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Tuning the π- acidity of N-heterocyclic compounds by variation of *meta*- and *para*-substituents in *N,N'*- diaryl moieties: a ^{77}Se NMR study

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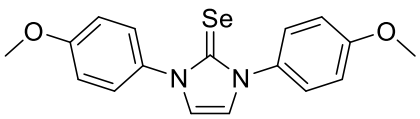
General Information

Chemicals were obtained from P&M Invest, Sigma-Aldrich and Acros Organics. The samples for the ESI-TOF-HRMS experiments were prepared in 1.8 mL glass vials with screw-top caps fitted with Teflon-lined septa (Agilent Technologies). NMR spectra were recorded by using Bruker Avance-NEO 300, Bruker Fourier 300HD, Bruker Avance 500 and Bruker Avance II 600 spectrometers operating at 300.1, 500, 600 MHz for ^{1}H, 75, 125, 151 MHz for ^{13}C, 57 MHz for ^{77}Se and 282.4 MHz for ^{19}F. ^{1}H and ^{13}C NMR chemical shifts are reported relative to the solvent signals as internal standards: 2.5 ppm/39.5 ppm for DMSO-d_6 and 7.26 ppm/77.16 for $CDCl_3$. ^{19}F NMR chemical shifts are reported relative to those of C_6F_6 (δ^{19}F = –162.9 with respect to $CFCl_3$). ^{77}Se chemical shifts are given in parts per million relative to internal standard Ph_2Se_2 ($\delta(^{77}Se)$ = 463.27).

General method of synthesis of selenones 2a-2h.

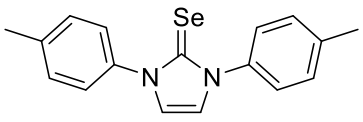
In vial, an imidazolium salt (1 mmol) and selenium (1.66 mmol) were combined in DMF (12 ml). Triethylamine (3 mmol) was added, and the reaction mixture was stirred at room temperature for 16 h. The solvent was removed under reduced pressure, and the residue was extracted with DCM and washed with water. The product was purified by precipitation from a DCM/Et_2O mixture, affording a white powder.

1,3-bis(4-methoxyphenyl)-1,3-dihydro-2H-imidazole-2-selenone (2a). Yield 86%, off-white powder.



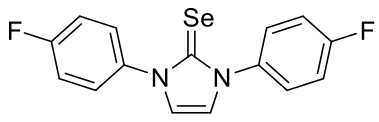
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.58 – 7.49 (m, 4H, 4H$_o$), 7.09 (s, 2H, Im), 7.06 – 6.99 (m, 4H, 4H$_m$), 3.86 (s, 6H, 2OCH_3). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 159.9, 158.8, 132.0, 128.1, 121.0, 114.5, 55.7. **^{77}Se NMR** (57 MHz, $CDCl_3$) δ: 51.6. ESI-(+) MS *m/z*: 329.0548, calcd for [$C_{17}H_{16}N_2Se$] 329.0551 $[M+H]^+$, (Δ = 0.9 ppm).

1,3-di-p-tolyl-1,3-dihydro-2H-imidazole-2-selenone (2b). Yield 73%, off-white powder.



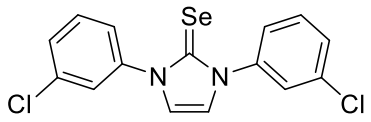
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.50 (d, J = 8.4 Hz, 4H, 4H$_o$), 7.37 – 7.29 (m, 4H, 4H$_m$), 7.10 (s, 2H, Im), 2.42 (s, 6H, 2CH_3). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 158.5, 139.2, 136.7, 129.9, 126.7, 121.0, 21.4. **^{77}Se NMR** (57 MHz, $CDCl_3$) δ: 54.5. ESI-(+) MS *m/z*: 361.0455, calcd for [$C_{17}H_{16}N_2O_2Se$] 361.0450 $[M+H]^+$, (Δ = 1.4 ppm).

1,3-bis(4-fluorophenyl)-1,3-dihydro-2*H*-imidazole-2-selenone (2c). Yield 57%, white powder.



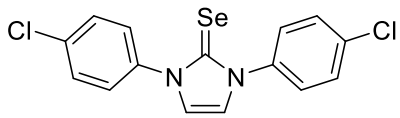
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.67 – 7.58 (m, 4H, 4H$_o$), 7.26 – 7.18 (m, 4H, 4H$_m$), 7.13 (s, 2H, Im). **^{13}C{^{1}H} NMR** (75 MHz, $CDCl_3$) δ: 162.6 (d, 2C$_{Ph}$-F, J = 249.7 Hz), 159.5 (C=Se), 135.0 (d, 2C$_{Ph}$-N, J = 3.3 Hz), 128.9 (d, 4CH$_o$, J = 8.8 Hz), 121.1 (2CH$_{Im}$), 116.4 (d, 4CH$_m$, J = 23.0 Hz). **^{19}F{^{1}H} NMR** (282.4 MHz, $CDCl_3$) δ: -112.58. **^{77}Se{^{1}H} NMR** (57 MHz, $CDCl_3$) δ: 62.32. ESI-(+) MS, *m/z*: 335.9974, calcd for [$C_{15}H_{10}F_2N_2Se$] 335.9972 $[M+H]^+$, (Δ = 0.6 ppm).

1,3-bis(3-chlorophenyl)-1,3-dihydro-2H-imidazole-2-selenone (2d). Yield 69%, white powder.



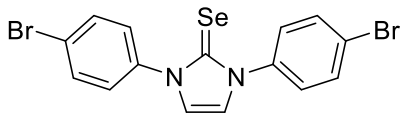
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.74 – 7.32 (m, 8H, 2Ph), 7.13 (s, 2H, Im). **^{13}C{^{1}H} NMR** (75 MHz, $CDCl_3$) δ: 159.4 (C=Se), 139.8 (2C$^{1}_{Ph}$), 135.0 (2C$^{3}_{Ph}$), 130.4 (2C$^{2}_{Ph}$), 129.4 (2C$^{4}_{Ph}$), 127.2 (2C$^{5}_{Ph}$), 125.3 (2C$^{6}_{Ph}$), 121.0 (2CH$_{Im}$). **^{77}Se{^{1}H} NMR** (57 MHz, $CDCl_3$) δ: 72.77. ESI-(+) MS, *m/z*: 367.9390, calcd for [$C_{15}H_{10}Cl_2N_2Se$] 367.9376 $[M+H]^+$, (Δ = 3.8 ppm).

1,3-bis(4-chlorophenyl)-1,3-dihydro-2H-imidazole-2-selenone (2e). Yield 67%, white powder.



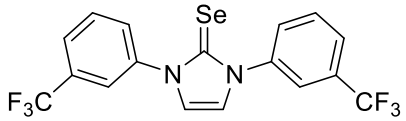
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.61 (d, J = 8.7 Hz, 4H, 4H$_o$), 7.55 – 7.47 (m, 4H, 4H$_m$), 7.14 (s, 2H, Im). **^{13}C{^{1}H} NMR** (75 MHz, $CDCl_3$) δ: 159.2 (C=Se), 137.3 (2C$_{Ph}$-N), 135.2 (2C$_{Ph}$-Cl), 129.6 (4CH$_o$), 128.2 (4CH$_m$), 121.0 (2CH$_{Im}$). **^{77}Se{^{1}H} NMR** (57 MHz, $CDCl_3$) δ: 68.10. ESI-(+) MS, *m/z*: 367.9383, calcd for [$C_{15}H_{10}Cl_2N_2Se$] 367.9376 $[M+H]^+$, (Δ = 1.9 ppm).

1,3-bis(4-bromophenyl)-1,3-dihydro-2H-imidazole-2-selenone (2f). Yield 88%, white powder.



^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.71 – 7.62 (m, 4H, 4H$_o$), 7.58 – 7.51 (m, 4H, 4H$_m$), 7.14 (s, 2H, Im). **^{13}C{^{1}H} NMR** (75 MHz, $CDCl_3$) δ: 159.1 (C=Se), 137.9 (2C$_{Ph}$-N), 132.6 (2C$_{Ph}$-Br), 128.5 (4CH$_o$), 123.3 (4CH$_m$), 121.0 (2CH$_{Im}$). **^{77}Se{^{1}H} NMR** (57 MHz, $CDCl_3$) δ: 69.54. ESI-(+) MS, *m/z*: 457.8351, calcd for [$C_{15}H_{10}Br_2N_2Se$] 457.8351 $[M+H]^+$, (Δ = 0.0 ppm).

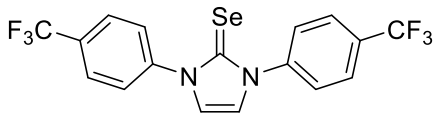
1,3-bis(3-(trifluoromethyl)phenyl)-1,3-dihydro-2H-imidazole-2-selenone (2g). Yield 95%, white powder.



^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.97 (d, 2H$^{4}_{Ph}$, J = 7.8 Hz, 2H), 7.90 (s, 2H$^{2}_{Ph}$, 2H), 7.71 (d, 2H$^{6}_{Ph}$, J = 17.0 Hz, 2H), 7.71 (t, 2H$^{5}_{Ph}$, J = 16.4 Hz, 2H), 7.21 (s, 2H, Im). **^{13}C{^{1}H} NMR** (75 MHz, $CDCl_3$) δ: 159.9 (C=Se), 139.2 (2C$^{1}_{Ph}$), 132.0 (q, 2C$^{3}_{Ph}$, J = 33.2 Hz), 130.6 (2C$^{5}_{Ph}$), 130.0 (2C$^{6}_{Ph}$), 126.0 (q, 2C$^{4}_{Ph}$, J = 3.7 Hz), 123.8 (q, 2C$^{2}_{Ph}$, J = 3.8 Hz), 123.5 (q, 2CF_3, J = 272.6 Hz), 121.1 (2CH$_{Im}$). **^{19}F{^{1}H}**

NMR (282.4 MHz, $CDCl_3$) δ: -63.80. **^{77}Se{^{1}H} NMR** (57 MHz, $CDCl_3$) δ: 74.65. ESI-(+) MS, *m/z*: 435.9915, calcd for $[C_{17}H_{10}F_6N_2Se]$ 435.9908 $[M+H]^+$, (Δ = 1.6 ppm).

1,3-bis(4-(trifluoromethyl)phenyl)-1,3-dihydro-2H-imidazole-2-selenone (2h). Yield 93%, white powder.



^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.83 (dd, J = 2.2 Hz, 8H, 2Ph), 7.20 (s, 2H, Im). **^{13}C{^{1}H} NMR** (75 MHz, $CDCl_3$) δ: 159.6 (C=Se), 141.7 ($2C_{Ph}$-N), 131.3 (q, $2C_{Ph}$-CF_3, J = 33.1 Hz), 127.3 ($4CH_o$), 126.7 (q, $4CH_m$, J = 3.7 Hz), 123.7 (q, $2CF_3$ J = 272.5 Hz), 121.1. **^{19}F{^{1}H} NMR** (282.4 MHz, $CDCl_3$) δ: -63.90. **^{77}Se{^{1}H} NMR** (57 MHz, $CDCl_3$) δ: 77.65. ESI-(+) MS, *m/z*: 435.9915, calcd for $[C_{17}H_{10}F_6N_2Se]$ 435.9908 $[M+H]^+$, (Δ = 1.6 ppm).

Characterization of the obtained compounds

^{1}H NMR Spectra of obtained compounds

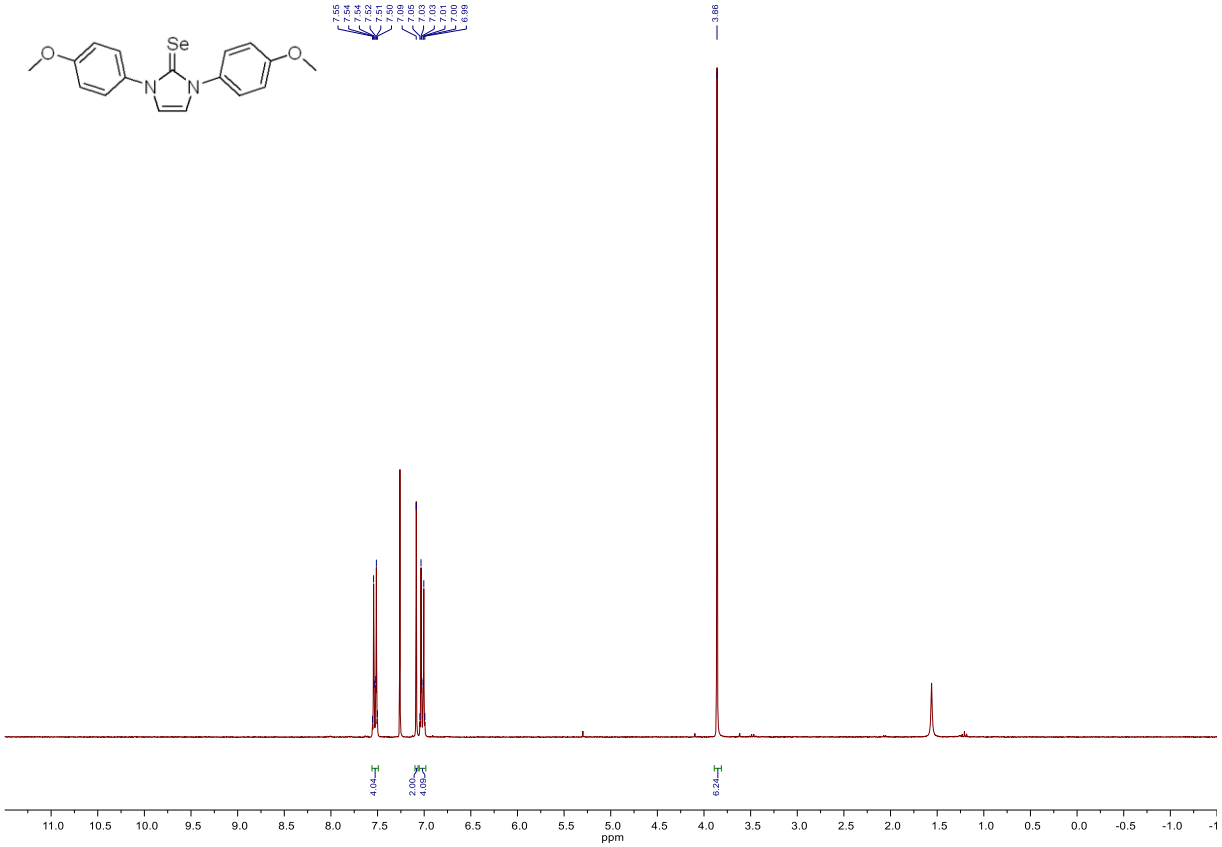


Figure S1. ^{1}H NMR spectrum of **2a**. Solvent: $CDCl_3$, 300 MHz.

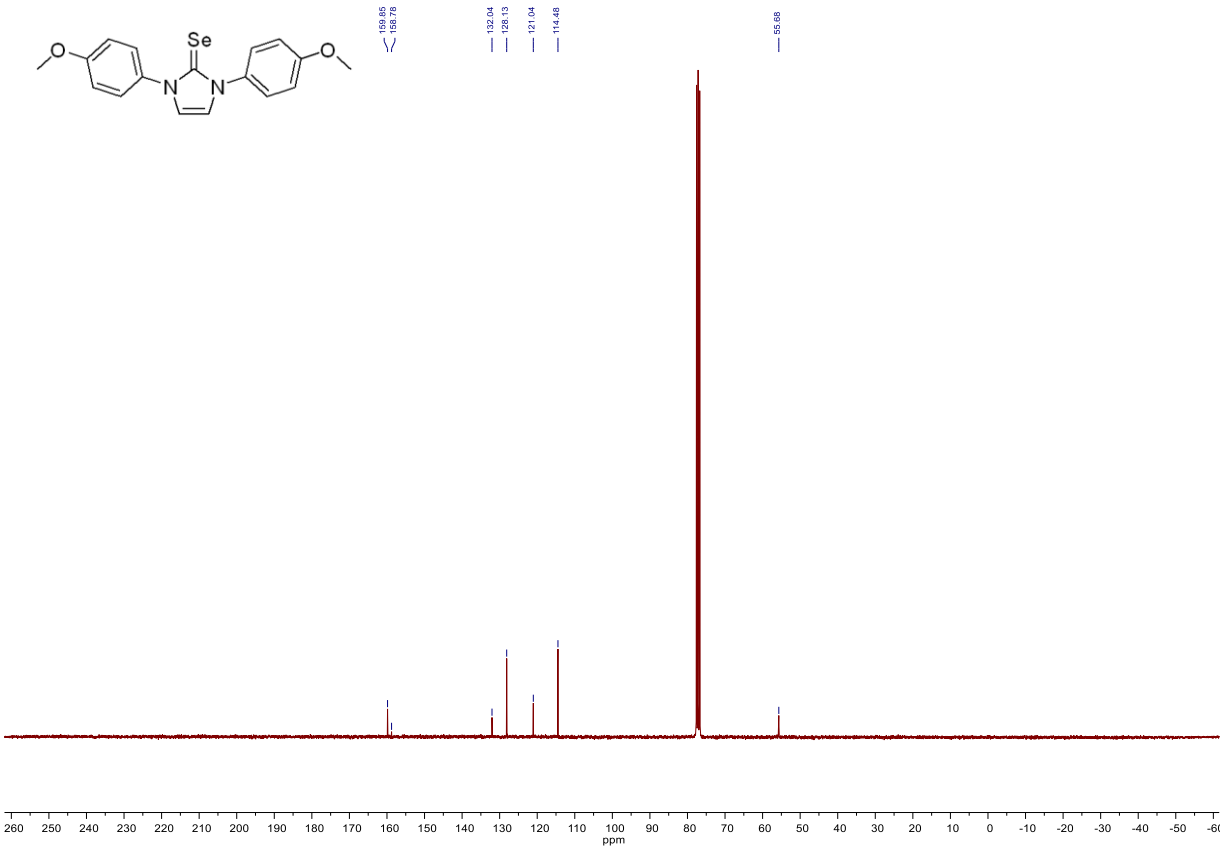


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **2a**. Solvent: $CDCl_3$, 282 MHz.

