Supporting Information

Rhodium-catalyzed Cascade Reactions of Triazoles with Organoselenium Compounds – A combined experimental and Mechanistic Study

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General Information

Unless otherwise noted, all commercially available compounds were used as provided without further purification. Chemicals used in this manuscript were purchased from Sigma Aldrich, Alfa Aesar, Fluorochem and Carl Roth.

Solvents used in reactions were p.A. grade. All reactions were performed under argon using degassed solvents. Solvents for chromatography were technical grade and distilled prior to use. Analytical thin-layer chromatography (TLC) was performed on Macherey-Nagel silica gel aluminium plates with F-254 indicator, visualised by irradiation with UV light. Column chromatography was performed using silica gel Merck 60 (particle size 0.063 – 0.2 mm). Solvent mixtures are understood as volume/volume.

^{1}H-NMR, ^{19}F-NMR and ^{13}C-NMR were recorded on a Varian AV600/AV400 or an Agilent DD2 400 NMR spectrometer in $CDCl_3$. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated br (broadened singlet), s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (*J*) are in Hertz (Hz).

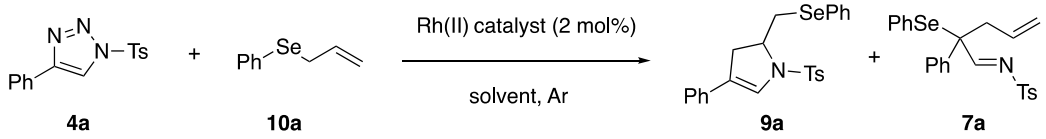
GC/MS were recorded on a Shimadzu GCMS-QP2010 SE Gas chromatograph mass spectrometer. GC column: Optima 5 MS column, 30 m. Carrier gas: Helium.

HRMS data were recorded on a ThermoFisher Scientific LTQ Orbitrap XL using ESI ionization or on a Finnigan MAT 95 using EI ionization at 70 eV.

HPLC was carried out on a JASCO UV- 2077 Plus with a PU-2080 Plus solvent pump. Operation and analysis were under control of JASCO ChromPass software. As chiral columns for determination of enantiomeric excess the following prefabricated columns from Daicel were used: Chiralcel OD-H (250 x 4.6 mm, 5 μm).

Reaction Optimization

Table S1. Optimization table for the cascade reaction of allyl selenide with triazole.



4a **10a** **9a** **7a**

Entry[a]	Catalyst	Solvent	Temperature	Conc. (M)	A:B	Yield(9a/7a) %[b]
1	$Rh_2(OAc)_4$	Toluene	100 °C	0.1	3:1	27 / -
2	$Rh_2(OAc)_4$	Toluene	100 °C	0.1	2:1	32 / -
3	$Rh_2(OAc)_4$	Toluene	100 °C	0.1	1:1	48 / -
4	$Rh_2(OAc)_4$	Toluene	100 °C	0.1	1:2	33 / 35
5	$Rh_2(OAc)_4$	Toluene	100 °C	0.1	1:3	10 / 61
6	$Rh_2(OAc)_4$	Toluene	100 °C	0.05	1:1	31 / 40
7	$Rh_2(OAc)_4$	Toluene	100 °C	0.1	1:1	47 / -
8	**$Rh_2(OAc)_4$**	**Toluene**	**100 °C**	**0.2**	**1:1**	**86 / -**
9	$Rh_2(OAc)_4$	Toluene	100 °C	0.2	1:3	63 / -
10	$Rh_2(OAc)_4$	*m*-xylene	100 °C	0.2	1:1	83 / -
11	$Rh_2(OAc)_4$	1,2-DCE	100 °C	0.2	1:1	65 / -
12	$Rh_2(OAc)_4$	1,4-dioxane	100 °C	0.2	1:1	42 / -
13	$Rh_2(OAc)_4$	MeCN	100 °C	0.2	1:1	*dec.*[c]
14	$Rh_2(Oct)_4$	Toluene	100 °C	0.2	1:1	21 / -
15	$Rh_2(esp)_4$	Toluene	100 °C	0.2	1:1	66 / -
16	$Rh_2(Piv)_4$	Toluene	100 °C	0.2	1:1	72 / -
17	$Rh_2(OAc)_4$	Toluene	80 °C	0.2	1:1	22 / -
18	$Rh_2(OAc)_4$	Toluene	120 °C	0.2	1:1	58 / -

19	$Rh_2(cap)_4$	Toluene	100 °C	0.2	1:1	dec. of **4a**
20	Rh_2(*S*-DOSP)$_4$	Toluene	100 °C	0.2	1:1	62 (*rac*)/ -
21	Rh_2(*S*-BTPCP)$_4$	Toluene	100 °C	0.2	1:1	36 (*rac*)/ -

Reaction condition: a) in an oven dried test tube **4a** (1.0 equiv., 0.2 mmol), **10a** (1.0 equiv.) and catalyst (2 mol%) were dissolved in solvent indicated and heated to 100 °C for 15 hours. b) Isolated yields. c) Decomposition of **4a**.

Experimental Procedures

General procedure for the synthesis of allyl selane (GP-I)[1]

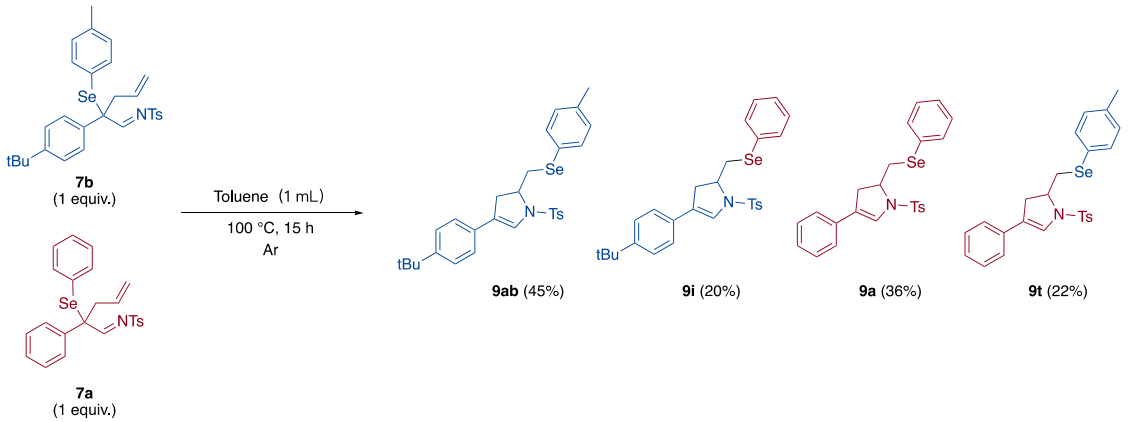
To a suspension of $NaBH_4$ (2.0 Eq.) in EtOH (20 mL) was added a solution of diselenide (5.0 mmol, 1.0 Eq.) in THF (40.0 mL) dropwise under an argon atmosphere. The mixture was kept under agitation at 0 ºC and allyl bromide (10.0 mmol, 2.0 Eq.) in THF (20 mL) was added. After 25 minutes, the reaction mixture was quenched with water and the organic phase was extracted with diethyl ether. The organic layers were combined, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by flash chromatography on silica gel using n-hexane as the eluent.

General procedure for the synthesis of dihydropyrroles (GP-II)

In a test tube and under Argon, the selenide **10** (0.2 mmol, 1.0 equiv.), triazole **4** (1.0 equiv.) and $Rh_2(OAc)_4$ (2 mol%) were dissolved in 1.0 mL toluene and stirred at the 100 °C in a preheated aluminum block for 15 h. Solvent was removed under reduced pressure, the crude reaction mixture was purified by column chromatography using *n*-hexane : ethyl acetate as eluent to afford the final product.

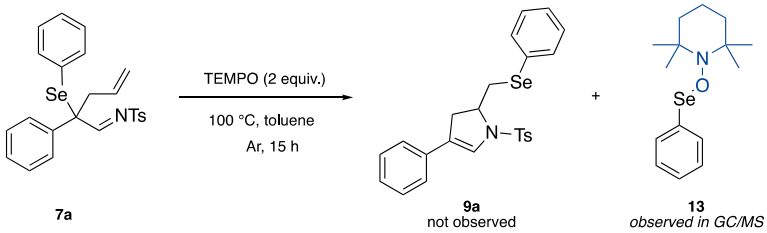
Control Experiments

a) cross-over experiment



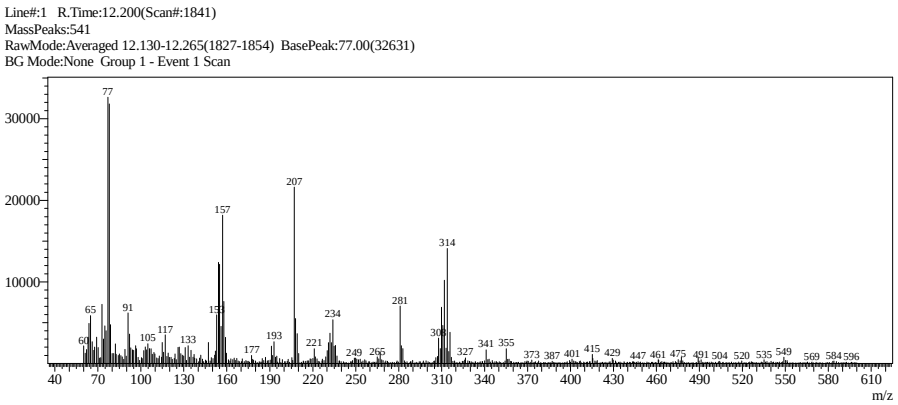
In a test tube and under Argon, the **7a** (0.2 mmol, 1.0 equiv.), **7b** (1.0 equiv.) were dissolved in 1.0 mL toluene and stirred at the 100 °C in a preheated aluminum block for 15 h. Solvent was removed under reduced pressure, and the crude reaction mixture was purified by column chromatography using *n*-hexane : ethyl acetate 40:1 → 10:1 as eluent to afford the final product.

b) TEMPO trapping experiment



In a test tube and under Argon, the **7a** (0.1 mmol), TEMPO (2.0 equiv.) were dissolved in 1.0 mL toluene and stirred at the 100 °C in a preheated aluminum block for 15 h. Solvent was removed under reduced pressure, and from the crude ^{1}H-NMR we have not observed any dihydropyrrole product **9a**. Then we also performed the GC/MS analysis of the crude reaction mixture.

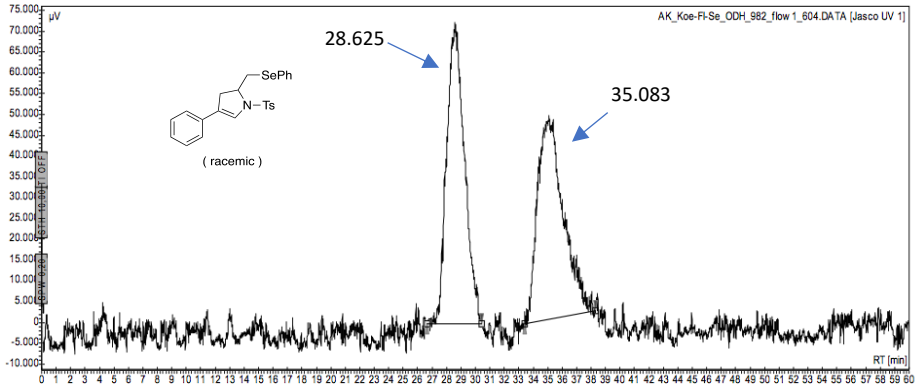
Analysis of the crude reaction mixture by GC/MS.
Method: 120 °C/5 min, 20 K/min, 300 °C/60 min.
Compound **13** was observed using GC/MS at a retention time of 10.130 min.
MS(EI): *m/z*: $[M]^+$ = 312 calc. 314 found, $[M\text{-}C_6H_5]^+$ = 236 calc. 234 found, $[M\text{-}C_9H_{18}NO]^+$ = 157 calc. 157 found, $[M\text{-}C_6H_{18}NOSe]^+$ = 77 calc. 77 found, $[M\text{-}C_{10}H_{19}NOSe]^+$ = 65 calc. 65 found .



Scheme S1. MS spectrum of compound **13**

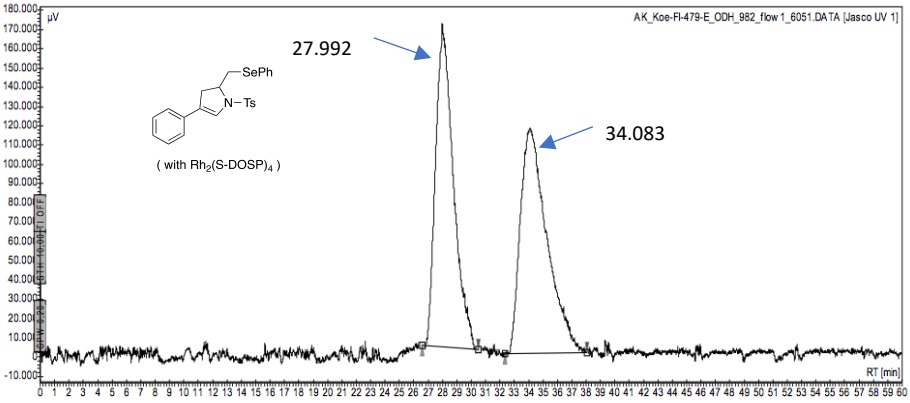
HPLC Spectra

HPLC analysis of **9a**.
Method: OD-H, eluent: Hexanes/i-PrOH = 98/2, 254 nm, flow rate: 1.0 mL/min, T = 25 ºC



AK_Koe-FI-Se_ODH_982_flow1_604.DATA [Jasco UV 1]

Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	26,653	28,625	30,434	50,536
2	33,409	35,083	38,306	49,464
Total				100,000



AK_Koe-FI-479-E_ODH_982_flow1_6051.DATA [Jasco UV 1]

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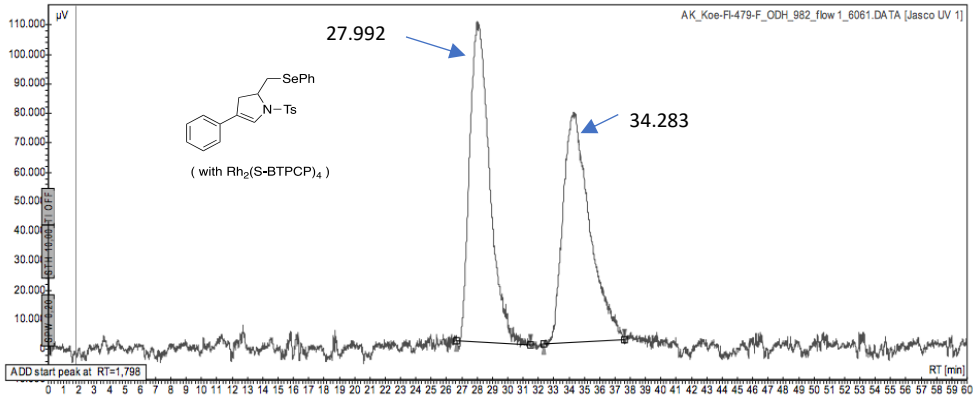
1	26,591	27,992	30,496	48,877
2	32,355	34,083	38,058	51,123
Total				100,000



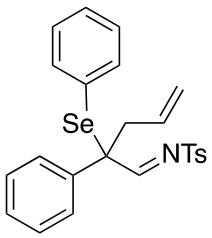
AK_Koe-FI-479-F_ODH_982_flow1_6061.DATA [Jasco UV 1]

Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	26,653	27,992	31,488	50,924
2	32,355	34,283	37,624	49,076
Total				100,000

Scheme S2. Chiral HPLC spectrum of **9a**

Physical Data

(*E*)-4-methyl-*N*-(2-phenyl-2-(phenylselanyl)pent-4-en-1-ylidene)benzenesulfonamide (7a)



Following the general procedure **II**, the selenide **10a** (0.2 mmol, 1.0 equiv.), triazole **4a** (1.0 equiv.) and $Rh_2(OAc)_4$ (2 mol%) were dissolved in 1.0 mL toluene and stirred at the 100 °C in a preheated aluminum block for 2 h. Solvent was removed under reduced pressure, and the crude reaction mixture was purified by silica gel column chromatography using *n*-pentane : ethyl acetate as eluent to afford the colorless oil (61%, 57 mg).

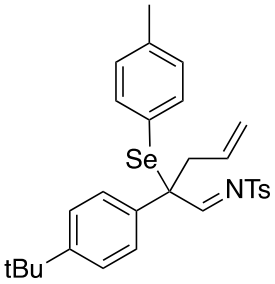
^{1}H NMR (400 MHz, Chloroform-*d*): δ = 8.81 (s, 1H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.20 (m, 10H), 7.14 – 6.97 (m, 2H), 5.55 (ddt, *J* = 17.1, 10.2, 6.9 Hz, 1H), 4.95 – 4.67 (m, 2H), 2.77 (dt, *J* = 7.0, 1.3 Hz, 2H), 2.45 (s, 3H) ppm.

^{13}C NMR (101 MHz, Chloroform-*d*): δ = 171.5, 144.3, 138.3, 137.0, 135.3, 132.7, 129.7, 129.6, 129.0, 128.8, 128.3, 128.1, 127.9, 125.5, 118.8, 58.7, 40.2, 21.6 ppm.

^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 503.20 ppm.

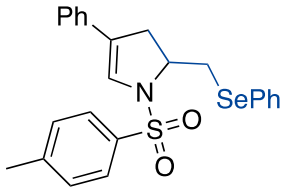
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{23}NSO_2SeNa^+$: 492.0506; Found: 492.0510.

(*E*)-*N*-(2-(4-(*tert*-butyl)phenyl)-2-(*p*-tolylselanyl)pent-4-en-1-ylidene)-4-methylbenzenesulfonamide (7b)



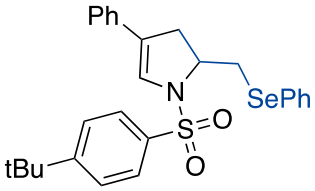
Following the general procedure **II**, the corresponding selenide (0.2 mmol, 1.0 equiv.), triazole (1.0 equiv.) and $Rh_2(OAc)_4$ (2 mol%) were dissolved in 1.0 mL toluene and stirred at the 100 °C in a preheated aluminum block for 2 h. Solvent was removed under reduced pressure, and the crude reaction mixture was purified by silica gel column chromatography using *n*-pentane : ethyl acetate as eluent to afford the colorless oil (65%, 70 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.84 (s, 1H), 7.85 – 7.75 (m, 2H), 7.40 – 7.37 (m, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.29 (m, 2H), 7.25 – 7.20 (m, 2H), 6.88 (d, *J* = 7.6 Hz, 2H), 5.68 – 5.54 (m, 1H), 5.00 – 4.77 (m, 2H), 2.79 (d, *J* = 6.9 Hz, 2H), 2.50 (s, 3H), 2.29 (s, 3H), 1.34 (s, 9H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 171.7, 151.4, 144.2, 139.9, 138.3, 135.6, 133.8, 133.2, 129.8, 129.6, 127.9, 127.8, 125.8, 122.4, 118.5, 58.5, 39.6, 34.6, 31.2, 21.6, 21.3 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 489.68 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{29}H_{23}NSO_2SeNa^+$: 562.1289; Found: 562.1269.

4-phenyl-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9a)



The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (86%, 80 mg).
^{1}H NMR (400 MHz, Chloroform-*d*): δ = 7.62 – 7.56 (m, 2H), 7.46 – 7.39 (m, 2H), 7.32 (dd, *J* = 5.0, 1.7 Hz, 3H), 7.29 – 7.24 (m, 2H), 7.23 – 7.18 (m, 3H), 7.18 – 7.13 (m, 2H), 6.81 (t, *J* = 1.8 Hz, 1H), 3.89 – 3.76 (m, 1H), 3.71 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.08 – 2.87 (m, 2H), 2.77 – 2.58 (m, 1H), 2.35 (s, 2H) ppm.
^{13}C NMR (101 MHz, Chloroform-*d*): δ = 143.8, 133.4, 132.99, 132.94, 129.7, 129.2, 128.57, 128.50, 127.4, 127.24, 127.22, 124.7, 123.6, 59.6, 37.3, 33.1, 21.5 ppm. Due to the overlap of aromatic carbon peaks, one carbon signal is missing.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.07 (d, *J* = 24.7 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{23}NSO_2SeNa^+$: 492.0506; Found: 492.0493.

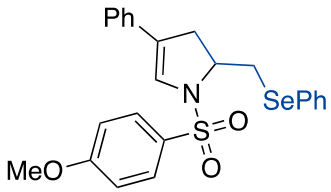
1-((4-(*tert*-butyl)phenyl)sulfonyl)-4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrole (9b)



The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 60:1 → 20:1 as light yellow solid (70%, 71 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.65 – 7.61 (m, 2H), 7.56 – 7.50 (m, 2H), 7.44 – 7.40 (m, 2H), 7.38 – 7.35 (m, 3H), 7.33 (m, 2H), 7.28 – 7.22 (m, 3H), 6.90 (t, *J* = 1.8 Hz, 1H), 3.91 (m, 1H), 3.76 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.09 – 2.94 (m, 2H), 2.75 (m, 1H), 1.32 (s, 9H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 156.7, 133.5, 133.1, 132.9, 129.3, 128.67, 128.63, 127.29, 127.26, 127.23, 126.1, 124.8, 124.7, 123.3, 59.7, 37.4, 35.1, 33.1, 31.0 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 259.91 ppm.

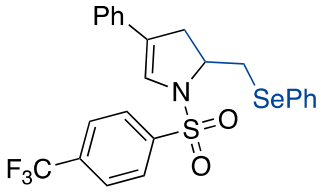
HRMS (ESI): m/z: $[M+H]^+$ Calcd. for $C_{27}H_{30}NSO_2Se^+$: 512.1157; Found: 512.1144.

1-((4-methoxyphenyl)sulfonyl)-4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrole (9c)



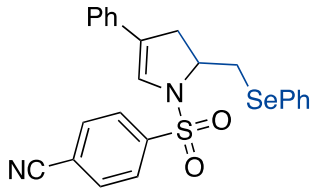
The titled compound was synthesized according to the general procedure **GP-II,** and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as light yellow solid (54%, 52 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.66 – 7.61 (m, 2H), 7.53 – 7.48 (m, 2H), 7.38 – 7.34 (m, 3H), 7.32 (m, 2H), 7.27 – 7.21 (m, 3H), 6.87 (m, 1H), 6.85 (m, 2H), 3.84 (m, 4H), 3.74 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.08 – 2.93 (m, 1H), 2.73 (m, 1H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 163.1, 133.5, 133.0, 129.5, 129.3, 128.6, 128.5, 127.6, 127.28, 127.24, 124.8, 124.7, 123.7, 114.3, 59.7, 55.5, 37.3, 33.2 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.39 (d, *J* = 24.9 Hz).
HRMS (ESI): m/z: $[M]^+$ Calcd. for $C_{24}H_{23}NSO_3Se^+$: 485.0558; Found: 485.0551.

4-phenyl-2-((phenylselanyl)methyl)-1-((4-(trifluoromethyl)phenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole (9d)



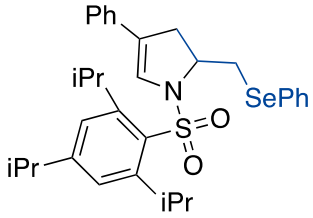
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as white solid (81%, 85 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.67 (s, 4H), 7.66 – 7.62 (m, 2H), 7.38 (m, 3H), 7.34 – 7.31 (m, 2H), 7.28 – 7.23 (m, 3H), 6.86 (t, *J* = 1.8 Hz, 1H), 3.83 (m, 1H), 3.74 (dd, *J* = 12.5, 3.0 Hz, 1H), 3.07 – 2.96 (m, 2H), 2.78 (m, 1H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 139.5, 134.6 (q, *J* = 33.1 Hz), 133.3, 132.9, 129.3, 128.6, 128.2, 127.8, 127.6, 127.5, 126.2 (q, *J* = 3.6 Hz), 124.8, 124.6, 123.8, 123.0 (q, *J* = 273.0 Hz), 59.8, 37.3, 33.1 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -63.17 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 264.14 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{20}NF_3SO_2SeNa^+$: 546.0224; Found: 546.0210.

4-((4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrol-1-yl)sulfonyl)benzonitrile (9e)



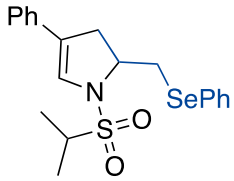
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as light yellow solid (65%, 63 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.62 – 7.57 (m, 2H), 7.55 – 7.48 (m, 4H), 7.32 – 7.25 (m, 3H), 7.25 – 7.20 (m, 2H), 7.19 – 7.13 (m, 3H), 6.73 (t, *J* = 1.8 Hz, 1H), 3.75 – 3.66 (m, 1H), 3.62 (dd, *J* = 12.6, 3.0 Hz, 1H), 2.97 – 2.81 (m, 2H), 2.73 – 2.59 (m, 1H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 140.1, 133.4, 132.87, 132.83, 129.4, 128.7, 128.1, 127.9, 127.7, 127.6, 125.0, 124.8, 123.5, 117.1, 116.7, 59.9, 37.3, 33.0 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 265.52 (d, *J* = 25.6 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{20}N_2SO_2SeNa^+$: 503.0302; Found: 503.0278.

4-phenyl-2-((phenylselanyl)methyl)-1-((2,4,6-triisopropylphenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole (9f)



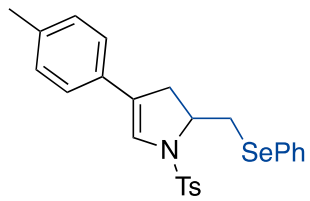
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 20:1 as colorless oil (24%, 28 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.45 – 7.40 (m, 2H), 7.25 – 7.22 (m, 2H), 7.22 – 7.19 (m, 3H), 7.18 – 7.13 (m, 3H), 7.12 (m, 2H), 6.66 (t, *J* = 1.8 Hz, 1H), 4.51 – 4.38 (m, 1H), 4.12 (p, *J* = 6.7 Hz, 2H), 3.33 (dd, *J* = 12.2, 3.3 Hz, 1H), 3.16 (m, 1H), 3.00 (dd, *J* = 12.2, 10.4 Hz, 1H), 2.85 (p, *J* = 6.9 Hz, 1H), 2.77 (m, 1H), 1.21 (d, *J* = 6.9 Hz, 6H), 1.18 (d, *J* = 6.8 Hz, 6H), 1.14 (d, *J* = 6.8 Hz, 6H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 153.6, 151.4, 133.7, 132.3, 131.0, 129.25, 129.23, 128.5, 127.1, 126.9, 124.6, 124.2, 122.5, 59.3, 37.3, 34.1, 32.9, 29.8, 25.0, 24.7, 23.5 ppm. Due to the overlap of aromatic carbon peaks, one carbon signal is missing.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 254.11 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{32}H_{39}NSO_2SeNa^+$: 604.1758; Found: 604.1750.

1-(isopropylsulfonyl)-4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrole (9g)



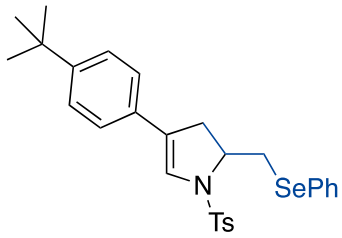
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (32%, 27 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.61 – 7.54 (m, 2H), 7.34 (m, 2H), 7.32 – 7.28 (m, 5H), 7.26 – 7.22 (m, 1H), 6.78 (t, *J* = 2.3 Hz, 1H), 4.44 (tt, *J* = 10.2, 3.7 Hz, 1H), 3.60 (dd, *J* = 12.5, 3.2 Hz, 1H), 3.38 – 3.24 (m, 2H), 3.06 (dd, *J* = 12.5, 10.3 Hz, 1H), 2.94 (m, 1H), 1.39 (d, *J* = 2.6 Hz, 3H), 1.37 (d, *J* = 2.7 Hz, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 133.6, 132.0, 129.3, 128.9, 128.6, 127.02, 127.01, 125.0, 124.5, 120.6, 60.5, 54.2, 36.8, 32.8, 16.8 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 251.53 (d, *J* = 21.5 Hz) ppm.
HRMS (ESI): m/z: $[M+H]^+$ Calcd. for $C_{20}H_{24}NSO_2Se^+$: 422.0687; Found: 422.0676.

2-((phenylselanyl)methyl)-4-(*p*-tolyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9h)



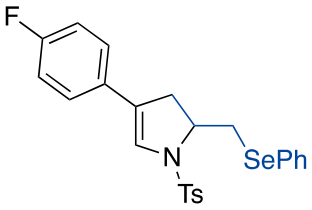
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as white solid (73%, 70 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.65 – 7.58 (m, 2H), 7.49 – 7.43 (m, 2H), 7.39 – 7.33 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.09 (m, 4H), 6.85 (t, *J* = 1.8 Hz, 1H), 3.89 – 3.82 (m, 1H), 3.74 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.00 (dd, *J* = 12.5, 10.8 Hz, 1H), 2.97 – 2.90 (m, 1H), 2.74 – 2.67 (m, 1H), 2.38 (s, 3H), 2.35 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 143.8, 137.1, 133.0, 132.9, 130.5, 129.7, 129.28, 129.26, 128.6, 127.4, 127.2, 124.7, 123.9, 123.8, 59.6, 37.3, 33.2, 21.5, 21.1 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.76 (d, *J* = 24.8 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_2SeNa^+$: 506.0663; Found: 506.0649.

4-(4-(*tert*-butyl)phenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9i)



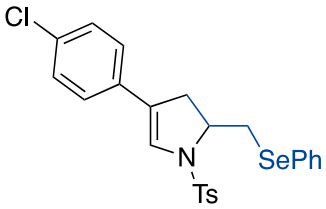
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (82%, 86 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.66 – 7.59 (m, 2H), 7.50 – 7.45 (m, 2H), 7.40 – 7.32 (m, 5H), 7.20 (dd, *J* = 8.4, 7.1 Hz, 4H), 6.83 (t, *J* = 1.9 Hz, 1H), 3.93 – 3.83 (m, 1H), 3.73 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.07 – 2.88 (m, 2H), 2.77 – 2.66 (m, 1H), 2.39 (s, 3H), 1.33 (s, 9H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 150.5, 143.8, 133.0, 132.9, 130.6, 129.7, 129.3, 128.6, 127.4, 127.2, 125.5, 124.5, 124.0, 123.7, 59.6, 37.3, 34.6, 33.2, 31.2, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.22 (d, *J* = 24.7 Hz) ppm.
HRMS (ESI): m/z: $[M+H]^+$ Calcd. for $C_{28}H_{32}NSO_2Se^+$: 526.1313; Found: 526.1302.

4-(4-fluorophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9j)



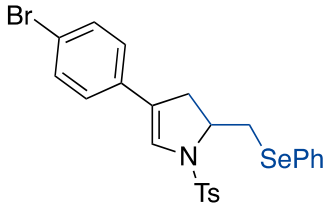
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (62%, 60 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.64 – 7.60 (m, 2H), 7.48 – 7.44 (m, 2H), 7.38 – 7.32 (m, 3H), 7.23 – 7.17 (m, 4H), 7.04 – 6.97 (m, 2H), 6.78 (t, *J* = 1.9 Hz, 1H), 3.93 – 3.83 (m, 1H), 3.74 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.00 (dd, *J* = 12.5, 10.8 Hz, 1H), 2.97 – 2.90 (m, 1H), 2.76 – 2.64 (m, 1H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 161.9 (d, *J* = 247.5 Hz), 143.9, 133.0, 129.7, 129.6 (d, *J* = 3.5 Hz), 129.3, 128.4, 127.4, 127.3, 126.3 (d, *J* = 7.9 Hz), 124.48, 124.47, 122.6, 115.5 (d, *J* = 21.7 Hz), 59.7, 37.5, 33.1, 21.5 ppm.
^{19}F NMR (376 MHz, Chloroform-*d*): δ = -114.31 (t, *J* = 5.0 Hz) ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.96 (d, *J* = 24.2 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{22}NFSO_2SeNa^+$: 510.0412; Found: 510.0398.

4-(4-chlorophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9k)



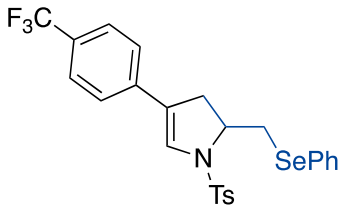
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (73%, 73 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.65 – 7.59 (m, 2H), 7.47 – 7.42 (m, 2H), 7.38 – 7.33 (m, 3H), 7.31 – 7.25 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.18 – 7.14 (m, 2H), 6.84 (t, *J* = 1.8 Hz, 1H), 3.92 – 3.82 (m, 1H), 3.74 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.07 – 2.90 (m, 2H), 2.77 – 2.61 (m, 1H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.0, 133.04, 133.02, 132.8, 131.9, 129.7, 129.3, 128.7, 128.4, 127.4, 127.3, 125.9, 125.3, 122.4, 59.7, 37.3, 33.1, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.23 (d, *J* = 24.9 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{22}NSClO_2SeNa^+$: 526.0117; Found: 526.0098.

4-(4-bromophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9l)



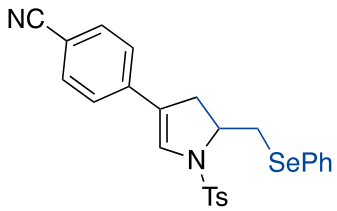
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (75%, 82 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.68 – 7.57 (m, 2H), 7.50 – 7.39 (m, 4H), 7.39 – 7.32 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.13 – 7.06 (m, 2H), 6.86 (t, *J* = 1.8 Hz, 1H), 3.92 – 3.81 (m, 1H), 3.74 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.06 – 2.88 (m, 2H), 2.76 – 2.63 (m, 1H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.0, 133.05, 133.01, 132.4, 131.6, 129.7, 129.3, 128.4, 127.4, 127.3, 126.2, 125.4, 122.4, 120.8, 59.7, 37.2, 33.1, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.30 (d, *J* = 24.6 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{22}NSO_2BrSeNa^+$: 569.9612; Found: 569.9595.

2-((phenylselanyl)methyl)-1-tosyl-4-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1*H*-pyrrole (9m)



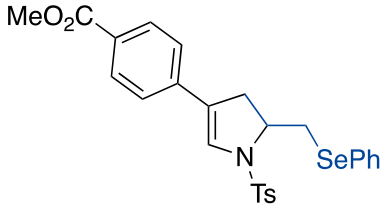
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (71%, 76 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.64 – 7.61 (m, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.39 – 7.35 (m, 3H), 7.34 – 7.31 (m, 2H), 7.23 – 7.19 (m, 2H), 6.97 (t, *J* = 1.8 Hz, 1H), 3.90 (m, 1H), 3.75 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.08 – 2.92 (m, 2H), 2.74 (m, 1H), 2.40 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.1, 137.0, 133.1, 133.0, 129.8, 129.3, 128.8 (d, *J* = 32.6 Hz), 128.3, 127.4, 127.3, 127.0, 125.5 (q, *J* = 3.8 Hz), 124.7, 124.0 (d, *J* = 271.9 Hz), 121.9, 59.8, 37.2, 33.1, 21.5 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -62.54 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.50 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{22}NF_3SO_2SeNa^+$: 560.0380; Found: 560.0367

4-(4-isocyanophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9n)



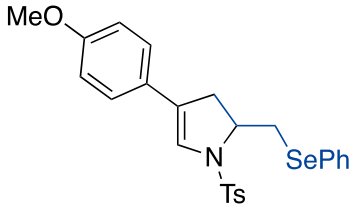
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as light yellow solid (66%, 65 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.57 – 7.50 (m, 2H), 7.50 – 7.46 (m, 2H), 7.39 – 7.32 (m, 2H), 7.28 – 7.27 (m, 2H), 7.23 – 7.17 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.92 (t, *J* = 1.7 Hz, 1H), 3.87 – 3.76 (m, 1H), 3.65 (dd, *J* = 12.6, 2.9 Hz, 1H), 2.98 – 2.84 (m, 2H), 2.72 – 2.59 (m, 1H), 2.31 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.2, 138.1, 133.1, 133.0, 132.3, 129.9, 129.3, 128.3, 128.2, 127.4, 127.3, 124.9, 121.2, 118.8, 110.0, 59.9, 37.1, 33.0, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.69 (d, *J* = 25.3 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{22}N_2SO_2SeNa^+$: 517.0459; Found: 517.0449.

methyl 4-(5-((phenylselanyl)methyl)-1-tosyl-4,5-dihydro-1*H*-pyrrol-3-yl)benzoate (9o)



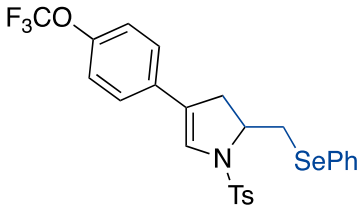
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 20:1 → 4:1 as colorless oil (61%, 65 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.87 (dd, *J* = 8.4, 1.6 Hz, 2H), 7.58 – 7.47 (m, 2H), 7.42 – 7.33 (m, 2H), 7.30 – 7.22 (m, 2H), 7.23 – 7.15 (m, 3H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.89 (t, *J* = 1.7 Hz, 1H), 3.83 (s, 3H), 3.82 – 3.77 (m, 1H), 3.65 (dd, *J* = 12.6, 3.0 Hz, 1H), 2.97 – 2.83 (m, 2H), 2.71 – 2.61 (m, 1H), 2.30 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 166.6, 144.1, 138.0, 133.12, 133.10, 129.89, 129.84, 129.3, 128.42, 128.40, 127.38, 127.37, 127.2, 124.4, 122.2, 59.8, 52.1, 37.2, 33.1, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.76 (d, *J* = 24.6 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{26}H_{25}NSO_4SeNa^+$: 550.0561; Found: 526.0551.

4-(4-methoxyphenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9p)



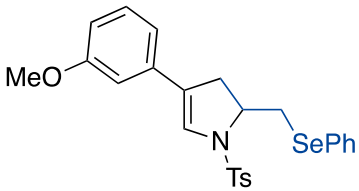
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 20:1 → 4:1 as colorless oil (43%, 43 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.56 – 7.50 (m, 2H), 7.40 – 7.35 (m, 2H), 7.30 – 7.24 (m, 3H), 7.12 – 7.02 (m, 4H), 6.79 – 6.70 (m, 2H), 6.62 (t, *J* = 1.8 Hz, 1H), 3.79 – 3.74 (m, 1H), 3.72 (s, 3H), 3.64 (dd, *J* = 12.5, 3.1 Hz, 1H), 2.91 (dd, *J* = 12.5, 10.8 Hz, 1H), 2.86 – 2.78 (m, 1H), 2.63 – 2.56 (m, 1H), 2.29 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 158.9, 143.7, 133.0, 132.9, 129.6, 129.2, 128.6, 127.4, 127.2, 126.1, 126.0, 123.6, 122.9, 114.0, 59.6, 55.3, 37.4, 33.2, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.62 (d, *J* = 26.2 Hz) ppm.
HRMS (ESI): m/z: $[M]^+$ Calcd. for $C_{25}H_{25}NSO_3^+$: 499.0714; Found: 499.0720.

2-((phenylselanyl)methyl)-1-tosyl-4-(4-(trifluoromethoxy)phenyl)-2,3-dihydro-1*H*-pyrrole (9q)



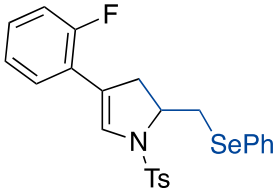
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (58%, 64 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.67 – 7.56 (m, 2H), 7.49 – 7.41 (m, 2H), 7.40 – 7.33 (m, 3H), 7.27 – 7.23 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.85 (t, *J* = 1.8 Hz, 1H), 3.93 – 3.84 (m, 1H), 3.74 (dd, *J* = 12.5, 3.0 Hz, 1H), 3.07 – 2.90 (m, 2H), 2.76 – 2.66 (m, 1H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 148.08, 148.07, 144.0, 133.0, 132.3, 129.7, 129.3, 128.4, 127.4, 127.3, 125.9, 125.5, 122.1, 121.1, 120.4 (q, *J* = 257.3 Hz), 59.7, 37.4, 33.1, 21.5 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*) δ = -57.92 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.94 (d, *J* = 24.1 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{22}NF_3SO_3SeNa^+$: 576.0329; Found: 576.0317.

4-(3-methoxyphenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9r)



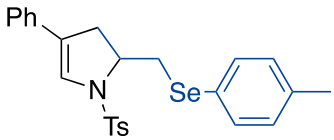
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 20:1 → 4:1 as colorless oil (69%, 69 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.56 – 7.48 (m, 2H), 7.39 – 7.34 (m, 2H), 7.30 – 7.22 (m, 3H), 7.16 – 7.07 (m, 3H), 6.78 – 6.73 (m, 2H), 6.69 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.67 – 6.65 (m, 1H), 3.82 – 3.73 (m, 1H), 3.73 (s, 3H), 3.64 (dd, *J* = 12.5, 3.0 Hz, 1H), 2.95 – 2.83 (m, 2H), 2.67 – 2.57 (m, 1H), 2.29 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 159.7, 143.9, 134.8, 133.0, 132.9, 129.7, 129.5, 129.2, 128.5, 127.4, 127.2, 125.1, 123.5, 117.3, 112.6, 110.4, 59.7, 55.2, 37.4, 33.2, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.94 (d, *J* = 24.6 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_3SeNa^+$: 522.0612; Found: 522.0601.

4-(2-fluorophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9s)



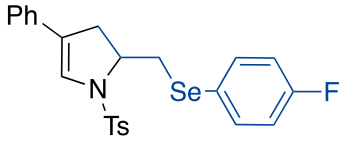
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as light yellow solid (75%, 73 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.56 – 7.51 (m, 2H), 7.41 – 7.37 (m, 2H), 7.30 – 7.23 (m, 3H), 7.14 – 7.05 (m, 3H), 7.02 – 6.91 (m, 4H), 3.77 – 3.70 (m, 1H), 3.68 (dd, *J* = 12.5, 3.0 Hz, 1H), 2.96 – 2.85 (m, 2H), 2.72 – 2.63 (m, 1H), 2.29 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 160.2 (d, *J* = 250.8 Hz), 143.9, 133.05, 133.02, 129.7, 129.3, 129.2, 128.5, 127.9 (d, *J* = 8.5 Hz), 127.4, 127.3, 127.2, 124.1 (d, *J* = 3.3 Hz), 121.7 (d, *J* = 13.2 Hz), 117.2 (d, *J* = 3.2 Hz), 115.7 (d, *J* = 22.4 Hz), 58.7, 38.1, 33.2, 21.5 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*) δ = -110.08 (dd, *J* = 12.3, 6.2 Hz) ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 261.03 (d, *J* = 25.0 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{22}NFSO_2SeNa^+$: 510.0412; Found: 510.0402.

4-phenyl-2-((*p*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9t)



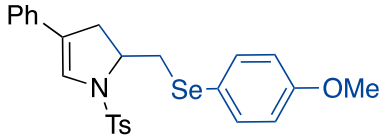
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as white solid (62%, 60 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.54 – 7.50 (m, 2H), 7.47 – 7.43 (m, 2H), 7.34 – 7.29 (m, 2H), 7.26 – 7.21 (m, 3H), 7.20 – 7.15 (m, 4H), 6.85 (t, *J* = 1.8 Hz, 1H), 3.88 – 3.79 (m, 1H), 3.69 (dd, *J* = 12.4, 3.1 Hz, 1H), 3.02 – 2.89 (m, 2H), 2.78 – 2.67 (m, 1H), 2.42 (s, 3H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 143.8, 137.3, 133.5, 133.0, 130.0, 129.6, 128.5, 127.4, 127.2, 124.8, 124.7, 124.6, 123.6, 59.7, 37.3, 33.4, 21.5, 21.1 ppm. Due to the overlap of aromatic carbon peaks, one carbon signal is missing.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 253.76 (d, *J* = 24.3 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_2SeNa^+$: 506.0663; Found: 506.0662.

2-(((4-fluorophenyl)selanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (9u)



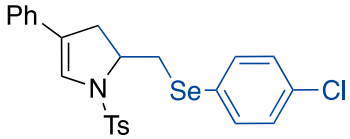
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as white solid (70%, 69 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.53 – 7.48 (m, 2H), 7.38 – 7.33 (m, 2H), 7.25 – 7.20 (m, 2H), 7.17 – 7.10 (m, 5H), 7.00 – 6.94 (m, 2H), 6.76 (t, *J* = 1.8 Hz, 1H), 3.75 – 3.66 (m, 1H), 3.56 (dd, *J* = 12.5, 3.1 Hz, 1H), 2.97 – 2.83 (m, 2H), 2.68 – 2.57 (m, 1H), 2.30 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 162.6 (d, *J* = 247.5 Hz), 144.0, 135.6 (d, *J* = 7.8 Hz), 133.4, 133.0, 129.7, 128.6, 127.3, 127.2, 124.8, 124.7, 123.6, 122.8 (d, *J* = 3.4 Hz), 116.4 (d, *J* = 21.4 Hz), 59.6, 37.3, 34.0, 21.5 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -114.20 (d, *J* = 5.0 Hz) ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 257.54 (d, *J* = 25.6 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{22}NFSO_2SeNa^+$: 510.0412; Found: 510.0392.

2-(((4-methoxyphenyl)selanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (9v)



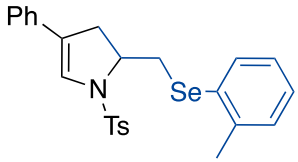
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as white solid (58%, 58 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.58 – 7.54 (m, 2H), 7.43 – 7.37 (m, 2H), 7.34 – 7.29 (m, 2H), 7.27 – 7.21 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.94 – 6.89 (m, 2H), 6.85 (t, *J* = 1.8 Hz, 1H), 3.88 (s, 3H), 3.82 – 3.73 (m, 1H), 3.64 (dd, *J* = 12.3, 3.1 Hz, 1H), 3.04 – 2.87 (m, 2H), 2.77 – 2.68 (m, 1H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 159.6, 143.8, 135.9, 133.5, 132.9, 129.6, 128.5, 127.4, 127.2, 124.9, 124.7, 123.5, 118.1, 114.9, 59.8, 55.3, 37.3, 34.1, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 251.59 (d, *J* = 25.4 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_3SeNa^+$: 522.0612; Found: 522.0603.

