{C}_6\text{H}_4\text{Cl}$); 131.1 (C_p , $\text{PhC}-2$); 130.1 (C_i , $\text{PhC}-2$); 129.7 (C-3,5, $\text{C}_6\text{H}_4\text{Cl}$); 128.9 (C_m , $\text{PhC}-2$); 128.6 (C_o , $\text{PhC}-2$); 128.4 (C-4, pyrroleselone); 88.7 (C-2, pyrroleselone); 35.6 (C-2,6, cyclohexyl); 24.1 (C-4, cyclohexyl); 20.9 (C-3,5, cyclohexyl). **$^{77}\text{Se NMR}$** could not be recorded (see General information for details). **IR** (neat): $\nu_{\text{max}} = 2928, 2855, 1718, 1672, 1600, 1582, 1515, 1496, 1462, 1451, 1416, 1356, 1274, 1250, 1229, 1216, 1174, 1158, 1133, 1091, 1074, 1029, 1013, 972, 931, 883, 838, 813, 752, 697, 663, 640, 613, 595, 533, 511 cm^{-1} . **HRMS** (ESI-TOF) calcd for $[\text{C}_{21}\text{H}_{20}\text{ClNSe} + \text{H}]^+$ 402.0528, found 402.0524.$

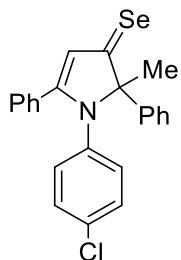
1-(4-Chlorophenyl)-2-(4-ethylphenyl)-1-azaspiro[4.5]dec-2-ene-4-selone (2s).



Yield: 0.304 g (71%); waxy product. **$^1\text{H NMR}$** (400.13 MHz, CDCl_3): δ 7.34 (d, 2H, H-2,6, $\text{C}_6\text{H}_4\text{Et}$, $^3J = 8.7$ Hz); 7.20 (d, 2H, H-2,6, $\text{C}_6\text{H}_4\text{Cl}$, $^3J = 8.2$ Hz); 7.14 (d, 2H, H-3,5, $\text{C}_6\text{H}_4\text{Et}$, $^3J = 8.7$ Hz); 7.08 (d, 2H, H-3,5, $\text{C}_6\text{H}_4\text{Cl}$, $^3J = 8.2$ Hz); 6.97 (s, 1H, H-4, pyrroleselone); 2.57 (q, 2H, MeCH_2 , $^3J = 7.6$ Hz); 2.36–2.28, 1.91–1.85 (m, 4H, H-2,6, cyclohexyl); 2.08–2.02, 1.28–1.23 (m, 4H, H-3,5, cyclohexyl); 1.52–1.43 (m, 2H, H-4, cyclohexyl); 1.19 (t, 3H, MeCH_2 , $^3J = 7.6$ Hz). **$^{13}\text{C}\{\text{H}\} \text{NMR}$** (100.62 MHz, CDCl_3): δ 222.8 ($\text{C}=\text{Se}$); 170.7 (C-5, pyrroleselone); 147.9 (C-4, $\text{C}_6\text{H}_4\text{Et}$); 138.7 (C-1, $\text{C}_6\text{H}_4\text{Cl}$); 134.9 (C-4, $\text{C}_6\text{H}_4\text{Cl}$); 131.4 (C-3,5, $\text{C}_6\text{H}_4\text{Et}$); 129.6 (C-2,6, $\text{C}_6\text{H}_4\text{Et}$); 128.8 (C-2,6, $\text{C}_6\text{H}_4\text{Cl}$); 128.4 (C-3,5, $\text{C}_6\text{H}_4\text{Cl}$); 128.3 (C-4, pyrroleselone); 126.9 (C-1, $\text{C}_6\text{H}_4\text{Et}$); 88.3 (C-2, pyrroleselone); 35.4 (C-2,6, cyclohexyl); 28.8 (MeCH_2); 24.0 (C-4, cyclohexyl); 20.8 (C-3,5, cyclohexyl); 14.8 (MeCH_2). **$^{15}\text{N NMR}$** (40.56 MHz, CDCl_3): δ -205.7. **$^{77}\text{Se NMR}$** (76.31 MHz, CDCl_3): δ 2400.4. **IR** (neat): $\nu_{\text{max}} = 2928, 2851, 1610, 1569,$

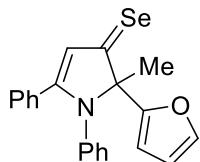
1529, 1492, 1476, 1448, 1401, 1374, 1335, 1306, 1272, 1203, 1187, 1170, 1144, 1091, 1061, 1051, 1028, 1016, 971, 939, 910, 856, 839, 820, 776, 732, 694, 667, 644, 618, 605, 566, 519 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₃H₂₄ClNSe + H]⁺ 430.0841, found 430.0840.

1-(4-Chlorophenyl)-2-methyl-2,5-diphenyl-1,2-dihydro-3H-pyrrole-3-selone (2t).



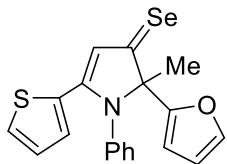
Yield: 0.262 g (62%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.44 (d, 2H, H_o, PhC-5, ³J = 7.7 Hz); 7.36–7.32 (m, 5H, H_m, PhC-2; H_{m,p}, PhC-5); 7.26–7.24 (m, 3H, H_{o,p}, PhC-2); 7.16 (d, 2H, H-3,5, C₆H₄Cl, ³J = 7.9 Hz); 7.06 (s, 1H, H-4, pyrroleselone); 6.66 (d, 2H, H-2,6, C₆H₄Cl, ³J = 8.2 Hz); 1.81 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 222.9 (C=Se); 171.5 (C-5, pyrroleselone); 138.8 (C-4, C₆H₄Cl); 136.3 (C_i, PhC-2); 134.4 (C-1, C₆H₄Cl); 131.7 (C_p, PhC-5); 129.6 (C_i, PhC-5); 129.4 (C-3,5, C₆H₄Cl); 129.1 (C_m, PhC-2); 129.0 (C_m, PhC-5); 128.9 (C_o, PhC-5); 128.4 (C_p, PhC-2); 128.3 (C-4, pyrroleselone); 128.0 (C_o, PhC-2); 127.2 (C-2,6, C₆H₄Cl); 90.3 (C-2, pyrroleselone); 24.0 (Me). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2478.1. **IR** (neat): ν_{max} = 2923, 2850, 1595, 1516, 1491, 1462, 1449, 1416, 1347, 1280, 1271, 1215, 1183, 1135, 1095, 1073, 1051, 1028, 1013, 970, 941, 910, 860, 825, 817, 768, 729, 694, 668, 642, 622, 607, 556, 535, 513 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₃H₁₈ClNSe + H]⁺ 424.0371, found 424.0369.

2-(Furan-2-yl)-2-methyl-1,5-diphenyl-1,2-dihydro-3H-pyrrole-3-selone (2u).⁶



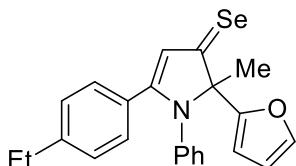
Yield: 0.204 g (54%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.45–7.40 (m, 4H, H-5, furyl; H_{o,p}, PhC-5); 7.30–7.26 (m, 3H, H_m, PhC-5; H_p, NPh); 7.23–7.19 (m, 2H, H_m, NPh); 7.05 (s, 1H, H-4, pyrroleselone); 6.67–6.65 (m, 2H, H_o, NPh); 6.40 (d, 1H, H-3, furyl, ³J_{3,4} = 3.3 Hz); 6.36 (dd, 1H, H-4, furyl, ³J_{4,3} = 3.3 Hz, ³J_{4,5} = 1.9 Hz); 1.82 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 217.7 (C=Se); 171.2 (C-5, pyrroleselone); 148.9 (C-2, furyl); 138.4 (C_i, PhC-5); 131.6 (C_p, PhC-5); 129.6 (C_i, NPh); 129.3 (C_m, NPh); 128.90, 128.88 (C_{o,m}, PhC-5; C_p, NPh); 128.4 (C-5, furyl); 127.9 (C-4, pyrroleselone); 127.6 (C_o, NPh); 110.7 (C-3, furyl); 110.6 (C-4, furyl); 87.2 (C-2, pyrroleselone); 23.5 (Me). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2446.9. **HRMS** (ESI-TOF) calcd for [C₂₁H₁₇NOSe + H]⁺ 380.0554, found 380.0552.

2-(Furan-2-yl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2v).



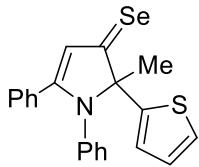
Yield: 0.200 g (52%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.62 (dd, 1H, H-5, thienyl, ³J₅₋₄ = 5.0 Hz, ⁴J₅₋₃ = 0.9 Hz); 7.49–7.42 (m, 1H, H_p, NPh); 7.39–7.35 (m, 4H, H-3, thienyl; H_m, NPh; H-5, furyl); 7.21 (s, 1H, H-4, pyrroleselone); 7.02 (dd, 1H, H-4, thienyl, ³J₄₋₃ = 3.9 Hz, ³J₄₋₅ = 5.0 Hz); 6.87 (m, 2H, H_o, NPh); 6.31 (dd, 1H, H-3, furyl, ³J₃₋₄ = 3.3 Hz, ⁴J₃₋₅ = 0.8 Hz); 6.31 (dd, 1H, H-4, furyl, ³J₄₋₃ = 3.3 Hz, ³J₄₋₅ = 1.8 Hz); 1.87 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 212.4 (C=Se); 163.4 (C-5, pyrroleselone); 148.9 (C-2, furyl); 137.3 (C-2, thienyl); 134.4 (C-3, thienyl); 134.3 (C-5, thienyl); 130.6 (C_i, NPh); 130.0 (C_p, NPh); 129.7 (C_m, NPh; C-5, furyl); 129.9 (C_o, NPh); 128.5 (C-4, thienyl); 125.0 (C-4, pyrroleselone); 110.8 (C-3, furyl); 110.6 (C-4, furyl); 86.8 (C-2, pyrroleselone); 23.1 (Me). **¹⁵N NMR** (40.56 MHz, CDCl₃): δ -213.5. **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2249.9. **IR** (neat): ν_{max} = 2923, 2850, 1595, 1535, 1497, 1478, 1431, 1410, 1378, 1339, 1319, 1271, 1248, 1221, 1157, 1140, 1091, 1074, 1026, 1004, 929, 911, 884, 863, 840, 796, 768, 729, 698, 637, 585, 508 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₁₉H₁₅NOSe + H]⁺ 386.0118, found 386.0120.

5-(4-Ethylphenyl)-2-(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2w).



Yield: 0.256 g (63%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.38 (dd, 1H, H-5, furyl, ³J₅₋₄ = 1.9 Hz, ⁴J₅₋₃ = 0.8 Hz); 7.28 (d, 2H, H-2,6, C₆H₄Et, ³J = 8.4 Hz); 7.25–7.18 (m, 3H, H_{m,p}, NPh); 7.08 (d, 2H, H-3,5, C₆H₄Et, ³J = 8.4 Hz); 7.04 (s, 1H, H-4, pyrroleselone); 6.66–6.64 (m, 2H, H_o, NPh); 6.32 (dd, 1H, H-3, furyl, ³J₃₋₄ = 3.4 Hz, ⁴J₃₋₅ = 0.8 Hz); 6.33 (dd, 1H, H-4, furyl, ³J₄₋₃ = 3.4 Hz, ³J₄₋₅ = 1.9 Hz); 2.57 (q, 2H, MeCH₂, ³J = 7.6 Hz); 1.79 (s, 3H, Me); 1.18 (t, 3H, MeCH₂, ³J = 7.6 Hz). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 216.6 (C=Se); 171.3 (C-5, pyrroleselone); 149.2 (C-2, furyl); 148.7 (C-4, C₆H₄Et); 142.8 (C-5, furyl); 138.6 (C_i, NPh); 129.3 (C_m, NPh); 129.2 (C-2,6, C₆H₄Et); 128.5 (C-3,5, C₆H₄Et); 128.4 (C_p, NPh); 127.7 (C-4, pyrroleselone); 127.6 (C_o, NPh); 126.7 (C-1, C₆H₄Et); 110.7 (C-3, furyl); 110.6 (C-4, furyl); 87.1 (C-2, pyrroleselone); 28.9 (MeCH₂); 23.5 (Me); 14.8 (MeCH₂). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 2460.9. **IR** (neat): ν_{max} = 2966, 2930, 2873, 1672, 1610, 1570, 1529, 1496, 1476, 1442, 1398, 1356, 1274, 1251, 1229, 1188, 1158, 1128, 1092, 1075, 1014, 931, 911, 883, 841, 809, 765, 734, 697, 646, 634, 614, 595 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₃H₂₁NOSe + H]⁺ 408.0867, found 408.0865.

2-Methyl-1,5-diphenyl-2-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2x).



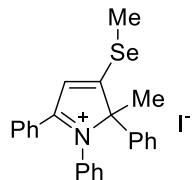
Yield: 0.197 g (50%); waxy product. **^1H NMR** (400.13 MHz, CDCl_3): δ 7.46–7.40 (m, 3H, $\text{H}_{o,p}$, PhC-5); 7.33–7.24 (m, 4H, H_p , NPh; H_m , PhC-5; H-5, thieryl); 7.20–7.17 (m, 2H, H_m , NPh); 7.05 (s, 1H, H-4, pyrroleselone); 7.01 (d, 1H, H-3, thieryl, $^3J_{3-4} = 3.4$ Hz); 6.93 (dd, 1H, H-4, thieryl, $^3J_{4-3} = 3.4$ Hz, $^3J_{4-5} = 4.4$ Hz); 6.74–6.72 (m, 2H, H_o , NPh); 1.89 (s, 3H, Me). **$^{13}\text{C}\{\text{H}\}$ NMR** (100.62 MHz, CDCl_3): δ 221.4 (C=Se); 170.4 (C-5, pyrroleselone); 141.0 (C-2, thieryl); 138.6 (C_i , NPh); 131.6 (C_p , PhC-5); 129.8 (C_i , PhC-5); 129.3 (C_m , NPh); 129.0 (C_o , PhC-5); 128.9 (C_m , PhC-5); 128.4 (C_p , NPh); 127.8 (C-4, pyrroleselone); 127.7 (C_o , NPh); 127.0 (C-3, thieryl); 126.7 (C-5, thieryl); 126.5 (C-4, furyl); 88.6 (C-2, pyrroleselone); 25.4 (Me). **^{15}N NMR** (40.56 MHz, CDCl_3): δ -205.7. **^{77}Se NMR** could not be recorded (see General information for details). **IR** (neat): $\nu_{\text{max}} = 2926, 2854, 1596, 1580, 1514, 1494, 1461, 1449, 1415, 1349, 1273, 1239, 1130, 1073, 1028, 1006, 969, 910, 857, 835, 816, 767, 729, 696, 647, 617, 572, 540, 523 cm^{-1} . **HRMS** (ESI-TOF) calcd for $[\text{C}_{21}\text{H}_{17}\text{NSSe} + \text{H}]^+$ 396.0325, found 396.0322.$

3. Alkylation of 1,2-dihydro-3*H*-pyrrole-3-selones 2a,c,f: General procedure and Spectral data

To 1,2-dihydro-3*H*-pyrrole-3-selone **2a,c,f** (1.0 mmol), methyl iodide or benzyl chloride (1 mL) was added. The mixture was stirred under an argon atmosphere at 20–25 °C for 5 min. The residue was re-precipitated from CHCl₃ to hexane to give 2*H*-pyrrolium iodide **6** or 2*H*-pyrrolium chloride **7**.

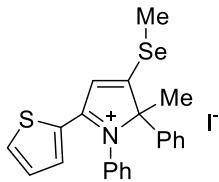
The transformation of selones **2** into their salts **6** and **7** is accompanied by the following changes in the NMR spectra. The chemical shifts of the methyl group protons and the H-4 proton are shifted downfield (by 0.2–0.36 ppm and 0.6 ppm, respectively). At the same time, the signals of the carbons of the methyl group, C-2, C-3, C-4 are shielded (0.4–1.0; 4–5; 35–37; 4–7 ppm, respectively). Unlike the shifts of other ring carbons, the C-5 resonance is shifted downfield by 3–4 ppm. The chemical shift of ⁷⁷Se for selones **2** (2350 ppm) during the formation of salts expectedly shifts significantly upfield (300–400 ppm). The minor change in the ¹⁵N chemical shift value (-206 → -184 ppm) can apparently be explained by two competing trends: a change in the hybridization of the nitrogen atom, leading to deshielding, and the presence of a charge on the sp²-hybridized nitrogen atom, which, on the contrary, causes significant shielding.

2-Methyl-3-(methylselanyl)-1,2,5-triphenyl-2*H*-pyrrolium iodide (**6a**).



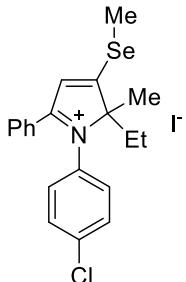
Yield: 0.504 g (95%); waxy product. ¹**H NMR** (400.13 MHz, CDCl₃): δ 7.94–7.93 (m, 2H, H_o, PhC-5); 7.87 (s, 1H, H-4, pyrrolium iodide); 7.58–7.54 (m, 1H, H_p, PhC-5); 7.52–7.39 (m, 6H, H_{m,p}, PhC-2; H_m, PhC-5; H_p, NPh); 7.31–7.27 (m, 2H, H_m, NPh); 7.24–7.22 (m, 2H, H_o, PhC-2); 6.80–6.79 (m, 2H, H_o, NPh); 2.94 (s, 3H, MeSe, ²J = 11.1 Hz); 2.07 (s, 3H, Me). ¹³**C{¹H} NMR** (100.62 MHz, CDCl₃): δ 187.2 (C-3, pyrrolium iodide); 174.4 (C-5, pyrrolium iodide); 135.5 (C_i, NPh); 135.0 (C_p, PhC-5); 132.7 (C_i, PhC-2); 132.4 (C_o, PhC-5); 131.0 (C_p, NPh); 130.9 (C_p, PhC-2); 130.3 (C_m, NPh); 130.0 (C_m, PhC-2); 129.5 (C_m, PhC-5); 127.5 (C_o, NPh); 126.7 (C_o, PhC-2); 125.8 (C_i, PhC-5); 123.6 (C-4, pyrrolium iodide); 87.1 (C-2, pyrrolium iodide); 22.7 (Me); 10.8 (MeSe). ¹⁵**N NMR** (40.56 MHz, CDCl₃): δ -172.9. ⁷⁷**Se NMR** (76.31 MHz, CDCl₃): δ 295.9. **IR** (neat): ν_{max} = 2924, 2852, 1598, 1582, 1556, 1492, 1455, 1382, 1340, 1319, 1282, 1221, 1188, 1158, 1130, 1092, 1075, 1028, 1004, 973, 918, 865, 845, 821, 770, 764, 728, 696, 668, 658, 640, 623, 610, 550, 519 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₄H₂₂NSe]⁺ 404.0917, found 404.0918.

2-Methyl-3-(methylselanyl)-1,2-diphenyl-5-(thiophen-2-yl)-2H-pyrrolium iodide (6b).



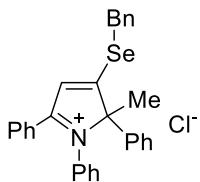
Yield: 0.499 g (93%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 9.54 (d, 1H, H-5, thienyl, ⁴J_{5,3} = 1.1 Hz); 8.51 (s, 1H, H-4, pyrrolium iodide); 7.85 (dd, 1H, H-3, thienyl, ³J_{3,4} = 5.0 Hz, ⁴J_{3,5} = 1.1 Hz); 7.62–7.60 (m, 2H, H_m, NPh); 7.48–7.29 (m, 7H, H_{m,p}, PhC-2; H_{o,p}, NPh; H-4, thienyl); 7.18–7.15 (m, 2H, H_o, PhC-2); 3.04 (s, 3H, MeSe, ²J = 10.9 Hz); 2.01 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 181.9 (C-3, pyrrolium iodide); 165.6 (C-5, pyrrolium iodide); 146.8 (C-5, thienyl); 142.2 (C-3, thienyl); 133.4 (C_i, PhC-2); 132.7 (C_i, NPh); 132.2 (C_p, NPh); 130.7 (C_m, NPh); 130.1 (C_p, PhC-2); 129.6 (C_m, PhC-2); 129.1 (C_o, NPh); 128.5 (C-4, thienyl); 127.0 (C-2, thienyl); 126.8 (C_o, PhC-2); 121.9 (C-4, pyrrolium iodide); 85.7 (C-2, pyrrolium iodide); 23.2 (Me); 11.2 (MeSe). **¹⁵N NMR** (40.56 MHz, CDCl₃): δ -185.4. **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 277.8. **IR** (neat): ν_{max} = 2925, 2852, 1593, 1559, 1508, 1494, 1466, 1453, 1417, 1387, 1341, 1320, 1280, 1223, 1190, 1158, 1104, 1097, 1075, 1041, 1027, 1003, 971, 917, 860, 845, 781, 759, 729, 706, 694, 654, 639, 614, 600, 568, 536, 505, 494 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₂H₂₀NSSe]⁺ 410.0482, found 410.0479.

1-(4-Chlorophenyl)-2-ethyl-2-methyl-3-(methylselanyl)-5-phenyl-2H-pyrrolium iodide (6c).



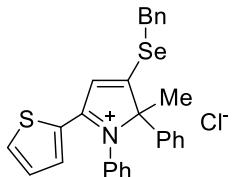
Yield: 0.475 g (92%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 7.81 (br.d, 2H, H_o, PhC-5, ³J = 7.7 Hz); 7.57 (s, 1H, H-4, pyrrolium iodide); 7.55 (t, 1H, H_p, PhC-5, ³J = 7.7 Hz); 7.50 (d, 2H, H-3,5, C₆H₄Cl, ³J = 8.8 Hz); 7.41 (t, 2H, H_m, PhC-5, ³J = 7.7 Hz); 7.37 (d, 2H, H-2,6, C₆H₄Cl, ³J = 8.8 Hz); 2.91 (s, 3H, MeSe, ²J = 10.0 Hz); 2.21, 1.93 (AB-dq, MeCH₂, ²J = 15.3 Hz, ³J = 7.2 Hz); 1.66 (s, 3H, Me); 0.84 (t, 3H, MeCH₂, ³J = 7.2 Hz). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 185.7 (C-3, pyrrolium iodide); 175.1 (C-5, pyrrolium iodide); 137.4 (C-1, C₆H₄Cl); 134.8 (C_p, PhC-5); 133.4 (C-4, C₆H₄Cl); 131.9 (C_o, PhC-5); 131.1 (C-3,5, C₆H₄Cl); 129.6 (C_m, PhC-5); 129.2 (C-2,6, C₆H₄Cl); 125.5 (C_i, PhC-5); 123.5 (C-4, pyrrolium iodide); 86.8 (C-2, pyrrolium iodide); 31.9 (MeCH₂); 25.4 (Me); 10.6 (MeSe); 7.6 (MeCH₂). **¹⁵N NMR** (40.56 MHz, CDCl₃): δ -183.9. **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 298.0. **IR** (neat): ν_{max} = 2970, 2924, 2851, 1598, 1581, 1490, 1454, 1385, 1334, 1323, 1297, 1276, 1226, 1190, 1160, 1113, 1091, 1075, 1058, 1013, 976, 918, 880, 837, 795, 773, 729, 707, 687, 640, 623, 591, 558, 526 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₀H₂₁ClNSe]⁺ 390.0527, found 390.0526.

3-(Benzylselanyl)-2-methyl-1,2,5-triphenyl-2*H*-pyrrolium chloride (7a).



Yield: 0.474 g (92%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 8.69 (s, 1H, H-4, pyrrolium chloride); 8.07–8.03 (m, 2H, H_o, PhC-5); 7.55–7.15 (m, 16H, H_{o,m,p}, PhCH₂; H_{o,m,p}, PhC-2; H_{m,p}, PhC-5; H_{m,p}, NPh); 6.75 (m, 2H, H_o, NPh); 5.17, 5.03 (AB-d, PhCH₂, ²J = 11.4 Hz); 1.98 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 186.1 (C-3, pyrrolium chloride); 174.8 (C-5, pyrrolium chloride); 135.7 (C_i, PhCH₂); 135.2 (C_i, NPh); 135.0 (C_p, PhC-5); 132.8 (C_i, PhC-2); 132.7 (C_o, PhC-5); 130.9 (C_p, NPh); 130.7 (C_p, PhC-2); 130.3 (C_m, PhC-5); 129.9 (C_o, NPh); 129.8 (C_o, PhCH₂); 129.5 (C_m, PhCH₂); 128.9 (C_m, PhC-2); 127.9 (C_p, PhCH₂); 127.5 (C_m, NPh); 126.7 (C_o, PhC-2); 126.0 (C_i, PhC-5); 124.6 (C-4, pyrrolium chloride); 87.0 (C-2, pyrrolium chloride); 34.2 (PhCH₂); 23.0 (Me). **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 402.1. **IR** (neat): ν_{max} = 3059, 3030, 3003, 2932, 1598, 1582, 1555, 1493, 1456, 1380, 1327, 1296, 1222, 1192, 1181, 1159, 1143, 1117, 1092, 1074, 1028, 1002, 972, 926, 866, 848, 762, 725, 697, 668, 658, 638, 623, 608, 550, 457, 418 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₃₀H₂₆NSe]⁺ 480.1230, found 480.1226.

3-(Benzylselanyl)-2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-2*H*-pyrrolium chloride (7b).



Yield: 0.485 g (93%); waxy product. **¹H NMR** (400.13 MHz, CDCl₃): δ 9.76 (d, 1H, H-5, thienyl, ³J_{5,4} = 4.1 Hz); 9.26 (s, 1H, H-4, pyrrolium chloride); 7.78 (d, 1H, H-3, thienyl, ³J_{3,4} = 5.0 Hz); 7.52–7.47 (m, 4H, H_o, NPh; H_m, PhCH₂); 7.36–7.13 (m, 10H, H_{m,p}, PhC-2; H_{m,p}, NPh; H_{o,p}, PhCH₂; H-4, thienyl); 6.99 (d, 2H, H_o, PhC-2, ³J = 8.0 Hz); 5.07, 5.01 (AB-d, PhCH₂, ²J = 11.5 Hz); 1.93 (s, 3H, Me). **¹³C{¹H} NMR** (100.62 MHz, CDCl₃): δ 180.0 (C-3, pyrrolium chloride); 166.1 (C-5, pyrrolium chloride); 147.8 (C-5, thienyl); 141.9 (C-3, thienyl); 135.7 (C_i, PhCH₂); 133.4 (C_i, NPh); 132.8 (C_i, PhC-2); 132.1 (C_p, NPh); 130.4 (C_p, PhC-2); 129.7 (C_o, NPh); 129.6 (C_o, PhCH₂); 129.4 (C_m, PhCH₂); 128.9 (C-4, thienyl); 128.6 (C_m, PhC-2); 127.6 (C_p, PhCH₂); 127.3 (C-2, thienyl); 126.8 (C_o, PhC-2); 126.7 (C_m, NPh); 123.3 (C-4, pyrrolium chloride); 85.7 (C-2, pyrrolium chloride); 33.8 (PhCH₂); 23.0 (Me). **¹⁵N NMR** (40.56 MHz, CDCl₃): δ -185.4. **⁷⁷Se NMR** (76.31 MHz, CDCl₃): δ 387.6. **IR** (neat): ν_{max} = 3051, 3003, 2934, 1593, 1559, 1509, 1495, 1468, 1453, 1418, 1387, 1341, 1287, 1225, 1193, 1166, 1106, 1075, 1041, 1028, 1002, 996, 969, 925, 875, 861, 843, 811, 780, 759, 730, 711, 704, 695, 669, 638, 614, 599, 570, 553, 536, 503, 493 cm⁻¹. **HRMS** (ESI-TOF) calcd for [C₂₈H₂₄NSSe]⁺ 486.0795, found 486.0796.

4. Quantum chemical computations

4.1 Computational details

The ground-state equilibrium structural parameters of selone **2a** and hypothetic hydrogenated selone ("H-selone") molecules (Figs. S1 and S2) have been obtained by means of the full geometry optimization performed using density-functional theory (DFT) with B3LYP functional⁷ and the cc-pVDZ (C,N,H),⁸ aug-cc-pVDZ-pp/ECP (Se) basis sets (basis A),⁹ followed by vibrational analysis in harmonic approximation to confirm the absence of imaginary frequencies. The optimal geometries in terms of the Cartesian coordinates are reported in Tables S5 and S6, whereas the selected bond length are shown in Figs. S3 and S4. For the equilibrium geometries found, the dipole moments have been evaluated at the Hartree-Fock (HF), B3LYP, second-order Møller-Plesset (MP2) and relaxed coupled-cluster singles and doubles (CCSD) levels of theory¹⁰ using basis A. The calculations have been carried out using the GAUSSIAN program package¹¹ except for the CCSD calculations which were performed using Orca program.¹² The results of the dipole moment calculations are shown in Table S1. For each molecule, the lowest four vertical ionization energies have been computed using the outer-valence Green's function (OVGF) method¹³ and the third-order algebraic-diagrammatic construction approximation for electron-propagator (IP-ADC(3))¹⁴ (Table S2). The calculations were done for basis A employing the GAUSSIAN and Q-Chem¹⁵ programs, respectively.

⁷ (a) A. D. Becke, Density-functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys.*, 1993, **98**, 5648–5652; (b) C. Lee, W. Yang and R. G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, *Phys. Rev. B*, 1988, **37**, 785–789.

⁸ T. H. Dunning, Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen, *J. Chem. Phys.*, 1989, **90**, 1007–1023.

⁹ (a) K. A. Peterson, D. Figgen, E. Goll, H. Stoll and M. Dolg, Systematically convergent basis sets with relativistic pseudopotentials. II. Small-core pseudopotentials and correlation consistent basis sets for the post-d group 16-18 elements, *J. Chem. Phys.*, 2003, **119**, 11113–11123; (b) B. P. Pritchard, D. Altarawy, B. Didier, T. D. Gibson and T. L. Windus, New Basis Set Exchange: An Open, Up-to-Date Resource for the Molecular Sciences Community, *J. Chem. Inf. Model.*, 2019, **59**, 4814–4820.

¹⁰ G. D. Purvis and R. J. Bartlett, A full coupled-cluster singles and doubles model: The inclusion of disconnected triples, *J. Chem. Phys.*, 1982, **76**, 1910–1918.

¹¹ M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc.: Wallingford, CT, USA, 2009.

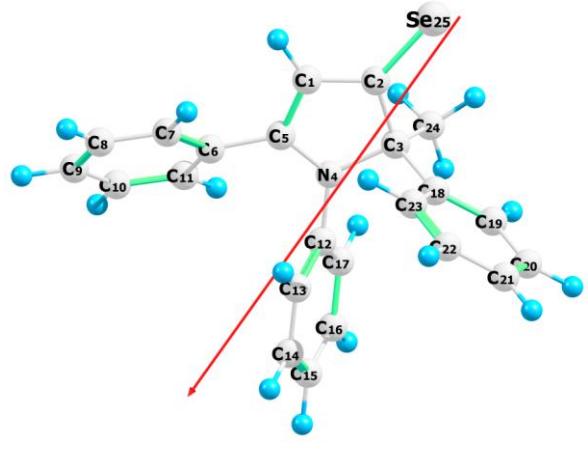
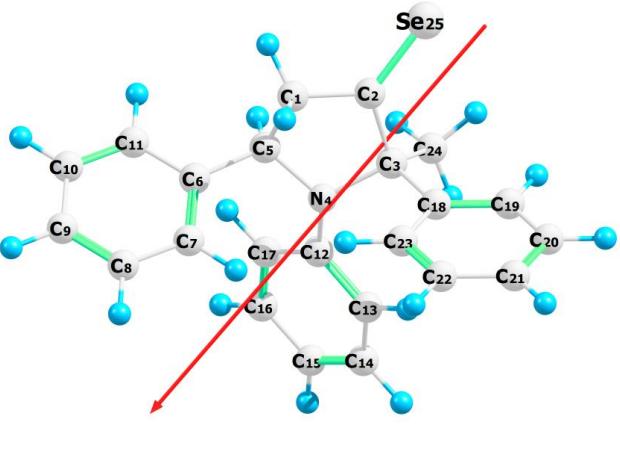
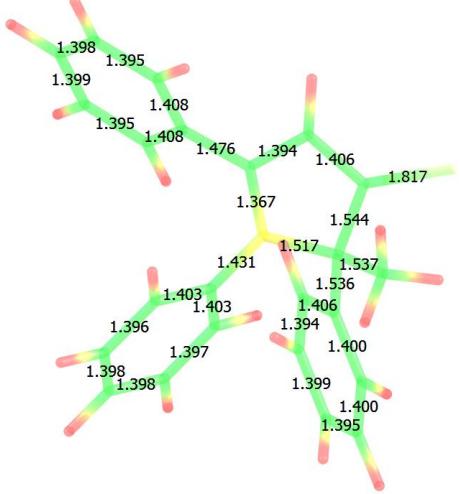
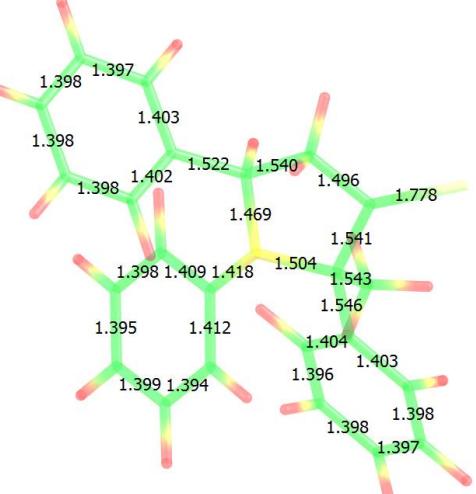
¹² F. Neese, Software update: The ORCA program system—Version 5.0, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2022, **12**, e1606.

¹³ W. von Niessen, J. Schirmer and L. S. Cederbaum, Computational methods for the one-particle Green's function, *Comput. Phys. Rep.*, 1984, **1**, 57–125.

¹⁴ (a) J. Schirmer, A. B. Trofimov and G. Stelter, A non-Dyson third-order approximation scheme for the electron propagator, *J. Chem. Phys.*, 1998, **109**, 4734–4744; (b) A. B. Trofimov and J. Schirmer, Molecular ionization energies and ground- and ionic-state properties using a non-Dyson electron propagator approach, *J. Chem. Phys.*, 2005, **123**, 144115; (c) A. L. Dempwolff, A. C. Paul, A. M. Belogolova, A. B. Trofimov and A. Dreuw, Intermediate state representation approach to physical properties of molecular electron-detached states. I. Theory and implementation, *J. Chem. Phys.*, 2020, **152**, 024113.

In order to obtain a more sensible information of atomic charges and bond orders for the molecules under consideration, additional calculations have been performed at the B3LYP level of theory using cc-pVTZ basis set (basis B).¹⁶ The optimized geometries and the results of the Mulliken analysis of B3LYP electron densities obtained are shown in Tables S7, S8 and Figures S6–S9.

4.2 Results of the quantum chemical computations

	
Figure S1. Schematic representation of selone molecule showing atom numbering used in the computations and spatial orientation of the dipole moment vector (red).	Figure S2. Schematic representation of <i>H</i> -selone showing atom numbering used in the computations and spatial orientation of the dipole moment vector (red).
	
Figure S3. Selected bond lengths (\AA) of selone computed at the B3LYP/basis A level of theory.	Figure S4. Selected bond lengths (\AA) of <i>H</i> -selone computed at the B3LYP/basis A level of theory.

¹⁵ (a) Y. Shao et al., Advances in methods and algorithms in a modern quantum chemistry program package, *Phys. Chem. Chem. Phys.*, 2006, **8**, 3172–3191; (b) A. I. Krylov and P. M. W. Gill, Q-Chem: an engine for innovation, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2013, **3**, 317–326.

¹⁶ A. K. Wilson, D. E. Woon, K. A. Peterson and T. H. Dunning, Gaussian basis sets for use in correlated molecular calculations. IX. The atoms gallium through krypton, *J. Chem. Phys.*, 1999, **110**, 7667–7676.

Table S1. Cartesian components and module of dipole moment (Debye) of selone and *H*-selone obtained using HF, MP2, B3LYP and CCSD methods with basis A (B3LYP/ basis A geometry). In the case of HF and B3LYP, basis B results also given for comparison (B3LYP/basis B geometry).

Molecule	Method	X	Y	Z	$ \mu $
Selone					
	HF (A)	-7.36	5.05	-0.48	8.94
	HF (B)	-7.16	4.94	-0.43	8.71
	B3LYP (A)	-5.99	4.47	-0.35	7.48
	B3LYP (B)	-5.75	4.29	-0.32	7.18
	MP2	-5.76	4.48	-0.38	7.31
	CCSD	-6.05	4.60	-0.38	7.60
H-Selone					
	HF (A)	-2.05	1.19	-0.66	2.46
	HF (B)	-2.02	1.06	-0.65	2.37
	B3LYP (A)	-1.45	0.67	-0.64	1.72
	B3LYP (B)	-1.38	0.50	-0.60	1.59
	MP2	-1.15	0.46	-0.49	1.33
	CCSD	-1.40	0.66	-0.48	1.61

Note the agreement of Basis A and B results both at the HF and B3LYP level of theory which implies that the results are rather good converged with respect to the basis set. The B3LYP and CCSD results for the same basis (A) are in excellent agreement with each other.

Table S2. Vertical ionization energies (eV) associated with HOMO, HOMO-1, HOMO-2, and HOMO-3 of selone and *H*-selone obtained using HF (Koopmans' theorem), OVGF and IP-ADC(3) methods with basis A (B3LYP/basis A geometry). The corresponding pole strengths (a.u.) for ionization transitions are shown in parentheses.

Molecule	Method	HOMO	HOMO-1	HOMO-2	HOMO-3
Selone					
	HF (A)	7.19 (1.00)	7.52 (1.00)	8.91 (1.00)	9.08 (1.00)
	HF (B)	7.23 (1.00)	7.55 (1.00)	8.98 (1.00)	9.14 (1.00)
	OVGF	6.63 (0.88)	6.89 (0.87)	8.41 (0.89)	8.70 (0.89)
	IP-ADC(3)	6.48 (0.84)	6.82 (0.84)	8.34 (0.84)	—
H-Selone					
	HF (A)	8.11 (1.00)	8.48 (1.00)	8.85 (1.00)	8.93 (1.00)
	HF (B)	8.10 (1.00)	8.49 (1.00)	8.89 (1.00)	8.96 (1.00)
	OVGF	7.38 (0.89)	7.86 (0.89)	8.43 (0.89)	8.46 (0.89)
	IP-ADC(3)	7.29 (0.88)	7.80 (0.87)	8.39 (0.87)	8.46 (0.87)

Here the HF results for Basis A and B are again in excellent agreement indicating that they are sufficiently converged with respect to the basis set and that the OVGF and IP-ADC(3) predictions obtained using smaller basis A should be already quite accurate.

Table S3. Localization properties of MOs in **selone** (Mulliken MOs population on atoms) for HOMO through HOMO-3 and LUMO computed at the HF/Basis B level of theory (Fig. S5) and their assignment in terms of the local symmetries (σ and π). Sum over all atoms is unity (atoms that contribute less than 0.10 are not shown).

Atom	HOMO (π)	HOMO-1 (σ_{LP} Se)	HOMO-2 (π)	HOMO-3 (π)	LUMO (π)
C ₁	0.17	0.01	0.02	0.00	0.02
C ₂	0.04	0.01	0.02	0.00	0.20
C ₅	0.06	0.00	0.00	0.00	0.22
C ₁₈	0.00	0.00	0.21	0.09	0.01
C ₁₉	0.00	0.00	0.01	0.30	0.00
C ₂₀	0.00	0.00	0.21	0.08	0.00
C ₂₁	0.00	0.00	0.21	0.08	0.00
C ₂₂	0.00	0.00	0.01	0.30	0.00
C ₂₃	0.00	0.00	0.21	0.09	0.00
Se ₂₅	0.59	0.93	0.01	0.00	0.14

Table S4. Localization properties of MOs in **H-selone** (Mulliken MOs population on atoms) for HOMO through HOMO-3 and LUMO computed at the HF/Basis B level of theory (Fig. S5) and their assignment in terms of the local symmetries (σ and π). Sum over all atoms is unity (atoms that contribute less than 0.10 are not shown).