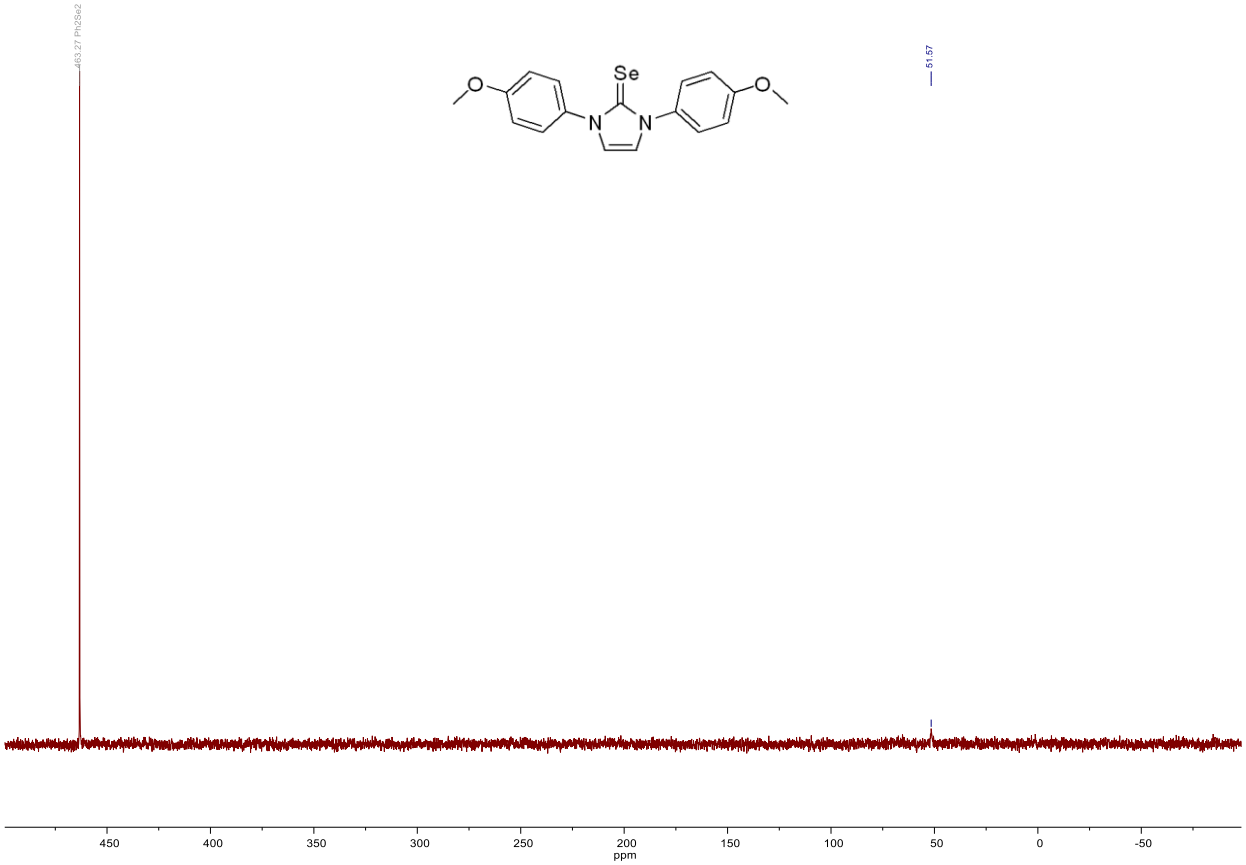


Figure S3. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2a.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

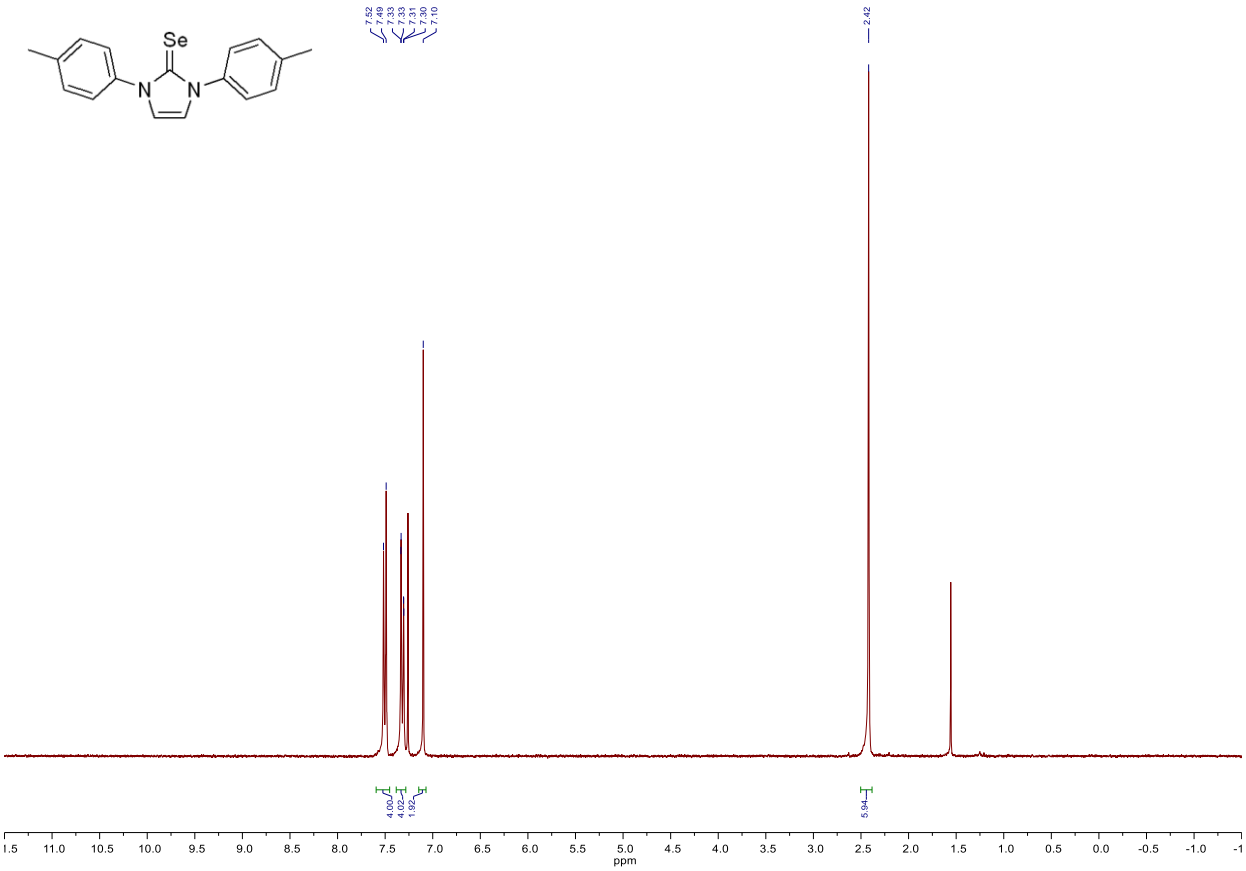


Figure S4. ^{1}H NMR spectrum of **2b**. Solvent: $CDCl_3$, 300 MHz.

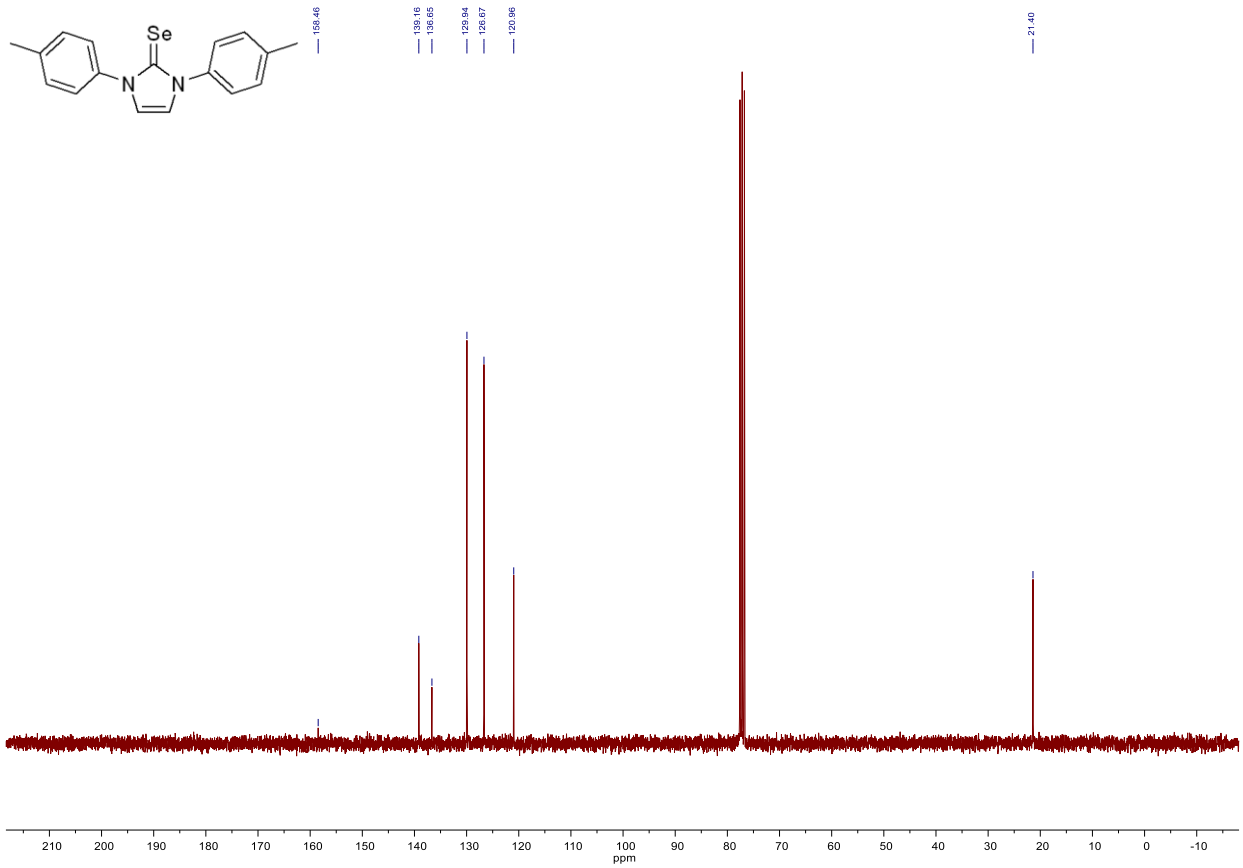


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **2b**. Solvent: $CDCl_3$, 282 MHz.

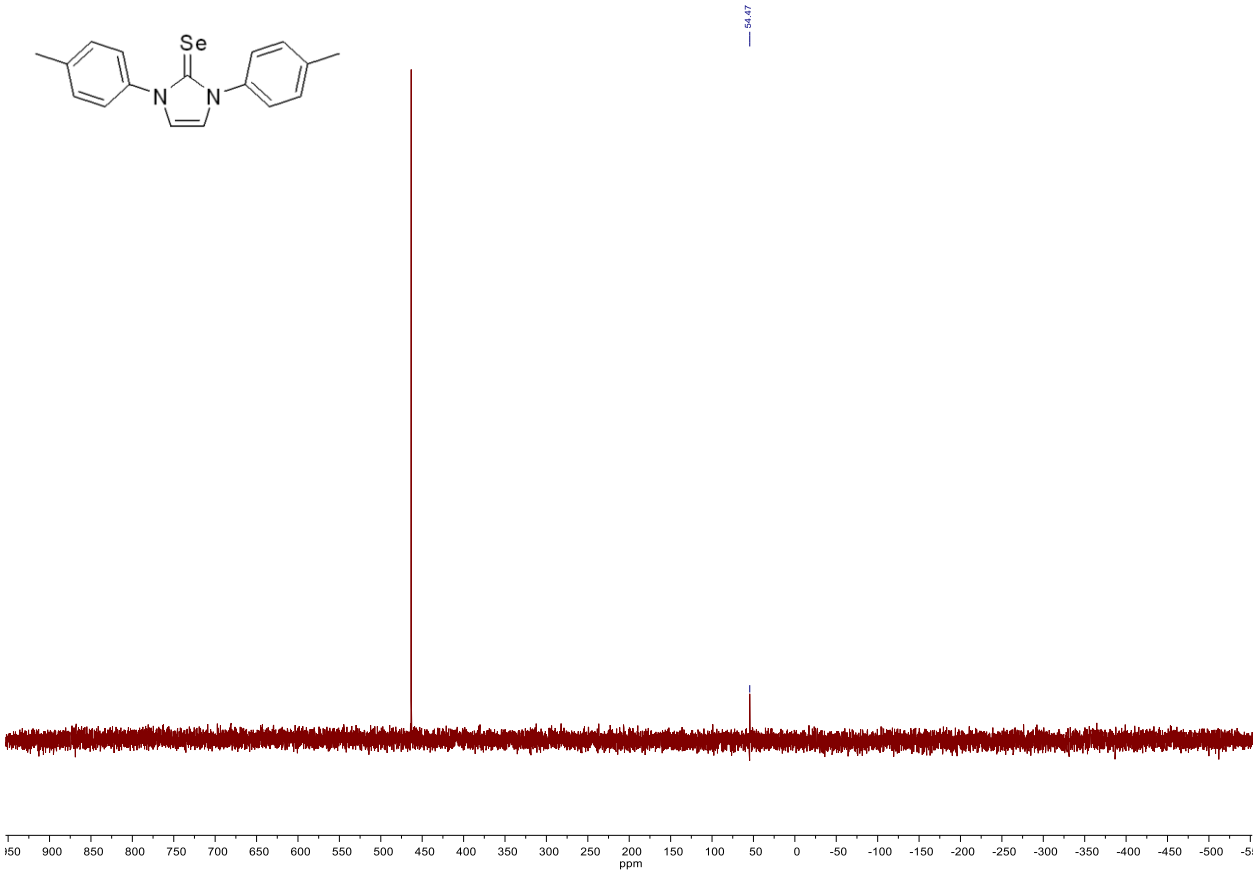


Figure S6. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2b.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

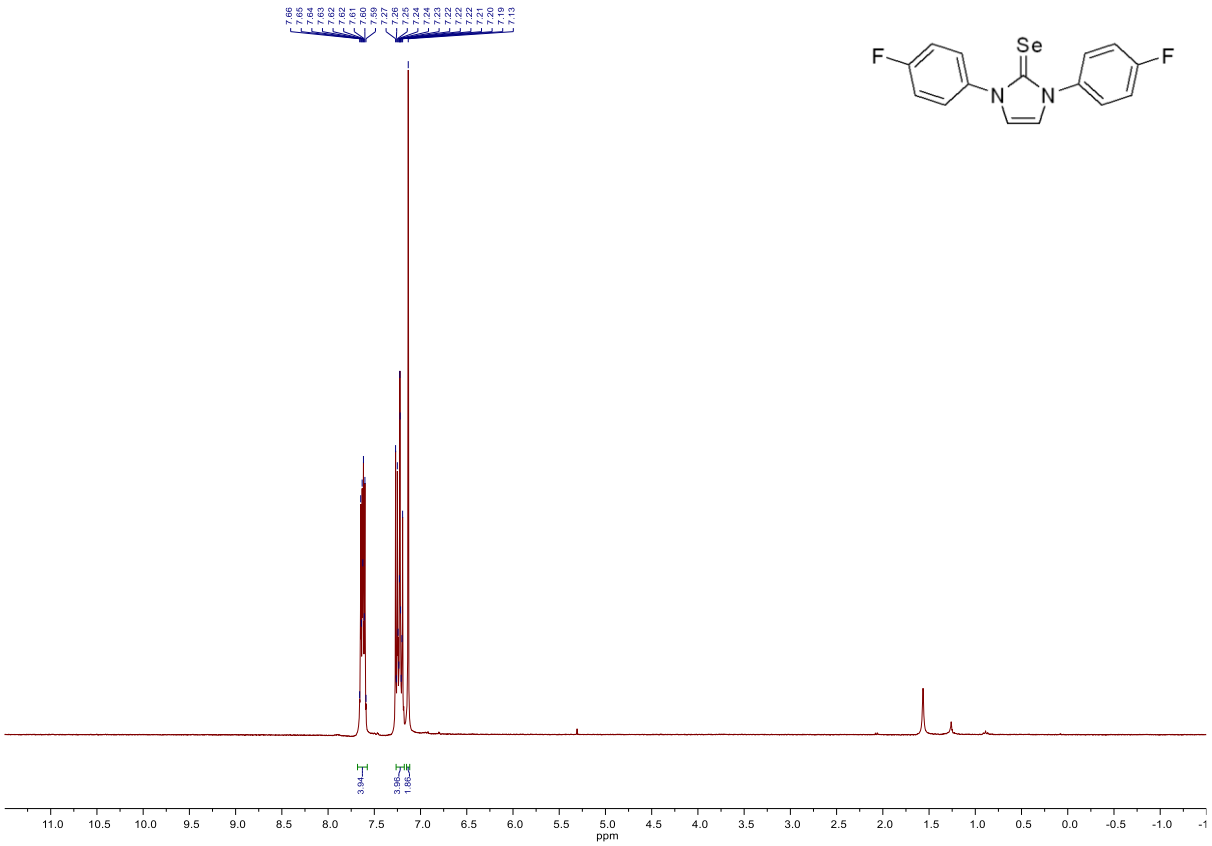


Figure S7. ^{1}H NMR spectrum of **2c**. Solvent: $CDCl_3$, 300 MHz.

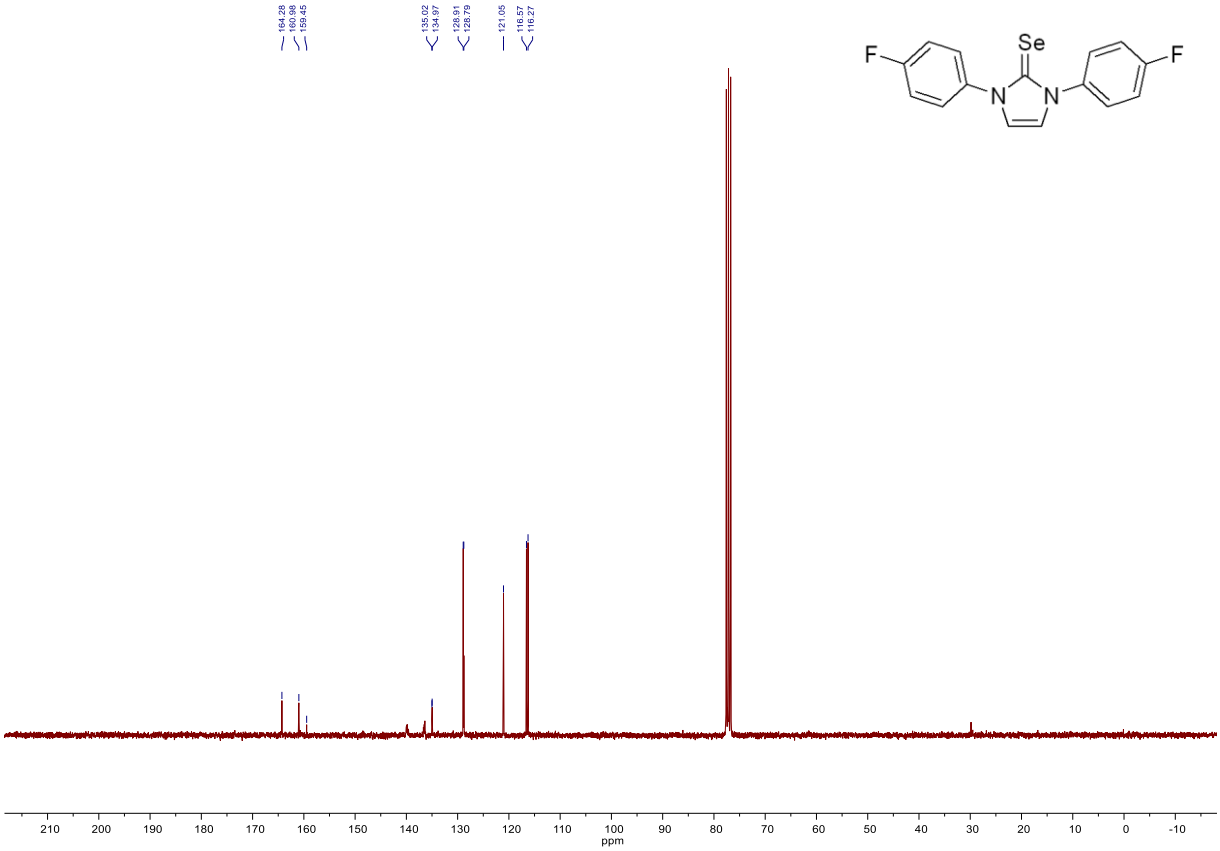


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **2c**. Solvent: $CDCl_3$, 282 MHz.

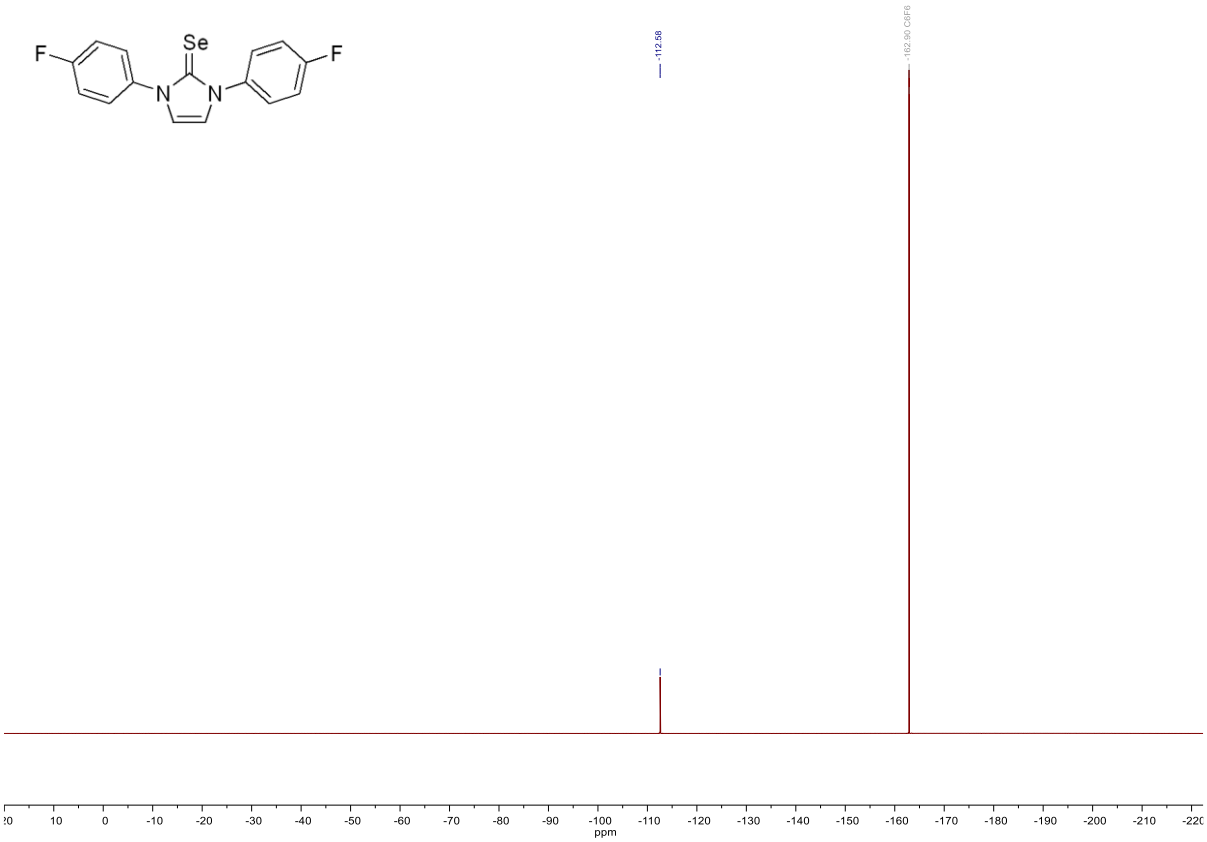


Figure S9. $^{19}F\{^{1}H\}$ NMR spectrum of **2c**. Solvent: $CDCl_3$, 282.4 MHz. Standard: C_6F_6 with respect to $CFCl_3$.