2-(((4-chlorophenyl)selanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (9w)



The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as white solid (57%, 58 mg).
^{1}H NMR (400 MHz, Chloroform-*d*): δ = 7.53 – 7.48 (m, 2H), 7.44 – 7.39 (m, 2H), 7.31 – 7.26 (m, 4H), 7.23 – 7.16 (m, 5H), 6.82 (t, *J* = 1.9 Hz, 1H), 3.81 – 3.70 (m, 1H), 3.66 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.03 – 2.85 (m, 2H), 2.72 – 2.62 (m, 1H), 2.36 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.0, 134.5, 133.6, 133.3, 132.9, 129.8, 129.4, 128.6, 127.38, 127.31, 126.6, 124.8, 124.7, 123.6, 59.5, 37.3, 33.6, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 260.59 (d, *J* = 25.3 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{22}NClSO_2SeNa^+$: 526.0117; Found: 526.0114.

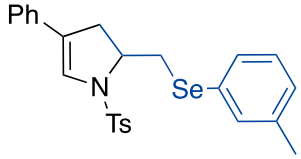
4-phenyl-2-((*o*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9x)



The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (46%, 45 mg).

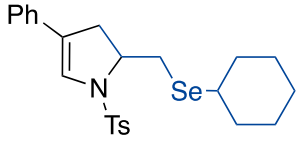
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.70 – 7.61 (m, 1H), 7.53 – 7.44 (m, 2H), 7.34 – 7.30 (m, 2H), 7.28 – 7.19 (m, 8H), 6.86 (t, *J* = 1.9 Hz, 1H), 3.92 – 3.83 (m, 1H), 3.71 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.05 – 2.91 (m, 2H), 2.79 – 2.70 (m, 1H), 2.47 (s, 3H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 143.8, 139.9, 133.4, 133.1, 132.3, 130.2, 129.7, 129.4, 128.5, 127.4, 127.26, 127.24, 126.6, 124.76, 124.72, 123.6, 59.5, 37.4, 32.0, 22.3, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 213.99 (d, *J* = 24.1 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_2SeNa^+$: 506.0663; Found: 506.0655.

4-phenyl-2-((*m*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9y)



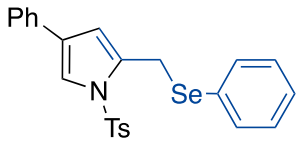
The titled compound was synthesized according to the general procedure **GP-II** and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (64%, 62 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.50 – 7.47 (m, 2H), 7.45 (s, 1H), 7.43 – 7.39 (m, 1H), 7.34 – 7.29 (m, 2H), 7.27 – 7.23 (m, 4H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.17 – 7.13 (m, 1H), 6.86 (t, *J* = 1.8 Hz, 1H), 3.94 – 3.83 (m, 1H), 3.74 (dd, *J* = 12.5, 3.1 Hz, 1H), 3.05 – 2.88 (m, 2H), 2.79 – 2.66 (m, 1H), 2.40 (s, 3H), 2.39 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 143.8, 139.1, 133.4, 133.2, 133.1, 129.76, 129.72, 129.0, 128.5, 128.3, 128.0, 127.4, 127.2, 124.7, 123.7, 59.7, 37.3, 33.0, 21.5, 21.2 ppm. Due to the overlap of aromatic carbon peaks, one carbon signal is missing.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 257.92 (d, *J* = 25.3 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_2SeNa^+$: 506.0663; Found: 506.0655.

2-((cyclohexylselanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole (9z)



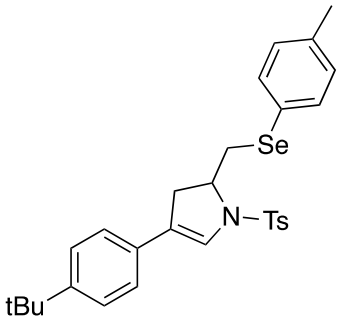
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 60:1 → 20:1 as colorless oil (55%, 52 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): 7.63 – 7.53 (m, 2H), 7.26 – 7.20 (m, 4H), 7.19 – 7.17 (m, 2H), 7.16 – 7.11 (m, 1H), 6.78 (t, *J* = 1.9 Hz, 1H), 3.98 – 3.86 (m, 1H), 3.14 (dd, *J* = 12.2, 3.3 Hz, 1H), 3.01 – 2.93 (m, 1H), 2.91 – 2.84 (m, 1H), 2.78 (dd, *J* = 12.2, 10.5 Hz, 1H), 2.63 – 2.57 (m, 1H), 2.34 (s, 3H), 2.08 – 1.92 (m, 2H), 1.78 – 1.65 (m, 2H), 1.62 – 1.56 (m, 1H), 1.47 – 1.40 (m, 2H), 1.35 – 1.21 (m, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 144.01, 133.6, 133.5, 129.8, 128.6, 127.4, 127.2, 124.7, 124.6, 123.7, 60.6, 39.4, 37.4, 34.7, 34.6, 28.6, 26.9, 25.8, 21.5 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{24}H_{29}NSO_2SeNa^+$: 498.09764; Found: 498.09796.

4-phenyl-2-((phenylselanyl)methyl)-1-tosyl-1*H*-pyrrole (9aa)



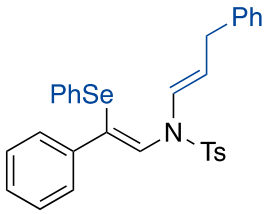
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (20%, 19 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.65 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.38 – 7.29 (m, 10H), 6.99 (s, 1H), 6.51 (s, 1H), 4.28 (d, *J* = 1.5 Hz, 2H), 2.46 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.1, 136.6, 134.9, 133.4, 129.8, 129.5, 128.7, 128.0, 127.4, 127.3, 127.2, 127.01, 124.9, 122.3, 122.2, 120.1, 48.8, 21.6 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 428.85 ppm.
HRMS (ESI): m/z: $[M-C_7H_8O_2S]^+$ Calcd. for $C_{17}H_{14}NSe^+$: 312.02860 ; Found: 312.02911.

4-(4-(*tert*-butyl)phenyl)-2-((*p*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9ab)



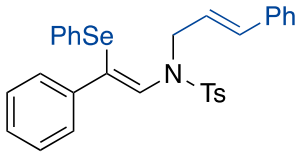
The titled compound was synthesized according to the general procedure **GP-II** and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 20:1 as colorless oil (45%, 48 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.51 (d, *J* = 8.1 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.36 – 7.32 (m, 2H), 7.22 – 7.15 (m, 6H), 6.82 – 6.79 (m, 1H), 3.83 (tdd, *J* = 10.5, 5.6, 3.1 Hz, 1H), 3.68 (dd, *J* = 12.4, 3.1 Hz, 1H), 3.02 – 2.85 (m, 2H), 2.76 – 2.60 (m, 1H), 2.41 (s, 3H), 2.39 (s, 3H), 1.32 (s, 9H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ =150.4, 143.7, 137.3, 133.4, 133.0, 130.6, 130.0, 129.6, 127.4, 125.5, 124.6, 124.5, 124.0, 123.7, 59.7, 37.2, 34.5, 33.5, 31.2, 21.5, 21.1 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 253.08 (d, *J* = 25.3 Hz) ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{29}H_{33}NSO_2SeNa^+$: 562.1289; Found: 562.1268.

4-methyl-*N*-((*Z*)-2-phenyl-2-(phenylselanyl)vinyl)-*N*-((*E*)-3-phenylprop-1-en-1-yl)benzenesulfonamide (8a')



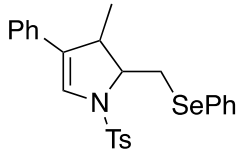
The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (29%, 31 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.77 – 7.62 (m, 2H), 7.34 – 7.25 (m, 6H), 7.24 – 7.21 (m, 1H), 7.16 – 6.98 (m, 10H), 6.89 (s, 1H), 5.89 (d, *J* = 15.8 Hz, 1H), 5.56 (dt, *J* = 15.9, 6.5 Hz, 1H), 3.76 (dd, *J* = 6.6, 1.4 Hz, 2H), 2.44 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 144.0, 137.9, 136.2, 135.9, 133.5, 132.4, 130.5, 129.8, 129.4, 128.9, 128.7, 128.5, 128.1, 127.9, 127.8, 127.4, 127.1, 126.4, 125.0, 123.3, 50.0, 21.6 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 482.05 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{30}H_{27}NSO_2SeNa^+$: 568.0819; Found: 568.0810.

***N*-cinnamyl-4-methyl-*N*-((*Z*)-2-phenyl-2-(phenylselanyl)vinyl)benzenesulfonamide (8a)**



The titled compound was synthesized according to the general procedure **GP-II**, and was obtained after silica gel column chromatography using *n*-hexane : ethyl acetate = 40:1 → 10:1 as colorless oil (30%, 33 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.77 (d, *J* = 8.3 Hz, 2H), 7.40 – 7.24 (m, 9H), 7.15 – 7.06 (m, 5H), 7.05 – 6.98 (m, 1H), 6.90 (t, *J* = 7.7 Hz, 2H), 6.64 – 6.54 (m, 1H), 6.29 (dt, *J* = 15.8, 6.7 Hz, 1H), 6.14 (s, 1H), 4.23 (dd, *J* = 6.7, 1.4 Hz, 2H), 2.45 (s, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 143.8, 141.0, 138.0, 136.3, 135.4, 134.0, 133.3, 129.7, 129.5, 128.9, 128.6, 128.5, 128.1, 127.93, 127.90, 127.7, 126.88, 126.87, 126.5, 123.8, 52.4, 21.5 ppm.
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 411.11 ppm.
HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{30}H_{27}NSO_2SeNa^+$: 568.0819; Found: 568.0812.

3-methyl-4-phenyl-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (15)



Following the general procedure **II**, the selenide **14** (0.2 mmol, 1.0 equiv.), triazole **4a** (1.0 equiv.) and $Rh_2(OAc)_4$ (2 mol%) were dissolved in 1.0 mL toluene and stirred at the 100 °C in a preheated aluminum block for 15 h. Solvent was removed under reduced pressure, and the crude reaction mixture was purified by silica gel column chromatography using *n*-pentane : ethyl acetate as eluent to afford the colorless oil (60%, 57 mg, d.r. = 1:1).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.69 – 7.64 (m, 2H), 7.63 – 7.59 (m, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.42 – 7.38 (m, 1H), 7.38 – 7.33 (m, 5H), 7.32 – 7.22 (m, 10H), 7.22 – 7.17 (m, 4H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.78 (s, 1H), 6.73 (s, 1H), 3.99 – 3.90 (m, 1H), 3.59 – 3.54 (m, 1H), 3.52 – 3.45 (m, 2H), 3.43 – 3.37 (m, 1H), 3.26 – 3.17 (m, 1H), 3.13 – 3.06 (m, 1H), 2.92 (dd, *J* = 12.6, 11.2 Hz, 1H), 2.35 (s, 3H), 2.34 (s, 3H), 1.12 (d, *J* = 6.0 Hz, 3H), 0.43 (d, *J* = 6.9 Hz, 3H) ppm.

^{13}C NMR (151 MHz, Chloroform-*d*): δ = 143.8, 134.2, 133.2, 132.7, 132.7, 131.3, 129.6, 129.5, 129.4, 129.2, 129.2, 128.8, 128.6, 127.76, 127.73, 127.3, 127.15, 127.11, 127.0, 125.5, 125.3, 125.1, 123.3, 66.7, 64.7, 43.7, 40.1, 32.2, 26.5, 21.53, 21.50, 21.0, 13.6 ppm.

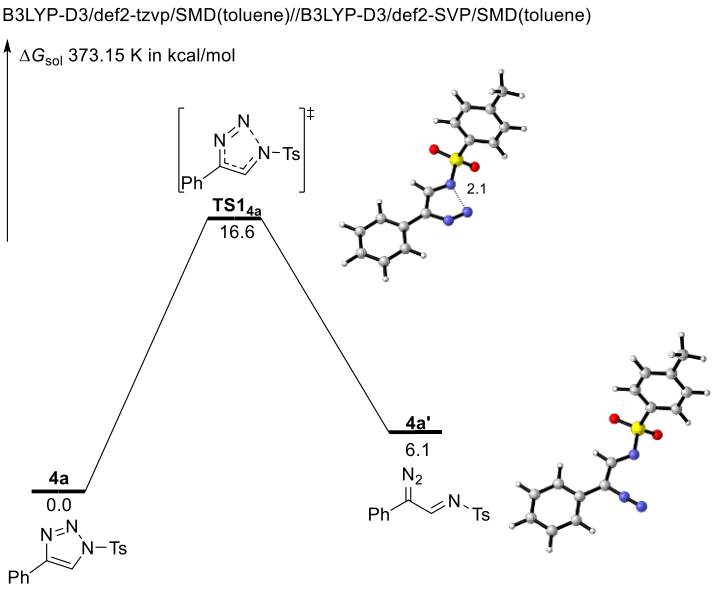
^{77}Se NMR (115 MHz, Chloroform-*d*): δ = 288.93 (d, *J* = 26.1 Hz), 247.12 (d, *J* = 25.8 Hz) ppm.

HRMS (ESI): m/z: $[M+Na]^+$ Calcd. for $C_{25}H_{25}NSO_2SeNa^+$: 506.0663; Found: 506.0652.

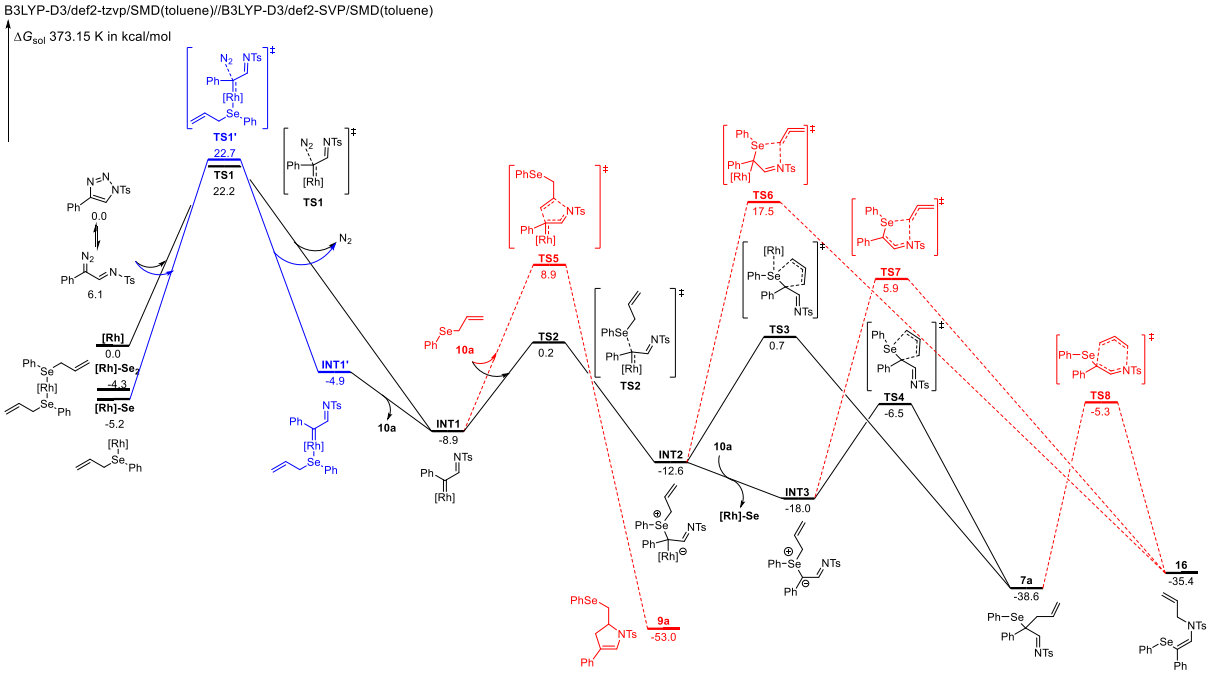
DFT Calculations

Computational Details

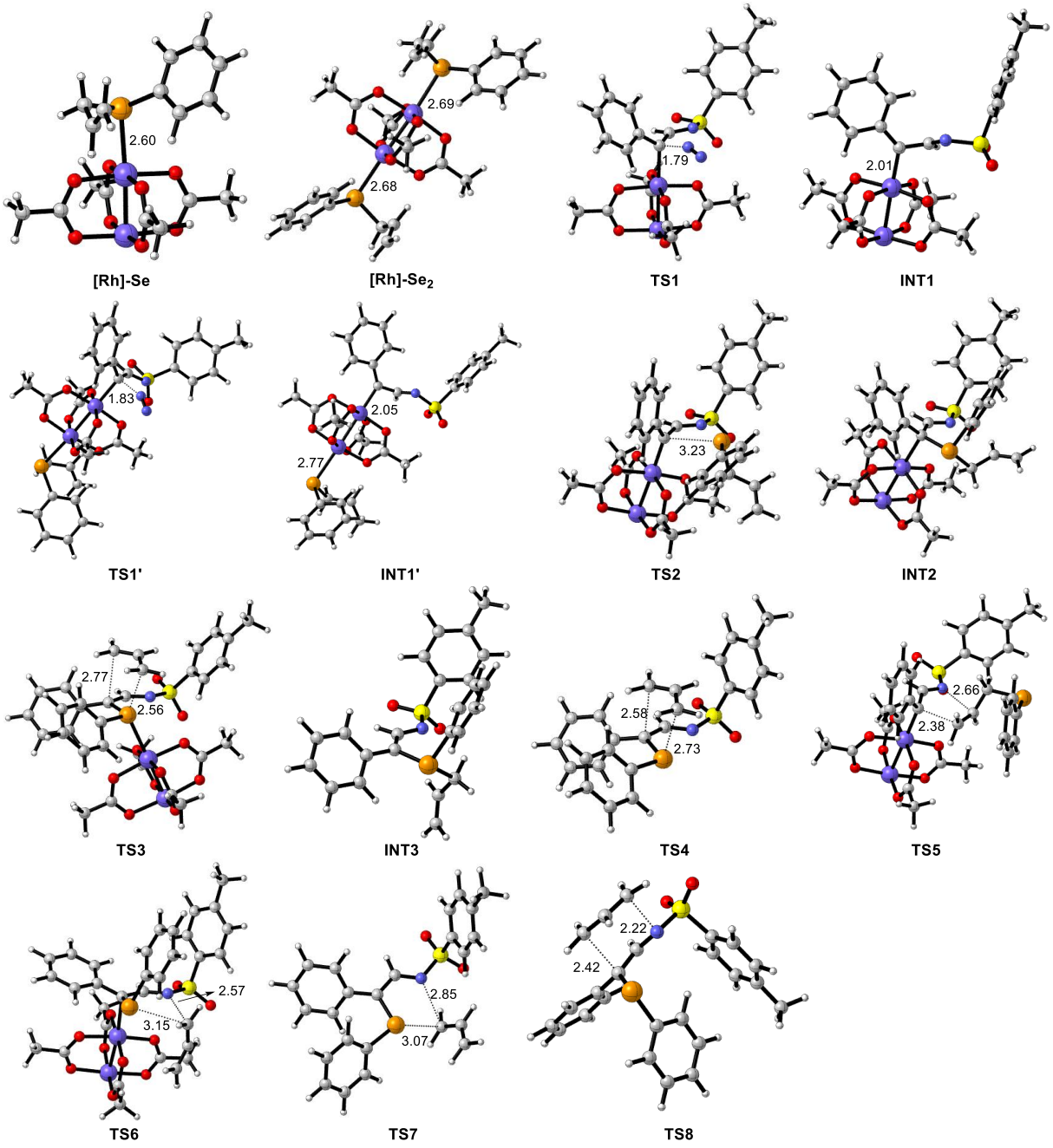
All the calculations were performed with the Gaussian 16 program.[2] The (U)B3LYP functional[3] together with Grimme's dispersion correction[4] (denoted (U)B3LYP-D3) and the def2-SVP basis set[5] were applied for the optimization of all stationary points at 373.15 K in the toluene, in which the solvent effects (ε = 2.3741) were evaluated by SMD solvation model.[6] Harmonic vibrational frequency calculations at the same level were performed for all of the stationary points to confirm them as a local minima or transition state structures. Key transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.[7] To improve the calculation accuracy, single point energy calculations using larger def2-TZVP basis set[5] at the (U)B3LYP-D3 level with SMD solvation model were performed based on the optimized geometries of all species at 373.15 K. The given Gibbs free energies in toluene were calculated according to the formula: G_{sol} = TCG + E_{sol} (kcal/mol). The CYL View software and GaussView 6.0 was employed to show the 3D structures of the studied species.[8]



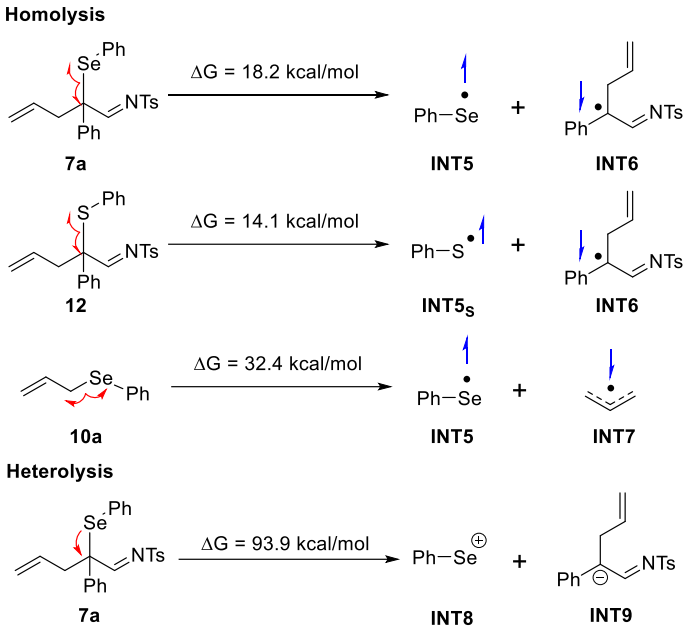
Scheme S3. Potential energy surfaces of Dimroth rearrangement of triazole **4a**.



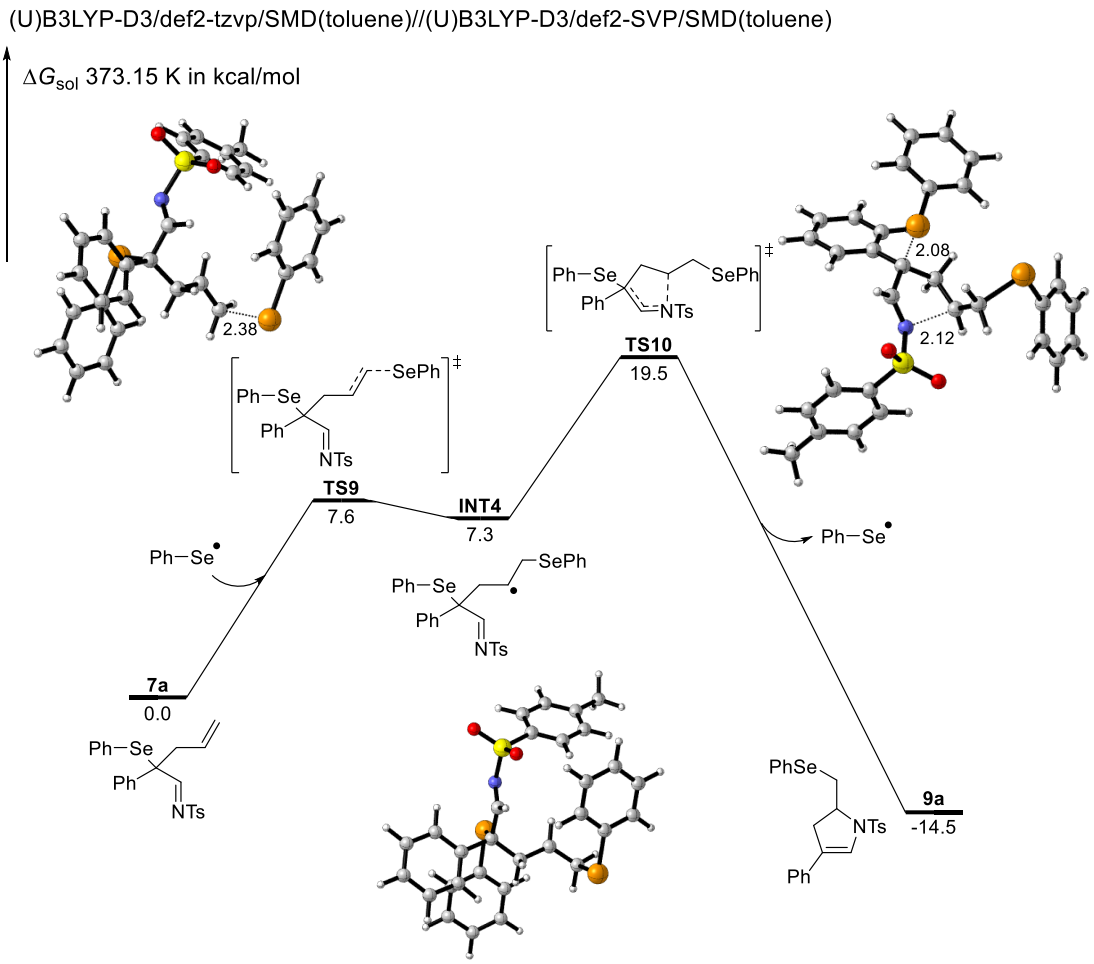
Scheme S4. Potential energy surfaces of Rh(II)-catalyzed rearrangement reaction of allyl selenide with triazole.



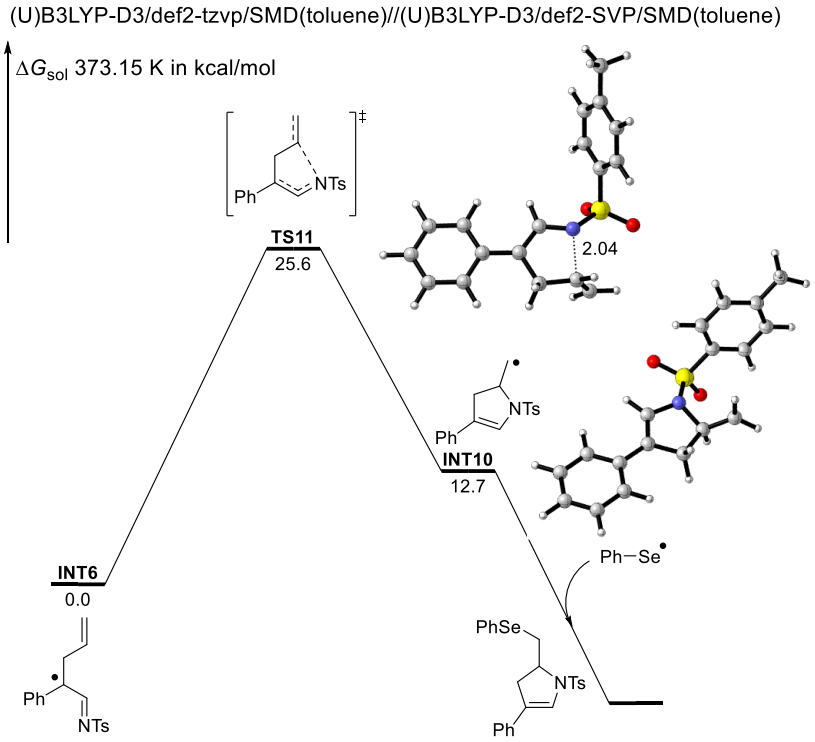
Scheme S5. 3D structures of key species in the Rh(II)-catalyzed rearrangement reaction. The bond lengths in the structures at the bottom are given in Å.



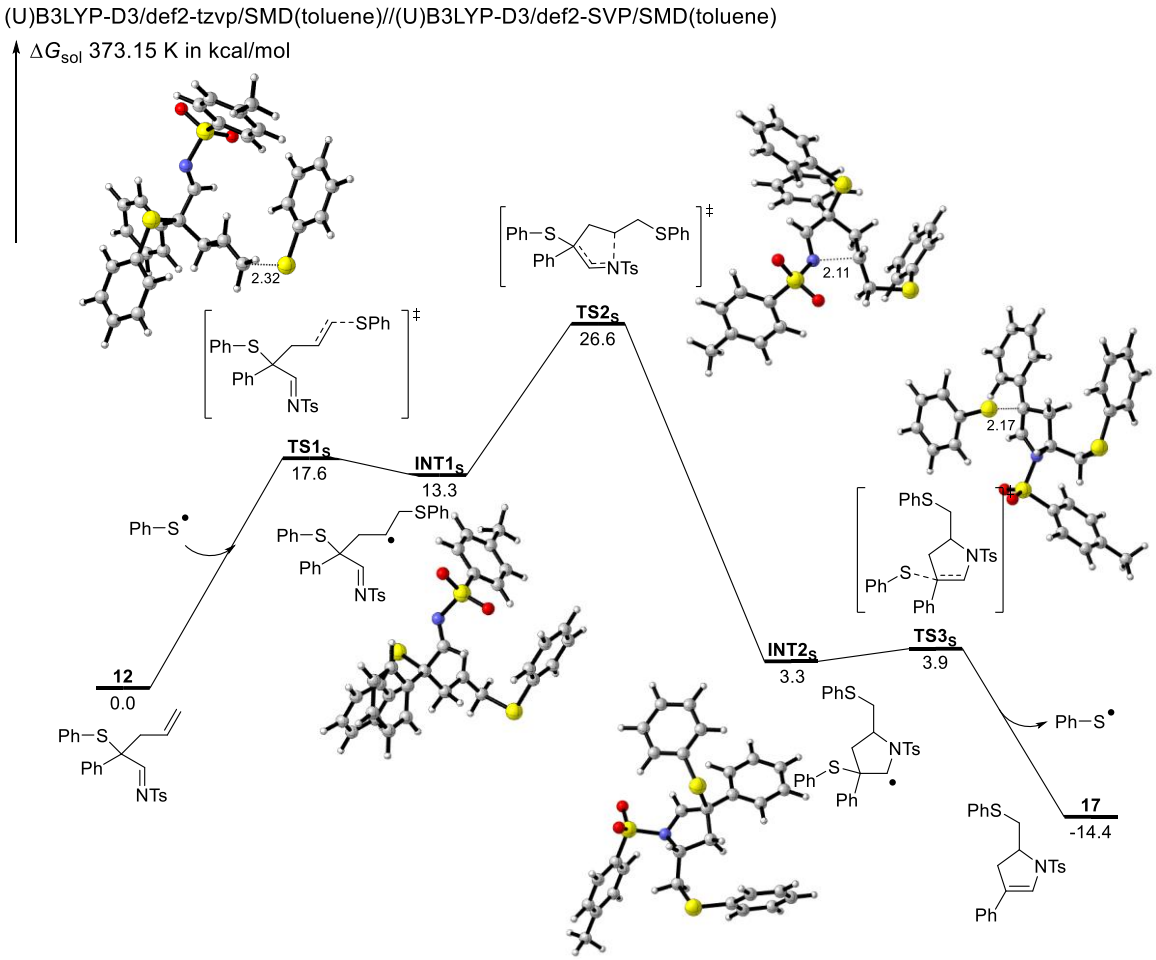
Scheme S6. Bond Dissociation Gibbs Free Energy (BDFE) illustration of **7a**, **12**, **10a**.



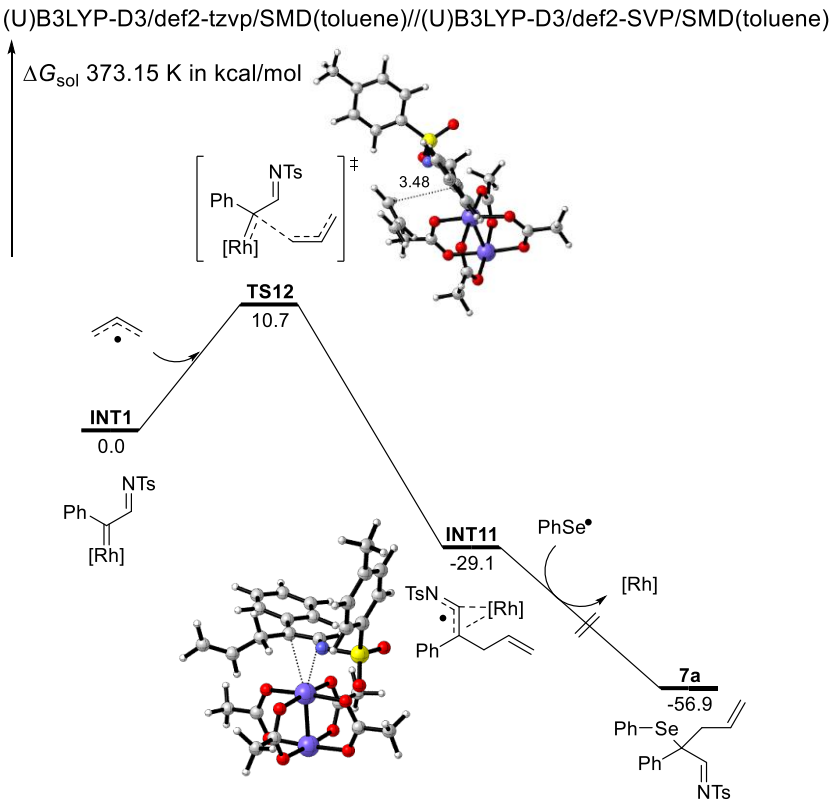
Scheme S7. Potential energy surface of cyclization reaction of homoallyl selenide and formation of the dihydropyrrole.



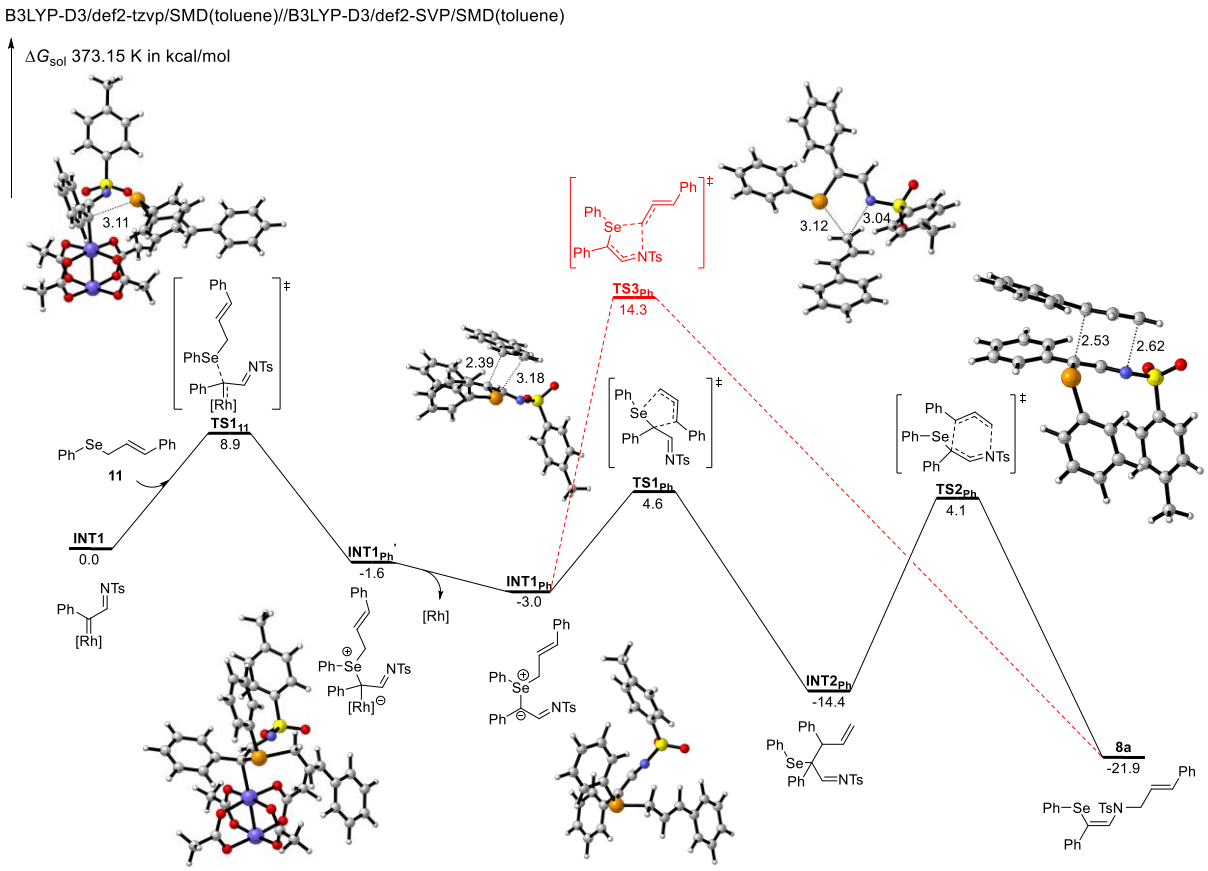
Scheme S8. Potential energy surface of the direct cyclization pathway of enamine radical.



Scheme S9. Potential energy surface of cyclization reaction of homoallyl sulfide.



Scheme S10. Potential energy surface of allyl radical addition to imino-carbene.



Scheme S11. Potential energy surface of formal 1,3-difunctionalization reaction with cinnamyl selenide.

Computed energies of all stationary points

Table S2. Thermal correction to Gibbs free energies (***TCG***, in Hartree), thermal correction to enthalpies (***TCH***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), single point energies in toluene computed at the (U)B3LYP-D3/def2-TZVP level (E_{sol}, in Hartree), and total spin-squared operator of open-shell species S^2.

Name	*TCG*/a.u.	*TCH*/a.u.	*G*/a.u.	E_{sol}/a.u.	S^2
4a	0.189923	0.286046	-1291.303580	-1292.674596	
TS1$_{4a}$	0.186111	0.283374	-1291.273240	-1292.644329	
4a'	0.185983	0.285347	-1291.288152	-1292.660888	
$Rh_2(OAc)_4$	0.138647	0.242039	-1134.523056	-1135.772779	
10a	0.110357	0.177486	-2749.908983	-2750.695390	
[Rh]-Se	0.276831	0.422521	-3884.446174	-3886.504259	
[Rh]-Se_2	0.414265	0.601598	-6634.359128	-6637.225328	
TS1	0.352794	0.526932	-2425.793738	-2428.436274	
INT1	0.347188	0.516616	-2316.382776	-2318.894358	
N_2	-0.018328	0.009816	-109.452028	-109.567446	
TS1'	0.488431	0.706983	-5175.707054	-5179.156146	
INT1'	0.483988	0.696738	-5066.290712	-5069.609887	
TS2	0.489336	0.695597	-5066.285831	-5069.607110	
INT2	0.490582	0.697389	-5066.308225	-5069.628738	
TS3	0.497281	0.695789	-5066.285984	-5069.614194	
7a	0.321344	0.453478	-3931.808233	-3933.858497	
INT3	0.317662	0.452341	-3931.770943	-3933.822041	
TS4	0.322314	0.450700	-3931.752890	-3933.808350	
TS5	0.489316	0.695670	-5066.271037	-5069.593131	
9a	0.327488	0.455639	-3931.837299	-3933.887688	
TS6	0.492799	0.695390	-5066.261003	-5069.582956	
16	0.324833	0.453713	-3931.806229	-3933.856912	
TS7	0.316203	0.449912	-3931.734270	-3933.782535	
TS8	0.324347	0.451170	-3931.754860	-3933.808506	
INT5	0.048477	0.099968	-2632.706863	-2633.300165	0.7530
INT6	0.243417	0.350455	-1299.067723	-1300.499828	0.7729
INT7	0.032899	0.072479	-117.148486	-117.314607	0.7787
INT8	0.050734	0.099700	-2632.461811	-2633.055832	
INT9	0.245251	0.349775	-1299.186344	-1300.627636	
TS9	0.395845	0.554148	-6564.507266	-6567.172611	0.7712
INT4	0.396324	0.555057	-6564.508923	-6567.173563	0.7579
TS10	0.395727	0.553656	-6564.491101	-6567.153485	0.7697
TS11	0.243452	0.347626	-1299.030014	-1300.459054	0.7783
INT10	0.245442	0.349846	-1299.054913	-1300.481675	0.7541
TS12	0.403627	0.590241	-2433.519317	-2436.215469	0.7772
INT11	0.411009	0.595138	-2433.588188	-2436.286213	0.7795

12	0.325135	0.454379	-1928.597321	-1930.494450	
INT5$_S$	0.050650	0.100262	-629.501752	-629.941078	0.7680
TS1$_S$	0.402112	0.555235	-2558.075376	-2560.433746	0.7742
INT1$_S$	0.401411	0.556209	-2558.083087	-2560.439901	0.7556
TS2$_S$	0.403257	0.555025	-2558.063441	-2560.420606	0.7704
INT2$_S$	0.408181	0.558436	-2558.107015	-2560.462642	0.7581
TS3$_S$	0.409152	0.557437	-2558.105800	-2560.462736	0.7627
17	0.329972	0.456331	-1928.625504	-1930.522313	
11	0.181434	0.266286	-2980.752752	-2981.854139	
TS1$_{11}$	0.560133	0.784393	-5297.130327	-5300.765808	
INT1$_{Ph}$'	0.565723	0.786391	-5297.149879	-5300.788173	
INT1$_{Ph}$	0.392416	0.541289	-4162.617020	-4164.982982	
TS1$_{Ph}$	0.394911	0.539753	-4162.606442	-4164.973358	
INT2$_{Ph}$	0.398452	0.542505	-4162.636734	-4165.007095	
TS2$_{Ph}$	0.395778	0.539462	-4162.606191	-4164.974951	
8a	0.395669	0.542525	-4162.650679	-4165.016237	
TS3$_{Ph}$	0.391049	0.539010	-4162.586733	-4164.954069	

Coordinates of all stationary points

4a

C	-5.36391300	-0.47372500	1.41899800
C	-4.06203900	-0.03542200	1.17221100
C	-3.44114400	-0.29658500	-0.06290200
C	-4.15576200	-1.00718200	-1.04471900
C	-5.45744200	-1.44414100	-0.79389300
C	-6.06732300	-1.18013600	0.43713700
H	-5.83231400	-0.26213800	2.38375200
H	-3.52493900	0.51524200	1.94860900
H	-3.67738000	-1.21012800	-2.00453400
H	-6.00022600	-1.99452400	-1.56689300
C	-2.07053900	0.15931000	-0.33556800
C	-1.19284300	0.88028600	0.45842100
H	-1.25033800	1.30161700	1.45697200
N	-0.24814900	0.41185200	-1.51703300
N	-1.43392100	-0.09842400	-1.52713700
N	-0.08621300	1.01237000	-0.32323600
S	1.44432400	1.79850700	0.08434300
C	2.55215300	0.41591300	0.13335300
C	3.14431200	-0.02034500	-1.05762600
C	2.79626800	-0.21324300	1.35660600
C	3.99814200	-1.11844200	-1.00773800
H	2.93151200	0.48898100	-1.99863000
C	3.65839600	-1.30952700	1.38026600
H	2.32560400	0.15429500	2.26999900
C	4.26977100	-1.77930500	0.20553700
H	4.46598900	-1.47334200	-1.92978300
H	3.86070300	-1.80913800	2.33102000
O	1.20303500	2.31548300	1.42802300
O	1.76077800	2.65507900	-1.04682400
H	-7.08707800	-1.52254600	0.63108900
C	5.21407000	-2.95119900	0.23267200
H	4.98744600	-3.66334000	-0.57691700
H	6.25394500	-2.61313400	0.08136500
H	5.17273300	-3.49059000	1.19016600

TS1$_{4a}$

C	5.21115600	-0.36260300	-1.60563900
C	3.92376400	-0.00944300	-1.19841900
C	3.47342300	-0.31676500	0.10036000
C	4.35196800	-0.98744100	0.97438200
C	5.63716700	-1.33784500	0.56104000
C	6.07589000	-1.02817900	-0.73079700
H	5.54016200	-0.11380300	-2.61792400

H	3.26726900	0.50993300	-1.90009900
H	4.02085500	-1.23335900	1.98675800
H	6.30218100	-1.85695800	1.25620900
C	2.12680900	0.04911300	0.53826400
C	1.08537200	0.73240800	-0.14415700
H	1.22033600	1.07995100	-1.17366200
N	0.61827500	-0.02433100	2.27305800
N	1.64691300	-0.24353300	1.77680800
N	-0.02552100	0.92452700	0.51216700
S	-1.35504400	1.73927500	-0.16946900
C	-2.57303000	0.43546900	-0.19734500
C	-3.30840700	0.17121900	0.95991600
C	-2.76330100	-0.30235300	-1.36976200
C	-4.24555400	-0.86268700	0.93856400
H	-3.14975000	0.77016500	1.85844300
C	-3.70600100	-1.32844400	-1.37066300
H	-2.18507600	-0.06383700	-2.26431100
C	-4.45928800	-1.62759200	-0.22027900
H	-4.82520300	-1.07687700	1.84024600
H	-3.86610200	-1.90882300	-2.28366500
O	-1.02521600	2.11921400	-1.55219800
O	-1.76103300	2.74993500	0.80487300
H	7.08338200	-1.30277600	-1.05265400
C	-5.47637900	-2.73849800	-0.25007900
H	-5.93768400	-2.89912300	0.73531700
H	-6.28235700	-2.51329000	-0.96909200
H	-5.01653300	-3.68759800	-0.57202100

4a'

C	5.95515900	-0.64833000	-1.21532900
C	4.92624700	0.03074200	-1.87412500
C	3.68059500	0.19895600	-1.26670700
C	3.43864200	-0.31032900	0.02410800
C	4.48310200	-0.99167600	0.68102800
C	5.72403600	-1.15845800	0.06586100
H	6.92790400	-0.77875700	-1.69541400
H	5.08904000	0.43551300	-2.87626800
H	2.89835500	0.72908400	-1.81194200
H	4.33350100	-1.39561000	1.68562700
H	6.51767100	-1.69044700	0.59669400
C	2.12059700	-0.13149700	0.66990000
N	1.69567600	-1.20298900	2.83591800
N	1.90698500	-0.71626100	1.83924800
N	-0.11299300	0.71447500	0.81339200
S	-1.32050700	1.68790000	0.10768700
O	-0.89492700	2.18205600	-1.21623400
O	-1.73832500	2.63727700	1.14216900
C	-2.61697300	0.48011100	-0.12542600
C	-2.78762900	-0.11590500	-1.37846700
C	-3.43723600	0.14992900	0.95530800
C	-3.79608800	-1.06407200	-1.54059800
H	-2.14209500	0.17263400	-2.21002800
C	-4.43976100	-0.80419000	0.77385300
H	-3.29345400	0.64078000	1.91955100
C	-4.63570000	-1.42539800	-0.47084500
H	-3.94006900	-1.53265900	-2.51832800
H	-5.08611100	-1.06796500	1.61519100
C	-5.72610000	-2.44483000	-0.67547500
H	-6.48654000	-2.06867800	-1.38113100
H	-6.23548400	-2.69541600	0.26657100
H	-5.32330400	-3.37652000	-1.10598900
C	1.00331100	0.62859900	0.17004200
H	1.15382800	1.13848900	-0.79368300