Atom	HOMO (π)	HOMO-1 (σ_{LP} Se)	HOMO-2 (π)	HOMO-3 (π)	LUMO (π)
C ₂	0.00	0.01	0.06	0.00	0.47
N ₄	0.17	0.02	0.00	0.00	0.00
C ₆	0.01	0.02	0.00	0.11	0.00
C ₉	0.00	0.02	0.00	0.11	0.00
C ₁₂	0.17	0.01	0.00	0.01	0.00
C ₁₃	0.11	0.01	0.00	0.12	0.00
C ₁₄	0.04	0.00	0.00	0.13	0.00
C ₁₅	0.23	0.01	0.00	0.01	0.00
C ₁₆	0.05	0.00	0.00	0.12	0.00
C ₁₇	0.10	0.00	0.00	0.13	0.00
C ₁₈	0.00	0.00	0.22	0.00	0.02
C ₂₁	0.00	0.01	0.21	0.00	0.02
Se ₂₅	0.04	0.75	0.21	0.03	0.34

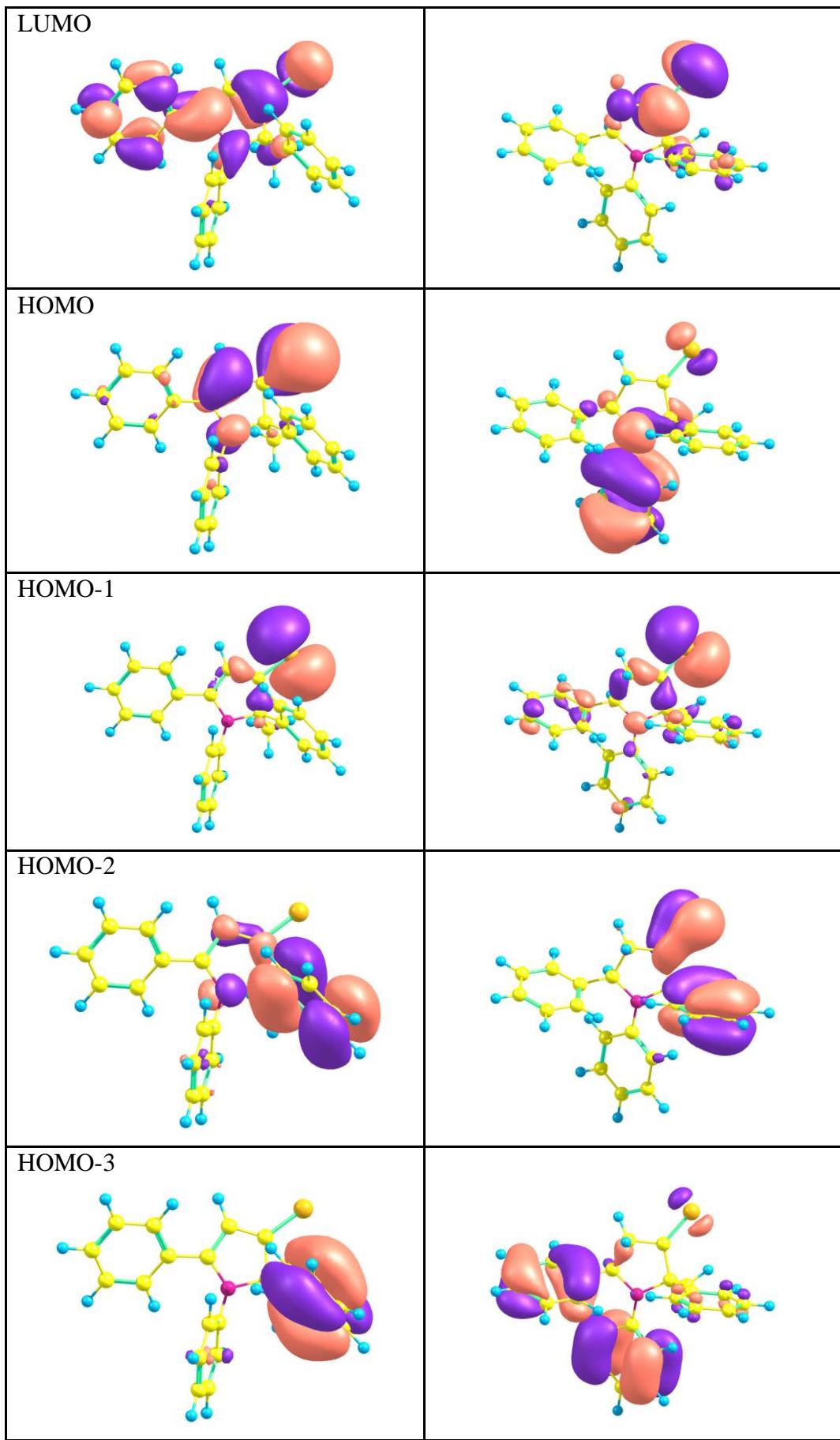


Figure S5. Molecular orbitals of selone (left) and *H*-selone (right), LUMO and HOMO through HOMO-3, obtained at the HF/basis B level of theory.

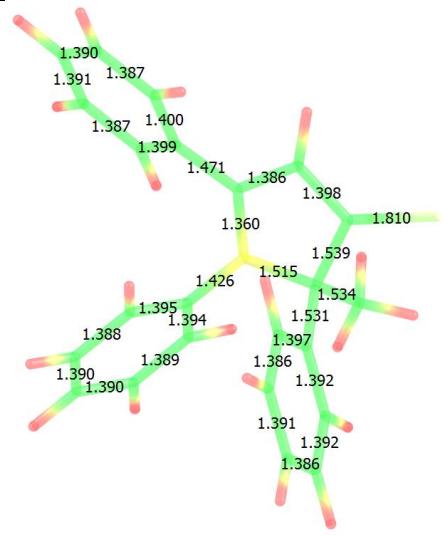


Figure S6. Selected bond lengths (\AA) of selone computed at the B3LYP/basis B level of theory.

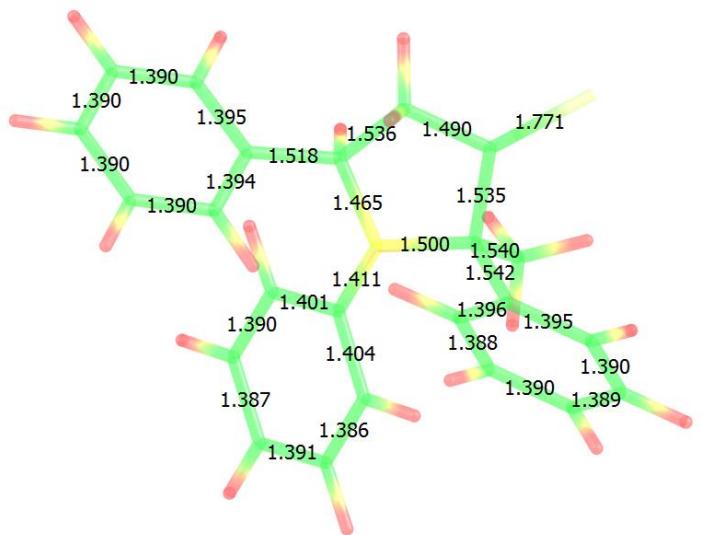


Figure S7. Selected bond lengths (\AA) of H -selone computed at the B3LYP/basis B level of theory.

Note good agreement with the results obtained using basis A. The differences concern third digit after the decimal point. The structural parameters are well converged with respect to basis set.

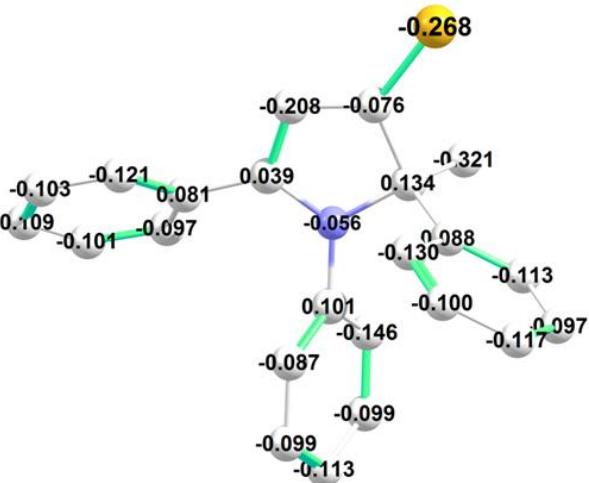


Figure S8. Mulliken charges on atoms in selone computed at the B3LYP/basis B level of theory.

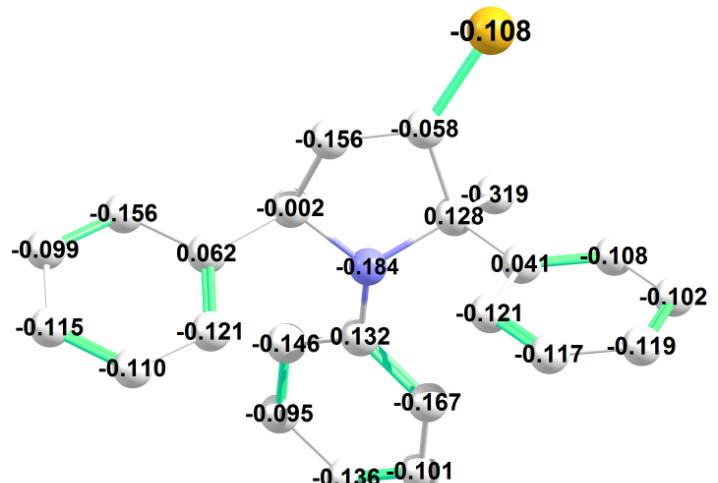


Figure S9. Mulliken charges on atoms in H -selone computed at the B3LYP/basis B level of theory.

Table S5. Optimized geometry of **selone** in terms of Cartesian coordinates (Å) obtained at the B3LYP/Basis A level of theory ($E_T = -1315.912158$ Hartree).

No.	Atomic No.	X	Y	Z
1	6	0.021707	-2.095907	-0.074017
2	6	1.286685	-1.613984	0.306156
3	6	1.104205	-0.144261	0.742079
4	7	-0.389075	0.053841	0.563271
5	6	-0.940699	-1.098028	0.074948
6	6	-2.382418	-1.278598	-0.184993
7	6	-2.788507	-2.077906	-1.270869
8	6	-4.142504	-2.308006	-1.516278
9	6	-5.112771	-1.754055	-0.675571
10	6	-4.719734	-0.966354	0.411136
11	6	-3.367613	-0.723609	0.653498
12	6	-0.997375	1.347941	0.518623
13	6	-1.441449	1.883174	-0.699678
14	6	-2.037313	3.144909	-0.735691
15	6	-2.181398	3.891306	0.437785
16	6	-1.735495	3.362594	1.652201
17	6	-1.152826	2.093212	1.696650
18	6	1.868171	0.820607	-0.177471
19	6	2.666227	1.855757	0.323126
20	6	3.340348	2.724168	-0.543566
21	6	3.225040	2.571510	-1.924975
22	6	2.433495	1.537454	-2.436727
23	6	1.767101	0.670670	-1.571456
24	6	1.467532	-0.016968	2.229854
25	34	2.863281	-2.515977	0.362248
26	1	-0.189567	-3.121413	-0.364643
27	1	-2.034412	-2.506022	-1.933718
28	1	-4.440542	-2.922672	-2.368335
29	1	-6.172670	-1.936859	-0.865631
30	1	-5.471752	-0.537924	1.077199
31	1	-3.073241	-0.115663	1.508826
32	1	-1.313420	1.306969	-1.616439
33	1	-2.380914	3.550771	-1.689611
34	1	-2.641636	4.881098	0.405857
35	1	-1.851709	3.934286	2.575520
36	1	-0.835584	1.667276	2.648673
37	1	2.780881	1.995929	1.397470
38	1	3.961232	3.521644	-0.128991
39	1	3.753556	3.247423	-2.600969
40	1	2.343671	1.398114	-3.516567
41	1	1.170566	-0.145129	-1.984757
42	1	2.522205	-0.297778	2.362401
43	1	1.312316	1.002985	2.606659
44	1	0.850531	-0.710443	2.819145

Table S6. Optimized geometry of **H-selone** in terms of Cartesian coordinates (Å) obtained at the B3LYP/Basis A level of theory (E_T = - 1317.101395 Hartree).

No.	Atomic No.	X	Y	Z
1	6	0.020940	-2.035080	0.089837
2	6	1.290237	-1.387790	0.545211
3	6	1.060484	0.135658	0.582493
4	7	-0.419068	0.252887	0.339948
5	6	-1.077955	-1.046720	0.523565
6	6	-2.361875	-1.243048	-0.269541
7	6	-2.606937	-0.575177	-1.477567
8	6	-3.764741	-0.841209	-2.213594
9	6	-4.693993	-1.779872	-1.755794
10	6	-4.460506	-2.447217	-0.550094
11	6	-3.304997	-2.175762	0.187261
12	6	-1.094942	1.434007	0.740056
13	6	-0.586347	2.700464	0.378647
14	6	-1.248320	3.869617	0.750983
15	6	-2.443755	3.818015	1.475693
16	6	-2.961792	2.570752	1.825654
17	6	-2.298404	1.392314	1.471049
18	6	1.878563	0.752805	-0.574714
19	6	3.141058	1.326096	-0.358242
20	6	3.886578	1.836355	-1.425350
21	6	3.389304	1.775908	-2.729151
22	6	2.135538	1.201326	-2.956566
23	6	1.389775	0.695615	-1.889940
24	6	1.457332	0.688712	1.967414
25	34	2.779510	-2.245887	0.999173
26	1	0.035546	-2.098219	-1.013825
27	1	-1.896106	0.172441	-1.831870
28	1	-3.944247	-0.305747	-3.148884
29	1	-5.599003	-1.985025	-2.331973
30	1	-5.182486	-3.177971	-0.178173
31	1	-3.133222	-2.695933	1.134246
32	1	0.330290	2.767062	-0.205906
33	1	-0.826706	4.834093	0.457370
34	1	-2.963844	4.735770	1.757170
35	1	-3.895268	2.502966	2.389654
36	1	-2.734539	0.439126	1.765121
37	1	3.557370	1.378941	0.646904
38	1	4.864430	2.283259	-1.231560
39	1	3.973398	2.174539	-3.561592
40	1	1.731416	1.149085	-3.970294
41	1	0.405590	0.265045	-2.073729
42	1	2.485777	0.397320	2.215326
43	1	1.371029	1.782832	1.996615
44	1	0.793205	0.268412	2.737236
45	1	-0.108009	-3.052107	0.479632
46	1	-1.305952	-1.240564	1.593152

Table S7. Optimized geometry of **selone** in terms of Cartesian coordinates (Å) obtained at the B3LYP/Basis B level of theory ($E_T = -3344.575053$ Hartree).

No.	Atomic No.	X	Y	Z
1	6	-0.001634	-2.085665	0.076305
2	6	-1.264388	-1.618243	-0.297887
3	6	-1.096645	-0.152917	-0.736069
4	7	0.391373	0.059320	-0.547786
5	6	0.947363	-1.086093	-0.069536
6	6	2.385847	-1.260010	0.183353
7	6	2.799671	-2.043086	1.267396
8	6	4.148197	-2.266610	1.504057
9	6	5.105533	-1.722314	0.655517
10	6	4.705128	-0.951040	-0.430007
11	6	3.358233	-0.715327	-0.663000
12	6	0.988736	1.353684	-0.500561
13	6	1.441354	1.877700	0.710216
14	6	2.024619	3.136325	0.752924
15	6	2.147769	3.892031	-0.407273
16	6	1.692629	3.375616	-1.614294
17	6	1.122364	2.109660	-1.664705
18	6	-1.876271	0.808974	0.165138
19	6	-2.644063	1.850659	-0.347110
20	6	-3.329474	2.716142	0.500984
21	6	-3.254347	2.554575	1.875976
22	6	-2.492151	1.515282	2.399755
23	6	-1.815297	0.651834	1.552436
24	6	-1.450281	-0.045677	-2.224724
25	34	-2.827209	-2.529182	-0.348865
26	1	0.217378	-3.099722	0.362214
27	1	2.058510	-2.464007	1.932501
28	1	4.451153	-2.866499	2.351505
29	1	6.156907	-1.899314	0.837724
30	1	5.444172	-0.532081	-1.099444
31	1	3.059545	-0.120849	-1.513503
32	1	1.329013	1.298640	1.615274
33	1	2.372681	3.531165	1.697853
34	1	2.596145	4.875484	-0.370874
35	1	1.791469	3.952638	-2.523886
36	1	0.799490	1.698453	-2.609502
37	1	-2.728162	1.996471	-1.413194
38	1	-3.925032	3.514728	0.078951
39	1	-3.789763	3.224738	2.535101
40	1	-2.435196	1.369513	3.470331
41	1	-1.247044	-0.165930	1.974188
42	1	-2.490397	-0.338550	-2.358020
43	1	-1.305126	0.961371	-2.608695
44	1	-0.827589	-0.732322	-2.795966

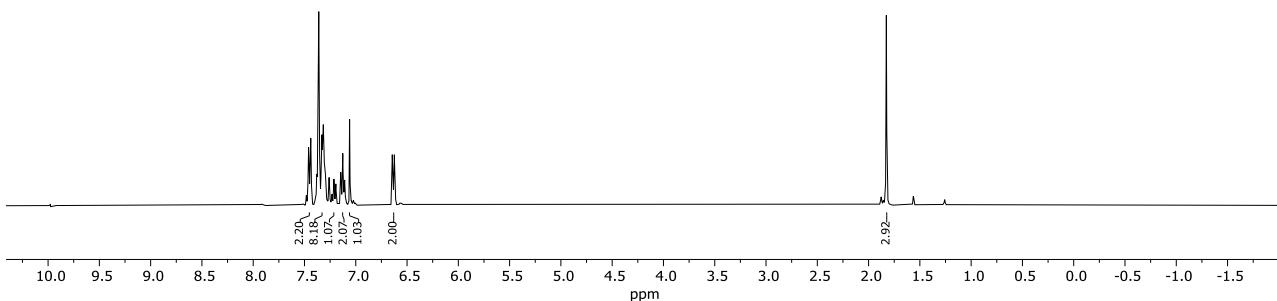
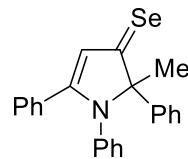
Table S8. Optimized geometry of **H-selone** in terms of Cartesian coordinates (Å) obtained at the B3LYP/Basis B level of theory ($E_T = -3345.766848$ Hartree).

No.	Atomic No.	X	Y	Z
1	6	-0.022810	-2.026192	-0.092638
2	6	-1.287671	-1.381323	-0.543540
3	6	-1.060240	0.136176	-0.581728
4	7	0.417982	0.254610	-0.355225
5	6	1.075764	-1.043266	-0.525835
6	6	2.353471	-1.241853	0.268616
7	6	2.593548	-0.587573	1.475477
8	6	3.743848	-0.854830	2.207927
9	6	4.670755	-1.782701	1.747475
10	6	4.442497	-2.437176	0.543062
11	6	3.294294	-2.163623	-0.190189
12	6	1.092688	1.431600	-0.743206
13	6	0.579503	2.692870	-0.399647
14	6	1.243519	3.854748	-0.760559
15	6	2.444822	3.803010	-1.459821
16	6	2.966639	2.562393	-1.795408
17	6	2.302209	1.391319	-1.449934
18	6	-1.873157	0.754734	0.573431
19	6	-3.134556	1.312614	0.362303
20	6	-3.873484	1.823147	1.423571
21	6	-3.370989	1.776985	2.717284
22	6	-2.119328	1.215854	2.940428
23	6	-1.380962	0.710202	1.878880
24	6	-1.463688	0.685611	-1.963177
25	34	-2.771067	-2.239021	-0.990502
26	1	-0.032925	-2.092521	1.000689
27	1	1.889071	0.150206	1.831558
28	1	3.919009	-0.330831	3.138256
29	1	5.566452	-1.987928	2.318154
30	1	5.159845	-3.156395	0.170545
31	1	3.128548	-2.671422	-1.133101
32	1	-0.338630	2.762928	0.162515
33	1	0.819949	4.810516	-0.480408
34	1	2.963655	4.711698	-1.732090
35	1	3.900450	2.494755	-2.338271
36	1	2.740673	0.447151	-1.731348
37	1	-3.554841	1.353639	-0.630587
38	1	-4.846632	2.256495	1.234296
39	1	-3.947266	2.174179	3.542036
40	1	-1.713233	1.173904	3.942481
41	1	-0.402415	0.291993	2.061047
42	1	-2.480763	0.389805	-2.204945
43	1	-1.384958	1.769539	-1.992794
44	1	-0.805498	0.271974	-2.726488
45	1	0.103624	-3.032986	-0.480668
46	1	1.306250	-1.238626	-1.583862

5. NMR Spectra

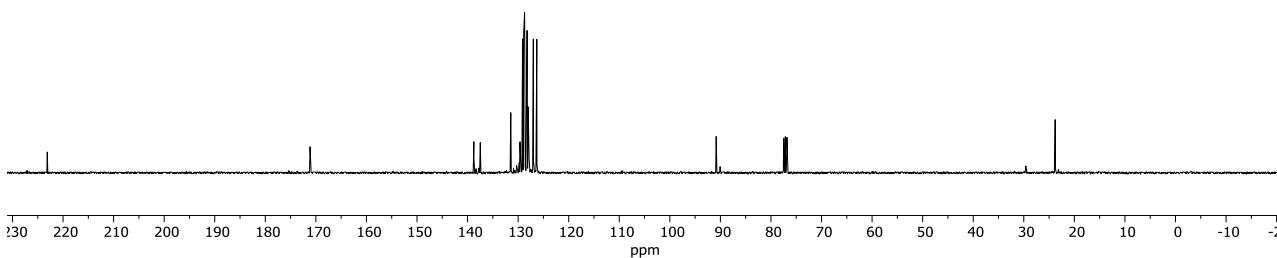
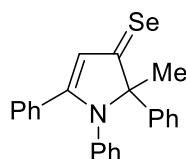
^1H NMR of 2-methyl-1,2,5-triphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2a)

NMR_1H

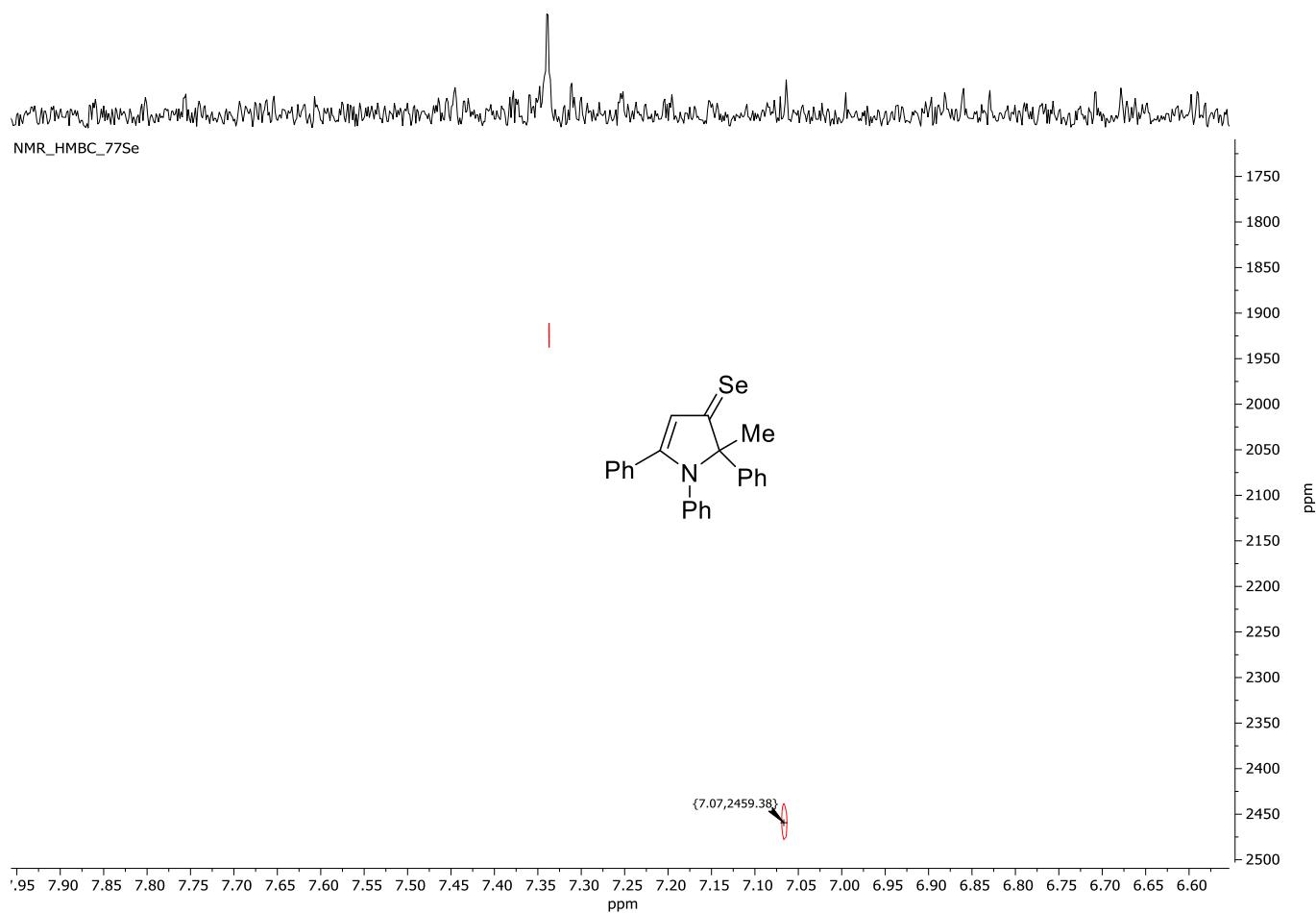


$^{13}\text{C}\{^1\text{H}\}$ NMR of 2-methyl-1,2,5-triphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2a)

NMR_13C

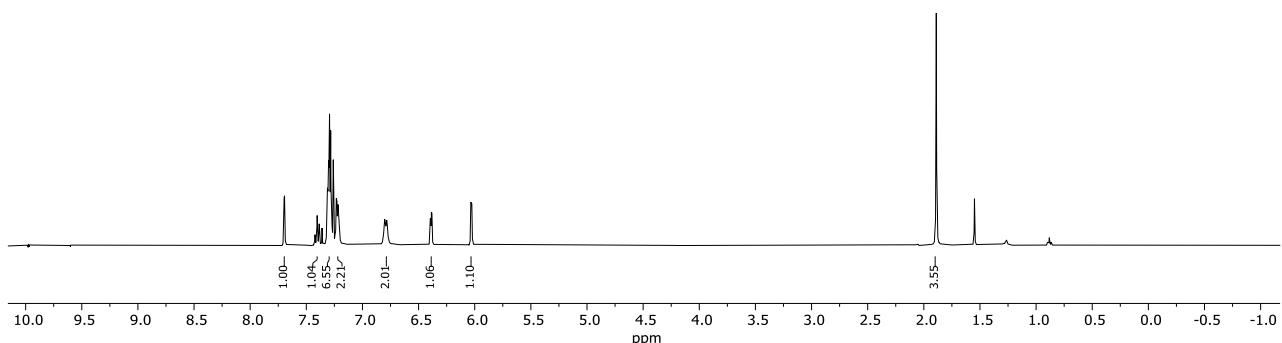
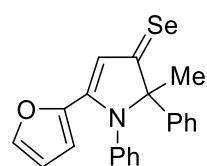


2D ^1H - ^{77}Se HMBC NMR of 2-methyl-1,2,5-triphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2a)



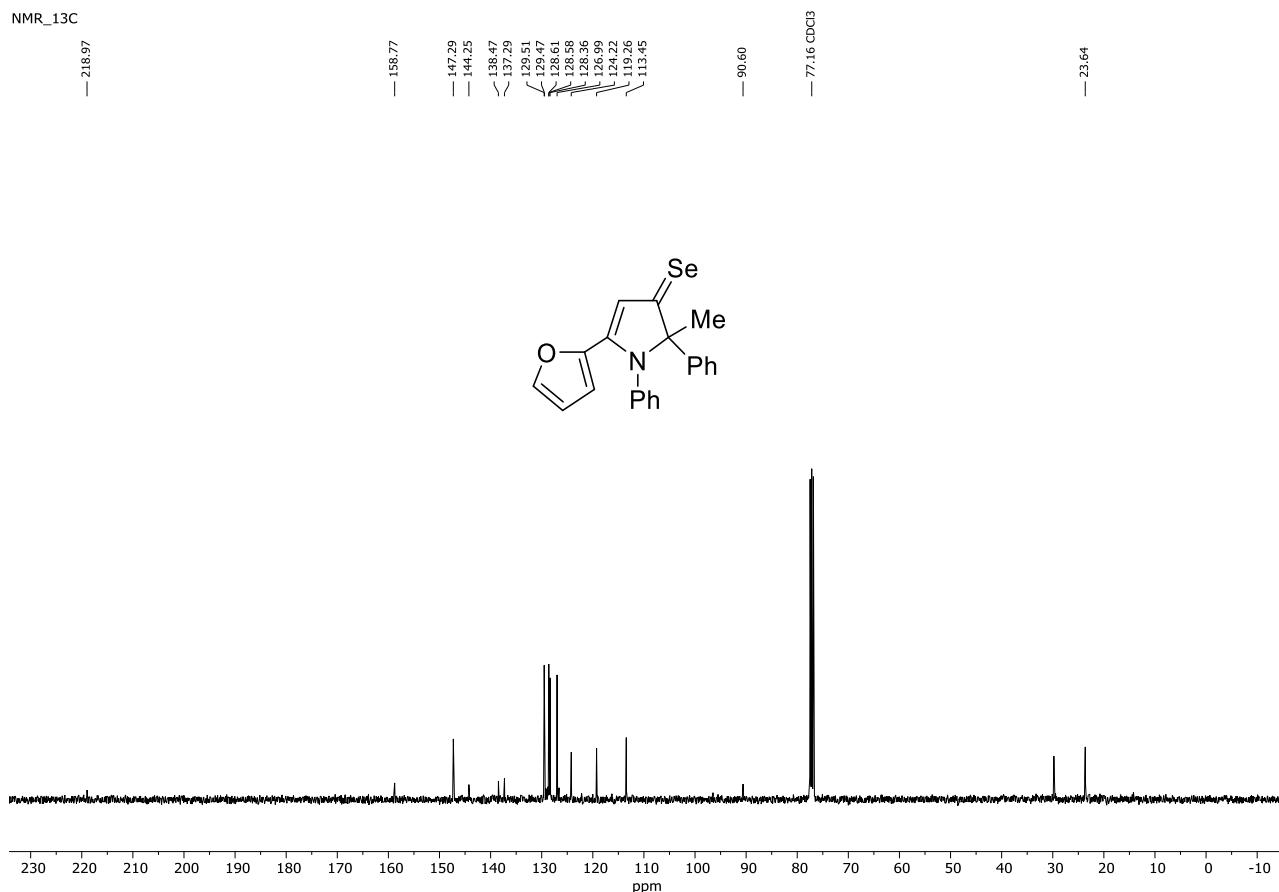
^1H NMR of 5-(furan-2-yl)-2-methyl-1,2-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2b)

NMR_1H



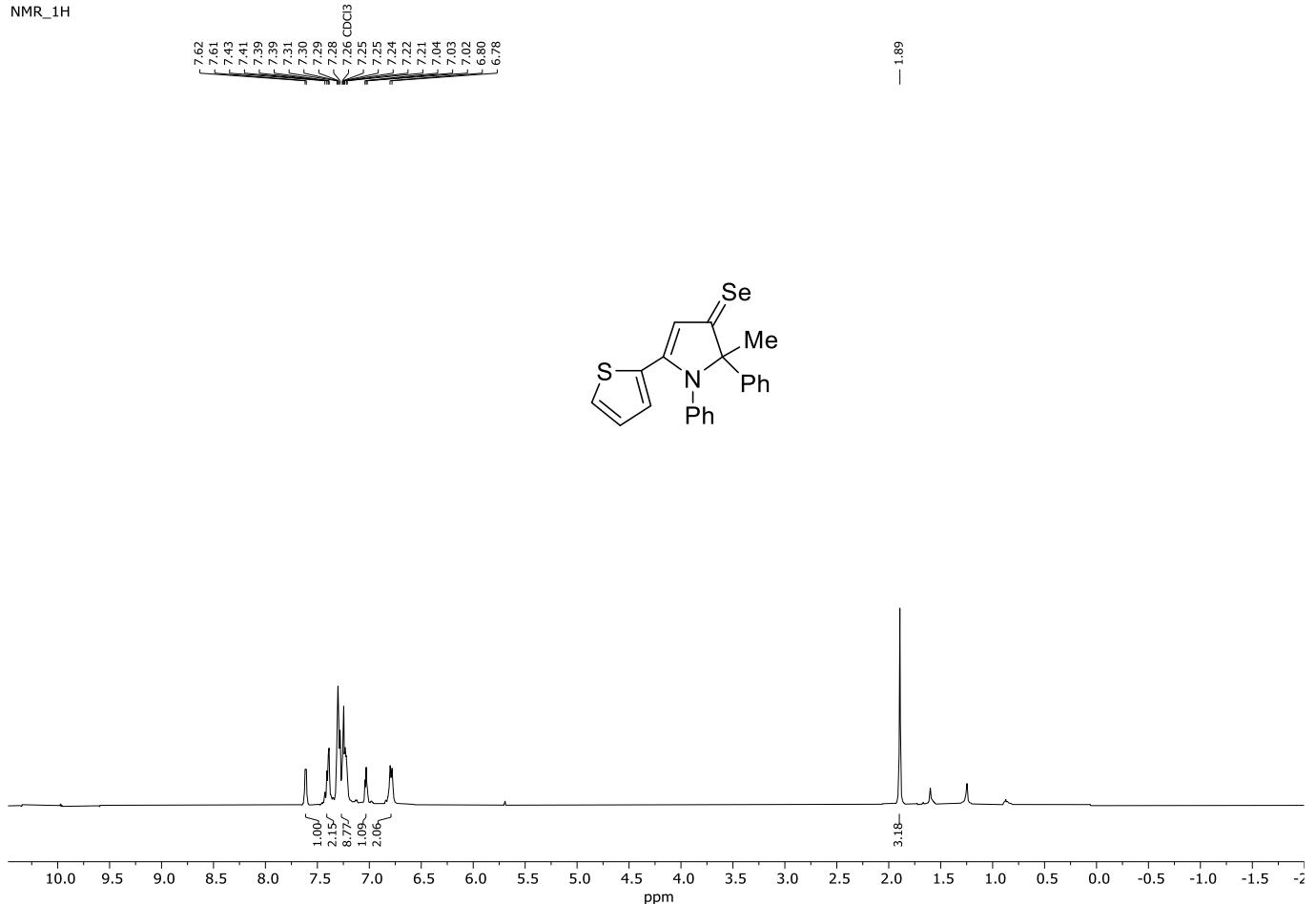
$^{13}\text{C}\{^1\text{H}\}$ NMR of 5-(furan-2-yl)-2-methyl-1,2-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2b)

NMR_13C



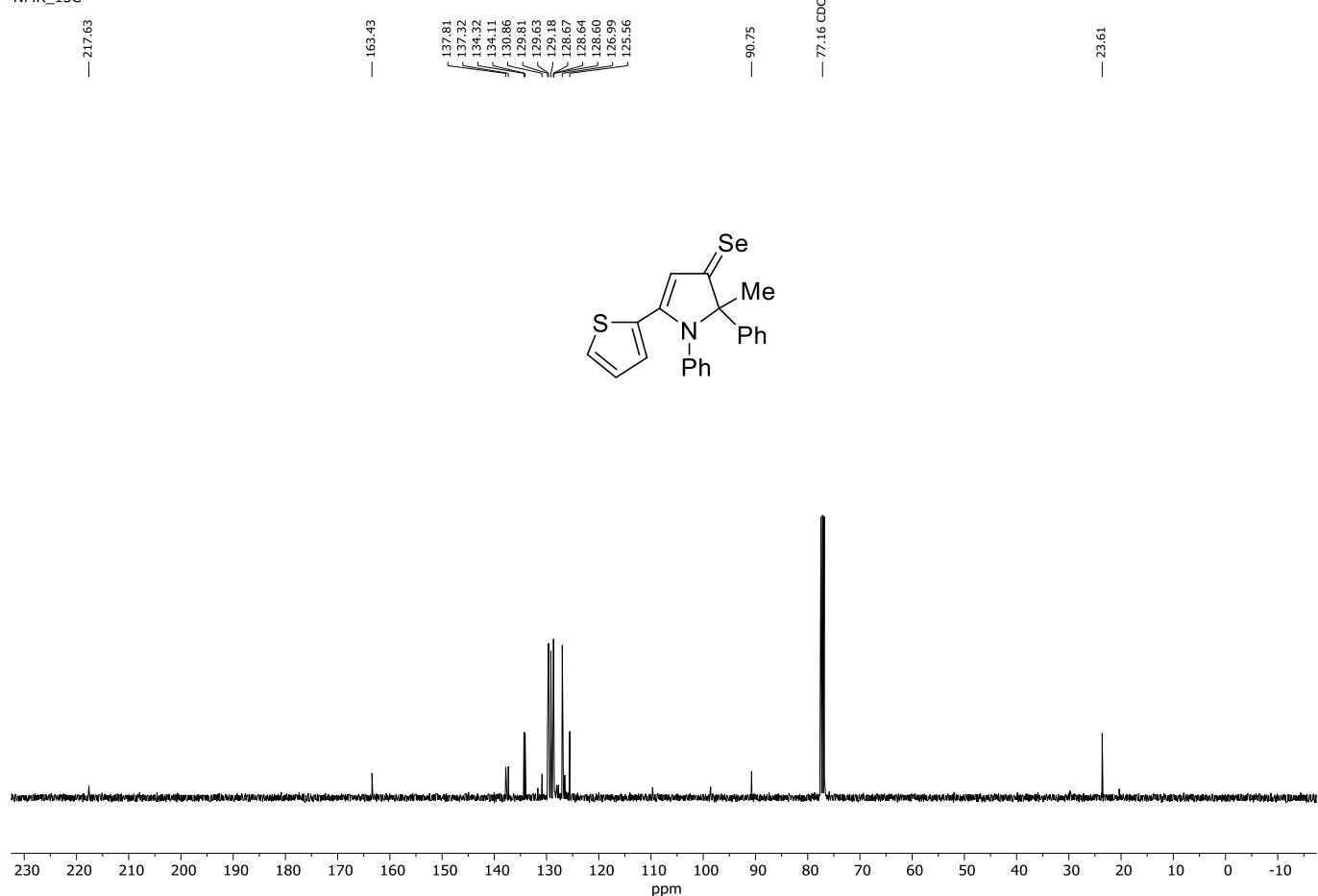
^1H NMR of 2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2c)

NMR_1H

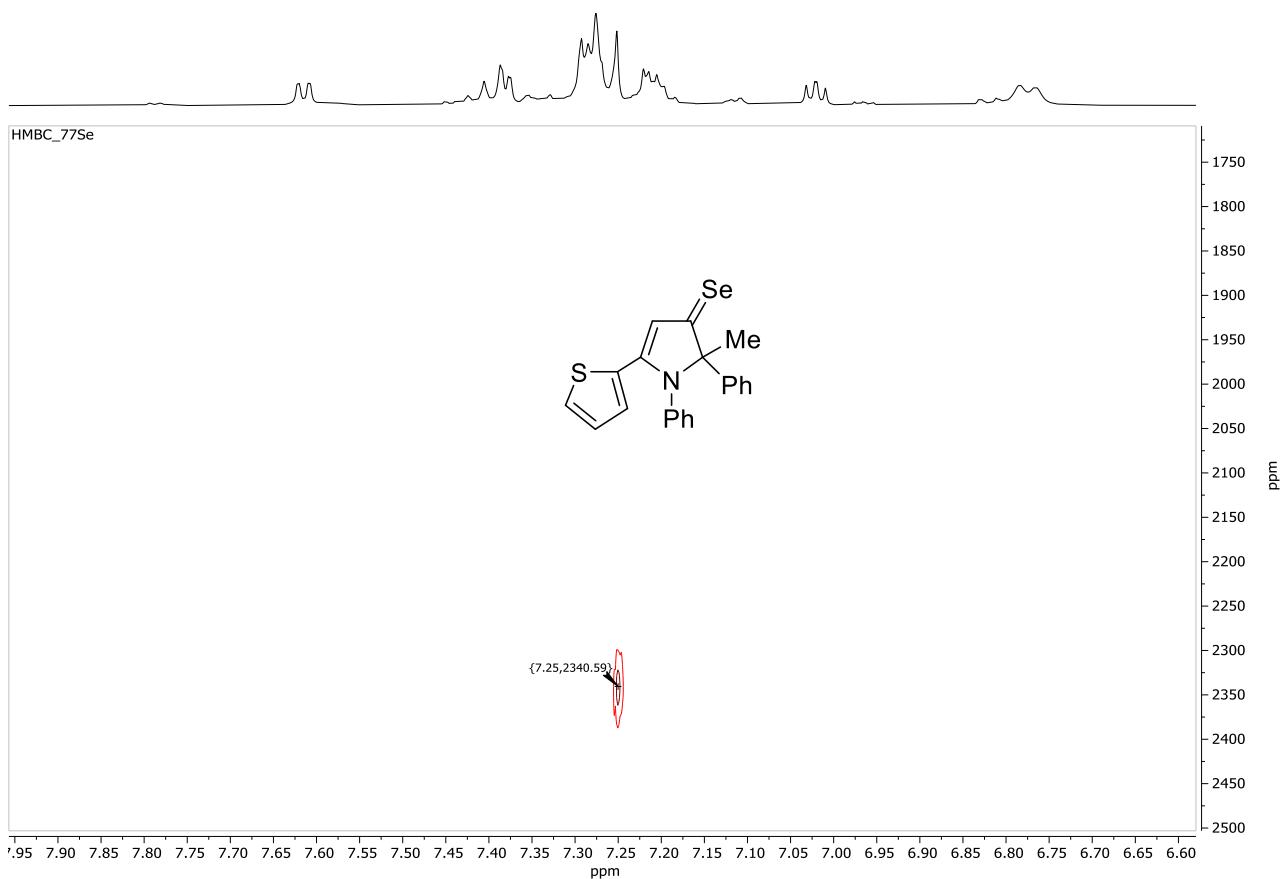


$^{13}\text{C}\{\text{H}\}$ NMR of 2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2c)

NMR_13C

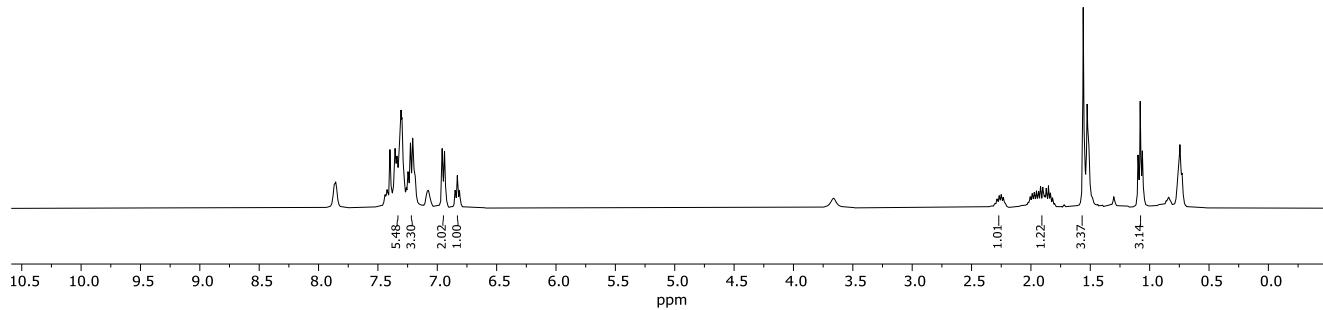
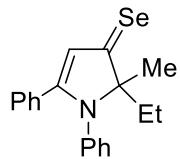


2D ^1H - ^{77}Se HMBC NMR of 2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2c)