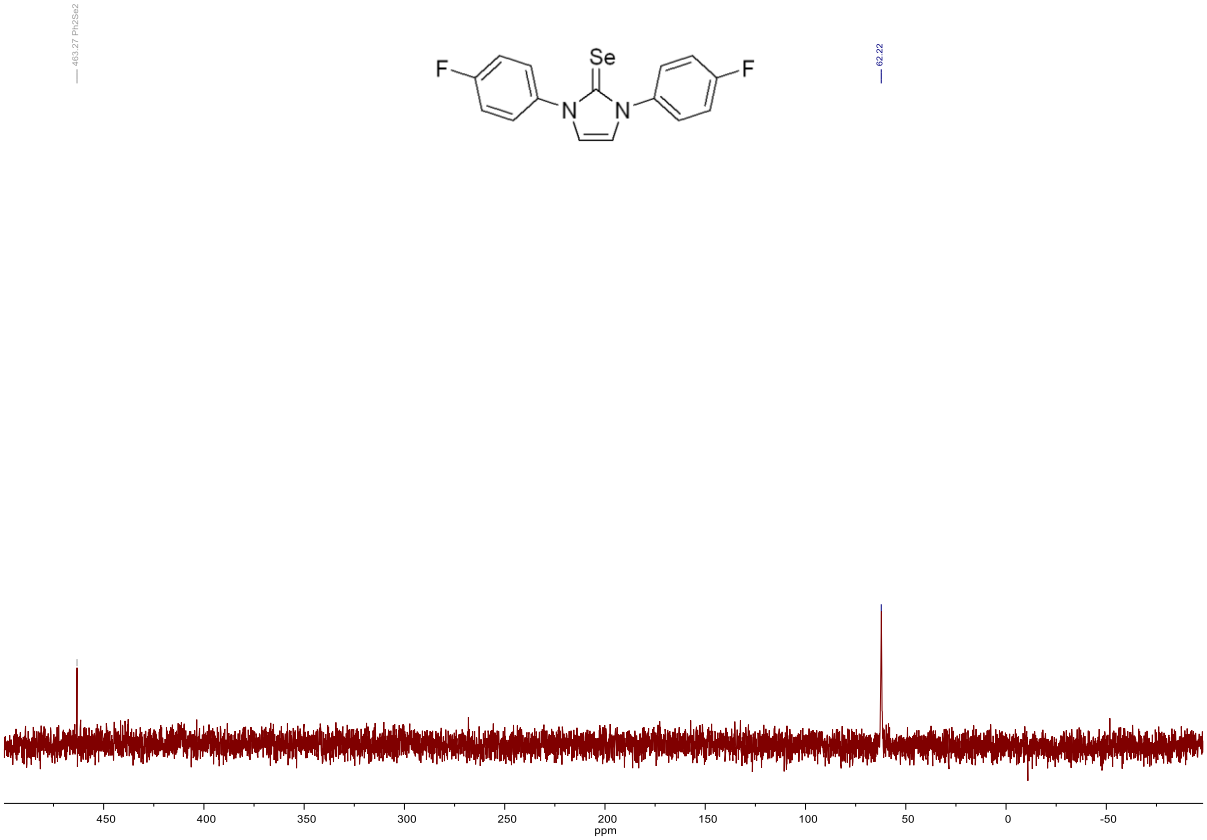


Figure S10. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2c.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

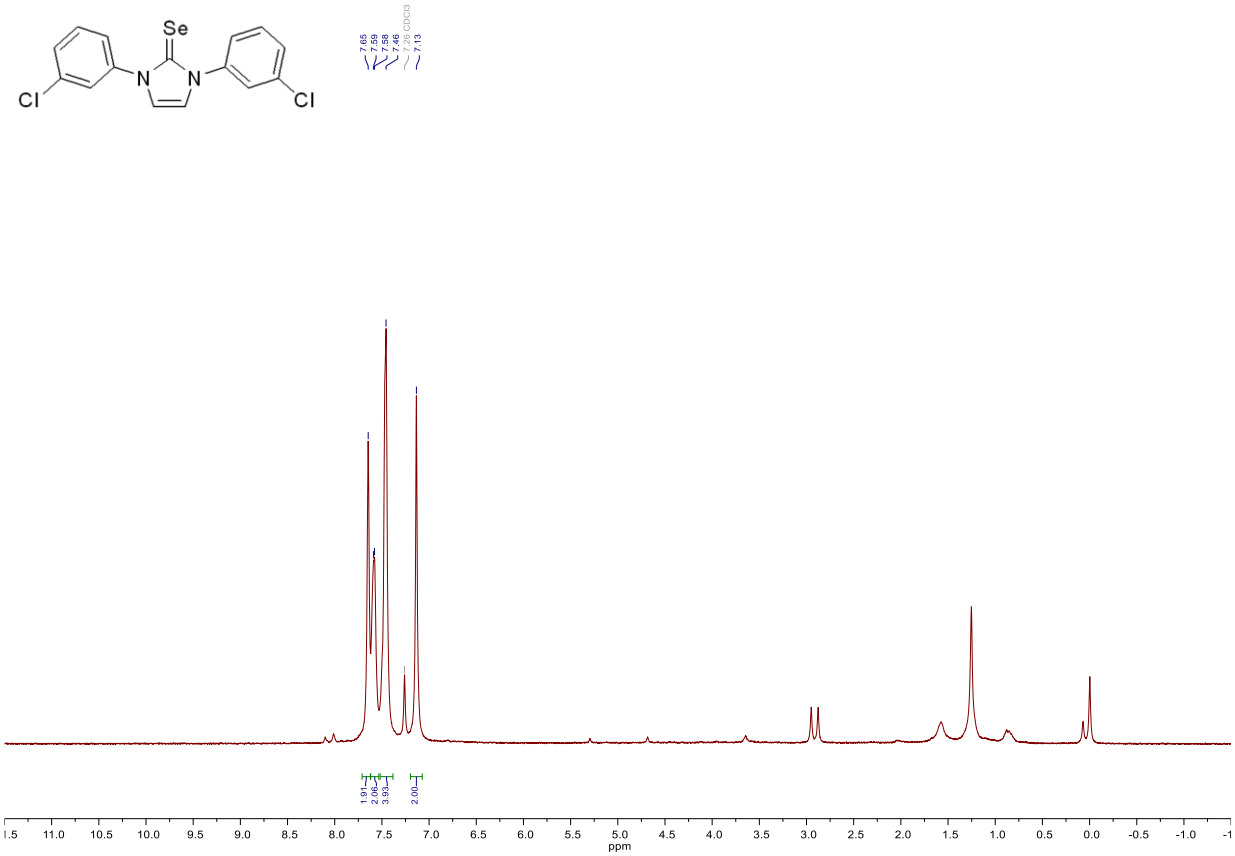


Figure S11. ^{1}H NMR spectrum of **2d**. Solvent: $CDCl_3$, 300 MHz.

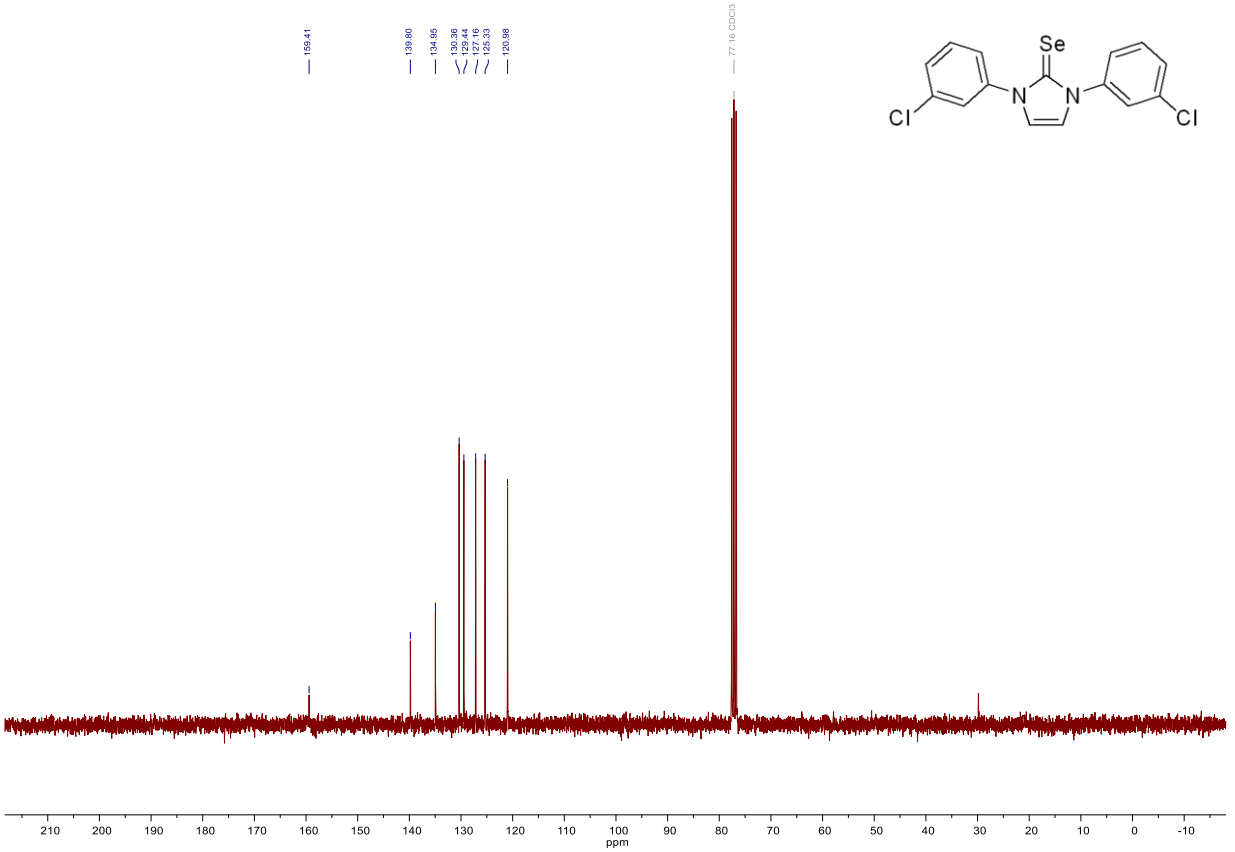


Figure S12. ^{13}C{^{1}H} NMR spectrum of **2d**. Solvent: $CDCl_3$, 75 MHz.

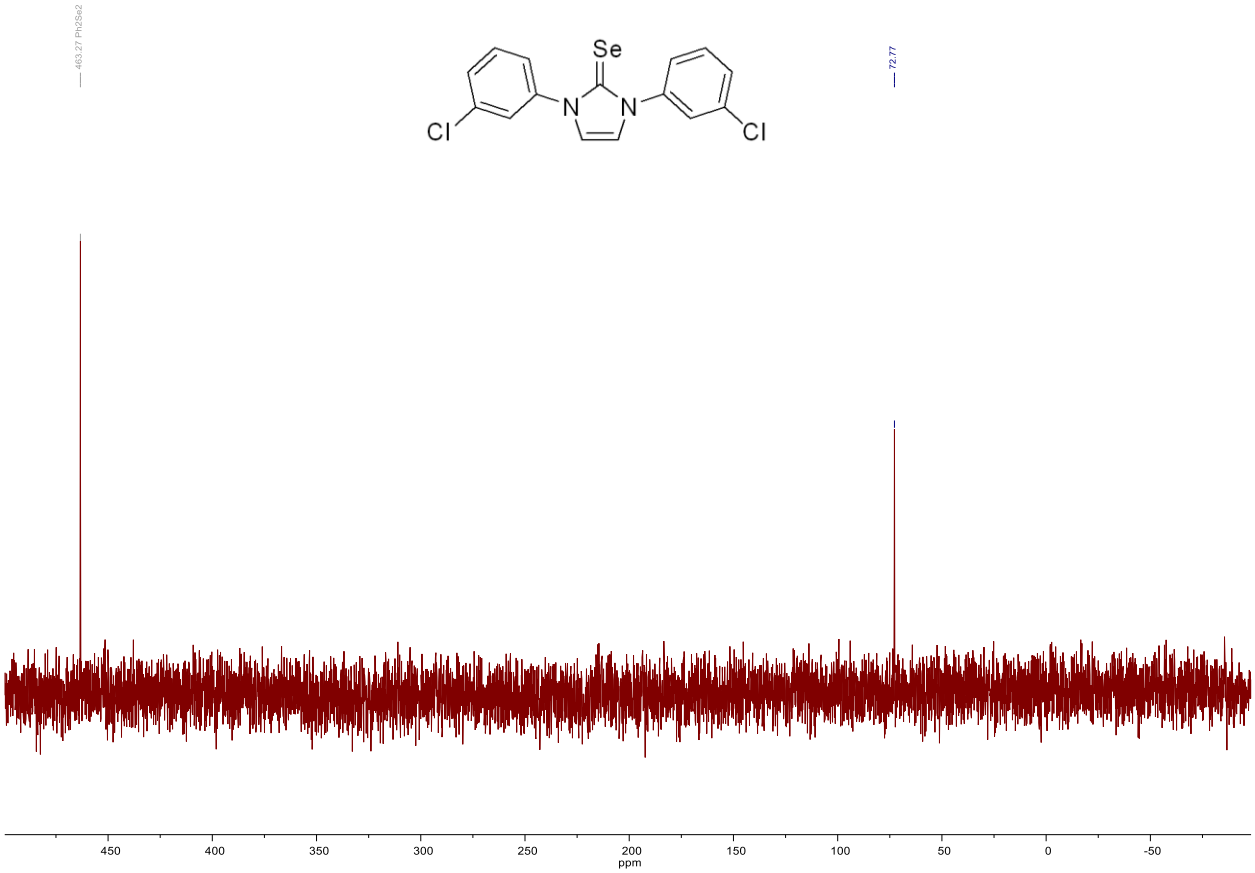


Figure S13. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2d.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

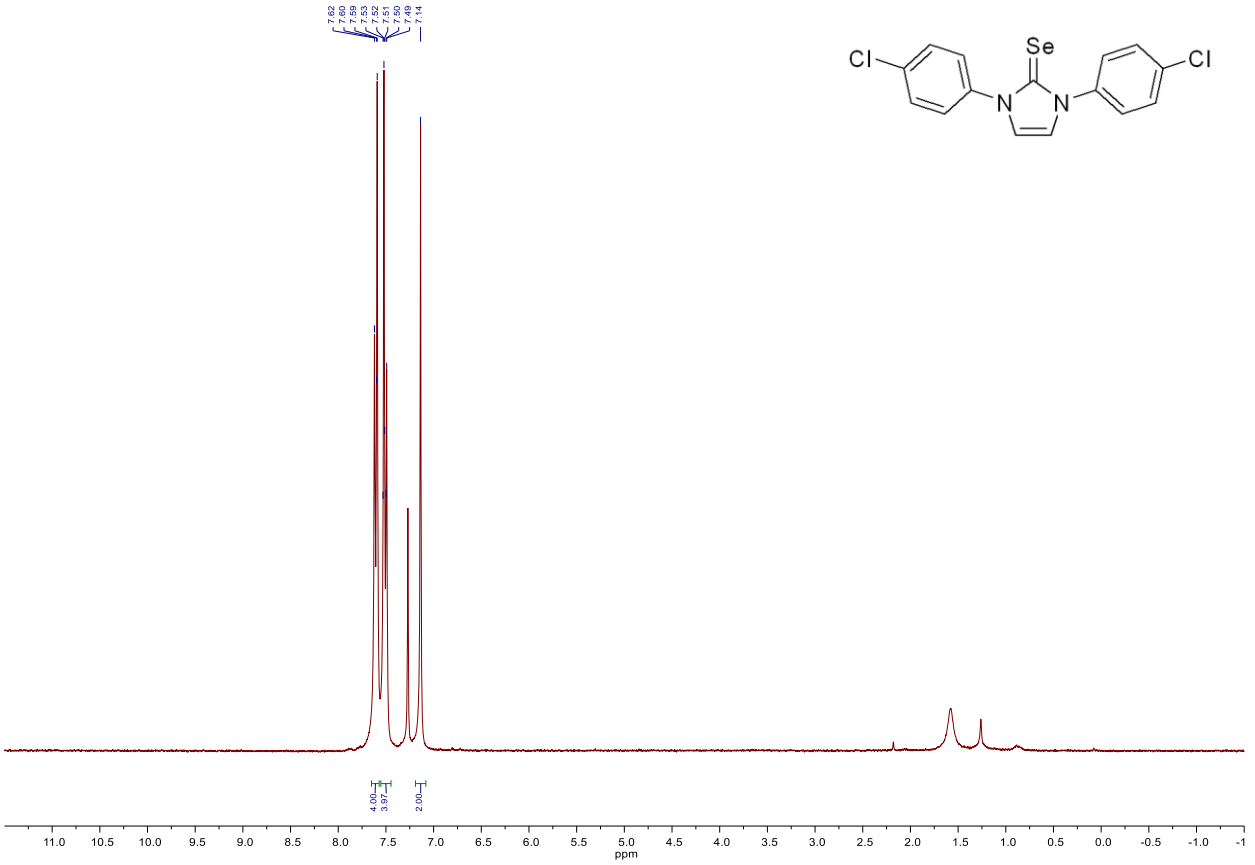


Figure S14. ^{1}H NMR spectrum of **2e**. Solvent: $CDCl_3$, 300 MHz.

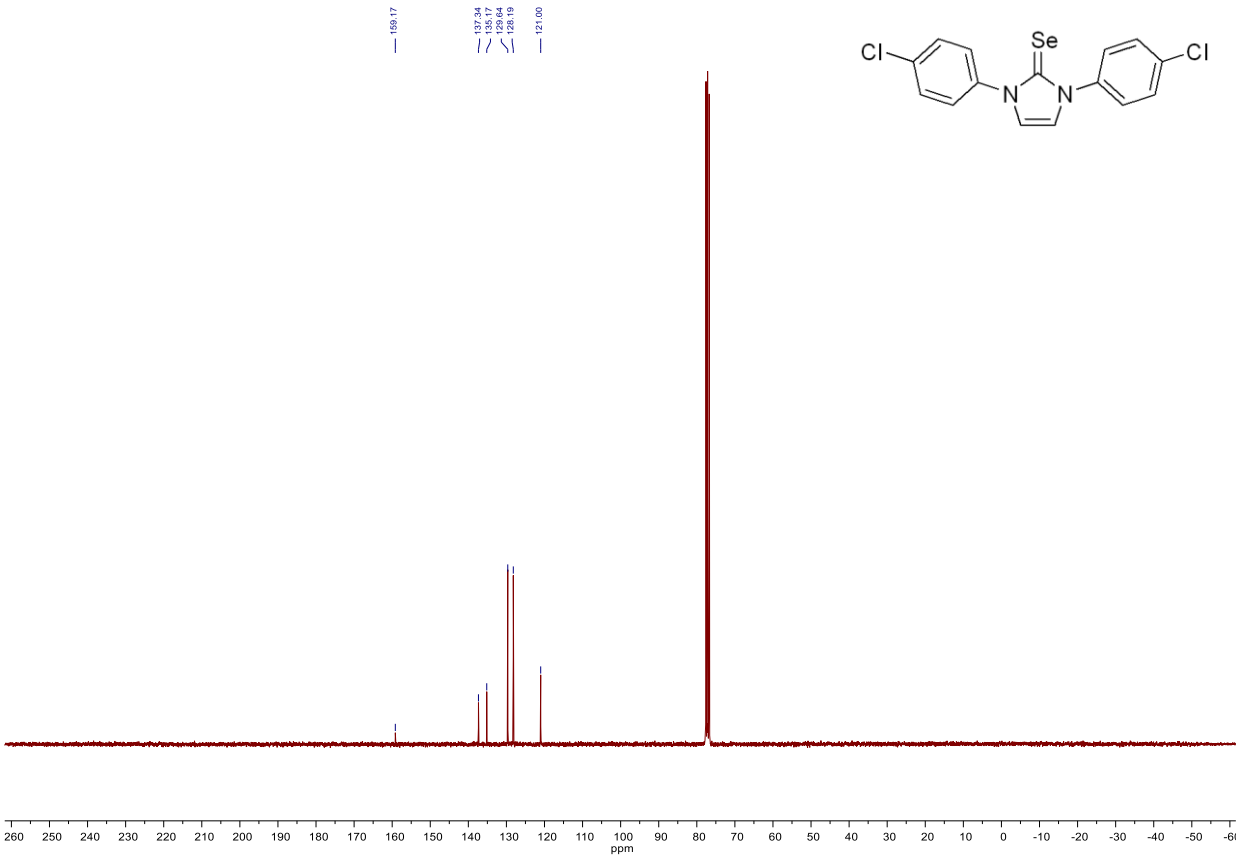


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of **2e**. Solvent: $CDCl_3$, 75 MHz.