$Rh_2(OAc)_4$

Rh	0.00048000	0.00031900	1.19505000
Rh	-0.00014600	-0.00073300	-1.19477800
O	-1.38280500	-1.52025100	-1.12500500
C	-1.78694800	-1.94109900	0.00173900
O	-1.38377800	-1.51764100	1.12789200
O	1.51840700	-1.38425200	1.12709500
C	1.94141000	-1.78694600	0.00078700
O	1.51949200	-1.38292000	-1.12579600
O	-1.51761500	1.38469400	1.12670200
C	-1.94111900	1.78655600	0.00026600
O	-1.51971700	1.38169100	-1.12618600
O	1.38448200	1.51837600	1.12465500
C	1.78705100	1.94092800	-0.00228100
O	1.38274600	1.51872300	-1.12823700
C	3.00221100	-2.85511700	-0.00330300
H	3.56594600	-2.84556600	0.93873900
H	2.50600100	-3.83464200	-0.10636400

H	3.67351200	-2.72230300	-0.86286400
C	-2.85702500	-2.99996100	0.00297100
H	-2.78107900	-3.62237400	0.90467900
H	-3.83899200	-2.49779700	0.01129000
H	-2.79150800	-3.61481500	-0.90462700
C	-3.00154500	2.85510500	-0.00361400
H	-3.57218100	2.83810100	0.93421400
H	-2.50408800	3.83526300	-0.09404900
H	-3.66647200	2.72981600	-0.86916100
C	2.85390500	3.00304900	0.00231400
H	2.70044100	3.69180300	0.84467300
H	3.83131800	2.51116700	0.13985000
H	2.86472800	3.54751700	-0.95085200

10a

C	-2.71254200	-0.49160800	1.03265600
C	-1.38573600	-0.91935700	0.92491200
C	-0.59093000	-0.48334600	-0.14688300
C	-1.13601000	0.37982600	-1.10961500
C	-2.46481100	0.80314200	-0.99816100
C	-3.25362200	0.36945000	0.07162900
H	-3.32635300	-0.83513000	1.86971000
H	-0.96352300	-1.59369300	1.67398400
H	-0.51882300	0.72032000	-1.94332300
H	-2.88306900	1.47642700	-1.75121800
H	-4.29176800	0.70142100	0.15650100
Se	1.24777900	-1.06484800	-0.28691300
C	2.05557700	0.42761900	0.78774700
H	1.56701100	0.41483000	1.77237200
H	3.10479200	0.11376700	0.90285000
C	1.92685400	1.74048400	0.09904700
H	2.56964200	1.88856800	-0.77740500
C	1.05419400	2.69360000	0.44831200
H	0.38082400	2.56756200	1.30304900
H	0.97895600	3.63190400	-0.10936000

[Rh]-Se

Rh	0.34604100	-0.05930400	-0.28856300
Rh	2.54390800	0.43871900	0.61653900
O	2.01423400	2.42837300	0.56390100
C	0.87204100	2.76212800	0.13318000
O	-0.01870300	1.96457000	-0.29800900
O	1.18186800	0.07759900	-2.16550400
C	2.41407800	0.36595200	-2.28107600
O	3.21627500	0.56227500	-1.32282000
O	-0.31005500	-0.15721100	1.66703300
C	0.50272200	0.03559200	2.62667200
O	1.73448700	0.28549400	2.50330900
O	0.86359900	-2.05423200	-0.20868000
C	2.01657200	-2.38735600	0.21540900
O	2.90994200	-1.58885800	0.61649200
C	2.95027800	0.52269000	-3.68114700
H	2.39201700	-0.11120500	-4.38309300
H	2.81838400	1.57417500	-3.98684800
H	4.02275800	0.28796700	-3.71081100
C	0.51221200	4.22571000	0.16535400
H	-0.14528900	4.47758600	-0.67797900
H	-0.04029000	4.42714200	1.09840200
H	1.41689400	4.84768200	0.15431500
C	-0.07567000	-0.00706800	4.01785800
H	-0.52500300	0.97595000	4.23767800
H	-0.87170700	-0.76246600	4.07697800
H	0.70810500	-0.20718000	4.75995300
C	2.33876000	-3.85976900	0.20333500
H	1.45506600	-4.44380300	0.49719900
H	2.60758700	-4.15058500	-0.82579800
H	3.18627900	-4.07911900	0.86539100
C	-5.57825900	1.23359100	-0.77851900
C	-4.50705100	0.54210600	-1.35212200
C	-3.36073700	0.27942300	-0.58806800
C	-3.27933500	0.70755800	0.74442600
C	-4.35694700	1.39946600	1.30680900
C	-5.50358300	1.66281900	0.55071000
H	-6.47125600	1.43990700	-1.37434300
H	-4.56249700	0.20990800	-2.39187600
H	-2.38282300	0.50218300	1.32918400
H	-4.29662600	1.73563900	2.34536600
H	-6.34074300	2.20608300	0.99698300
Se	-1.90304500	-0.66857800	-1.43189800
C	-2.24852100	-2.51008600	-0.69829300
H	-3.19821900	-2.83416700	-1.14665900
H	-1.41131200	-3.07668600	-1.13058700
C	-2.25223500	-2.55898800	0.78657800

H	-1.27767800	-2.43522600	1.26635100
C	-3.36007400	-2.68140300	1.52704800
H	-4.35220500	-2.76954400	1.07087000
H	-3.31427900	-2.69454700	2.62021700

[Rh]-Se$_2$

Rh	-1.21261000	-0.61590500	0.09962200
Rh	1.21459800	-0.59549600	-0.21014700
O	1.12070400	1.46206400	-0.02355200
C	0.00972800	2.03193300	0.18804400
O	-1.10914600	1.44511400	0.27342900
O	-1.38382900	-0.41400900	-1.94624400
C	-0.34206300	-0.35676500	-2.66183500
O	0.85231200	-0.42672900	-2.23642600
O	-0.85106700	-0.79664900	2.12543300
C	0.34323100	-0.82274200	2.55537500
O	1.38524800	-0.75051900	1.84115700
O	-1.12218100	-2.66471700	-0.09603400
C	-0.00368900	-3.23370500	-0.27213500
O	1.11610600	-2.64801700	-0.36473600
C	-0.52106800	-0.15596300	-4.14591900
H	-1.55983600	-0.34355100	-4.44591000
H	-0.25683400	0.88576700	-4.39256700
H	0.16558600	-0.81222800	-4.70010300
C	0.02996700	3.52540600	0.39374700
H	-0.93395600	3.97172700	0.11486400
H	0.20480700	3.72412400	1.46463500
H	0.85133300	3.98057400	-0.17632800
C	0.52828800	-0.98592200	4.04332600
H	-0.26249300	-0.44959100	4.58645600
H	0.44159400	-2.05728600	4.29013600
H	1.52094300	-0.63458800	4.35375200
C	-0.00146100	-4.74072300	-0.33713600
H	0.10624100	-5.13214200	0.68840800
H	-0.95122700	-5.11022900	-0.74674700
H	0.84729500	-5.10106600	-0.93364200
C	-6.91411900	1.32164400	-1.33436800
C	-6.18837400	0.33292300	-0.66268300
C	-4.83229200	0.54023000	-0.37060800
C	-4.20104100	1.73337500	-0.75101200
C	-4.93582100	2.71565800	-1.42309300
C	-6.28839200	2.51327700	-1.71545500
H	-7.97072900	1.15759900	-1.56234900
H	-6.67544400	-0.59979900	-0.36726100
H	-3.14681200	1.88697300	-0.51981100
H	-4.44426900	3.64599100	-1.72042300
H	-6.85635000	3.28443200	-2.24280100
Se	-3.85210400	-0.85369400	0.54265200
C	-3.96912500	-0.14121600	2.41947600
H	-5.02496200	-0.21609000	2.71551300
H	-3.36712600	-0.87919600	2.96941100
C	-3.42048800	1.23360700	2.55158300
H	-2.33652400	1.32247500	2.43927700
C	-4.17236100	2.32603900	2.73074300
H	-5.26379100	2.26875800	2.80775000
H	-3.72212900	3.32090500	2.80107200
C	6.90447300	1.08666300	1.53936200
C	6.18018400	0.21783900	0.71717200
C	4.82862800	0.47761000	0.44665700
C	4.20026100	1.60337000	0.99883100
C	4.93396500	2.46603600	1.81996200
C	6.28193100	2.21112800	2.09155500
H	7.95754400	0.88169400	1.74994700
H	6.66509900	-0.66211200	0.28702500
H	3.14943300	1.79864300	0.78418300
H	4.44496100	3.34410200	2.25063300
H	6.84887000	2.88843900	2.73593200
Se	3.85295800	-0.75286500	-0.68208000
C	3.97672300	0.25601400	-2.41732700
H	5.03820100	0.25019600	-2.70236800
H	3.39993700	-0.39472900	-3.09054800
C	3.40019400	1.62360200	-2.33700000
H	2.31186200	1.67228500	-2.24514900
C	4.13108100	2.74435800	-2.31178400
H	5.22518400	2.72091600	-2.36451800
H	3.65976900	3.72870000	-2.23134300

TS1

Rh	-3.01080500	-1.59860000	-0.11939900
Rh	-1.26497400	0.09193300	0.07840000
C	-3.25132300	0.16043300	2.19126900
O	-2.19359100	0.75161900	1.78972700

O	-3.80028800	-0.82164200	1.62292000
C	-3.89622900	0.71891000	3.43348100
H	-4.42538000	1.64885300	3.16667600
H	-4.61747300	0.00587400	3.85248100
H	-3.12670000	0.97353100	4.17622400
C	-0.65032700	-2.44479500	1.33872400
O	-1.77646600	-2.86289200	0.94600700
O	-0.22015800	-1.25409000	1.20115000
C	0.29433900	-3.40416800	2.00941800
H	-0.15602800	-4.39916600	2.11308600
H	1.21119200	-3.45126200	1.40015100
H	0.57716500	-3.00907600	2.99741800
C	-0.99859000	-1.73044200	-2.18991400
O	-0.47310500	-0.71156200	-1.63688300
O	-2.07525700	-2.28078900	-1.82572700
C	-0.25979600	-2.28176900	-3.38026200
H	0.82214100	-2.21463900	-3.19547400
H	-0.56568700	-3.31572000	-3.58539200
H	-0.49088800	-1.65858300	-4.26012200
C	-3.59222800	0.91765100	-1.45071200
O	-4.08877000	-0.21910700	-1.20872600
O	-2.45535500	1.33149100	-1.05686200
C	-4.39175500	1.86504100	-2.30922600
H	-5.46219400	1.62628500	-2.25746900
H	-4.20710300	2.90491100	-2.00627800
H	-4.05837100	1.75158800	-3.35437200
C	-0.36913800	5.69808900	-0.44604400
C	0.81766400	5.11449700	-0.90404200
C	1.06662900	3.76427300	-0.66147700
C	0.11395400	2.97275400	0.01485300
C	-1.08128200	3.57130900	0.46688100
C	-1.31153600	4.92726100	0.24645600
H	-0.56004400	6.75889600	-0.62859100
H	1.55451600	5.71627700	-1.44149400
H	2.00280900	3.31527200	-1.00162600
H	-1.81701500	2.95823600	0.98756000
H	-2.23647400	5.38615200	0.60417900
C	0.34169900	1.53521100	0.22298500
N	0.40782600	1.24094200	3.02522100
N	0.70821300	1.35349000	1.96782300
N	2.30259500	0.10496900	0.22637000
S	3.16015900	-1.01809900	-0.73764300
O	2.99650500	-0.73692100	-2.17744900
O	2.81719700	-2.34779600	-0.21761100
C	4.84089900	-0.63663500	-0.27108600
C	5.63115500	0.13805800	-1.12081800
C	5.33423400	-1.11924000	0.94581000
C	6.93990600	0.43926000	-0.73686400
H	5.22502200	0.48995800	-2.07079200
C	6.64060100	-0.80502600	1.31263700
H	4.70082400	-1.73536100	1.58658200
C	7.46418000	-0.02271800	0.48093600
H	7.56652700	1.04259900	-1.39908300
H	7.03525100	-1.17698700	2.26234400
C	8.87960800	0.28745200	0.89370700
H	9.49439500	-0.62901300	0.90061200
H	8.91438800	0.70343600	1.91401400
H	9.35733900	1.00742400	0.21303300
C	1.43418000	0.81801900	-0.39626700
H	1.35213400	0.80724900	-1.49735500

INT1

C	1.34540100	5.29226200	0.01696100
C	2.36679800	4.38984300	-0.31727700
C	2.08243300	3.03585200	-0.42576000
C	0.75998600	2.55155800	-0.19994300
C	-0.25928600	3.48698600	0.13779800
C	0.03826800	4.83990300	0.24471000
H	1.57229800	6.35859300	0.10080600
H	3.38269500	4.75227100	-0.49034300
H	2.87692900	2.33078800	-0.67552600
H	-1.26904900	3.12409100	0.31434800
H	-0.74744500	5.55200800	0.50711200
C	0.46598900	1.15942400	-0.30055100
N	2.33779000	-0.14390600	0.36359600
S	3.19348100	-1.61444700	0.11220900
O	3.03148800	-2.40026600	1.34053300
O	2.85703300	-2.21070300	-1.19409600
C	4.86677100	-0.99170900	0.04557000
C	5.51864800	-0.66755600	1.24027800
C	5.48932500	-0.82643200	-1.19251300
C	6.81491000	-0.16125100	1.18109100
H	5.01340600	-0.81756800	2.19613300
C	6.79081600	-0.32115400	-1.23029800

H	4.96116800	-1.09931200	-2.10795500
C	7.47201400	0.02029500	-0.05068800
H	7.33328400	0.09548800	2.10921400
H	7.28757200	-0.19359900	-2.19580700
C	8.88127700	0.55171000	-0.08579800
H	8.97363000	1.47523800	0.50898200
H	9.58530900	-0.17961700	0.34719100
H	9.21225700	0.76924300	-1.11196300
C	1.47015800	0.14451900	-0.54319800
H	1.34098200	-0.47103900	-1.45342100
Rh	-3.39046200	-1.04425000	0.14240100
Rh	-1.28011400	0.19432500	-0.09194500
C	-2.84815000	0.85577500	2.26932100
O	-1.77620200	1.16456500	1.64921600
O	-3.69100400	-0.00417000	1.89664500
C	-3.08855900	1.56957300	3.57457600
H	-2.75591700	2.61476300	3.50627100
H	-4.14783500	1.51478500	3.85695300
H	-2.48672600	1.07613700	4.35580900
C	-1.09050400	-2.32723100	1.35665400
O	-2.32773500	-2.48806800	1.16218800
O	-0.41228000	-1.31529100	0.98174400
C	-0.33140900	-3.38198500	2.11645900
H	-0.74494000	-4.37673500	1.90010200
H	0.73866200	-3.32857600	1.87375200
H	-0.45577300	-3.18774000	3.19512300
C	-1.82980500	-1.74917200	-2.19939400
O	-0.97400000	-0.88210300	-1.81878800
O	-2.92267400	-1.99907600	-1.62443500
C	-1.46543300	-2.53524900	-3.43139700
H	-0.61071800	-3.18756600	-3.18919200
H	-2.31113900	-3.14687100	-3.76966200
H	-1.14110000	-1.85069400	-4.22916000
C	-3.60217600	1.44943100	-1.33238200
O	-4.29386400	0.48565300	-0.90662700
O	-2.34720700	1.59944900	-1.15855500
C	-4.29318300	2.50988100	-2.15145700
H	-5.36866500	2.52753700	-1.93185700
H	-3.84039400	3.49416300	-1.96835800
H	-4.15693900	2.26780200	-3.21874300

N_2

N	0.00000000	0.00000000	0.55004200
N	0.00000000	0.00000000	-0.55004200

TS1'

Rh	0.24913900	1.08317100	0.06935500
Rh	-2.05267200	0.35109000	-0.36042400
O	-1.54458500	-1.40086900	0.62374700
C	-0.38349200	-1.54260800	1.11190000
O	0.51805500	-0.65218100	1.11612500
O	0.73768000	0.10435300	-1.67313700
C	-0.13100400	-0.52315000	-2.34935500
O	-1.37271100	-0.54144300	-2.09843300
O	-0.44231500	1.97752500	1.78941900
C	-1.67223900	1.87029500	2.10044400
O	-2.54857300	1.25728800	1.42951900
O	-0.19111800	2.78531600	-1.00400500
C	-1.35991100	2.95278000	-1.46922700
O	-2.32837300	2.14783200	-1.34469600
C	0.37581300	-1.27908500	-3.54904700
H	0.44633600	-0.58341800	-4.40190000
H	1.38449800	-1.66057600	-3.33566600
H	-0.31139800	-2.09320900	-3.81495800
C	-0.01475300	-2.86758200	1.72168800
H	0.84331800	-3.26564400	1.15685800
H	0.31756600	-2.71372100	2.75996800
H	-0.85859900	-3.56849800	1.69255500
C	-2.11086600	2.56593600	3.36414100
H	-1.34306900	2.45511500	4.14294700
H	-2.22107500	3.64216900	3.15031800
H	-3.07540100	2.17362200	3.71092900
C	-1.59708800	4.21029700	-2.26834900
H	-1.00664700	5.04077300	-1.85703700
H	-1.25813300	4.03375200	-3.30286000
H	-2.66531500	4.46293700	-2.28934800
C	-7.46396400	-1.87870800	1.66364400
C	-6.83135700	-1.25405700	0.58426100
C	-5.43118100	-1.25269200	0.50139900
C	-4.66346100	-1.87425700	1.49722000
C	-5.30603400	-2.49669500	2.57253000
C	-6.70190200	-2.50030000	2.65854300

H	-8.55547500	-1.87753400	1.72678000
H	-7.42544400	-0.76713100	-0.19318200
H	-3.57541400	-1.86961200	1.42677400
H	-4.70775200	-2.98186400	3.34852200
H	-7.19773100	-2.98723100	3.50260900
Se	-4.58490000	-0.36713700	-0.99437800
C	-4.23355300	-1.97358900	-2.15275400
H	-5.21611900	-2.33486700	-2.48768300
H	-3.68981100	-1.51966600	-2.99401400
C	-3.42814500	-3.02020300	-1.47056300
H	-2.38104500	-2.76682300	-1.28459800
C	-3.92704700	-4.18501300	-1.04005600
H	-4.98155100	-4.44801400	-1.17974300
H	-3.29675200	-4.91740300	-0.52648200
C	3.52994000	5.78329400	0.13161700
C	4.38766100	4.78596200	-0.34743900
C	4.02840600	3.44434200	-0.22722300
C	2.78744200	3.08482700	0.34318600
C	1.92799300	4.10133100	0.81448800
C	2.30630700	5.43838500	0.71995000
H	3.81690000	6.83477300	0.04634100
H	5.34267800	5.05589000	-0.80476500
H	4.70624600	2.66454900	-0.58277900
H	0.96840900	3.82083000	1.24993300
H	1.63946900	6.21975600	1.09276500
C	2.36460500	1.68482500	0.41520500
N	2.03120200	1.15899900	3.19574800
N	2.47427200	1.21923300	2.18443500
N	3.45538500	-0.48804300	0.33299200
S	3.73303200	-1.79508800	-0.71822200
O	3.79820900	-1.36743800	-2.13106700
O	2.78936500	-2.85527000	-0.33561700
C	5.37250100	-2.28920500	-0.20462300
C	6.47461700	-1.92865500	-0.98030600
C	5.52270200	-3.02562300	0.97510400
C	7.75107000	-2.30938800	-0.55944400
H	6.32770400	-1.36392200	-1.90267600
C	6.80379400	-3.39247100	1.38096200
H	4.64410700	-3.30696500	1.55848600
C	7.93743600	-3.04252300	0.62328700
H	8.61882000	-2.03283500	-1.16444000
H	6.93074400	-3.96643700	2.30325700
C	9.31081000	-3.47112400	1.07127600
H	9.43803800	-4.56114000	0.95210800
H	9.47198500	-3.24468000	2.13783200
H	10.10426300	-2.97679300	0.49143400
C	3.04258400	0.59895500	-0.22739900
H	3.02555100	0.70811600	-1.32720100

INT1'

Rh	0.30423000	0.99802100	-0.14254600
Rh	-2.10485100	0.47229000	-0.33816000
O	-1.64076100	-1.37570300	0.47997300
C	-0.44709300	-1.65099300	0.79852600
O	0.53797100	-0.85951000	0.68341200
O	0.50248700	0.15790400	-2.01622800
C	-0.49894200	-0.33627700	-2.62330600
O	-1.69170000	-0.30795400	-2.20824400
O	-0.12890900	1.78809600	1.70548900
C	-1.31982600	1.75160300	2.15503300
O	-2.32056400	1.27776700	1.55028800
O	-0.14778300	2.81944100	-1.00026000
C	-1.34659700	3.10257100	-1.31943100
O	-2.34861100	2.35232500	-1.15966200
C	-0.21190800	-1.00969400	-3.94009800
H	0.26777200	-0.29082300	-4.62221900
H	0.50464800	-1.82868700	-3.77017300
H	-1.13182700	-1.40177500	-4.39136500
C	-0.15489900	-3.00483500	1.38781600
H	0.89802400	-3.26968200	1.21933900
H	-0.33252500	-2.95468800	2.47534400
H	-0.83463800	-3.75765900	0.96499300
C	-1.52837700	2.29203800	3.54691500
H	-1.25723100	1.50348700	4.26849800
H	-0.86996900	3.15320000	3.72675700
H	-2.58013900	2.56465900	3.70340500
C	-1.56686700	4.44245200	-1.97615700
H	-0.90776800	5.19986500	-1.52920600
H	-1.30331200	4.35457700	-3.04333300
H	-2.61882000	4.74584300	-1.89694600
C	-7.43847700	-1.65845800	2.13326600
C	-6.89954400	-0.96123300	1.04748400
C	-5.52292500	-1.03013100	0.78648600
C	-4.68536500	-1.79541600	1.61201600

C	-5.23472100	-2.49067400	2.69445000
C	-6.60667200	-2.42391500	2.95738600
H	-8.51153800	-1.60168200	2.33523900
H	-7.54822800	-0.36305100	0.40267400
H	-3.61581600	-1.84465600	1.40510600
H	-4.58194500	-3.08802000	3.33680100
H	-7.02917100	-2.96780800	3.80656600
Se	-4.80094100	-0.04157500	-0.70994100
C	-4.68372200	-1.54167400	-2.04414700
H	-5.71701000	-1.83244400	-2.28056600
H	-4.22913300	-1.03322200	-2.90716200
C	-3.85352200	-2.67950900	-1.56852100
H	-2.77995500	-2.48528300	-1.49684900
C	-4.35235200	-3.85995100	-1.18291000
H	-5.42780400	-4.06793900	-1.20899500
H	-3.70096100	-4.66092700	-0.82014100
C	4.30266600	4.96762500	1.10386500
C	5.05363200	3.86686800	0.66343000
C	4.40606600	2.70055200	0.27953100
C	2.98449500	2.60888700	0.33259800
C	2.24491500	3.73797200	0.78510800
C	2.90372000	4.90134800	1.16482900
H	4.81531800	5.88578900	1.40362900
H	6.14362900	3.92853400	0.62331000
H	4.98488100	1.83729100	-0.05423400
H	1.15999200	3.66968300	0.83161600
H	2.33167900	5.76447400	1.51311800
C	2.31193000	1.40708900	-0.03842300
N	3.58364100	-0.54727900	0.43909200
S	3.92691500	-2.13866500	-0.08081500
O	3.57096400	-2.33256500	-1.50066200
O	3.37883000	-3.04598300	0.93567000
C	5.70980400	-2.14571300	0.06469700
C	6.49485300	-1.98735300	-1.07783600
C	6.28707100	-2.30111200	1.32959700
C	7.88563100	-1.97904400	-0.94587800
H	6.01835100	-1.88202900	-2.05422300
C	7.67539000	-2.28606400	1.44135100
H	5.65081000	-2.43736500	2.20593100
C	8.49699400	-2.12498200	0.30956700
H	8.50714100	-1.86125300	-1.83762900
H	8.13573900	-2.40699500	2.42609200
C	9.99648100	-2.12481400	0.45753300
H	10.35413700	-3.09942200	0.83119100
H	10.32342600	-1.36424500	1.18600200
H	10.50312200	-1.92323700	-0.49780100
C	2.97346000	0.19334300	-0.42886300
H	2.77574000	-0.15890300	-1.45932600

TS2

C	-0.93719600	2.58417500	4.46893100
C	-1.84720900	1.54726000	4.21148800
C	-1.60992700	0.66365900	3.16706500
C	-0.44100600	0.78712900	2.36625700
C	0.47197300	1.83718900	2.65066700
C	0.21546900	2.72901400	3.68553900
H	-1.13235200	3.28651300	5.28368300
H	-2.74542500	1.44241900	4.82457700
H	-2.32812400	-0.12956200	2.94722800
H	1.35886500	1.94405700	2.02988800
H	0.91215000	3.54641100	3.88518400
C	-0.20107400	-0.10758800	1.27499700
N	-2.00899400	-1.01896900	-0.04468300
S	-2.67186400	-2.44939700	-0.69709700
O	-2.55216800	-2.30849100	-2.15542800
O	-2.14476200	-3.65489100	-0.03036700
C	-4.38567800	-2.23478100	-0.24302800
C	-5.14055700	-1.25203600	-0.89423100
C	-4.93647900	-3.02846200	0.76313400
C	-6.46698700	-1.06446800	-0.51469700
H	-4.69062300	-0.64562500	-1.68230500
C	-6.27144900	-2.82936800	1.12433100
H	-4.32566400	-3.79147500	1.24899600
C	-7.05466200	-1.84747100	0.49740400
H	-7.06376600	-0.29592700	-1.01380200
H	-6.71192400	-3.45067400	1.90871000
C	-8.49649300	-1.63289200	0.87784700
H	-8.69285900	-0.57292300	1.10900400
H	-9.16613300	-1.90793100	0.04497200
H	-8.78355600	-2.23379100	1.75325700
C	-1.10543000	-1.15902200	0.86004700
H	-0.84079500	-2.15993300	1.25663100
Rh	3.69534100	-1.23185800	-0.67808800

Rh	1.57164100	-0.55486400	0.36613700
C	3.03483200	1.57352700	-1.00487400
O	1.95355800	1.33644400	-0.36431800
O	3.92061800	0.72368700	-1.27993600
C	3.24915000	2.99803000	-1.44979200
H	3.32992700	3.64531000	-0.56250900
H	4.16300000	3.08148700	-2.05065000
H	2.38085200	3.34467300	-2.02933500
C	1.36819800	-1.51083400	-2.38153400
O	2.62420100	-1.63959100	-2.39259200
O	0.67883000	-1.10958100	-1.38718600
C	0.59037100	-1.81253300	-3.63367600
H	1.15402100	-2.49167200	-4.28667200
H	-0.39285100	-2.22708400	-3.37011800
H	0.42268600	-0.86375800	-4.17117100
C	2.27744000	-3.37878200	0.64315900
O	1.42773100	-2.50186600	1.01408100
O	3.31813600	-3.14746600	-0.02831400
C	1.97301200	-4.79684000	1.04715800
H	1.04232200	-5.10983900	0.54725300
H	2.79307500	-5.46969500	0.76744300
H	1.79363900	-4.84210300	2.13201300
C	3.92220000	-0.32636900	2.07378600
O	4.60693100	-0.77768100	1.11522300
O	2.66801300	-0.09997700	2.05211900
C	4.62756300	-0.05858500	3.37920000
H	5.69031700	0.15670300	3.20628800
H	4.14303300	0.76678400	3.91834000
H	4.55352900	-0.96426100	4.00421500
C	0.41816600	5.33052500	-0.11510700
C	-0.00312700	4.00269700	-0.23214900
C	-1.35893100	3.71488600	-0.45418200
C	-2.28705200	4.76330900	-0.54098100
C	-1.86074100	6.08922100	-0.40816500
C	-0.50801200	6.37610000	-0.19881800
H	1.47708900	5.54931700	0.04931600
H	0.71181600	3.18314900	-0.15203000
H	-3.34213400	4.54266200	-0.72099900
H	-2.58917200	6.90167400	-0.47891700
H	-0.17598800	7.41319200	-0.10176500
Se	-1.96684300	1.88298000	-0.55727300
C	-1.00253800	1.31245800	-2.20787300
H	0.06929100	1.34666800	-1.97963000
H	-1.30924600	0.26009200	-2.28434900
C	-1.38127400	2.12408800	-3.39407000
H	-2.41455700	2.01504900	-3.74614400
C	-0.55655100	2.97341400	-4.01929800
H	0.47727300	3.11451900	-3.68551700
H	-0.88116400	3.55528000	-4.88714900

INT2

C	-0.41552500	3.93972600	3.55639400
C	-1.16173800	2.76639300	3.69404900
C	-1.15011100	1.80020600	2.68494800
C	-0.36176900	1.96648500	1.52808300
C	0.38781100	3.15538500	1.40719900
C	0.35162100	4.13165100	2.40155100
H	-0.43500000	4.70178700	4.33980200
H	-1.77559800	2.60692400	4.58463500
H	-1.77569700	0.91208100	2.79462600
H	1.02288900	3.29941400	0.53286500
H	0.94190100	5.04420500	2.28159500
C	-0.35336000	0.92737500	0.45536200
N	-1.68323700	-0.99436200	-0.14925500
S	-2.11552700	-2.57626900	0.18818600
O	-2.05613600	-3.31078900	-1.08730300
O	-1.42841200	-3.11393100	1.37695900
C	-3.84872200	-2.34738500	0.59967500
C	-4.79846100	-2.29153200	-0.42524800
C	-4.21584700	-2.15940900	1.93323300
C	-6.12850000	-2.02467700	-0.10249200
H	-4.49283600	-2.46101400	-1.45920600
C	-5.55311700	-1.89686500	2.23916300
H	-3.46033700	-2.22373300	2.71885500
C	-6.52803600	-1.81975400	1.23123000
H	-6.87556700	-1.97939100	-0.90018700
H	-5.84487000	-1.75080000	3.28265900
C	-7.97233400	-1.53551700	1.55425000
H	-8.34013100	-0.66039000	0.99275700
H	-8.61394100	-2.38797100	1.27355200
H	-8.12172900	-1.33915500	2.62611700
C	-0.94608600	-0.35318400	0.70674200
H	-0.66823600	-0.81179900	1.66958600

Rh	3.99008100	-0.95358400	-0.22416000
Rh	1.77615500	0.00066100	0.14727100
C	3.09826900	0.91221300	-2.28006500
O	2.02605200	1.05984800	-1.60585100
O	4.07234100	0.18205500	-1.95431900
C	3.17481100	1.64764200	-3.59446700
H	2.62199700	2.59564900	-3.54161400
H	4.22049700	1.82405200	-3.87886900
H	2.70740400	1.01870400	-4.37099400
C	1.83118900	-2.47267400	-1.41543200
O	3.08656900	-2.47759100	-1.27807000
O	1.04796400	-1.58395800	-0.94623100
C	1.18643300	-3.56730300	-2.22222100
H	1.81207200	-4.46968900	-2.21959700
H	0.17725300	-3.77154400	-1.83899200
H	1.08767100	-3.21525100	-3.26342600
C	2.64910700	-1.89624300	2.16541500
O	1.69501500	-1.10813000	1.87251600
O	3.72248600	-2.02822400	1.50941700
C	2.45267800	-2.74665000	3.39341200
H	1.61916500	-3.44219600	3.20489800
H	3.36229000	-3.31150500	3.63286600
H	2.16273500	-2.10898100	4.24208700
C	3.97965400	1.47647400	1.34421300
O	4.76473400	0.61143100	0.85834000
O	2.71861300	1.49758500	1.19975300
C	4.58248900	2.55948700	2.20354000
H	5.61418600	2.77085000	1.89164500
H	3.96788300	3.46889300	2.16908600
H	4.60371800	2.20050000	3.24611100
C	-4.33425500	4.04763600	-1.20267000
C	-3.01110800	3.61110200	-1.32407200
C	-2.70937800	2.26030600	-1.10363700
C	-3.71352600	1.34387700	-0.76350800
C	-5.02970700	1.79417700	-0.64312300
C	-5.34180900	3.14079300	-0.86171000
H	-4.57336600	5.10058600	-1.37115200
H	-2.22212600	4.32203700	-1.58170400
H	-3.46172600	0.29907400	-0.59453300
H	-5.81269400	1.07998900	-0.37663300
H	-6.37459600	3.48530900	-0.76454100
Se	-0.83140100	1.80226900	-1.26258300
C	-0.76102000	0.38595400	-2.71067700
H	-0.27316300	0.95771300	-3.51204900
H	-0.06583800	-0.34613100	-2.28389100
C	-2.05250200	-0.21632200	-3.13158500
H	-2.36266400	-1.09795700	-2.56665700
C	-2.79380900	0.25184500	-4.14256100
H	-2.50199700	1.14150400	-4.71216200
H	-3.72530700	-0.24016900	-4.43754300

TS3

C	2.46626400	5.01213300	2.66183200
C	1.09146500	5.26811200	2.68563600
C	0.20443100	4.41412800	2.02592800
C	0.67194300	3.27308200	1.34323300
C	2.05955300	3.01449100	1.34599000
C	2.94340100	3.88151700	1.98917600
H	3.16097900	5.68723900	3.16824600
H	0.70574700	6.14563000	3.21159800
H	-0.86547600	4.63173700	2.03191000
H	2.43874200	2.11445300	0.85832900
H	4.01465100	3.66277500	1.97583000
C	-0.27700700	2.34214500	0.70657800
N	-1.99229700	0.73659600	0.80645400
S	-3.12253700	-0.11790000	1.65377500
O	-2.63779200	-1.49551200	1.87645400
O	-3.62066900	0.62165300	2.83337400
C	-4.41855800	-0.19178000	0.42030800
C	-4.11254500	-0.67682900	-0.85862800
C	-5.70537900	0.23084200	0.74516900
C	-5.12191700	-0.72962800	-1.81595700
H	-3.09154200	-0.98840200	-1.08865300
C	-6.70761100	0.16486100	-0.22933700
H	-5.91196300	0.61304000	1.74666600
C	-6.43537400	-0.31304700	-1.51930700
H	-4.89168200	-1.10170900	-2.81879300
H	-7.71951300	0.49499900	0.02099100
C	-7.50928000	-0.38907900	-2.57409200
H	-7.21849900	0.17066000	-3.47890200
H	-7.68189000	-1.43325500	-2.88616300
H	-8.46617100	0.01798400	-2.21527000
C	-1.32646000	1.70164400	1.39571700

H	-1.54649400	2.02095800	2.42654300
Rh	1.80907800	-3.07535900	0.54742800
Rh	0.96697300	-0.95536700	-0.22738900
C	2.20075900	-2.57868100	-2.29203700
O	1.60037000	-1.46905700	-2.12383900
O	2.44400000	-3.42464400	-1.38454900
C	2.62150700	-2.91994500	-3.69823800
H	2.86785200	-2.00867500	-4.26026600
H	3.47155700	-3.61492400	-3.68936500
H	1.77451700	-3.41431600	-4.20281700
C	-0.94458200	-3.13232300	-0.32925500
O	-0.02276700	-3.87750400	0.12069900
O	-0.81299200	-1.90337100	-0.62357800
C	-2.30879600	-3.73803500	-0.51032800
H	-2.26877400	-4.82965700	-0.40729100
H	-2.95738300	-3.30904200	0.26917800
H	-2.72360300	-3.46004400	-1.48972400
C	0.55792000	-1.49539000	2.60031100
O	0.45356400	-0.58706300	1.72104800
O	1.10016500	-2.62635900	2.41451100
C	-0.03537300	-1.19463400	3.94757600
H	-1.13022500	-1.23029000	3.83041200
H	0.28534200	-1.92917600	4.69697800
H	0.23860800	-0.17589600	4.25853700
C	3.71142400	-0.89113000	0.71867200
O	3.59011200	-2.12362500	0.97195600
O	2.81899400	-0.15832900	0.18393600
C	4.99721200	-0.20666400	1.10235100
H	5.80085300	-0.93749200	1.25912100
H	5.27923400	0.52497200	0.33183400
H	4.82679800	0.34472200	2.04216700
C	3.49515800	2.49194100	-3.02980700
C	2.48959300	1.77237000	-2.37574400
C	1.44436200	2.46934400	-1.75664900
C	1.39179700	3.86919300	-1.79917800
C	2.40500100	4.57538700	-2.45074700
C	3.45781700	3.88877700	-3.06570100
H	4.31522000	1.95199600	-3.51002300
H	2.52695700	0.68309800	-2.34054400
H	0.58266900	4.41053400	-1.30842600
H	2.37162600	5.66748000	-2.47321200
H	4.24978500	4.44497800	-3.57362000
Se	0.03526700	1.43527500	-0.92342300
C	-1.95307300	2.43950300	-2.18590300
H	-1.25232200	3.12466700	-2.67139500
H	-2.26394500	1.57457400	-2.77809300
C	-2.74726700	2.88473000	-1.11452100
H	-3.60033300	2.26839400	-0.81888500
C	-2.34259700	3.90033000	-0.28477400
H	-1.49425600	4.54091300	-0.53260700
H	-2.92840600	4.17689300	0.59499600

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C	-4.07282300	3.42597900	0.04044400
C	-4.27590800	2.41327100	0.97891900
C	-3.29256300	1.44138700	1.19759000
C	-2.09061700	1.46264000	0.47396200
C	-1.89775500	2.48941700	-0.47167300
C	-2.87504700	3.46063700	-0.68430500
H	-4.84139700	4.18465200	-0.12813400
H	-5.20813800	2.37077100	1.54819000
H	-3.48762800	0.65884700	1.93015600
H	-0.97842100	2.51506600	-1.06100100
H	-2.70187500	4.24732700	-1.42310600
C	-1.01145300	0.39347000	0.64904400
N	1.18304500	1.01491100	-0.21081300
S	2.63919800	1.92718700	-0.00899000
O	2.72847100	2.77347700	-1.20037800
O	2.70431100	2.52293200	1.33626200
C	3.82915100	0.60411800	-0.11931100
C	4.16450800	0.09972100	-1.38046700
C	4.38694700	0.08298000	1.04900500
C	5.07183000	-0.95339700	-1.45975300
H	3.72014200	0.53215400	-2.27873100
C	5.29750700	-0.97099300	0.94717200
H	4.11521100	0.50474500	2.01832200
C	5.65123400	-1.50646700	-0.30181400
H	5.34073000	-1.35710600	-2.43980100
H	5.74293600	-1.38312900	1.85637400
C	6.63237900	-2.64330000	-0.41879600
H	6.18338100	-3.49798400	-0.95178100
H	7.52106600	-2.33735300	-0.99637400
H	6.97243800	-2.99540000	0.56605900
C	0.31972500	1.09559200	0.72027000

H	0.49391800	1.69526100	1.63302000
C	-5.13587200	-1.40264700	-1.04194800
C	-3.86339400	-0.84705900	-1.20785200
C	-2.72788600	-1.55104700	-0.77646200
C	-2.87671300	-2.81948000	-0.19327000
C	-4.15148000	-3.37359400	-0.03634100
C	-5.28194500	-2.66478400	-0.45678200
H	-6.01602100	-0.84614600	-1.37484500
H	-3.74917400	0.13672200	-1.66695100
H	-1.99251500	-3.36532100	0.14288400
H	-4.26079800	-4.36236200	0.41747000
H	-6.27780000	-3.09820500	-0.33146900
Se	-0.96190800	-0.79685400	-1.00776500
C	-0.30000600	-2.72019300	2.58234600
H	-1.31082000	-3.10884400	2.74802200
H	0.53173100	-3.40517000	2.77225600
C	-0.09104100	-1.46814500	2.16727400
H	0.94071800	-1.12905300	2.00997600
C	-1.18086900	-0.45766900	1.92907500
H	-2.15514800	-0.96589400	1.90482300
H	-1.21585700	0.24619000	2.78313700

INT3

C	5.14777500	-0.89177400	-2.93051800
C	3.84359900	-1.16278600	-3.35687800
C	2.76372300	-0.98981500	-2.48895200
C	2.95836000	-0.57157600	-1.15348000
C	4.28347700	-0.31151300	-0.73905900
C	5.35843200	-0.45865300	-1.61697600
H	5.99102400	-1.01505600	-3.61478000
H	3.66040400	-1.49434400	-4.38273800
H	1.74818000	-1.16726400	-2.85060500
H	4.47656300	-0.01042800	0.29408700
H	6.37271600	-0.25114400	-1.26478400
C	1.80008100	-0.44948300	-0.24573000
N	-0.34428600	-1.19615700	0.54270900
S	-1.49395000	-2.37924200	0.53311400
O	-1.77683500	-2.73939200	1.93272800
O	-1.19749200	-3.45332700	-0.43921900
C	-2.91267000	-1.45840200	-0.07916100
C	-3.67907200	-0.70618500	0.81416200
C	-3.18785800	-1.44467300	-1.44891900
C	-4.72479900	0.07788000	0.32219900
H	-3.45521600	-0.74433800	1.88194600
C	-4.23841700	-0.65935700	-1.92440900
H	-2.58141200	-2.04869400	-2.12671300
C	-5.02188800	0.11596100	-1.05112700
H	-5.32576500	0.66886200	1.01931400
H	-4.45669500	-0.64725200	-2.99615400
C	-6.17221800	0.93850000	-1.57362000
H	-6.40941800	1.77977100	-0.90428500
H	-7.08480300	0.32253400	-1.66061200
H	-5.95917600	1.34370300	-2.57526600
C	0.72441200	-1.32741600	-0.23041700
H	0.81265100	-2.20821300	-0.88878600
C	-0.10787300	4.52367500	-0.34448900
C	0.83808000	3.58904100	0.08976500
C	0.43007400	2.27410000	0.34756300
C	-0.90318700	1.87862600	0.17636300
C	-1.83505900	2.82390900	-0.25923300
C	-1.44147000	4.14173200	-0.51896000
H	0.20246200	5.55164500	-0.54794800
H	1.88168800	3.88655900	0.22129300
H	-1.19366400	0.84539800	0.36945900
H	-2.87499700	2.51769500	-0.39682200
H	-2.17717500	4.87409600	-0.86104100
Se	1.83326300	1.04923400	0.92721700
C	1.04739100	0.41880000	2.67174300
H	-0.03313000	0.37270900	2.50302800
H	1.31364400	1.24003200	3.35312100
C	1.61664700	-0.89836200	3.07093500
H	1.10663800	-1.76996800	2.64995800
C	2.66787300	-1.04049600	3.88600900
H	3.18830800	-0.17658600	4.31533300
H	3.04155100	-2.03135200	4.15986900

TS4

C	-4.13669100	3.30434200	1.29006900
C	-2.89194000	3.28468000	1.92663400
C	-1.87453100	2.44814000	1.46335100
C	-2.06857900	1.61704600	0.33972200
C	-3.32259900	1.66834500	-0.30387200

C	-4.34390000	2.49196000	0.17089000
H	-4.93611200	3.95188000	1.65908100
H	-2.71083200	3.91894100	2.79852600
H	-0.91554600	2.43668900	1.98294000
H	-3.49341300	1.06533200	-1.19661100
H	-5.30577700	2.50714200	-0.34832100
C	-0.95977000	0.77828300	-0.17442300
N	1.20701300	0.70035400	-1.17082700
S	2.69068300	1.44159300	-1.41754300
O	3.04903500	1.23810900	-2.82502700
O	2.72478300	2.80349700	-0.84454500
C	3.75229200	0.39691100	-0.41796300
C	4.09074200	-0.87596600	-0.89004400
C	4.17569300	0.83752000	0.83579300
C	4.84912400	-1.71757700	-0.07934900
H	3.75568000	-1.19491000	-1.87883900
C	4.94036500	-0.01803800	1.63397700
H	3.90437600	1.83872200	1.17563900
C	5.28504500	-1.30595900	1.19488100
H	5.11401900	-2.71574300	-0.44003000
H	5.27532500	0.32328400	2.61733700
C	6.11635700	-2.23014300	2.04677200
H	5.65215700	-3.22702400	2.12446100
H	7.11716200	-2.37636100	1.60487500
H	6.25401700	-1.83635600	3.06468500
C	0.30951900	1.34999800	-0.47579000
H	0.50101200	2.37065900	-0.10686100
C	-4.93642500	-2.70691000	-0.95402200
C	-3.70849000	-2.17249400	-1.35747500
C	-2.90114200	-1.50191600	-0.42787400
C	-3.32141000	-1.37186300	0.90351900
C	-4.55312700	-1.90063300	1.29550400
C	-5.36234000	-2.56926500	0.37018400
H	-5.56417500	-3.22609300	-1.68276000
H	-3.38617700	-2.27141500	-2.39751400
H	-2.70255100	-0.84375000	1.62860500
H	-4.88144900	-1.78721400	2.33178500
H	-6.32522400	-2.98146600	0.68206100
Se	-1.18314600	-0.87683700	-1.06142700
C	0.21978400	-2.18759500	0.88017300
H	-0.76716200	-2.44572500	1.27125800
H	0.73440300	-2.96543600	0.30985600
C	0.91076100	-1.08143900	1.35469500
H	1.95399000	-0.95624500	1.05530000
C	0.26309600	-0.01096000	1.95131400
H	-0.75350000	-0.10195300	2.33690500
H	0.82517300	0.86989100	2.26921400