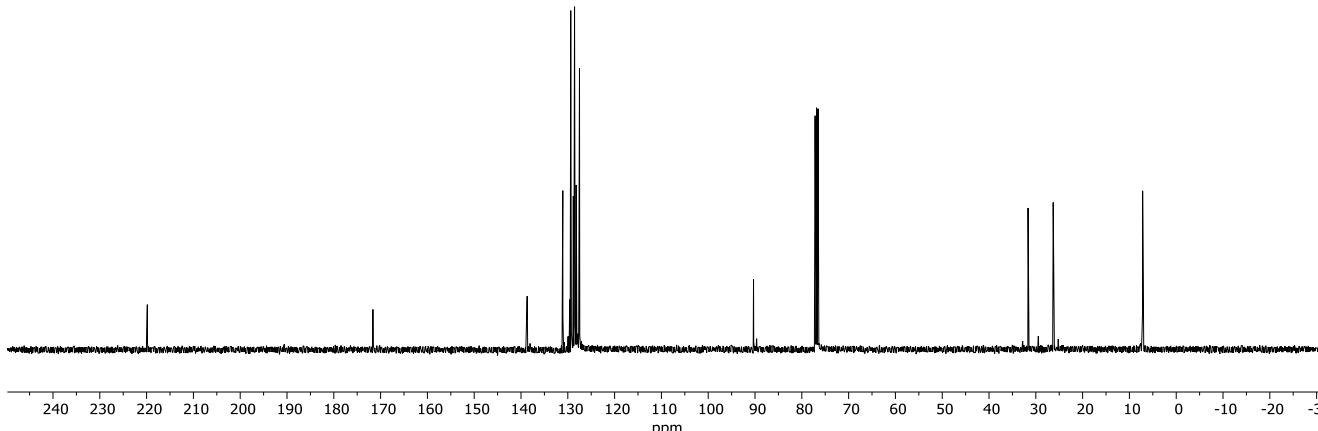
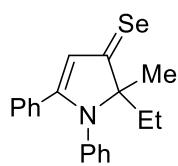
¹H NMR of 2-ethyl-2-methyl-1,5-diphenyl-1,2-dihydro-3H-pyrrole-3-selone (2d)

NMR_1H



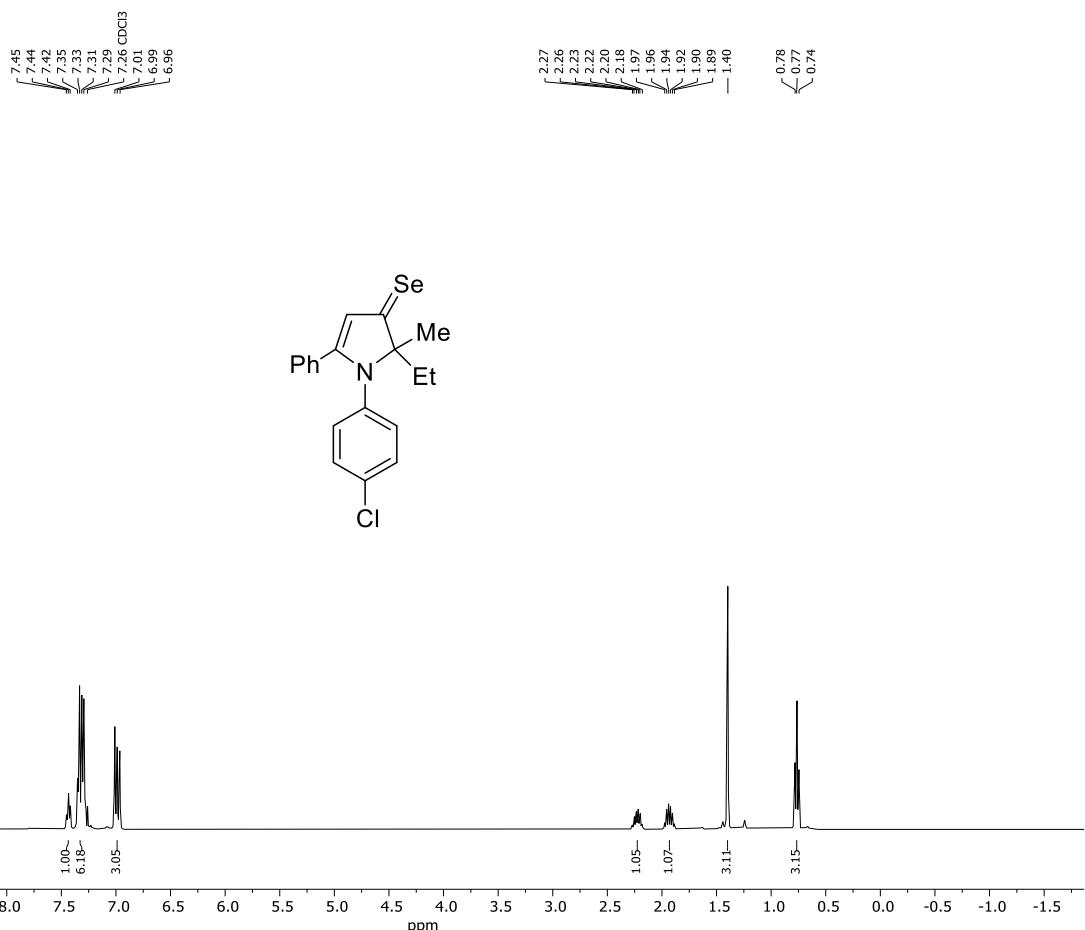
¹³C{¹H} NMR of 2-ethyl-2-methyl-1,5-diphenyl-1,2-dihydro-3H-pyrrole-3-selone (2d)

NMR_13C



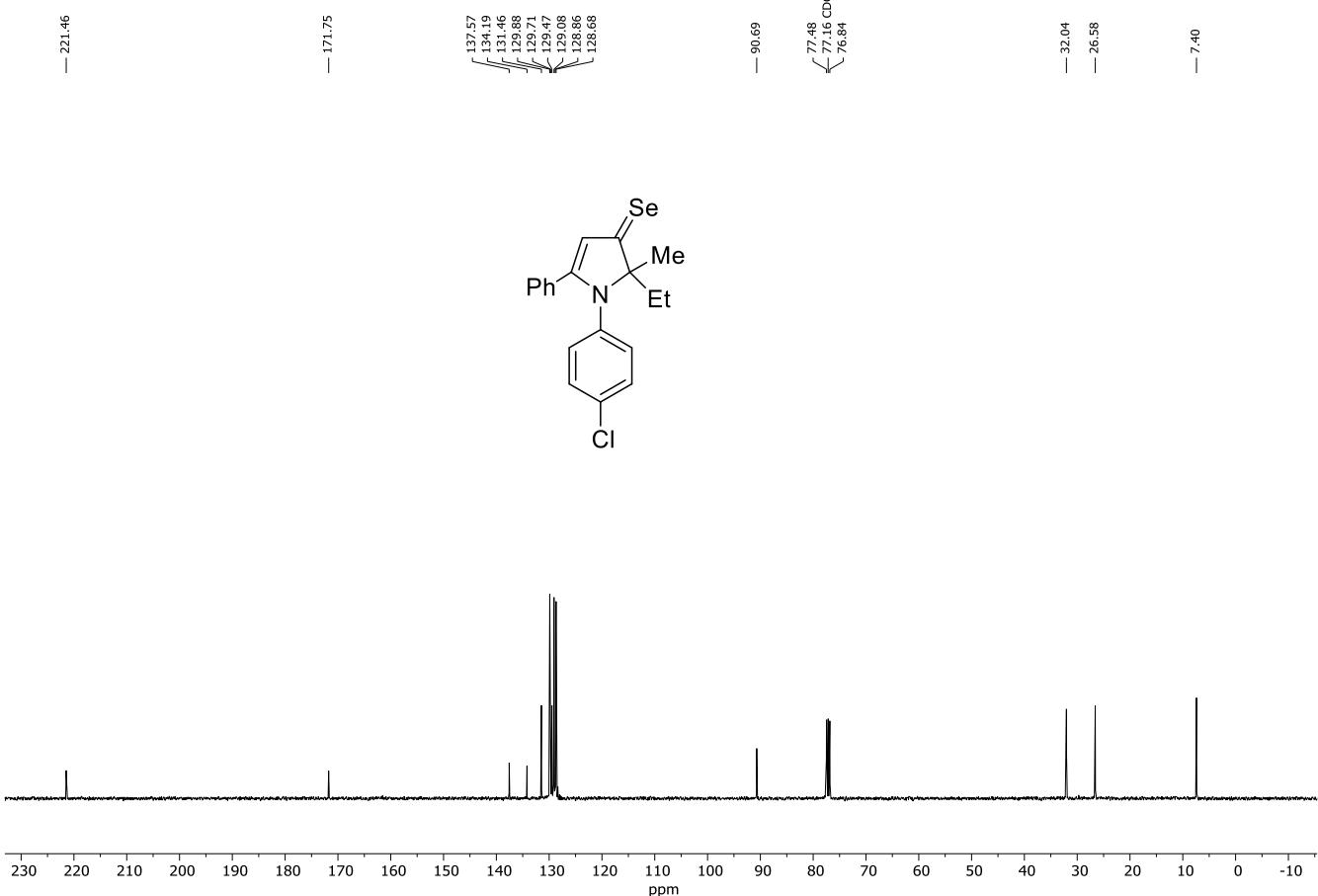
¹H NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-5-phenyl-1,2-dihydro-3H-pyrrole-3-selone (2f)

NMR_1H



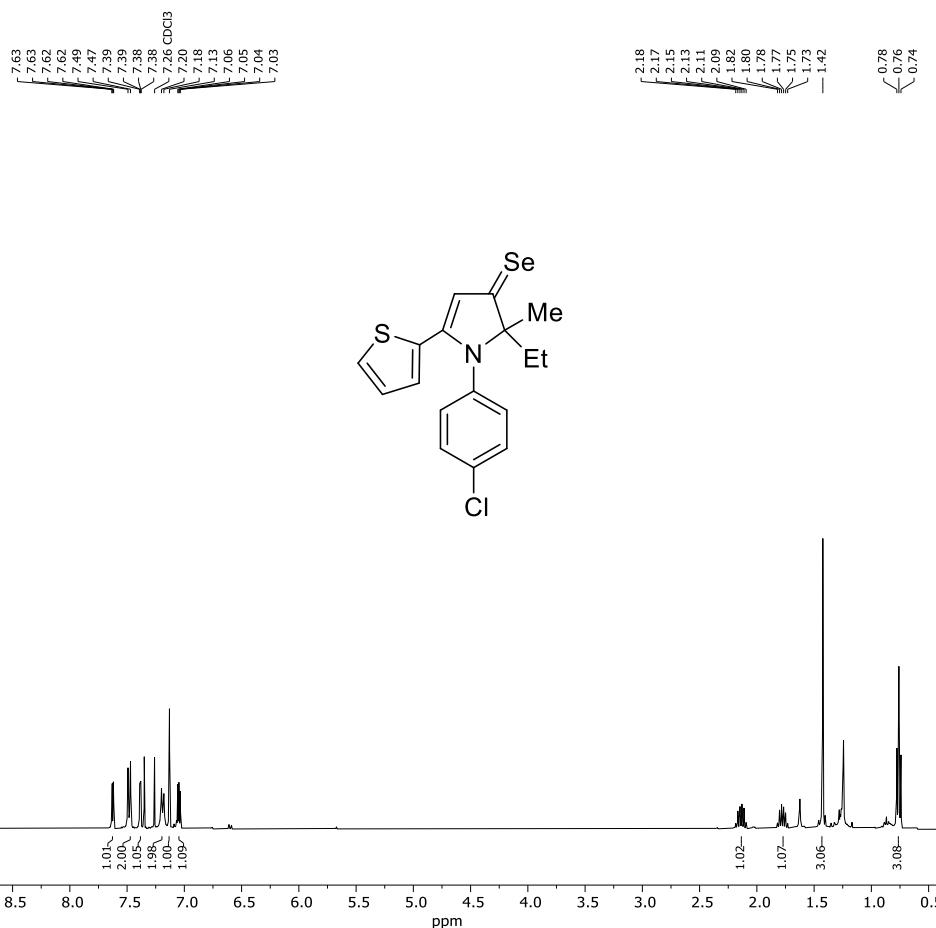
¹³C{¹H} NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-5-phenyl-1,2-dihydro-3H-pyrrole-3-selone (2f)

NMR_13C



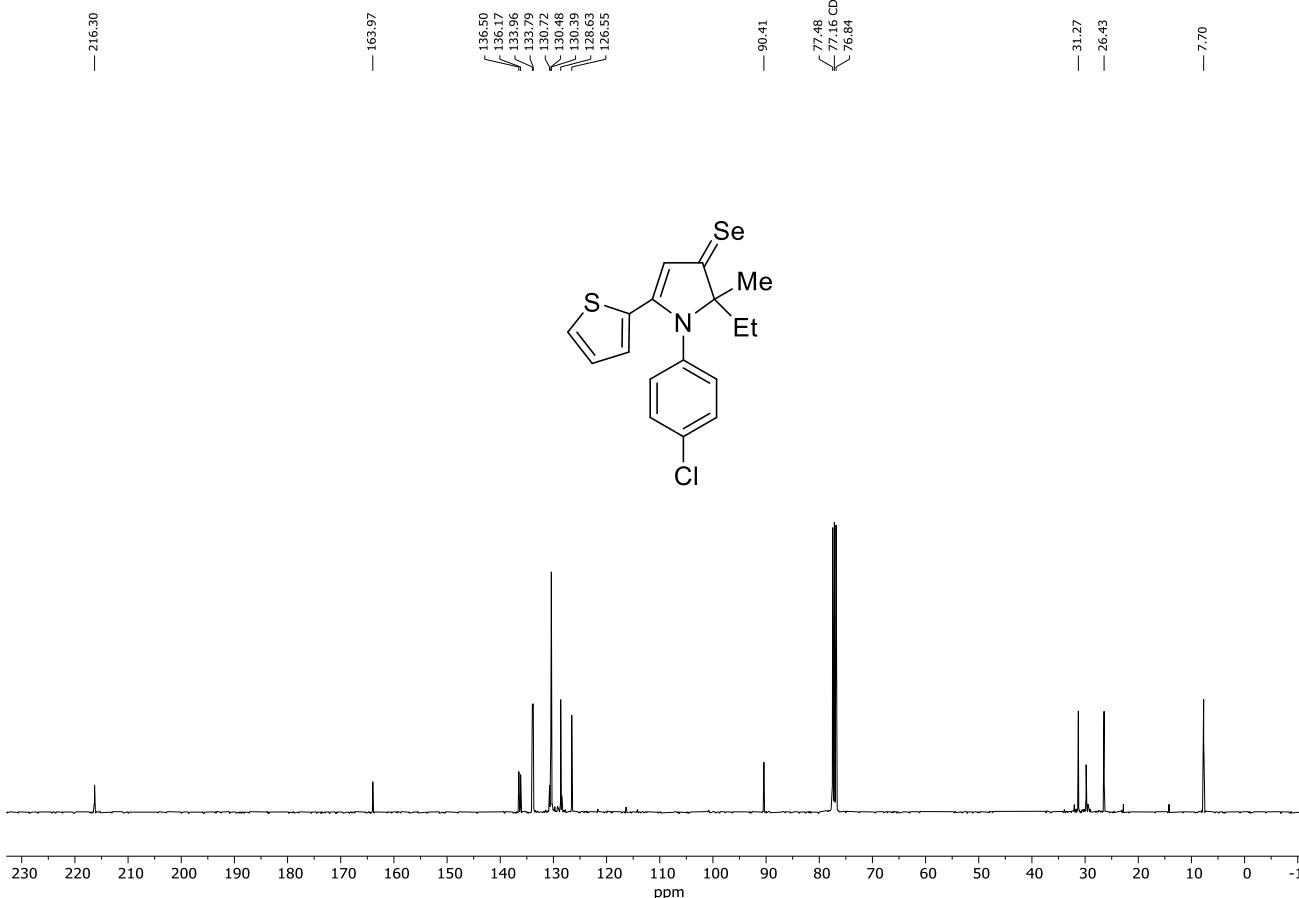
^1H NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2g)

NMR_1H



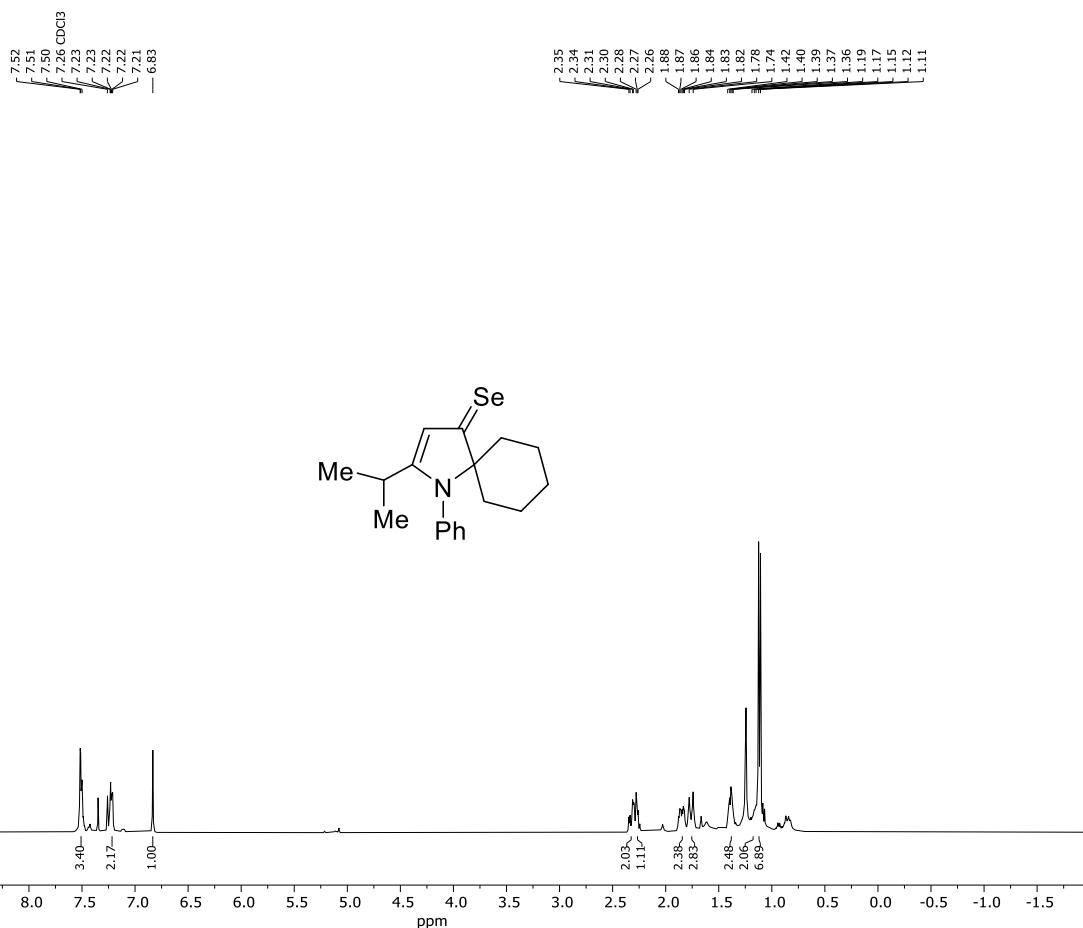
$^{13}\text{C}\{^1\text{H}\}$ NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2g)

NMR_13C



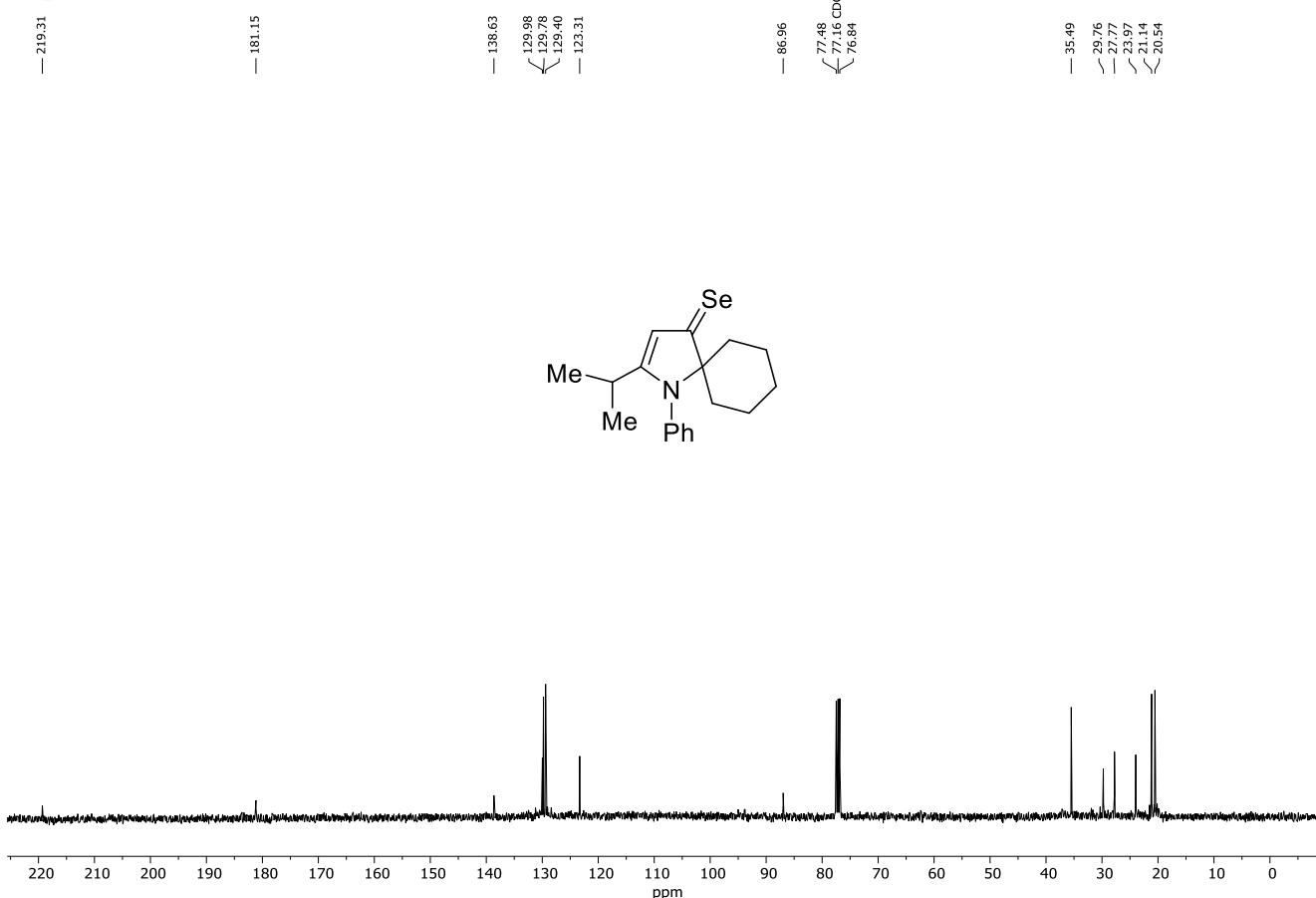
¹H NMR of 1-phenyl-2-(propan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2h)

NMR_1H

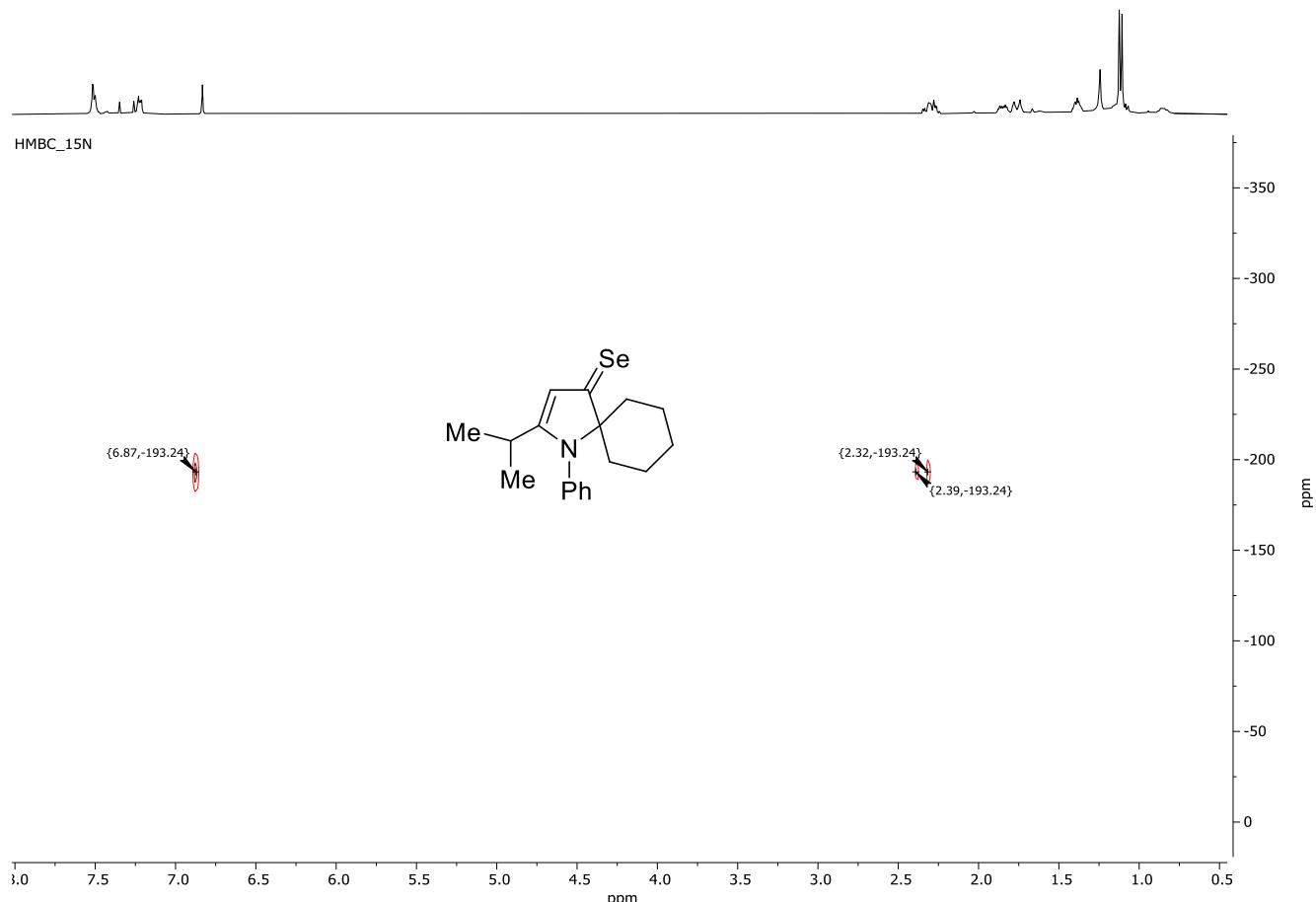


¹³C{¹H} NMR of 1-phenyl-2-(propan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2h)

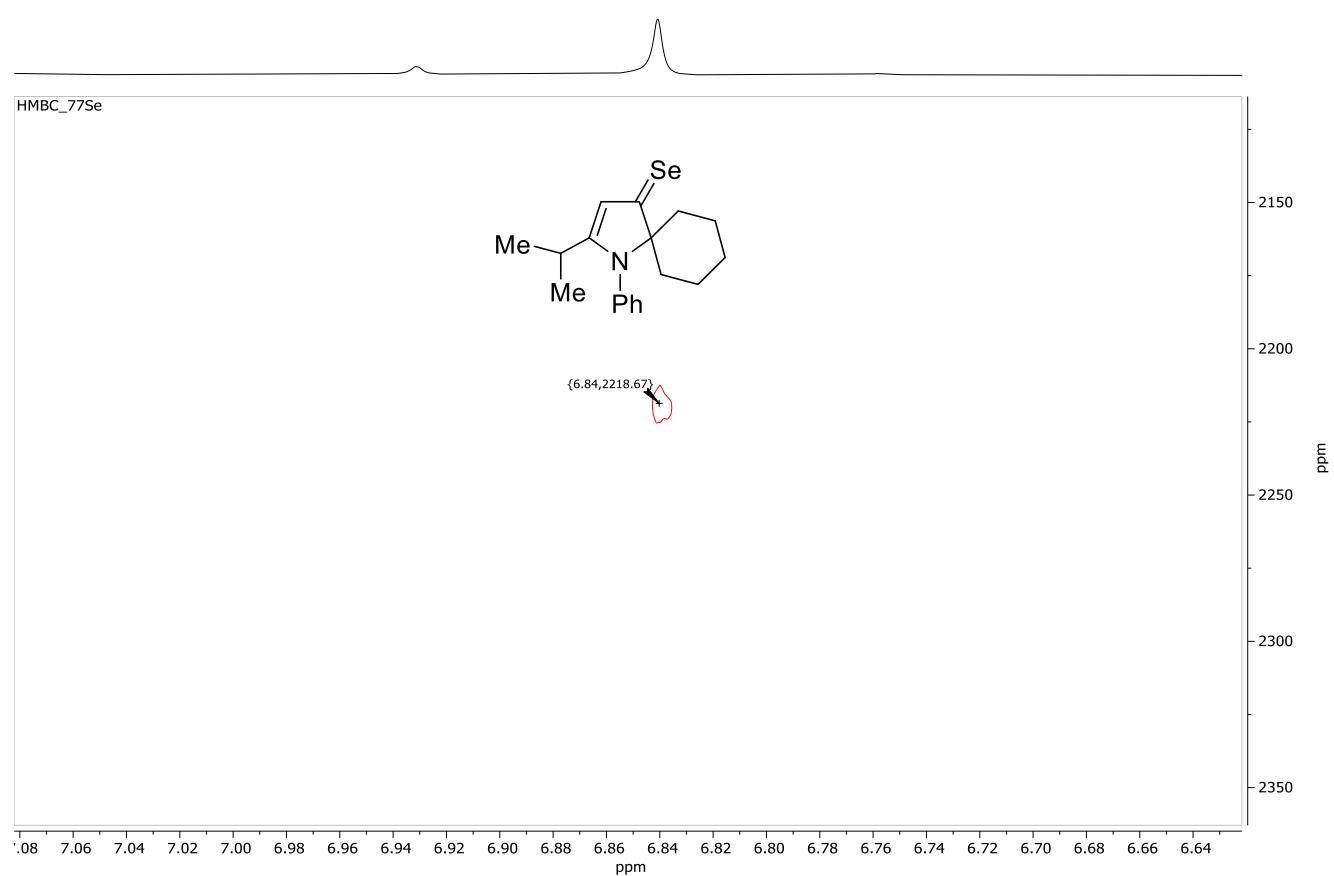
NMR_13C



2D ^1H - ^{15}N HMBC NMR of 1-phenyl-2-(propan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2h)

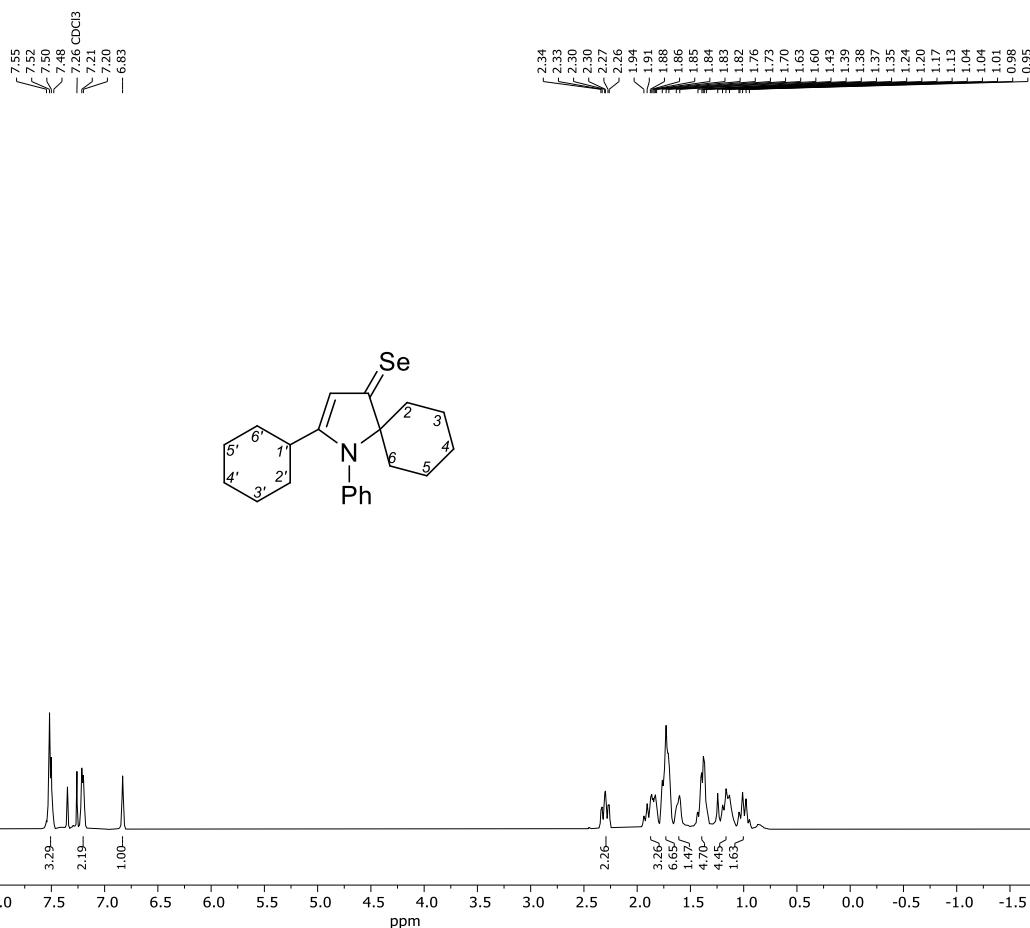


2D ^1H - ^{77}Se HMBC NMR of 1-phenyl-2-(propan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2h)



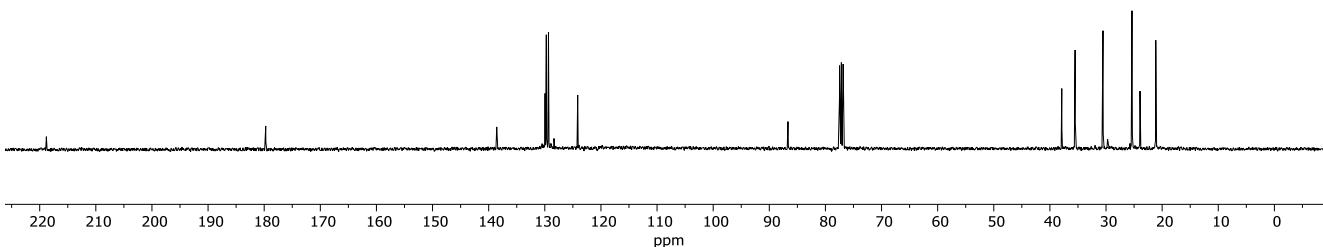
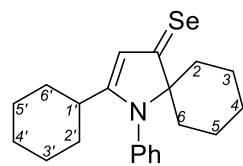
¹H NMR of 2-cyclohexyl-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2i)

NMR_1H

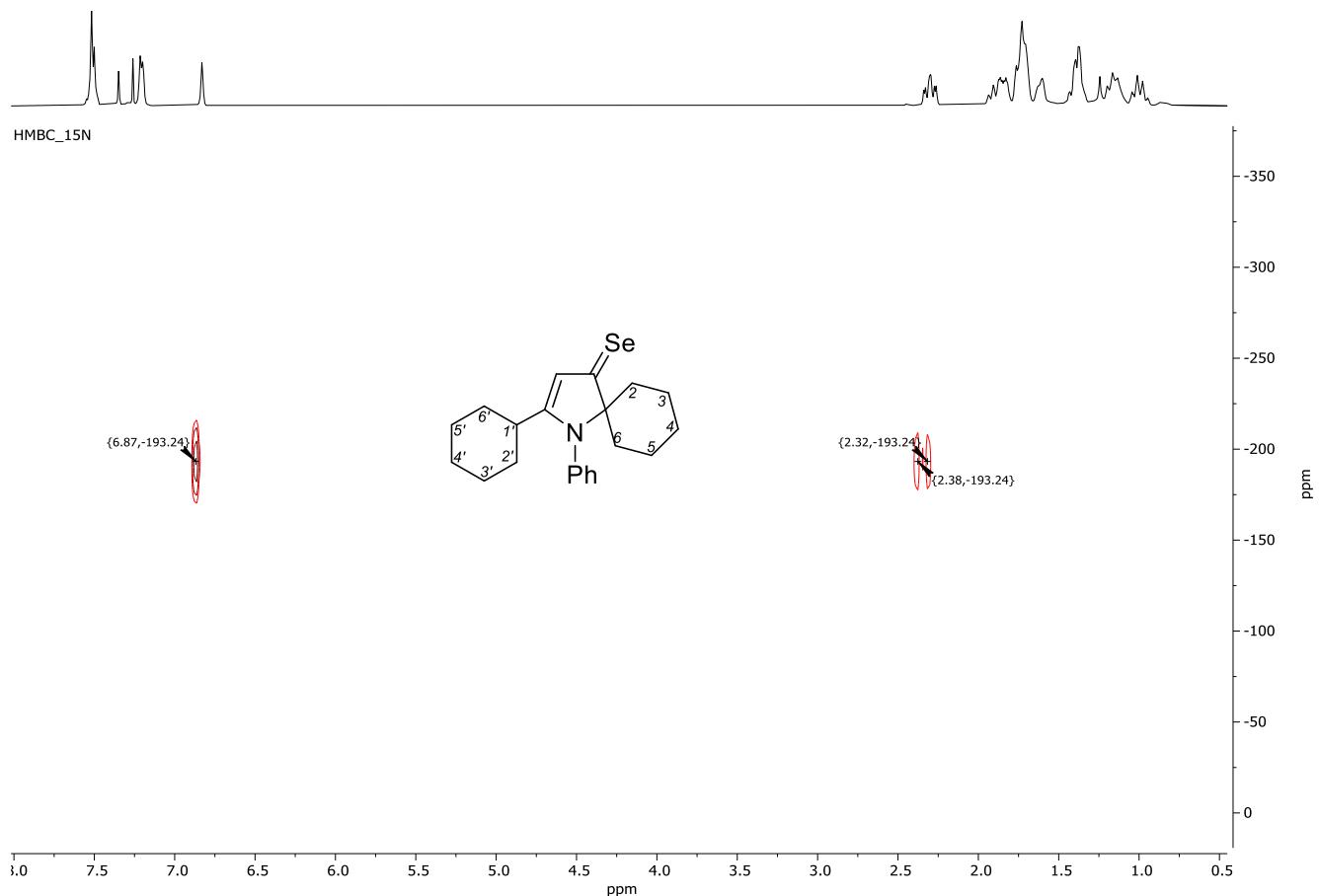


¹³C{¹H} NMR of 2-cyclohexyl-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2i)

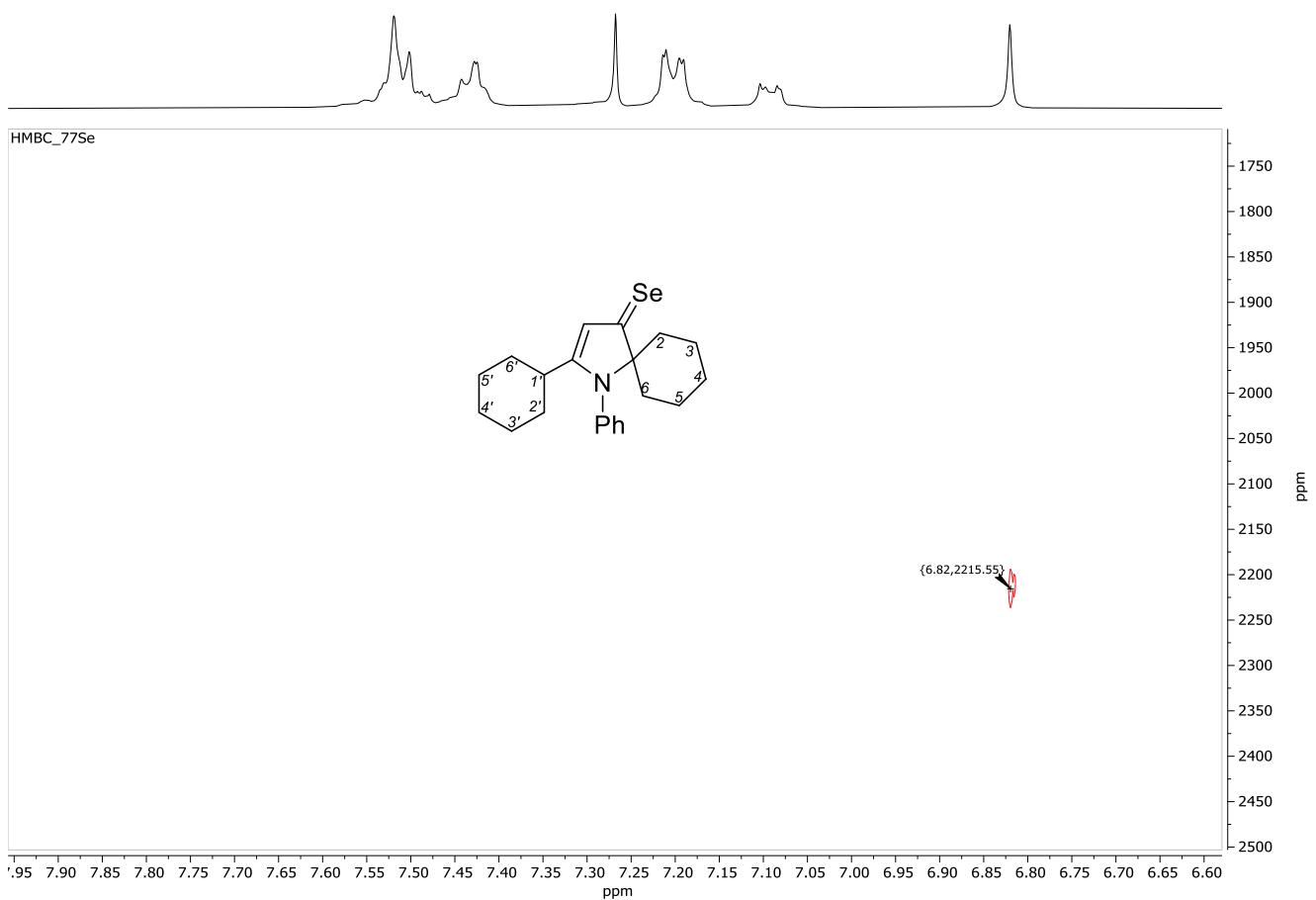
NMR_13C



2D ^1H - ^{15}N HMBC NMR of 2-cyclohexyl-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2i)

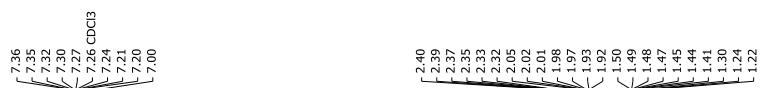


2D ^1H - ^{77}Se HMBC NMR of 2-cyclohexyl-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2i)