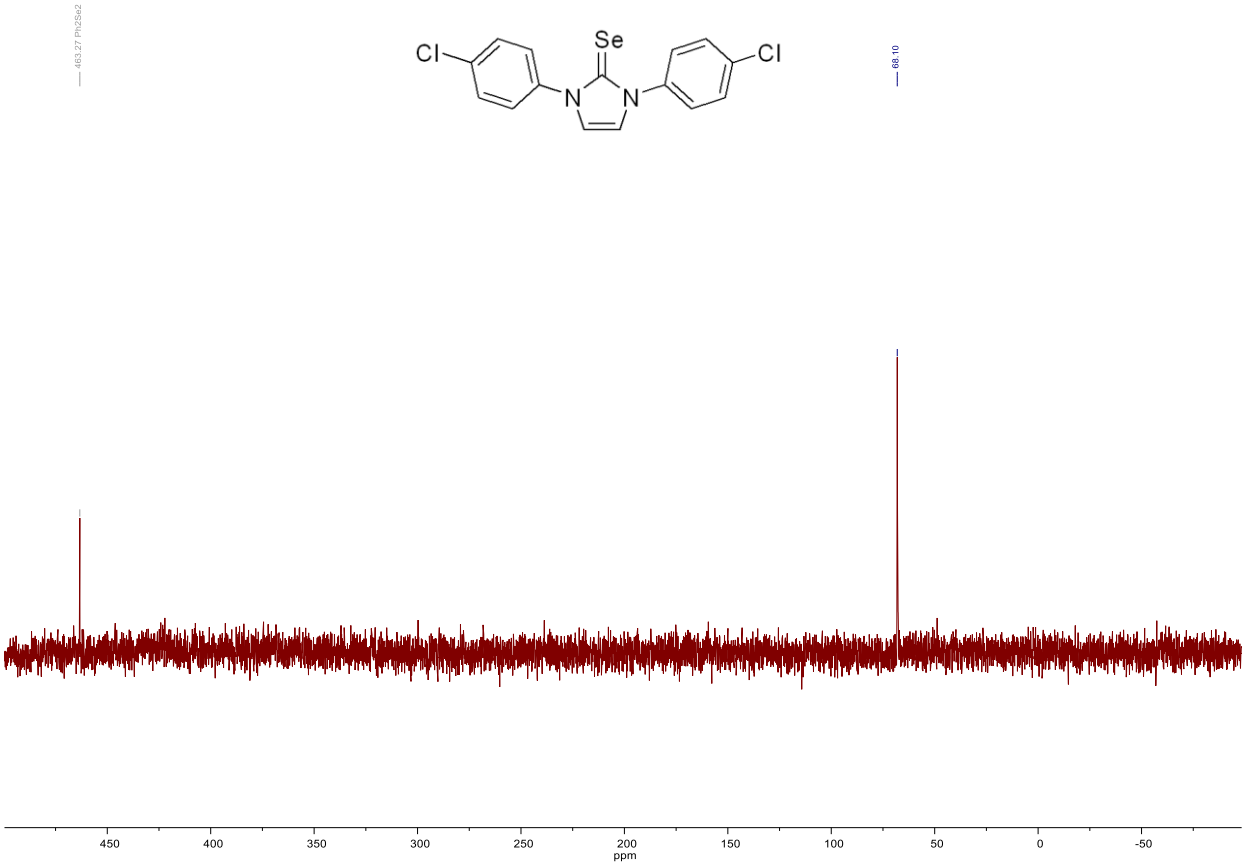


Figure S16. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2e.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

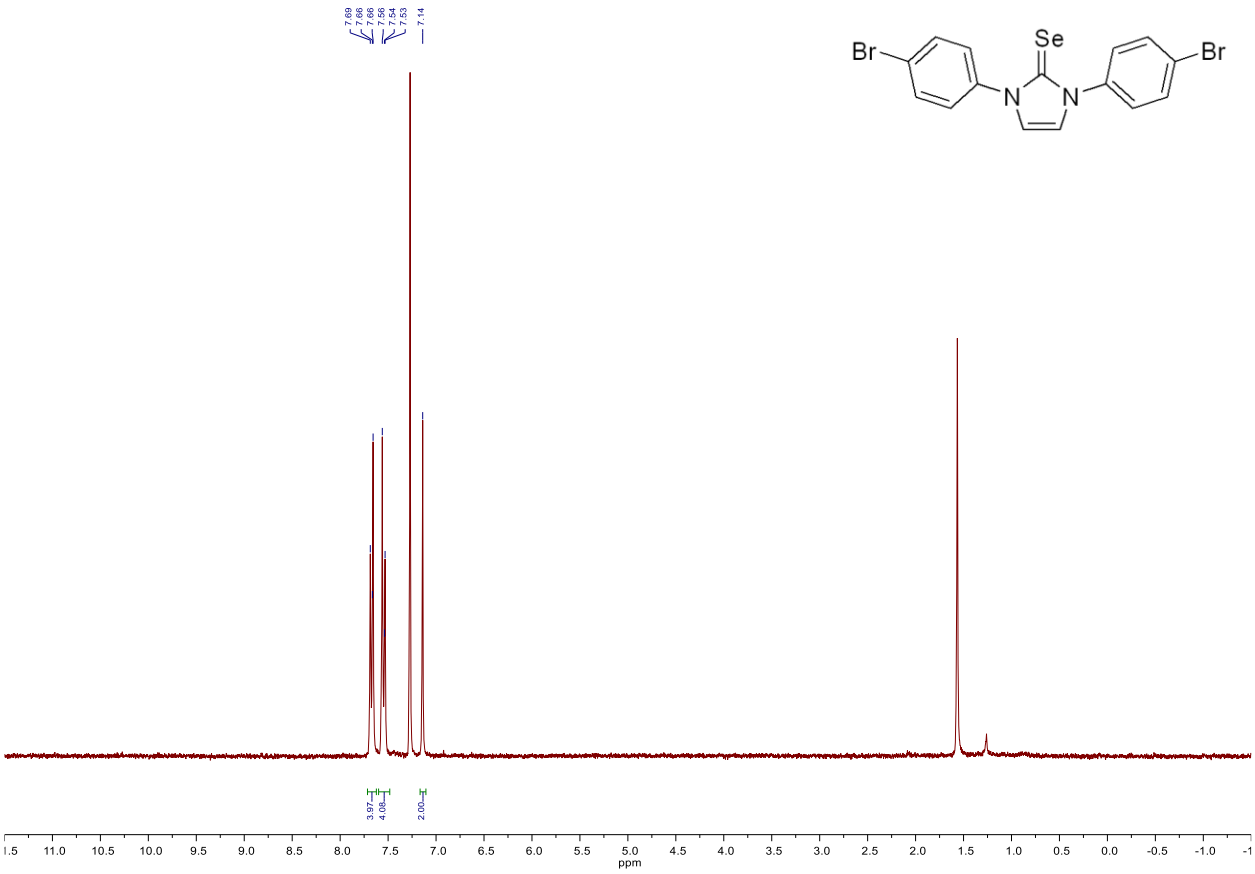


Figure S17. ^{1}H NMR spectrum of **2f**. Solvent: $CDCl_3$, 300 MHz.

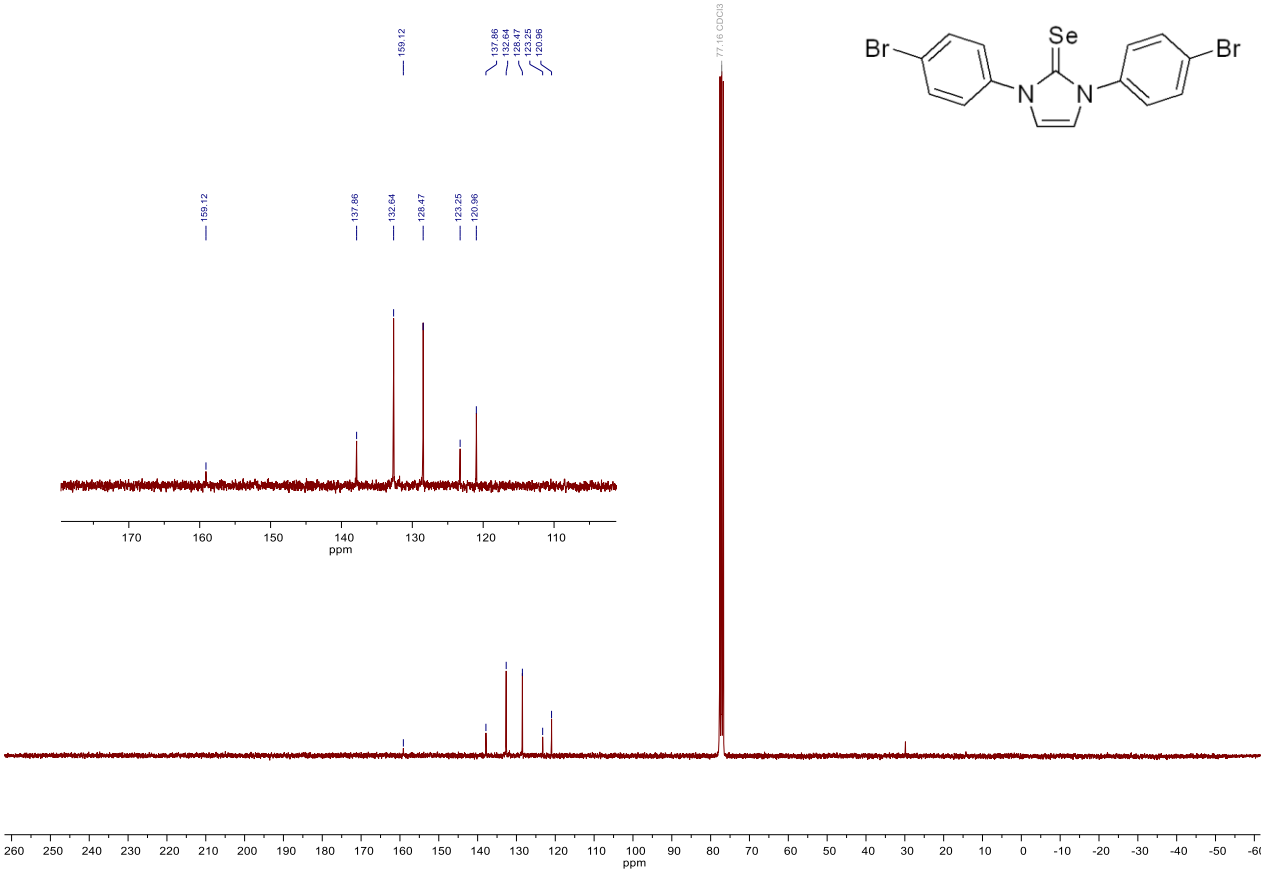


Figure S18. ^{13}C{^{1}H} NMR spectrum of **2f**. Solvent: $CDCl_3$, 75 MHz.

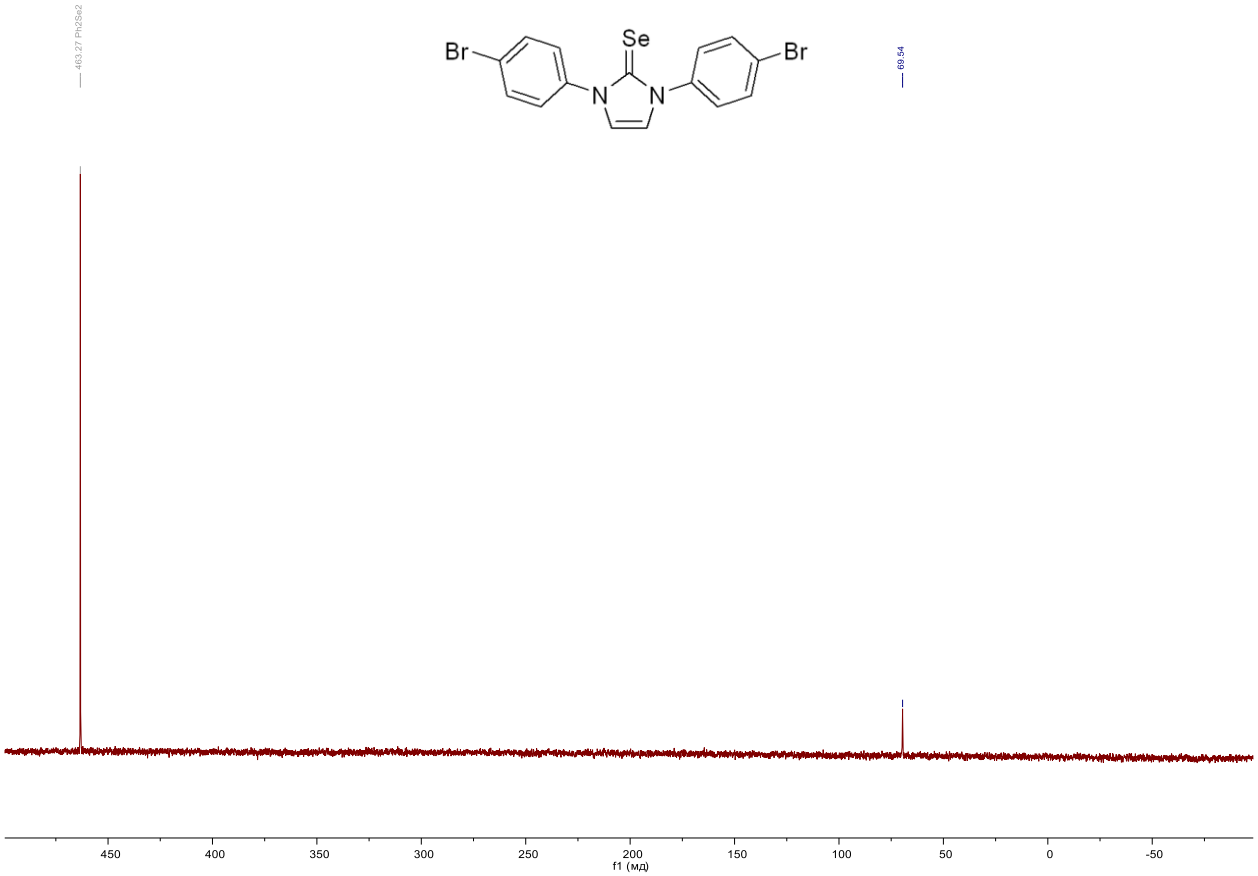


Figure S19. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2f.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

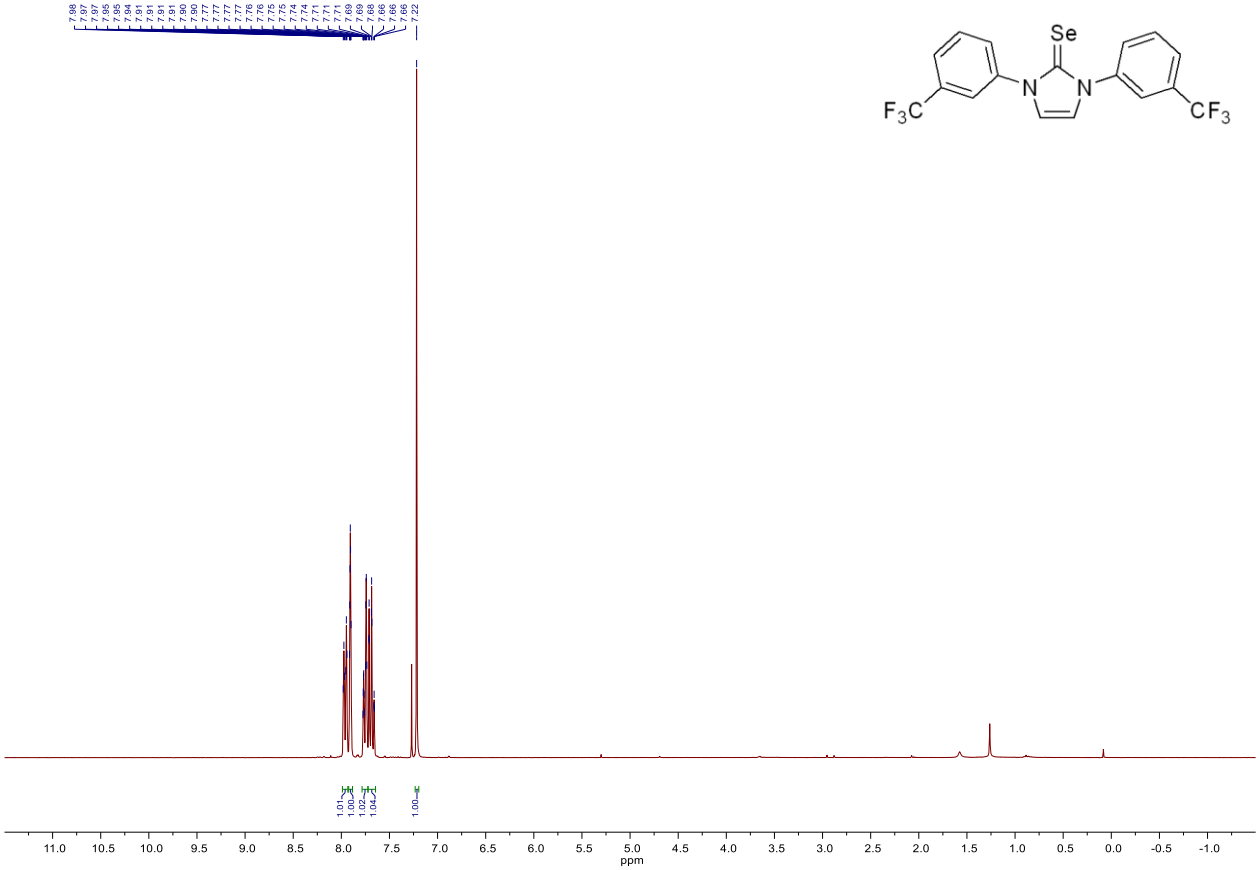


Figure S20. ^{1}H NMR spectrum of **2g**. Solvent: $CDCl_3$, 300 MHz.

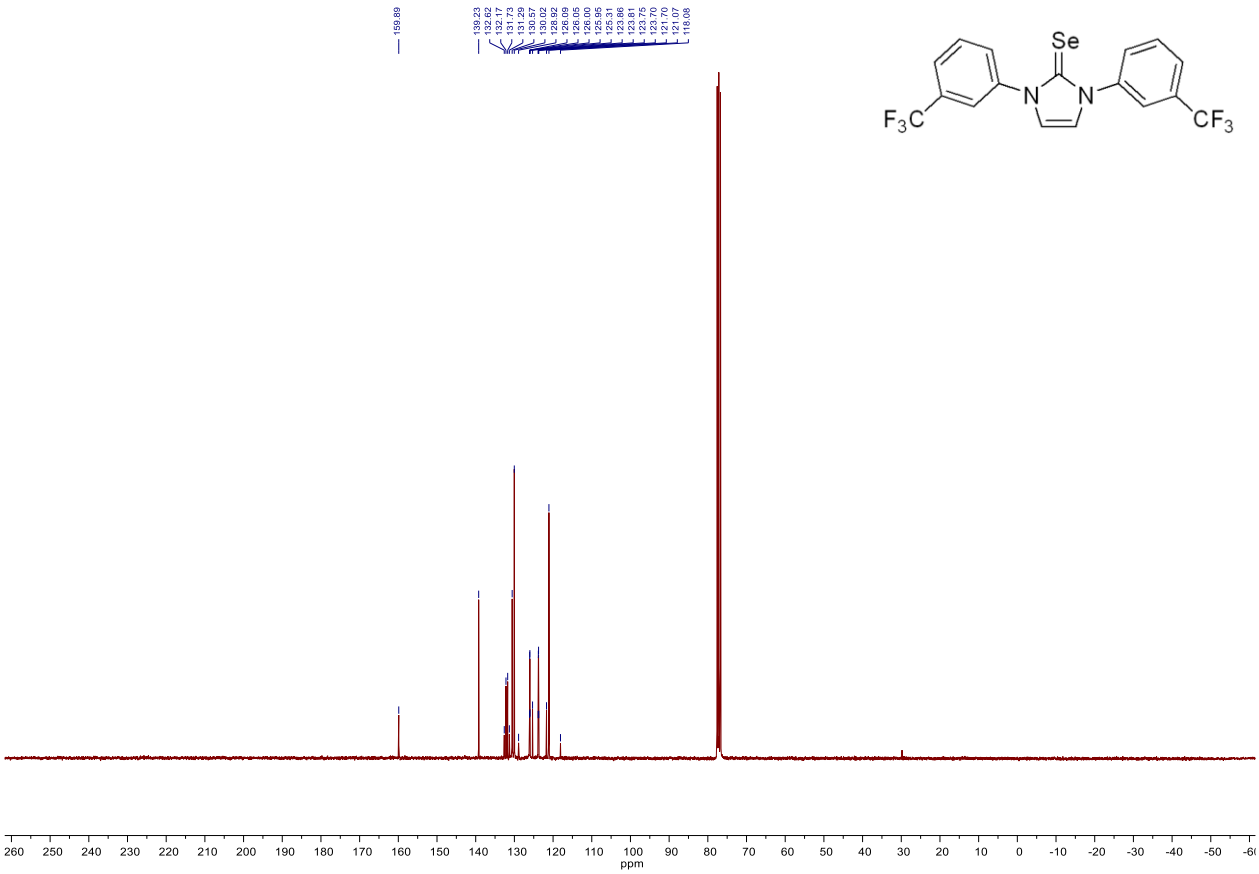


Figure S21. ^{13}C NMR spectrum of **2g**. Solvent: $CDCl_3$, 75 MHz.