TS5

C	0.14436400	-2.96204000	4.58577800
C	0.97353200	-1.83564000	4.50023200
C	0.85797500	-0.97124800	3.41546500
C	-0.10164000	-1.20590700	2.39908400
C	-0.92912500	-2.34930800	2.50238400
C	-0.80113800	-3.21655100	3.58411200
H	0.23712800	-3.64371400	5.43543100
H	1.71145300	-1.63697300	5.28140000
H	1.51470900	-0.10032600	3.34402900
H	-1.65611900	-2.54316300	1.71549300
H	-1.44423500	-4.09751000	3.65225600
C	-0.22949900	-0.29806600	1.27057000
N	1.15115900	1.57190400	0.47239300
S	1.30421000	3.26535800	0.54552400
O	0.73919600	3.79878100	-0.70405300
O	0.85423400	3.80929100	1.83949500
C	3.08630000	3.37598800	0.45105000
C	3.70285000	3.34340100	-0.80391600
C	3.83475200	3.40815800	1.62781400
C	5.09462200	3.32558500	-0.86983800
H	3.09274600	3.32986600	-1.70876300
C	5.22893700	3.39348100	1.54180200
H	3.32841900	3.44481300	2.59437800
C	5.87991600	3.34434500	0.29834800
H	5.58583200	3.29680800	-1.84648900
H	5.82250100	3.41958400	2.45950900
C	7.38274500	3.31627600	0.19819500
H	7.86027300	3.31727000	1.18892300
H	7.72405500	2.41892600	-0.34461900
H	7.75682000	4.19044100	-0.36084500
C	0.35178500	1.02011200	1.31256800
H	-0.11745800	1.62598700	2.11314500
Rh	-3.99396400	0.42264300	-1.18256900
Rh	-1.96525200	-0.00059900	0.13396200

C	-3.13794400	-2.35646200	-1.12758600
O	-2.13489900	-1.97949200	-0.43408300
O	-4.05042800	-1.60662300	-1.56482500
C	-3.23362500	-3.83507900	-1.40751100
H	-3.60984500	-4.33892200	-0.50151300
H	-3.92645000	-4.03102900	-2.23582700
H	-2.23802500	-4.24551500	-1.62864800
C	-1.51599800	0.67517900	-2.66339900
O	-2.76800700	0.72012800	-2.81528900
O	-0.90961900	0.38544200	-1.58251000
C	-0.63375800	0.99902200	-3.84200100
H	-1.23077000	1.17800200	-4.74490500
H	-0.04399800	1.89709700	-3.59880500
H	0.07376400	0.17311500	-4.01255300
C	-2.82492200	2.79070700	0.00020500
O	-1.99903900	2.00744000	0.57285000
O	-3.77596500	2.42449800	-0.74423300
C	-2.59997400	4.25814000	0.24282800
H	-1.61368800	4.52066700	-0.17171000
H	-3.38925200	4.86323300	-0.22036500
H	-2.55250700	4.44859000	1.32562900
C	-4.45448800	-0.20528100	1.61820400
O	-5.05939100	0.11253900	0.55678900
O	-3.19602200	-0.36045300	1.74151300
C	-5.27456400	-0.38998200	2.87028000
H	-6.32129500	-0.60740500	2.62078000
H	-4.84718800	-1.18825800	3.49301100
H	-5.23771200	0.54696300	3.45075600
C	4.01862400	-5.10896700	0.44953300
C	4.46115900	-3.82511400	0.11660600
C	3.98005800	-3.19604900	-1.04184900
C	3.06431000	-3.86380300	-1.86840900
C	2.63147000	-5.15159600	-1.53481300
C	3.10420200	-5.77347400	-0.37533300
H	4.39332300	-5.59331600	1.35520300
H	5.17842900	-3.30799400	0.75870700
H	2.68435200	-3.37155000	-2.76603300
H	1.91625000	-5.66632000	-2.18184900
H	2.76122100	-6.77791400	-0.11379200
Se	4.54516800	-1.39762800	-1.47448500
C	3.26350400	-0.44740100	-0.25654100
H	3.43383600	-0.82506100	0.76107400
H	3.56971500	0.60451500	-0.31969300
C	1.88484600	-0.67334300	-0.74154500
H	1.54277000	-0.07312300	-1.58575900
C	1.05625300	-1.62545400	-0.22900600
H	1.42268700	-2.30510700	0.54239000
H	0.12811500	-1.89452900	-0.73034300

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C	5.36413900	-3.51650900	0.82614000
C	4.22543100	-4.30986200	0.63008700
C	3.00412500	-3.72447100	0.30434800
C	2.88007100	-2.32348300	0.16693100
C	4.03624900	-1.53965900	0.36520200
C	5.26074600	-2.13006500	0.69093700
H	6.32191200	-3.97853800	1.07889200
H	4.29326800	-5.39686900	0.72757800
H	2.13269800	-4.36376900	0.14391100
H	3.97967600	-0.45303100	0.27230600
H	6.14021400	-1.49774200	0.84077500
C	1.60493500	-1.68682800	-0.17104600
N	-0.63503700	-1.31314900	-0.47216200
S	-2.10382700	-1.82210300	-1.16179400
O	-2.24436900	-1.21291800	-2.49057300
O	-2.15754500	-3.27724600	-0.98705900
C	-3.31957900	-1.07383600	-0.08303700
C	-4.27778100	-0.21603500	-0.62165700
C	-3.31605900	-1.39720500	1.27897600
C	-5.24059700	0.34039700	0.22568100
H	-4.26222900	0.01599100	-1.68784200
C	-4.28057000	-0.83125600	2.10704900
H	-2.56339800	-2.07635700	1.68456700
C	-5.25752600	0.04696300	1.59707800
H	-5.99138400	1.01677800	-0.19109600
H	-4.28119400	-1.07319700	3.17357100
C	-6.28882500	0.64507500	2.51778600
H	-5.80874300	1.21785200	3.32893600
H	-6.97391000	1.31970900	1.98384000
H	-6.89237000	-0.14385600	2.99747000
C	0.37961000	-2.25142900	-0.19471200
H	0.09248600	-3.28232200	0.00246600
C	2.66734400	3.22955400	2.08579500

C	1.49464000	3.14160500	1.33048500
C	1.56507800	3.05283000	-0.06813800
C	2.81401100	3.08735900	-0.70423100
C	3.98413300	3.19587000	0.05553600
C	3.91438300	3.25641900	1.45075400
H	2.60581500	3.28597200	3.17588200
H	0.52276000	3.13606200	1.83013800
H	2.87272500	3.01120600	-1.79256300
H	4.95449400	3.21997900	-0.44750100
H	4.82990200	3.32863500	2.04341900
Se	-0.04447700	2.89604800	-1.13382700
C	-0.73992800	1.18382400	-0.42846700
H	-0.74333100	1.21943100	0.67085100
H	-1.78377500	1.17927000	-0.77095500
C	0.00398600	-0.04374100	-0.94080300
H	-0.01548500	-0.04163200	-2.04317200
C	1.45709000	-0.20205800	-0.43560700
H	1.61211800	0.36670700	0.49688100
H	2.18113300	0.19034200	-1.16384400

TS6

C	-0.35434500	4.52310100	-2.74681300
C	0.20842200	3.33762300	-3.22798500
C	0.50192500	2.28531000	-2.35853600
C	0.22603400	2.37371400	-0.97648000
C	-0.33607900	3.58032100	-0.51196900
C	-0.61778900	4.63606000	-1.37794400
H	-0.57540400	5.34984200	-3.42693900
H	0.43609000	3.23029800	-4.29232800
H	0.95390900	1.38487700	-2.77437300
H	-0.57116900	3.68451300	0.54742400
H	-1.05628100	5.55444500	-0.97752000
C	0.51070500	1.23765600	-0.04938300
N	1.79369100	-0.82958300	0.12677500
S	2.27432100	-2.21893900	-0.66682300
O	2.27214100	-3.31179300	0.32716100
O	1.58698600	-2.41653500	-1.95652700
C	3.99199200	-1.82949000	-1.01785600
C	4.97539900	-2.12161000	-0.06973500
C	4.31579800	-1.18864900	-2.21586200
C	6.29454800	-1.74493500	-0.32051600
H	4.70658300	-2.65024500	0.84655400
C	5.64110900	-0.81956000	-2.45181700
H	3.53784300	-0.99088500	-2.95584500
C	6.64907000	-1.08180400	-1.50822500
H	7.06680100	-1.97160300	0.41984300
H	5.89850600	-0.31982300	-3.38977500
C	8.06960600	-0.63711000	-1.74269300
H	8.27639100	-0.47377700	-2.81112800
H	8.26806800	0.31473700	-1.21853000
H	8.79327300	-1.37342400	-1.35915000
C	1.05329100	0.03025800	-0.54409600
H	0.82155000	-0.20226100	-1.59256000
Rh	-3.88491100	-0.97147400	-0.17801800
Rh	-1.66819300	0.01865400	-0.03586100
C	-3.07338800	-0.17940100	2.50178100
O	-1.94312100	0.14154100	2.01144300
O	-4.03221500	-0.69578100	1.86310700
C	-3.28436900	0.05869800	3.97751000
H	-2.47373300	0.66380800	4.40263000
H	-4.24977000	0.56335200	4.13020000
H	-3.33798900	-0.91031100	4.49926600
C	-1.74768300	-2.89657300	0.09786000
O	-3.01171500	-2.81814200	0.06764500
O	-0.95188800	-1.90847200	0.10215900
C	-1.13128300	-4.27133900	0.15962700
H	-1.65422200	-4.94197700	-0.53731900
H	-0.06045300	-4.22606300	-0.07374400
H	-1.26767800	-4.68148700	1.17408700
C	-2.51678500	-0.70197100	-2.71451800
O	-1.57721600	-0.13266300	-2.07635700
O	-3.58607800	-1.14690000	-2.20432200
C	-2.30853300	-0.87170900	-4.19648900
H	-1.55012700	-1.65635000	-4.35277300
H	-3.24164900	-1.16252500	-4.69534400
H	-1.91443500	0.06149900	-4.62468600
C	-3.85315700	1.90684800	-0.39920800
O	-4.64154500	0.91794500	-0.45841900
O	-2.60524600	1.84111800	-0.18262800
C	-4.42147900	3.28343100	-0.63109300
H	-4.00606500	3.98869200	0.10301700
H	-4.10499200	3.62526800	-1.62998400
H	-5.51767800	3.27158100	-0.58015300

C	4.95600000	2.10069000	0.52536500
C	3.56577100	1.96263000	0.50246100
C	2.85181700	1.89584400	1.70664500
C	3.54078800	1.97602800	2.92872300
C	4.93138500	2.11549700	2.94194300
C	5.64522900	2.17389900	1.74023700
H	5.50310300	2.14667900	-0.41967300
H	3.04310800	1.90556700	-0.45283400
H	2.99285900	1.93227000	3.87524900
H	5.45824500	2.17678100	3.89813400
H	6.73305500	2.27830600	1.75077200
C	1.73735700	-1.25611400	2.65779000
H	1.76851900	-0.41939100	3.35361900
H	2.67264300	-1.55291100	2.19412800
Se	0.93459300	1.66721800	1.79243100
C	0.61732800	-2.10456500	2.62337300
H	0.65722800	-2.96236000	1.95351700
C	-0.47973500	-1.84338000	3.38467800
H	-0.53177400	-0.95656800	4.01949700
H	-1.34030000	-2.51787600	3.39360000

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C	-3.07658100	2.89857500	2.70759300
C	-2.10366900	2.04266700	3.23276700
C	-1.08114500	1.55684600	2.41494900
C	-1.01135500	1.92469700	1.05758400
C	-2.00162500	2.77846200	0.53825100
C	-3.02082300	3.26424700	1.35797100
H	-3.88108400	3.27355000	3.34562600
H	-2.14622800	1.74130100	4.28271100
H	-0.33786500	0.86689500	2.82116900
H	-1.96535900	3.05959000	-0.51636800
H	-3.77906300	3.93126500	0.93957700
C	0.08870800	1.39698200	0.21402800
N	2.44246100	0.78737400	-0.06094500
S	3.11769000	-0.56854100	0.73970800
O	4.27555800	-0.98365700	-0.06190400
O	3.28602000	-0.28691100	2.17371800
C	1.81184800	-1.77665500	0.56261500
C	1.46667300	-2.22553200	-0.71709200
C	1.20137500	-2.29651600	1.70371700
C	0.48471100	-3.20336900	-0.84328200
H	1.95450500	-1.80423100	-1.59685700
C	0.22154400	-3.28262400	1.55671500
H	1.49518600	-1.93122100	2.68900800
C	-0.15302600	-3.74831500	0.28731700
H	0.19599000	-3.54796000	-1.83980800
H	-0.26345900	-3.69154500	2.44697100
C	-1.23577000	-4.77971000	0.11542100
H	-2.10203000	-4.34248500	-0.40938500
H	-0.88414800	-5.62888400	-0.49343600
H	-1.58653000	-5.17234700	1.08118800
C	1.36101500	1.36666800	0.66228500
H	1.60154300	1.81751600	1.63402900
C	-4.17715200	-0.77382000	-1.95482700
C	-2.99648100	-0.05203500	-2.15853800
C	-1.95126300	-0.14543100	-1.22842500
C	-2.09496700	-0.95737900	-0.09419900
C	-3.28691800	-1.65546100	0.11438000
C	-4.32895500	-1.57128400	-0.81601000
H	-4.98794100	-0.69849400	-2.68443100
H	-2.89462900	0.59148200	-3.03639300
H	-1.27864000	-1.04609200	0.62305600
H	-3.39465500	-2.27719000	1.00701800
H	-5.25790700	-2.12341600	-0.65219800
Se	-0.30432700	0.79904900	-1.58047600
C	2.48657400	3.56738400	-2.12088600
H	2.61330800	4.30710300	-1.32239700
H	2.06520700	3.92422100	-3.06546300
C	2.83265200	2.28959100	-1.94772700
H	2.67837400	1.56203700	-2.75335600
C	3.40499100	1.72812800	-0.67794300
H	4.32022900	1.15856600	-0.89732200
H	3.66724900	2.53555300	0.03003800

TS7

C	-3.92712500	3.85664800	-0.41826200
C	-2.63502700	4.07815900	0.06966800
C	-1.69786500	3.04333300	0.07535500
C	-2.02874300	1.76257600	-0.41773100
C	-3.33349200	1.55878800	-0.91423000
C	-4.26977700	2.59224900	-0.91099600

H	-4.66301100	4.66491000	-0.41587600
H	-2.35633100	5.06126500	0.45849500
H	-0.69742000	3.21635600	0.47922600
H	-3.60723800	0.58287700	-1.31691800
H	-5.27377200	2.41076200	-1.30362700
C	-1.00556000	0.70695000	-0.43184600
N	1.17026300	-0.08314100	-0.93125000
S	2.66043700	0.22608900	-1.60781600
O	3.06315200	-0.98041600	-2.35362500
O	2.71496600	1.52730700	-2.30373300
C	3.70669700	0.34426600	-0.15160500
C	3.69934800	-0.68416800	0.79936100
C	4.54130200	1.45142100	-0.00379800
C	4.54246100	-0.59172300	1.90328600
H	3.02431600	-1.53440400	0.68432100
C	5.38408600	1.52629900	1.10966800
H	4.52414100	2.24371300	-0.75419900
C	5.40086300	0.51156800	2.07738700
H	4.53604500	-1.38942500	2.65183100
H	6.03987400	2.39355500	1.22571900
C	6.30547100	0.58467000	3.28055400
H	5.72423400	0.54041100	4.21704700
H	7.00720200	-0.26648300	3.29948500
H	6.89785100	1.51153400	3.29242500
C	0.27775300	0.91123400	-0.92532400
H	0.51680700	1.88317400	-1.38127400
C	-5.31635200	-1.99861000	0.73700300
C	-4.02136600	-1.95414300	0.20945000
C	-3.07278900	-1.08442400	0.76411100
C	-3.41695800	-0.26698900	1.85067500
C	-4.71474500	-0.31002100	2.36499500
C	-5.66577100	-1.17428100	1.81066600
H	-6.05537000	-2.67536400	0.30016000
H	-3.75648800	-2.58683300	-0.64165200
H	-2.67763700	0.40953900	2.28423400
H	-4.98323900	0.33541000	3.20528000
H	-6.67998100	-1.20503500	2.21690200
Se	-1.26435500	-1.10512600	0.07289500
C	0.69094200	-4.05541000	-0.31867600
H	-0.37161800	-4.30411900	-0.22646300
H	1.38178000	-4.55595000	0.36510300
C	1.13630700	-3.16116000	-1.25085600
H	2.19456800	-2.88897300	-1.28268200
C	0.30069400	-2.49516100	-2.16691500
H	0.73712300	-1.79964400	-2.88220200
H	-0.73966000	-2.79599700	-2.30273600

TS8

C	-4.45922000	-0.83850600	2.69695000
C	-3.12938300	-0.69990600	3.10371900
C	-2.17330200	-0.18049300	2.22791600
C	-2.52566300	0.21813400	0.92212900
C	-3.86660400	0.05280300	0.52230100
C	-4.82160400	-0.46205700	1.39892300
H	-5.20612400	-1.24752400	3.38217300
H	-2.82716300	-1.01023600	4.10750500
H	-1.13419200	-0.11159400	2.55556000
H	-4.15670300	0.32379300	-0.49470900
H	-5.85640600	-0.57375200	1.06442600
C	-1.50186400	0.75973000	-0.01140800
N	0.60910300	1.85626700	-0.31604900
S	2.02907700	2.36011100	0.47140800
O	2.72084600	3.26943900	-0.44893800
O	1.76935100	2.78780400	1.86005900
C	2.90345500	0.79722700	0.50883500
C	3.48895500	0.32405900	-0.67018700
C	2.90752100	0.03763100	1.67832600
C	4.07383600	-0.93959500	-0.66975500
H	3.47071400	0.93836700	-1.57204800
C	3.50116100	-1.22740200	1.65979800
H	2.44779500	0.43376700	2.58560200
C	4.08408300	-1.73829900	0.48953800
H	4.52464000	-1.32276900	-1.58936200
H	3.50444500	-1.83026400	2.57176000
C	4.69702200	-3.11396600	0.45332300
H	5.77457000	-3.06099400	0.22287200
H	4.58187500	-3.64011600	1.41244200
H	4.23196300	-3.73017400	-0.33415200
C	-0.36227700	1.40175300	0.47781200
H	-0.35342100	1.67546800	1.54432700
C	-1.25996500	-4.18830300	-1.16745500
C	-1.67596800	-2.90783900	-1.55005700
C	-0.88707500	-1.79348200	-1.23396700
C	0.31466800	-1.96318500	-0.52870000

C	0.71316300	-3.24255300	-0.13306700
C	-0.06951600	-4.35773900	-0.45460700
H	-1.87883300	-5.05440300	-1.41715200
H	-2.61966200	-2.77433500	-2.08423700
H	0.93834800	-1.10014600	-0.28927400
H	1.64655900	-3.36335600	0.42209900
H	0.24801100	-5.35768800	-0.14737300
Se	-1.44699800	-0.02608600	-1.80390500
C	-2.39375200	2.89748100	-0.70352600
H	-2.40140200	3.23683500	0.33459100
H	-3.32770600	2.46936900	-1.07235300
C	-1.39920600	3.30770300	-1.57688600
H	-1.47466600	3.02616900	-2.63214300
C	-0.17912700	3.77852600	-1.10233900
H	0.65001200	3.99450300	-1.77668700
H	-0.11130500	4.22206300	-0.10596300

INT5

C	-2.17116400	-1.20757400	0.00000300
C	-0.77340400	-1.21558700	0.00002000
C	-0.06796800	-0.00004300	-0.00002700
C	-0.77335900	1.21556200	0.00000000
C	-2.17109500	1.20761400	0.00002400
C	-2.87645100	0.00002500	-0.00002200
H	-2.71101100	-2.15847700	0.00000200
H	-0.23657300	-2.16772600	0.00002500
H	-0.23645600	2.16766200	0.00000100
H	-2.71093200	2.15852200	0.00002100
H	-3.96917100	0.00007000	-0.00003500
Se	1.84896400	-0.00000100	0.00000000

INT6

C	-5.89857300	0.19602100	-1.22066800
C	-5.49049300	1.27709300	-0.42966600
C	-4.25069100	1.25925600	0.20220400
C	-3.36111400	0.15905900	0.05794800
C	-3.80252400	-0.92725200	-0.75008500
C	-5.04551900	-0.90581400	-1.37236300
H	-6.87432300	0.20937600	-1.71248400
H	-6.14671000	2.14215400	-0.30492000
H	-3.95886000	2.11916000	0.80590800
H	-3.17331900	-1.80887500	-0.87689000
H	-5.35746200	-1.75935700	-1.97949700
C	-2.06812500	0.15980100	0.71510500
N	0.09443300	-0.80055400	0.97212800
S	1.26106500	-1.90346200	0.40454900
O	1.73273700	-2.64654700	1.57690600
O	0.78834600	-2.63345200	-0.78711700
C	2.52514700	-0.74343000	-0.09765500
C	3.40836600	-0.24325300	0.86505600
C	2.58659900	-0.32560800	-1.42783900
C	4.36066700	0.69759500	0.47963600
H	3.34478500	-0.59542000	1.89625700
C	3.54941800	0.61649300	-1.79537100
H	1.89152800	-0.73879200	-2.16110200
C	4.44639000	1.14451100	-0.85254500
H	5.05612500	1.09422900	1.22477100
H	3.60493400	0.94725700	-2.83591000
C	5.49300700	2.15426200	-1.24594000
H	5.46223800	3.03666700	-0.58570800
H	6.50528800	1.72372000	-1.15706700
H	5.36331100	2.49724400	-2.28300700
C	-1.05988400	-0.79080900	0.36346200
H	-1.24892100	-1.49743000	-0.45708400
C	0.30109100	2.64844700	1.05002000
H	0.99134700	2.01265100	1.61351900
H	0.73280200	3.49446200	0.50608900
C	-1.00994300	2.39603200	1.01348300
H	-1.66679600	3.03510900	0.40988000
C	-1.68112000	1.23001200	1.71143900
H	-0.98290100	0.79358700	2.43889400
H	-2.56599800	1.57902000	2.26502900

INT7

C	1.23241500	-0.19651200	-0.00011500
H	1.30166300	-1.28949700	0.00031300
H	2.16754200	0.36938000	0.00024100
C	-0.00008100	0.44286700	0.00003400
H	0.00003500	1.54076400	-0.00007600
C	-1.23223600	-0.19641500	0.00001000
H	-1.30217800	-1.28937600	-0.00014400
H	-2.16765000	0.36909200	0.00009000

INT8

C	-2.11963300	-1.23749900	-0.00000700
C	-0.74271000	-1.25147500	-0.00000400
C	-0.01206400	0.00000000	-0.00000100
C	-0.74271000	1.25147500	-0.00000600
C	-2.11963300	1.23749900	-0.00000800
C	-2.80444900	0.00000000	-0.00000800
H	-2.68515800	-2.17120900	-0.00000900
H	-0.18281000	-2.18909700	-0.00000400
H	-0.18280900	2.18909600	-0.00000700
H	-2.68515700	2.17120900	-0.00001000
H	-3.89889200	0.00000000	-0.00001000
Se	1.79064800	0.00000000	0.00000700

INT9

C	-5.65745400	-0.53267100	1.48595100
C	-5.26639400	-1.43794700	0.49465500
C	-4.09311100	-1.23927800	-0.23649800
C	-3.24463800	-0.12055600	-0.01662400
C	-3.67784000	0.79156300	0.98718600
C	-4.84319700	0.58526600	1.72059100
H	-6.57623600	-0.68732800	2.05807600
H	-5.88062700	-2.32032600	0.28753500
H	-3.82022300	-1.98321100	-0.98737300
H	-3.09470700	1.69466600	1.17806200
H	-5.13101500	1.31986600	2.47966400
C	-2.01631800	0.07365800	-0.78737300
N	0.12948300	1.13179900	-1.05278800
S	1.31595700	1.97383300	-0.34087200
O	2.04968900	2.73077500	-1.37427200
O	0.89848400	2.70633800	0.88452400
C	2.45160000	0.67719300	0.21407200
C	3.28559300	0.05086600	-0.71977200
C	2.44726200	0.26074600	1.54520900
C	4.10344000	-1.00165000	-0.31442400
H	3.28493600	0.40108400	-1.75404200
C	3.27382600	-0.79659200	1.94024700
H	1.79880900	0.77158000	2.25982600
C	4.10966500	-1.44762400	1.02116000
H	4.75383000	-1.49159800	-1.04615500
H	3.26771800	-1.12078900	2.98545900
C	4.99630400	-2.59606500	1.43529600
H	4.72826200	-3.52112000	0.89596900
H	6.05568600	-2.38876700	1.20567900
H	4.91978100	-2.80361800	2.51359000
C	-1.01122000	0.91907600	-0.35920700
H	-1.13454000	1.44715600	0.59806100
C	0.33467800	-2.14601000	-2.09023400
H	0.89048700	-1.36208900	-2.61437400
H	0.88743000	-3.04833500	-1.80752700
C	-0.95245400	-1.97802100	-1.76918200
H	-1.46655000	-2.76460600	-1.19930300
C	-1.75899300	-0.73365400	-2.05255400
H	-1.20274400	-0.10483500	-2.76477600
H	-2.71186500	-1.00836700	-2.53791000

TS9

C	4.78732600	1.20354600	-3.22459800
C	4.65927200	-0.07409500	-2.67777000
C	3.60583100	-0.36953600	-1.80475400
C	2.66598900	0.61334600	-1.45927700
C	2.80554700	1.89941300	-2.01732900
C	3.85200500	2.19102900	-2.89109300
H	5.61026800	1.43192400	-3.90670900
H	5.38422600	-0.85347600	-2.92638700
H	3.53996400	-1.37483900	-1.38981500
H	2.09519600	2.68426700	-1.74754800
H	3.93979900	3.19609400	-3.31155800
C	1.52686900	0.34576300	-0.47824300
N	-0.31792500	1.93098100	-0.58246400
S	-1.75309900	2.48180200	-1.37663000
O	-1.49771700	3.88160600	-1.72115200
O	-2.17311700	1.52562800	-2.41528700
C	-2.88731500	2.39726000	-0.00302300
C	-3.05071300	3.52060000	0.81315700
C	-3.56618000	1.20400500	0.24943800
C	-3.91510800	3.43537000	1.90268900
H	-2.50974700	4.44137800	0.58802700
C	-4.42477900	1.13874800	1.34765100
H	-3.43212800	0.34218700	-0.40480200
C	-4.61305200	2.24720500	2.18960700
H	-4.05338100	4.30839800	2.54658000

H	-4.95967900	0.20714600	1.54963200
C	-5.54171900	2.18296500	3.37380500
H	-5.00775200	2.42714200	4.30737100
H	-6.35964800	2.91619200	3.27229800
H	-5.99166800	1.18594900	3.48875800
C	0.25925600	0.90703100	-1.06945700
H	-0.13508600	0.37131700	-1.95240700
C	5.83451900	-0.01518700	1.60147600
C	4.69525300	0.70823700	1.23514400
C	3.44337300	0.36352000	1.76858600
C	3.34477800	-0.70069300	2.67922100
C	4.48855800	-1.41693000	3.04677100
C	5.73338100	-1.07701300	2.50634900
H	6.80537900	0.25506800	1.17786000
H	4.77441800	1.53729500	0.52932000
H	2.36991900	-0.96917400	3.09296100
H	4.40556700	-2.24388800	3.75718100
H	6.62627100	-1.63886200	2.79311800
Se	1.86153900	1.35638100	1.26624300
C	0.00869600	-2.62025200	1.43895200
H	0.90855900	-3.20480000	1.66172100
H	-0.79269200	-2.70681800	2.17717600
C	0.14802500	-1.41805800	0.74723400
H	-0.69830000	-0.72425500	0.73769200
C	1.29788600	-1.14601200	-0.17069700
H	2.21689100	-1.58581800	0.24504300
H	1.12479100	-1.67638600	-1.12953600
C	-3.29340500	-1.57511300	-2.24753800
C	-2.18948000	-2.30231300	-1.79345300
C	-2.32411400	-3.21510900	-0.73106000
C	-3.58529400	-3.38745100	-0.13159600
C	-4.68999900	-2.66812200	-0.59681400
C	-4.54714000	-1.76166100	-1.65395500
H	-3.16685300	-0.84324700	-3.04751200
H	-1.21488000	-2.16520000	-2.26729600
H	-3.69681700	-4.09105600	0.69681300
H	-5.66757000	-2.81534800	-0.12941300
H	-5.40952500	-1.19166900	-2.00885200
Se	-0.80958000	-4.22008700	-0.11628500

INT4

C	-4.79339400	-1.17187200	-3.22398200
C	-4.69621200	0.08803200	-2.63137200
C	-3.64167500	0.38213400	-1.75940800
C	-2.66928800	-0.58439100	-1.46011100
C	-2.77871200	-1.85295100	-2.06315900
C	-3.82618900	-2.14282600	-2.93648800
H	-5.61706100	-1.39924700	-3.90558600
H	-5.44670800	0.85413000	-2.84283500
H	-3.60031100	1.37250100	-1.30705700
H	-2.04390600	-2.62676400	-1.82988700
H	-3.88962000	-3.13413800	-3.39254000
C	-1.53028400	-0.31685100	-0.47856900
N	0.32559900	-1.88548900	-0.62718000
S	1.76433400	-2.40259900	-1.43373400
O	1.50849000	-3.78460400	-1.84457300
O	2.19536700	-1.40149000	-2.42478900
C	2.88928000	-2.38608700	-0.04982100
C	3.04597500	-3.54829600	0.71134100
C	3.56747600	-1.20764900	0.26579600
C	3.90247200	-3.51765000	1.80989400
H	2.50586100	-4.45621900	0.43739700
C	4.41878700	-1.19737700	1.37163600
H	3.43768600	-0.31458600	-0.34585500
C	4.59949600	-2.34596200	2.15980100
H	4.03533200	-4.42143500	2.41111100
H	4.95366000	-0.27759300	1.62230400
C	5.51752000	-2.34142300	3.35407200
H	4.97079400	-2.61508900	4.27202800
H	6.32674100	-3.08097600	3.23158100
H	5.97905100	-1.35593400	3.51349900
C	-0.25431400	-0.84696100	-1.07959500
H	0.14281500	-0.27748100	-1.93969900
C	-5.84116200	-0.06549600	1.63544900
C	-4.69516800	-0.76874100	1.25103000
C	-3.44240500	-0.40886200	1.77223600
C	-3.34984500	0.65120900	2.68857700
C	-4.49982000	1.34803500	3.07349600
C	-5.74565300	0.99229000	2.54557000
H	-6.81267300	-0.34788700	1.22130500
H	-4.76952200	-1.59373600	0.53991400

H	-2.37428000	0.93114400	3.09318000
H	-4.42118200	2.17194900	3.78795300
H	-6.64356000	1.53875000	2.84614300
Se	-1.85213300	-1.37316000	1.24295400
C	0.05580400	2.78520900	1.29213200
H	-0.86864600	3.29069200	1.61357500
H	0.80870400	2.82168900	2.08916700
C	-0.16014900	1.45637800	0.74547500
H	0.65139300	0.72714000	0.81758000
C	-1.32224500	1.17227300	-0.14719400
H	-2.24218100	1.58310500	0.30072500
H	-1.19981100	1.72515300	-1.10264500
C	3.46264600	1.60670300	-2.10589000
C	2.29665600	2.27199000	-1.71328300
C	2.33296500	3.20600200	-0.66552400
C	3.54942600	3.46880200	-0.01509900
C	4.71466900	2.80548700	-0.41328600
C	4.67345600	1.87613900	-1.45883400
H	3.41273000	0.85673100	-2.89732900
H	1.35413100	2.06546100	-2.22487700
H	3.58214400	4.19585600	0.79991800
H	5.65920100	3.01832800	0.09486500
H	5.58358300	1.35359500	-1.76437800
Se	0.72582600	4.14021600	-0.14013000

TS10

C	-0.17376500	-3.25867600	3.84080100
C	1.06947700	-3.03021100	3.23787100
C	1.15140600	-2.32856100	2.03517600
C	-0.00833600	-1.83618900	1.40780500
C	-1.24975200	-2.07017100	2.02281200
C	-1.33143400	-2.77521500	3.22796600
H	-0.23633400	-3.80932200	4.78301000
H	1.98363900	-3.40121600	3.70900700
H	2.12881900	-2.17241400	1.57543400
H	-2.16602700	-1.70301600	1.55807100
H	-2.30908800	-2.94670500	3.68591200
C	0.08130800	-1.09899400	0.09511200
N	-0.82713300	0.98881900	-0.54337400
S	-1.96908500	1.87494600	-1.47422500
O	-1.16871600	2.73352200	-2.35581500
O	-3.00300200	0.99056500	-2.04036000
C	-2.71577900	2.88911900	-0.20574000
C	-2.03438000	4.02507900	0.24438800
C	-3.95354700	2.52519900	0.32459800
C	-2.60713600	4.79619000	1.25285300
H	-1.07498500	4.29864100	-0.19850600
C	-4.51317900	3.31319400	1.33324400
H	-4.47043900	1.64199600	-0.05506300
C	-3.85182800	4.45383300	1.81513300
H	-2.08271600	5.68646800	1.61137100
H	-5.48454800	3.03632400	1.75137000
C	-4.44837900	5.30580800	2.90508900
H	-5.41914100	4.91665700	3.24550000
H	-3.77605200	5.35626600	3.77809100
H	-4.59935200	6.34172500	2.55762500
C	-1.09587700	-0.27602900	-0.29977000
H	-2.04080100	-0.73841700	-0.60568500
C	-3.78718200	-3.69751800	-1.66259100
C	-2.57124100	-3.03991900	-1.87448300
C	-1.42749900	-3.43411900	-1.15924500
C	-1.50963800	-4.49232400	-0.23942800
C	-2.72789400	-5.14665600	-0.03544700
C	-3.86673500	-4.75030900	-0.74479000
H	-4.67442700	-3.38383900	-2.21882300
H	-2.51141300	-2.21315500	-2.58577900
H	-0.62227600	-4.79486900	0.31990800
H	-2.78640700	-5.96772300	0.68390200
H	-4.81834500	-5.26349000	-0.58267400
Se	0.24616500	-2.52324200	-1.43365700
C	1.34693900	-0.21115600	-0.06238700
H	2.23040300	-0.84437400	-0.24831300
H	1.52944500	0.29960100	0.89555200
C	1.75638100	2.15262100	-1.03145100
H	1.63436900	2.57868900	-0.02559200
H	1.33635200	2.84150800	-1.77685700
C	1.18123100	0.80853900	-1.14971300
H	1.02858100	0.42859800	-2.16510100
C	4.51747500	0.75073800	2.45582200
C	4.11969200	1.54847500	1.37941500
C	4.34333300	1.11751500	0.06209100
C	4.99543800	-0.10447700	-0.16401800
C	5.41068200	-0.88965000	0.91712700

C	5.16410000	-0.46959500	2.22821900
H	4.32740200	1.08802400	3.47827000
H	3.62710000	2.50633100	1.56388400
H	5.16191500	-0.44926000	-1.18737500
H	5.91731700	-1.84051300	0.73110300
H	5.47773500	-1.08970000	3.07193000
Se	3.74721800	2.17690000	-1.44070500

TS11

C	-5.33059800	2.46047000	-0.22512300
C	-5.54369500	1.26816400	0.47011300
C	-4.49814500	0.36067200	0.65736100
C	-3.20259200	0.61846900	0.15528300
C	-3.00744100	1.83757200	-0.53880400
C	-4.05194300	2.73758500	-0.72801400
H	-6.14860100	3.16992300	-0.37325200
H	-6.53336200	1.03852100	0.87405300
H	-4.69731900	-0.55764800	1.21178100
H	-2.02287300	2.08539300	-0.93997500
H	-3.86837100	3.66768200	-1.27263200
C	-2.11386000	-0.33981700	0.36213300
N	0.08936700	-1.10602500	0.36268700
S	1.40592500	-1.48435000	-0.64691200
O	1.95126900	-2.74251500	-0.12448000
O	1.05301200	-1.35641300	-2.07022800
C	2.53637700	-0.15797600	-0.22926400
C	3.18194600	-0.18065400	1.01300800
C	2.75771100	0.87220200	-1.14353800
C	4.05219700	0.85609300	1.33726900
H	3.00291000	-1.00439200	1.70659600
C	3.63745200	1.90274600	-0.80087700
H	2.25438100	0.85553300	-2.11192400
C	4.29431900	1.91415400	0.43915000
H	4.56144500	0.84729600	2.30513200
H	3.81868900	2.71084000	-1.51460300
C	5.24907600	3.01789300	0.81263500
H	4.95981800	3.48538100	1.76858000
H	6.27106600	2.62393400	0.94590300
H	5.28769900	3.80490500	0.04519200
C	-0.82824800	-0.18103000	-0.06286700
H	-0.50822300	0.62136500	-0.73536400
C	-1.11799500	-3.52026800	-0.14839000
H	-1.78727000	-3.42084200	-1.00873900
H	-0.31715200	-4.25943700	-0.20553600
C	-1.17110900	-2.61604200	0.90259300
H	-0.57853700	-2.84179000	1.79115600
C	-2.35159200	-1.66842800	1.07195900
H	-3.26089300	-2.14268100	0.66924100
H	-2.53918700	-1.49161000	2.14606000

INT10

C	-6.43584000	-0.14924300	0.92718800
C	-5.90058300	-1.28775800	0.32071700
C	-4.55183800	-1.32712800	-0.04473600
C	-3.69988300	-0.22717800	0.18751500
C	-4.26048600	0.91771900	0.79869800
C	-5.60426200	0.95400500	1.16337200
H	-7.49060400	-0.11699400	1.21181200
H	-6.53603000	-2.15669200	0.12871600
H	-4.15683700	-2.23115100	-0.51292400
H	-3.63654200	1.79536200	0.98307400
H	-6.01067500	1.85404700	1.63286200
C	-2.28828900	-0.28498000	-0.20144600
N	-0.05020800	0.18294600	-0.35308100
S	1.15372100	1.34667700	-0.67611900
O	1.30971500	1.49669600	-2.12839200
O	0.82914100	2.50095200	0.16912400
C	2.62084900	0.55479300	-0.03638000
C	3.57092000	0.04497100	-0.92100000
C	2.78972800	0.46360000	1.34949200
C	4.70867900	-0.57847400	-0.40260300
H	3.41502500	0.13604500	-1.99684100
C	3.92847100	-0.16418300	1.84669800
H	2.03839100	0.87978300	2.02343000
C	4.90532200	-0.69570000	0.98207200
H	5.45678200	-0.98183200	-1.09012100
H	4.06887500	-0.24294200	2.92832700
C	6.13978200	-1.35012100	1.54490000
H	6.69899400	-1.90098700	0.77425800
H	6.81915300	-0.59375300	1.97512600
H	5.88649700	-2.05160700	2.35608600
C	-1.31189900	0.59359300	0.11192100
H	-1.37596700	1.51325600	0.69045000

C	0.84003100	-1.96101700	-1.23880000
H	1.18184500	-2.30544900	-0.25938900
H	1.20860000	-2.45914800	-2.13783700
C	-0.23613200	-0.94147800	-1.32196300
H	-0.27159800	-0.50832000	-2.33651900
C	-1.66384500	-1.45213400	-0.94502400
H	-2.22162300	-1.75632300	-1.84353400
H	-1.59755700	-2.33765300	-0.28708400

TS12

C	0.57029600	5.35175800	-1.36312900
C	1.73318100	4.56624900	-1.32007500
C	1.63028600	3.19155400	-1.16312100
C	0.35569000	2.57219700	-1.01872500
C	-0.80775900	3.38795400	-1.05873300
C	-0.69430300	4.76190900	-1.23991200
H	0.65361100	6.43390000	-1.49506500
H	2.71495000	5.03588100	-1.41470300
H	2.53102000	2.57549900	-1.11788400
H	-1.78310300	2.91665800	-0.95951800
H	-1.59244300	5.38244900	-1.28062100
C	0.25385500	1.16563500	-0.80358300
N	2.17217600	-0.20270400	-0.20308900
S	3.04788400	-1.59088700	-0.69546900
O	2.64598800	-2.66582300	0.22436600
O	2.95761500	-1.81078000	-2.15133100
C	4.70841900	-1.07660800	-0.29016100
C	5.11280500	-1.08159600	1.04902500
C	5.56687700	-0.66161000	-1.30881900
C	6.39991800	-0.65150100	1.36304100
H	4.42633200	-1.42151400	1.82655900
C	6.85521800	-0.23859100	-0.97403800
H	5.22746700	-0.67759100	-2.34605100
C	7.29140100	-0.22443300	0.36062800
H	6.72496700	-0.64972500	2.40716000
H	7.53518900	0.08448300	-1.76684800
C	8.68746900	0.21140500	0.72234700
H	9.18804100	0.71999900	-0.11490100
H	8.68234800	0.89372100	1.58764600
H	9.30612700	-0.65872200	1.00317000
C	1.33942600	0.24643500	-1.07053400
H	1.29716300	-0.17403100	-2.09686200
Rh	-3.17261100	-1.41914900	0.46812100
Rh	-1.32993100	0.04485600	-0.24253300
C	-3.36735900	1.32066600	1.40911900
O	-2.24453000	1.53798300	0.84277100
O	-4.00145500	0.23216100	1.39006200
C	-3.94438900	2.47033300	2.19486500
H	-3.74865200	3.42228100	1.68157800
H	-5.02048200	2.32924700	2.35874400
H	-3.43881700	2.50704100	3.17438100
C	-0.93029300	-1.38105200	2.27922200
O	-2.09910800	-1.84467500	2.17129100
O	-0.36767300	-0.59269700	1.45228300
C	-0.09655600	-1.77722800	3.46900300
H	-0.66437200	-2.42268100	4.15063000
H	0.79887800	-2.30586800	3.10599500
H	0.24493800	-0.87243400	3.99483700
C	-1.08700900	-2.73976600	-1.05928000
O	-0.59195200	-1.57956400	-1.25363200
O	-2.16433800	-2.97364800	-0.44766900
C	-0.27315900	-3.88435000	-1.59729000
H	0.68766100	-3.89535200	-1.05692400
H	-0.79746700	-4.83967000	-1.47096400
H	-0.04082900	-3.70679200	-2.65806500
C	-3.59520400	-0.03894600	-2.05861000
O	-4.11135900	-0.89730900	-1.29347300
O	-2.48269300	0.55642300	-1.86640700
C	-4.32218200	0.30386100	-3.33376500
H	-3.88070000	-0.28621700	-4.15416600
H	-5.38729600	0.05126500	-3.25192100
H	-4.19114600	1.36767900	-3.57622800
C	1.68652300	1.75226100	2.31450600
H	1.65700800	0.66696600	2.21767500
H	2.66581400	2.24382200	2.31725900
C	0.51321300	2.49116100	2.36494100
H	-0.42596300	1.93160700	2.31901700
C	0.43668000	3.87605900	2.40597100
H	1.33916300	4.49650200	2.41609400
H	-0.52858600	4.38877900	2.41417800

INT11

C	-1.13531800	4.99272500	-1.93376200
C	-0.69146900	3.82539600	-2.56969100
C	-0.05298000	2.82739100	-1.84526100
C	0.16533900	2.95525900	-0.44360500
C	-0.29523600	4.14876600	0.17614700
C	-0.92885100	5.14635500	-0.55691600
H	-1.63946800	5.77508800	-2.50677500
H	-0.85371200	3.68926200	-3.64176300
H	0.24342700	1.92170200	-2.37010500
H	-0.15539100	4.29043400	1.24564400
H	-1.26787200	6.05333300	-0.05003400
C	0.84043200	1.92882100	0.33680000
N	2.31707800	0.04710400	0.33895300
S	3.10655000	-1.17527600	-0.54102300
O	2.87947900	-2.42507100	0.19868600
O	2.82849000	-1.10765000	-1.98738400
C	4.80496300	-0.67892900	-0.27846400
C	5.41093400	-0.94767400	0.95398900
C	5.49722600	-0.02769200	-1.30058000
C	6.72872300	-0.54547900	1.15785400
H	4.85287200	-1.46955600	1.73343500
C	6.81907900	0.36434500	-1.07872400
H	5.00472300	0.15956400	-2.25638800
C	7.45451400	0.11528800	0.14849900
H	7.21009400	-0.75045200	2.11828200
H	7.36783300	0.87138800	-1.87693300
C	8.88688000	0.51870900	0.38406300
H	9.25610600	1.19676600	-0.39958900
H	9.00644800	1.02010000	1.35812700
H	9.54454000	-0.36790500	0.39677000
C	1.55378400	0.86957100	-0.32848500
H	1.48207200	0.77198200	-1.41937600
Rh	-2.95241400	-1.66957700	0.10544600
Rh	-1.16769500	-0.07469700	-0.03850100
C	-3.64958000	0.99363400	1.01251900
O	-2.46538900	1.33470200	0.70424100
O	-4.13459700	-0.16850500	0.87267400
C	-4.52467500	2.05168500	1.62999200
H	-4.26771300	3.04129300	1.22846500
H	-5.58614700	1.82446500	1.46558300
H	-4.33459500	2.06435500	2.71651500
C	-1.28889700	-1.52181000	2.46584900
O	-2.30216000	-2.12589700	2.00078200
O	-0.63667500	-0.61578400	1.86070200
C	-0.79164100	-1.91688400	3.82948000
H	-1.56873900	-2.45028400	4.39173800
H	0.07798700	-2.58214700	3.69929100
H	-0.45291600	-1.02582900	4.37686900
C	-0.48923300	-2.73699800	-0.95809000
O	-0.01191000	-1.57089400	-0.80126300
O	-1.67553500	-3.07757700	-0.65948500
C	0.43149100	-3.76665700	-1.54653000
H	1.34537400	-3.80598300	-0.93640500
H	-0.05605000	-4.74781500	-1.60172100
H	0.73712500	-3.43404500	-2.55058300
C	-2.80985800	-0.25167400	-2.41522700
O	-3.49217600	-1.12457700	-1.79951300
O	-1.79990400	0.35542400	-1.94265700
C	-3.20218300	0.06932500	-3.83283100
H	-2.63373900	-0.59234600	-4.50771200
H	-4.27328600	-0.11499700	-3.98916400
H	-2.94519700	1.10969100	-4.07391100
C	1.06637000	2.05747700	1.83122300
H	1.50024500	1.10087000	2.15812200
H	1.85320900	2.81971200	1.98941400
C	-0.11322500	2.35108900	2.72342600
H	-1.02770000	1.80066600	2.49432500
C	-0.07557100	3.17147800	3.77816000
H	0.82348900	3.74337400	4.03633300
H	-0.94556700	3.29986800	4.42950100

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C	-2.23538800	-3.78794700	-1.51046100
C	-3.02405100	-2.81046700	-2.12964700
C	-2.70561800	-1.46006500	-1.99076000
C	-1.59103900	-1.05518900	-1.23560600
C	-0.80329100	-2.04307800	-0.62646200
C	-1.12472600	-3.39897400	-0.76054500
H	-2.48739700	-4.84641700	-1.61438300
H	-3.89661400	-3.10243100	-2.71992700
H	-3.33980000	-0.70252400	-2.45666000