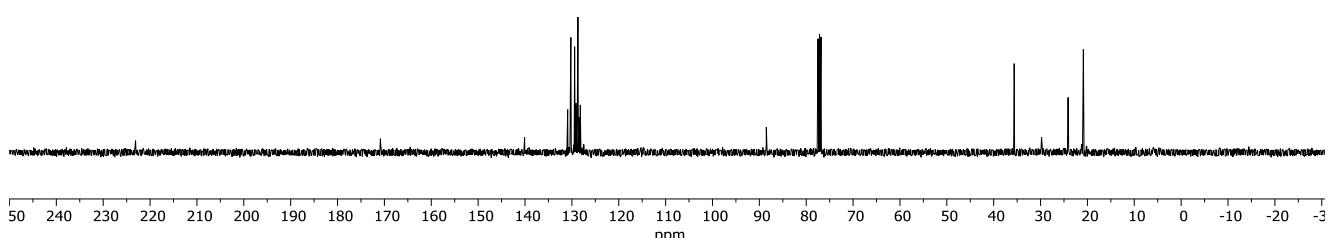
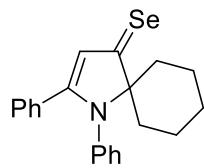
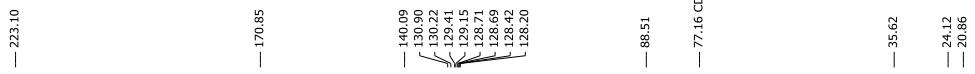
¹H NMR of 1,2-diphenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2j)

NMR_1H

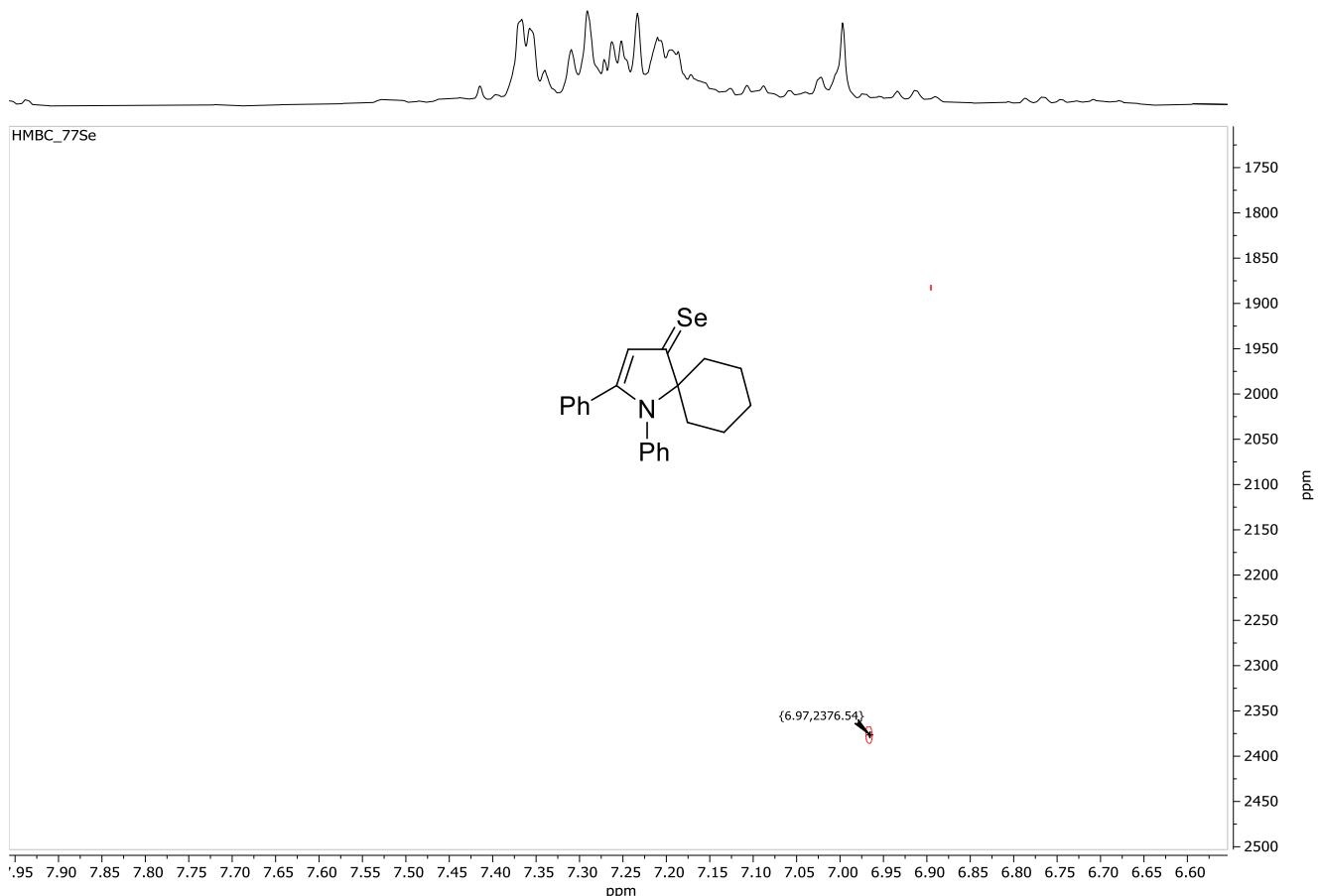


¹³C{¹H} NMR of 1,2-diphenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2j)

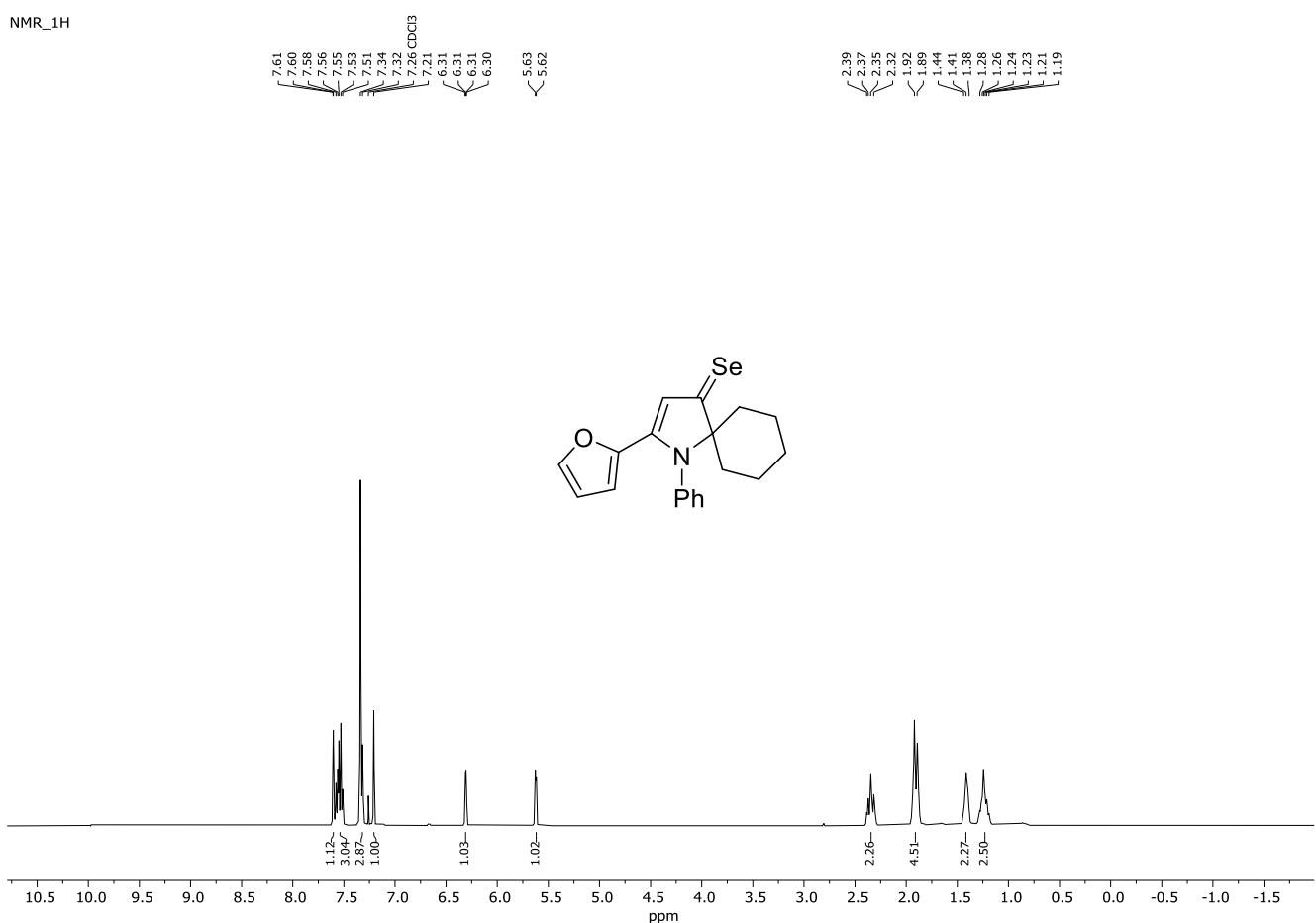
NMR_13C



2D ^1H - ^{77}Se HMBC NMR of 1,2-diphenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2j)

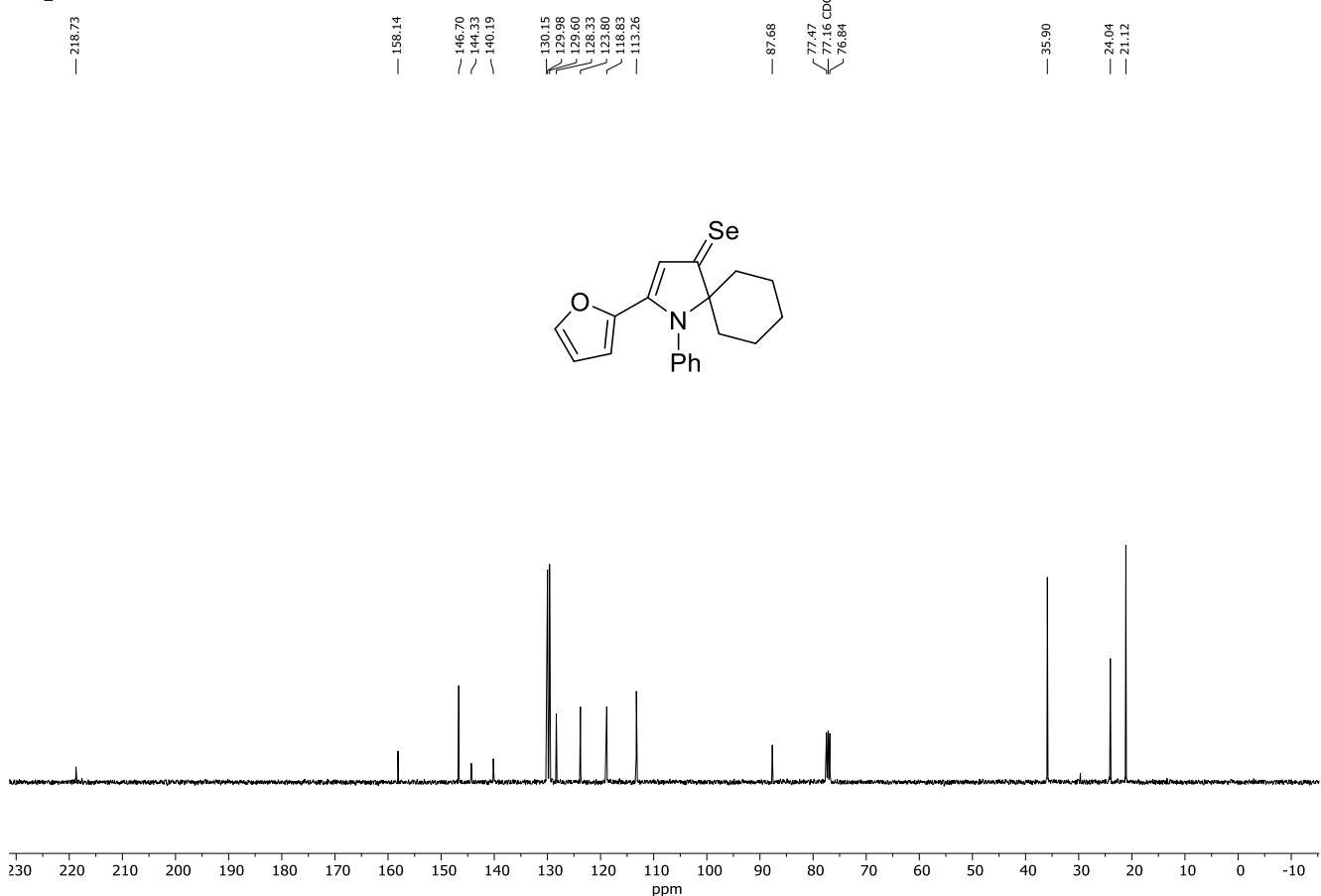


^1H NMR of 2-(furan-2-yl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2k)



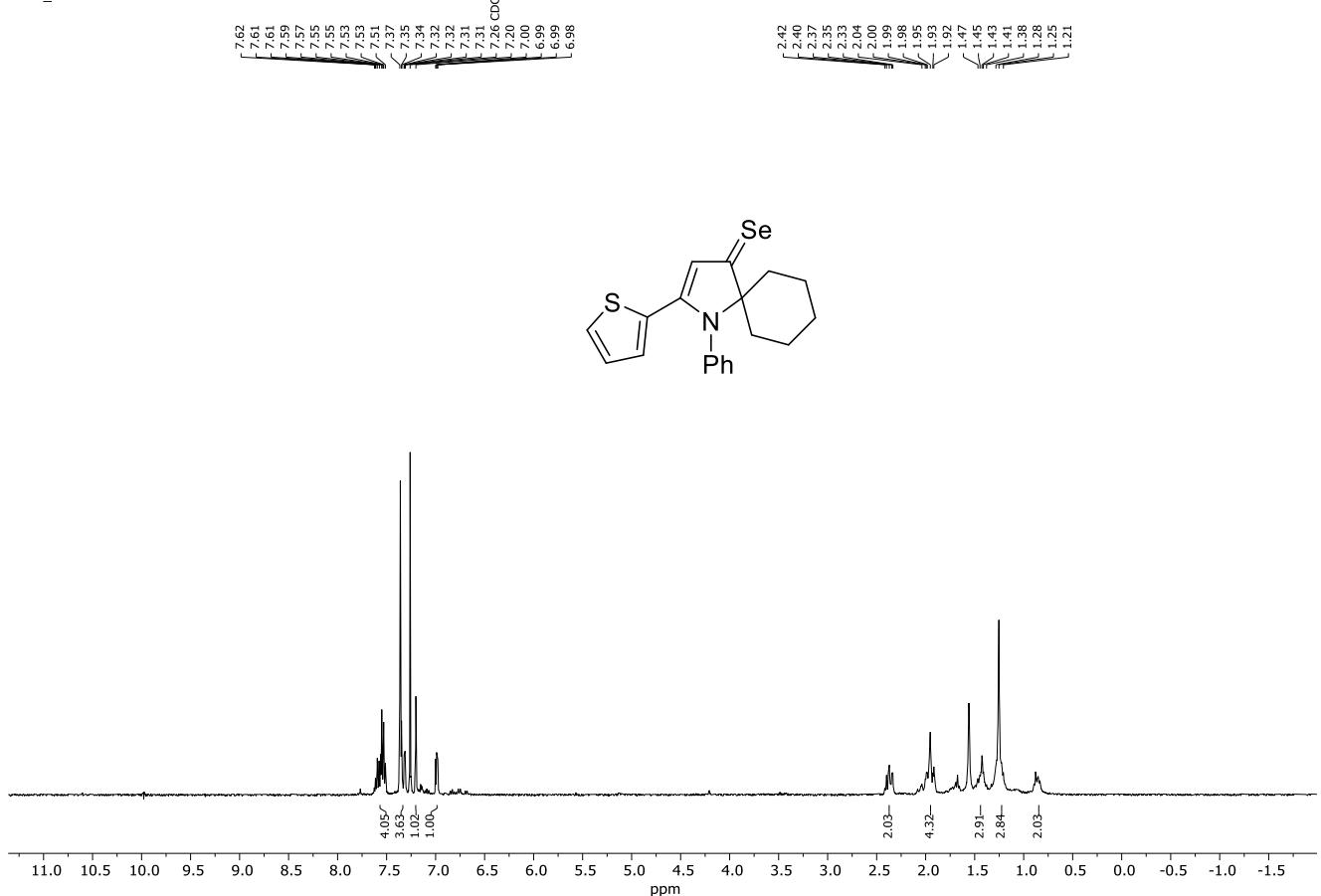
$^{13}\text{C}\{\text{H}\}$ NMR of 2-(furan-2-yl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2k)

NMR_13C



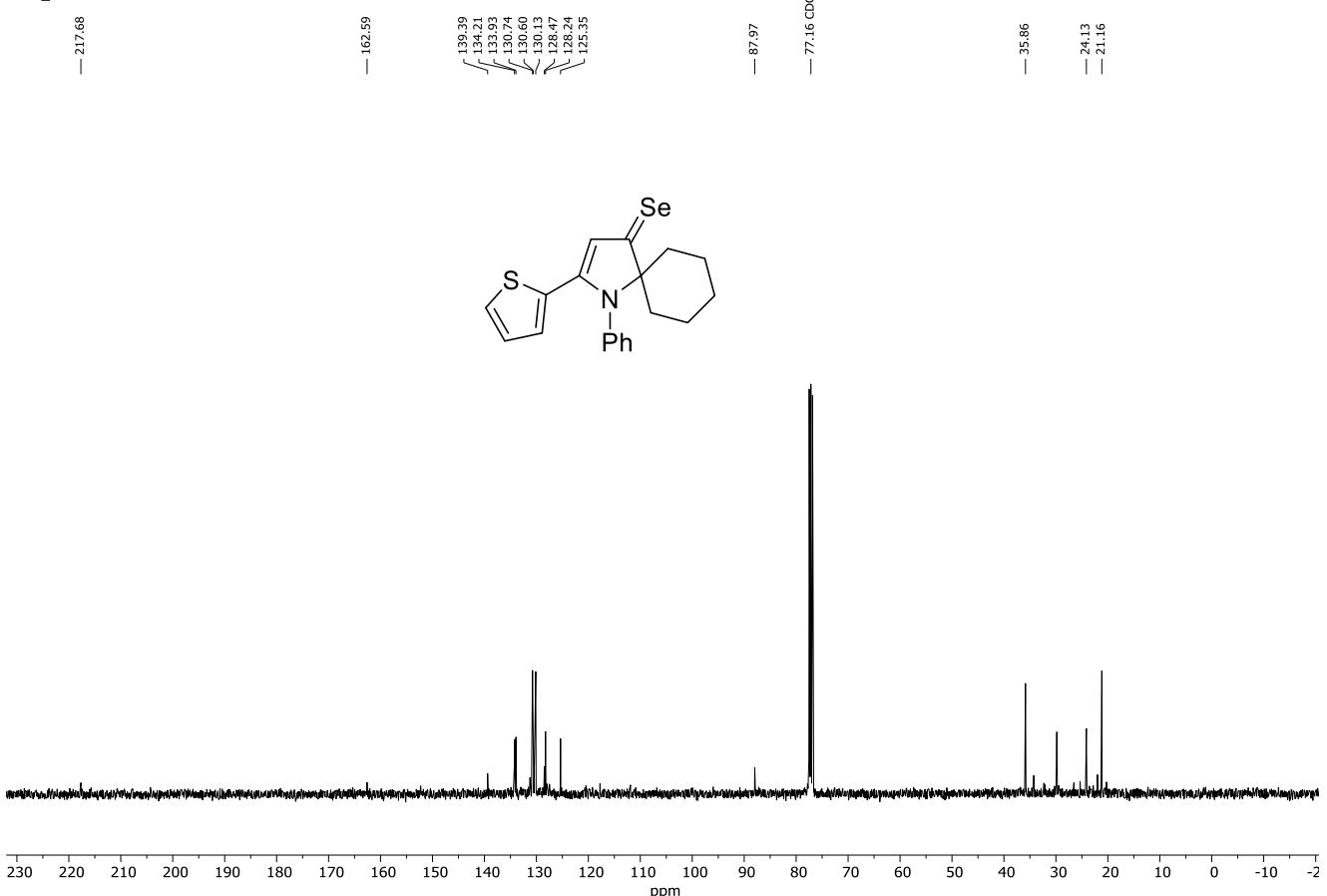
^1H NMR of 1-phenyl-2-(thiophen-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2l)

NMR_1H



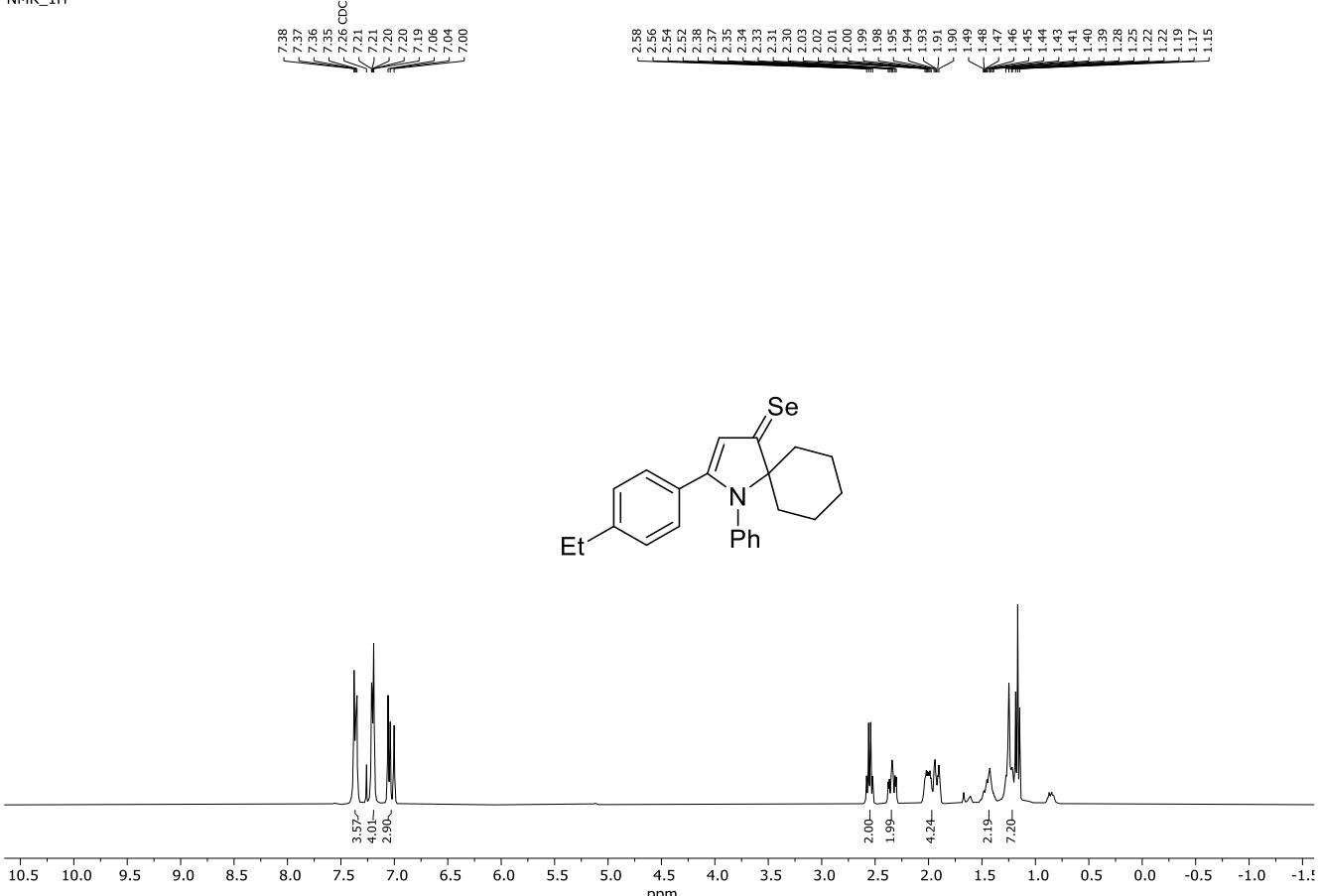
$^{13}\text{C}\{\text{H}\}$ NMR of 1-phenyl-2-(thiophen-2-yl)-1-azaspiro[4.5]dec-2-ene-4-selone (2l)

NMR_13C

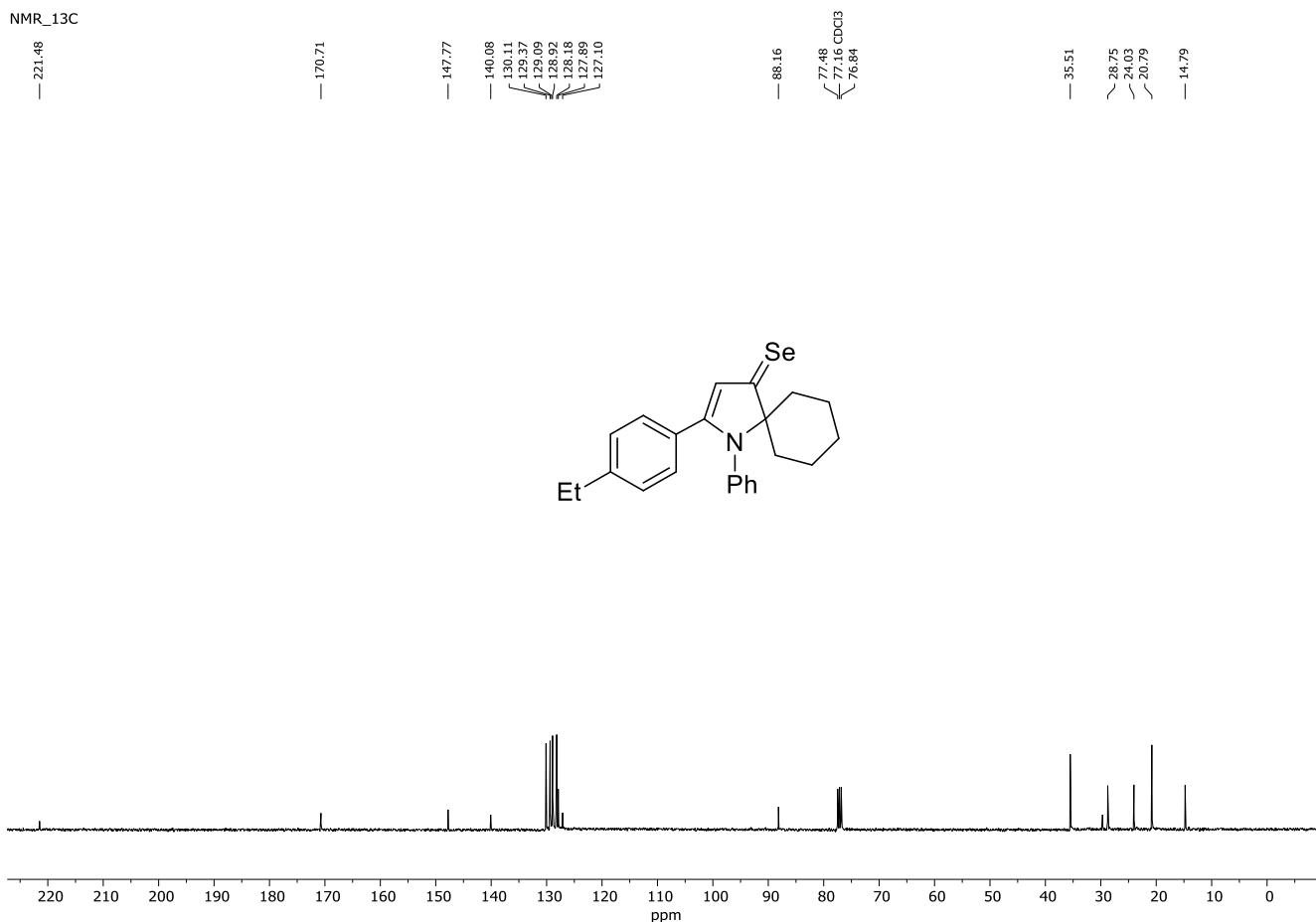


^1H NMR of 2-(4-ethylphenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2m)

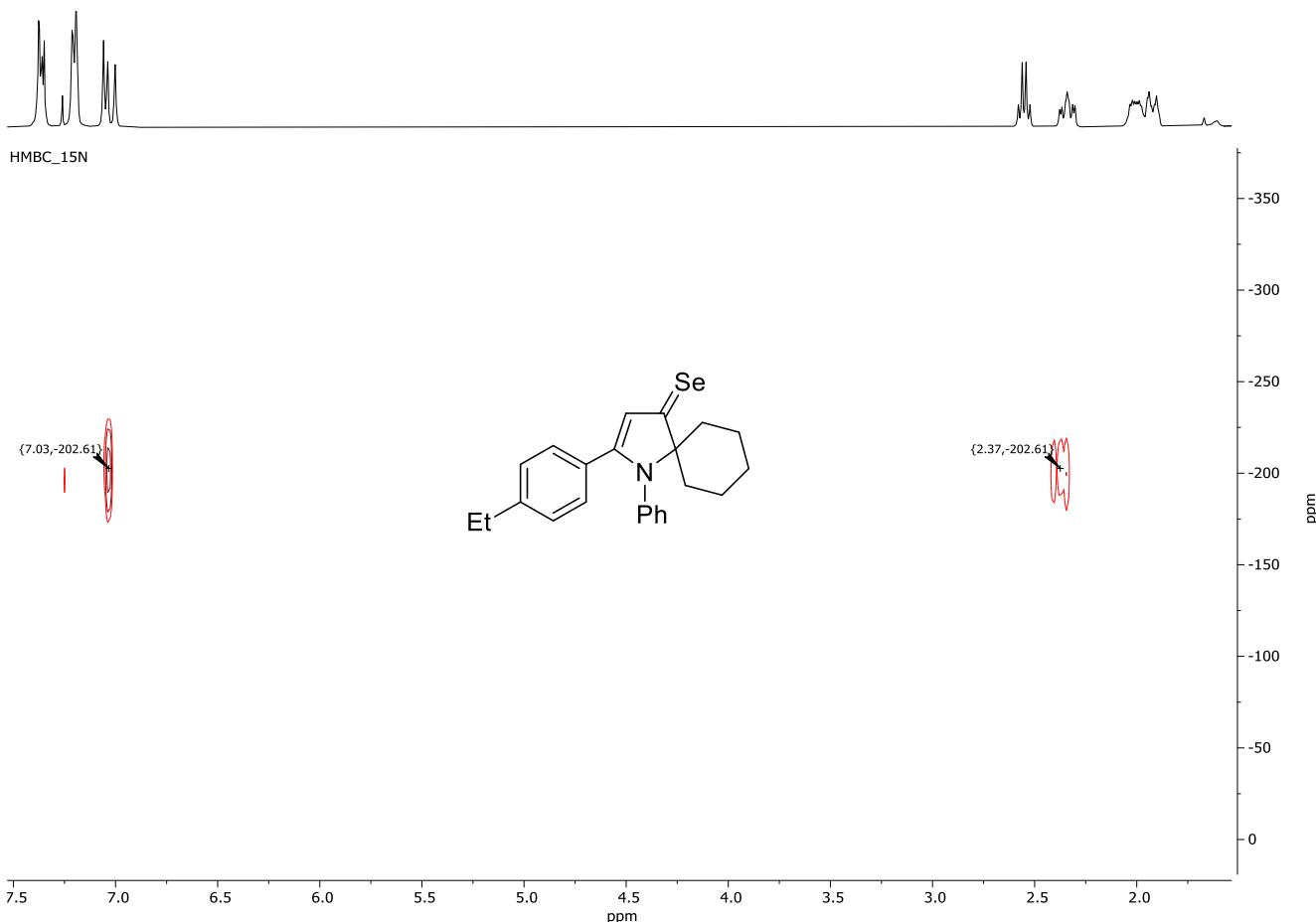
NMR_1H



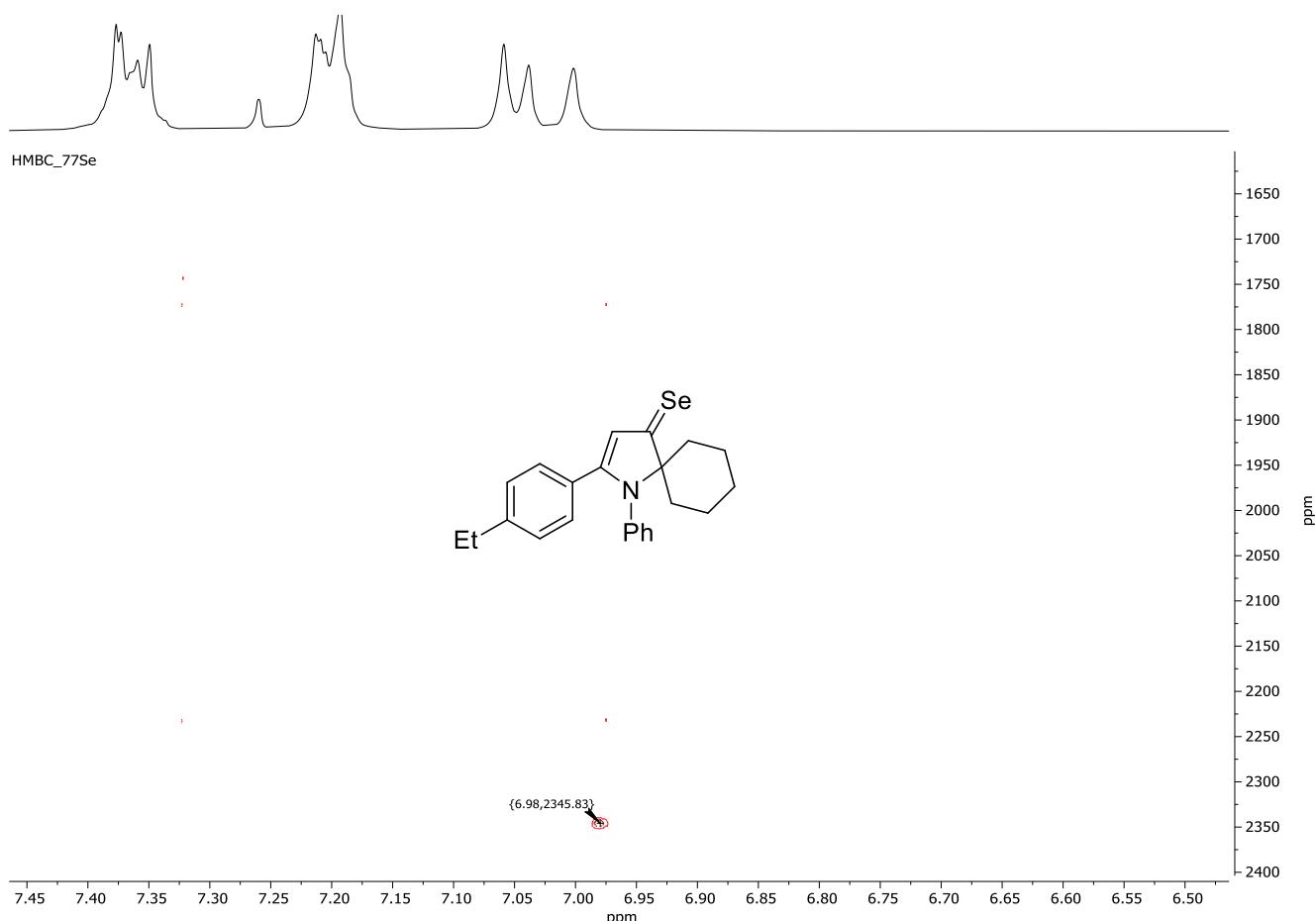
$^{13}\text{C}\{\text{H}\}$ NMR of 2-(4-ethylphenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2m)



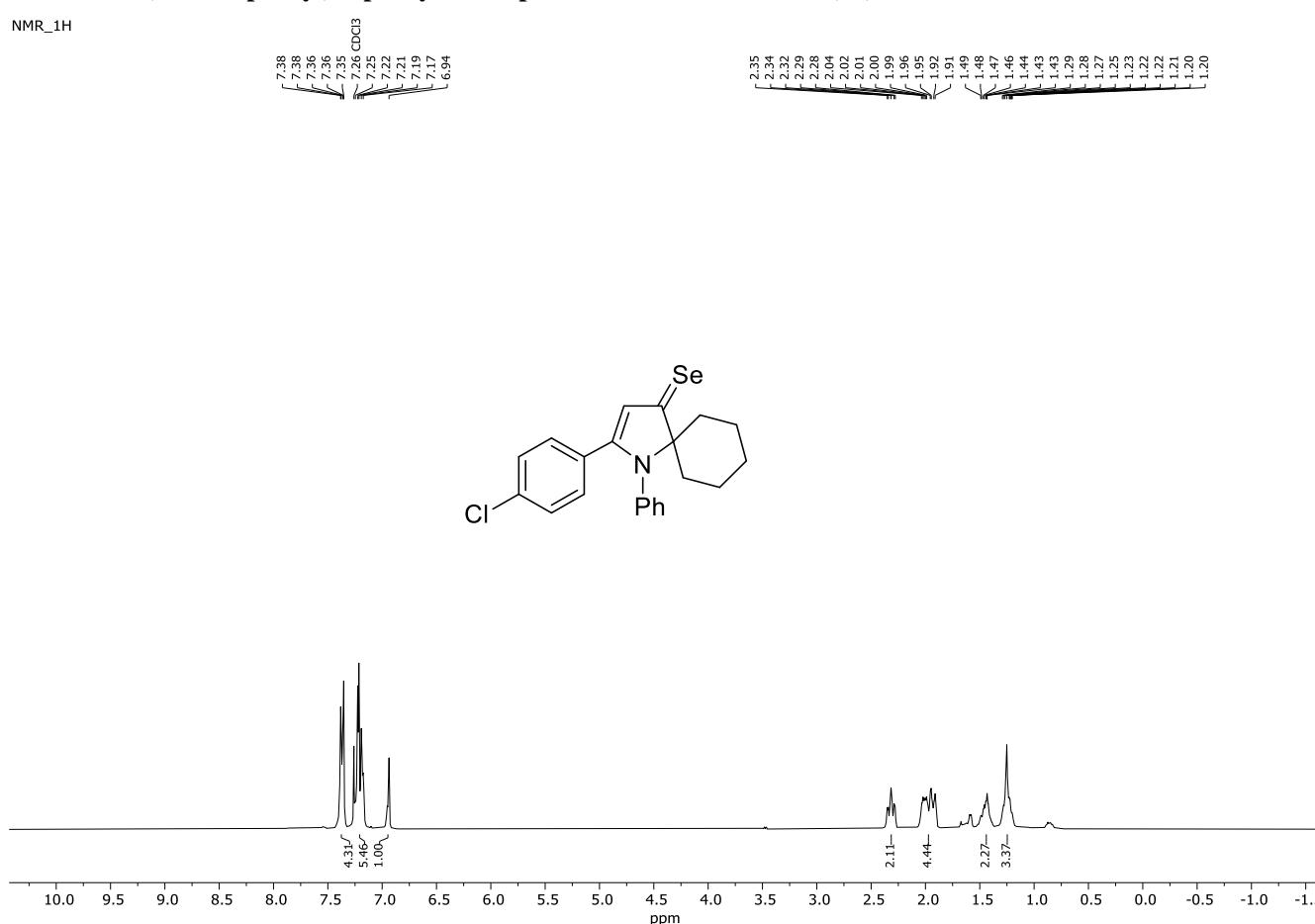
2D ^1H - ^{15}N HMBC NMR of 2-(4-ethylphenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2m)



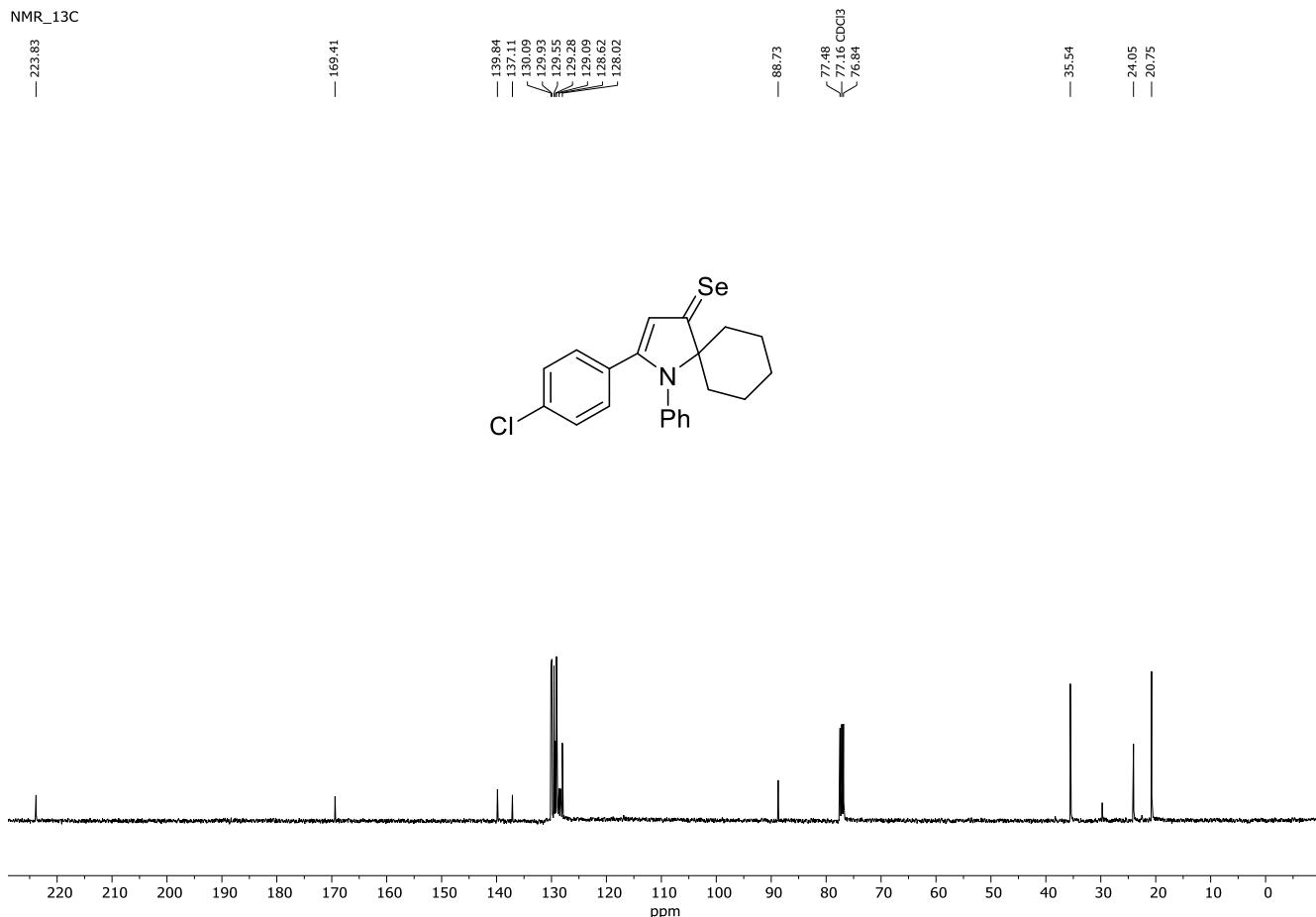
2D ^1H - ^{77}Se HMBC NMR of 2-(4-ethylphenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2m)