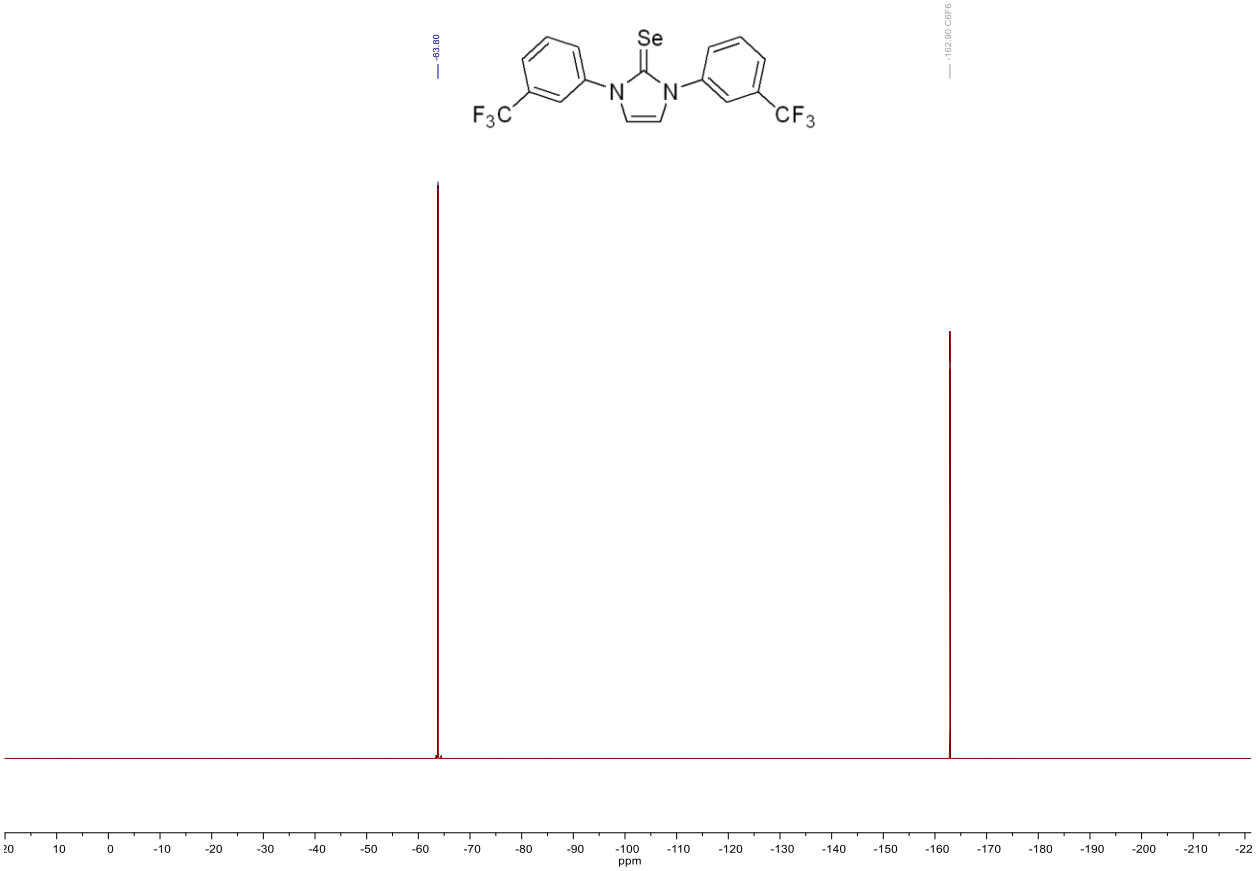


Figure S22. $^{19}F\{^1H\}$ NMR spectrum of **2g**. Solvent: $CDCl_3$, 282.4 MHz. Standard: C_6F_6 with respect to $CFCl_3$.

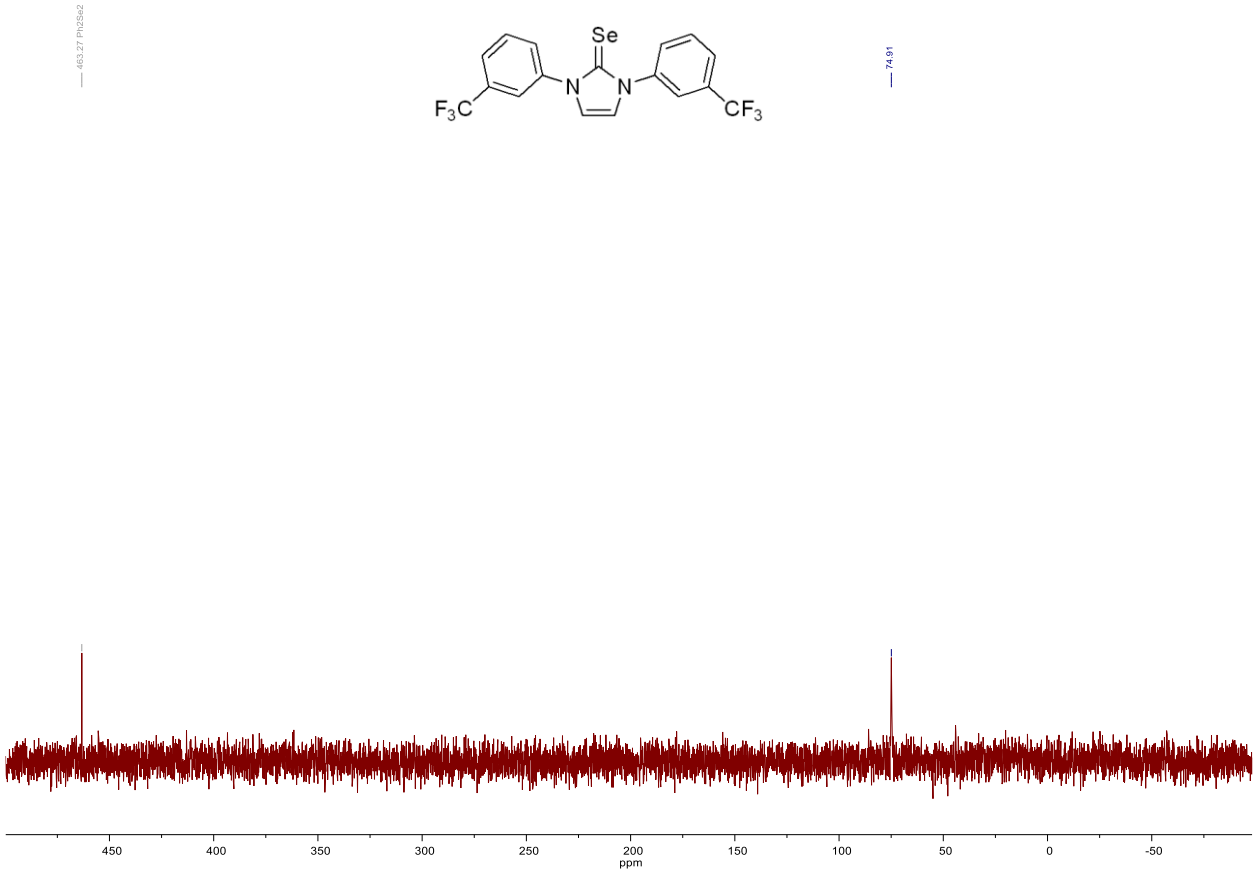


Figure S23. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2g.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

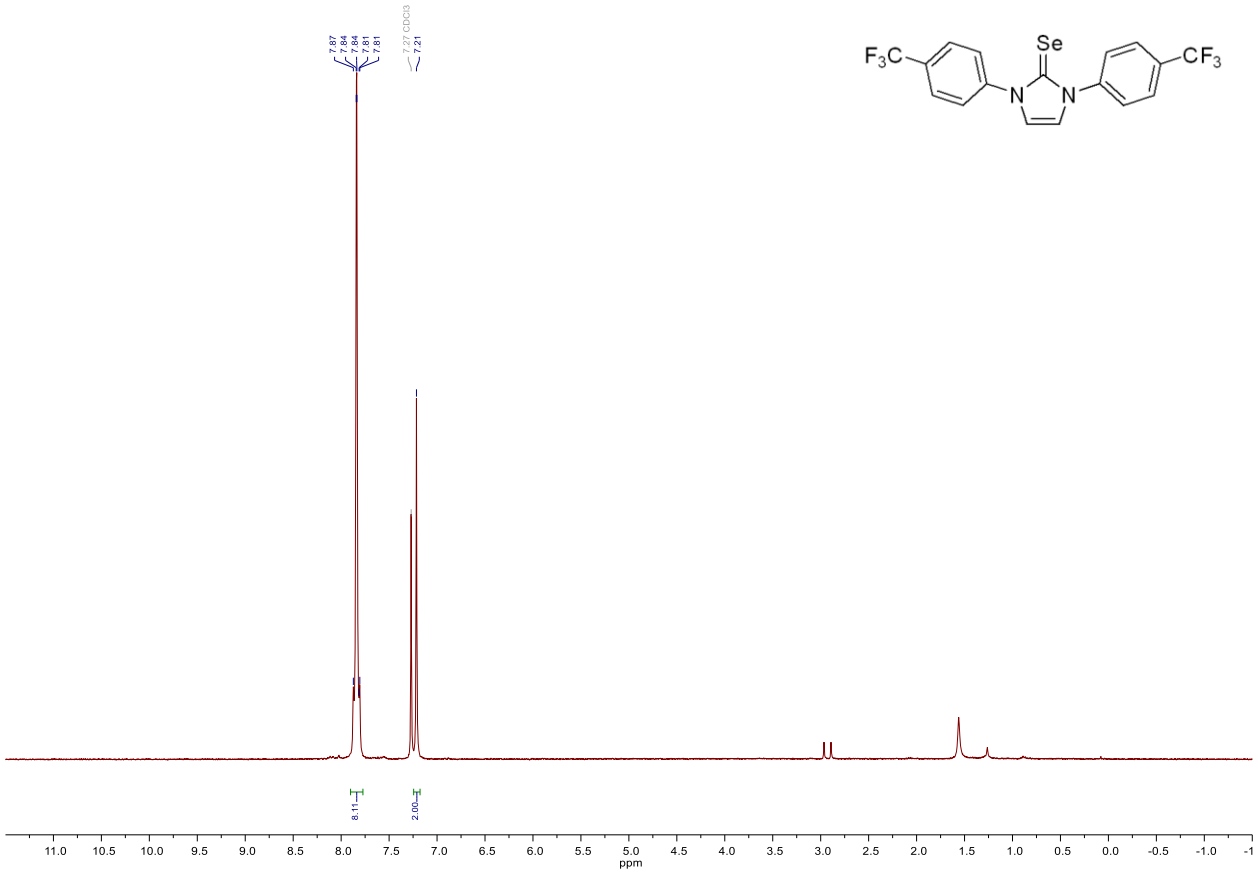


Figure S24. ^{1}H NMR spectrum of **2h**. Solvent: $CDCl_3$, 300 MHz.

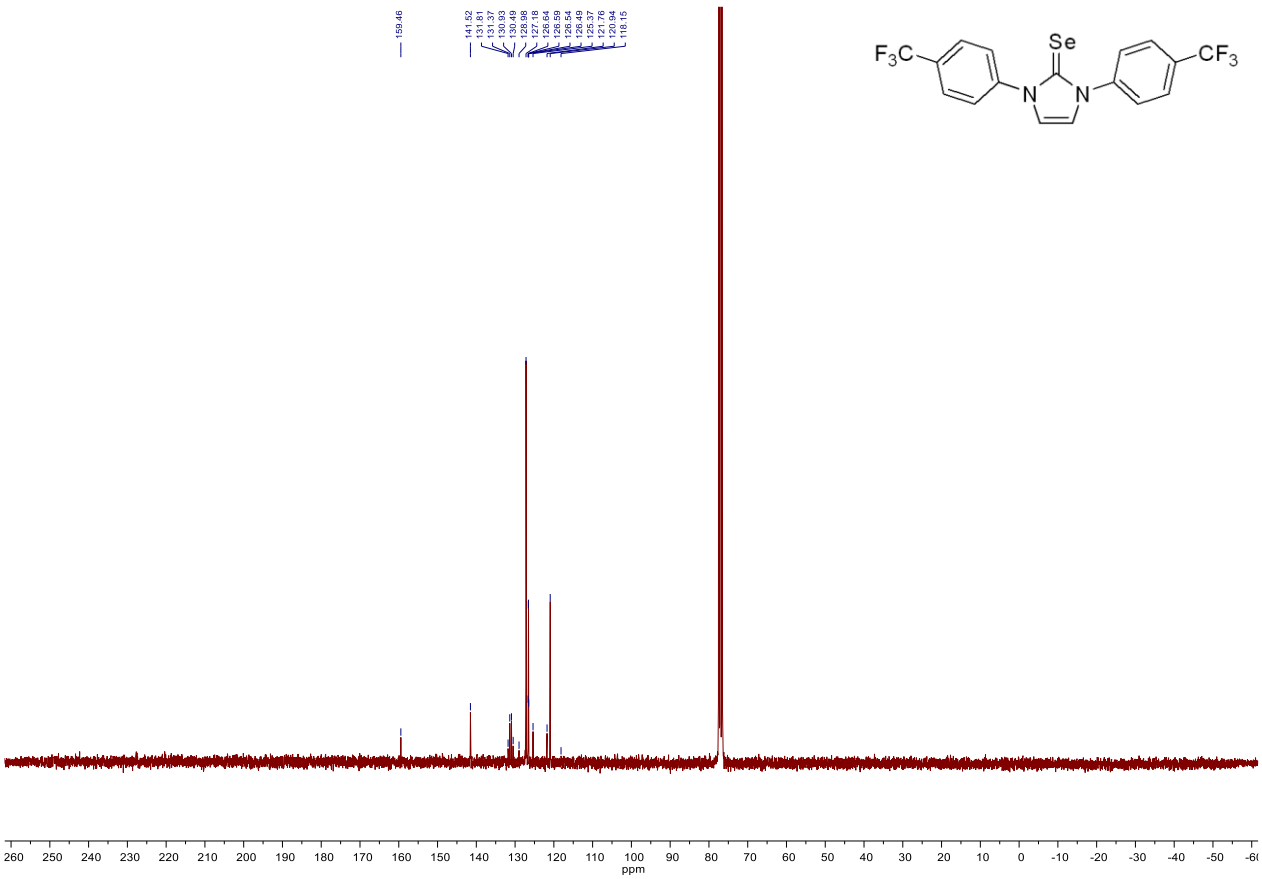


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of **2h**. Solvent: $CDCl_3$, 75 MHz.

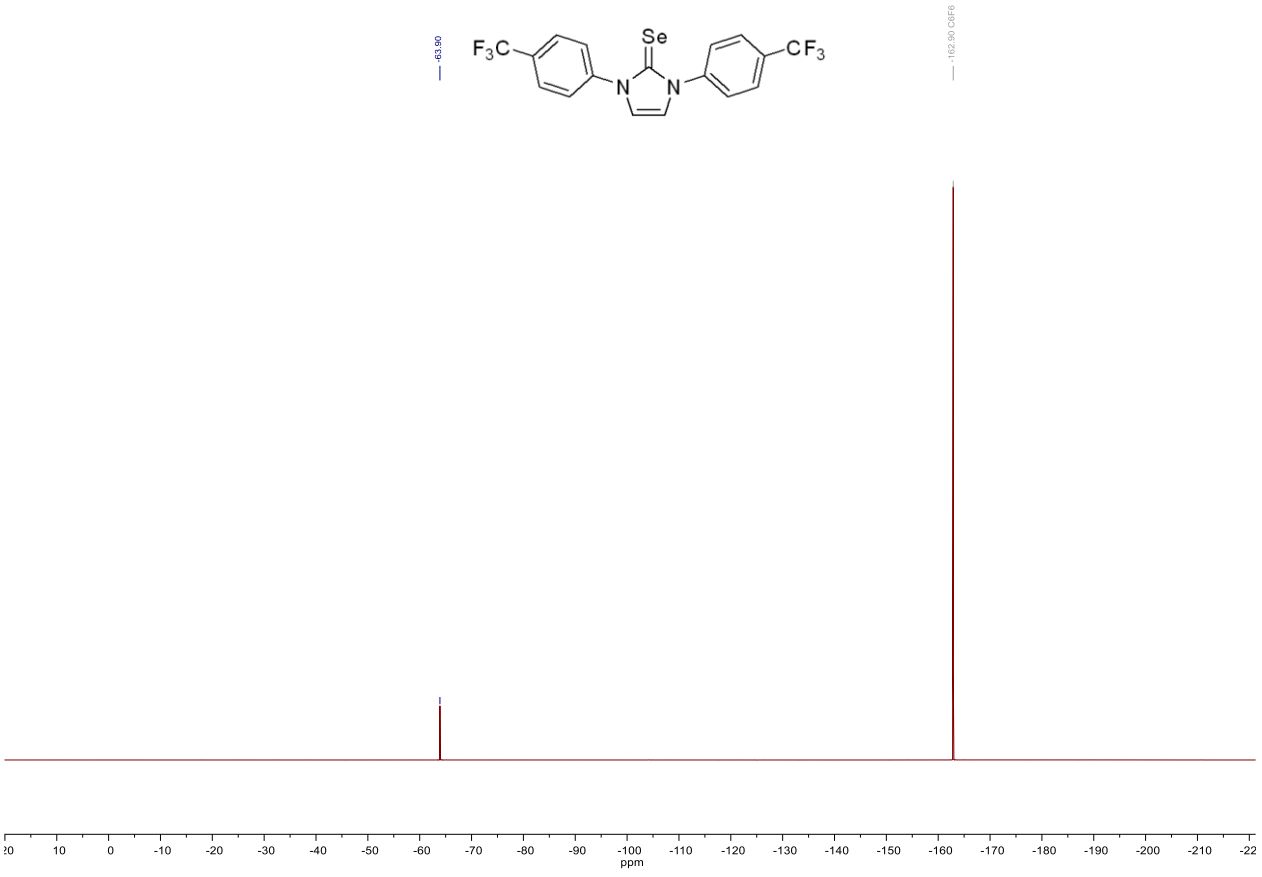


Figure S26. $^{19}F\{^{1}H\}$ NMR spectrum of **2h**. Solvent: $CDCl_3$, 282.4 MHz. Standard: C_6F_6 with respect to $CFCl_3$.