H	0.08131100	-1.76825000	-0.04794900
H	-0.49785500	-4.15147700	-0.27521700
C	-1.23017400	0.42335400	-1.13034200
N	0.95603000	1.16216200	-0.34486200
S	1.98486300	1.48556900	1.00264500
O	2.42440900	2.87140100	0.82784900
O	1.35458400	1.05828400	2.26526700
C	3.33687300	0.38024100	0.63229800
C	4.28119100	0.76229000	-0.32318500
C	3.41965700	-0.85051100	1.29013900
C	5.32171900	-0.11586300	-0.62842200
H	4.20063000	1.73386100	-0.81402700
C	4.46850700	-1.71229400	0.97324700
H	2.67510400	-1.11656700	2.04278200
C	5.43328300	-1.36237400	0.01100700
H	6.06427900	0.17409700	-1.37646100
H	4.54406700	-2.67591800	1.48468600
C	6.57127300	-2.29945100	-0.29897500
H	7.09704200	-2.01417400	-1.22213000
H	7.31067800	-2.29686100	0.52088100
H	6.21725400	-3.33699900	-0.40903400
C	-0.18358900	0.65681000	-0.07386600
H	-0.45705300	0.37387600	0.95571400
C	-4.60548600	-1.06701200	2.04645300
C	-4.18111500	-0.41792600	0.88419300
C	-3.21820100	0.60171000	0.95922000
C	-2.70498800	0.97939900	2.21209700
C	-3.13243900	0.32539600	3.37087100
C	-4.08014200	-0.69989400	3.28965600
H	-5.35152500	-1.86309100	1.97865100
H	-4.59349400	-0.70322500	-0.08420700
H	-1.96498800	1.78003300	2.27713700
H	-2.72170700	0.62097900	4.33959800
H	-4.41318100	-1.21052600	4.19701700
C	-1.38811100	3.27528300	-3.40218200
H	-2.16875200	2.87017500	-4.05635600
H	-1.22637200	4.35708400	-3.43704700
C	-0.66724700	2.48943700	-2.59705900
H	0.10142000	2.92698900	-1.95229400
C	-0.82967500	0.99448300	-2.51776400
H	-1.57434500	0.66156900	-3.25516200
H	0.12515700	0.50502600	-2.77712900
S	-2.69807300	1.47493200	-0.52094500

INT5S

C	-1.53979200	-1.21689300	0.00000400
C	-0.14927700	-1.22247300	0.00000800
C	0.58045200	-0.00000600	-0.00003500
C	-0.14927500	1.22247200	0.00000600
C	-1.53977900	1.21690200	0.00000500
C	-2.23917700	-0.00000100	-0.00000800
H	-2.08874100	-2.16193700	0.00001600
H	0.40477400	-2.16356400	0.00002300
H	0.40480200	2.16354700	0.00002000
H	-2.08874800	2.16193400	0.00001900
H	-3.33228000	0.00001600	-0.00000900
S	2.30758000	0.00000000	0.00000400

TS1S

C	-4.85790900	-1.47642200	-2.94605600
C	-4.75733000	-0.13808300	-2.56329700
C	-3.71223900	0.28522700	-1.73358400
C	-2.75617600	-0.62875500	-1.26828600
C	-2.86509500	-1.97591300	-1.66279400
C	-3.90339300	-2.39563500	-2.49327700
H	-5.67427100	-1.80447100	-3.59462700
H	-5.49700700	0.58894400	-2.90838900
H	-3.66652000	1.33574200	-1.44787400
H	-2.13571000	-2.70344000	-1.29981900
H	-3.96870500	-3.44628200	-2.78737200
C	-1.62223000	-0.22388600	-0.31973600
N	0.29563500	-1.73349900	-0.40349500
S	1.72778900	-2.25071500	-1.22479200
O	1.52011900	-3.66976700	-1.51973000
O	2.07889700	-1.31184500	-2.30462500
C	2.89995400	-2.07948100	0.10861600
C	3.13168600	-3.16940100	0.95304200
C	3.54179400	-0.85509000	0.30150200
C	4.02641200	-3.01778200	2.01034200
H	2.61887300	-4.11608000	0.77447400
C	4.43213500	-0.72316800	1.36808100
H	3.35421900	-0.02013300	-0.37400600
C	4.68801800	-1.79640600	2.23746600

H	4.21802900	-3.86395500	2.67607700
H	4.93836100	0.23319500	1.52312800
C	5.64885800	-1.66087000	3.38958400
H	5.14995100	-1.88595400	4.34708500
H	6.48546600	-2.37292200	3.29008300
H	6.07101700	-0.64740700	3.45507300
C	-0.33787400	-0.75556700	-0.91276700
H	0.00767200	-0.23815500	-1.82619100
C	-5.78372800	-0.08875100	1.88475200
C	-4.61027300	-0.71476400	1.45538100
C	-3.36122400	-0.24033500	1.88880100
C	-3.30182200	0.85310300	2.76856900
C	-4.47920600	1.47048800	3.20118800
C	-5.72071000	1.00309300	2.75708800
H	-6.75182000	-0.46012200	1.53872400
H	-4.65662200	-1.57018200	0.77914300
H	-2.32864900	1.21814600	3.10465700
H	-4.42561400	2.32018300	3.88701200
H	-6.64051200	1.48797200	3.09462100
C	-0.21010200	2.97162100	1.27746200
H	-1.11586500	3.57088900	1.42140000
H	0.60355200	3.17815100	1.97717100
C	-0.32066000	1.70266400	0.72743800
H	0.54181700	1.03162400	0.79014800
C	-1.46818400	1.29948100	-0.14470200
H	-2.40435800	1.72602500	0.24604200
H	-1.32921200	1.75623500	-1.14472500
C	3.16398400	1.81413700	-2.25423000
C	1.99181500	2.47789600	-1.88659000
C	2.01443300	3.48630200	-0.90093800
C	3.24454800	3.81192000	-0.29244700
C	4.41703400	3.15384900	-0.66965700
C	4.38058800	2.15443800	-1.65012600
H	3.12026400	1.01139600	-2.99272600
H	1.04451200	2.22144300	-2.36592800
H	3.26868200	4.59004100	0.47417100
H	5.36526800	3.42160400	-0.19552200
H	5.29740800	1.63305300	-1.93689200
S	-1.84848300	-1.04937900	1.36583500
S	0.53129300	4.33311900	-0.44545400

INT1s

C	-4.84900700	-1.40884100	-2.97114500
C	-4.76089300	-0.08498400	-2.53796400
C	-3.71677500	0.31761900	-1.69687800
C	-2.74871700	-0.60275700	-1.27024500
C	-2.84650900	-1.93542900	-1.71379400
C	-3.88356600	-2.33439700	-2.55619100
H	-5.66443000	-1.72070600	-3.62884200
H	-5.50991600	0.64660100	-2.85195500
H	-3.68116100	1.35655600	-1.37028700
H	-2.10973800	-2.66923300	-1.37944800
H	-3.93948700	-3.37401900	-2.88894700
C	-1.61667100	-0.22063000	-0.31007300
N	0.30307400	-1.72663300	-0.41272200
S	1.74444200	-2.21983400	-1.22960500
O	1.55861900	-3.64020700	-1.53313400
O	2.08894300	-1.27126900	-2.30326700
C	2.90858700	-2.03979100	0.11031700
C	3.15684800	-3.13315600	0.94544700
C	3.52685500	-0.80561600	0.31759000
C	4.04421700	-2.97539500	2.00810000
H	2.66196200	-4.08717500	0.75566900
C	4.41031500	-0.66780600	1.38919300
H	3.32633400	0.03201800	-0.35078300
C	4.68227300	-1.74436600	2.24954900
H	4.24847200	-3.82425300	2.66664300
H	4.89875500	0.29591700	1.55533200
C	5.63523100	-1.60198000	3.40743500
H	5.13463900	-1.83986900	4.36098800
H	6.48254200	-2.30128600	3.30831500
H	6.04233300	-0.58293300	3.48125500
C	-0.32806000	-0.73816000	-0.90500300
H	0.02400600	-0.20113500	-1.80410100
C	-5.78611600	-0.11625200	1.89521600
C	-4.61719500	-0.74284600	1.45419100
C	-3.36419400	-0.28160100	1.89027900
C	-3.29677800	0.80043900	2.78369100
C	-4.46928200	1.41924600	3.22722700
C	-5.71466600	0.96414700	2.78098000
H	-6.75724400	-0.47767600	1.54710100
H	-4.66977900	-1.58852300	0.76619400

H	-2.32021400	1.15446100	3.12220700
H	-4.40918800	2.25997500	3.92351500
H	-6.63083800	1.44977700	3.12724800
C	-0.06251800	3.09841600	1.09085400
H	-0.98332200	3.60862000	1.42393100
H	0.71083900	3.22332700	1.86174900
C	-0.29701000	1.68761000	0.74841800
H	0.48471600	0.95593500	0.96813100
C	-1.45627600	1.29827100	-0.10580400
H	-2.38813600	1.71380600	0.31556000
H	-1.35964500	1.77627200	-1.10220100
C	3.17647600	1.80269500	-2.28593500
C	1.97805700	2.40196200	-1.88618300
C	1.97534600	3.38048100	-0.87903800
C	3.18861300	3.75521700	-0.27801500
C	4.38565300	3.15550300	-0.68000900
C	4.38161700	2.18100400	-1.68492500
H	3.15883200	1.01850200	-3.04469000
H	1.03714400	2.11268100	-2.35889600
H	3.18878300	4.52254800	0.49995500
H	5.32630800	3.45482900	-0.20987900
H	5.31759900	1.70908100	-1.99452500
S	-1.85762700	-1.09076200	1.35188400
S	0.44210400	4.17200200	-0.39369700

TS2$_S$

C	-1.93664400	2.43788900	3.75281900
C	-2.87787000	1.70978000	3.01380100
C	-2.53880800	1.18174500	1.76803200
C	-1.25046400	1.36798700	1.23486200
C	-0.31534100	2.09804200	1.98374100
C	-0.65513700	2.62858200	3.23321400
H	-2.20408500	2.85264500	4.72819200
H	-3.88394900	1.55243800	3.41166900
H	-3.28887300	0.62808300	1.19995400
H	0.68967900	2.25959300	1.58995000
H	0.08894300	3.19602300	3.79827700
C	-0.90174500	0.82004200	-0.13357400
N	1.02938000	-0.41719200	-0.72494700
S	2.52067300	-0.52237700	-1.57790800
O	2.36423500	-1.65573100	-2.49734400
O	2.93901200	0.79424800	-2.08899600
C	3.62327600	-1.00141100	-0.25527800
C	3.66730000	-2.34235900	0.14086600
C	4.41033700	-0.03220600	0.36725100
C	4.51051700	-2.70564600	1.18815600
H	3.05506800	-3.08519700	-0.37367100
C	5.25143000	-0.41681600	1.41405300
H	4.36817800	1.00450100	0.02848500
C	5.31384700	-1.75235600	1.84243200
H	4.55321400	-3.75150100	1.50508700
H	5.87406100	0.33623800	1.90433900
C	6.22240600	-2.17496200	2.96737500
H	6.75084000	-1.31910600	3.41231800
H	5.65403700	-2.67928000	3.76659300
H	6.97975900	-2.89376300	2.61118100
C	0.55561700	0.78384300	-0.48321100
H	1.09307600	1.69386600	-0.77356200
C	0.70099600	5.17214700	-1.72010700
C	0.12531300	3.91870300	-1.94813000
C	-0.98081700	3.50402300	-1.18625600
C	-1.50841400	4.35859400	-0.20319700
C	-0.92629200	5.60858300	0.02106800
C	0.17778900	6.01676800	-0.73550700
H	1.56235400	5.48723100	-2.31473400
H	0.53486400	3.25373900	-2.71172700
H	-2.36912500	4.03581000	0.38523200
H	-1.33883200	6.26672800	0.79015900
H	0.62980200	6.99641400	-0.55915100
C	-1.46407500	-0.61514400	-0.38197900
H	-2.53997600	-0.55442200	-0.61486300
H	-1.38084900	-1.18012200	0.55790500
C	-0.46269600	-2.78538200	-1.38474400
H	-0.13334100	-3.08685400	-0.37863900
H	0.30553500	-3.08988000	-2.10978300
C	-0.71622500	-1.33231900	-1.46473300
H	-0.75448900	-0.89620900	-2.46821700
C	-3.59455800	-3.41373500	1.87827600
C	-2.73186200	-3.75057100	0.83275700
C	-3.07013400	-3.43257500	-0.49338700
C	-4.29852200	-2.80680900	-0.75888700
C	-5.16935900	-2.49166700	0.28931600
C	-4.81535100	-2.78303700	1.61043400

H	-3.31561800	-3.65273500	2.90796600
H	-1.78638100	-4.25553200	1.04504900
H	-4.55948100	-2.55140500	-1.78858700
H	-6.12254700	-2.00262400	0.07118800
H	-5.49026800	-2.52410700	2.43023100
S	-1.72523600	1.90724100	-1.48656100
S	-1.96233300	-3.81278600	-1.84942300

INT2$_S$

C	4.93316000	1.46966600	2.42007500
C	4.25834700	2.37234400	1.59121100
C	3.14878500	1.95722400	0.85195800
C	2.68724900	0.63109700	0.92919200
C	3.37326500	-0.26753800	1.76562100
C	4.48588400	0.14794200	2.50193600
H	5.80239200	1.79485600	2.99770200
H	4.59818800	3.40898200	1.51801100
H	2.64447400	2.67548000	0.20265400
H	3.04826400	-1.30623400	1.83621300
H	5.00577400	-0.56934800	3.14258200
C	1.51290700	0.17616900	0.10683800
N	-0.65198800	-0.74726600	0.18539800
S	-1.45447600	-2.20690400	-0.29727000
O	-1.45618000	-2.31683300	-1.76319300
O	-0.86091800	-3.26710200	0.52364600
C	-3.12598700	-1.91091900	0.24869400
C	-4.16161100	-1.91577200	-0.68561800
C	-3.36879600	-1.69739000	1.61028900
C	-5.46753000	-1.68794100	-0.24385900
H	-3.94203400	-2.08295400	-1.74141600
C	-4.67598900	-1.46768800	2.02922100
H	-2.54436900	-1.70211700	2.32612500
C	-5.74581700	-1.45809800	1.11243000
H	-6.28405600	-1.68566700	-0.97053500
H	-4.87618100	-1.29139400	3.08964800
C	-7.15345000	-1.22489700	1.59414900
H	-7.20314400	-0.36464500	2.28098600
H	-7.84690200	-1.04158900	0.76042300
H	-7.52301000	-2.10295500	2.15177600
C	0.64987800	-0.85430600	0.67557100
H	0.94026700	-1.74431500	1.22511600
C	2.81518200	-4.36328400	-0.62960800
C	2.23557100	-3.16572300	-1.05698900
C	3.01670600	-2.00011800	-1.15679600
C	4.38631600	-2.05627800	-0.84154100
C	4.96280900	-3.26036000	-0.42852600
C	4.17796900	-4.41374000	-0.31599700
H	2.19538100	-5.25964000	-0.54397200
H	1.17588000	-3.12870600	-1.31081600
H	4.98949400	-1.14907400	-0.91403100
H	6.02837300	-3.29549100	-0.18607900
H	4.62960300	-5.35321200	0.01385800
C	0.50210800	1.24326900	-0.33954900
H	0.84457100	1.86217200	-1.17812000
H	0.31025100	1.91665700	0.50900500
C	-2.07822500	1.21403000	-0.42250600
H	-2.14362400	1.51831600	0.63326700
H	-2.94658500	0.57423900	-0.63062700
C	-0.77522400	0.45848100	-0.68854100
H	-0.74413000	0.13230800	-1.73962600
C	-0.42198900	5.24819200	0.99945100
C	-1.31436400	4.29937200	0.49514300
C	-1.21904100	3.88363400	-0.84275700
C	-0.24763800	4.45726400	-1.67680700
C	0.62831800	5.42443000	-1.17288800
C	0.55182100	5.81365400	0.16778400
H	-0.49442000	5.55552300	2.04606200
H	-2.08396400	3.87529000	1.14458100
H	-0.16761800	4.12978700	-2.71608300
H	1.38351000	5.86326000	-1.83027200
H	1.24613200	6.55883500	0.56415500
S	2.27208100	-0.46532200	-1.65582400
S	-2.34044900	2.65958300	-1.52487300

TS3$_S$

C	4.85188800	1.61783800	2.51831900
C	4.12154500	2.52405900	1.74241200
C	3.03075000	2.08812800	0.98740900
C	2.64445700	0.73530500	0.99569700
C	3.38559700	-0.16738500	1.78176300
C	4.47856300	0.27019900	2.53265300
H	5.70682300	1.95971500	3.10746500

H	4.40327100	3.58031400	1.72264800
H	2.48118300	2.81053400	0.38079400
H	3.11938300	-1.22508500	1.79692500
H	5.04301700	-0.44964600	3.13133900
C	1.49246900	0.26644200	0.17157500
N	-0.59225100	-0.77302500	0.09419000
S	-1.37272800	-2.25304300	-0.33654700
O	-1.42463200	-2.36323000	-1.80016200
O	-0.72238700	-3.28977300	0.46981300
C	-3.02997800	-1.99798200	0.27140800
C	-4.10245200	-2.07653900	-0.61655500
C	-3.22585800	-1.76173000	1.63715600
C	-5.39829700	-1.89805200	-0.12473200
H	-3.92070100	-2.26470900	-1.67599800
C	-4.52366800	-1.58208500	2.10595400
H	-2.37394400	-1.71315700	2.31839400
C	-5.63023800	-1.64499700	1.23564500
H	-6.24351300	-1.95517100	-0.81536600
H	-4.68822400	-1.39077700	3.16996400
C	-7.02306000	-1.44000300	1.77003400
H	-7.13310600	-0.43082600	2.20186500
H	-7.78482600	-1.55867800	0.98588000
H	-7.24579100	-2.15872000	2.57615900
C	0.68999400	-0.82682200	0.63002800
H	0.99166800	-1.69330800	1.21072700
C	2.88513600	-4.24346400	-0.66932500
C	2.33694700	-3.04142200	-1.12300700
C	3.12870900	-1.87800500	-1.18620300
C	4.48275600	-1.94923300	-0.80370500
C	5.02971400	-3.15860100	-0.36792500
C	4.23165200	-4.30643700	-0.29280100
H	2.25329400	-5.13368400	-0.61154800
H	1.29091600	-2.99686600	-1.42775200
H	5.09554300	-1.04634700	-0.84366400
H	6.08257200	-3.20250200	-0.07591500
H	4.65959200	-5.24972700	0.05711100
C	0.47191800	1.27797500	-0.35076600
H	0.84391100	1.91698700	-1.16079300
H	0.17629700	1.93806700	0.47984700
C	-2.09095400	1.09165800	-0.64828300
H	-2.27632000	1.37465600	0.39882900
H	-2.89495700	0.40567000	-0.94774000
C	-0.72606100	0.42047900	-0.79689900
H	-0.58554000	0.08948600	-1.83747300
C	-0.87857000	5.18766000	1.00834500
C	-1.64224000	4.19270900	0.39377400
C	-1.37501700	3.81827300	-0.93295000
C	-0.36290400	4.47733500	-1.64661500
C	0.38360600	5.48909400	-1.03367000
C	0.13638900	5.83879600	0.29723600
H	-1.08466900	5.46352200	2.04591300
H	-2.44564600	3.70073700	0.94738500
H	-0.14926900	4.18247200	-2.67669200
H	1.17218000	5.99463900	-1.59721700
H	0.72939000	6.62002200	0.77939700
S	2.41832300	-0.34036900	-1.69536500
S	-2.32918000	2.53893900	-1.75389200

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C	-3.16702600	5.01587300	0.53949600
C	-3.78358900	3.76368300	0.48643500
C	-3.03993800	2.62081400	0.17832700
C	-1.65615400	2.70194300	-0.08379700
C	-1.05016900	3.97723300	-0.02971000
C	-1.79347400	5.11422200	0.27855800
H	-3.74859900	5.90975100	0.77914900
H	-4.85445800	3.67113000	0.68725300
H	-3.54414300	1.65256300	0.14987400
H	0.01665400	4.08007800	-0.24206000
H	-1.29938500	6.08910600	0.31122500
C	-0.89324100	1.49291000	-0.40433700
N	0.83994300	0.02517200	-0.73362300
S	2.27864500	-0.25486300	-1.60405500
O	2.16963100	-1.62767000	-2.11122200
O	2.53894400	0.86192000	-2.51990100
C	3.51103500	-0.20260900	-0.30841700
C	3.48571900	-1.17295300	0.70098600
C	4.49919700	0.78044300	-0.34314800
C	4.46352800	-1.14051200	1.68999500
H	2.70692400	-1.93809800	0.71412900
C	5.47430200	0.79568700	0.65885600
H	4.50222500	1.51980700	-1.14569000
C	5.47373500	-0.15785500	1.68708900

H	4.44954500	-1.89307400	2.48334800
H	6.25053000	1.56499700	0.63602600
C	6.51929200	-0.14783300	2.77133500
H	7.24871000	0.66321400	2.63063900
H	6.05579500	-0.02119700	3.76430400
H	7.07094400	-1.10258200	2.79543100
C	0.44481500	1.35580000	-0.49524500
H	1.21347100	2.11806300	-0.37415700
C	-1.53344400	0.13168300	-0.58273700
H	-2.35417800	0.13417000	-1.31554100
H	-1.97038700	-0.20657300	0.37028600
C	-0.30361200	-2.13730900	-0.27501800
H	-0.27947300	-1.97630600	0.81412600
H	0.61325500	-2.66735100	-0.56812500
C	-0.37510800	-0.80350600	-1.01755900
H	-0.42859000	-1.00566700	-2.09887700
C	-4.15841300	-2.01276200	2.24668600
C	-3.05905500	-2.55479100	1.57696800
C	-3.05620000	-2.63371600	0.17467900
C	-4.18066100	-2.20127400	-0.54379600
C	-5.28783800	-1.67836700	0.13265600
C	-5.27547900	-1.57225200	1.52677100
H	-4.14720400	-1.94359200	3.33767100
H	-2.19527700	-2.91325000	2.14218000
H	-4.17760800	-2.25908200	-1.63473700
H	-6.15862500	-1.34121900	-0.43587300
H	-6.13641000	-1.15248500	2.05326000
S	-1.64934700	-3.31013300	-0.71219000

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C	-2.07001100	2.80456900	0.71714800
C	-2.53190800	1.48717200	0.63708300
C	-1.96174400	0.59720700	-0.28675700
C	-0.93292600	1.03906700	-1.13252300
C	-0.47416100	2.35794400	-1.04854200
C	-1.03985400	3.24078400	-0.12367800
H	-2.51733700	3.49267700	1.43953300
H	-3.33384300	1.14522600	1.29595400
H	-0.48406200	0.34736900	-1.84778000
H	0.33386600	2.69156900	-1.70475000
H	-0.67885200	4.27059800	-0.05795300
Se	-2.55478100	-1.24076200	-0.35630000
C	-1.25265300	-1.94407100	1.02025200
H	-1.46085600	-1.40199200	1.95311300
H	-1.55689100	-2.99541800	1.13522300
C	0.14876400	-1.79218100	0.56056900
H	0.48877700	-2.50996000	-0.19370700
C	0.94640500	-0.77539700	0.94380800
H	0.54032800	-0.05494500	1.66346800
C	2.30782000	-0.47986200	0.47646400
C	2.90898800	0.73584700	0.86139900
C	3.04713500	-1.34604100	-0.35698200
C	4.19119200	1.07933200	0.42719700
H	2.35173800	1.42331400	1.50413800
C	4.32774700	-1.00408100	-0.78924200
H	2.61809600	-2.30179800	-0.66605900
C	4.90762500	0.21078000	-0.40122900
H	4.63268500	2.03014600	0.73783000
H	4.88212700	-1.69226400	-1.43318400
H	5.91226900	0.47498400	-0.74142900

TS1$_{11}$

C	-0.78267100	1.24798300	5.41283100
C	-0.59361200	2.39446600	4.62806200
C	-0.68707700	2.30845000	3.24399700
C	-0.99202700	1.07130900	2.61398300
C	-1.18679300	-0.07481800	3.42814000
C	-1.07361100	0.01613700	4.81023000
H	-0.69804000	1.31489900	6.50070600
H	-0.36341100	3.35133800	5.10255000
H	-0.51577500	3.19551200	2.62988700
H	-1.41134300	-1.02532000	2.94949100
H	-1.21012700	-0.87477000	5.42769500
C	-1.07626500	0.97597900	1.18398600
N	0.25254000	2.38135600	-0.26713800
S	0.20684000	3.44054800	-1.60205400
O	0.97981900	2.77124000	-2.65908800
O	-1.16100900	3.91503800	-1.88190900
C	1.17605300	4.79915500	-0.96615000
C	2.55308800	4.62257300	-0.78589300
C	0.54800500	6.00212600	-0.64388600
C	3.30118800	5.67444600	-0.26409700

H	3.02465400	3.67412600	-1.04929500
C	1.31776300	7.04793000	-0.12783500
H	-0.52623100	6.11386500	-0.80163700
C	2.69942400	6.90234500	0.07256100
H	4.37693400	5.54523800	-0.11541200
H	0.83316200	7.99549100	0.12215100
C	3.53623200	8.02664000	0.62533700
H	4.09628200	7.70168900	1.51794300
H	4.28202900	8.36156400	-0.11553200
H	2.92327900	8.89635200	0.90414300
C	-0.87158300	2.09564900	0.28882900
H	-1.81110300	2.59574200	-0.02174800
Rh	-3.34326700	-1.96841500	-1.37128000
Rh	-2.06806100	-0.40842500	0.04182300
C	-1.07088900	-3.15122600	-0.01039200
O	-0.83815200	-1.99764400	0.48704400
O	-2.02048300	-3.43458400	-0.78753200
C	-0.12906600	-4.25695400	0.39323900
H	-0.33824300	-4.53982300	1.43738800
H	-0.26763700	-5.13412800	-0.25103800
H	0.91092700	-3.90458300	0.35237700
C	-1.19245700	-0.58794300	-2.73677600
O	-2.07968900	-1.46683100	-2.92129700
O	-0.98009500	0.02242500	-1.63817600
C	-0.27059500	-0.23575700	-3.87278100
H	-0.74845200	-0.44967000	-4.83794000
H	0.03619700	0.81638400	-3.79676200
H	0.63552300	-0.85903400	-3.78507400
C	-4.33830400	0.74904900	-1.39064800
O	-3.43766800	1.01860900	-0.52791200
O	-4.55694800	-0.38820200	-1.88803800
C	-5.18203200	1.91180100	-1.84213600
H	-4.53620100	2.62092000	-2.38480100
H	-5.99710000	1.57566200	-2.49502300
H	-5.58582500	2.44010000	-0.96539200
C	-4.27293900	-1.77860500	1.37235300
O	-4.51650100	-2.35699200	0.27816200
O	-3.32377100	-0.95524500	1.58469500
C	-5.19943400	-2.04733800	2.53136000
H	-6.01611100	-1.30668300	2.49949000
H	-5.64051300	-3.04951000	2.44681900
H	-4.67047100	-1.93115100	3.48690100
C	2.27922000	-3.21150800	3.13322700
C	1.77271000	-2.10596300	2.44185900
C	2.65037800	-1.14625100	1.91700600
C	4.03450300	-1.30051300	2.09204500
C	4.53587200	-2.41133500	2.77808000
C	3.65929100	-3.36784300	3.30059100
H	1.59057000	-3.95877800	3.53735000
H	0.70117100	-1.99654100	2.27857700
H	4.72082800	-0.55794300	1.67929800
H	5.61578700	-2.53133100	2.89798500
H	4.05211700	-4.23587000	3.83681900
Se	1.97013900	0.39343400	0.95792600
C	1.91765000	-0.42990300	-0.87669000
H	1.15164400	-1.21115800	-0.82046900
H	1.54411100	0.40481400	-1.48292000
C	3.25117300	-0.92410600	-1.28690000
H	3.96950700	-0.16650100	-1.61845200
C	3.62139700	-2.21632800	-1.18282300
H	2.87968300	-2.92470000	-0.79514400
C	4.93495000	-2.79994800	-1.48508100
C	5.20240500	-4.12214700	-1.07561100
C	5.95798800	-2.09756300	-2.15694200
C	6.44296100	-4.71722100	-1.31453200
H	4.42306200	-4.68326800	-0.55211300
C	7.19608100	-2.69217500	-2.39706700
H	5.77869800	-1.07784900	-2.50514700
C	7.44728400	-4.00458800	-1.97621700
H	6.62564300	-5.74304500	-0.98314900
H	7.97259500	-2.12964600	-2.92265500
H	8.41844000	-4.46819300	-2.16813900

INT1$_{Ph}$'

C	-1.81922300	-5.23805600	-1.03972000
C	-2.34925500	-4.14027400	-1.72283500
C	-2.01960900	-2.83985800	-1.33480200
C	-1.11846200	-2.59933900	-0.27649900
C	-0.59644600	-3.71995100	0.40349000
C	-0.94937200	-5.01739800	0.03329100
H	-2.08738500	-6.25575300	-1.33495000
H	-3.04285300	-4.29310000	-2.55413500
H	-2.48349600	-2.00213700	-1.85831700

H	0.11440500	-3.57215800	1.21511600
H	-0.52731200	-5.86504900	0.58010500
C	-0.77479600	-1.19949900	0.12948700
N	-1.77056200	0.98642700	-0.28262600
S	-2.07592000	2.16681600	-1.44101700
O	-1.73441100	3.47055600	-0.84350900
O	-1.54009800	1.81822800	-2.76998000
C	-3.86638200	2.05948400	-1.51805300
C	-4.63742500	2.72010900	-0.55901300
C	-4.46174200	1.26367500	-2.50029600
C	-6.02517500	2.56893200	-0.58293400
H	-4.15279100	3.34870300	0.19035500
C	-5.84977500	1.12525600	-2.51096800
H	-3.83868200	0.76626900	-3.24624100
C	-6.65391900	1.77194600	-1.55542300
H	-6.63310100	3.08412100	0.16592400
H	-6.32064200	0.50509100	-3.27889700
C	-8.15455600	1.63969300	-1.59928100
H	-8.46319400	0.63412400	-1.92550700
H	-8.61113600	1.84086800	-0.61824400
H	-8.58679800	2.35957700	-2.31657000
C	-1.23677200	-0.12291700	-0.69819500
H	-1.04403900	-0.27908500	-1.77217500
C	-4.64692800	-2.98936500	3.15706800
C	-3.30753900	-2.59842100	3.05511100
C	-2.96928600	-1.52745200	2.22022800
C	-3.94696700	-0.84824600	1.47984500
C	-5.27996600	-1.24987700	1.59112400
C	-5.63060100	-2.31661300	2.42703300
H	-4.91761200	-3.82638600	3.80539800
H	-2.53547700	-3.13102100	3.61564100
H	-3.67089200	-0.02404900	0.82056300
H	-6.04651800	-0.72567400	1.01553400
H	-6.67555400	-2.62712600	2.50580000
Se	-1.08789900	-1.06151500	2.09055600
C	-0.00632700	2.79095000	1.85786200
H	-0.87287400	3.03503400	1.23891200
C	-0.06207300	1.69417500	2.63584300
H	0.78266700	1.40363000	3.26328600
C	-1.28239400	0.86496200	2.71568800
H	-2.11703400	1.26662400	2.13553600
H	-1.58873800	0.64841700	3.75174500
C	1.11692400	3.72713400	1.74018100
C	2.43927000	3.38710000	2.08655300
C	0.87461400	5.01472000	1.22182600
C	3.47924700	4.30201300	1.92693600
H	2.65947000	2.38673900	2.45654600
C	1.91156500	5.93787800	1.07864900
H	-0.13983600	5.27883200	0.91303800
C	3.21945100	5.58429400	1.42736000
H	4.50104400	4.00768100	2.17967300
H	1.70173100	6.93192900	0.67501000
H	4.03617200	6.29945200	1.29921900
Rh	3.81950700	-0.32798000	-0.80182100
Rh	1.47123100	-0.74729200	-0.28721500
C	3.22676400	-3.08494000	-0.17908600
O	2.02434300	-2.71685600	-0.00477700
O	4.18675500	-2.33434700	-0.51344200
C	3.51708900	-4.54666100	0.05993800
H	2.75762100	-5.16203500	-0.44448600
H	4.52236500	-4.81115100	-0.29181700
H	3.44487900	-4.75109800	1.14077200
C	3.13809600	-0.17528000	2.02320300
O	4.10173400	-0.02239600	1.22275000
O	1.93255000	-0.42315800	1.69923600
C	3.45190700	-0.09745700	3.49824900
H	4.21891700	0.66632800	3.68687700
H	2.55075300	0.10308000	4.09196100
H	3.86531600	-1.07051000	3.81213100
C	2.11107500	1.98642200	-1.06734600
O	1.15682800	1.25362900	-0.66078700
O	3.32812100	1.63873100	-1.11798200
C	1.75747000	3.35711300	-1.57602500
H	0.71656500	3.60636500	-1.34389800
H	2.44429900	4.10279800	-1.15305900
H	1.89418100	3.35182500	-2.67013900
C	2.15721800	-0.97422700	-3.09575000
O	3.34588500	-0.68619000	-2.77669200
O	1.18350400	-1.10218300	-2.28741200
C	1.83750800	-1.16134400	-4.55682900
H	1.20930000	-2.05412200	-4.69061600
H	1.25435300	-0.29065700	-4.89907600
H	2.75501300	-1.24189900	-5.15336700

INT1$_{Ph}$

C	2.89568300	3.97629800	3.33797300
C	1.80842000	3.20810000	3.76622500
C	1.12321500	2.38767300	2.86784800
C	1.52506000	2.28477200	1.51754900
C	2.63146900	3.06053500	1.10697500
C	3.29808400	3.90067300	2.00019800
H	3.42364500	4.62807900	4.03867100
H	1.47599200	3.26093200	4.80667600
H	0.25157200	1.82460100	3.20957400
H	2.99001800	2.98933100	0.07652100
H	4.15260000	4.48720300	1.65145000
C	0.80846800	1.36725200	0.60559300
N	-0.33152300	-0.72882300	0.22821600
S	-0.65037700	-2.23846900	0.80805900
O	-0.22516700	-3.22057400	-0.21343900
O	-0.18939400	-2.43302000	2.19911000
C	-2.44600000	-2.22955000	0.80821100
C	-3.13423100	-2.50441100	-0.37525500
C	-3.13153000	-1.87906000	1.97462700
C	-4.52825600	-2.41376600	-0.38843400
H	-2.57910400	-2.79213500	-1.26998800
C	-4.52326500	-1.79649200	1.94549200
H	-2.57136500	-1.67873200	2.89010400
C	-5.24485500	-2.05836000	0.76671000
H	-5.07035800	-2.62961000	-1.31344000
H	-5.06402900	-1.52428700	2.85654600
C	-6.75044300	-1.98422500	0.76106500
H	-7.15511600	-1.95941500	-0.26195300
H	-7.18758900	-2.86136800	1.26957700
H	-7.11114200	-1.09084500	1.29591400
C	0.37253900	0.10469100	0.98331300
H	0.68238600	-0.21798900	1.99151400
C	-3.19316100	3.74621600	-2.06142800
C	-1.83021100	3.51520800	-1.84739600
C	-1.41218600	2.25113600	-1.41161200
C	-2.33157300	1.21874300	-1.18292500
C	-3.68945500	1.46730500	-1.39870700
C	-4.12086000	2.72440600	-1.83731700
H	-3.52730800	4.72952100	-2.40199300
H	-1.10567000	4.31592600	-2.01664600
H	-1.98112100	0.24875600	-0.82693300
H	-4.41038700	0.66621000	-1.21762300
H	-5.18525100	2.90938500	-2.00352300
Se	0.50939500	2.04066400	-1.14704700
C	0.85621100	0.48957300	-2.41699800
H	0.02348300	-0.20400300	-2.26206700
H	0.77138900	1.00023800	-3.38812700
C	2.18281700	-0.11443400	-2.15336100
H	3.06689600	0.47561200	-2.41815300
C	2.29371200	-1.31999000	-1.55976600
H	1.36727200	-1.83400000	-1.29050400
C	3.51431000	-2.03483100	-1.17539300
C	4.80996200	-1.64782400	-1.57569500
C	3.37636200	-3.16264800	-0.33898300
C	5.92826400	-2.36145400	-1.14722700
H	4.94326500	-0.78711600	-2.23580400
C	4.49898100	-3.87180700	0.09287900
H	2.37371100	-3.46437400	-0.02215900
C	5.77794200	-3.47492800	-0.30960300
H	6.92613700	-2.05120100	-1.46900900
H	4.37342000	-4.73872200	0.74684900
H	6.65756000	-4.03134300	0.02494400

TS1$_{Ph}$

C	-4.21699900	1.19009000	-2.61686100
C	-4.45880000	0.65964800	-1.34412300
C	-3.39800600	0.24422600	-0.54151700
C	-2.06223200	0.33973100	-0.98701100
C	-1.83767800	0.86960400	-2.27452700
C	-2.90146600	1.29388700	-3.07532000
H	-5.04868600	1.51818000	-3.24555500
H	-5.48233700	0.57215000	-0.97066200
H	-3.60647800	-0.15461100	0.45126200
H	-0.82052100	0.93999700	-2.66449500
H	-2.69617200	1.70277700	-4.06809200
C	-0.92710000	-0.05441100	-0.12687000
N	1.43011400	0.04306900	0.25639300
S	2.80409900	1.01453900	0.25036300
O	3.04180600	1.42752600	1.64766800
O	2.74725200	2.05708500	-0.79317200
C	4.05708700	-0.17754000	-0.19671800

C	4.51149600	-1.08291800	0.76811800
C	4.55493900	-0.19397100	-1.49932900
C	5.47339300	-2.02328400	0.40769500
H	4.11516300	-1.04173900	1.78426000
C	5.52262800	-1.14212600	-1.84104400
H	4.18921600	0.53093300	-2.22873200
C	5.99439200	-2.07001300	-0.89949000
H	5.83343500	-2.73646400	1.15470600
H	5.91877100	-1.15917400	-2.85993900
C	7.04483400	-3.08878600	-1.25931200
H	7.27091500	-3.08213600	-2.33586000
H	6.72296500	-4.10641600	-0.98285000
H	7.98500700	-2.89174800	-0.71593600
C	0.36421100	0.53586800	-0.30779000
H	0.41016300	1.47974800	-0.87103000
C	-4.11017700	-3.54622700	-1.20117400
C	-2.87717000	-2.93322500	-0.96622800
C	-2.50862500	-2.58520600	0.34170200
C	-3.36609800	-2.87679200	1.41190800
C	-4.59459300	-3.50131900	1.17103000
C	-4.97069300	-3.83026900	-0.13488500
H	-4.39818800	-3.80533900	-2.22328000
H	-2.20636500	-2.71272400	-1.79899300
H	-3.07864500	-2.60958400	2.43161300
H	-5.26117800	-3.72557200	2.00796500
H	-5.93377900	-4.31220400	-0.32214700
Se	-0.78272100	-1.78995500	0.70002300
C	-0.70153700	-0.09186900	3.39087200
H	-1.73583300	-0.44577900	3.40263900
H	-0.00213400	-0.57770000	4.07639100
C	-0.32030100	0.95592200	2.61773300
H	0.71996500	1.28933400	2.66050500
C	-1.19195900	1.53062800	1.64115900
H	-2.22670800	1.18545000	1.66540100
C	-0.99360900	2.84153600	1.02671600
C	-2.06025700	3.43866200	0.31753800
C	0.24190700	3.52829800	1.07759200
C	-1.89928300	4.66892400	-0.31899700
H	-3.01993700	2.92076100	0.26249700
C	0.39807600	4.75489500	0.43660400
H	1.09888600	3.08809200	1.58855600
C	-0.66873800	5.33240500	-0.26391800
H	-2.73765800	5.10983100	-0.86453000
H	1.36704300	5.25870100	0.47407300
H	-0.53908900	6.29451600	-0.76640200

INT2$_{Ph}$

C	4.59171300	2.22247900	-1.46687800
C	4.25805700	2.55612800	-0.14968900
C	3.16506800	1.95231900	0.47559700
C	2.38468600	0.99670700	-0.19755800
C	2.73749200	0.66404900	-1.51672800
C	3.82561000	1.27427700	-2.14770100
H	5.44326500	2.70020200	-1.95821100
H	4.84807200	3.29811700	0.39476700
H	2.90044300	2.23997400	1.49396900
H	2.17834000	-0.10017100	-2.06127900
H	4.07683400	0.99641700	-3.17436900
C	1.24928900	0.24687800	0.48752400
N	-0.45918300	-1.27988900	-0.35413400
S	-1.60025100	-1.67016500	-1.57746900
O	-1.40197300	-3.09917200	-1.83119000
O	-1.54489800	-0.70457000	-2.68896300
C	-3.12882500	-1.43311100	-0.68589500
C	-3.46702400	-2.32504600	0.33478500
C	-3.95784100	-0.35933800	-1.02095700
C	-4.65315400	-2.12113600	1.04079600
H	-2.81147500	-3.16531100	0.57074300
C	-5.14338500	-0.17825400	-0.31016600
H	-3.66579100	0.31953000	-1.82345800
C	-5.50823500	-1.04915300	0.73259800
H	-4.92259000	-2.81072200	1.84496600
H	-5.80132800	0.65672000	-0.56752500
C	-6.79663900	-0.83354900	1.48301700
H	-6.86238800	0.19621900	1.87130200
H	-6.89864000	-1.52647500	2.33100900
H	-7.66545800	-0.98150400	0.81898800
C	0.20816900	-0.20266500	-0.50420800
H	0.02865500	0.46815500	-1.35961700
C	-0.64822800	4.31857900	-1.31408100
C	-0.00178400	3.54529900	-0.34540200
C	-0.71833900	2.56241300	0.35497200
C	-2.08393800	2.37384100	0.09490000

C	-2.72744800	3.16346700	-0.86315900
C	-2.01042900	4.13139000	-1.57308000
H	-0.08386000	5.07557100	-1.86496200
H	1.05892400	3.69904100	-0.14084100
H	-2.63865600	1.60046200	0.62973800
H	-3.79149200	3.01169800	-1.06225300
H	-2.51257300	4.74063500	-2.32901100
Se	0.13923600	1.47591100	1.71219400
C	1.91607200	-0.69075500	3.89241800
H	0.97395700	-1.22825100	4.04628600
H	2.43766400	-0.33720800	4.78710700
C	2.40798500	-0.47511900	2.66887700
H	3.35188900	0.06786600	2.56120300
C	1.73719400	-0.94567300	1.39989600
H	0.82155100	-1.48078000	1.68500600
C	2.61575800	-1.92312800	0.61498300
C	2.05926700	-3.09522200	0.07601200
C	3.98475500	-1.68084200	0.40714400
C	2.84532400	-3.99489900	-0.65008600
H	0.99403900	-3.29254300	0.20231100
C	4.77211700	-2.58014200	-0.31621100
H	4.44623300	-0.77369600	0.79991900
C	4.20551100	-3.74212300	-0.84875200
H	2.38641600	-4.89623800	-1.06507300
H	5.83395600	-2.36754700	-0.46669600
H	4.82048000	-4.44534900	-1.41677000

TS2$_{Ph}$

C	3.80869100	1.76143000	3.24100900
C	3.09118900	0.59383300	3.52943300
C	2.22516100	0.04322500	2.58712100
C	2.02497500	0.65080700	1.32150800
C	2.77416100	1.81521300	1.04740800
C	3.64657100	2.36193900	1.99099700
H	4.49159500	2.18867500	3.97963700
H	3.21513700	0.09903000	4.49650700
H	1.71087900	-0.88537600	2.83970100
H	2.66451300	2.29646900	0.07510300
H	4.20725000	3.26594600	1.73897500
C	1.11123600	0.05294600	0.32645100
N	-0.81337700	-1.33627200	-0.08269900
S	-2.01806400	-2.29316100	0.62695300
O	-2.27041200	-3.41771400	-0.28478000
O	-1.72221300	-2.57321800	2.04784200
C	-3.43908800	-1.20277900	0.55822000
C	-4.36285700	-1.35177700	-0.47908100
C	-3.60896800	-0.22927000	1.54424100
C	-5.46857200	-0.50401300	-0.52573000
H	-4.20946100	-2.12748100	-1.23092500
C	-4.71569700	0.61731900	1.47495100
H	-2.88486600	-0.13559100	2.35570500
C	-5.66061900	0.49590500	0.44310800
H	-6.19522800	-0.61465600	-1.33584500
H	-4.84645500	1.39018700	2.23685900
C	-6.85362300	1.41291100	0.36272900
H	-7.78727100	0.86633400	0.58155100
H	-6.77848600	2.24590200	1.07735300
H	-6.96195000	1.83711300	-0.64908100
C	0.05892400	-0.79659200	0.74084100
H	0.01369800	-1.06027400	1.80826600
C	-2.21146500	3.35105800	-0.19567900
C	-0.95595700	2.75310000	-0.33716600
C	-0.79385100	1.66997800	-1.21334400
C	-1.88703100	1.18997600	-1.94573500
C	-3.13529000	1.80638700	-1.81435500
C	-3.30097000	2.88276200	-0.93827400
H	-2.33621400	4.19038500	0.49387600
H	-0.10313400	3.12481000	0.23546600
H	-1.76464500	0.32284800	-2.59741900
H	-3.98737500	1.42546900	-2.38172900
H	-4.28208600	3.35141100	-0.82665800
Se	0.94642200	0.84914800	-1.44630800
C	2.56599200	-1.89504700	-0.36543300
H	2.48521900	-2.24662900	0.66598600
C	1.70087300	-2.49401300	-1.31122600
H	1.78930500	-2.21451700	-2.36363300
C	0.67374100	-3.31000500	-0.93928000
H	-0.03666500	-3.71382800	-1.66093200
H	0.56875000	-3.65916800	0.09026400
C	3.77131200	-1.14655300	-0.67764900
C	4.68795200	-0.85711000	0.35895000
C	4.06214900	-0.66665900	-1.97780200
C	5.84695500	-0.12323100	0.10996100

H	4.47872700	-1.21370500	1.36901700
C	5.21779400	0.07018000	-2.22044400
H	3.37412100	-0.86394200	-2.80097900
C	6.11578400	0.34498700	-1.17938500
H	6.53784400	0.09080300	0.92886400
H	5.42339400	0.43559100	-3.22971700
H	7.02185600	0.92364100	-1.37665400