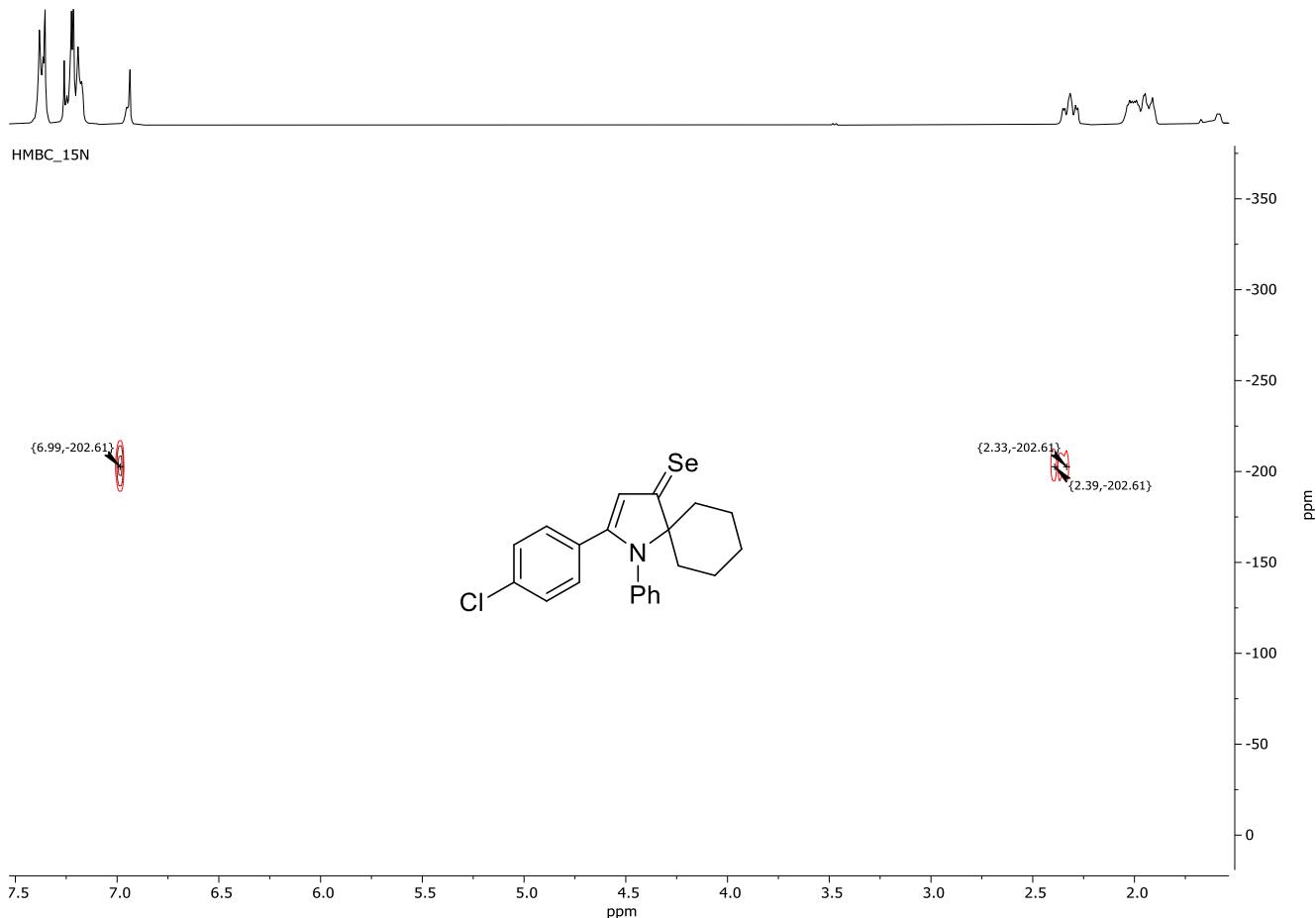
^1H NMR of 2-(4-chlorophenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2n)



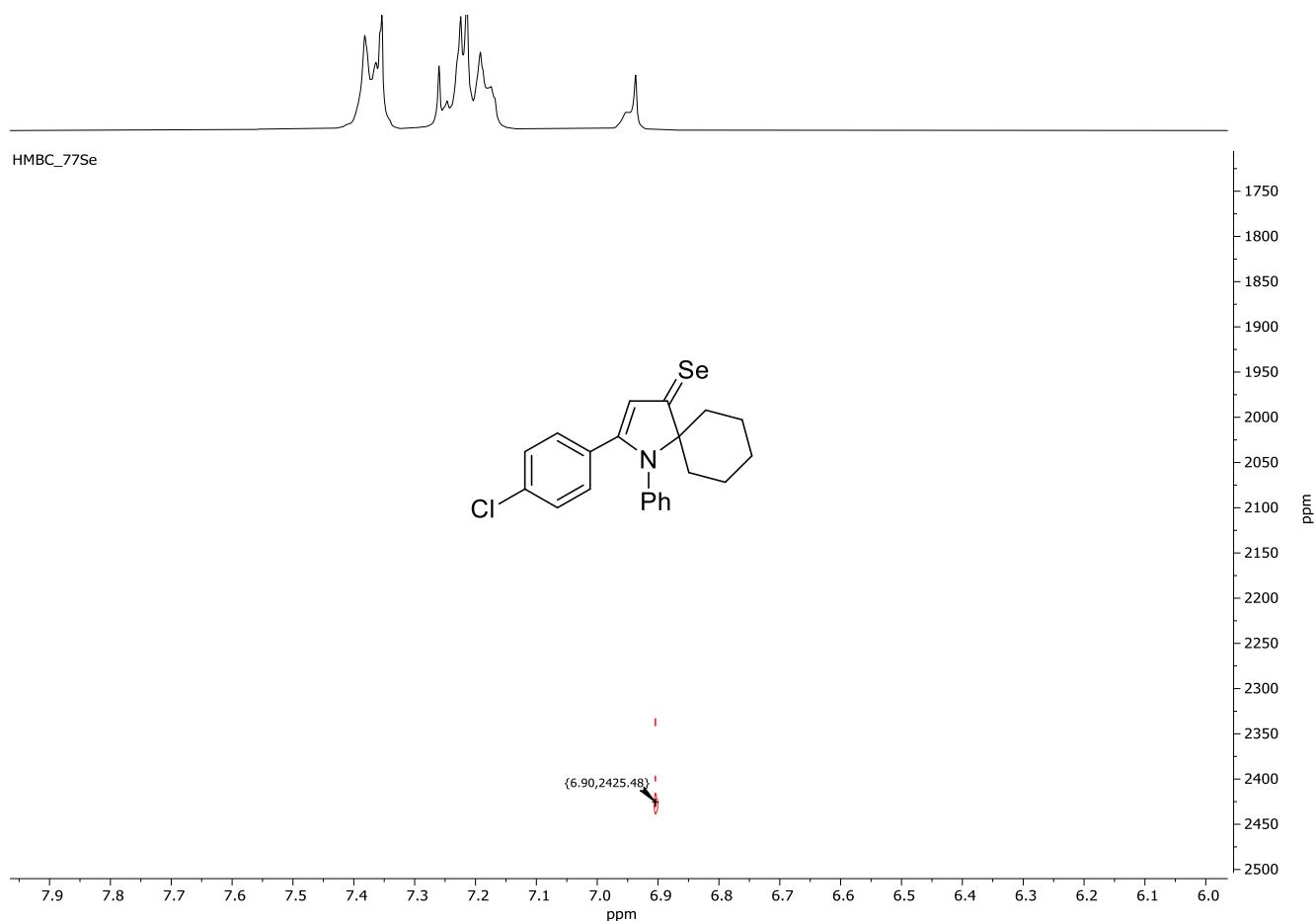
$^{13}\text{C}\{^1\text{H}\}$ NMR of 2-(4-chlorophenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2n)



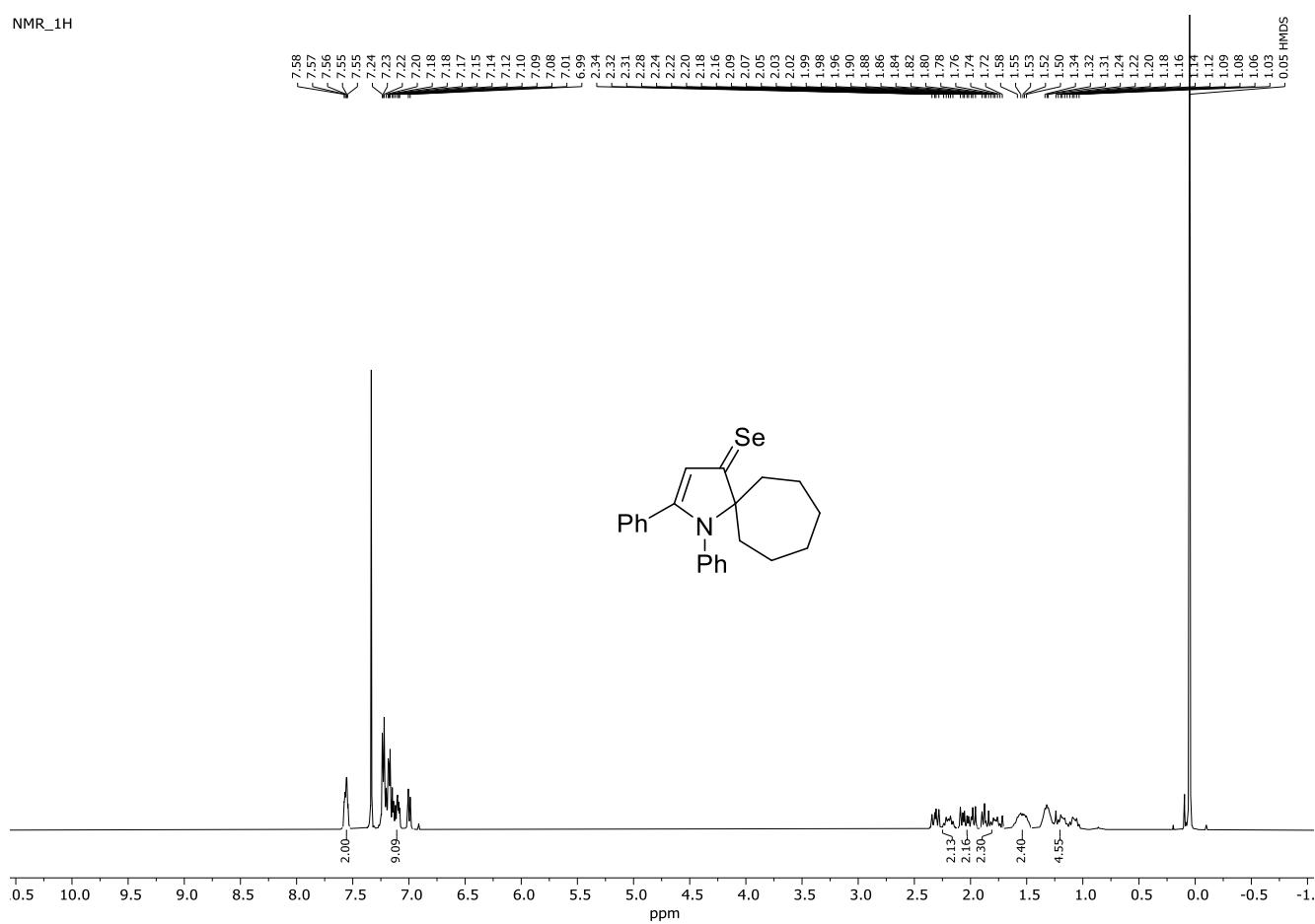
2D ^1H - ^{15}N HMBC NMR of 2-(4-chlorophenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2n)



2D ^1H - ^{77}Se HMBC NMR of 2-(4-chlorophenyl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2n)

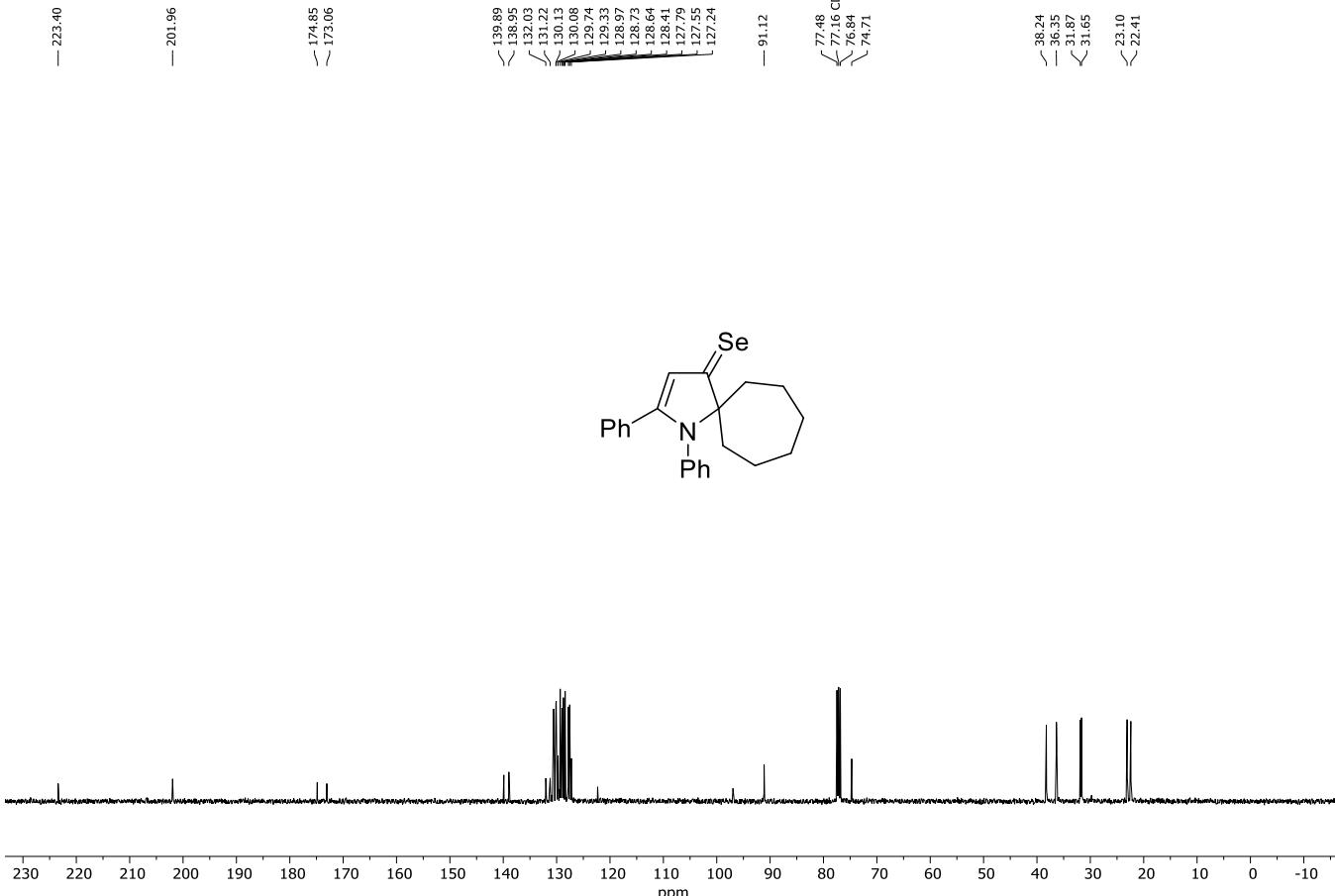


^1H NMR of 1,2-diphenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2o)

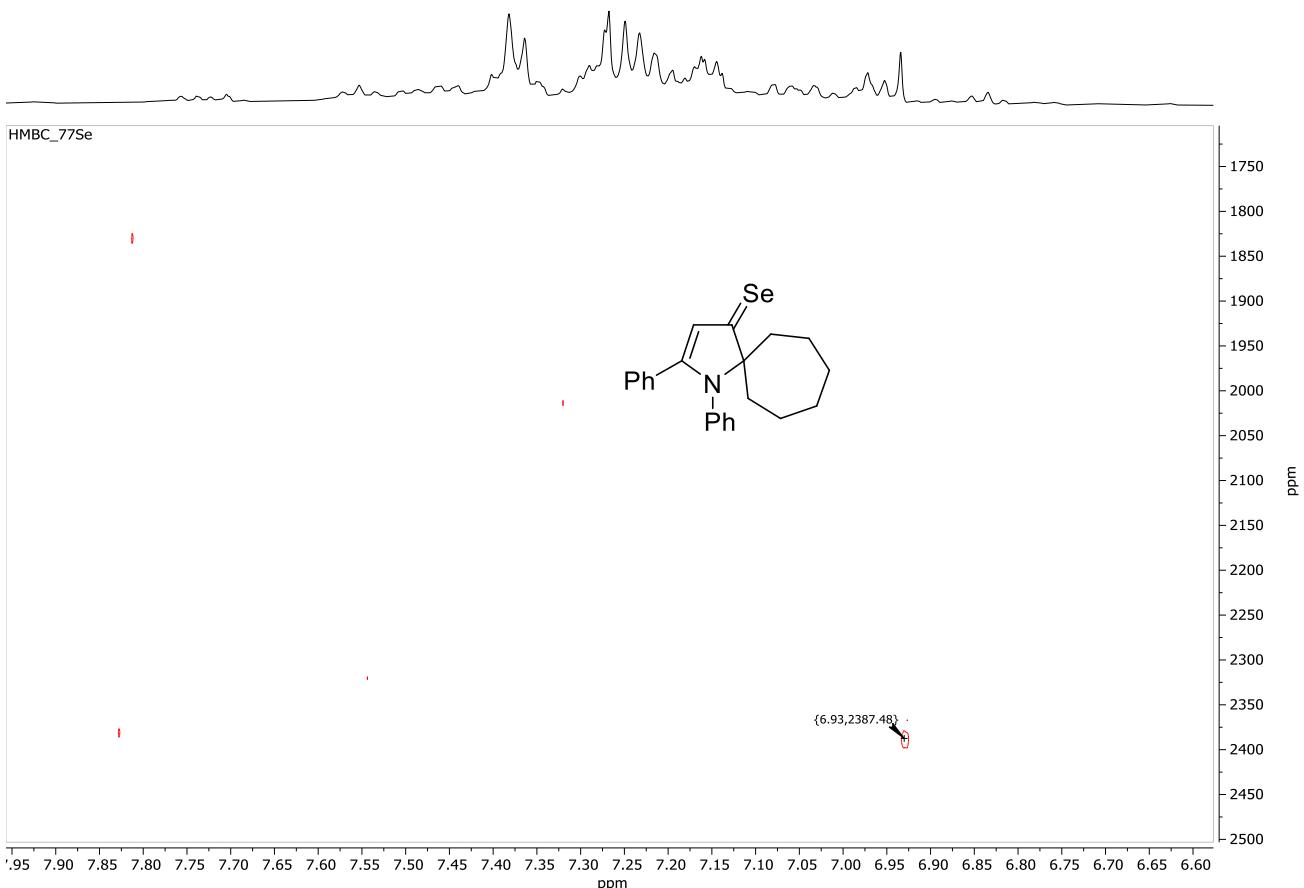


$^{13}\text{C}\{\text{H}\}$ NMR of 1,2-diphenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2o)

NMR_13C

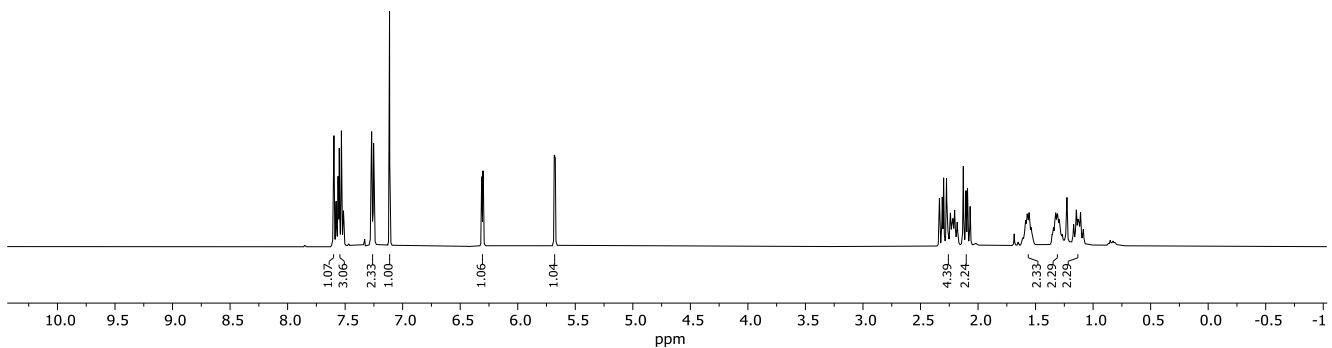
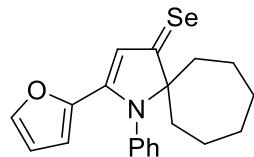
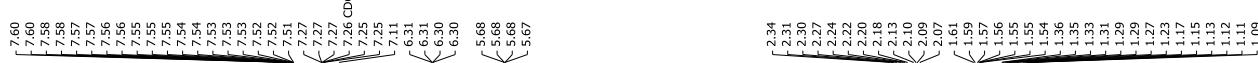


2D ^1H - ^{77}Se HMBC NMR of 1,2-diphenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2o)



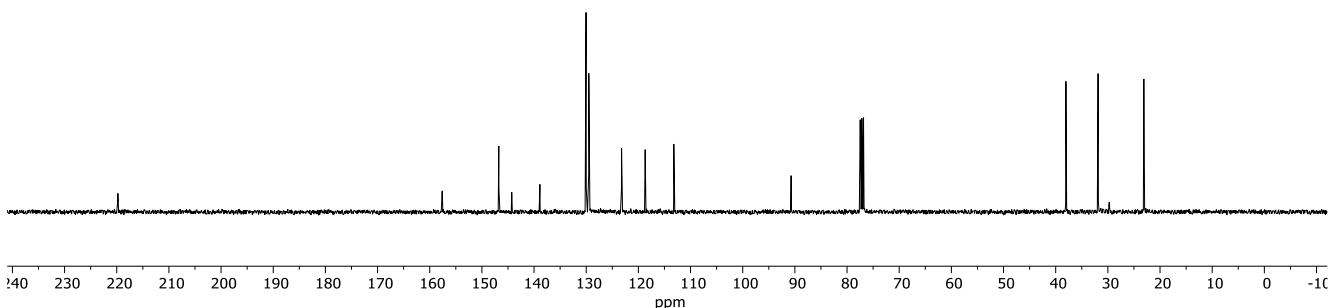
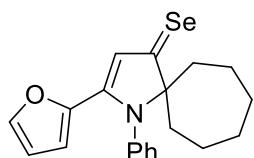
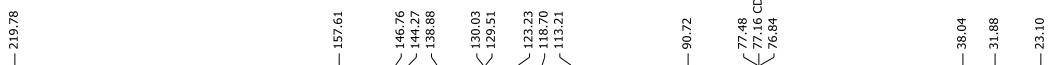
¹H NMR of 2-(furan-2-yl)-1-phenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2p)

NMR_1H

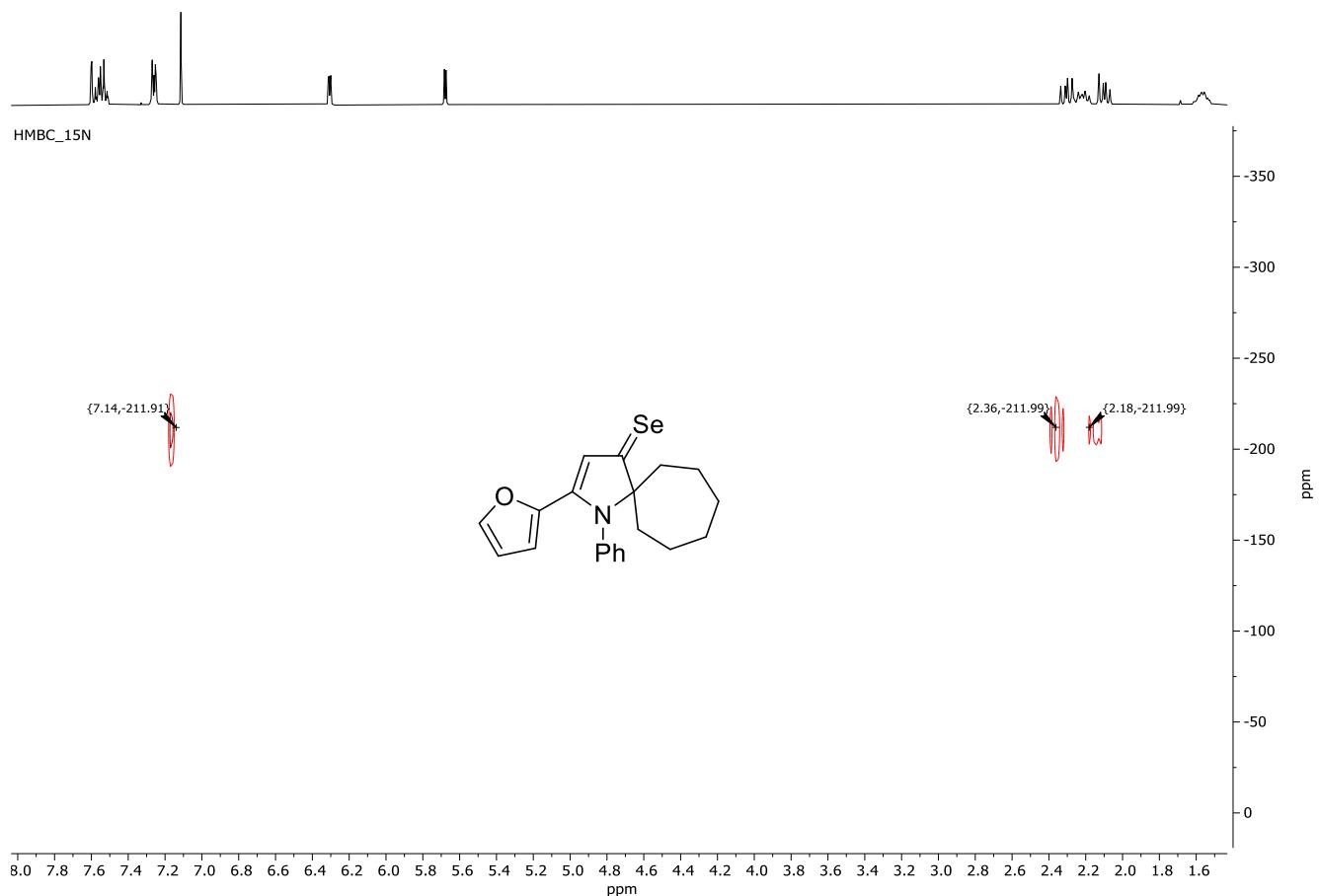


¹³C{¹H} NMR of 2-(furan-2-yl)-1-phenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2p)

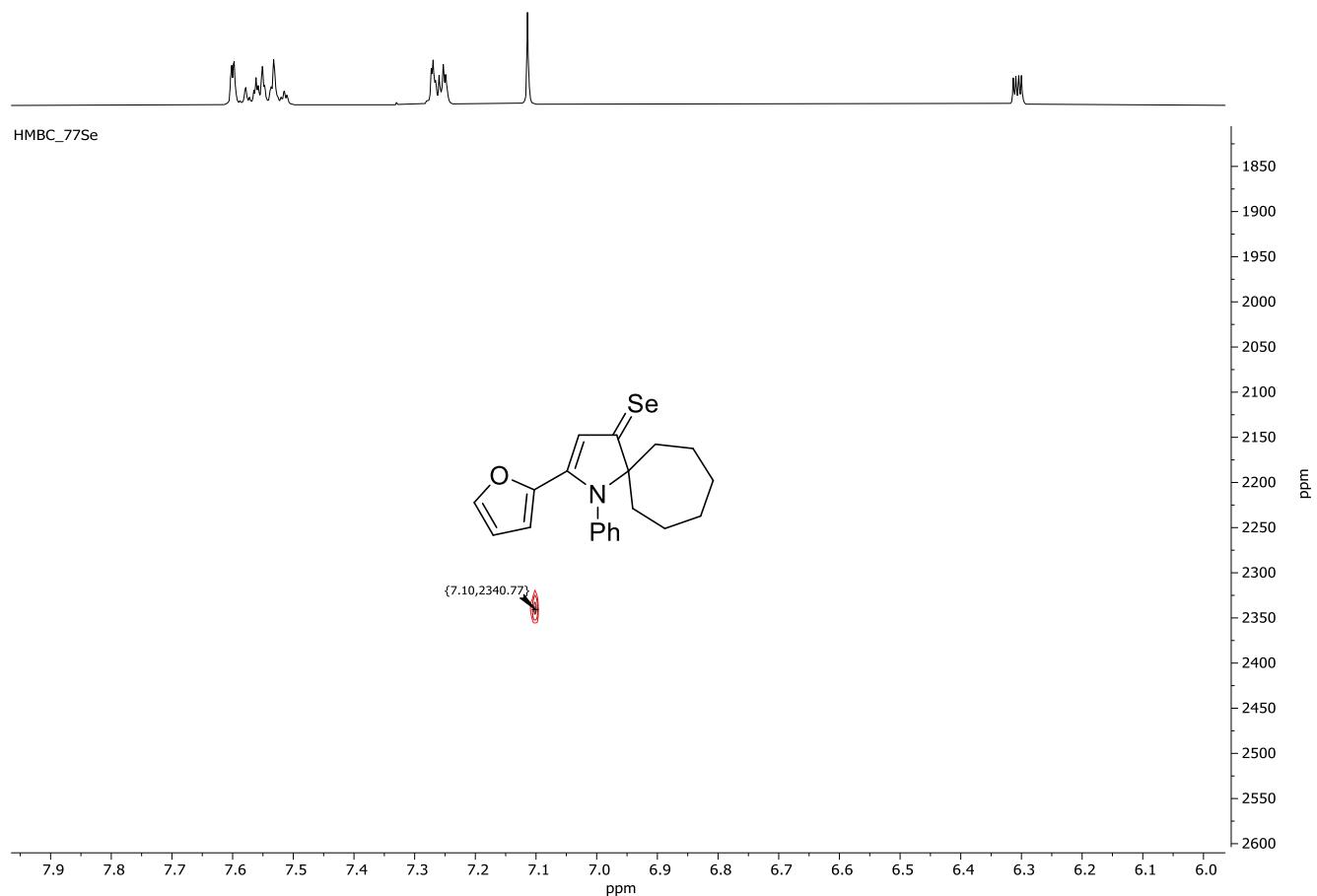
NMR_13C



2D ^1H - ^{15}N HMBC NMR of 2-(furan-2-yl)-1-phenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2p)

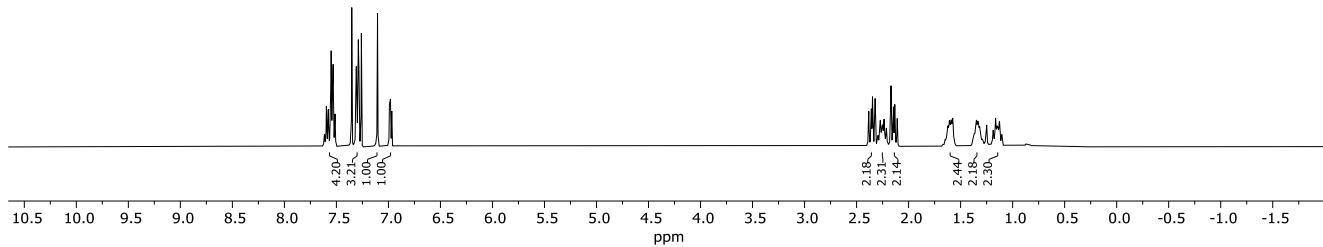
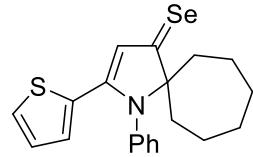


2D ^1H - ^{77}Se HMBC NMR of 2-(furan-2-yl)-1-phenyl-1-azaspiro[4.6]undec-2-ene-4-selone (2p)



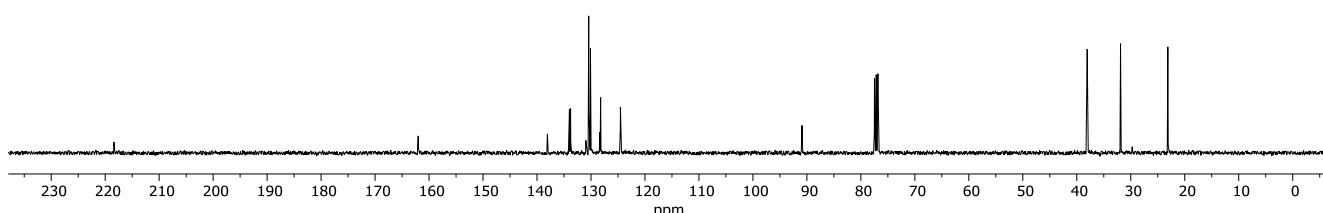
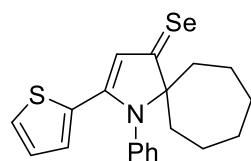
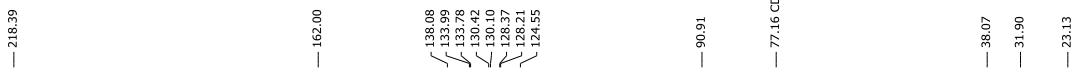
¹H NMR of 1-phenyl-2-(thiophen-2-yl)-1-azaspiro[4.6]undec-2-ene-4-selone (2q)

NMR_1H

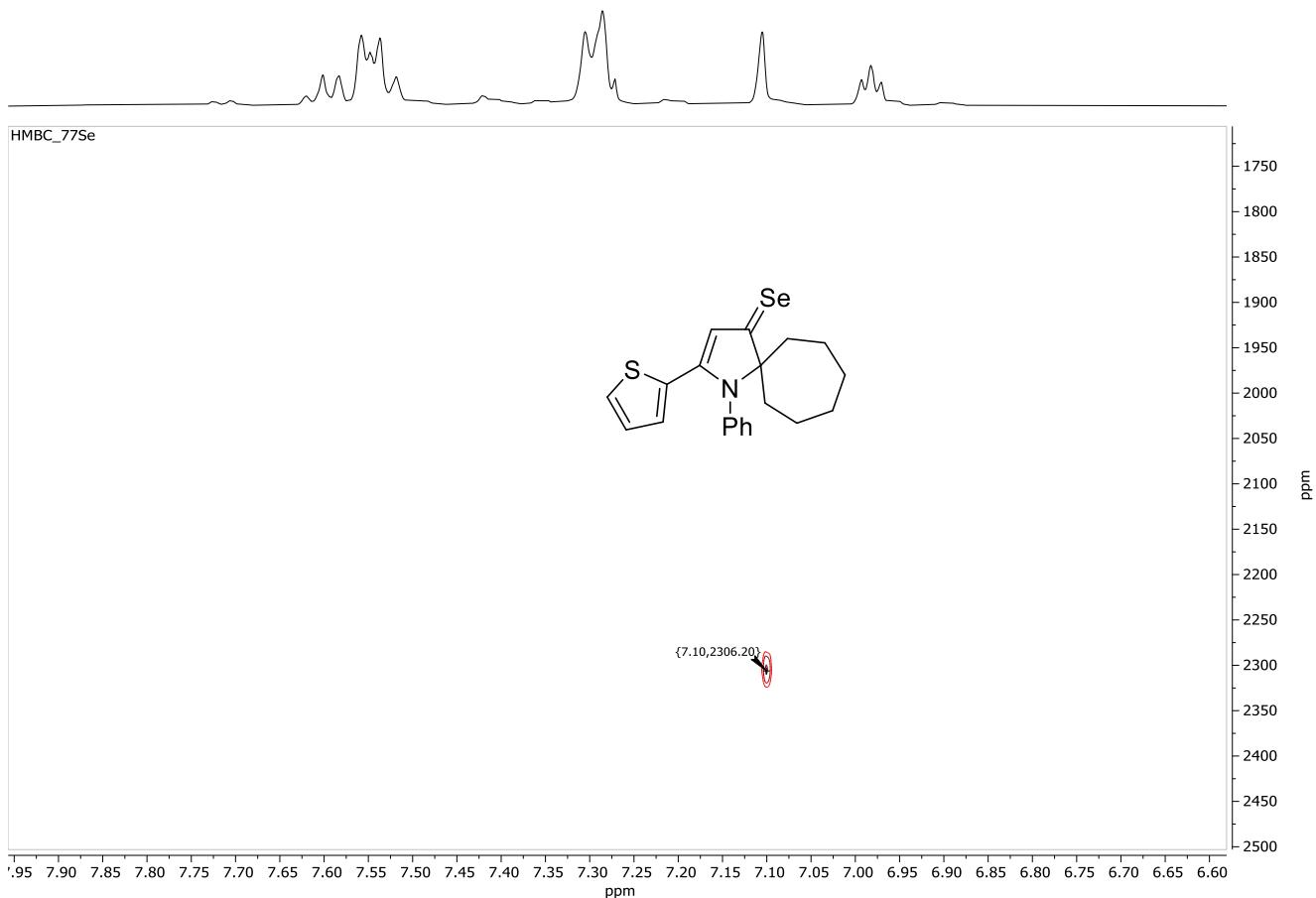


¹³C{¹H} NMR of 1-phenyl-2-(thiophen-2-yl)-1-azaspiro[4.6]undec-2-ene-4-selone (2q)

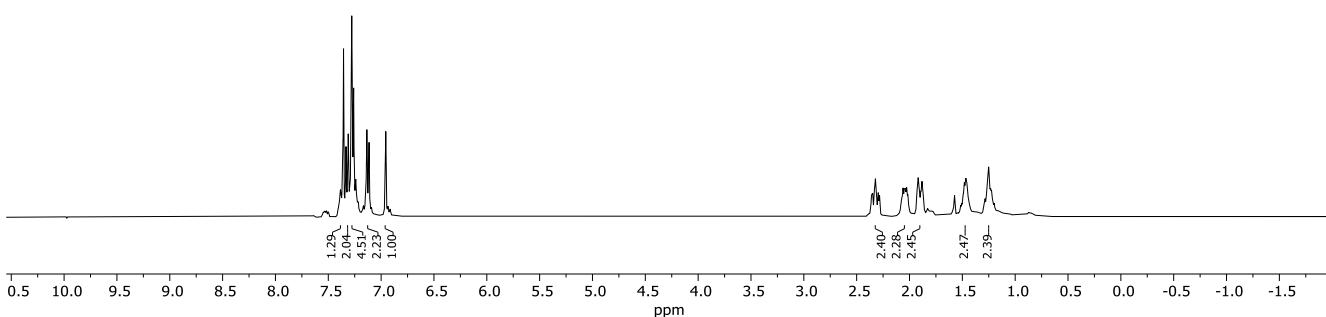
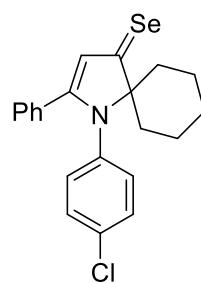
NMR_13C



2D ^1H - ^{77}Se HMBC NMR of 1-phenyl-2-(thiophen-2-yl)-1-azaspiro[4.6]undec-2-ene-4-selone (2q)

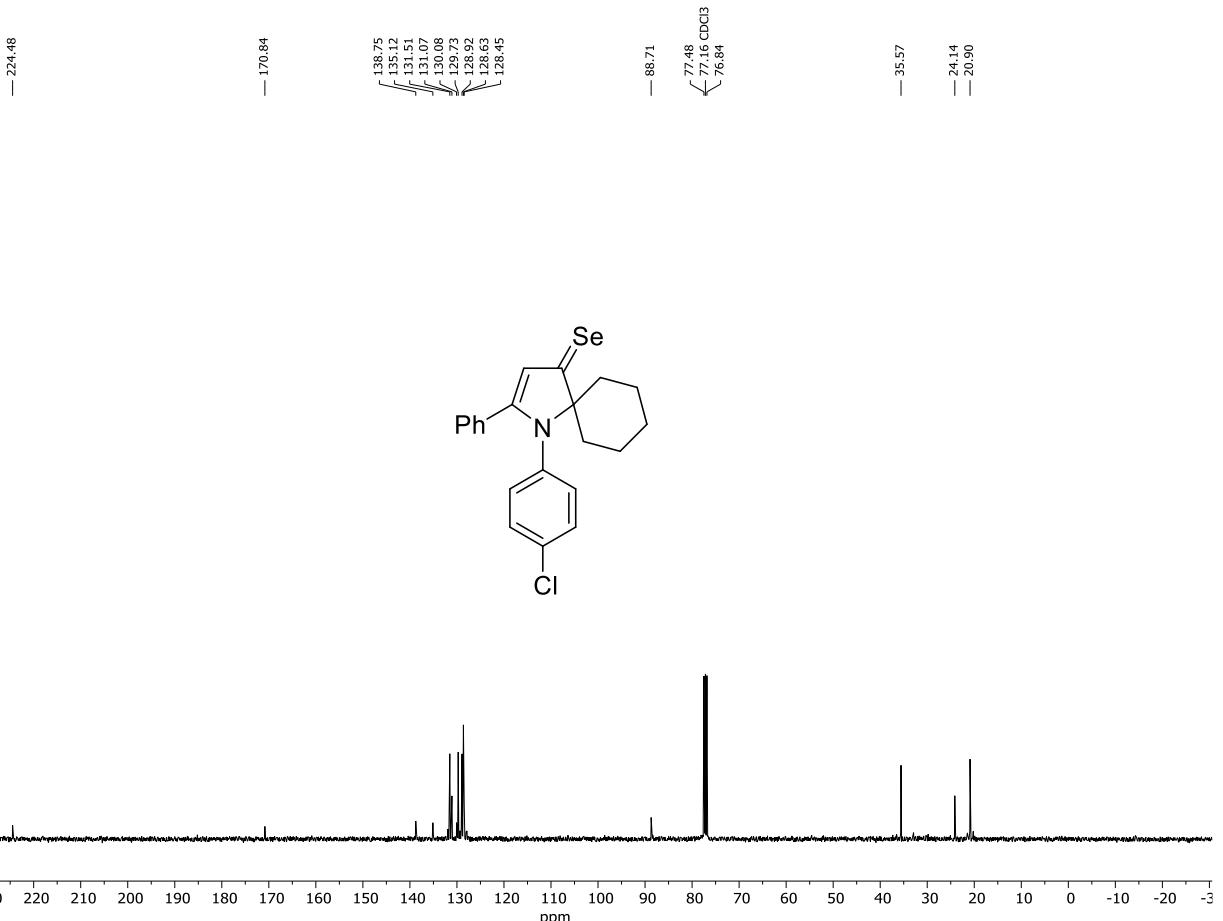


^1H NMR of 1-(4-chlorophenyl)-2-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2r)