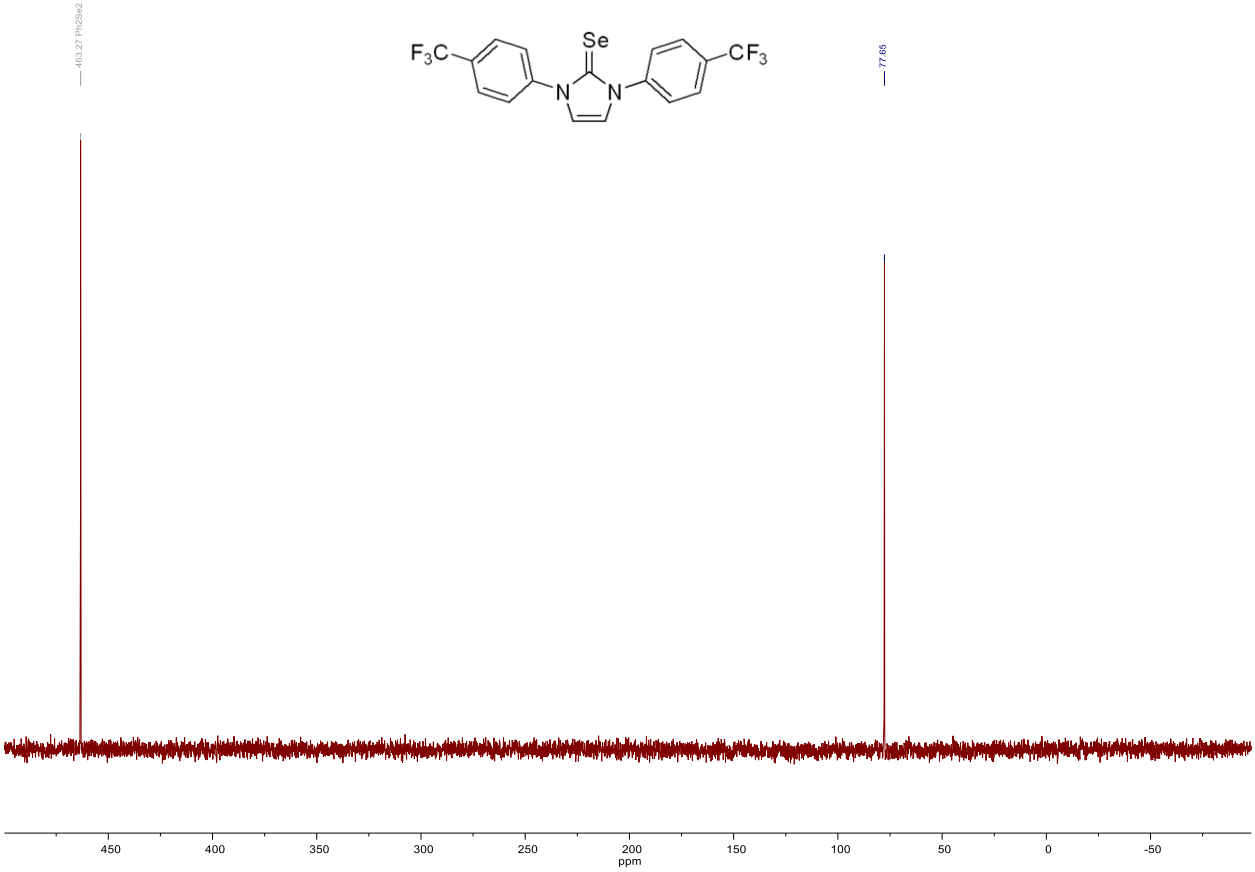


Figure S27. $^{77}Se\{^{1}H\}$ NMR spectrum of compound **2h.** Solvent: $CDCl_3$, 57 MHz. Standard: Ph_2Se_2.

ESI-HRMS spectra of the obtained compounds

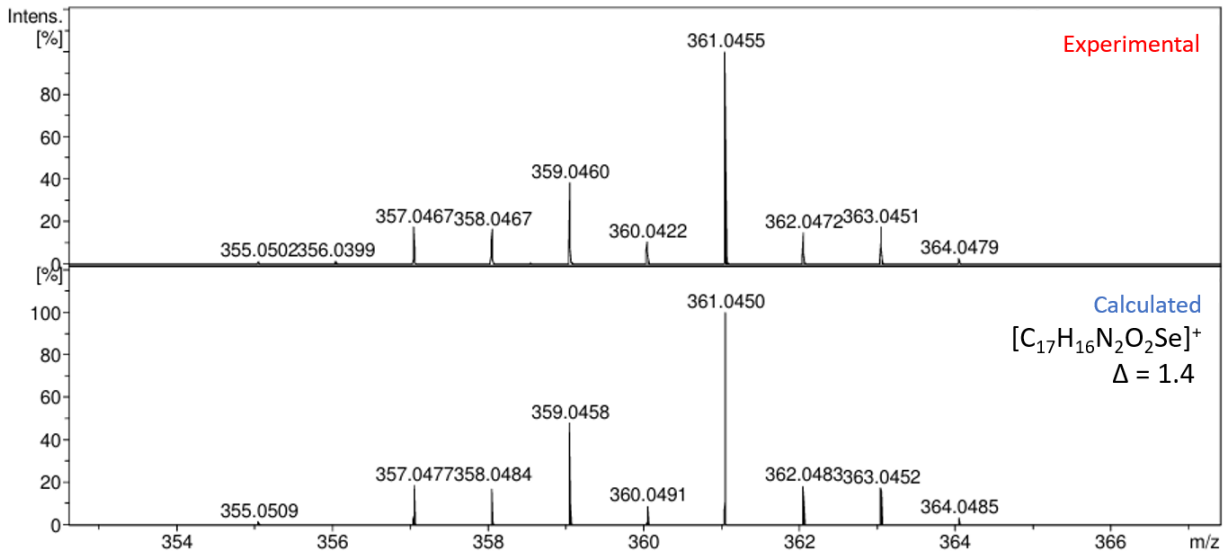


Figure S28. Experimental and theoretical ESI-(+)HRMS spectrum of **2a** in CH_3CN solution: experimental peak $[M+H]^+$ = 361.0455 Da, calculated for $[C_{17}H_{16}N_2O_2Se]^+$ = 361.0450, Δ = 1.4 ppm.

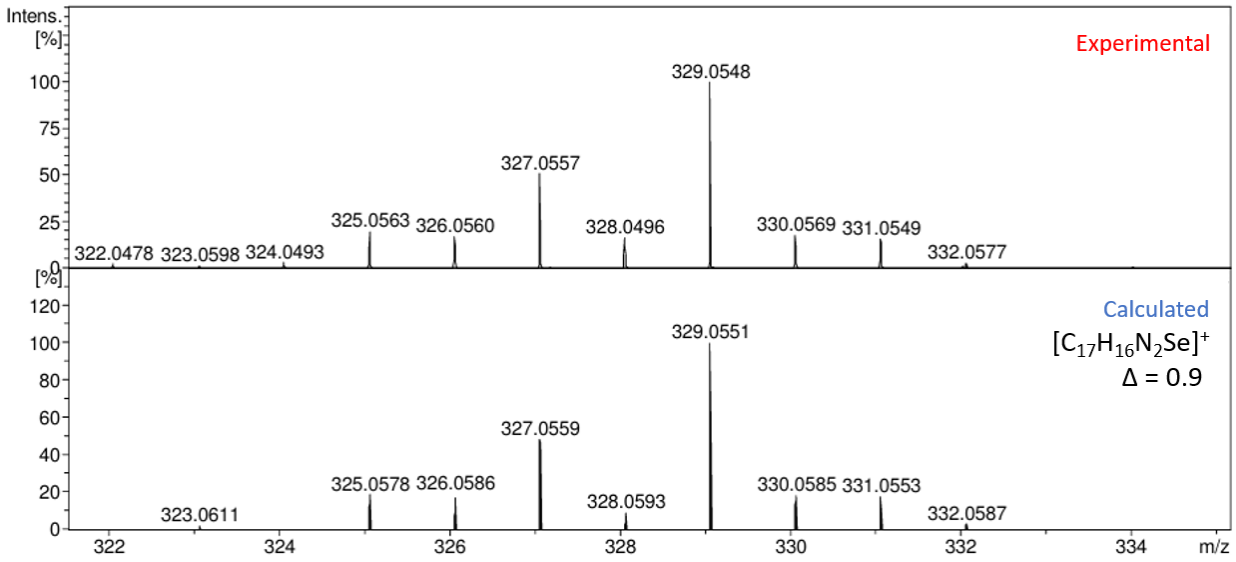


Figure S29. Experimental and theoretical ESI-(+)HRMS spectrum of **2b** in CH_3CN solution: experimental peak $[M+H]^+$ = 329.0548 Da, calculated for $[C_{17}H_{16}N_2Se]^+$ = 329.0551, Δ = 0.9 ppm.

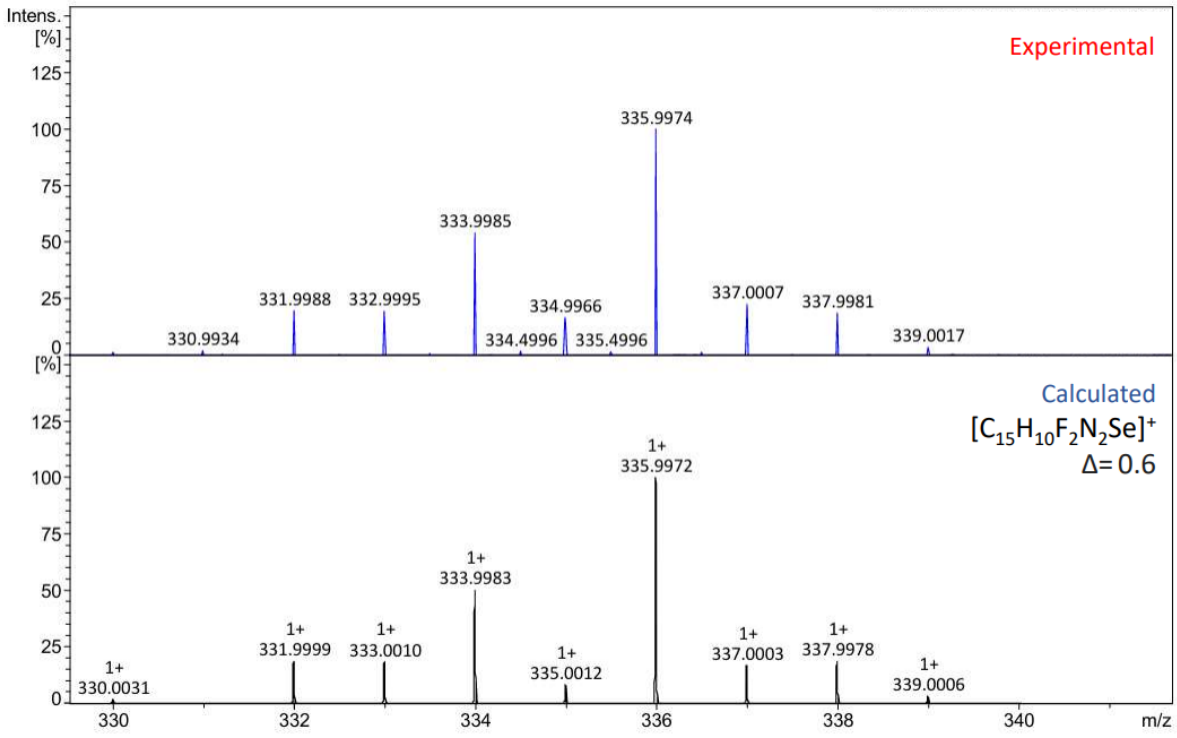


Figure S30. Experimental and theoretical ESI-(+)HRMS spectrum of **2c** in CH_3CN solution: experimental peak $[M+H]^+$ = 335.9974 Da, calculated for $[C_{15}H_{10}F_2N_2Se]^+$ = 335.9972, Δ = 0.6 ppm.

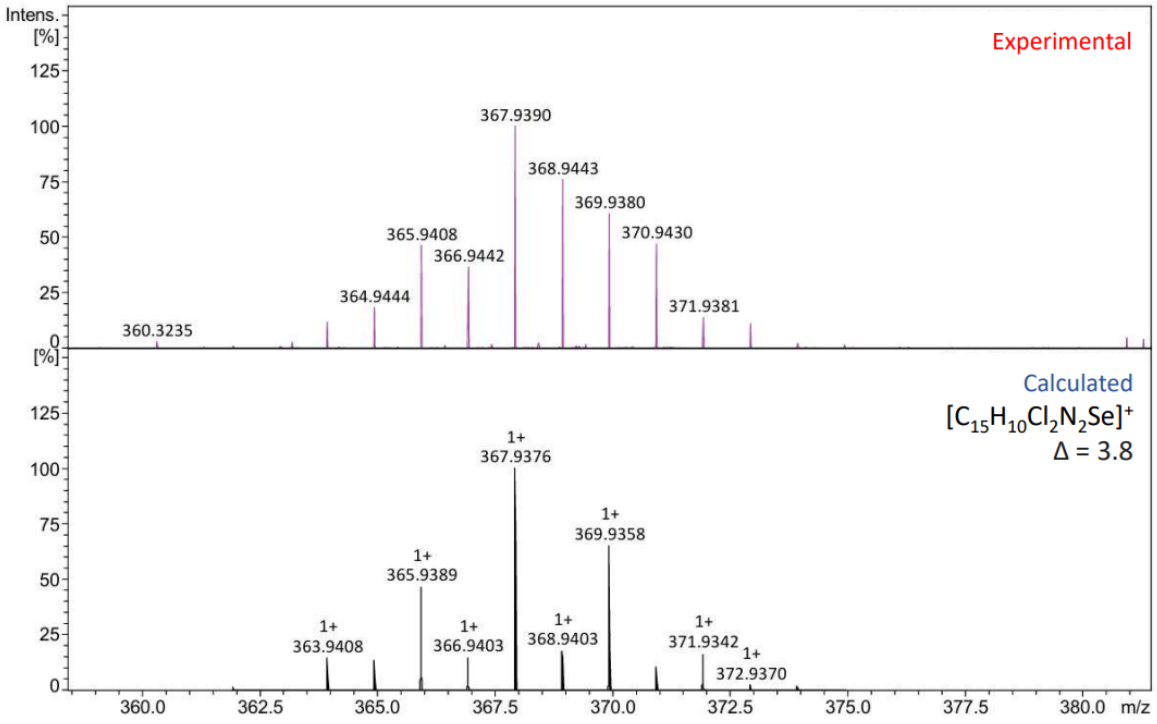


Figure S31. Experimental and theoretical ESI-(+)HRMS spectrum of **2d** in CH_3CN solution: experimental peak $[M+H]^+$ = 367.9390 Da, calculated for $[C_{15}H_{10}Cl_2N_2Se]^+$ = 367.9376, Δ = 3.8 ppm.

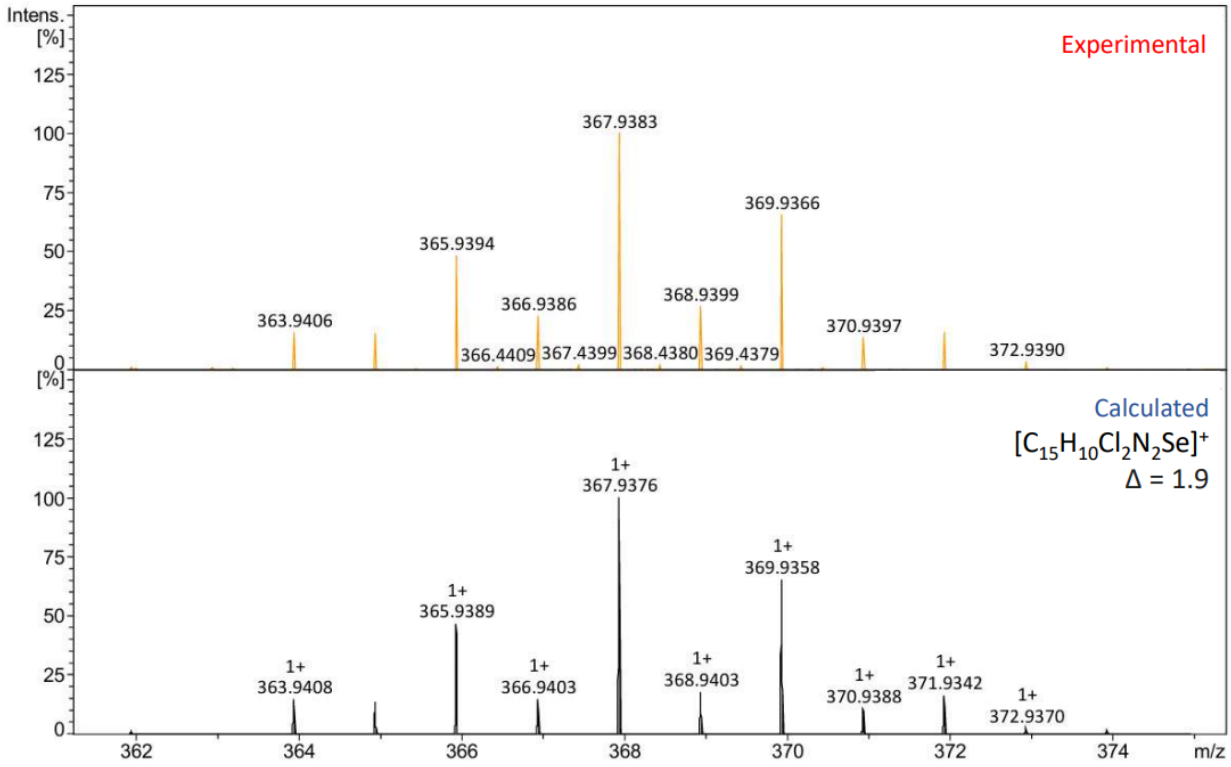


Figure S32. Experimental and theoretical ESI-(+)HRMS spectrum of **2e** in CH_3CN solution: experimental peak $[M+H]^+$ = 367.9383 Da, calculated for $[C_{15}H_{10}Cl_2N_2Se]^+$ = 367.9376, Δ = 1.9 ppm.

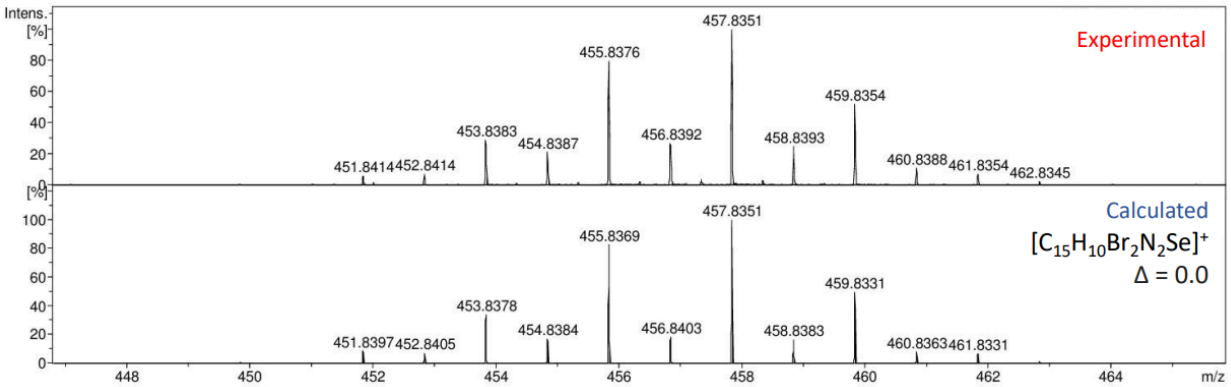


Figure S33. Experimental and theoretical ESI-(+)HRMS spectrum of **2f** in CH_3CN solution: experimental peak $[M+H]^+$ = 457.8351 Da, calculated for $[C_{15}H_{10}Br_2N_2Se]^+$ = 457.8351, Δ = 0.0 ppm.

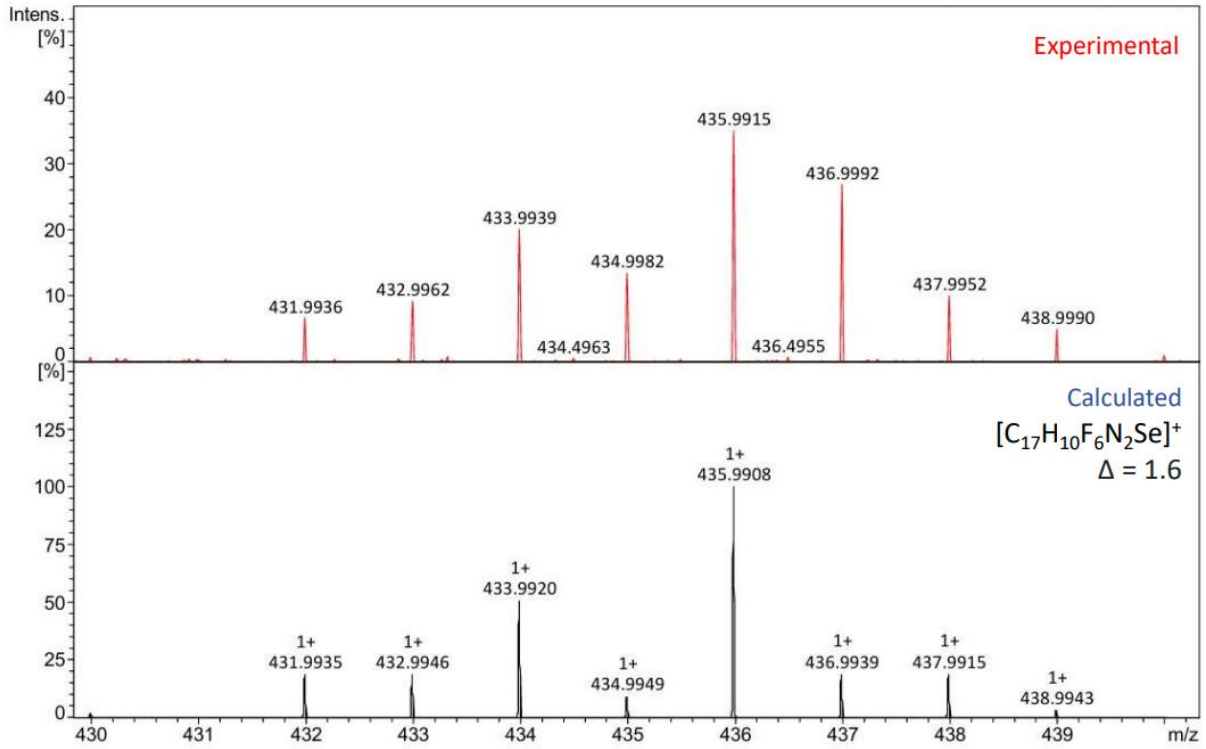


Figure S34. Experimental and theoretical ESI-(+)HRMS spectrum of **2g** in CH_3CN solution: experimental peak $[M+H]^+$ = 435.9915 Da, calculated for $[C_{17}H_{10}F_6N_2Se]^+$ = 435.9908, Δ = 1.6 ppm.