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C	-0.12126600	-3.29833700	-3.87726000
C	-1.07146300	-2.27269600	-3.88709400
C	-0.97596200	-1.21893600	-2.97532600
C	0.07592200	-1.17227600	-2.04116300
C	1.02128300	-2.21426700	-2.03441400
C	0.92512600	-3.26402300	-2.94851400
H	-0.19925100	-4.12649800	-4.58649700
H	-1.89878600	-2.29729000	-4.60125000
H	-1.73305400	-0.43130000	-2.96783500
H	1.83533400	-2.19236800	-1.30652700
H	1.67106600	-4.06295600	-2.93412900
C	0.15969800	-0.03894500	-1.08809000
N	0.00445900	2.35418000	-0.61860600
S	-1.47978400	3.19915600	-0.59188600
O	-1.27348200	4.36469900	0.27681900
O	-1.99101000	3.38796200	-1.95817500
C	-2.53956100	2.02003000	0.23650500
C	-2.27624200	1.68547800	1.56965700
C	-3.63481100	1.48725000	-0.44262200
C	-3.12525000	0.79421400	2.21875900
H	-1.41272300	2.11092700	2.08235600
C	-4.47885500	0.59694500	0.22780300
H	-3.81785200	1.77003900	-1.48045400
C	-4.23774300	0.23500300	1.56173300
H	-2.91808700	0.51433400	3.25505600
H	-5.33660100	0.17228200	-0.30038600
C	-5.11649900	-0.75386600	2.28021100
H	-5.50632200	-0.33011000	3.22053900
H	-5.97296200	-1.06559400	1.66438100
H	-4.54141600	-1.65658200	2.54687400
C	-0.00633500	1.23581200	-1.49861500
H	-0.13528200	1.44684300	-2.56819900
C	-0.82923100	-4.15946100	1.99376700
C	-0.02177400	-3.04415800	1.74743500
C	-0.52956300	-1.96298100	1.01331700
C	-1.84261100	-2.00507800	0.52250800
C	-2.63429400	-3.13309000	0.75206000
C	-2.13379000	-4.21025600	1.49232400
H	-0.42877600	-4.99918900	2.56809900
H	1.00681400	-3.02104400	2.11691600
H	-2.24661400	-1.15955400	-0.03506300
H	-3.65295600	-3.16303100	0.35651600
H	-2.75816500	-5.08853400	1.67524000
Se	0.58269000	-0.40487500	0.76113500
C	3.32709100	1.79161900	-0.34917800
H	3.44803100	1.85780900	-1.43744100
C	2.28911200	2.44138900	0.20469800
H	2.10958300	2.39792800	1.28359000
C	1.24552700	3.16900500	-0.58725600
H	0.99043400	4.12662700	-0.11154500
H	1.59352700	3.37690100	-1.61507900
C	4.32600400	0.95770700	0.33632100
C	5.38469800	0.40586700	-0.41131600
C	4.25993700	0.65500600	1.71272600
C	6.34608400	-0.41056200	0.18909000
H	5.44973100	0.62222400	-1.48154000
C	5.21921600	-0.15918900	2.31260500
H	3.44435800	1.05384900	2.31922700
C	6.26821400	-0.69615000	1.55496900
H	7.15833200	-0.82617600	-0.41316400
H	5.14772800	-0.38151200	3.38073000
H	7.01772300	-1.33564100	2.02843800

TS3$_{Ph}$

C	5.64070600	-2.90147400	0.69720800
C	4.44859500	-3.41247000	1.22136200
C	3.22885000	-2.80278500	0.92266500
C	3.16853600	-1.67117300	0.07920400
C	4.38053800	-1.17413000	-0.44702900
C	5.59812100	-1.77973400	-0.13894300
H	6.59648400	-3.37407600	0.93795400
H	4.46822700	-4.28651100	1.87805000
H	2.30567900	-3.19272300	1.35805900
H	4.36050400	-0.31139100	-1.11423500

H	6.52205200	-1.37639100	-0.56199900
C	1.86573200	-1.07613100	-0.24615900
N	-0.39441000	-1.25202700	-0.93950100
S	-1.63647200	-2.20600100	-1.46452500
O	-2.28190200	-1.51170100	-2.59772300
O	-1.25129100	-3.61960500	-1.65564100
C	-2.78338300	-2.14487900	-0.07790600
C	-2.98782600	-0.95017800	0.62319700
C	-3.50711400	-3.29370500	0.24350700
C	-3.93486800	-0.91364100	1.64423700
H	-2.39625000	-0.06599700	0.38229900
C	-4.45384000	-3.23988000	1.27089500
H	-3.32172700	-4.21977000	-0.30397200
C	-4.68646300	-2.05438700	1.98426200
H	-4.09364300	0.01990400	2.19191700
H	-5.02066300	-4.14056100	1.52269300
C	-5.69764100	-1.99247200	3.10035800
H	-6.40373700	-1.15840600	2.95277600
H	-6.28039400	-2.92248100	3.17712700
H	-5.20252200	-1.82406700	4.07227400
C	0.76337600	-1.83617000	-0.62145500
H	0.88600000	-2.92533700	-0.71908100
C	4.88858800	3.19650000	0.22355200
C	3.76876400	2.56434600	-0.32755400
C	3.09602000	1.57433900	0.40213700
C	3.54243400	1.22255000	1.68481300
C	4.66794900	1.84985900	2.22323900
C	5.34251300	2.83739800	1.49605100
H	5.41229900	3.96586600	-0.34999700
H	3.42873400	2.83325400	-1.33113200
H	3.01885700	0.45247700	2.25488100
H	5.01856200	1.56552600	3.21881100
H	6.22237300	3.32622300	1.92217200
Se	1.49443600	0.79013500	-0.34848400
C	-1.39522600	2.62532000	-1.47140300
H	-0.51296500	3.27511700	-1.50632500
C	-1.34405200	1.43457400	-2.18868400
H	-2.16427200	0.71751900	-2.12682500
C	-0.24204000	1.03916300	-2.92441800
H	-0.24490100	0.06407000	-3.41312100
H	0.59727200	1.71286300	-3.11086400
C	-2.49029000	3.08970700	-0.65941100
C	-2.35166300	4.30351500	0.06152500
C	-3.71231400	2.37690100	-0.53565900
C	-3.37854300	4.77849800	0.87223900
H	-1.41789500	4.86639500	-0.02150500
C	-4.73356200	2.85607800	0.27662700
H	-3.85529500	1.44119300	-1.07763100
C	-4.57337100	4.05630000	0.98577700
H	-3.25025500	5.71467500	1.42122600
H	-5.66479000	2.29050800	0.36179700
H	-5.37975500	4.42713800	1.62354100

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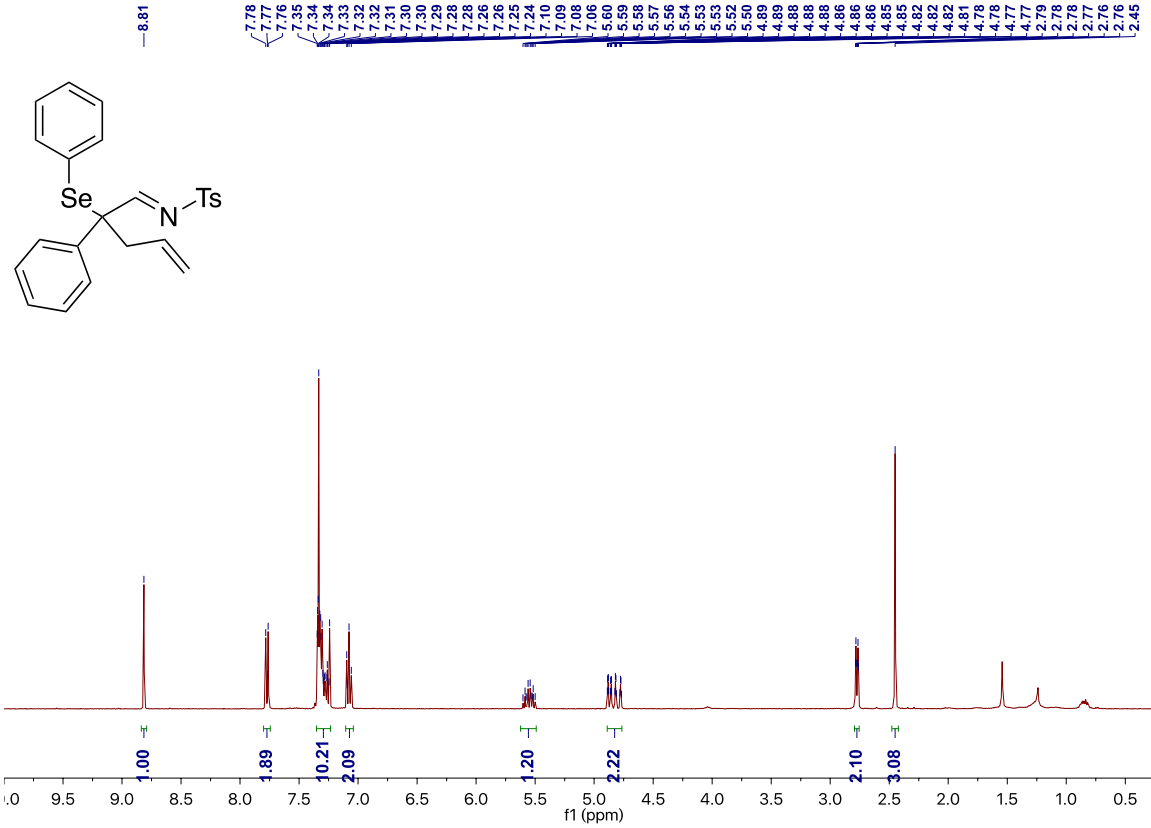
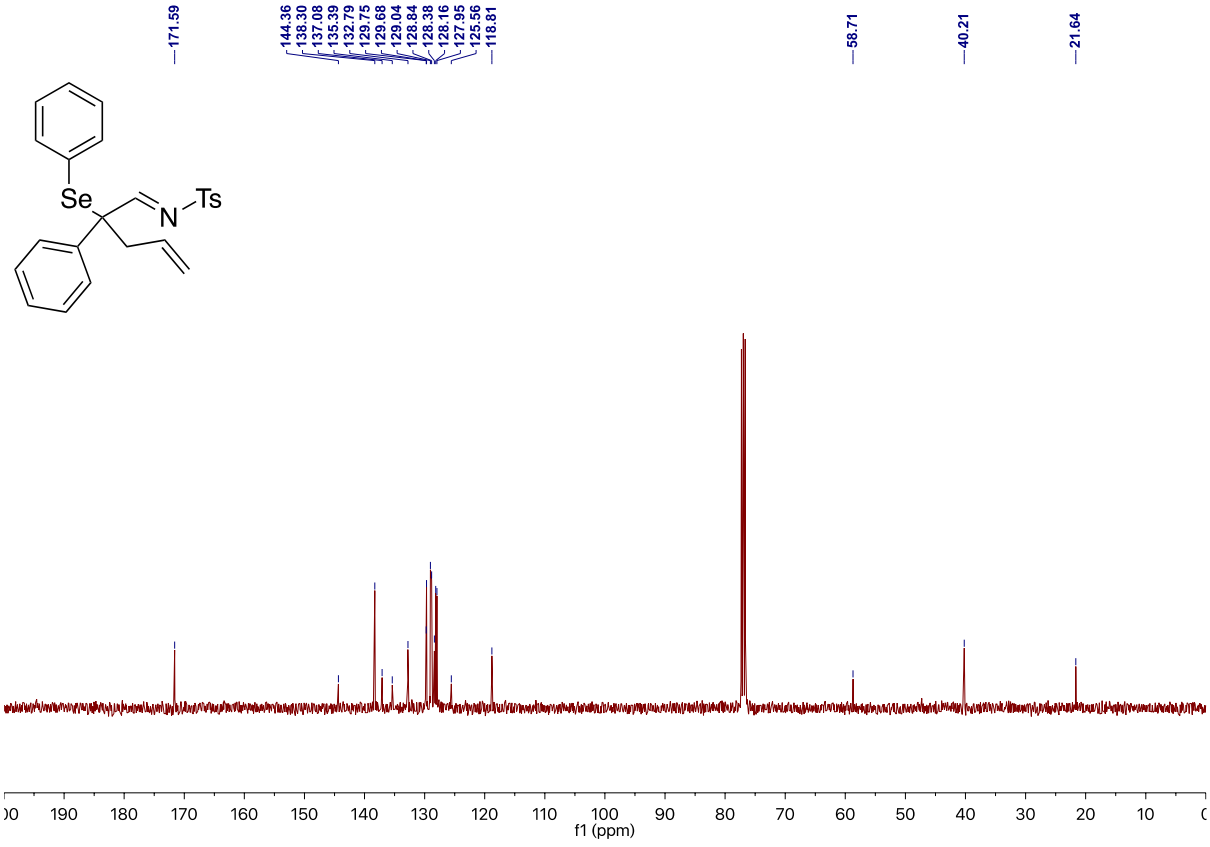
Spectra of Compounds

(*E*)-4-methyl-*N*-(2-phenyl-2-(phenylselanyl)pent-4-en-1-ylidene)benzenesulfonamide (7a)

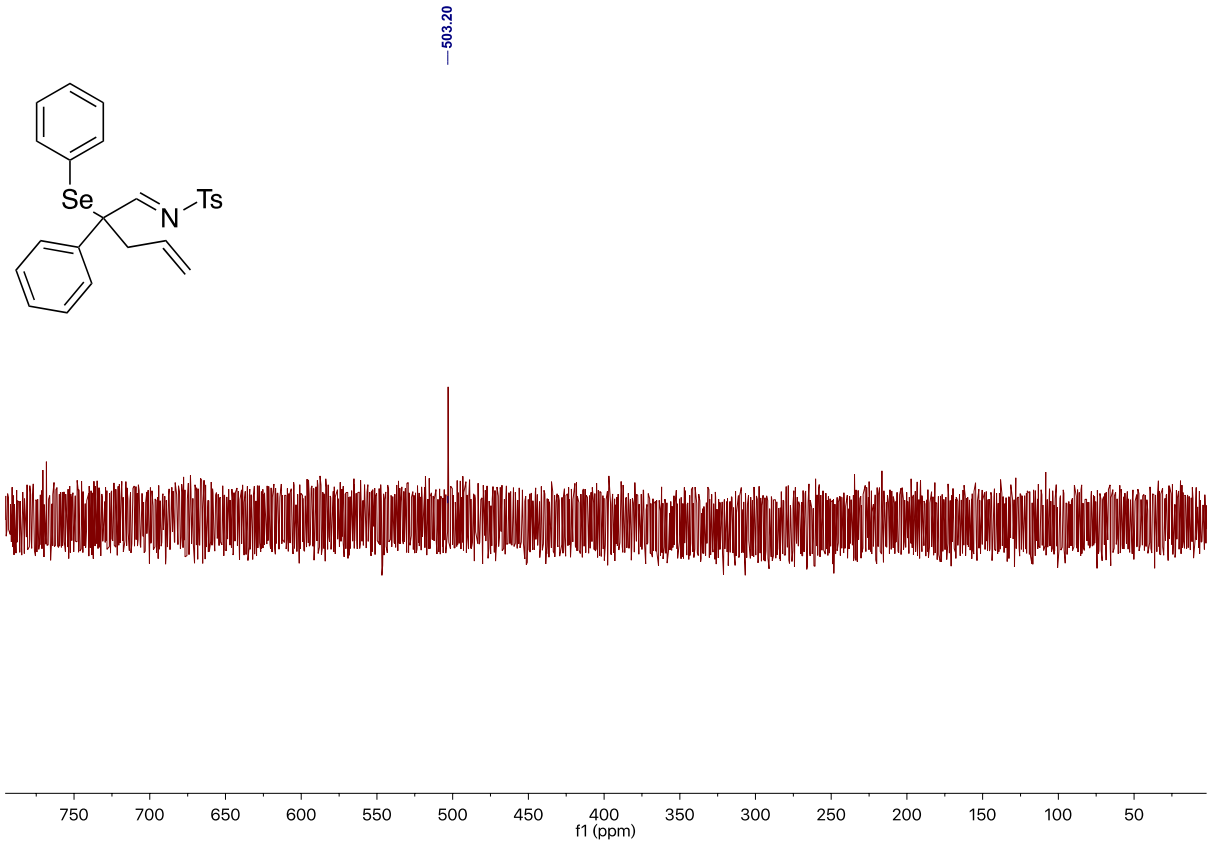
^{1}H NMR (400 MHz, Chloroform-*d*)



^{13}C NMR (101 MHz, Chloroform-*d*)

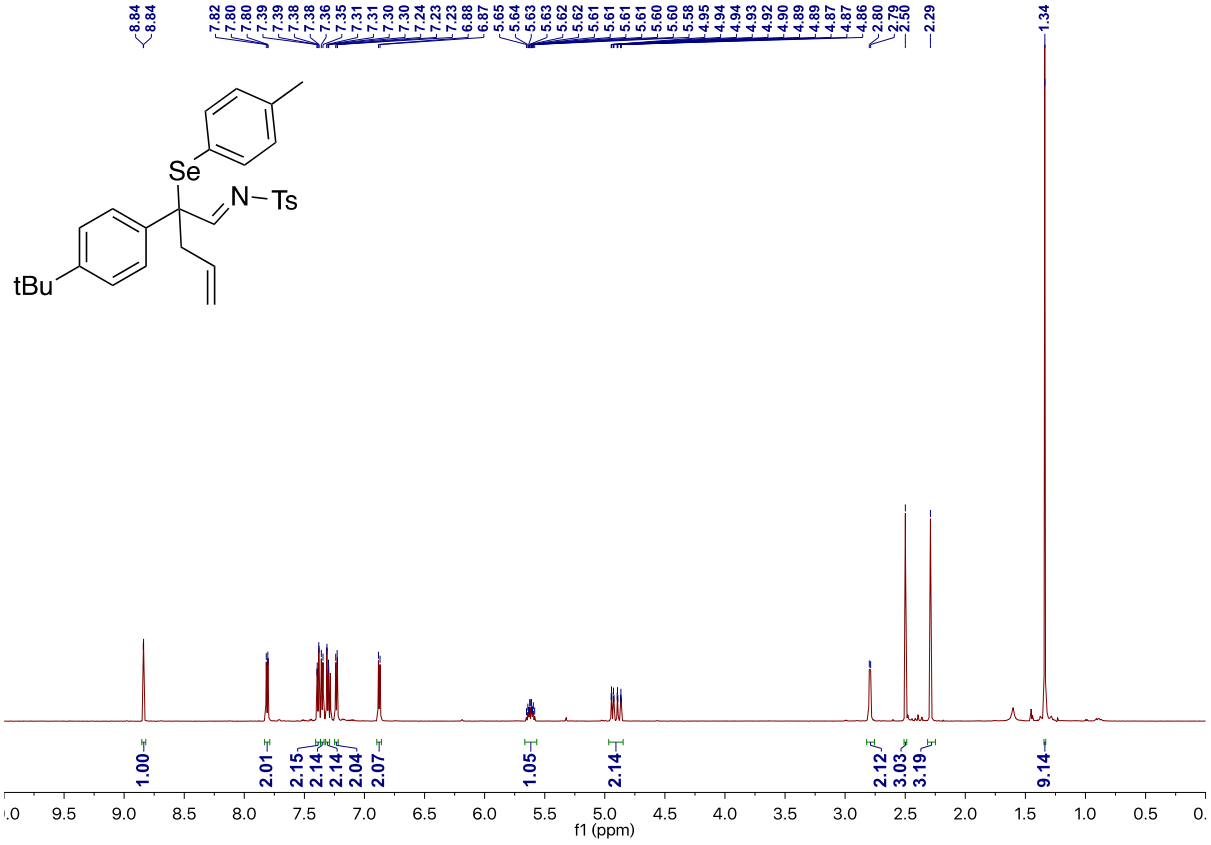


^{77}Se NMR (565 MHz, Chloroform-*d*)

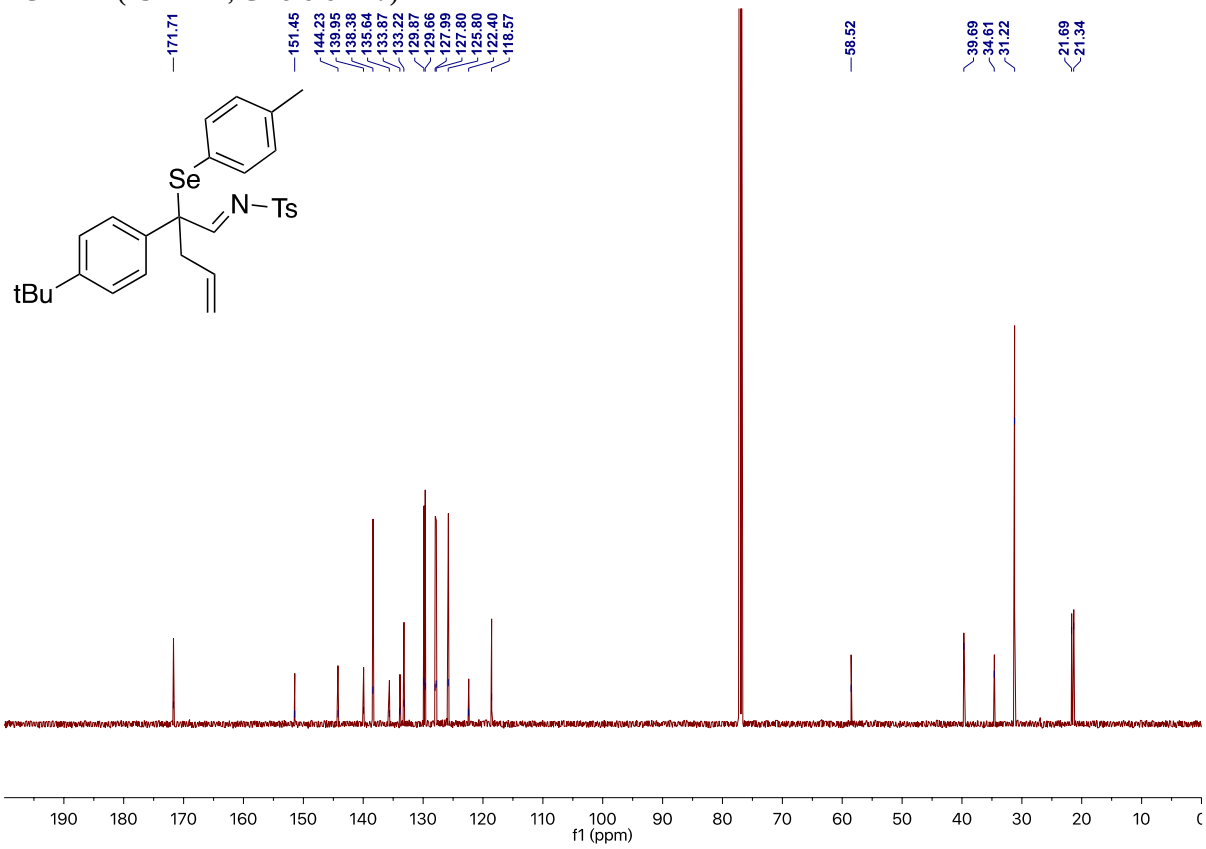


(*E*)-*N*-(2-(4-(*tert*-butyl)phenyl)-2-(*p*-tolylselanyl)pent-4-en-1-ylidene)-4-methylbenzenesulfonamide (7b)

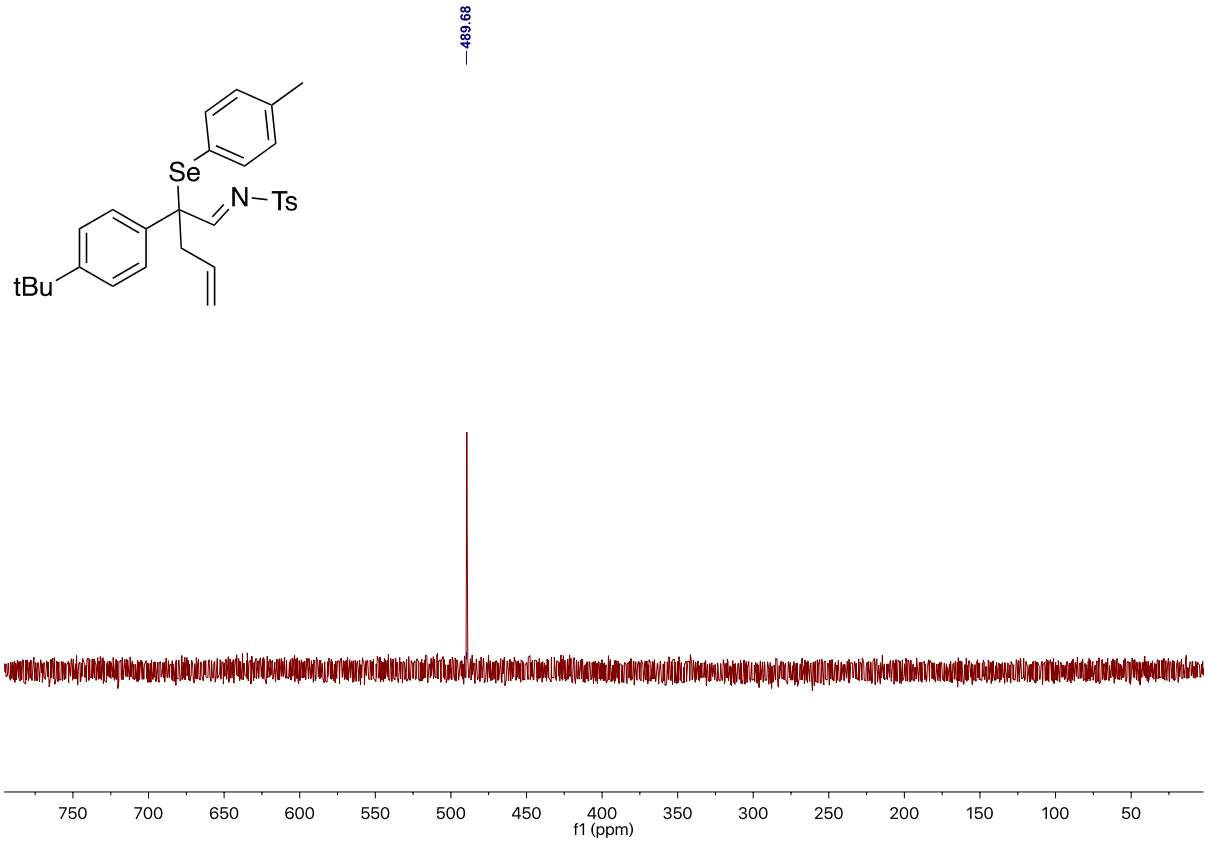
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

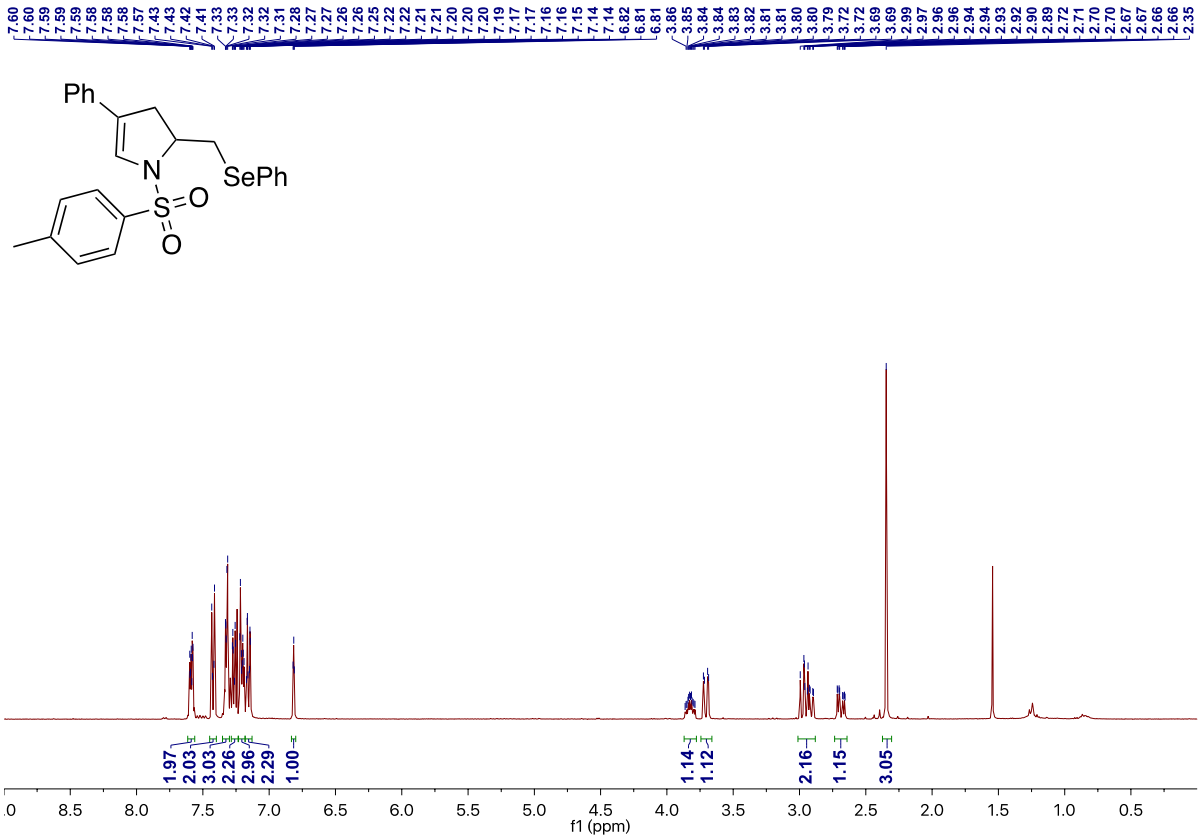


^{77}Se NMR (115 MHz, Chloroform-*d*)

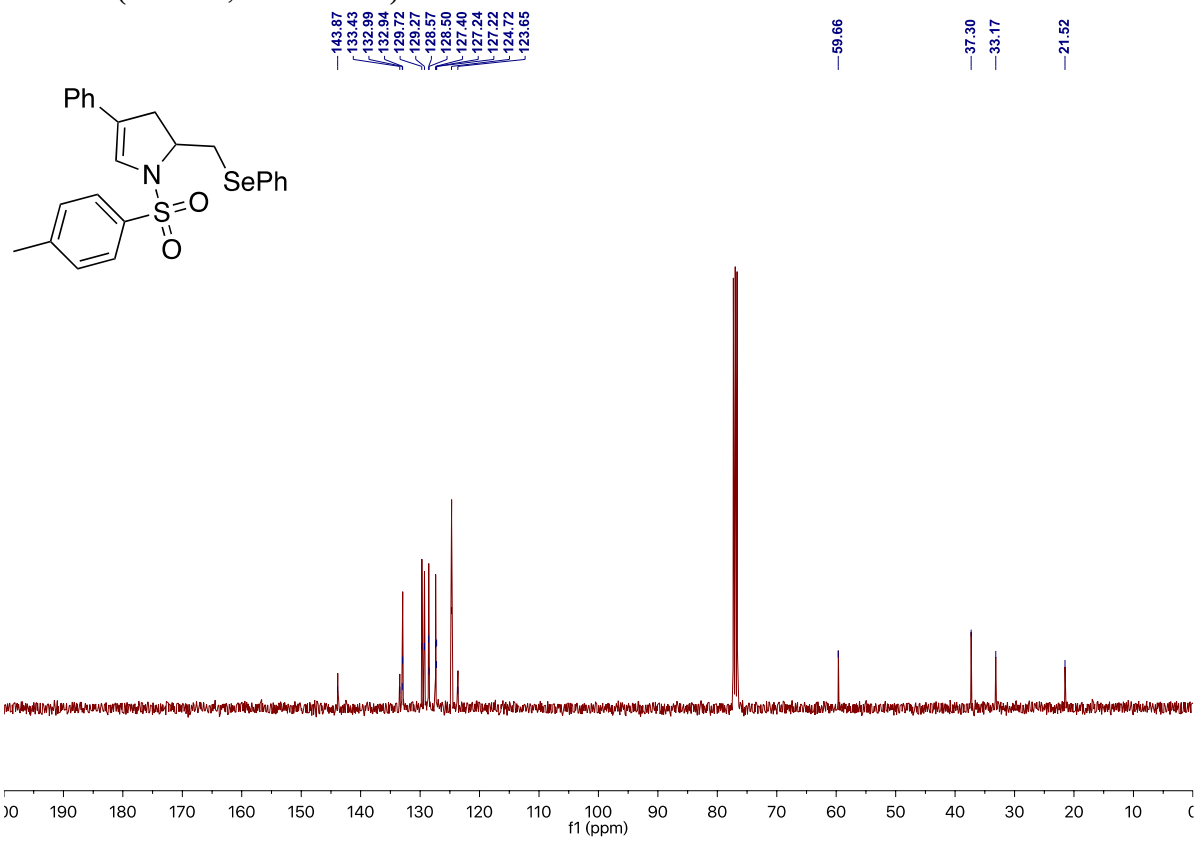


4-phenyl-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9a)

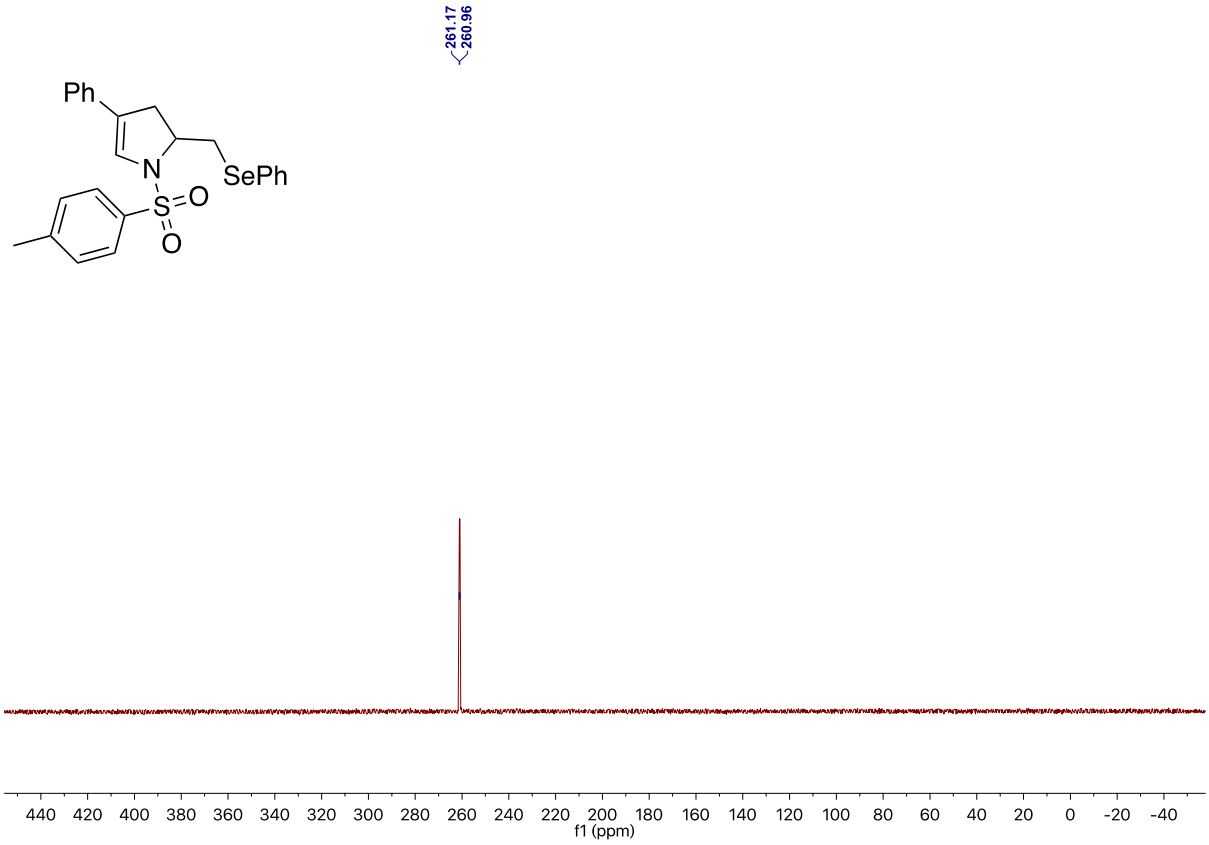
^{1}H NMR (400 MHz, Chloroform-*d*)



^{13}C NMR (101 MHz, Chloroform-*d*)

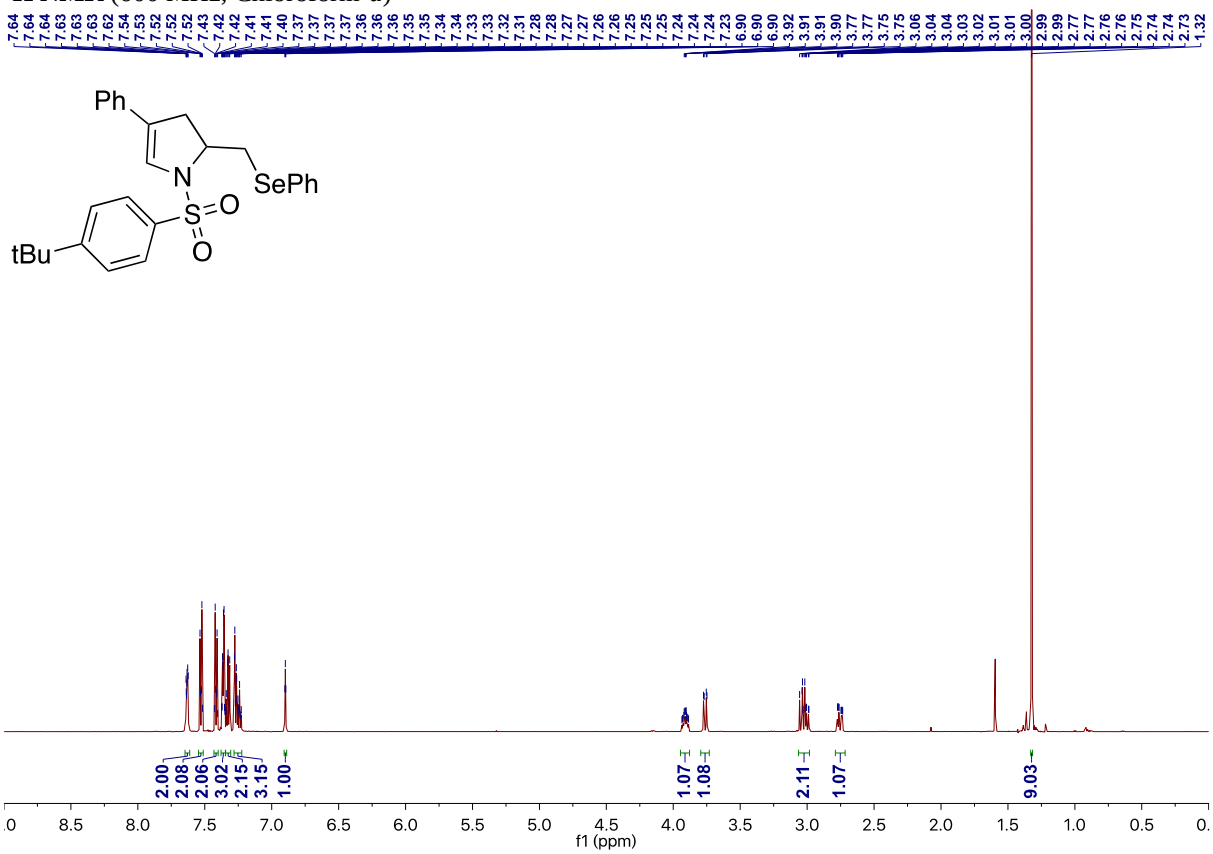


^{77}Se NMR (565 MHz, Chloroform-*d*)

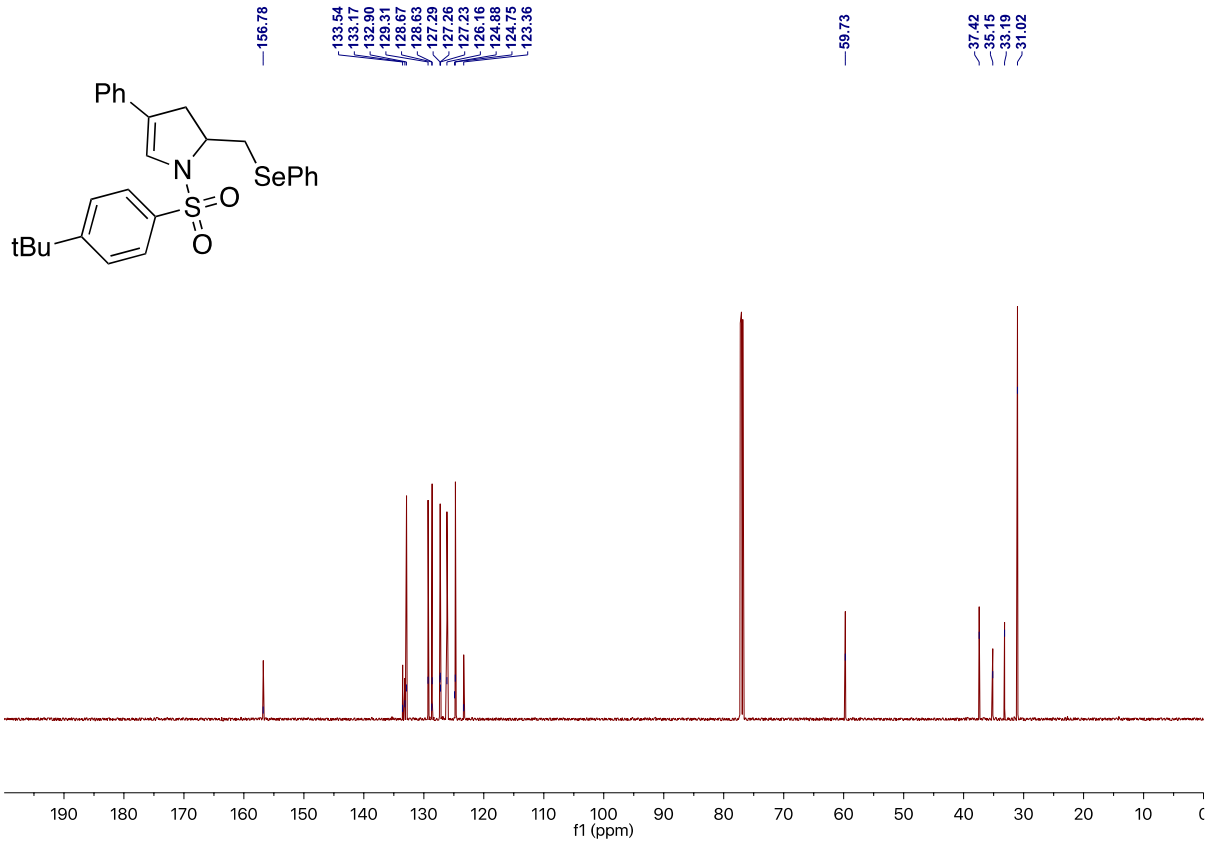


1-((4-(*tert*-butyl)phenyl)sulfonyl)-4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrole (9b)

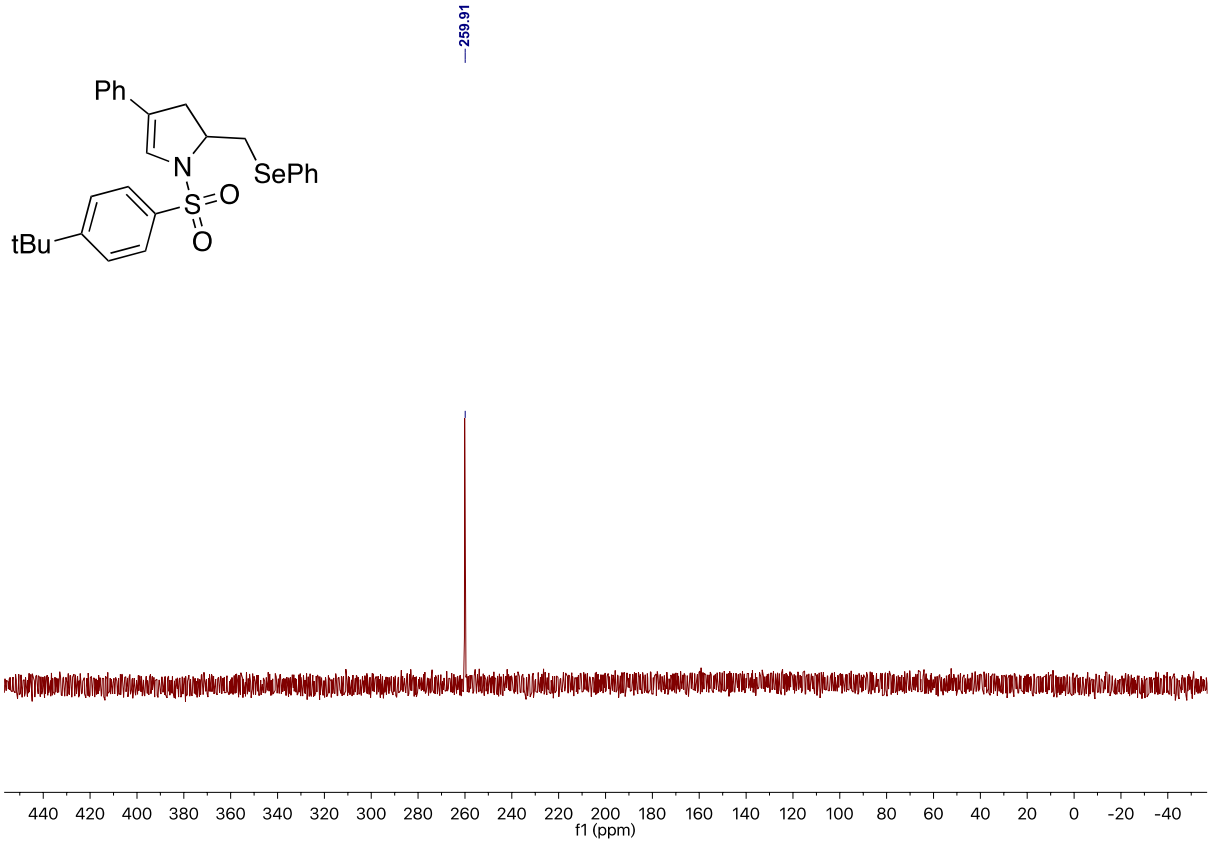
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