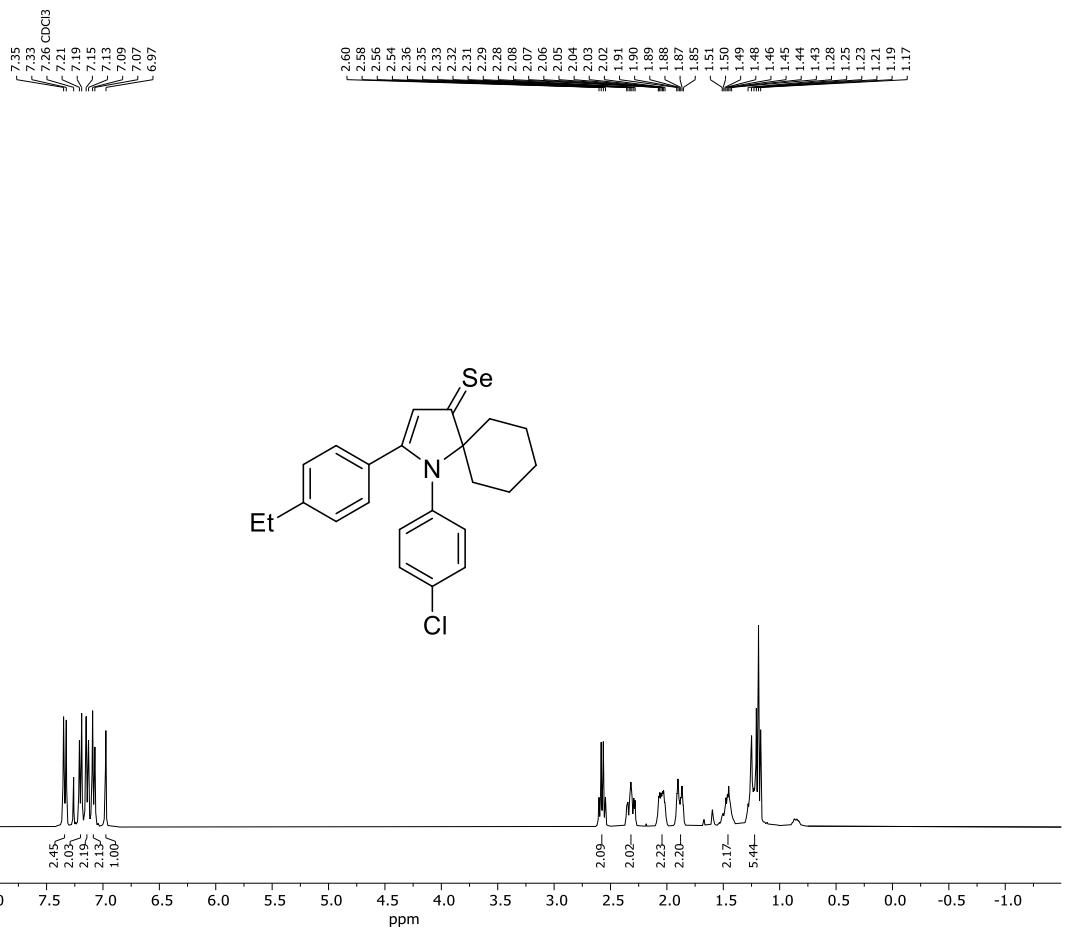
$^{13}\text{C}\{\text{H}\}$ NMR of 1-(4-chlorophenyl)-2-phenyl-1-azaspiro[4.5]dec-2-ene-4-selone (2r)

NMR_13C

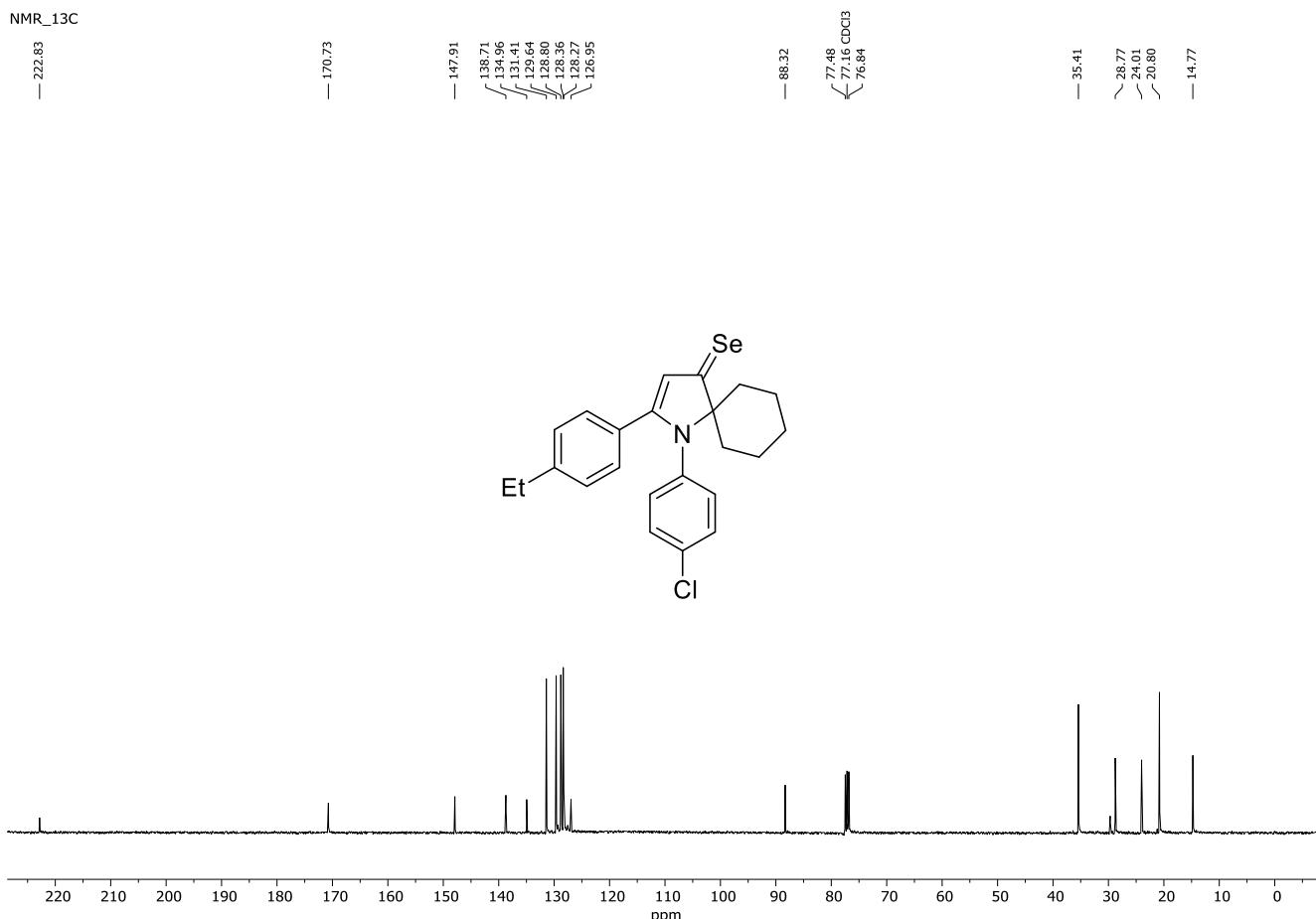


^1H NMR of 1-(4-chlorophenyl)-2-(4-ethylphenyl)-1-azaspiro[4.5]dec-2-ene-4-selone (2s)

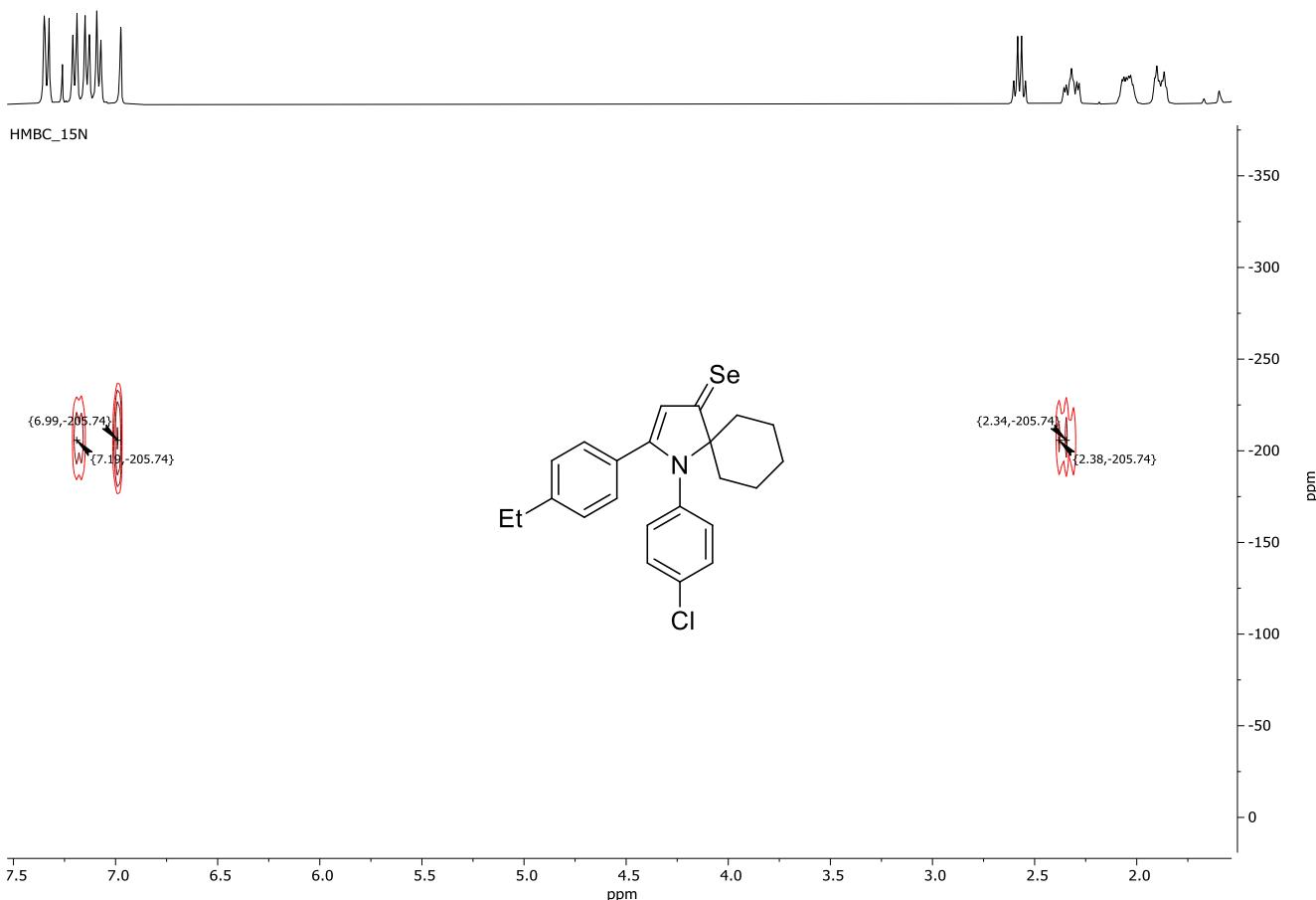
NMR_1H



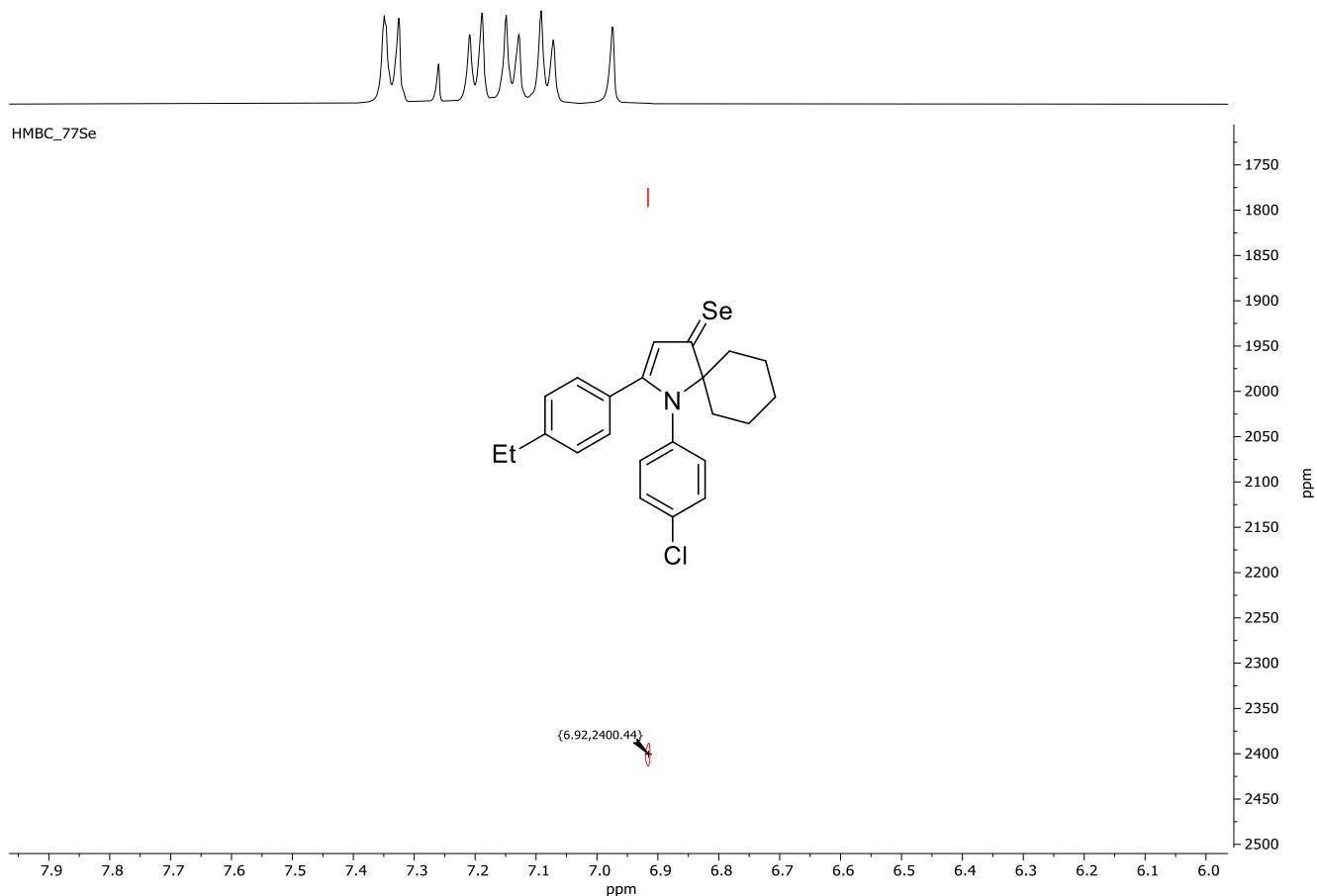
$^{13}\text{C}\{^1\text{H}\}$ NMR of 1-(4-chlorophenyl)-2-(4-ethylphenyl)-1-azaspiro[4.5]dec-2-ene-4-selone (2s)



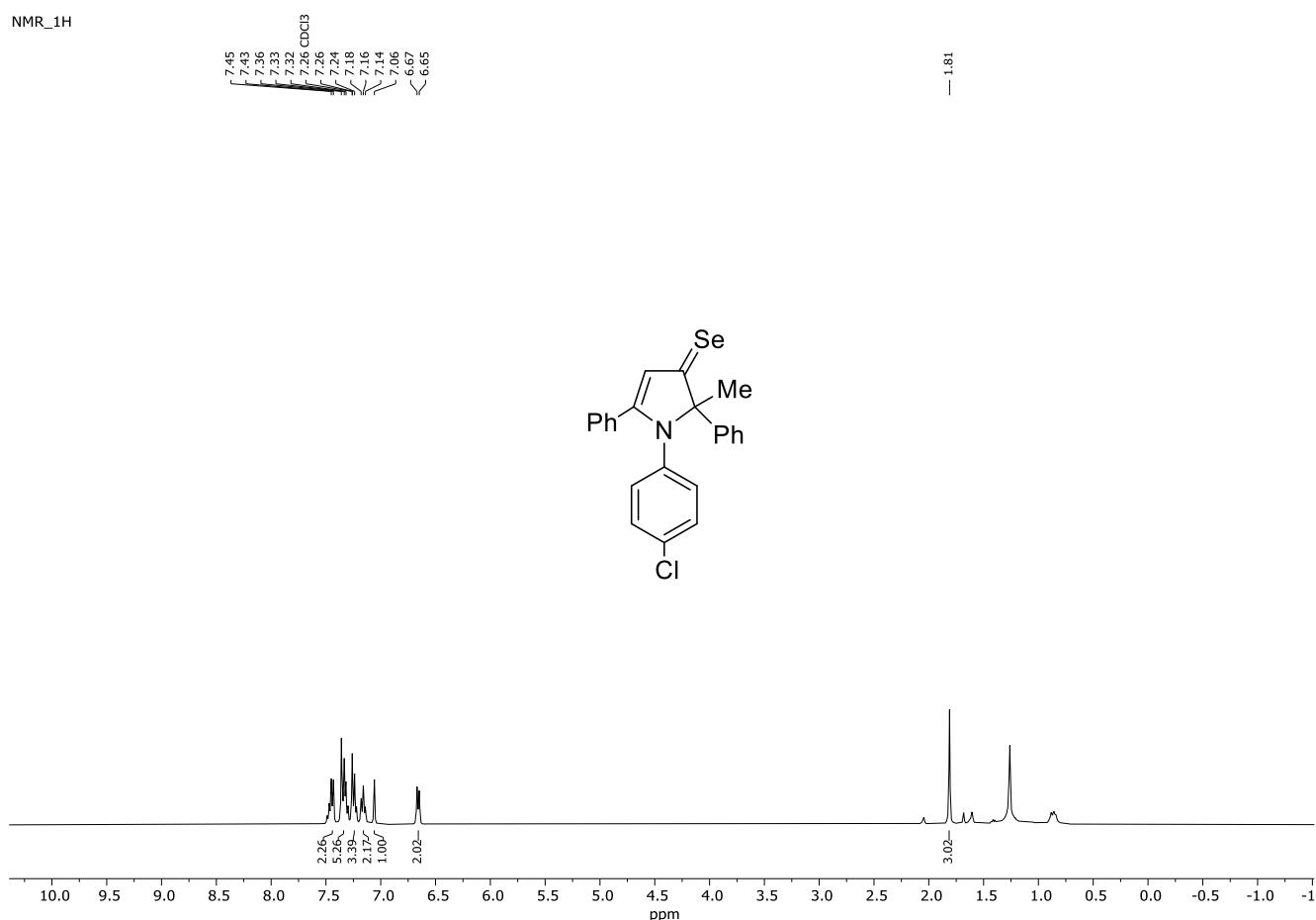
2D ^1H - ^{15}N HMBC NMR of 1-(4-chlorophenyl)-2-(4-ethylphenyl)-1-azaspiro[4.5]dec-2-ene-4-selone (2s)



2D ^1H - ^{77}Se HMBC NMR of 1-(4-chlorophenyl)-2-(4-ethylphenyl)-1-azaspiro[4.5]dec-2-ene-4-selone (2s)

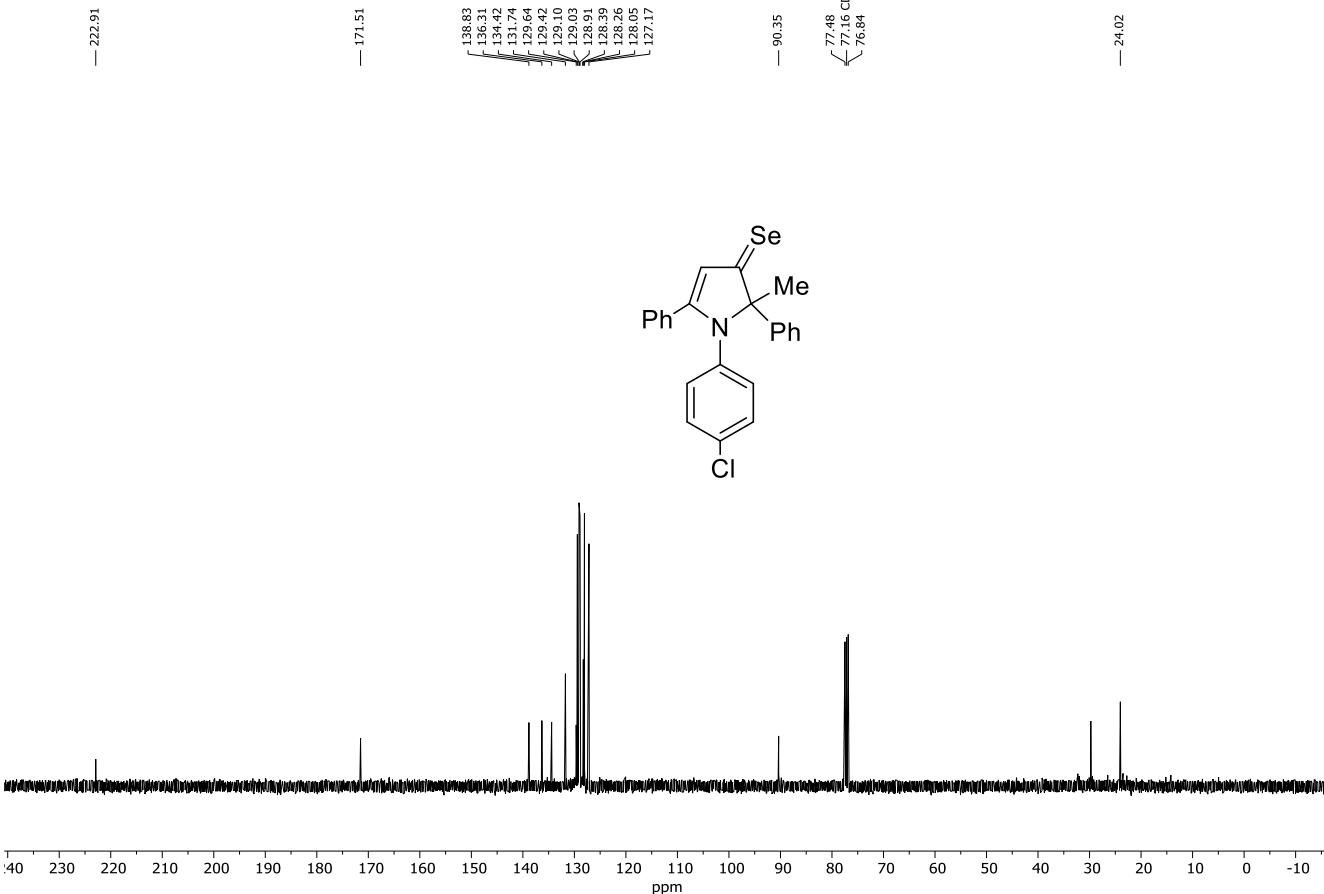


^1H NMR of 1-(4-chlorophenyl)-2-methyl-2,5-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2t)

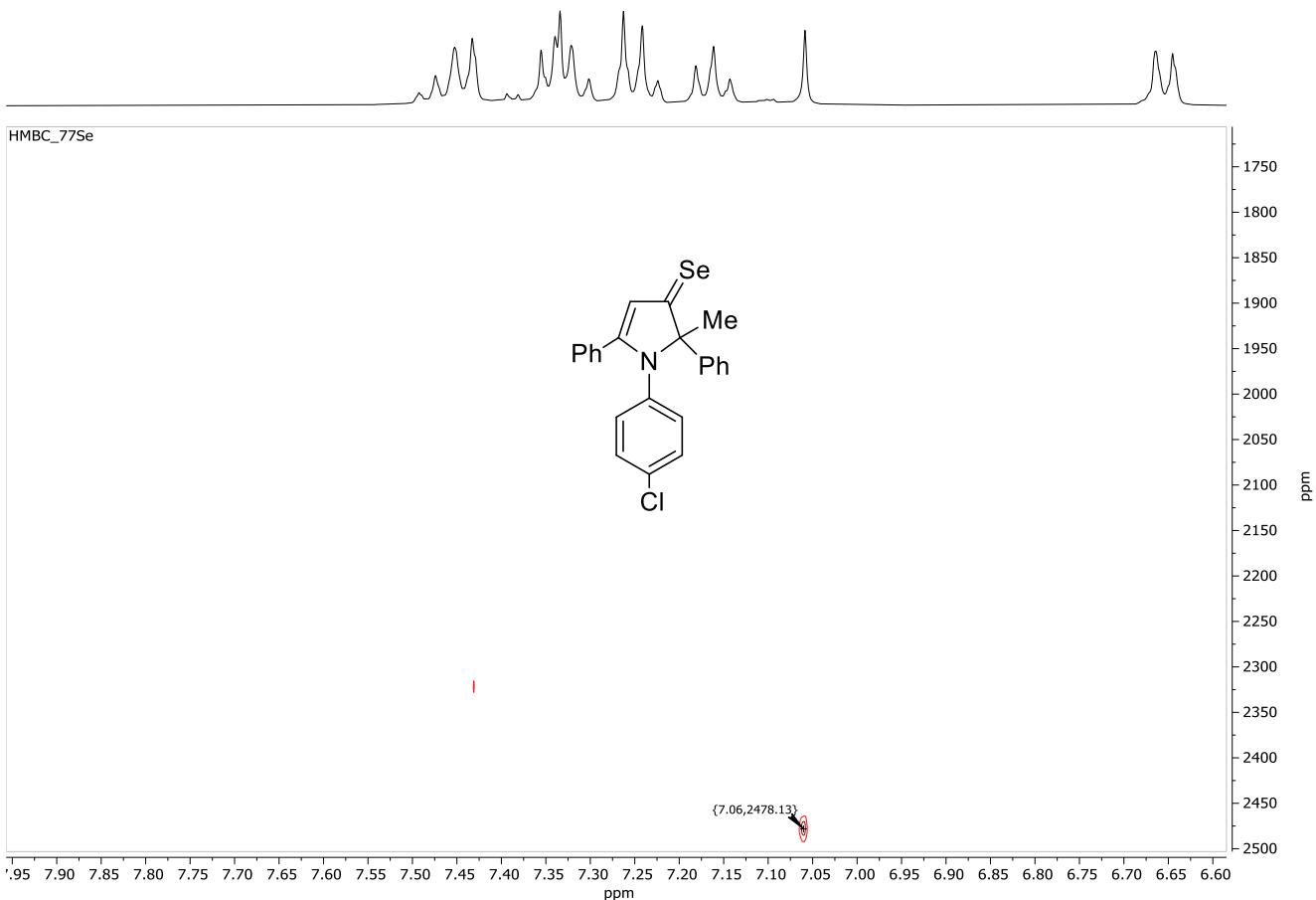


$^{13}\text{C}\{\text{H}\}$ NMR of 1-(4-chlorophenyl)-2-methyl-2,5-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2t)

NMR_13C

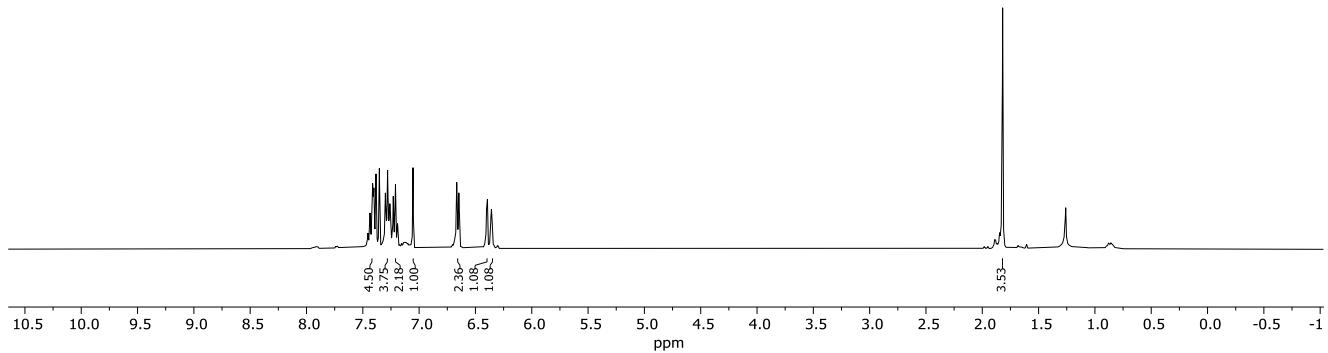
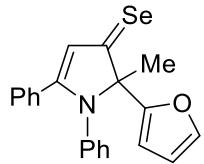


2D ^1H - ^{77}Se HMBC NMR of 1-(4-chlorophenyl)-2-methyl-2,5-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2t)



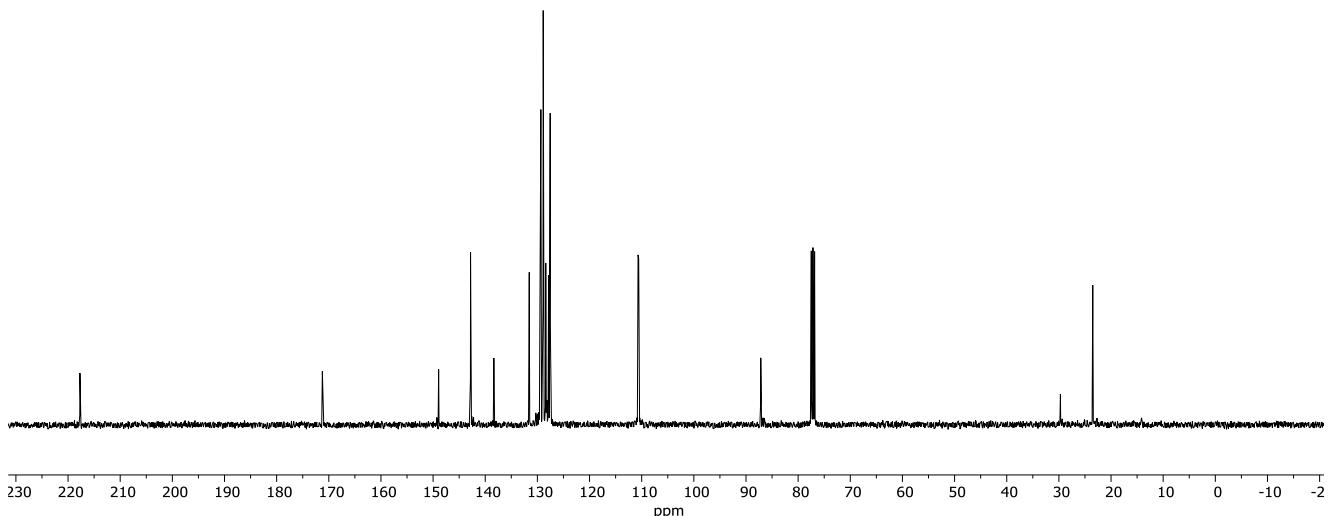
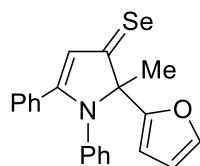
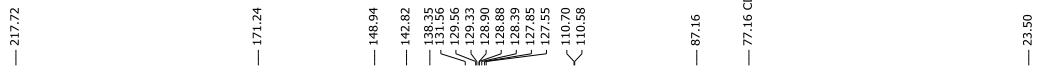
¹H NMR of 2-(furan-2-yl)-2-methyl-1,5-diphenyl-1,2-dihydro-3H-pyrrole-3-selone (2u)

NMR_1H

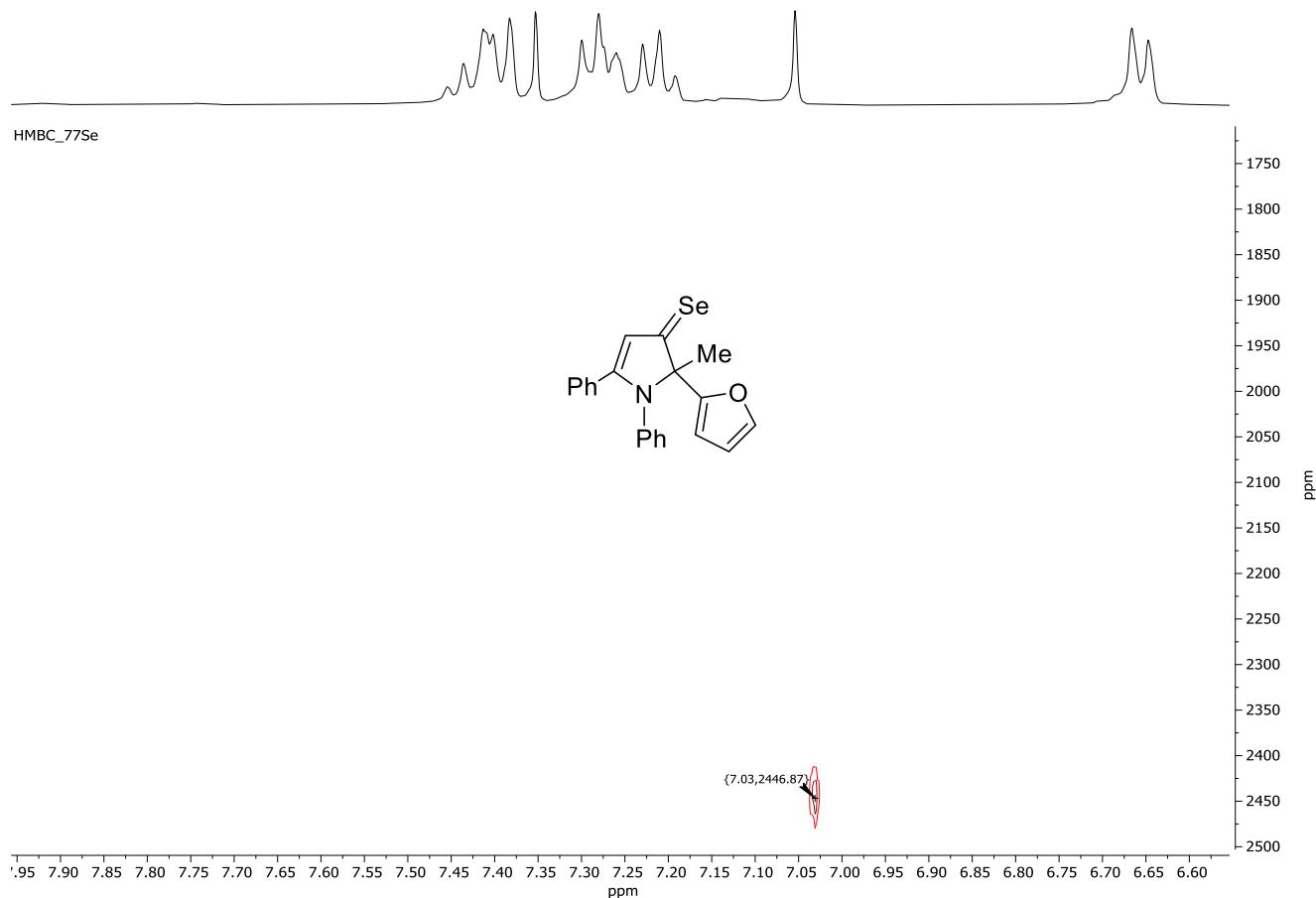


¹³C{¹H} NMR of 2-(furan-2-yl)-2-methyl-1,5-diphenyl-1,2-dihydro-3H-pyrrole-3-selone (2u)

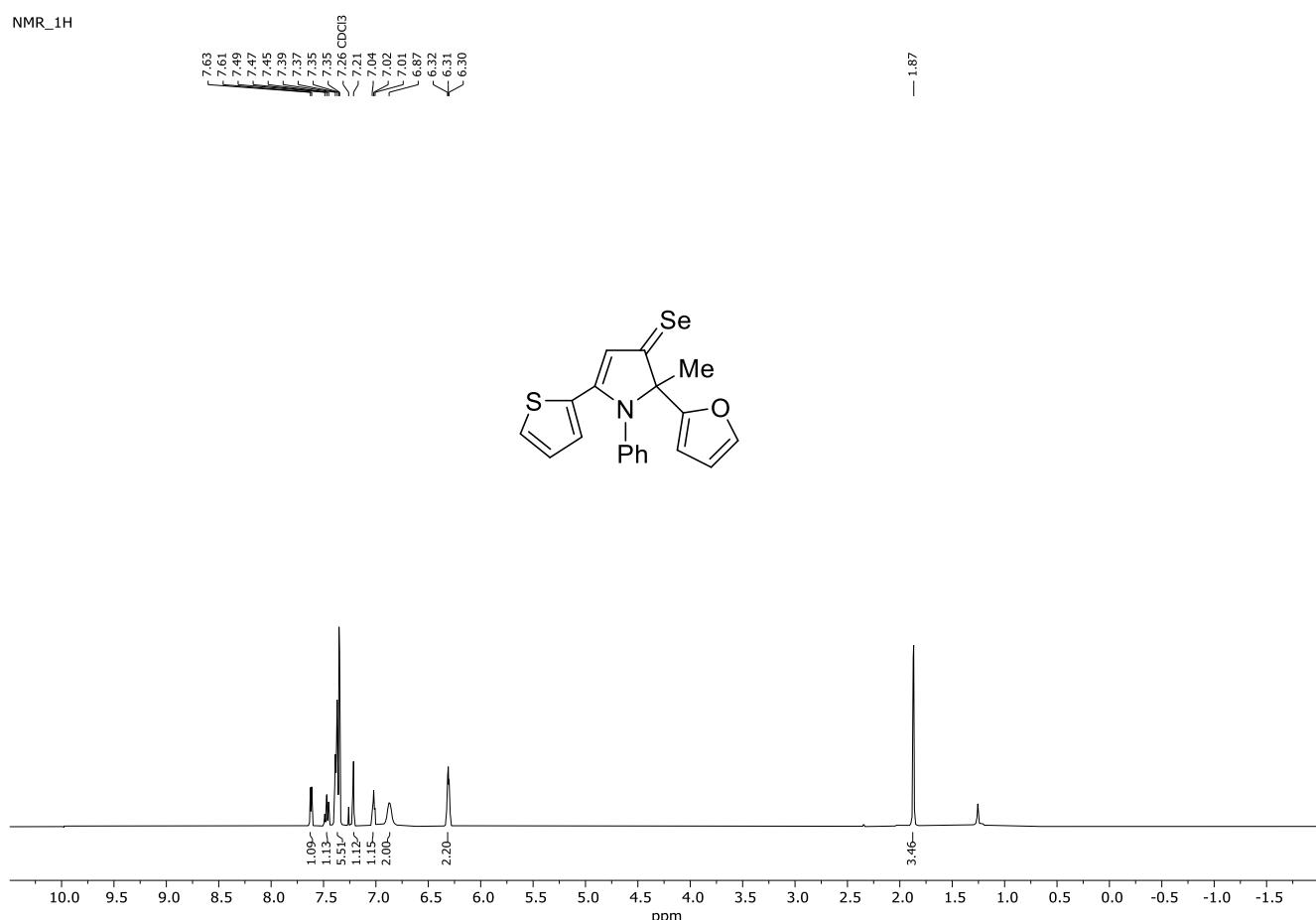
NMR_13C



2D ^1H - ^{77}Se HMBC NMR of 2-(furan-2-yl)-2-methyl-1,5-diphenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2u)

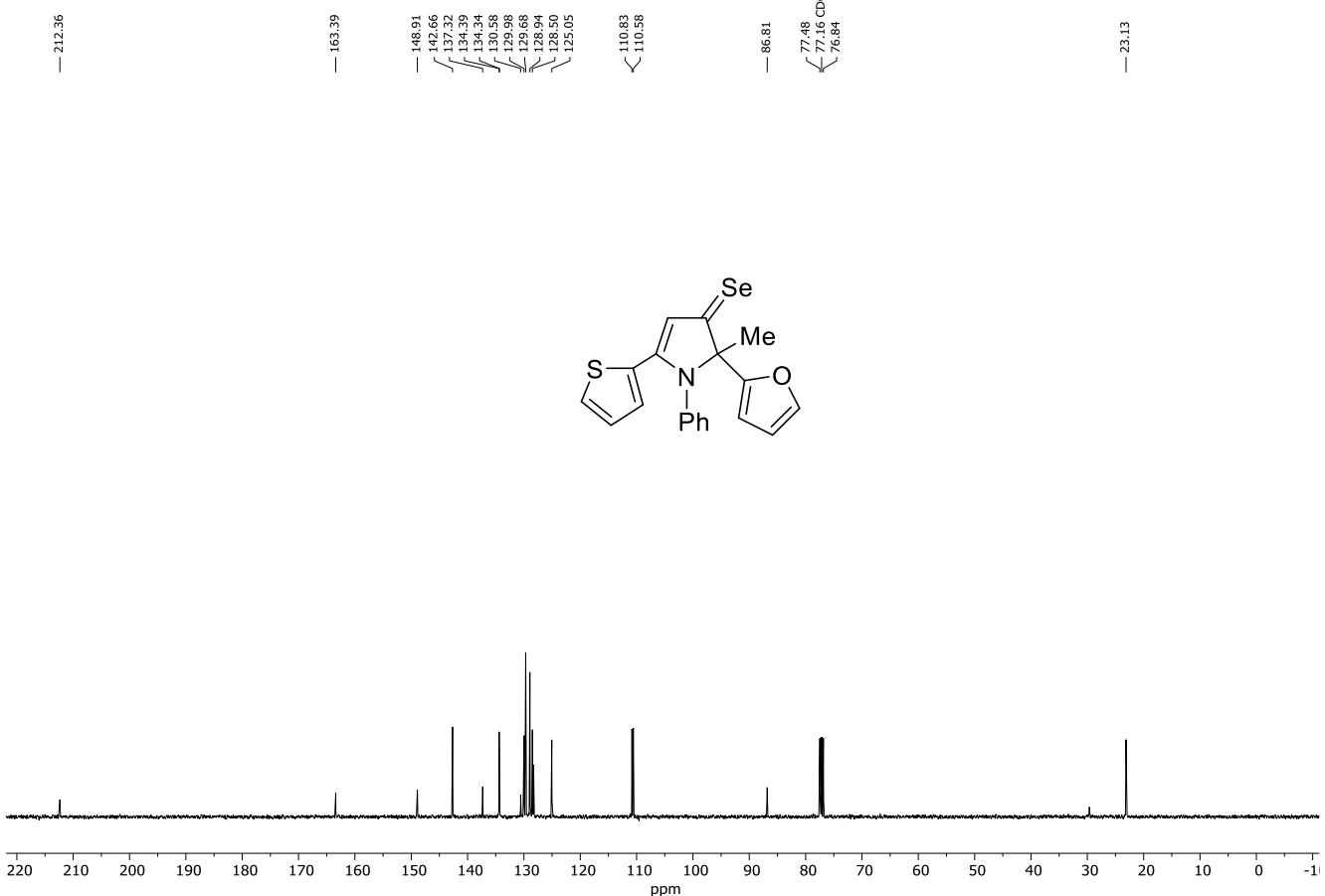


^1H NMR of 2-(furan-2-yl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2v)