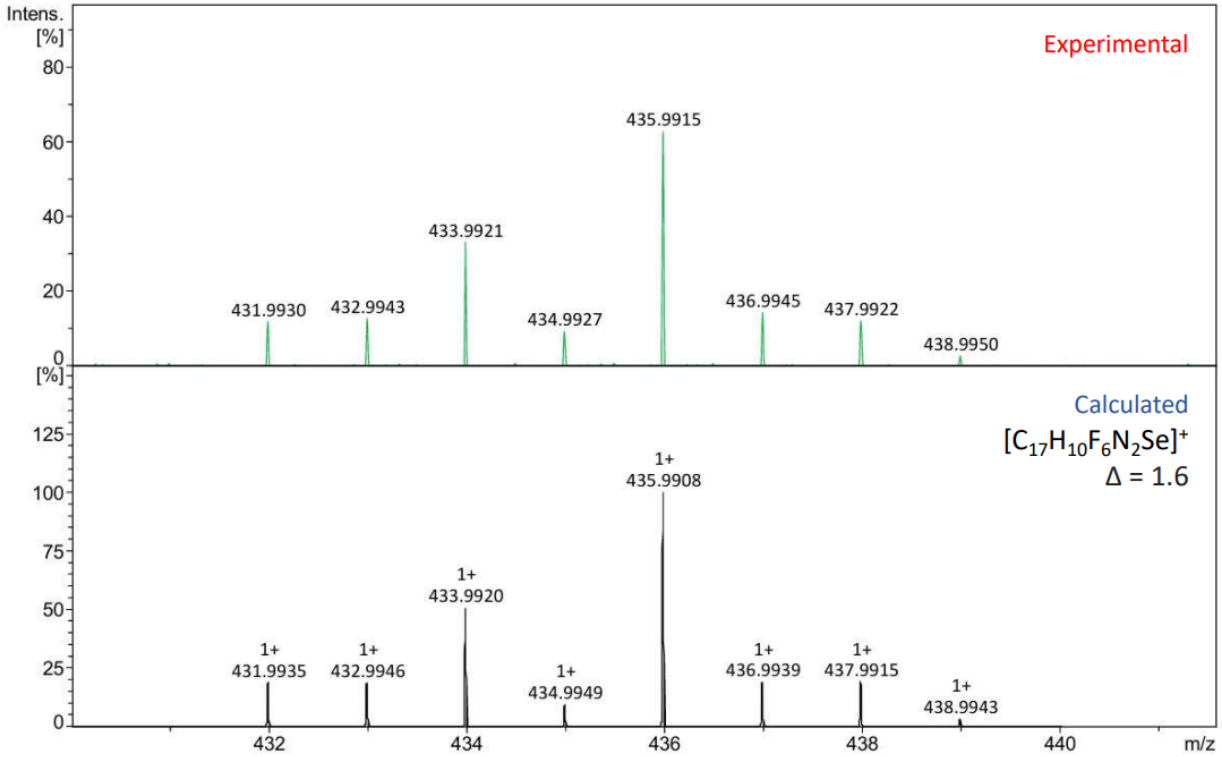


Figure S35. Experimental and theoretical ESI-(+)HRMS spectrum of **2h** in CH_3CN solution: experimental peak $[M+H]^+$ = 435.9915 Da, calculated for $[C_{17}H_{10}F_6N_2Se]^+$ = 435.9908, Δ = 1.6 ppm.

X-ray structure determination

X-ray crystallographic data and refinement details.

X-ray diffraction data were collected on a four-circle Rigaku XtaLAB Synergy-S diffractometer equipped with a HyPix-6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Mo Kα-radiation. The intensity data were integrated and analytically corrected for absorption and decay by the CrysAlisPro program.[1] The structures were solved by direct methods using SHELXT-2018/2[2] and refined by the full-matrix least-squares minimization method on F^2 using SHELXL-2025/1[3] in the OLEX2 program (ver. 1.5-ac7-016).[4] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters taken as U_{iso}(H)=1.2U_{eq}(C).

Crystals **2h** completely decay between 100K and 140K.

References:

1. CrysAlisPro. Version 1.171.44. *Rigaku Oxford Diffraction*, **2026**.
2. Sheldrick, G. M. SHELXT - Integrated space-group and crystal-structure determination. *Acta Cryst.* **2015**, A71(1), 3-8. http://doi.org/10.1107/S2053273314026370
3. Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Cryst.* **2015**, C71(1), 3-8. http://doi.org/10.1107/S2053229614024218
4. Dolomanov O.V.; Bourhis L.J.; Gildea R.J.; Howard J.A.K.; Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, 42(2), 339-341. http://doi.org/10.1107/S0021889808042726

Table S1. Crystal data and structure refinement for **2e** and **2h**.

Identification code	**2e**	**2h**
Empirical formula	$C_{15}H_{10}Cl_2N_2Se$	$C_{17}H_{10}F_6N_2Se$
Formula weight	368.11	435.23
Temperature, K	100.0(1)	150.0(1)
Wavelength, Å	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic
Space group	Pnc2	$P2_1/n$
Unit cell dimensions		
a, Å	5.57191(14)	4.74274(13)
b, Å	16.6697(4)	32.8081(8)
c, Å	7.65365(18)	10.4119(3)
β, °	90	91.625(2)
Volume, $Å^3$	710.89(3)	1619.44(8)
Z	2	4
Calcd density, $g•cm^{-3}$	1.720	1.785
Absorption coefficient, mm^{-1}	3.006	2.386
F(000)	364	856
Crystal size, mm	0.345×0.267×0.129	0.229×0.165×0.048
θ range for data collection, °	2.444 to 34.233	2.053 to 34.238
Index ranges	$-8 \le h \le 8$, $-25 \le k \le 24$, $-11 \le l \le 11$	$-7 \le h \le 6$, $-51 \le k \le 51$, $-16 \le l \le 16$
Reflections		
Collected	15104	27754
Independent [R_{int}]	2700 [0.0272]	6134 [0.0440]
Observed reflections	2567	4817
Completeness to θ_{full} / θ_{max}	1.000 / 0.951	1.000 / 0.909
T_{max} / T_{min}	1.000 / 0.335	1.000 / 0.634
Data / restraints / parameters	2700 / 1 / 97	6134 / 259 / 298
Goodness-of-fit on F^2	1.030	1.059
R_1 / wR_2 ($I>2\sigma(I)$)	0.0210 / 0.048	0.0411 / 0.0800
R_1 / wR_2 (all data)	0.0234 / 0.0496	0.0613 / 0.0870
Largest diff. peak / hole, $ē•Å^{-3}$	0.345 / -0.260	0.521 / -0.313
CCDC deposition number	2557100	2557101

The structure **2e**.

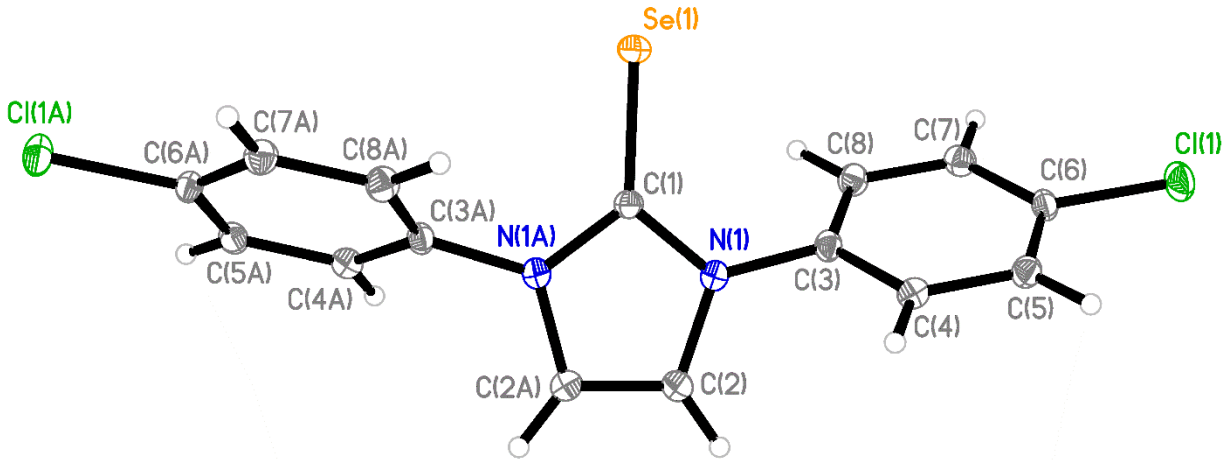


Figure S36. The structure of **2e**. The displacement ellipsoids for non-hydrogen atoms are set to a 50% probability level. The molecule is located on a 2-fold rotation axis.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2e**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	0	5000	2369(1)	18(1)
Cl(1)	6250(1)	8544(1)	4212(1)	21(1)
N(1)	1042(3)	5548(1)	5855(2)	14(1)
C(1)	0	5000	4762(3)	12(1)
C(2)	647(4)	5344(1)	7598(2)	16(1)
C(3)	2266(3)	6267(1)	5351(2)	13(1)
C(4)	1319(3)	6995(1)	5909(2)	14(1)
C(5)	2546(3)	7704(1)	5547(2)	15(1)
C(6)	4694(3)	7660(1)	4638(2)	14(1)
C(7)	5636(3)	6936(1)	4060(3)	16(1)
C(8)	4399(3)	6229(1)	4416(3)	15(1)

Table S3. Bond distances for **2e**, Å.

Se(1)-C(1)	1.832(3)	C(2)-H(2)	0.92(3)	C(5)-C(6)	1.387(3)
Cl(1)-C(6)	1.7408(17)	C(3)-C(4)	1.391(2)	C(6)-C(7)	1.388(2)
N(1)-C(1)	1.367(2)	C(3)-C(8)	1.389(3)	C(7)-H(7)	0.95(3)
N(1)-C(2)	1.394(2)	C(4)-H(4)	0.95(2)	C(7)-C(8)	1.392(2)
N(1)-C(3)	1.433(2)	C(4)-C(5)	1.393(2)	C(8)-H(8)	0.97(3)
C(2)-C(2)#1	1.354(4)	C(5)-H(5)	0.95(3)	C(5)-C(6)	1.387(3)

Symmetry transformation to generate equivalent atoms: #1 -x, -y+1, z

Table S4. Bond and angles for **2e**, °.

C(1)-N(1)-C(2)	110.80(16)	C(4)-C(3)-N(1)	117.83(16)	C(5)-C(6)-Cl(1)	118.59(13)
C(1)-N(1)-C(3)	126.61(16)	C(8)-C(3)-N(1)	120.56(15)	C(5)-C(6)-C(7)	122.20(16)
C(2)-N(1)-C(3)	122.49(15)	C(8)-C(3)-C(4)	121.52(16)	C(7)-C(6)-Cl(1)	119.22(14)
N(1)-C(1)-Se(1)	127.70(11)	C(3)-C(4)-H(4)	120.2	C(6)-C(7)-H(7)	120.5
N(1)#1-C(1)-Se(1)	127.70(11)	C(3)-C(4)-C(5)	119.53(16)	C(6)-C(7)-C(8)	119.09(17)
N(1)-C(1)-N(1)#1	104.6(2)	C(5)-C(4)-H(4)	120.2	C(8)-C(7)-H(7)	120.5
N(1)-C(2)-H(2)	126.6	C(4)-C(5)-H(5)	120.7	C(3)-C(8)-C(7)	119.09(16)
C(2)#1-C(2)-N(1)	106.89(10)	C(6)-C(5)-C(4)	118.56(16)	C(3)-C(8)-H(8)	120.5
C(2)#1-C(2)-H(2)	126.6	C(6)-C(5)-H(5)	120.7	C(7)-C(8)-H(8)	120.5

Symmetry transformation to generate equivalent atoms: #1 -x, -y+1, z

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2e**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	23(1)	20(1)	11(1)	0	0	-6(1)
Cl(1)	22(1)	17(1)	24(1)	3(1)	0(1)	-7(1)
N(1)	17(1)	12(1)	14(1)	-1(1)	0(1)	-2(1)
C(1)	13(1)	12(1)	11(1)	0	0	0(1)
C(2)	20(1)	15(1)	14(1)	1(1)	-1(1)	-1(1)
C(3)	13(1)	12(1)	14(1)	0(1)	-2(1)	-2(1)
C(4)	14(1)	14(1)	14(1)	-1(1)	0(1)	0(1)
C(5)	16(1)	13(1)	15(1)	-1(1)	-2(1)	-1(1)
C(6)	17(1)	12(1)	14(1)	2(1)	-3(1)	-3(1)
C(7)	14(1)	17(1)	16(1)	1(1)	0(1)	-1(1)
C(8)	15(1)	14(1)	17(1)	0(1)	-1(1)	1(1)

Table S6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters (Å$\times 10^3$) for **2e**.

Atom	x	y	z	U(eq)
H(2)	1169(16)	5623(8)	8570(30)	19
H(4)	-160(40)	7009(1)	6536(16)	17
H(5)	1920(17)	8210(14)	5916(10)	18
H(7)	7100(40)	6923(1)	3434(19)	19
H(8)	5016(18)	5719(15)	4017(12)	18

Table S7. Torsion angles for **2e**, °.

Cl(1)-C(6)-C(7)-C(8)	179.46(15)	C(3)-N(1)-C(1)-Se(1)	3.37(19)
N(1)-C(3)-C(4)-C(5)	175.69(16)	C(3)-N(1)-C(1)-N(1)#1	-176.64(19)
N(1)-C(3)-C(8)-C(7)	-175.21(17)	C(3)-N(1)-C(2)-C(2)#1	177.01(19)
C(1)-N(1)-C(2)-C(2)#1	0.3(3)	C(3)-C(4)-C(5)-C(6)	-0.3(3)
C(1)-N(1)-C(3)-C(4)	117.82(18)	C(4)-C(3)-C(8)-C(7)	1.2(3)
C(1)-N(1)-C(3)-C(8)	-65.6(2)	C(4)-C(5)-C(6)-Cl(1)	-179.08(14)
C(2)-N(1)-C(1)-Se(1)	179.87(10)	C(4)-C(5)-C(6)-C(7)	1.0(3)
C(2)-N(1)-C(1)-N(1)#1	-0.13(10)	C(5)-C(6)-C(7)-C(8)	-0.6(3)
C(2)-N(1)-C(3)-C(4)	-58.3(2)	C(6)-C(7)-C(8)-C(3)	-0.5(3)
C(2)-N(1)-C(3)-C(8)	118.2(2)	C(8)-C(3)-C(4)-C(5)	-0.8(3)

Symmetry transformation to generate equivalent atoms: #1 -x, -y+1, z

The dihedral C_3N_2-Ph angle between planes defined by atoms C(1), N(1), C(2) N(1)#1, C(2)#1 and atoms C(3) through C(8) is 61.76(5)°. Atom Se(1) is located on a 2-fold rotation axes, therefore its deviation from the C_3N_2 plane is 0.0000(0) Å. A deviation of atom Cl1 from the Ph plane (carbon atoms C(3)..C(8)) is 0.026(3)Å.

The structure **2h**.

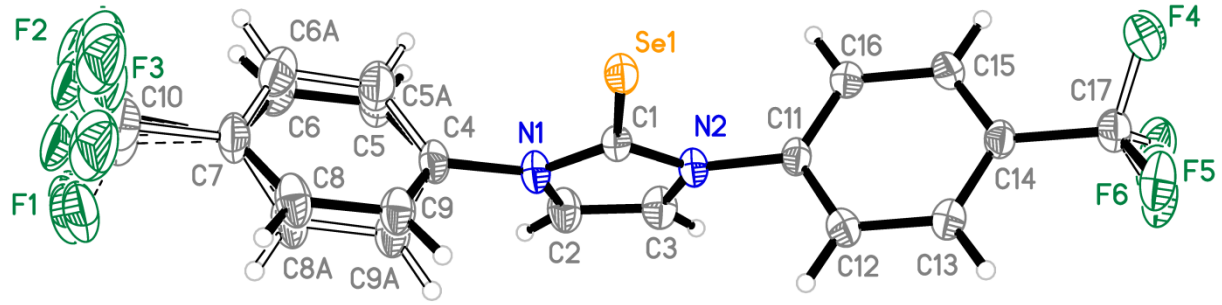


Figure S37. The structure of **2h**. The displacement ellipsoids for non-hydrogen atoms are set to a 50% probability level. The disorder ratio for carbon atoms of a phenyl ring (atoms C(4), C(5), C(6), C(7), C(8), C(9) / C(4), C(5A), C(6A), C(7), C(8A), C(9A)) is 0.573(12) : 0.427(12). The disorder ratio for its CF_3 group (atoms C(10), F(1), F(2), F(3) / C(10A), F(1A), F(2A), F(3A) / C(10A), F(1A), F(2A), F(3A) / C(10A), F(1A), F(2A), F(3A)) is 0.507(3) : 0.272(3) : 0.109(3) : 0.112(3). The disorder ratio for the second CF_3 group (atoms F(4), F(5), F(6) / F(4A), F(5A), F(6A)) is 0.624(15) : 0.376(15).

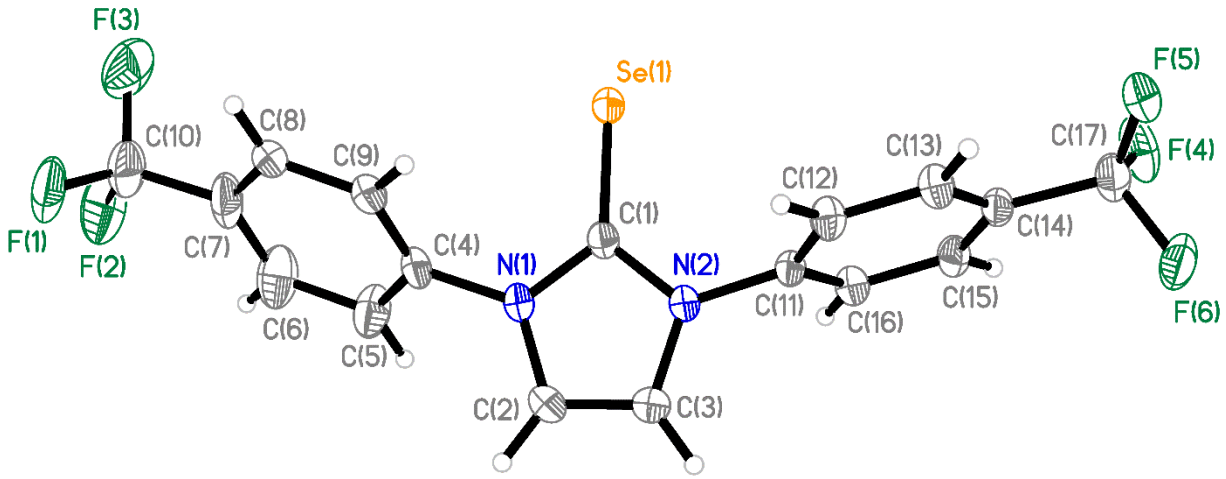


Figure S38. The structure of **2h**. The displacement ellipsoids for non-hydrogen atoms are set to a 50% probability level. All disorder is omitted for clarity.