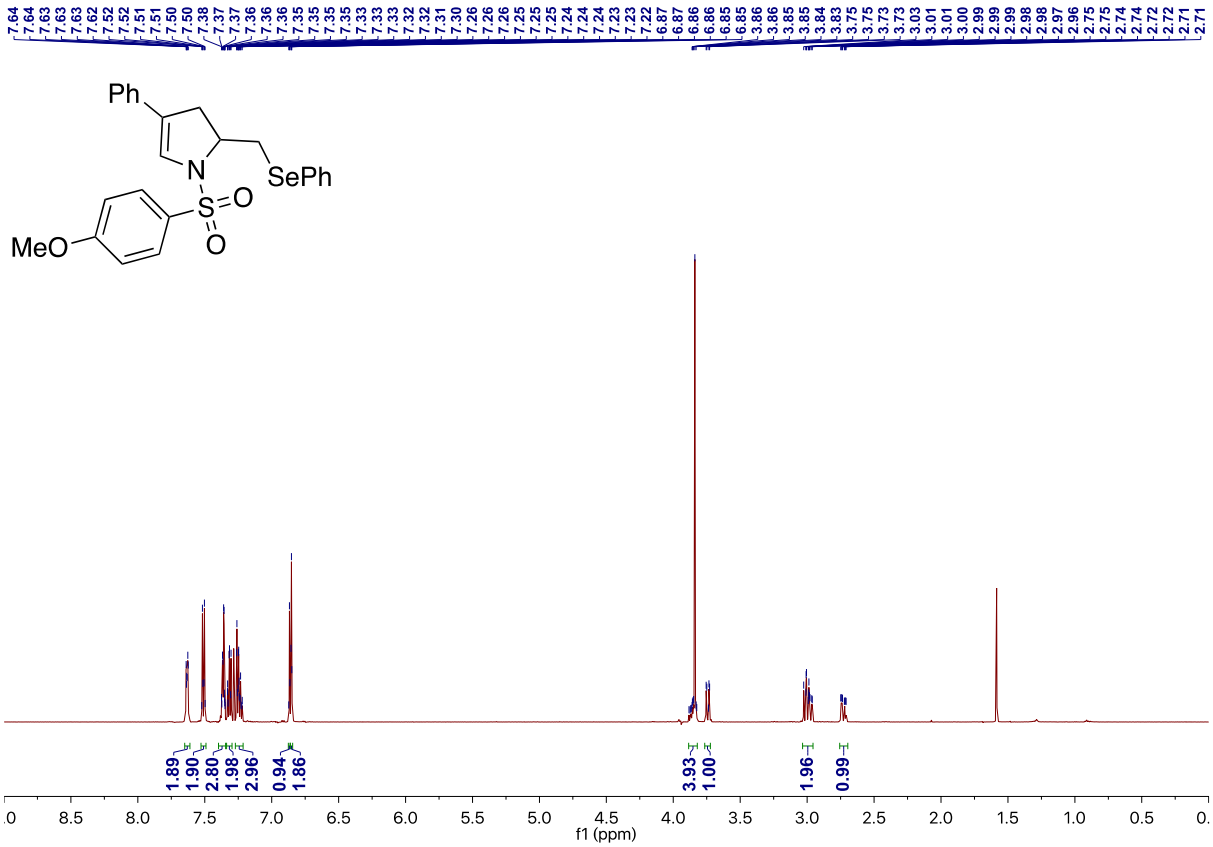


^{77}Se NMR (115 MHz, Chloroform-*d*)

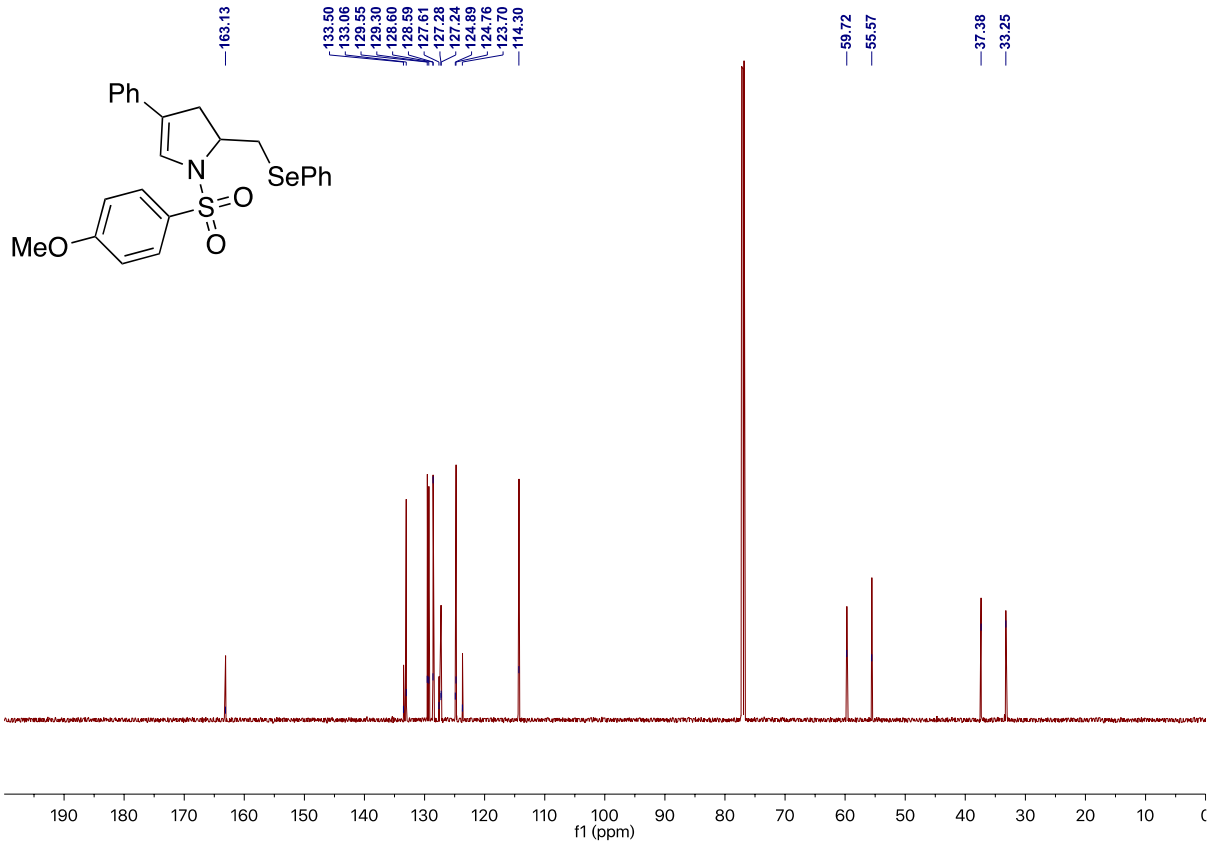


1-((4-methoxyphenyl)sulfonyl)-4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrole (9c)

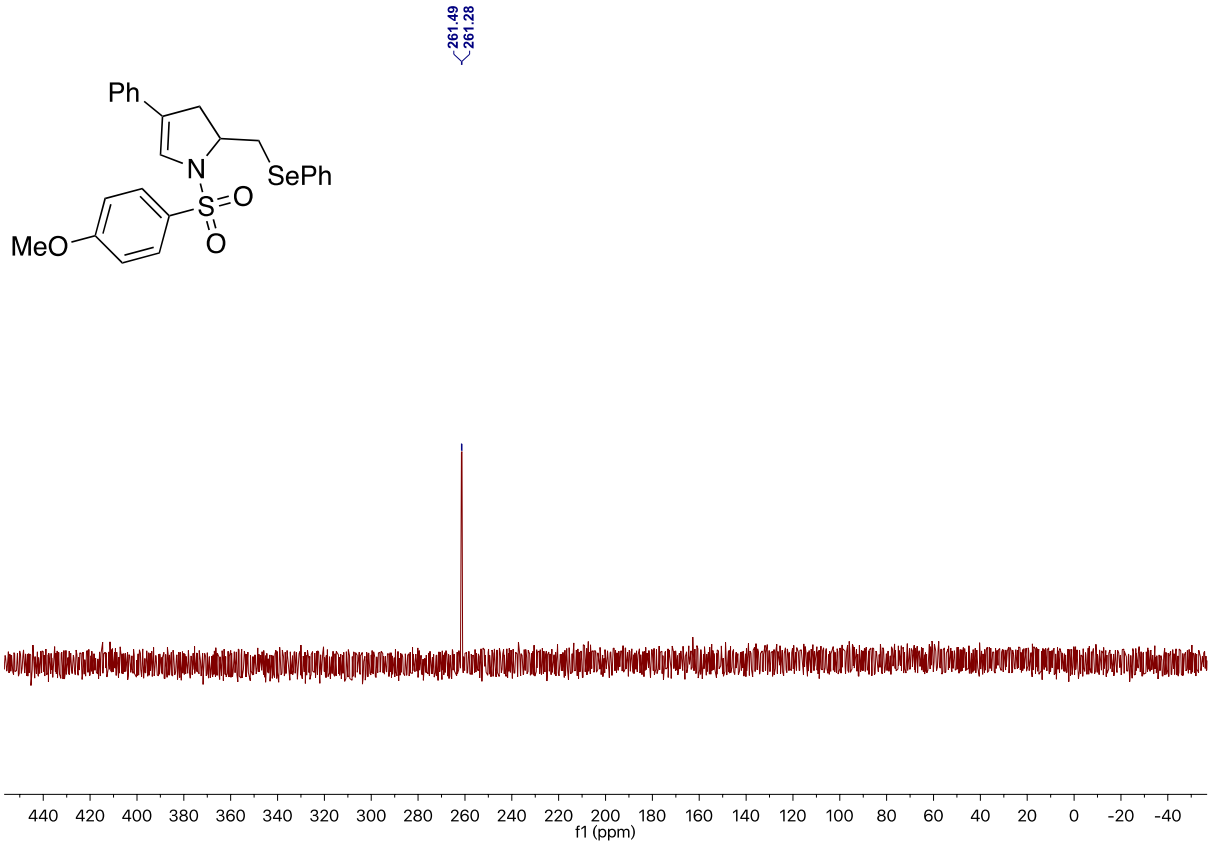
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

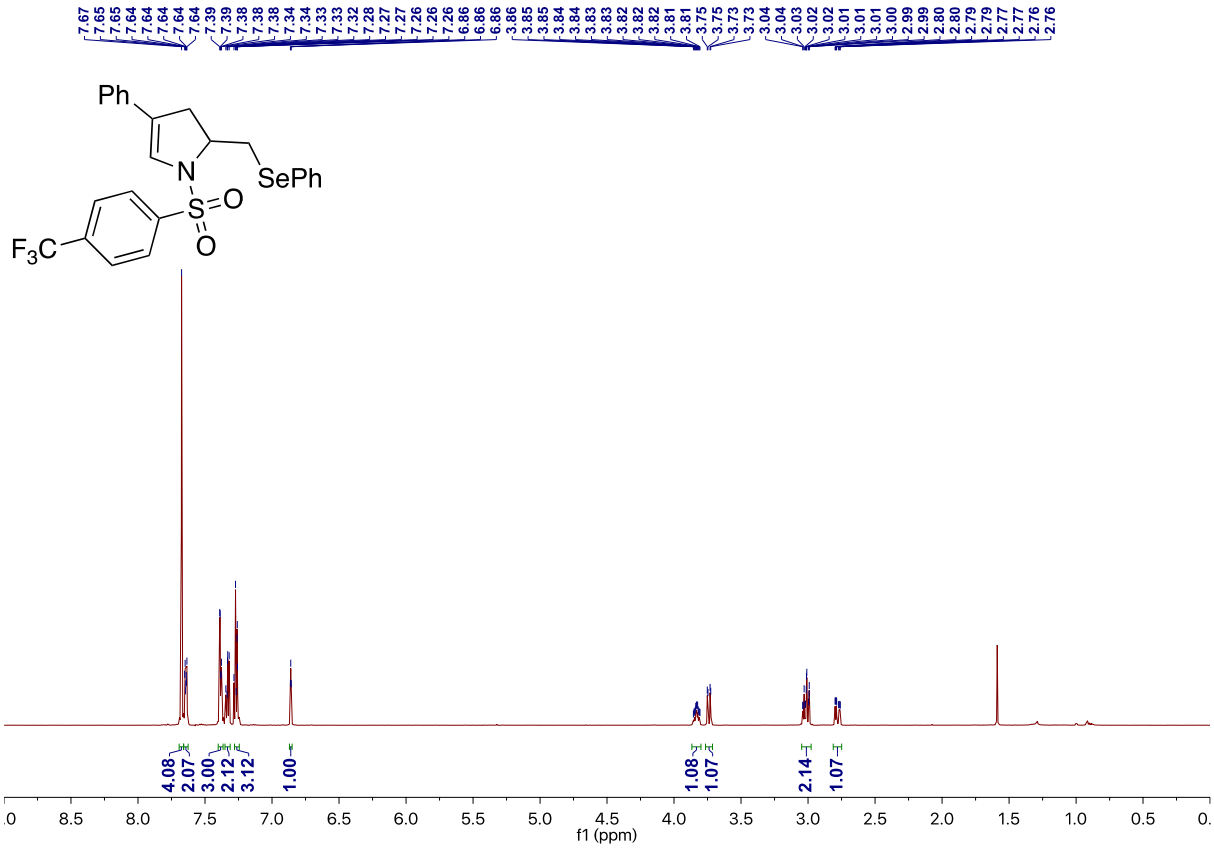


^{77}Se NMR (115 MHz, Chloroform-*d*)

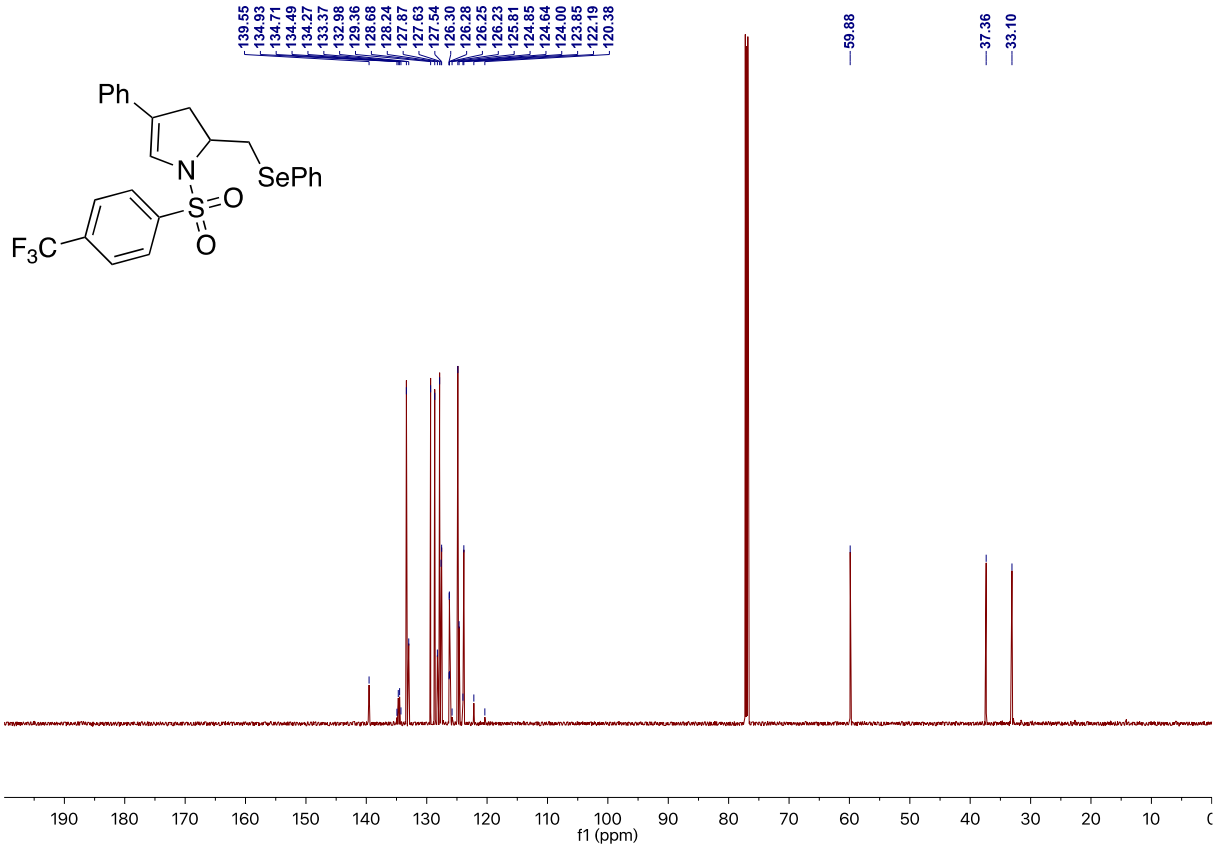


4-phenyl-2-((phenylselanyl)methyl)-1-((4-(trifluoromethyl)phenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole (9d)

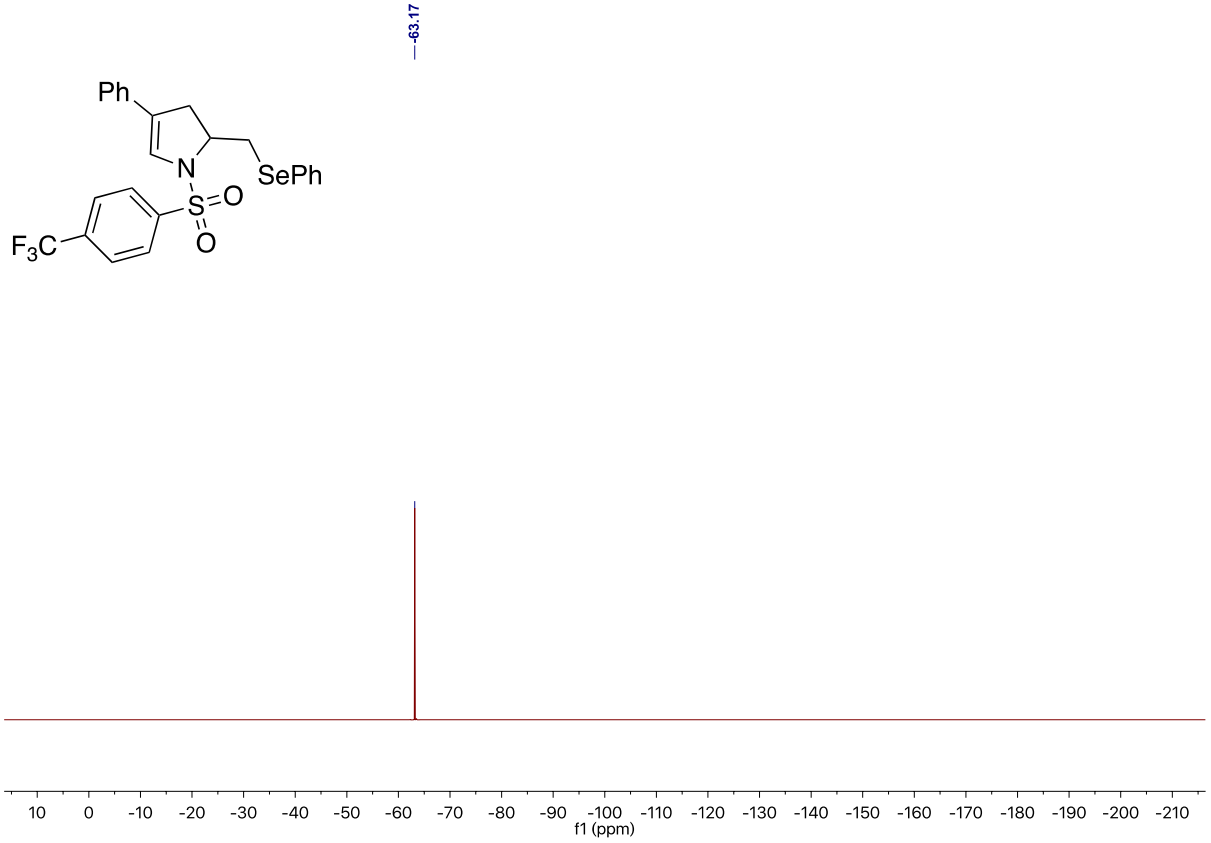
^{1}H NMR (600 MHz, Chloroform-*d*)



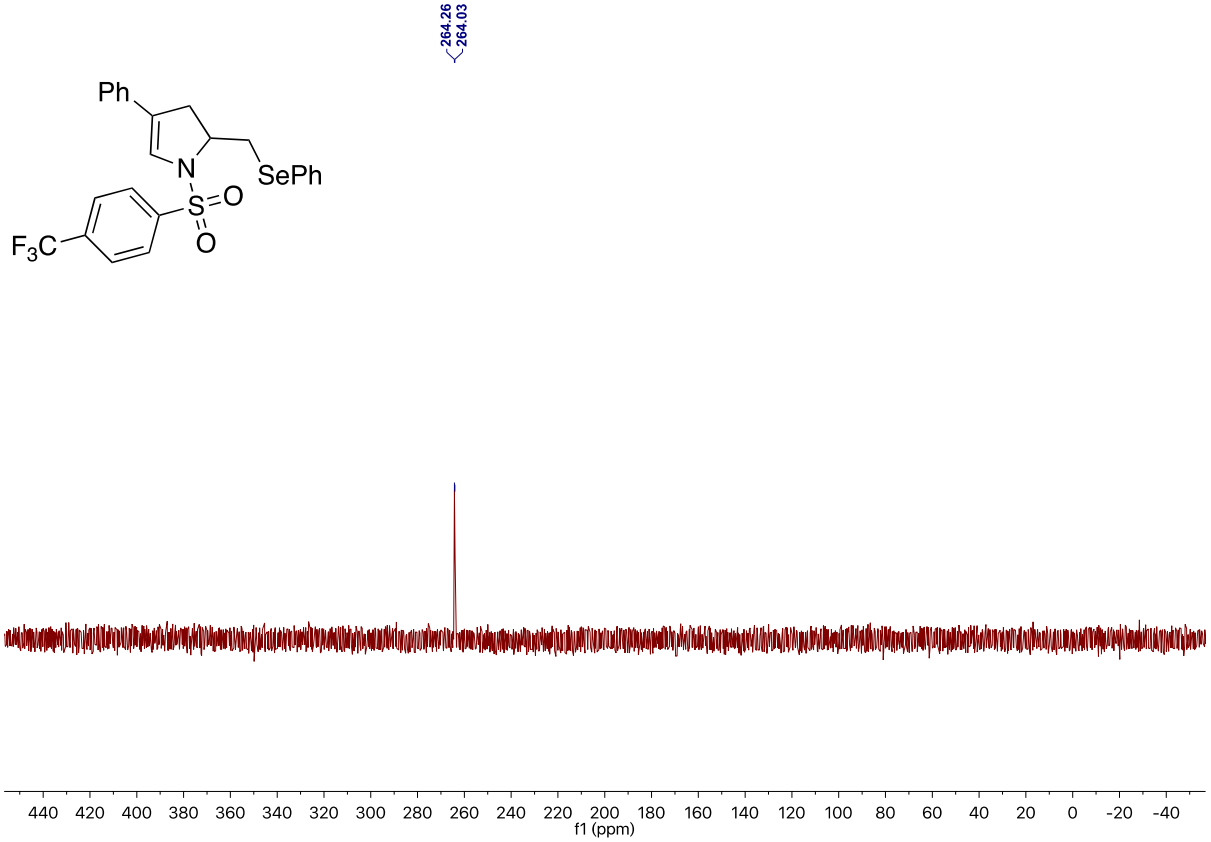
^{13}C NMR (151 MHz, Chloroform-*d*)



^{19}F NMR (565 MHz, Chloroform-*d*)

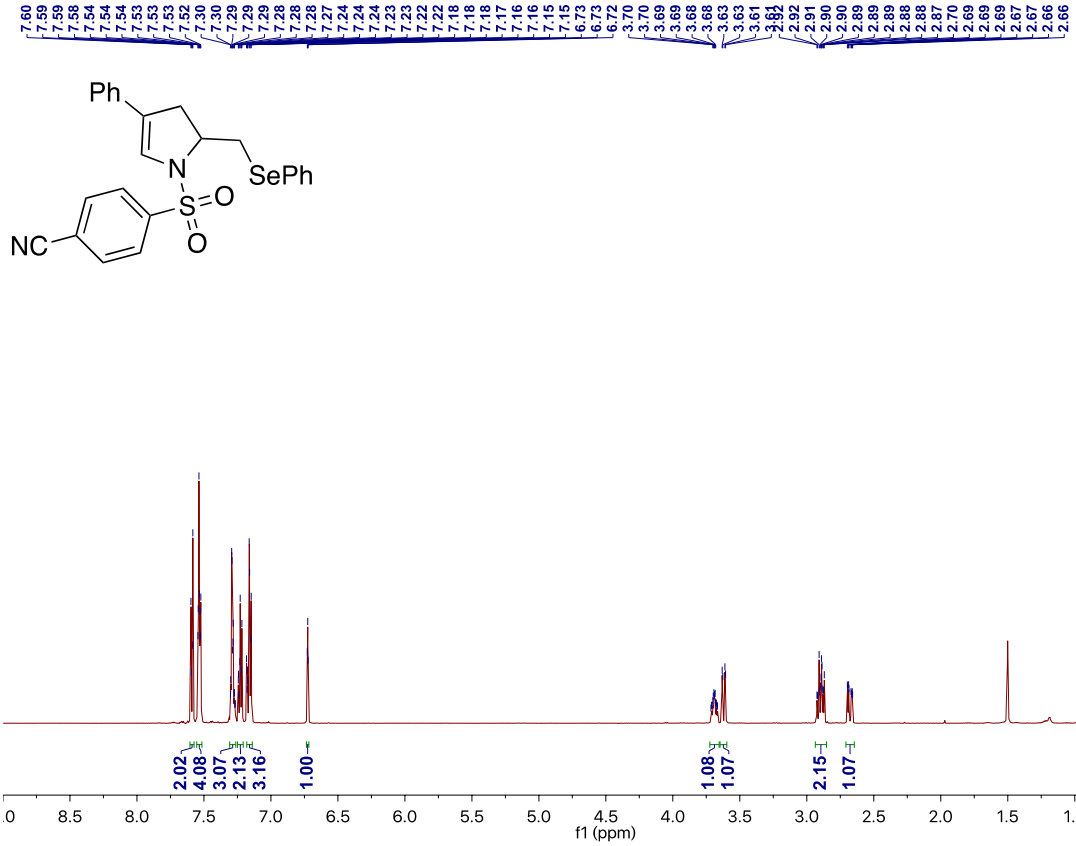


^{77}Se NMR (115 MHz, Chloroform-*d*)

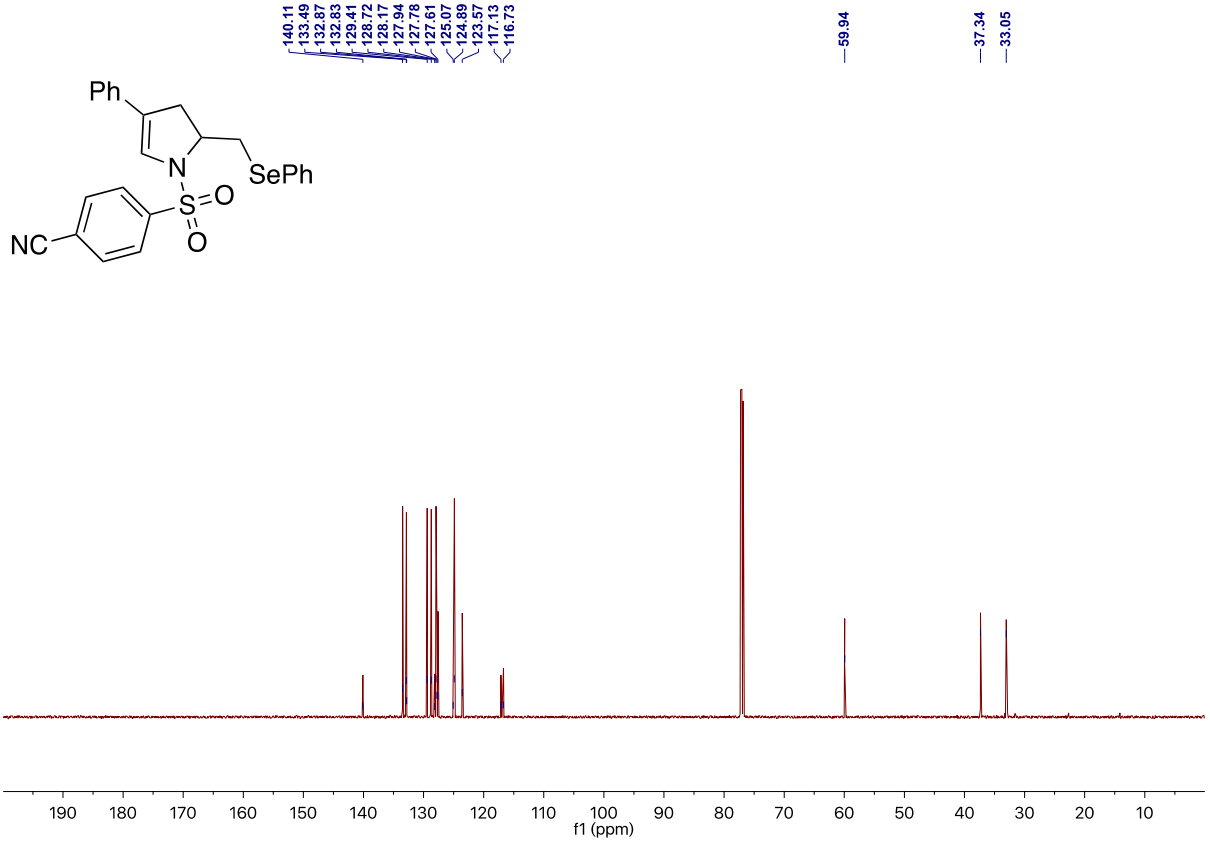


4-((4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrol-1-yl)sulfonyl)benzonitrile (9e)

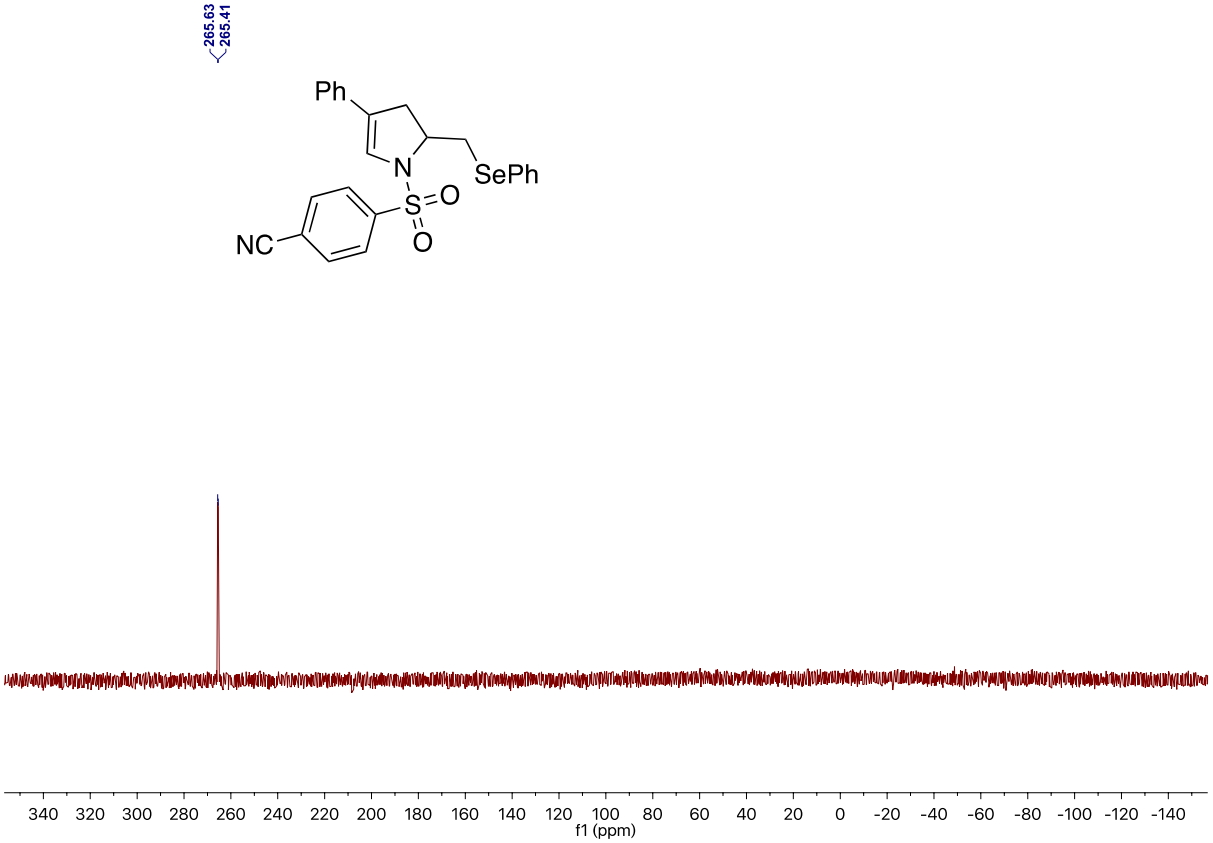
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

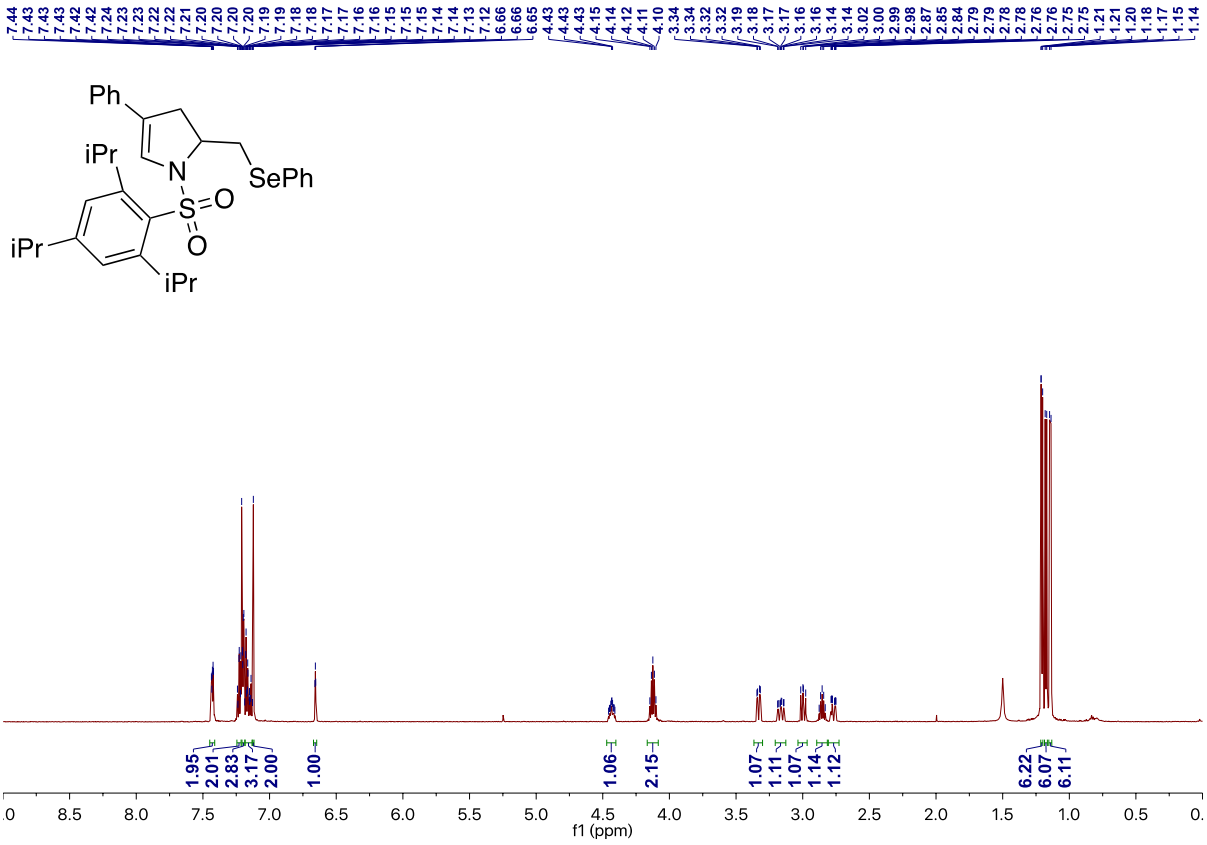


^{77}Se NMR (115 MHz, Chloroform-*d*)

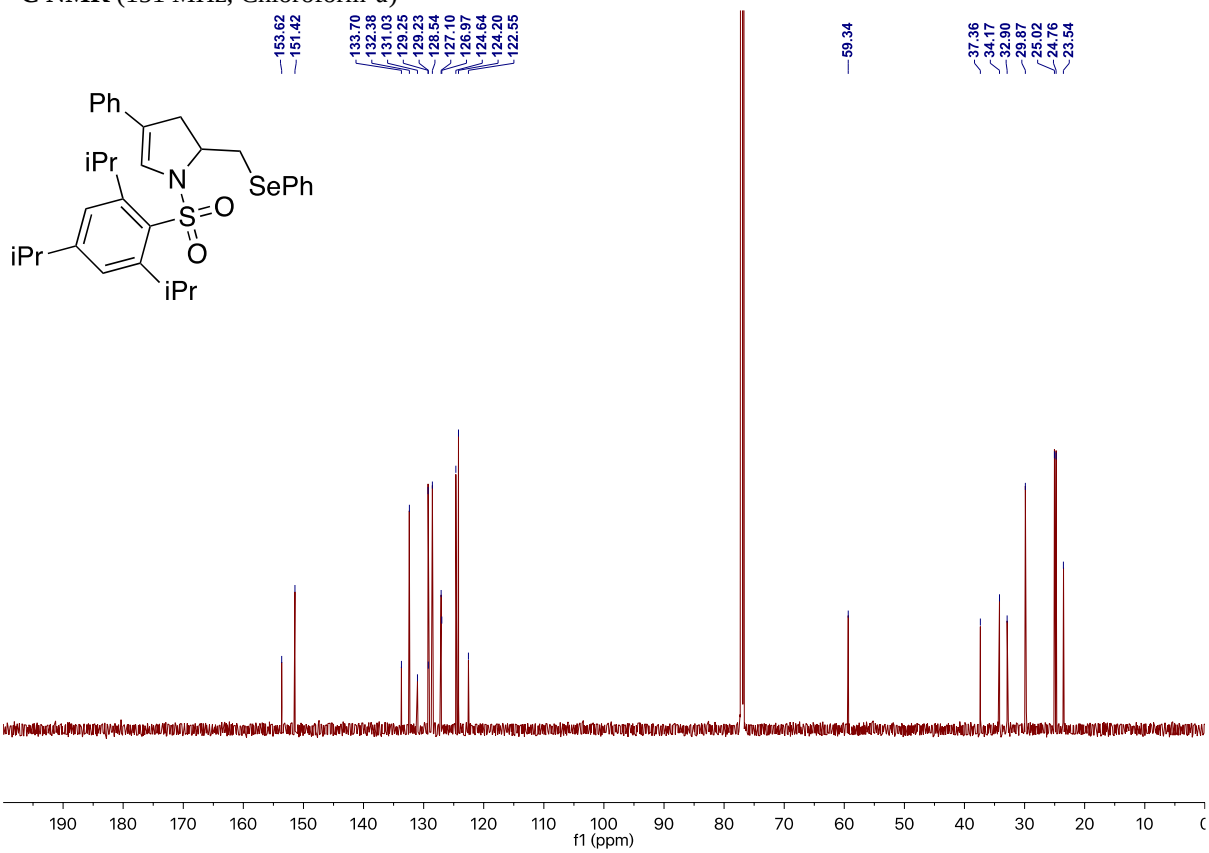


4-phenyl-2-((phenylselanyl)methyl)-1-((2,4,6-triisopropylphenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole (9f)

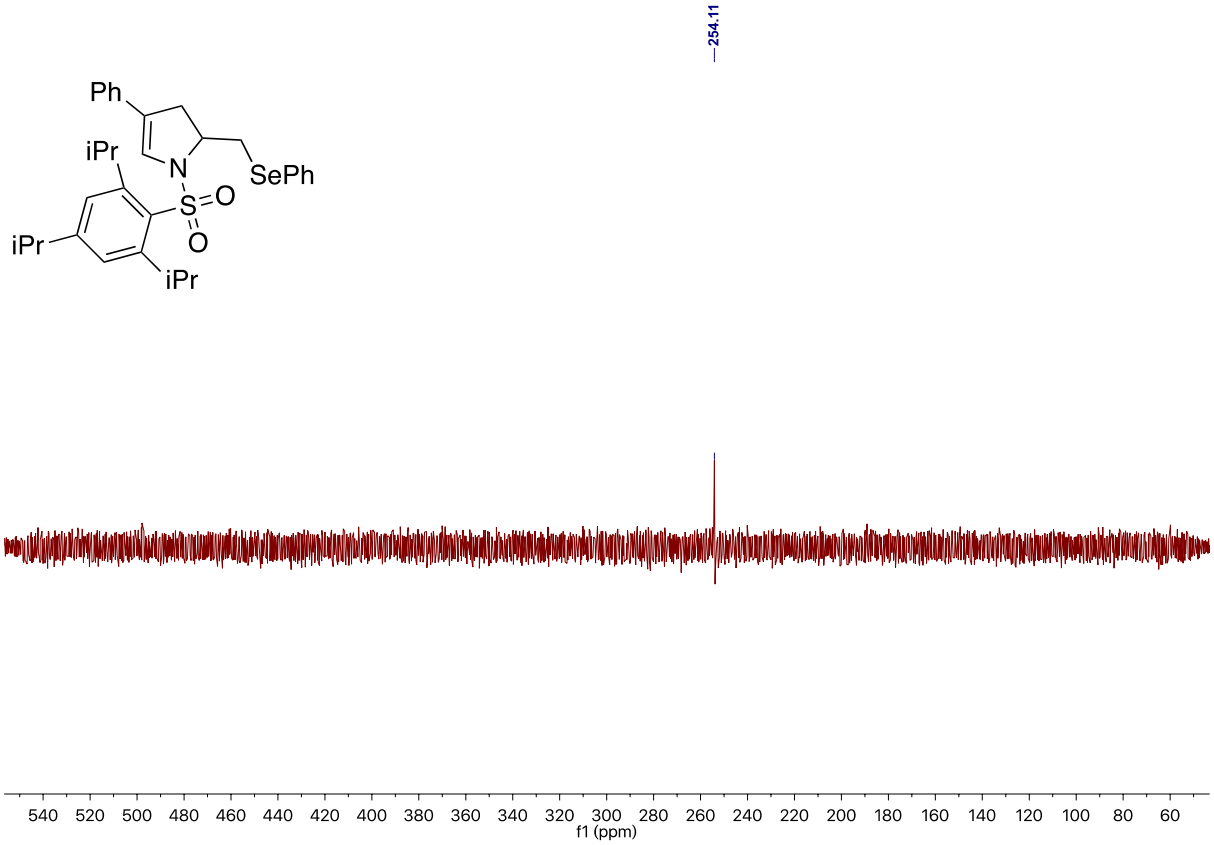
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

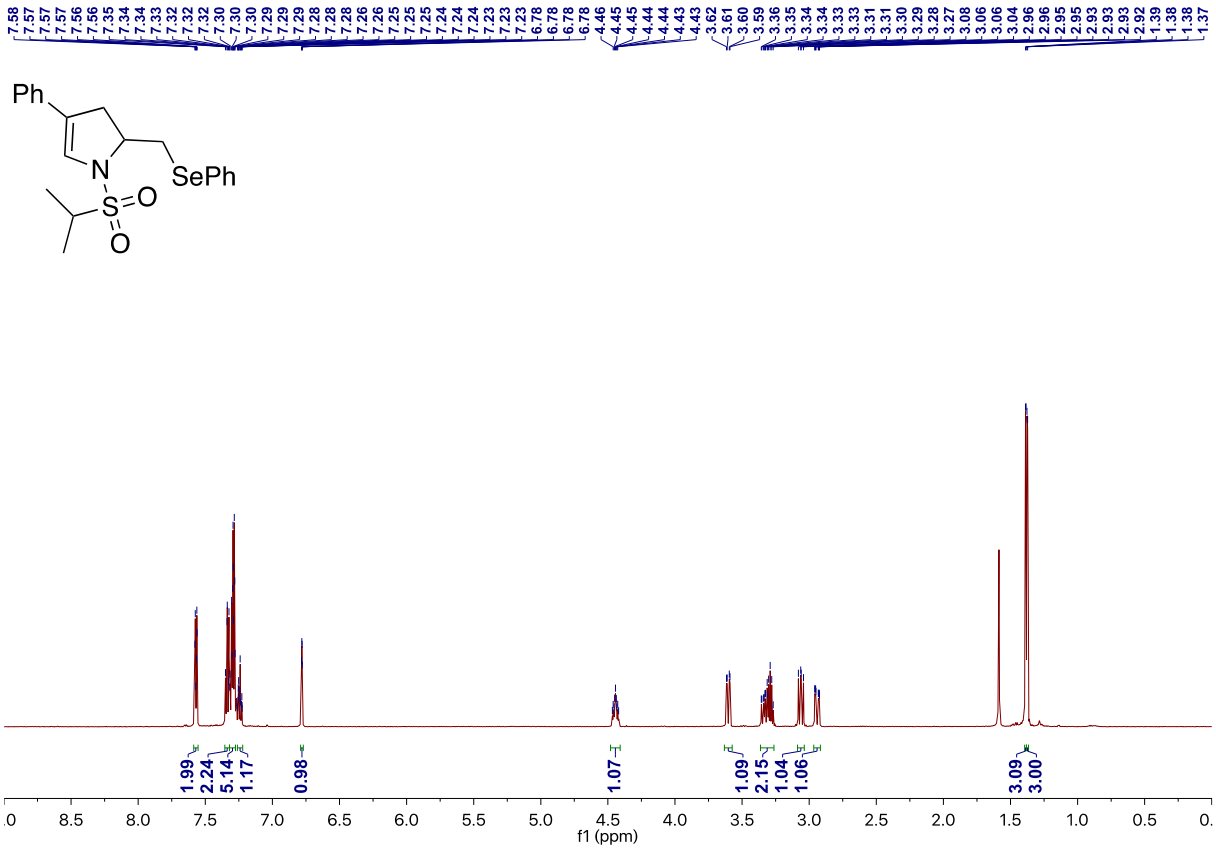


^{77}Se NMR (115 MHz, Chloroform-*d*)