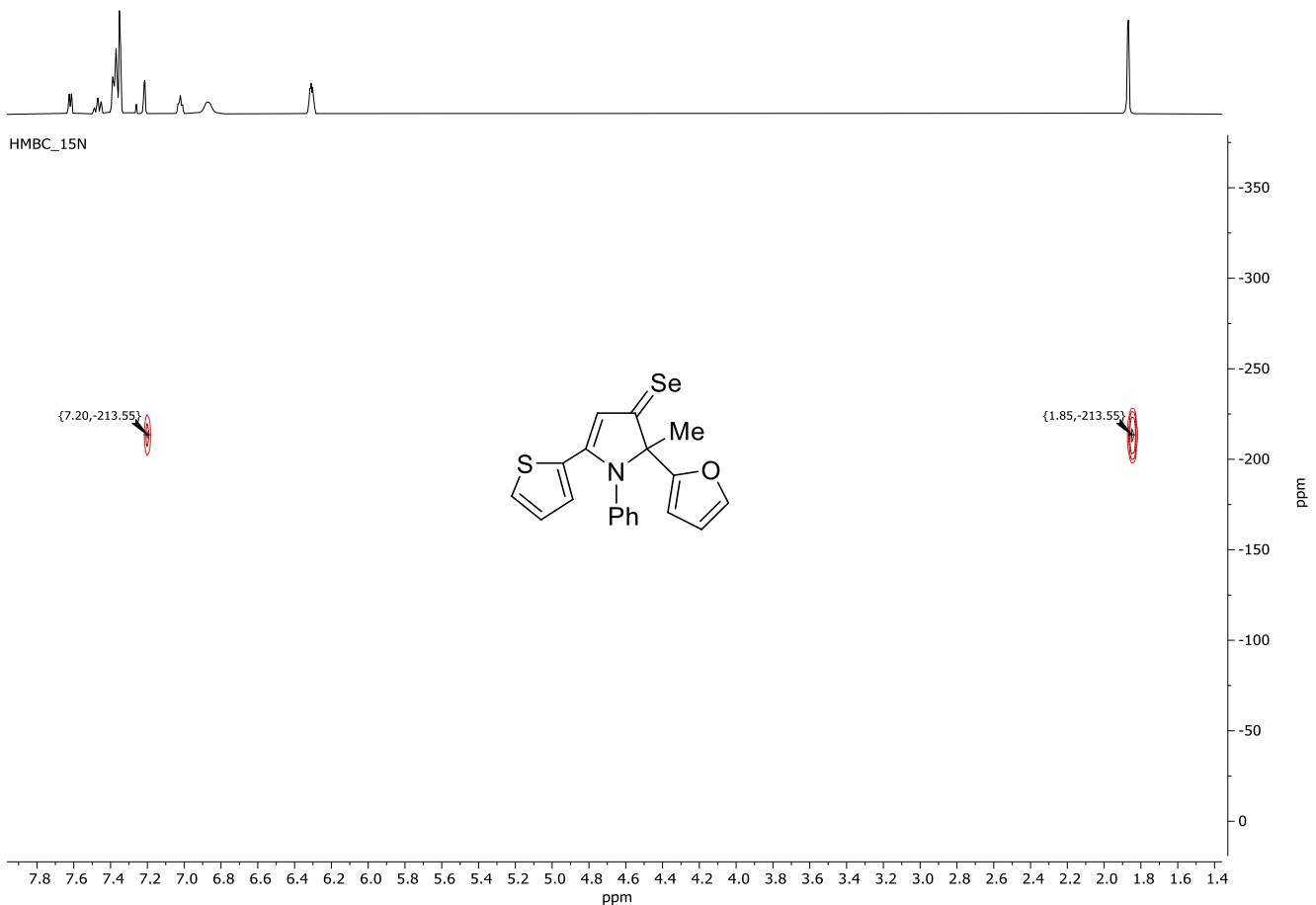


$^{13}\text{C}\{^1\text{H}\}$ NMR of 2-(furan-2-yl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2v)

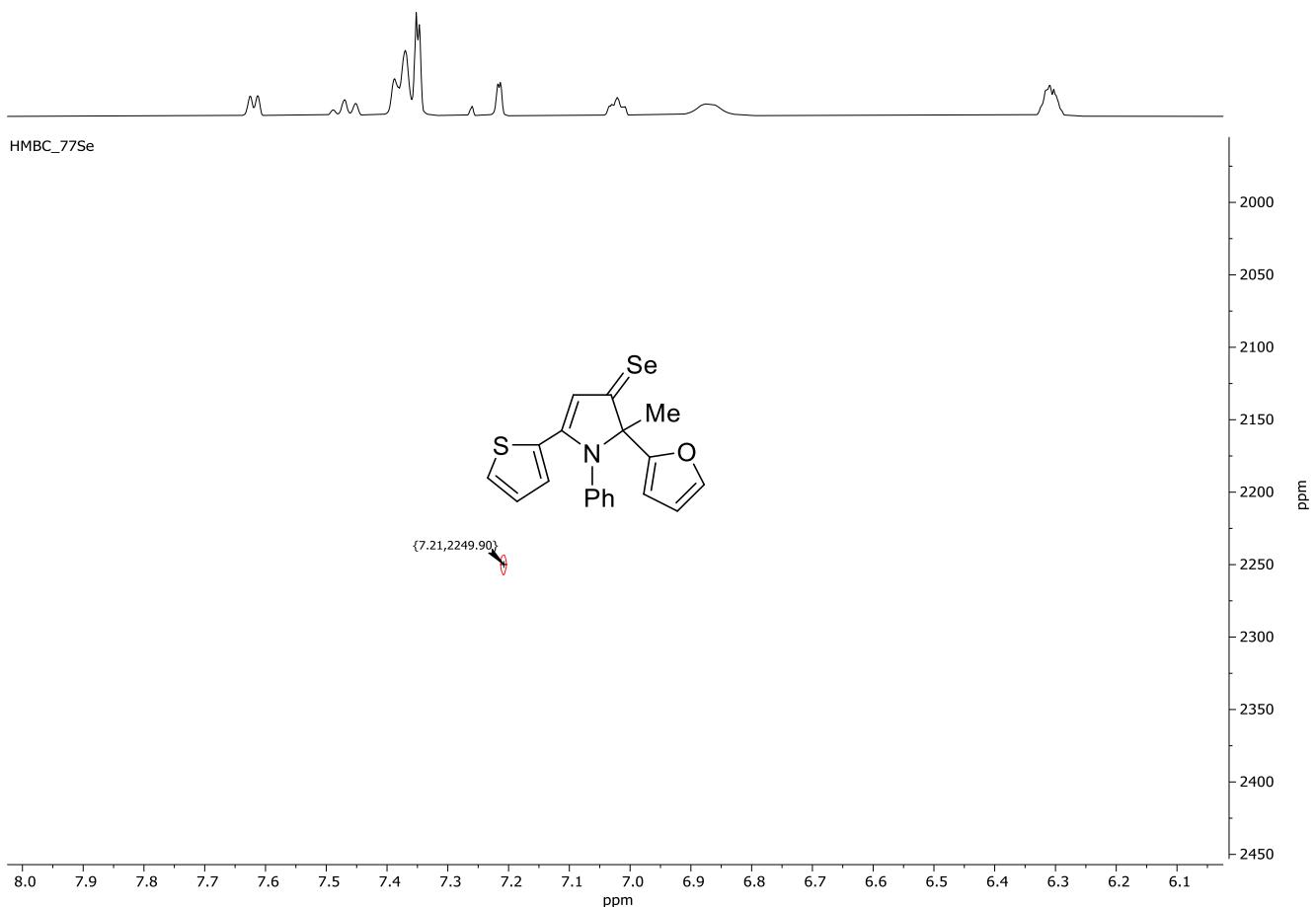
NMR_13C



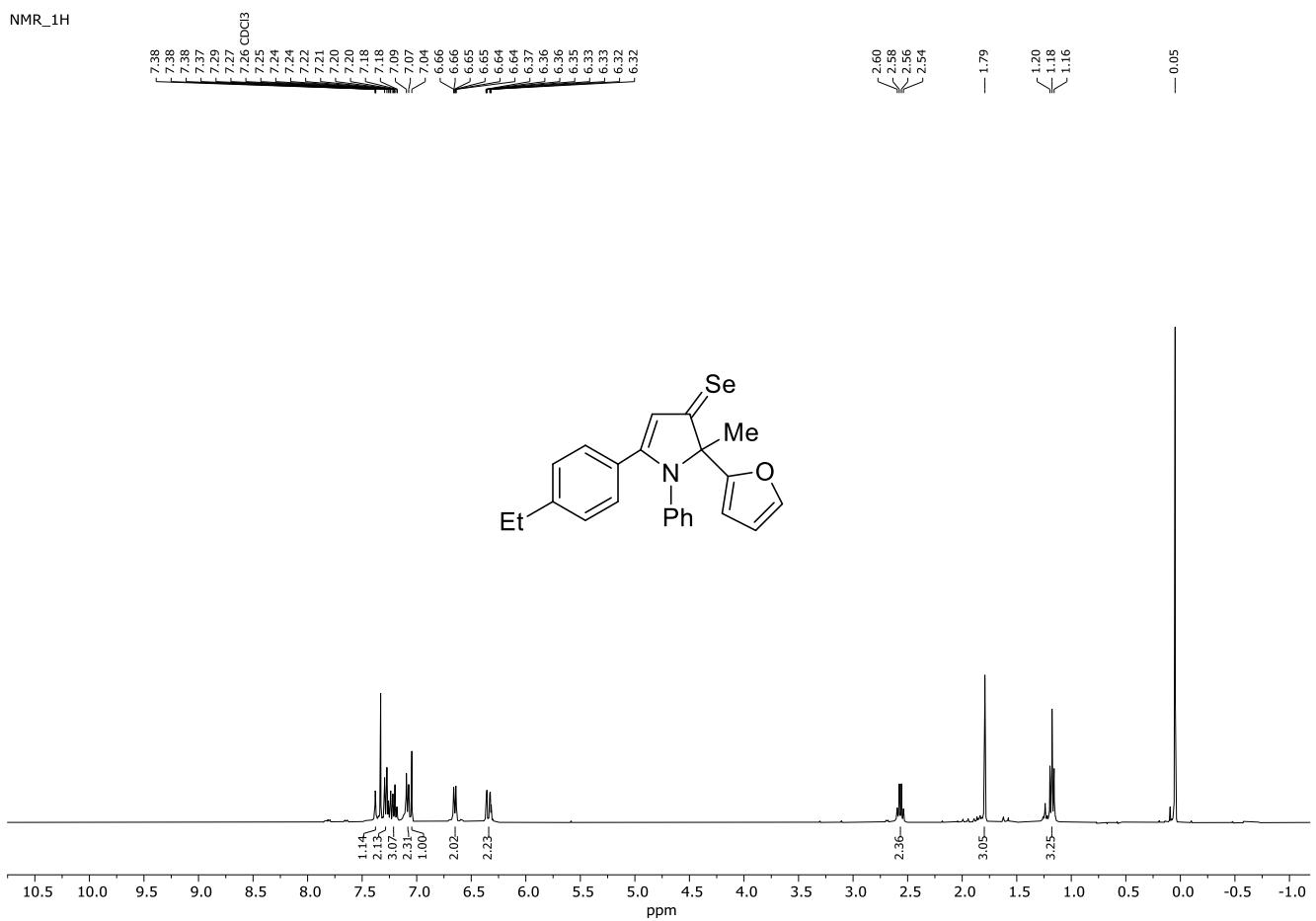
2D ^1H - ^{15}N HMBC NMR of 2-(furan-2-yl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2v)



2D ^1H - ^{77}Se HMBC NMR of 2-(furan-2-yl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2v)

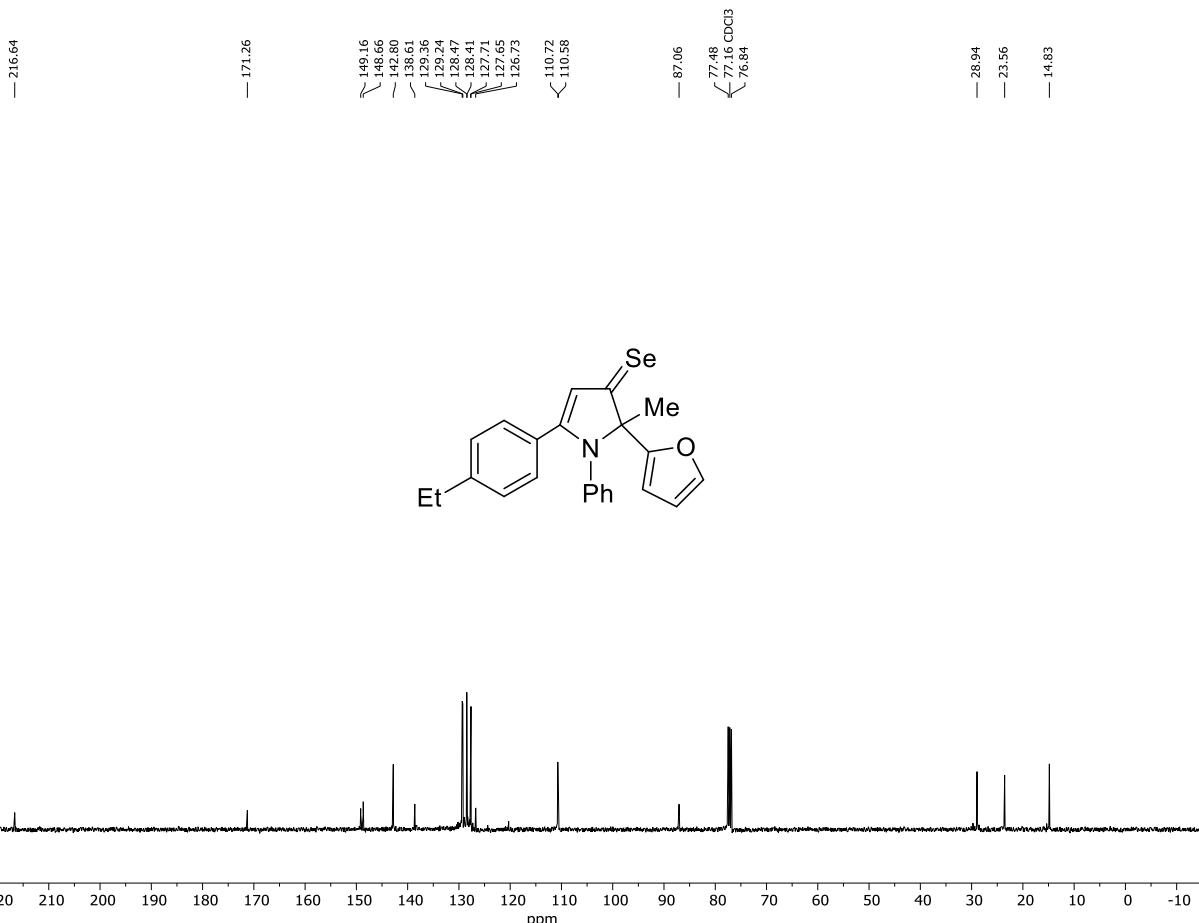


^1H NMR of 5-(4-ethylphenyl)-2-(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2w)

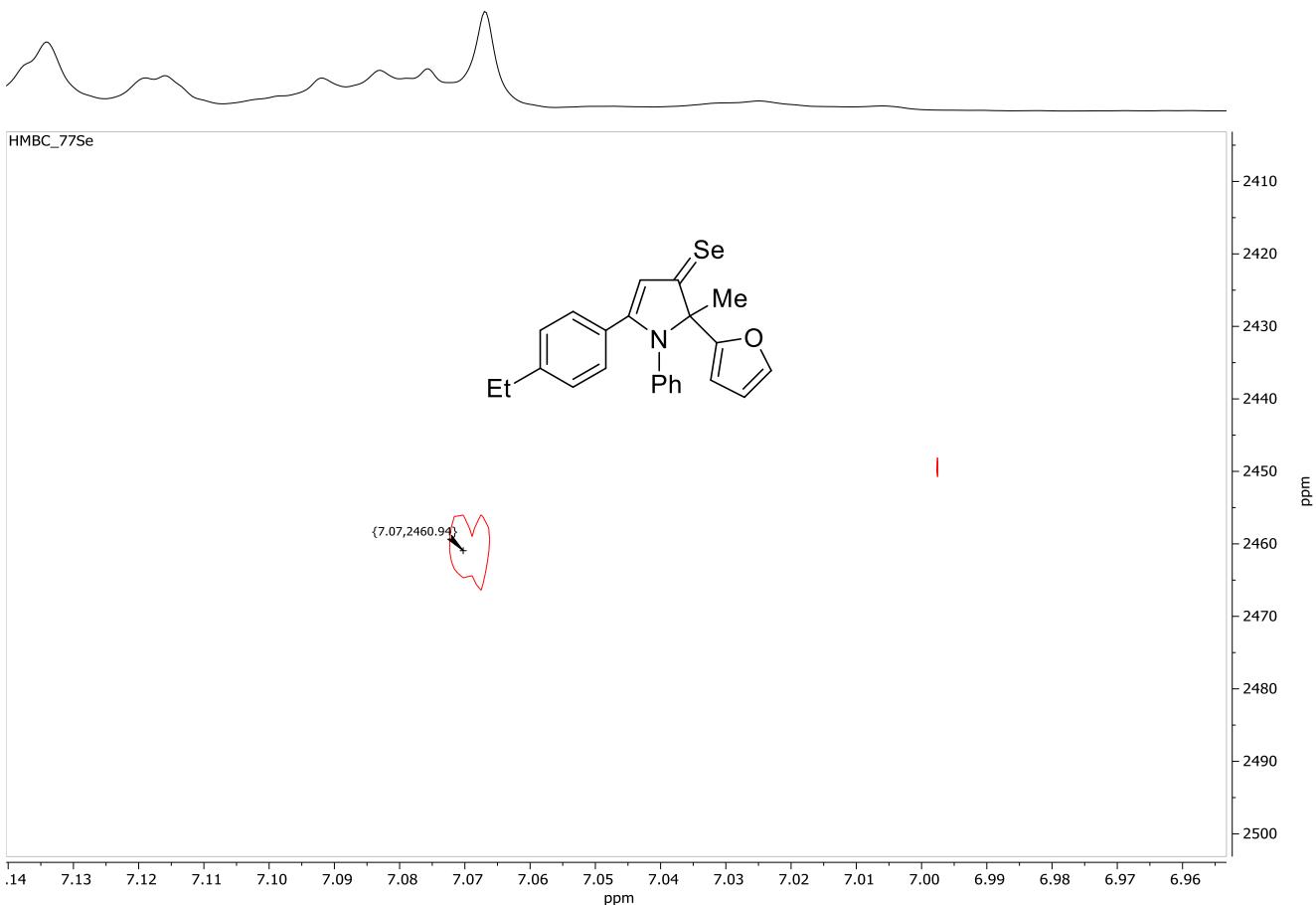


$^{13}\text{C}\{\text{H}\}$ NMR of 5-(4-ethylphenyl)-2-(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2w)

NMR_13C

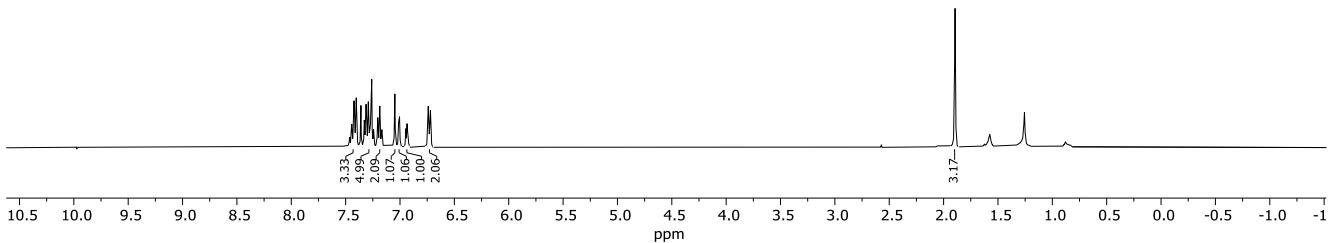
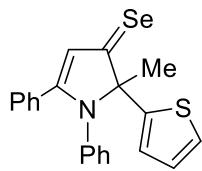
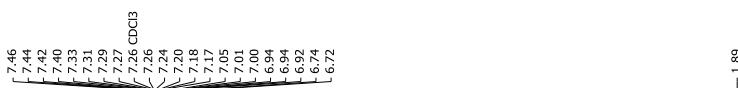


2D ^1H - ^{77}Se HMBC NMR of 5-(4-ethylphenyl)-2-(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3*H*-pyrrole-3-selone (2w)



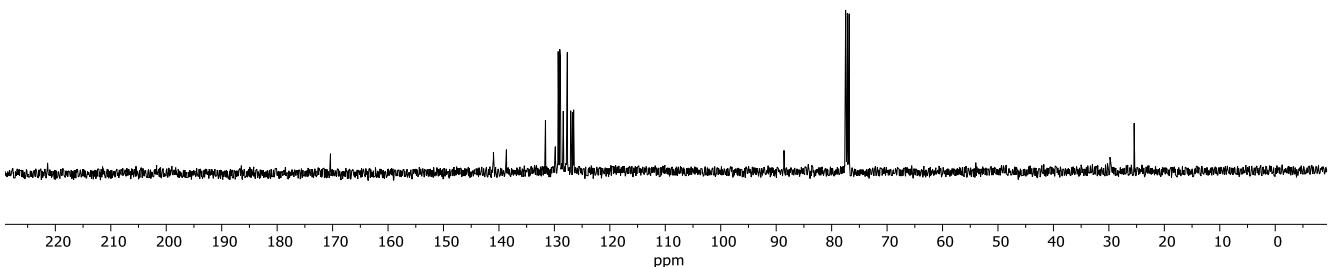
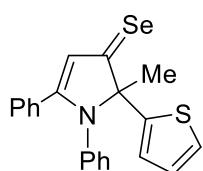
¹H NMR of 2-methyl-1,5-diphenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-selone (2x)

NMR_1H

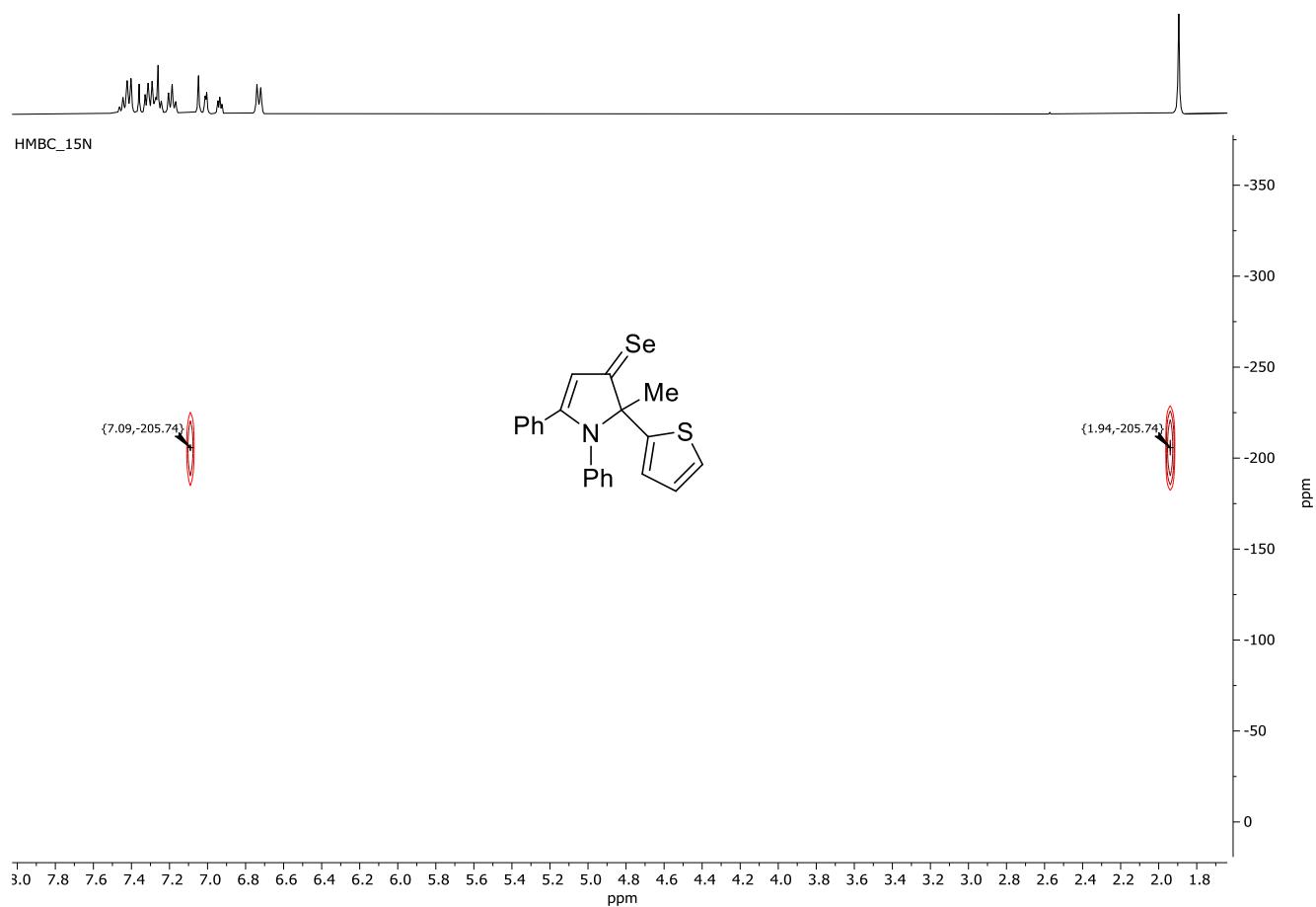


¹³C{¹H} NMR of 2-methyl-1,5-diphenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-selone (2x)

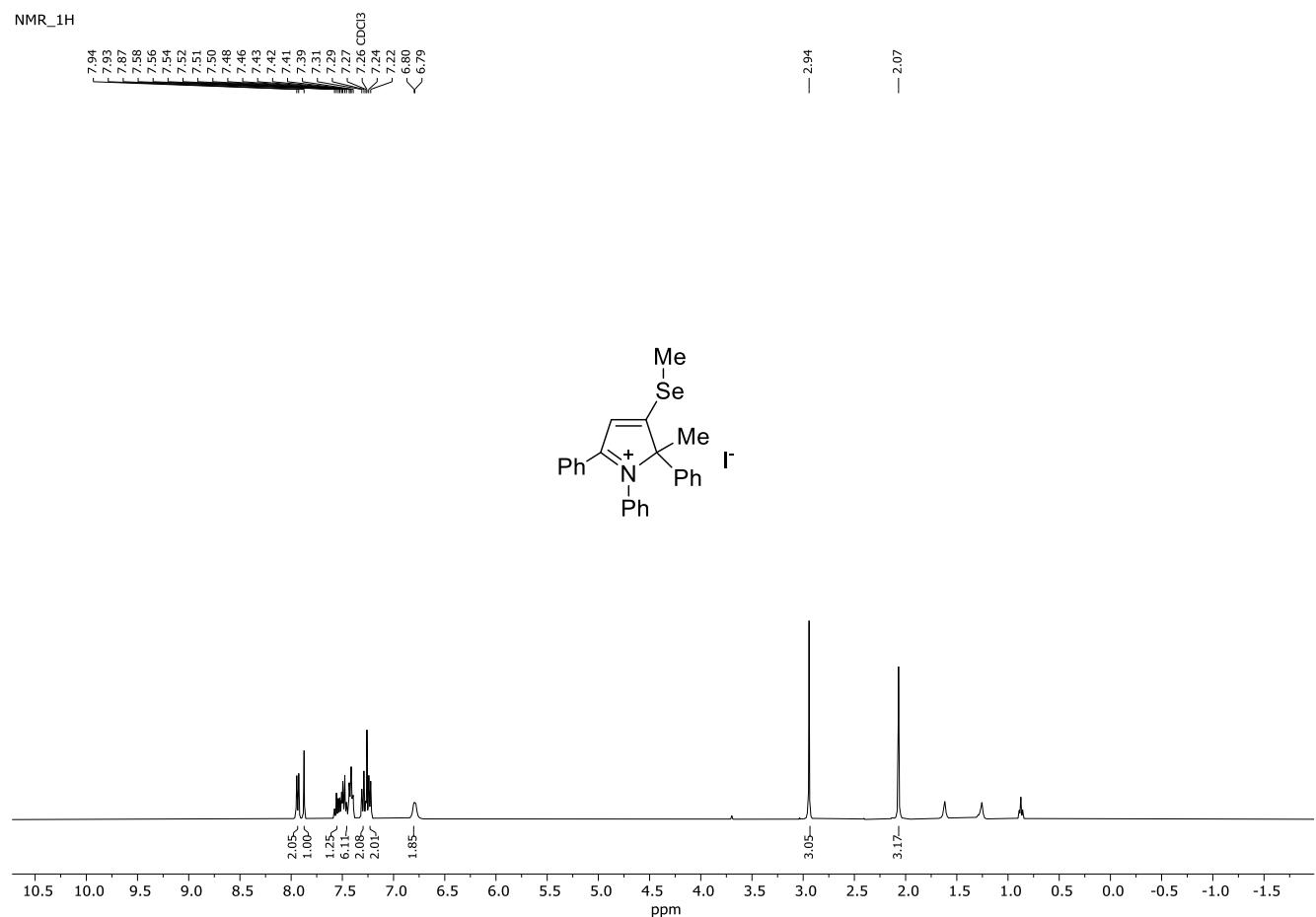
NMR_13C



2D ^1H - ^{15}N HMBC NMR of 2-methyl-1,5-diphenyl-2-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrole-3-selone (2x)

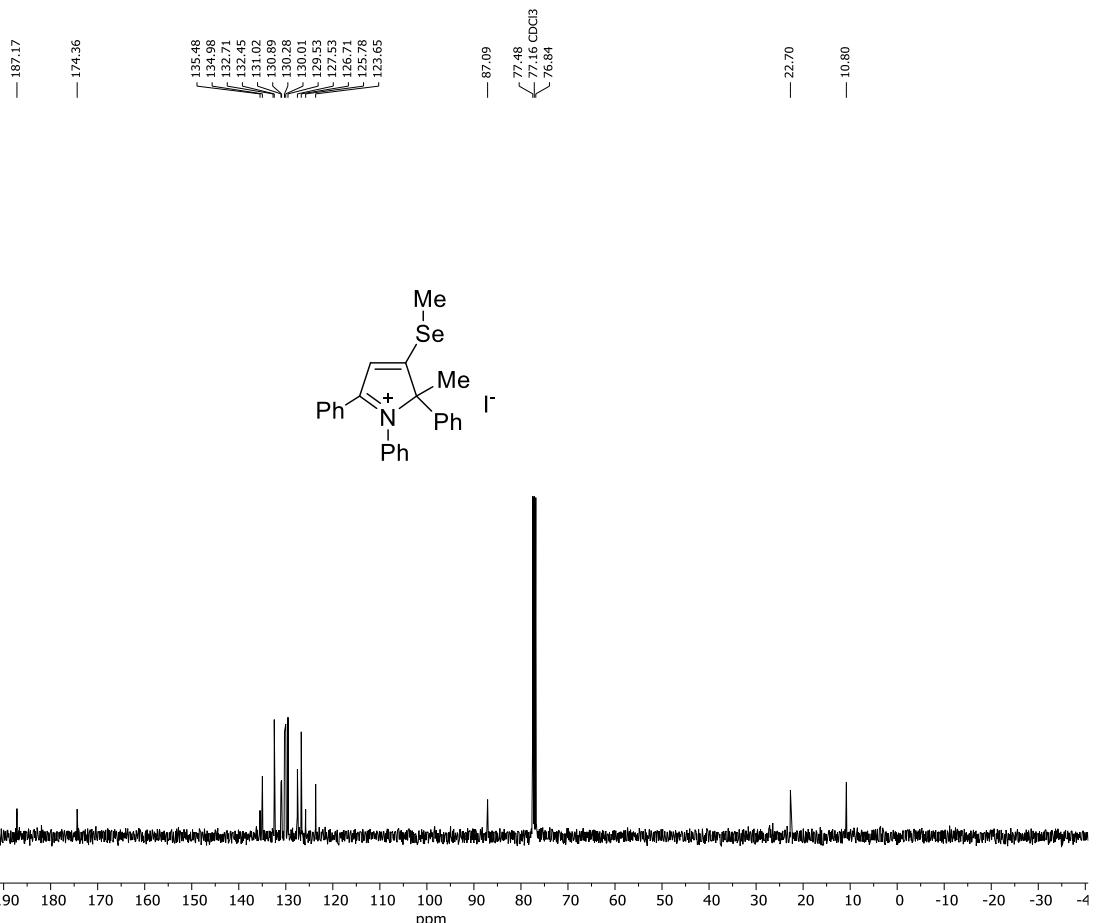


^1H NMR of 2-methyl-3-(methylselanyl)-1,2,5-triphenyl-2*H*-pyrrolium iodide (6a)

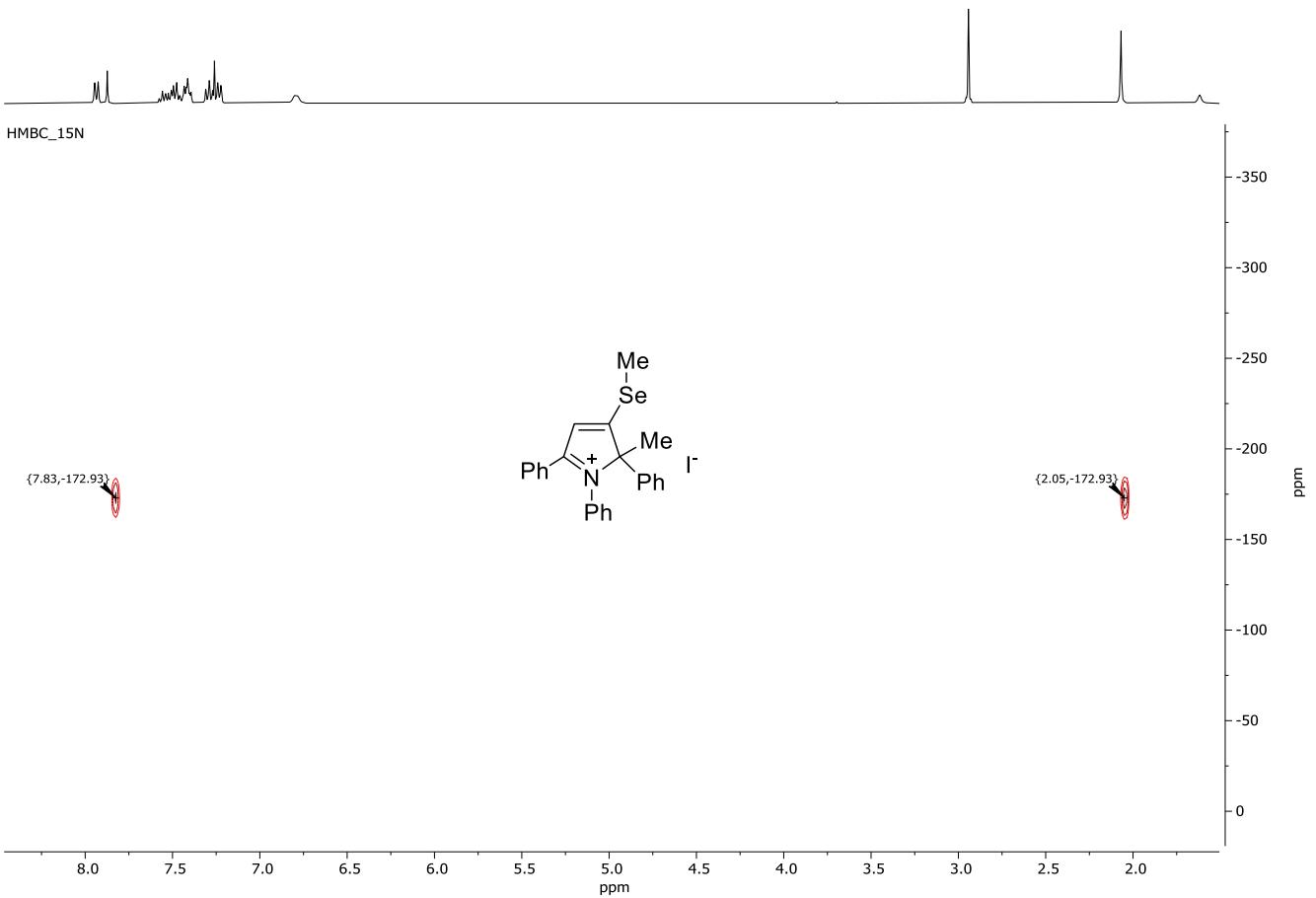


$^{13}\text{C}\{^1\text{H}\}$ NMR of 2-methyl-3-(methylselanyl)-1,2,5-triphenyl-2*H*-pyrrolium iodide (**6a**)

NMR_13C



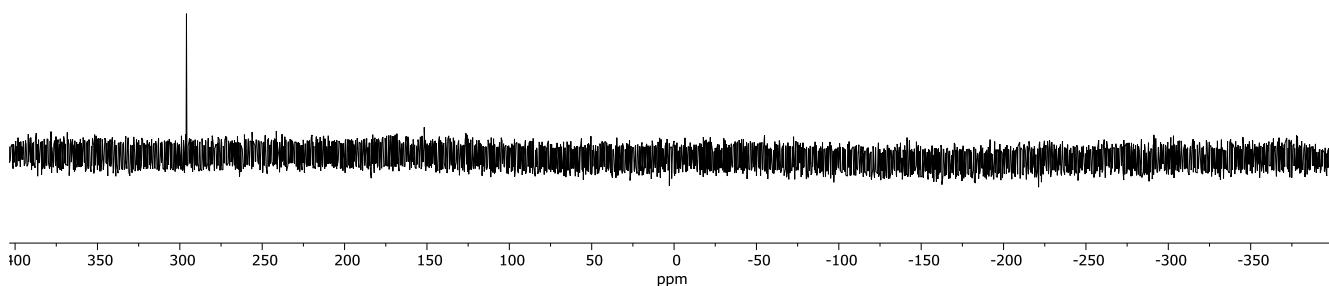
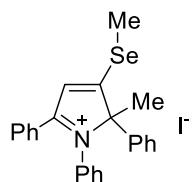
2D ^1H - ^{15}N HMBC NMR of 2-methyl-3-(methylselanyl)-1,2,5-triphenyl-2*H*-pyrrolium iodide (**6a**)



⁷⁷Se NMR of 2-methyl-3-(methylselanyl)-1,2,5-triphenyl-2H-pyrrolium iodide (**6a**)