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2h**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	2491(1)	6924(1)	7323(1)	24(1)
N(1)	5698(3)	6511(1)	5401(2)	25(1)
N(2)	5709(3)	7165(1)	5154(1)	22(1)
C(1)	4751(4)	6866(1)	5932(2)	22(1)
C(2)	7188(4)	6595(1)	4305(2)	31(1)
C(3)	7204(4)	7002(1)	4151(2)	29(1)
C(4)	5206(4)	6112(1)	5918(2)	27(1)
C(5)	3683(14)	5843(2)	5126(8)	40(1)
C(6)	3193(15)	5457(3)	5651(8)	49(1)
C(5A)	3124(18)	5860(3)	5443(10)	40(1)
C(6A)	2560(20)	5481(4)	5936(9)	49(1)
C(7)	4166(4)	5357(1)	6923(2)	41(1)
C(8)	5705(15)	5632(2)	7639(8)	33(1)
C(9)	6214(16)	6015(2)	7118(6)	29(1)
C(9A)	6900(20)	5982(3)	6968(8)	29(1)
C(8A)	6330(20)	5600(3)	7469(11)	33(1)
C(10)	3398(18)	4935(2)	7385(8)	44(1)
F(1)	5768(8)	4720(1)	7590(6)	55(2)
F(2)	1674(12)	4711(2)	6631(8)	64(1)
F(3)	2240(30)	4977(5)	8546(11)	66(2)
C(10A)	3540(30)	4974(4)	7726(15)	44(1)

Table S8 (*cont.*). Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2h**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1A)	5795(19)	4784(3)	8226(10)	55(2)
F(2A)	2490(30)	4700(4)	6849(16)	64(1)
F(3A)	1580(50)	4983(10)	8610(20)	66(2)
C(10B)	3840(50)	4932(5)	7438(18)	44(1)
F(1B)	5800(50)	4691(7)	7000(20)	55(2)
F(2B)	1280(40)	4823(6)	7060(30)	64(1)
F(3B)	3830(60)	4944(6)	8704(16)	66(2)
C(10C)	3960(50)	4958(5)	7672(17)	44(1)
F(1C)	5580(40)	4879(5)	8702(16)	55(2)
F(2C)	4180(50)	4640(4)	6870(16)	64(1)
F(3C)	1320(40)	4935(7)	8070(20)	66(2)
C(11)	5362(4)	7595(1)	5394(2)	22(1)
C(12)	7110(4)	7781(1)	6298(2)	26(1)
C(13)	6844(4)	8199(1)	6502(2)	27(1)
C(14)	4835(4)	8419(1)	5799(2)	24(1)
C(15)	3080(4)	8228(1)	4898(2)	26(1)
C(16)	3340(4)	7810(1)	4695(2)	25(1)
C(17)	4591(4)	8870(1)	5973(2)	32(1)
F(4)	1910(10)	9006(2)	5840(9)	49(1)
F(5)	5656(19)	8996(4)	7113(7)	40(1)
F(6)	6035(16)	9075(3)	5066(7)	42(1)
F(4A)	1952(19)	8967(3)	6305(11)	49(1)
F(5A)	6160(30)	9010(7)	6969(12)	40(1)
F(6A)	5270(20)	9082(5)	4966(12)	42(1)

Table S9. Bond distances for **2h,** Å.

Se(1)-C(1)	1.8356(18)	C(6A)-C(7)	1.325(10)	C(10B)-F(3B)	1.318(14)
N(1)-C(1)	1.368(2)	C(7)-C(8)	1.368(7)	C(10C)-F(1C)	1.326(13)
N(1)-C(2)	1.386(2)	C(7)-C(8A)	1.409(10)	C(10C)-F(2C)	1.342(14)
N(1)-C(4)	1.439(2)	C(7)-C(10)	1.513(8)	C(10C)-F(3C)	1.331(14)
N(2)-C(1)	1.361(2)	C(7)-C(10A)	1.542(12)	C(11)-C(12)	1.380(3)
N(2)-C(3)	1.387(2)	C(7)-C(10B)	1.504(15)	C(11)-C(16)	1.381(3)
N(2)-C(11)	1.441(2)	C(7)-C(10C)	1.528(14)	C(12)-H(12)	0.9500
C(2)-H(2)	0.9500	C(8)-H(8)	0.9500	C(12)-C(13)	1.392(2)
C(2)-C(3)	1.345(3)	C(8)-C(9)	1.391(8)	C(13)-H(13)	0.9500
C(3)-H(3)	0.9500	C(9)-H(9)	0.9500	C(13)-C(14)	1.387(3)
C(4)-C(5)	1.396(7)	C(9A)-H(9A)	0.9500	C(14)-C(15)	1.386(3)
C(4)-C(5A)	1.368(9)	C(9A)-C(8A)	1.385(11)	C(14)-C(17)	1.498(2)
C(4)-C(9)	1.363(7)	C(8A)-H(8A)	0.9500	C(15)-H(15)	0.9500
C(4)-C(9A)	1.404(9)	C(10)-F(1)	1.339(8)	C(15)-C(16)	1.394(2)
C(5)-H(5)	0.9500	C(10)-F(2)	1.336(8)	C(16)-H(16)	0.9500
C(5)-C(6)	1.400(8)	C(10)-F(3)	1.348(8)	C(17)-F(4)	1.350(5)
C(6)-H(6)	0.9500	C(10A)-F(1A)	1.329(12)	C(17)-F(5)	1.341(7)
C(6)-C(7)	1.429(8)	C(10A)-F(2A)	1.367(12)	C(17)-F(6)	1.358(6)
C(5A)-H(5A)	0.9500	C(10A)-F(3A)	1.328(12)	C(17)-F(4A)	1.346(9)
C(5A)-C(6A)	1.376(11)	C(10B)-F(1B)	1.314(14)	C(17)-F(5A)	1.340(11)
C(6A)-H(6A)	0.9500	C(10B)-F(2B)	1.316(14)	C(17)-F(6A)	1.305(10)

Table S10. Bond angles in **2h**, °.

C(1)-N(1)-C(2)	110.26(15)	C(6A)-C(7)-C(10A)	123.8(8)	F(1C)-C(10C)-F(2C)	107.3(14)
C(1)-N(1)-C(4)	124.30(15)	C(8)-C(7)-C(6)	120.4(5)	F(1C)-C(10C)-F(3C)	105.4(15)
C(2)-N(1)-C(4)	125.44(15)	C(8)-C(7)-C(10)	124.1(5)	F(2C)-C(10C)-C(7)	109.9(12)
C(1)-N(2)-C(3)	110.83(15)	C(8A)-C(7)-C(10A)	113.1(8)	F(3C)-C(10C)-C(7)	106.3(15)
C(1)-N(2)-C(11)	124.14(15)	C(7)-C(8)-H(8)	120.7	F(3C)-C(10C)-F(2C)	103.9(16)
C(3)-N(2)-C(11)	124.91(15)	C(7)-C(8)-C(9)	118.6(7)	C(12)-C(11)-N(2)	118.90(15)
N(1)-C(1)-Se(1)	127.83(13)	C(9)-C(8)-H(8)	120.7	C(12)-C(11)-C(16)	121.82(16)
N(2)-C(1)-Se(1)	127.36(13)	C(4)-C(9)-C(8)	120.6(7)	C(16)-C(11)-N(2)	119.27(16)
N(2)-C(1)-N(1)	104.69(15)	C(4)-C(9)-H(9)	119.7	C(11)-C(12)-H(12)	120.5
N(1)-C(2)-H(2)	126.3	C(8)-C(9)-H(9)	119.7	C(11)-C(12)-C(13)	119.04(17)
C(3)-C(2)-N(1)	107.40(16)	C(4)-C(9A)-H(9A)	121.4	C(13)-C(12)-H(12)	120.5
C(3)-C(2)-H(2)	126.3	C(8A)-C(9A)-C(4)	117.2(10)	C(12)-C(13)-H(13)	120.2
N(2)-C(3)-H(3)	126.6	C(8A)-C(9A)-H(9A)	121.4	C(14)-C(13)-C(12)	119.67(17)
C(2)-C(3)-N(2)	106.82(17)	C(7)-C(8A)-H(8A)	119.8	C(14)-C(13)-H(13)	120.2
C(2)-C(3)-H(3)	126.6	C(9A)-C(8A)-C(7)	120.4(10)	C(13)-C(14)-C(17)	120.32(17)

Table S10(cont.). Bond angles in **2h**, °.

C(5)-C(4)-N(1)	116.2(4)	C(9A)-C(8A)-H(8A)	119.8	C(15)-C(14)-C(13)	120.81(16)
C(5A)-C(4)-N(1)	122.5(5)	F(1)-C(10)-C(7)	108.9(6)	C(15)-C(14)-C(17)	118.84(17)
C(5A)-C(4)-C(9A)	119.2(7)	F(1)-C(10)-F(3)	105.8(8)	C(14)-C(15)-H(15)	120.2
C(9)-C(4)-N(1)	120.0(4)	F(2)-C(10)-C(7)	117.7(6)	C(14)-C(15)-C(16)	119.59(17)
C(9)-C(4)-C(5)	123.7(5)	F(2)-C(10)-F(1)	107.6(6)	C(16)-C(15)-H(15)	120.2
C(9A)-C(4)-N(1)	118.3(5)	F(2)-C(10)-F(3)	109.0(8)	C(11)-C(16)-C(15)	119.08(17)
C(4)-C(5)-H(5)	122.3	F(3)-C(10)-C(7)	107.3(8)	C(11)-C(16)-H(16)	120.5
C(4)-C(5)-C(6)	115.5(7)	F(1A)-C(10A)-C(7)	115.5(10)	C(15)-C(16)-H(16)	120.5
C(6)-C(5)-H(5)	122.3	F(1A)-C(10A)-F(2A)	103.1(11)	F(4)-C(17)-C(14)	112.8(3)
C(5)-C(6)-H(6)	119.4	F(2A)-C(10A)-C(7)	104.2(11)	F(4)-C(17)-F(6)	105.0(3)
C(5)-C(6)-C(7)	121.1(7)	F(3A)-C(10A)-C(7)	120.4(17)	F(5)-C(17)-C(14)	112.4(6)
C(7)-C(6)-H(6)	119.4	F(3A)-C(10A)-F(1A)	108.1(14)	F(5)-C(17)-F(4)	108.7(5)
C(4)-C(5A)-H(5A)	118.1	F(3A)-C(10A)-F(2A)	103.2(15)	F(5)-C(17)-F(6)	106.2(5)
C(4)-C(5A)-C(6A)	123.8(10)	F(1B)-C(10B)-C(7)	110.7(15)	F(6)-C(17)-C(14)	111.2(4)
C(6A)-C(5A)-H(5A)	118.1	F(1B)-C(10B)-F(2B)	112.8(17)	F(4A)-C(17)-C(14)	109.8(5)
C(5A)-C(6A)-H(6A)	121.5	F(1B)-C(10B)-F(3B)	113.0(16)	F(5A)-C(17)-C(14)	112.8(10)
C(7)-C(6A)-C(5A)	117.0(10)	F(2B)-C(10B)-C(7)	104.3(14)	F(5A)-C(17)-F(4A)	102.8(9)
C(7)-C(6A)-H(6A)	121.5	F(2B)-C(10B)-F(3B)	106.3(16)	F(6A)-C(17)-C(14)	114.1(8)
C(6)-C(7)-C(10)	115.5(5)	F(3B)-C(10B)-C(7)	109.3(14)	F(6A)-C(17)-F(4A)	109.5(7)
C(6A)-C(7)-C(8A)	122.4(8)	F(1C)-C(10C)-C(7)	122.4(14)	F(6A)-C(17)-F(5A)	107.1(10)

Table S11. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2h**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	27(1)	19(1)	26(1)	1(1)	5(1)	1(1)
N(1)	34(1)	16(1)	27(1)	0(1)	4(1)	2(1)
N(2)	28(1)	16(1)	24(1)	0(1)	3(1)	1(1)
C(1)	24(1)	17(1)	26(1)	0(1)	1(1)	0(1)
C(2)	40(1)	23(1)	29(1)	-5(1)	8(1)	3(1)
C(3)	36(1)	25(1)	26(1)	-1(1)	9(1)	1(1)
C(4)	34(1)	16(1)	33(1)	-2(1)	4(1)	2(1)
C(5)	49(2)	26(1)	43(3)	6(2)	-11(2)	-5(2)
C(6)	47(3)	28(1)	69(3)	6(2)	-11(2)	-11(2)
C(5A)	49(2)	26(1)	43(3)	6(2)	-11(2)	-5(2)
C(6A)	47(3)	28(1)	69(3)	6(2)	-11(2)	-11(2)
C(7)	42(1)	18(1)	65(2)	7(1)	10(1)	1(1)
C(8)	47(3)	23(1)	30(2)	1(1)	13(2)	7(2)
C(9)	38(3)	20(1)	29(2)	-3(1)	6(2)	1(2)
C(9A)	38(3)	20(1)	29(2)	-3(1)	6(2)	1(2)
C(8A)	47(3)	23(1)	30(2)	1(1)	13(2)	7(2)
C(10)	45(2)	24(2)	63(3)	8(2)	2(2)	-5(1)
F(1)	58(1)	30(2)	79(4)	25(3)	7(3)	8(1)
F(2)	67(4)	29(1)	95(3)	10(2)	-17(3)	-26(3)
F(3)	73(6)	51(1)	76(2)	26(2)	27(3)	-8(4)
C(10A)	45(2)	24(2)	63(3)	8(2)	2(2)	-5(1)
F(1A)	58(1)	30(2)	79(4)	25(3)	7(3)	8(1)
F(2A)	67(4)	29(1)	95(3)	10(2)	-17(3)	-26(3)
F(3A)	73(6)	51(1)	76(2)	26(2)	27(3)	-8(4)
C(10B)	45(2)	24(2)	63(3)	8(2)	2(2)	-5(1)
F(1B)	58(1)	30(2)	79(4)	25(3)	7(3)	8(1)
F(2B)	67(4)	29(1)	95(3)	10(2)	-17(3)	-26(3)
F(3B)	73(6)	51(1)	76(2)	26(2)	27(3)	-8(4)
C(10C)	45(2)	24(2)	63(3)	8(2)	2(2)	-5(1)
F(1C)	58(1)	30(2)	79(4)	25(3)	7(3)	8(1)
F(2C)	67(4)	29(1)	95(3)	10(2)	-17(3)	-26(3)
F(3C)	73(6)	51(1)	76(2)	26(2)	27(3)	-8(4)
C(11)	25(1)	16(1)	25(1)	1(1)	5(1)	-1(1)
C(12)	28(1)	21(1)	30(1)	2(1)	-1(1)	3(1)
C(13)	30(1)	21(1)	31(1)	-2(1)	0(1)	-2(1)
C(14)	25(1)	17(1)	29(1)	1(1)	6(1)	-1(1)

Table S11 (*cont.*). Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2h**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

_	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(15)	27(1)	20(1)	31(1)	3(1)	0(1)	3(1)
C(16)	26(1)	21(1)	28(1)	-1(1)	0(1)	0(1)
C(17)	32(1)	21(1)	42(1)	0(1)	4(1)	0(1)
F(4)	36(1)	25(1)	84(4)	-9(2)	-1(2)	9(1)
F(5)	58(3)	23(1)	40(2)	-6(2)	4(2)	-5(2)
F(6)	54(3)	25(1)	46(1)	11(1)	0(2)	-5(2)
F(4A)	36(1)	25(1)	84(4)	-9(2)	-1(2)	9(1)
F(5A)	58(3)	23(1)	40(2)	-6(2)	4(2)	-5(2)
F(6A)	54(3)	25(1)	46(1)	11(1)	0(2)	-5(2)

Table S12. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **2h**.

	x	y	z	U(eq)
H(2)	8041	6400	3763	37
H(3)	8072	7149	3483	35
H(5)	3024	5916	4287	48
H(6)	2196	5259	5152	58
H(5A)	2001	5954	4733	48
H(6A)	1091	5315	5584	58
H(8)	6411	5563	8474	40
H(9)	7272	6210	7603	35
H(9A)	8360	6149	7321	35
H(8A)	7419	5502	8185	40
H(12)	8475	7627	6775	32
H(13)	8032	8333	7119	33
H(15)	1709	8381	4422	31
H(16)	2142	7674	4085	30

Table S13. Torsion angles for **2h,** °.

N(1)-C(2)-C(3)-N(2)	-0.2(2)	C(5A)-C(6A)-C(7)-C(8A)	0.8(5)
N(1)-C(4)-C(5)-C(6)	-179.22(17)	C(5A)-C(6A)-C(7)-C(10A)	169.9(8)
N(1)-C(4)-C(5A)-C(6A)	-178.52(19)	C(6A)-C(7)-C(8A)-C(9A)	-1.0(6)
N(1)-C(4)-C(9)-C(8)	178.8(3)	C(6A)-C(7)-C(10A)-F(1A)	149.3(10)
N(1)-C(4)-C(9A)-C(8A)	178.5(3)	C(6A)-C(7)-C(10A)-F(2A)	37.0(14)
N(1)-C(2)-C(3)-N(2)	-0.2(2)	C(6A)-C(7)-C(10A)-F(3A)	-77.9(18)
N(2)-C(11)-C(12)-C(13)	177.86(16)	C(7)-C(8)-C(9)-C(4)	-0.2(5)
N(2)-C(11)-C(16)-C(15)	-177.70(16)	C(8)-C(7)-C(10)-F(1)	-63.2(8)
C(1)-N(1)-C(2)-C(3)	0.5(2)	C(8)-C(7)-C(10)-F(2)	174.1(6)
C(1)-N(1)-C(4)-C(5)	118.8(4)	C(8)-C(7)-C(10)-F(3)	50.8(10)
C(1)-N(1)-C(4)-C(5A)	99.4(4)	C(9)-C(4)-C(5)-C(6)	0.91(19)
C(1)-N(1)-C(4)-C(9)	-61.3(4)	C(9A)-C(4)-C(5A)-C(6A)	0.0(2)
C(1)-N(1)-C(4)-C(9A)	-79.1(4)	C(8A)-C(7)-C(10A)-F(1A)	-40.7(15)
C(1)-N(2)-C(3)-C(2)	-0.2(2)	C(8A)-C(7)-C(10A)-F(2A)	-153.0(10)
C(1)-N(2)-C(11)-C(12)	77.9(2)	C(8A)-C(7)-C(10A)-F(3A)	92.0(17)
C(1)-N(2)-C(11)-C(16)	-103.6(2)	C(10)-C(7)-C(8)-C(9)	-178.4(4)
C(2)-N(1)-C(1)-Se(1)	175.72(14)	C(10A)-C(7)-C(8A)-C(9A)	-171.1(8)
C(2)-N(1)-C(1)-N(2)	-0.6(2)	C(11)-N(2)-C(1)-Se(1)	7.8(3)
C(2)-N(1)-C(4)-C(5)	-61.3(4)	C(11)-N(2)-C(1)-N(1)	-175.80(16)
C(2)-N(1)-C(4)-C(5A)	-80.8(4)	C(11)-N(2)-C(3)-C(2)	176.08(17)
C(2)-N(1)-C(4)-C(9)	118.5(4)	C(11)-C(12)-C(13)-C(14)	0.1(3)
C(2)-N(1)-C(4)-C(9A)	100.7(4)	C(12)-C(11)-C(16)-C(15)	0.8(3)
C(3)-N(2)-C(1)-Se(1)	-175.87(14)	C(12)-C(13)-C(14)-C(15)	0.2(3)
C(3)-N(2)-C(1)-N(1)	0.5(2)	C(12)-C(13)-C(14)-C(17)	-177.80(18)
C(3)-N(2)-C(11)-C(12)	-97.9(2)	C(13)-C(14)-C(15)-C(16)	-0.1(3)
C(3)-N(2)-C(11)-C(16)	80.6(2)	C(13)-C(14)-C(17)-F(4)	-146.0(5)
C(4)-N(1)-C(1)-Se(1)	-4.4(3)	C(13)-C(14)-C(17)-F(5)	-22.7(5)
C(4)-N(1)-C(1)-N(2)	179.25(16)	C(13)-C(14)-C(17)-F(6)	96.3(4)
C(4)-N(1)-C(2)-C(3)	-179.34(18)	C(13)-C(14)-C(17)-F(4A)	-123.3(6)
C(4)-C(5)-C(6)-C(7)	1.08(18)	C(13)-C(14)-C(17)-F(5A)	-9.2(8)
C(4)-C(5A)-C(6A)-C(7)	-0.3(2)	C(13)-C(14)-C(17)-F(6A)	113.4(6)
C(4)-C(9A)-C(8A)-C(7)	0.6(6)	C(14)-C(15)-C(16)-C(11)	-0.4(3)
C(5)-C(4)-C(9)-C(8)	-1.4(4)	C(15)-C(14)-C(17)-F(4)	35.9(5)
C(5)-C(6)-C(7)-C(8)	-2.7(4)	C(15)-C(14)-C(17)-F(5)	159.3(5)
C(5)-C(6)-C(7)-C(10)	177.9(4)	C(15)-C(14)-C(17)-F(6)	-81.8(4)
C(6)-C(7)-C(8)-C(9)	2.2(5)	C(15)-C(14)-C(17)-F(4A)	58.7(6)
C(6)-C(7)-C(10)-F(1)	116.2(6)	C(15)-C(14)-C(17)-F(5A)	172.7(7)
C(6)-C(7)-C(10)-F(2)	-6.4(9)	C(15)-C(14)-C(17)-F(6A)	-64.7(6)

Table S13 (*cont.*). Torsion angles [°] for **2h**.

C(6)-C(7)-C(10)-F(3)	-129.7(8)	C(16)-C(11)-C(12)-C(13)	-0.6(3)
C(5A)-C(4)-C(9A)-C(8A)	-0.1(5)	C(17)-C(14)-C(15)-C(16)	177.98(17)

The deviation of atom Se(1) from the plane C(1), N(1), C(2), C(3), N(2) is 0.108(3)Å.

Table S14. Dihedral angles between planes [°] for **2h**.

Plane 1	Plane 2	
C(1), N(1), C(2), C(3), N(2)	C(4), C(5), C(6), C(7), C(8), C(9)	61.2(2)
C(1), N(1), C(2), C(3), N(2)	C(4), C(5A), C(6A), C(7), C(8A), C(9A)	79.8(3)
C(1), N(1), C(2), C(3), N(2)	C(11)…C(17)	79.22(6)
C(4), C(5), C(6), C(7), C(8), C(9)	C(4), C(5A), C(6A), C(7), C(8A), C(9A)	18.6(6)