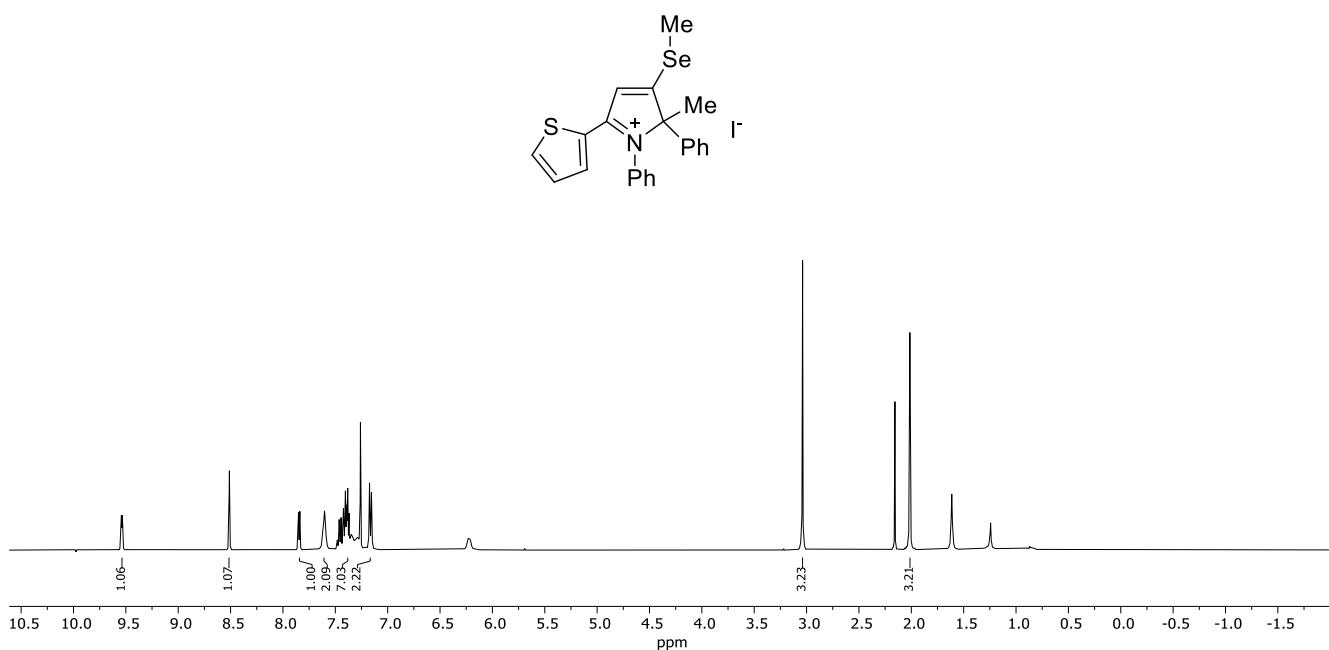
NMR_77Se

— 295.97



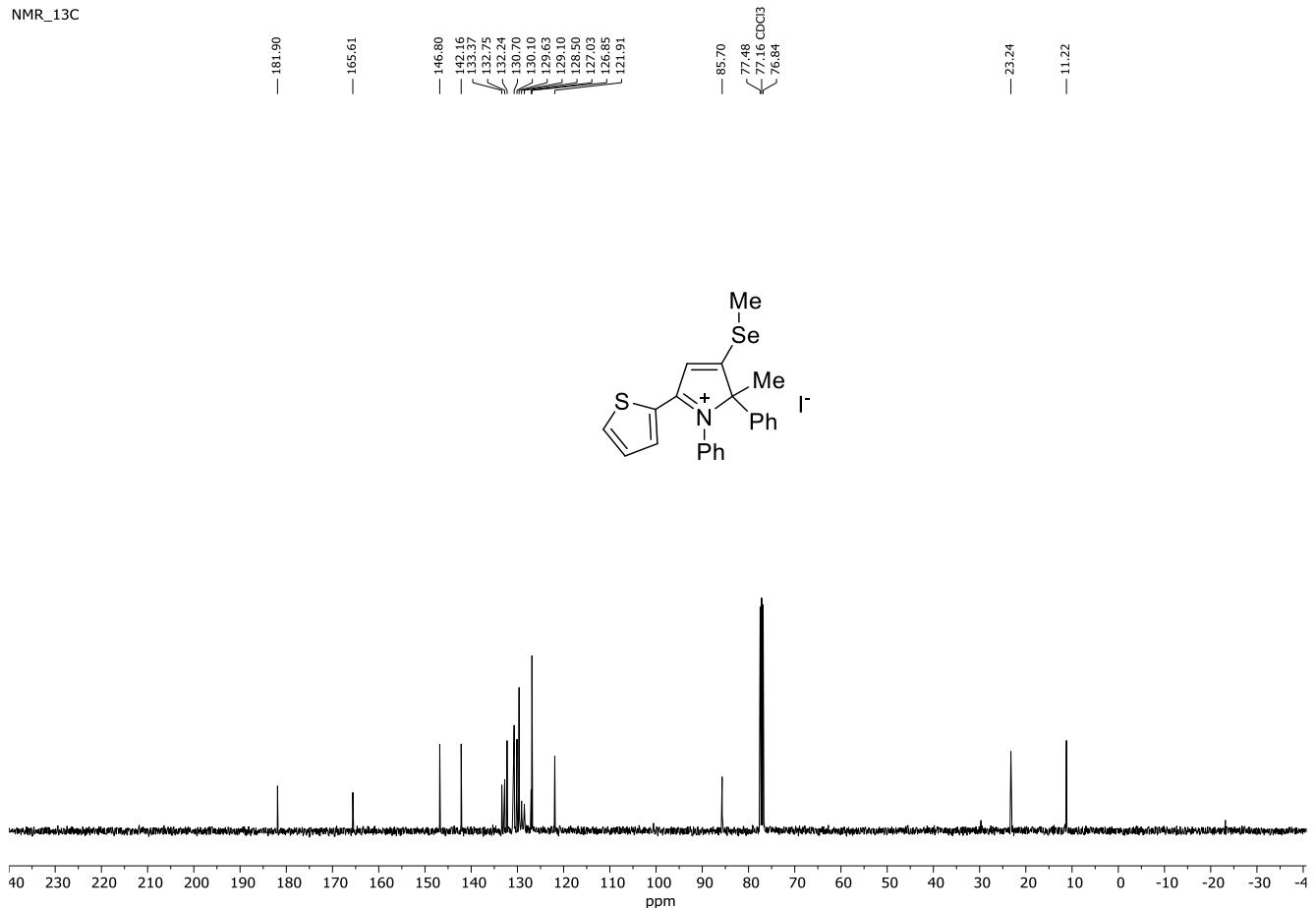
¹H NMR of 2-methyl-3-(methylselanyl)-1,2-diphenyl-5-(thiophen-2-yl)-2H-pyrrolium iodide (**6b**)

NMR_1H

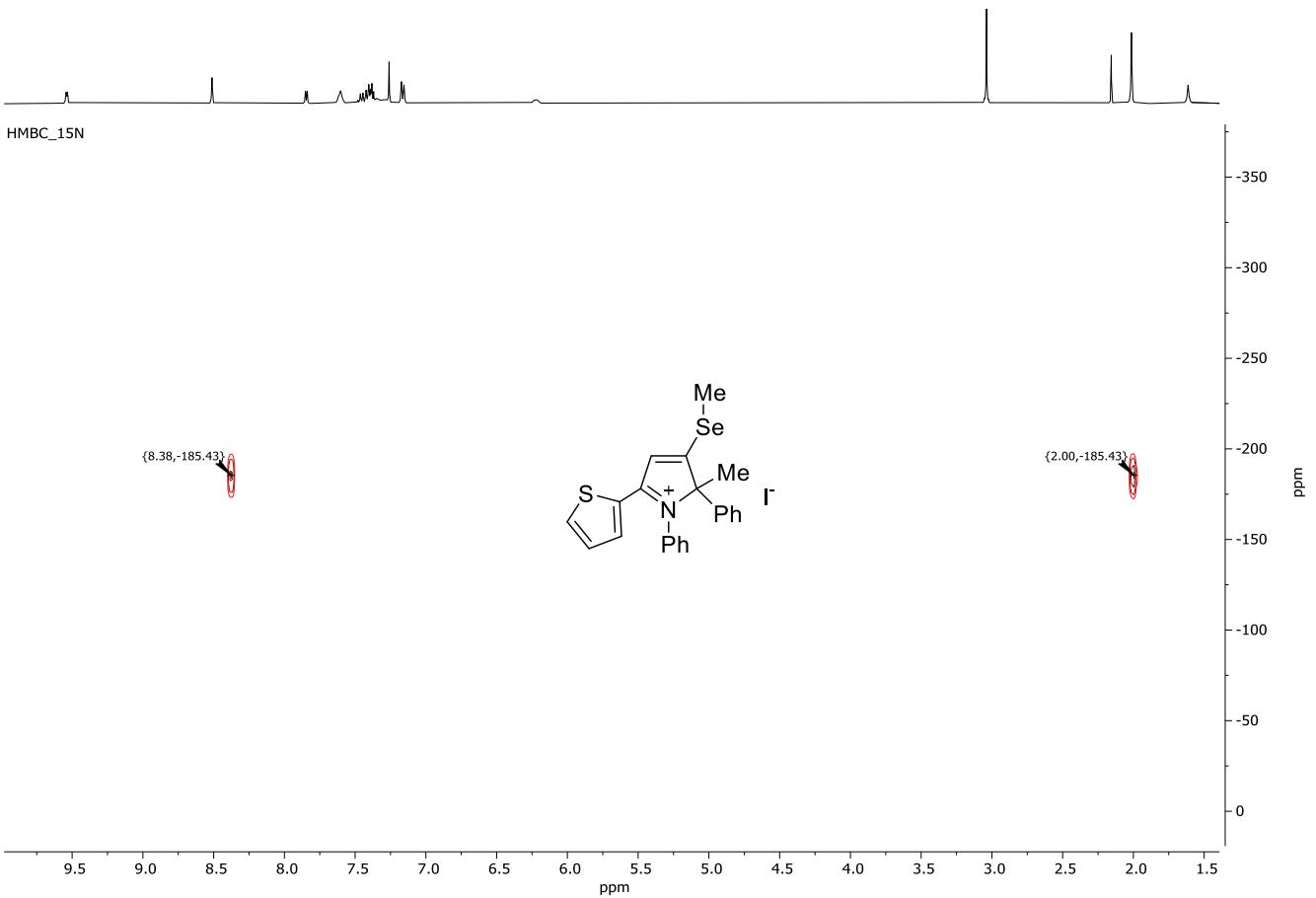


$^{13}\text{C}\{^1\text{H}\}$ NMR of 2-methyl-3-(methylselanyl)-1,2-diphenyl-5-(thiophen-2-yl)-2*H*-pyrrolonium iodide (**6b**)

NMR_13C



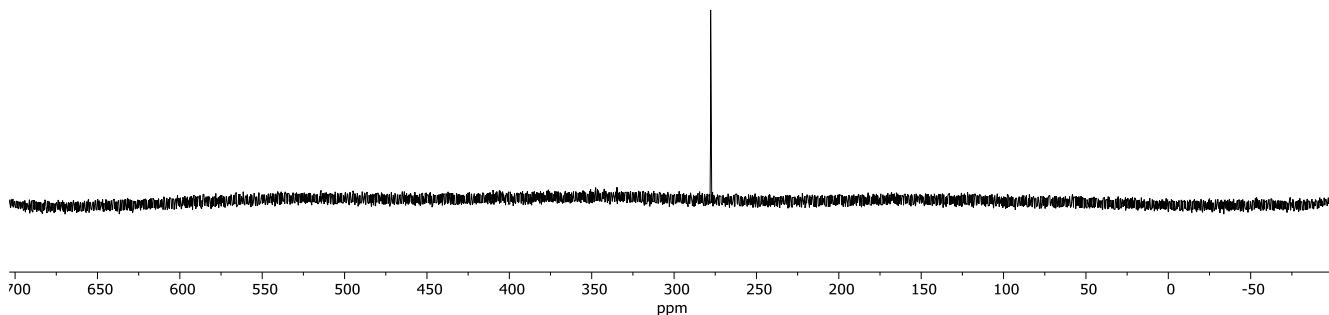
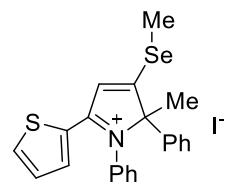
2D ^1H - ^{15}N HMBC NMR of 2-methyl-3-(methylselanyl)-1,2-diphenyl-5-(thiophen-2-yl)-2*H*-pyrrolonium iodide (**6b**)



⁷⁷Se NMR of 2-methyl-3-(methylselanyl)-1,2-diphenyl-5-(thiophen-2-yl)-2H-pyrrolium iodide (6b)

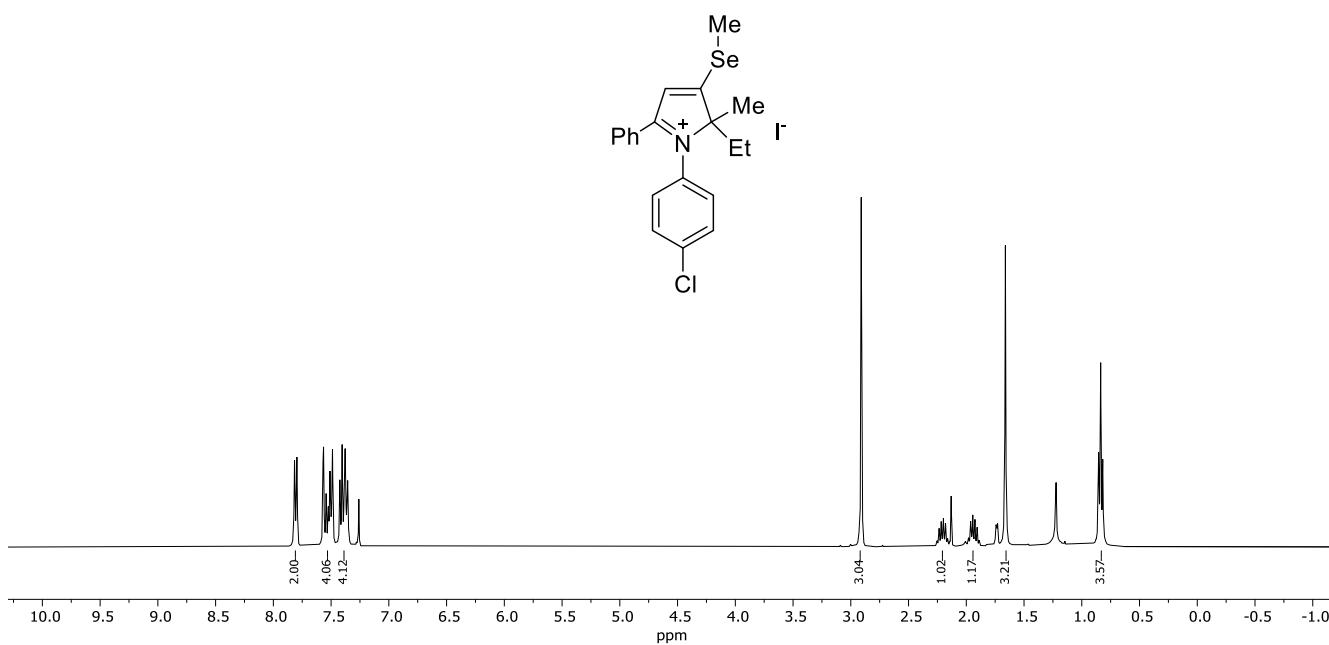
NMR_77Se

— 277.81



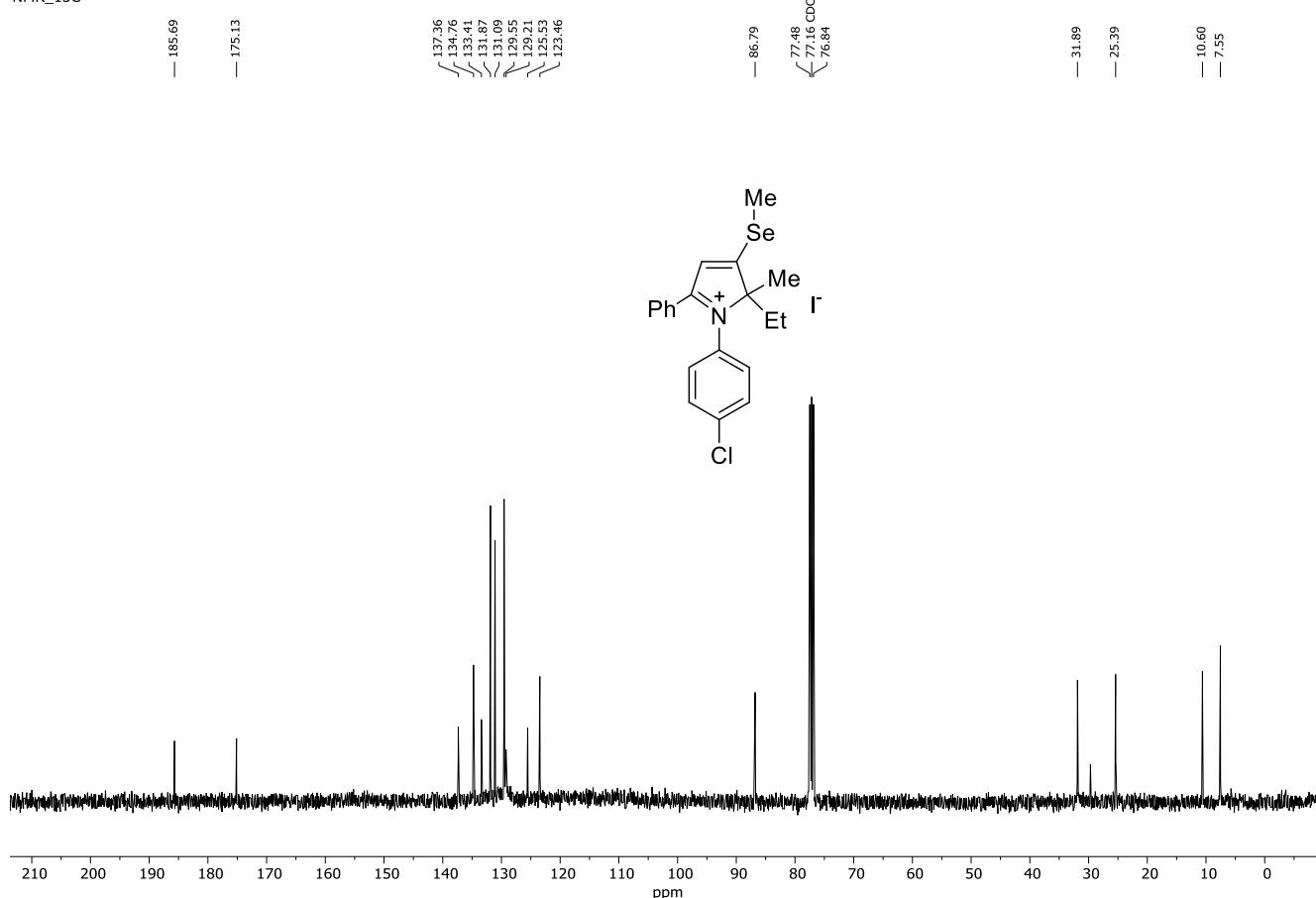
¹H NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-3-(methylselanyl)-5-phenyl-2H-pyrrolium iodide (6c)

NMR_1H

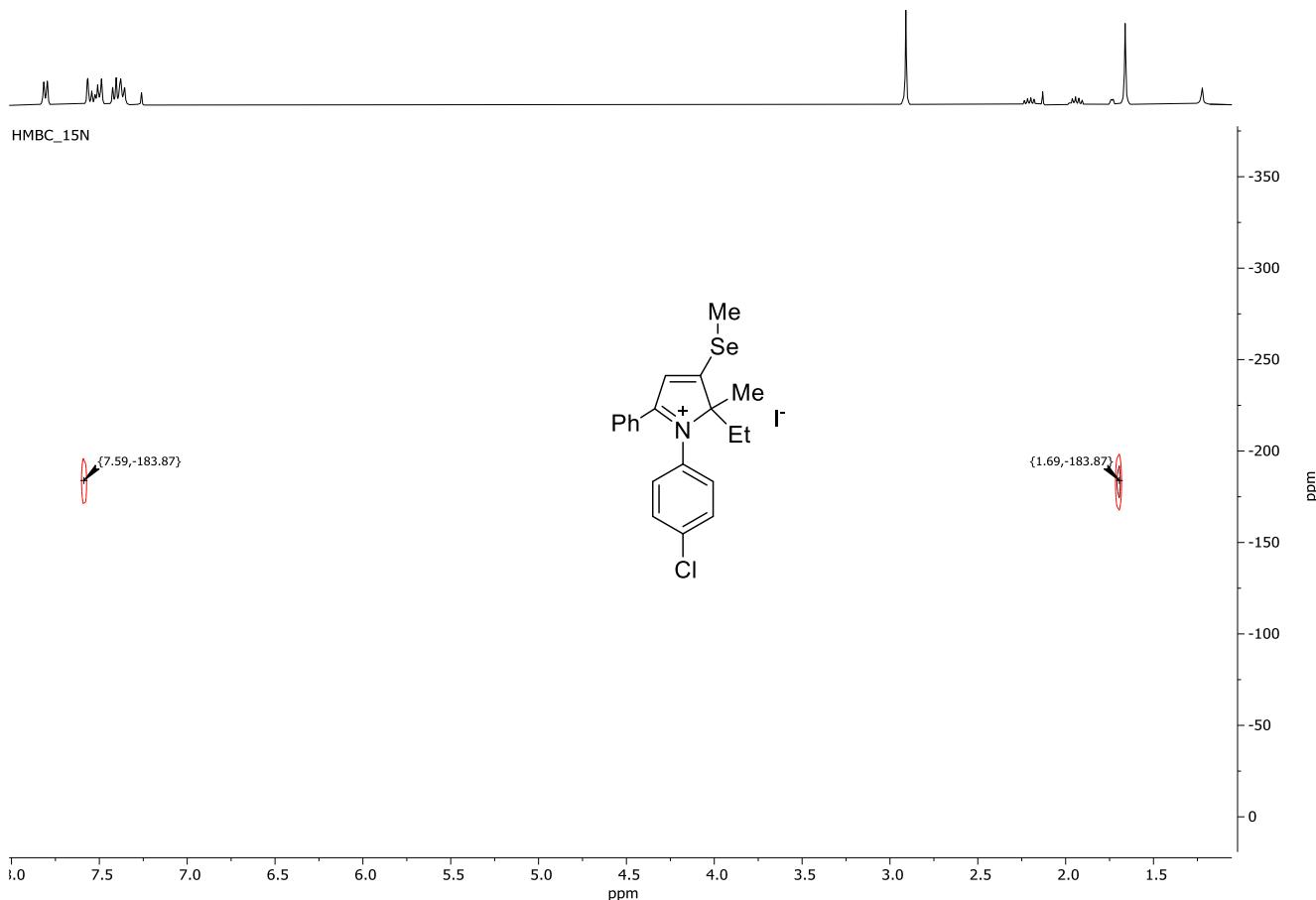


$^{13}\text{C}\{^1\text{H}\}$ NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-3-(methylselanyl)-5-phenyl-2*H*-pyrrolium iodide (**6c**)

NMR_13C



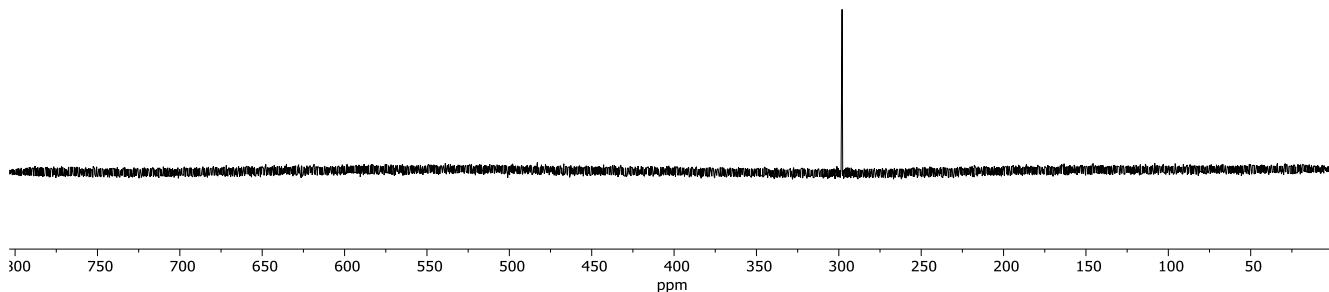
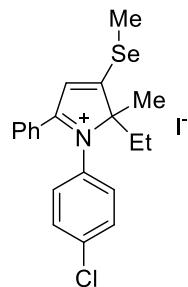
2D ^1H - ^{15}N HMBC NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-3-(methylselanyl)-5-phenyl-2*H*-pyrrolium iodide (**6c**)



⁷⁷Se NMR of 1-(4-chlorophenyl)-2-ethyl-2-methyl-3-(methylselanyl)-5-phenyl-2H-pyrrolium iodide (6c)

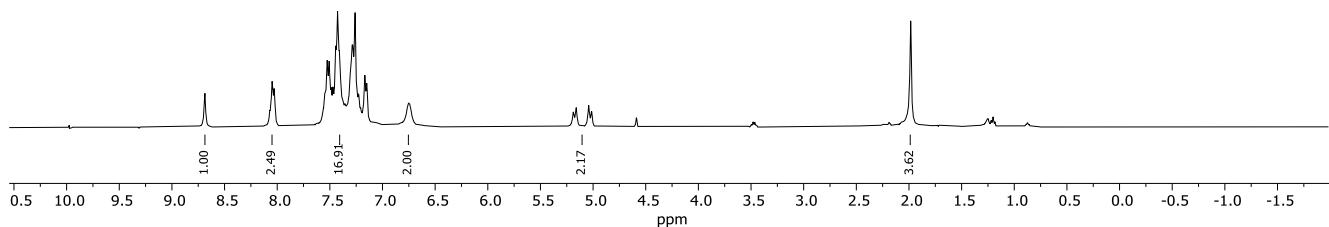
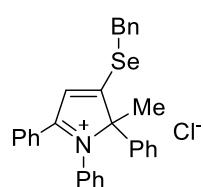
NMR_77Se

— 298.03



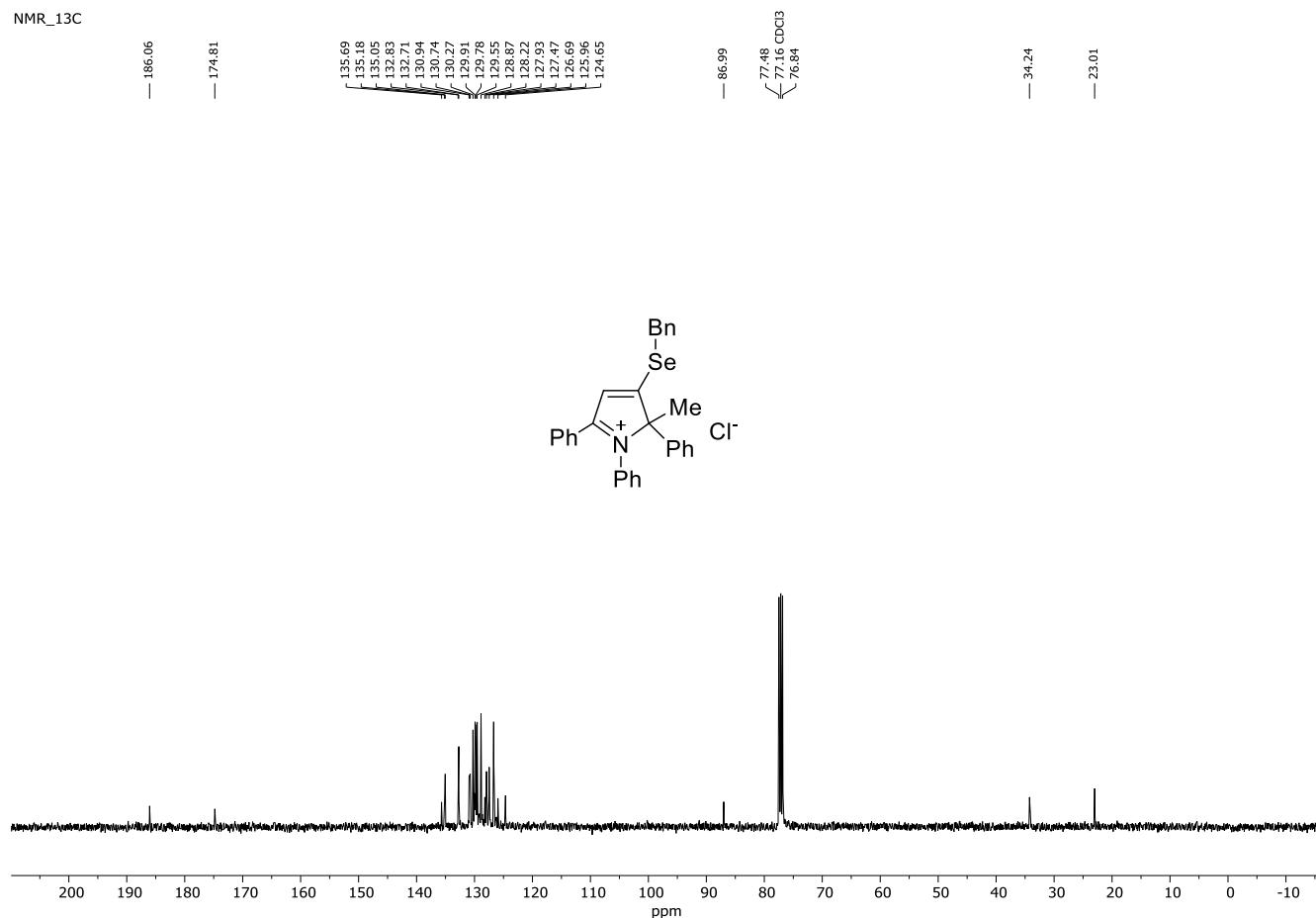
¹H NMR of 3-(benzylselanyl)-2-methyl-1,2,5-triphenyl-2H-pyrrolium chloride (7a)

NMR_1H



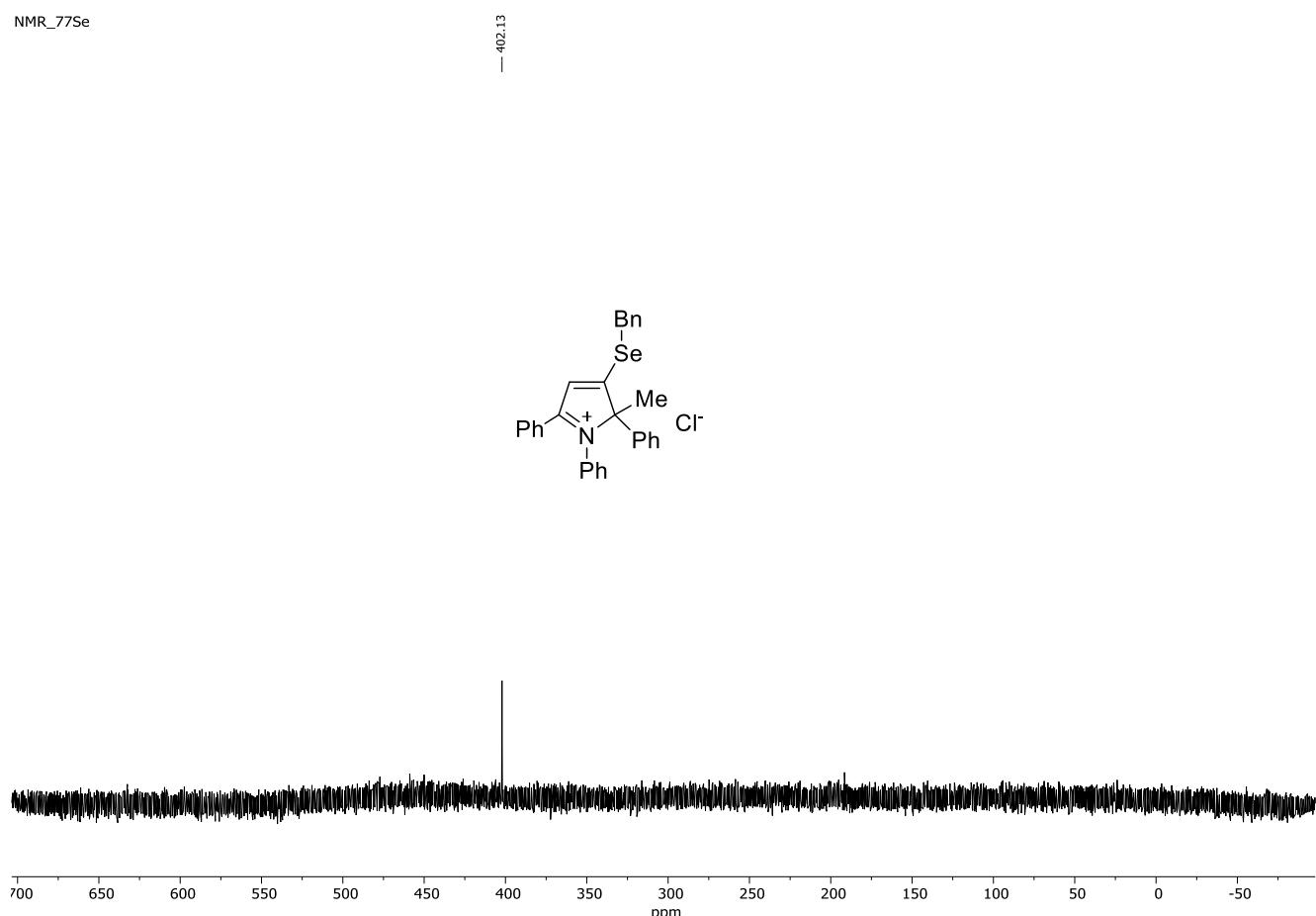
$^{13}\text{C}\{\text{H}\}$ NMR of 3-(benzylselanyl)-2-methyl-1,2,5-triphenyl-2H-pyrrolium chloride (7a)

NMR_13C



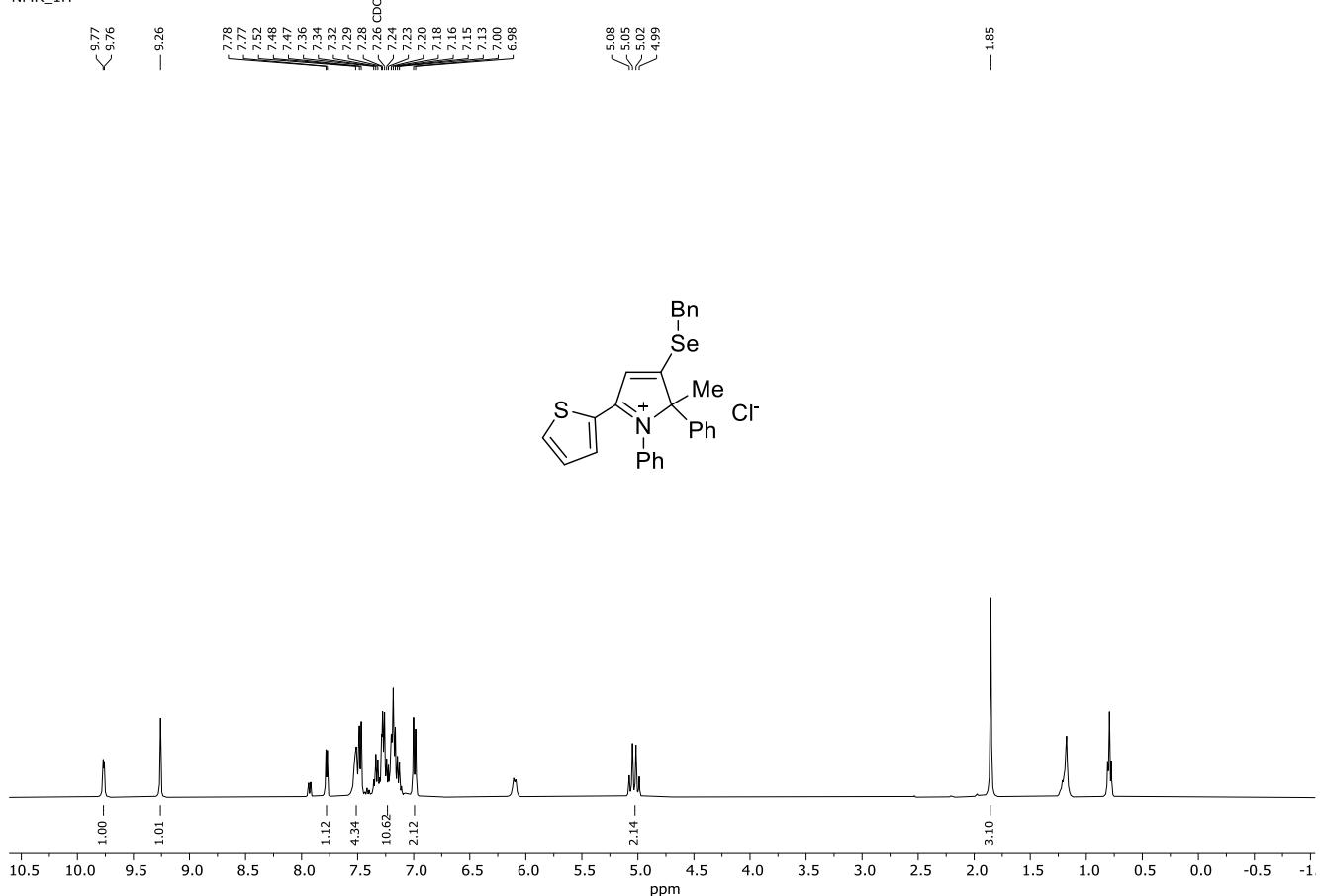
^{77}Se NMR of 3-(benzylselanyl)-2-methyl-1,2,5-triphenyl-2H-pyrrolium chloride (7a)

NMR_77Se



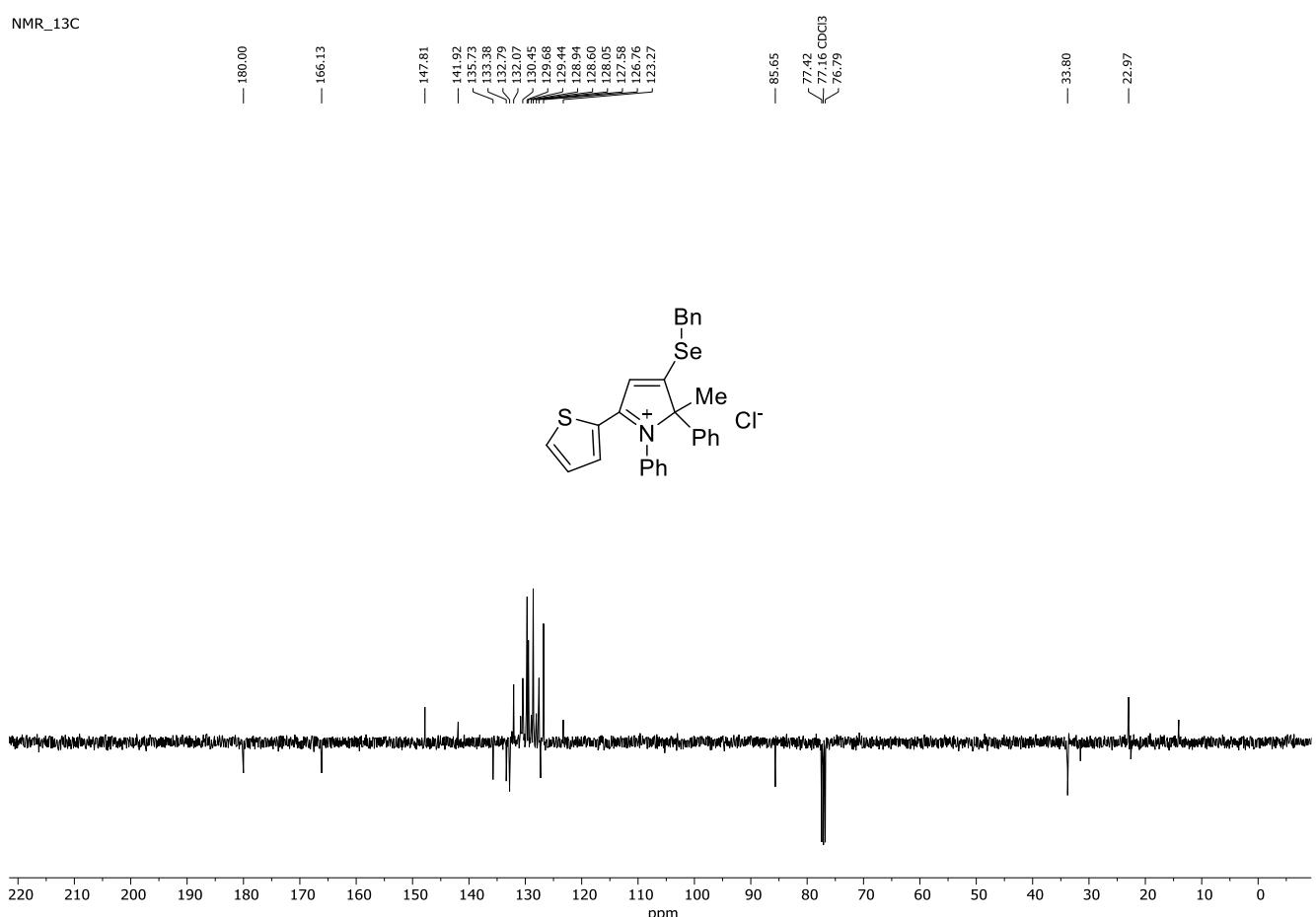
¹H NMR of 3-(benzylselanyl)-2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-2H-pyrrolium chloride (7b)

NMR_1H

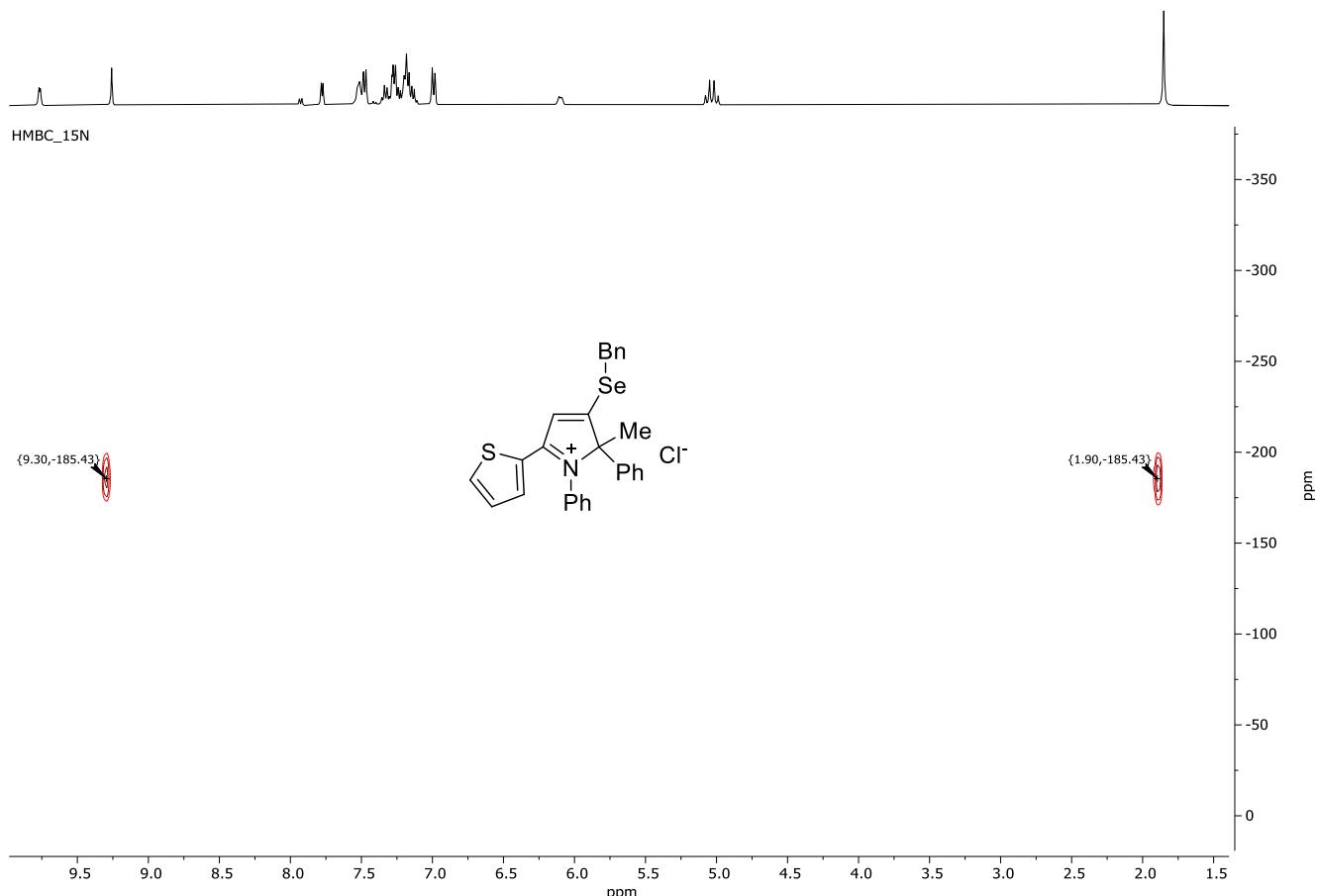


¹³C{¹H} NMR of 3-(benzylselanyl)-2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-2H-pyrrolium chloride (7b)

NMR_13C



2D ^1H - ^{15}N HMBC NMR of 3-(benzylselanyl)-2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-2*H*-pyrrolium chloride (7b)



^{77}Se NMR of 3-(benzylselanyl)-2-methyl-1,2-diphenyl-5-(thiophen-2-yl)-2*H*-pyrrolium chloride (7b)