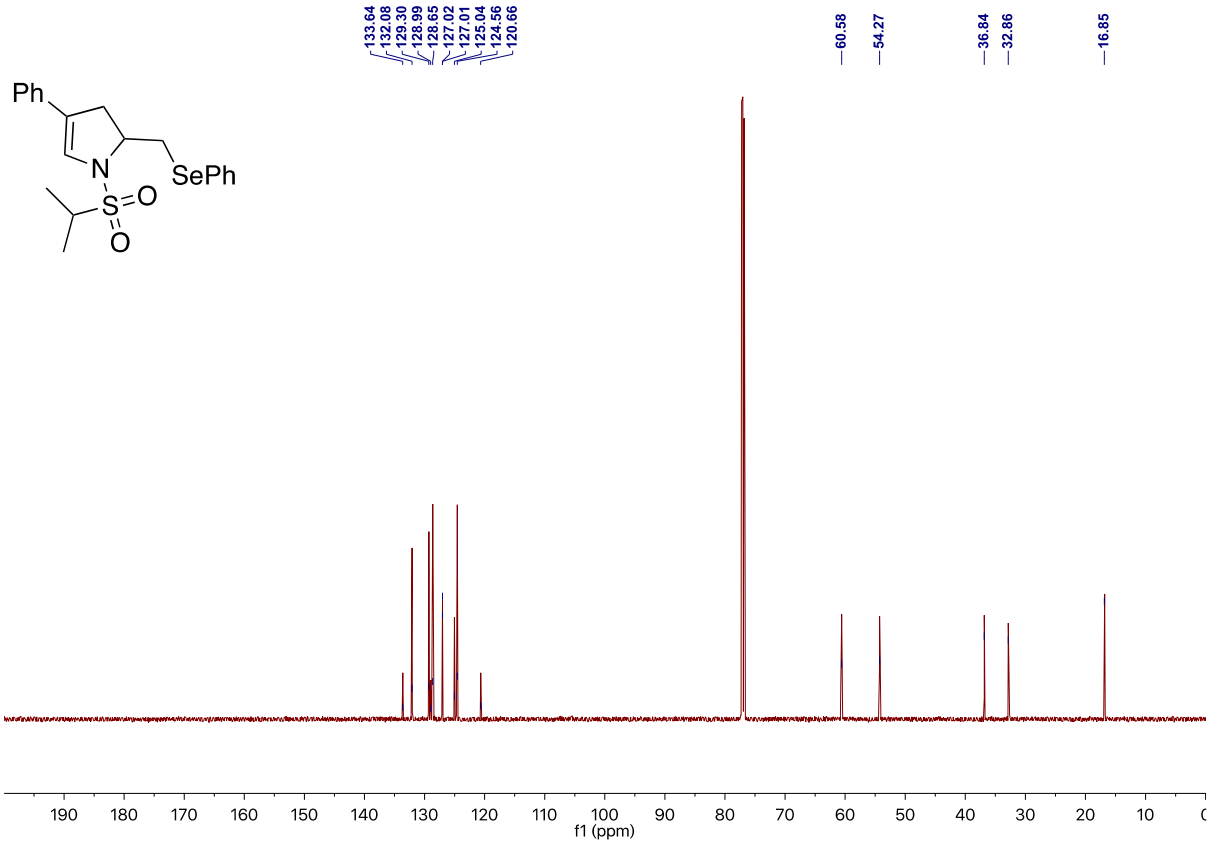


1-(isopropylsulfonyl)-4-phenyl-2-((phenylselanyl)methyl)-2,3-dihydro-1*H*-pyrrole (9g)

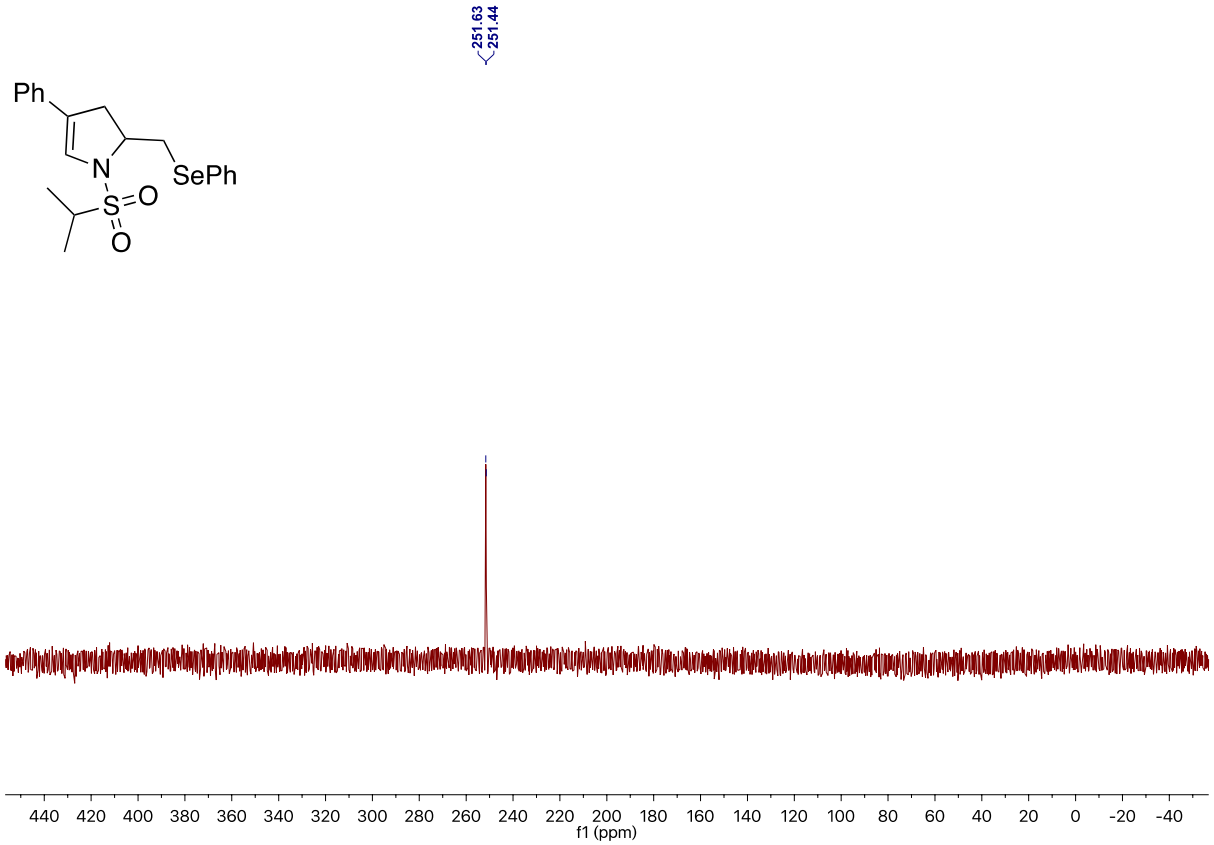
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

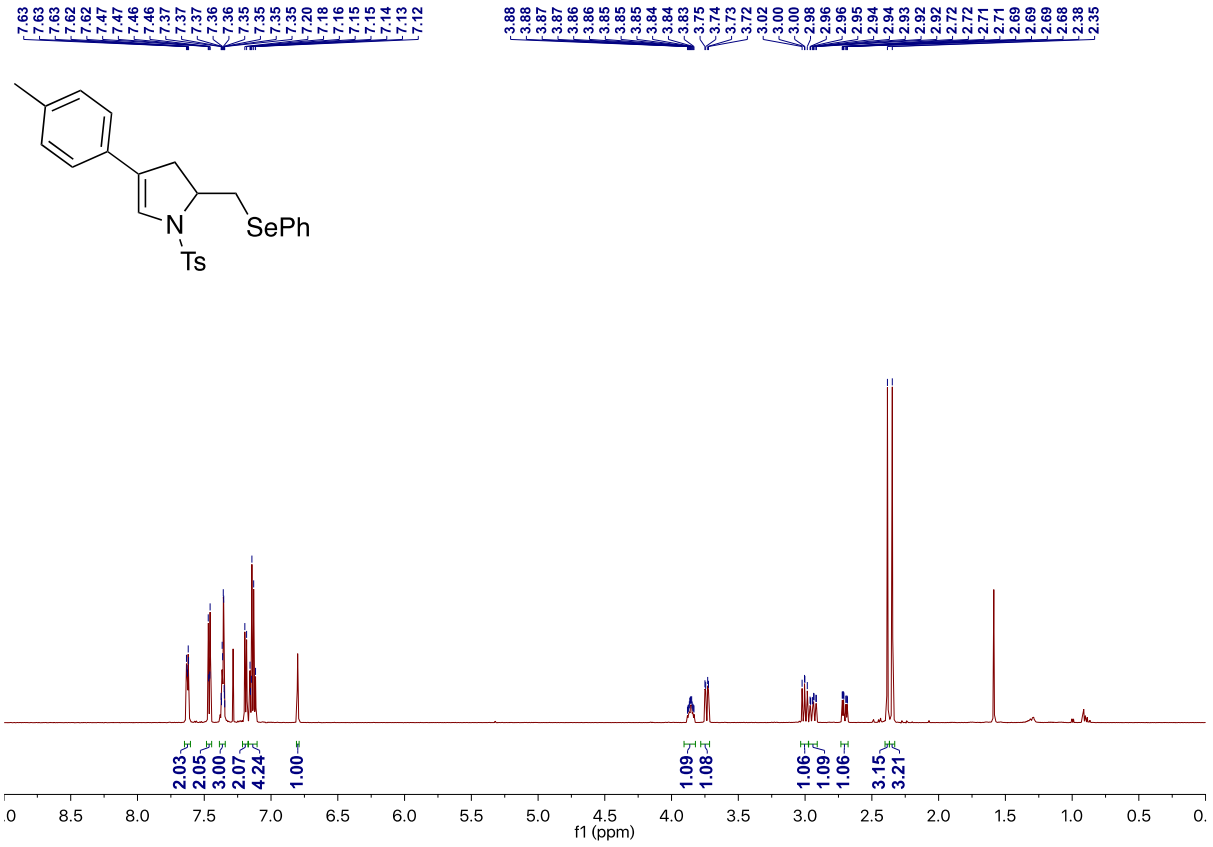


^{77}Se NMR (115 MHz, Chloroform-*d*)

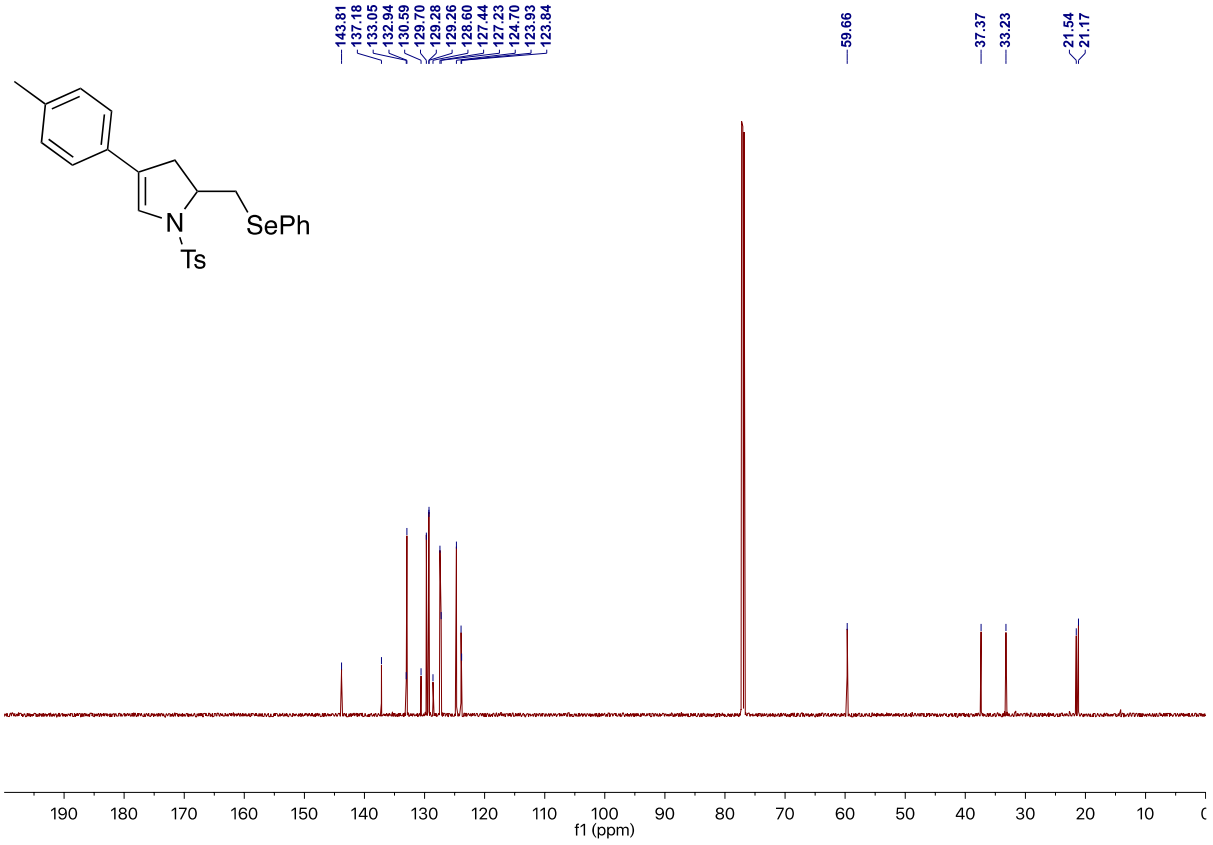


2-((phenylselanyl)methyl)-4-(*p*-tolyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9h)

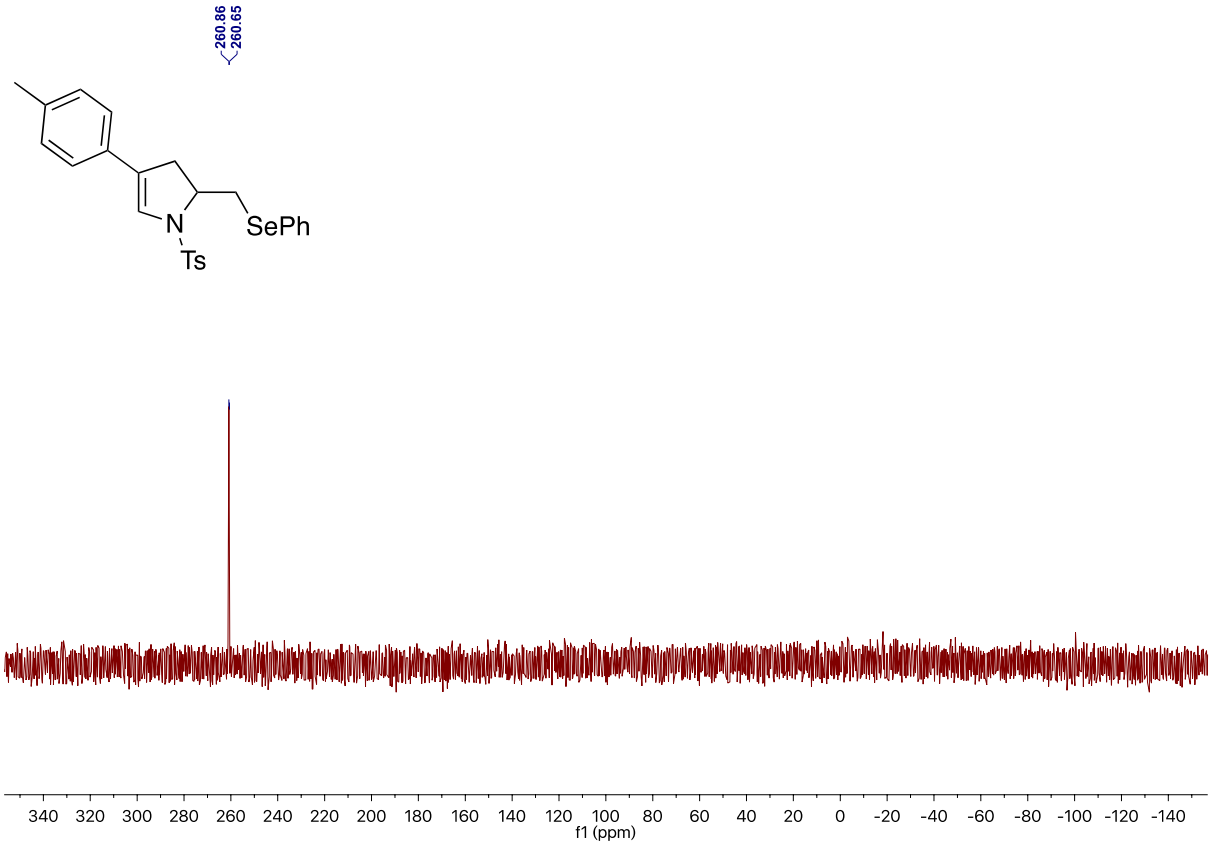
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

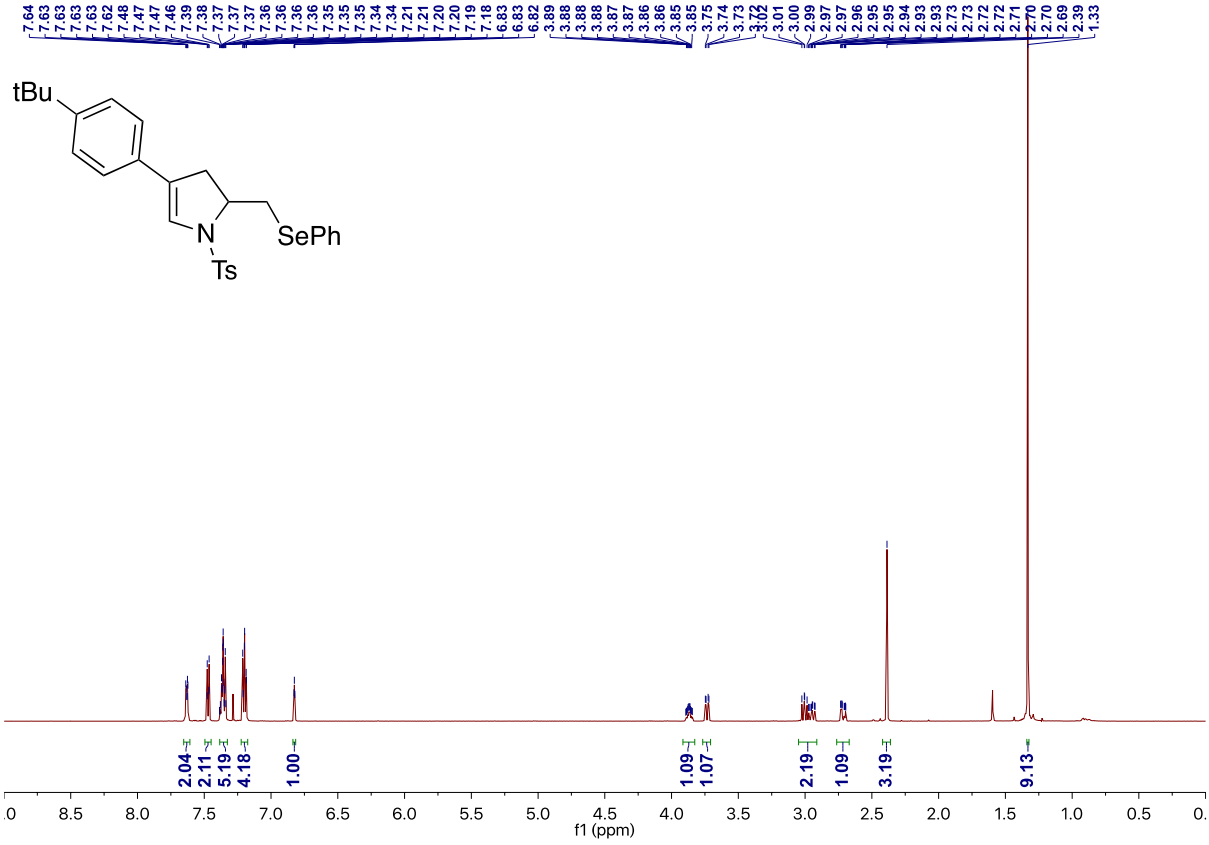


^{77}Se NMR (115 MHz, Chloroform-*d*)

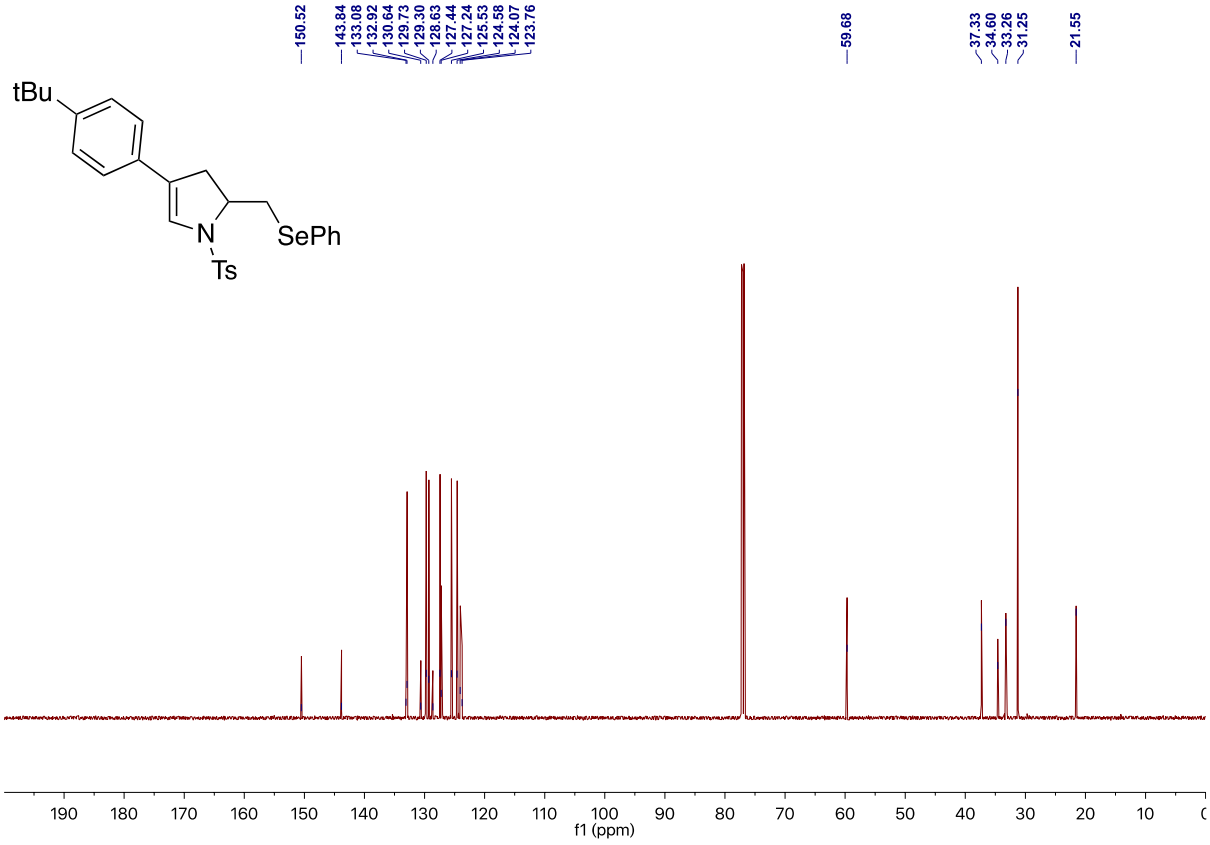


4-(4-(*tert*-butyl)phenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9i)

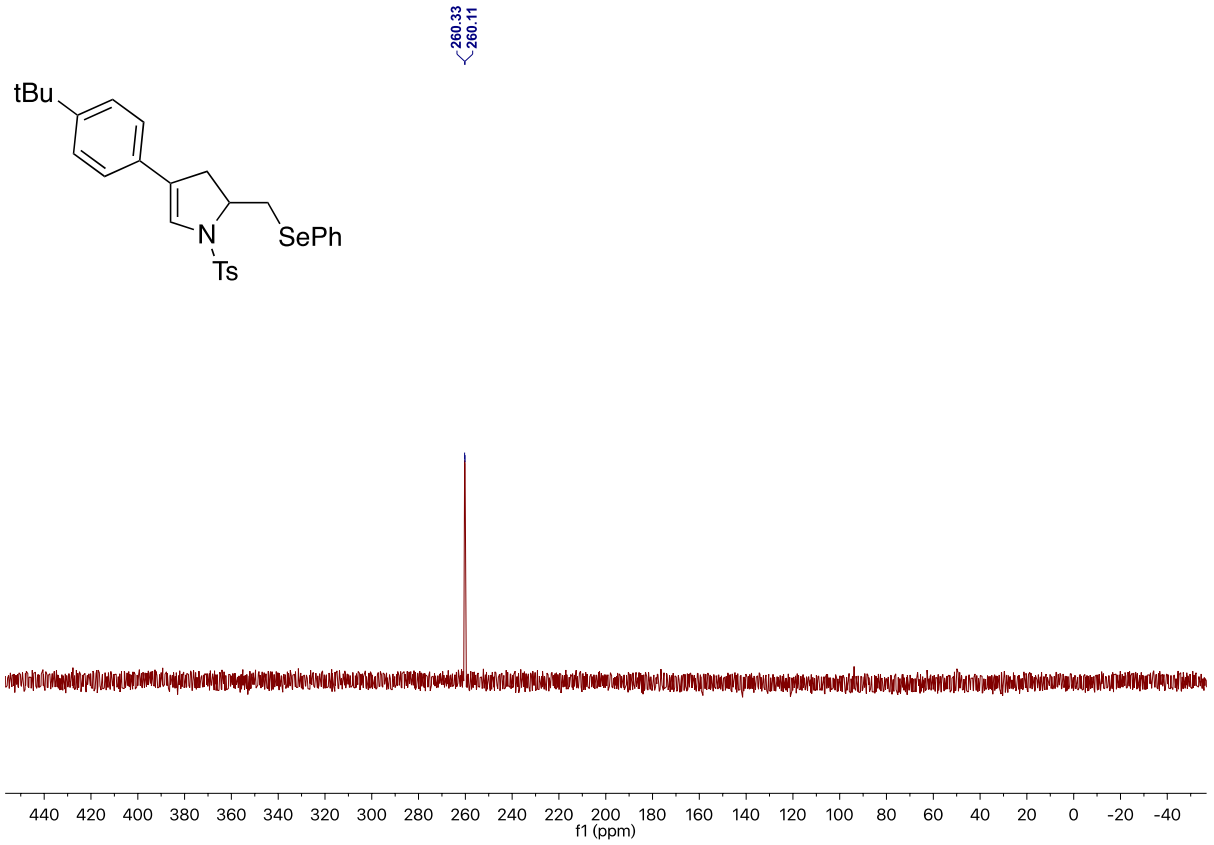
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

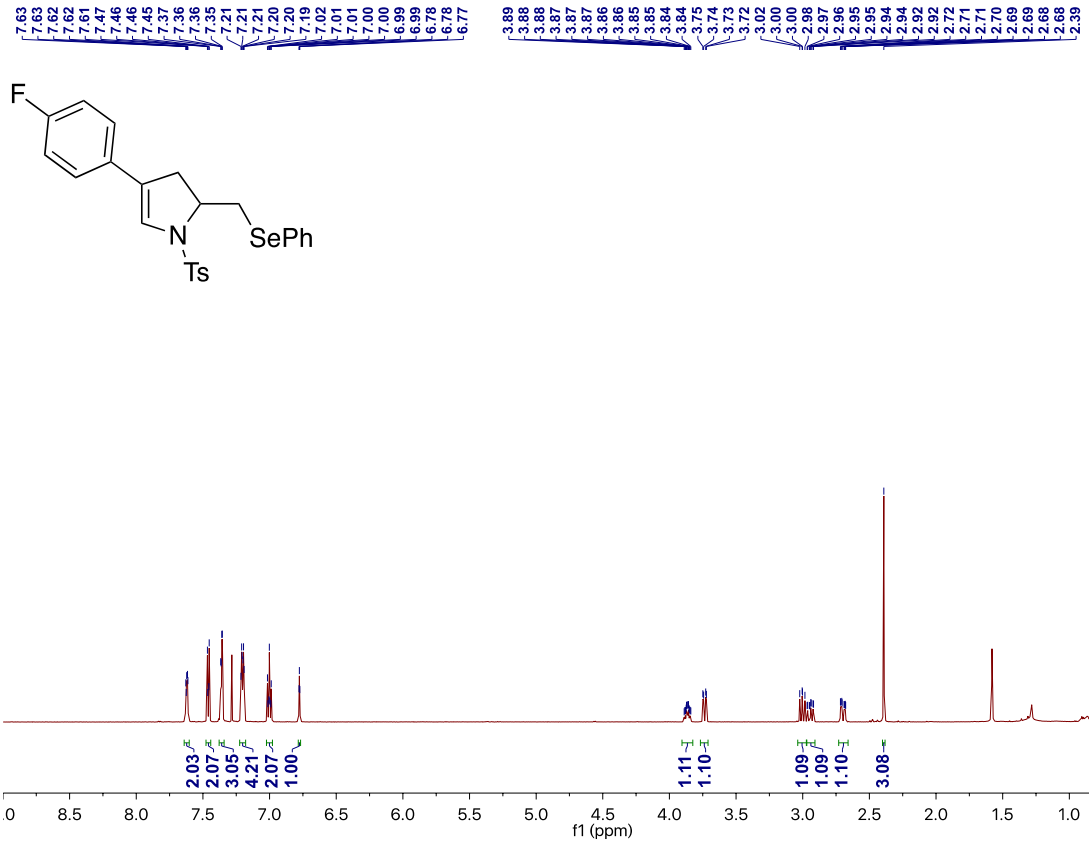


^{77}Se NMR (115 MHz, Chloroform-*d*)

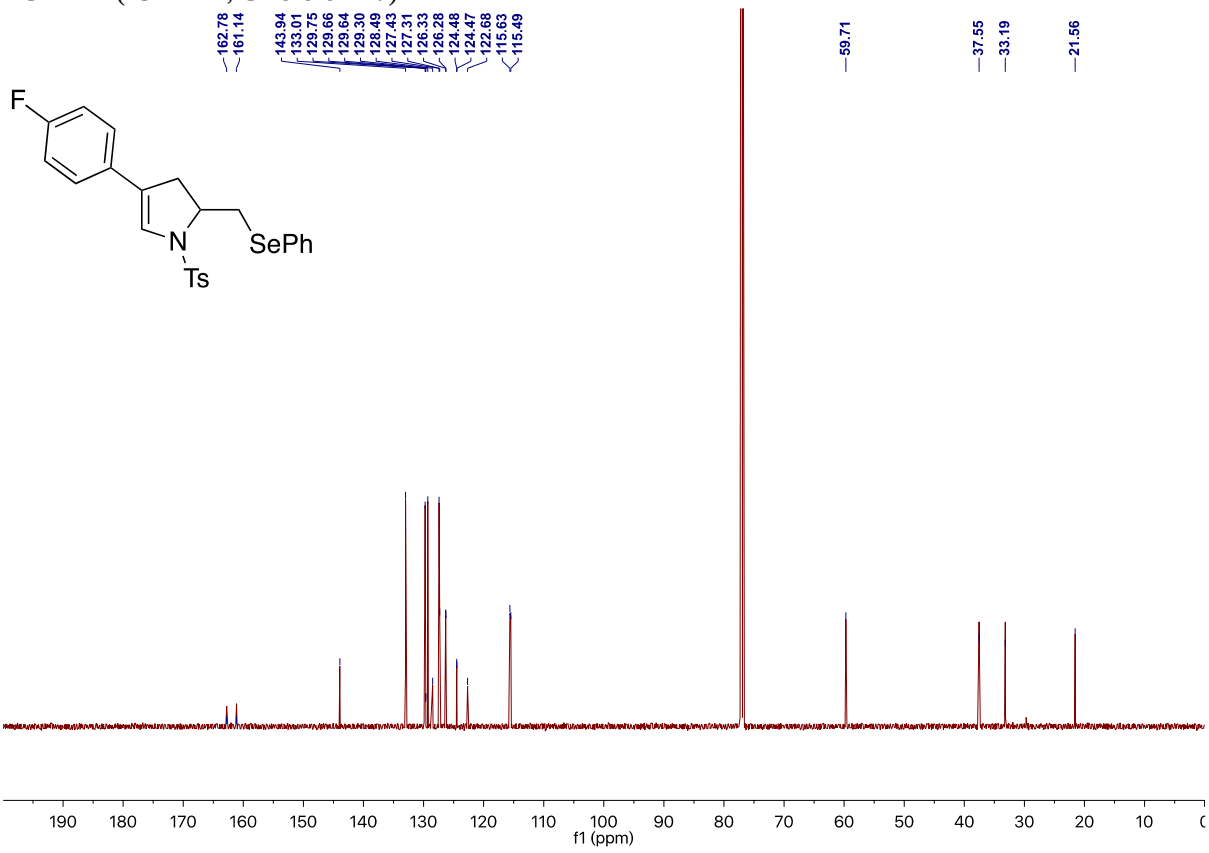


4-(4-fluorophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9j)

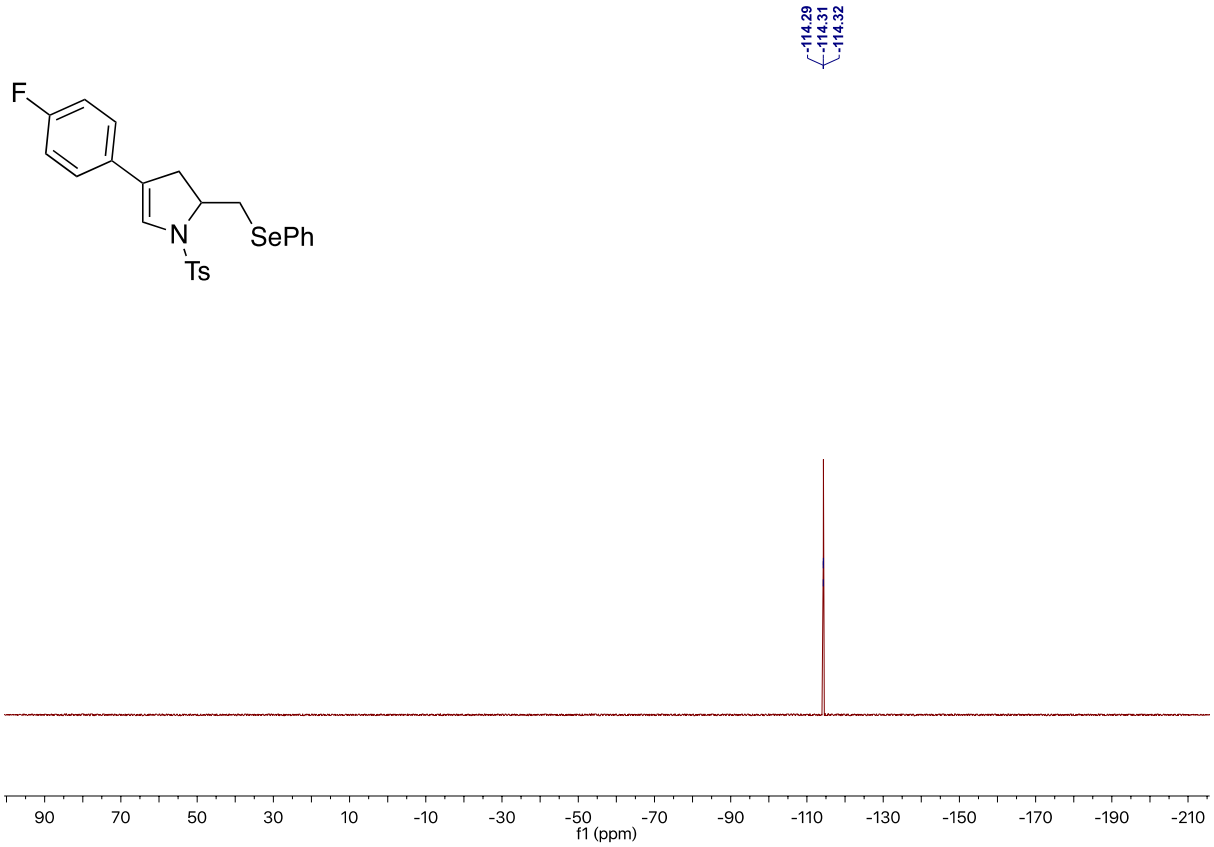
^{1}H NMR (600 MHz, Chloroform-*d*)



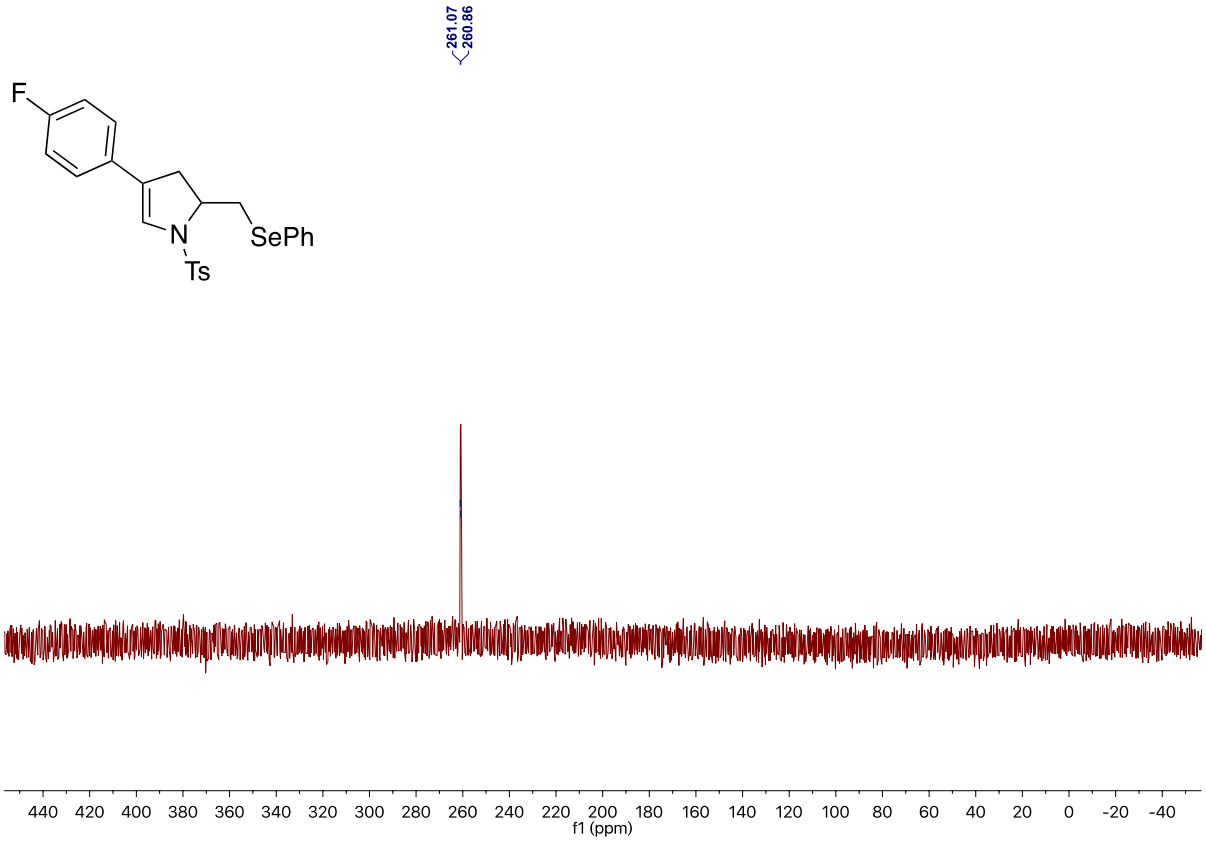
^{13}C NMR (151 MHz, Chloroform-*d*)



^{19}F NMR (376 MHz, Chloroform-*d*)

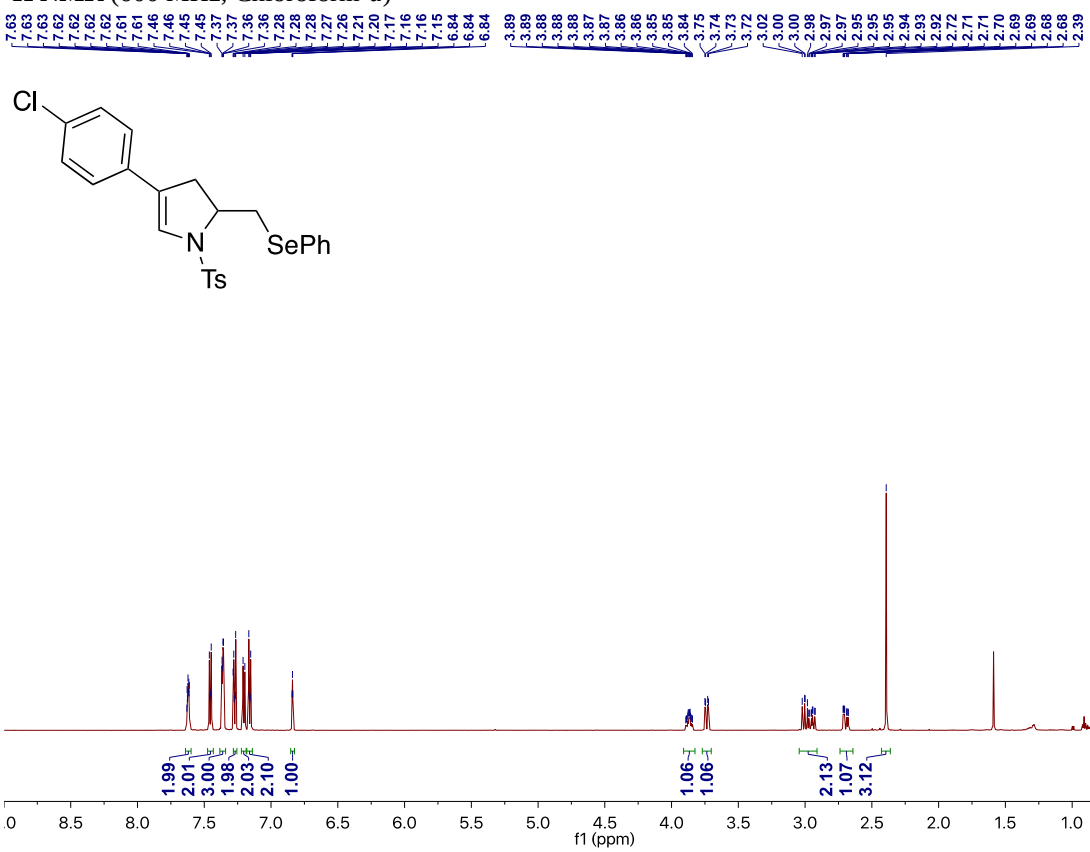


^{77}Se NMR (115 MHz, Chloroform-*d*)

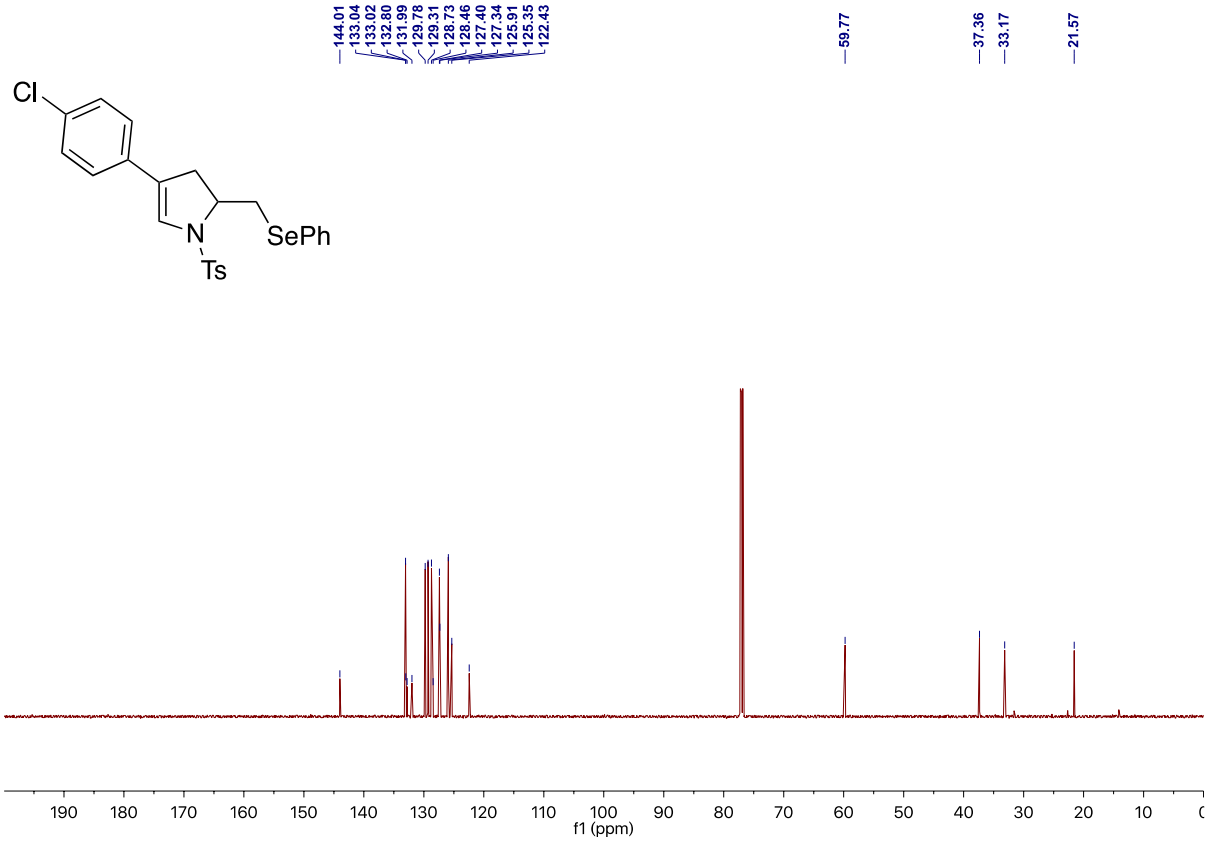


4-(4-chlorophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9k)

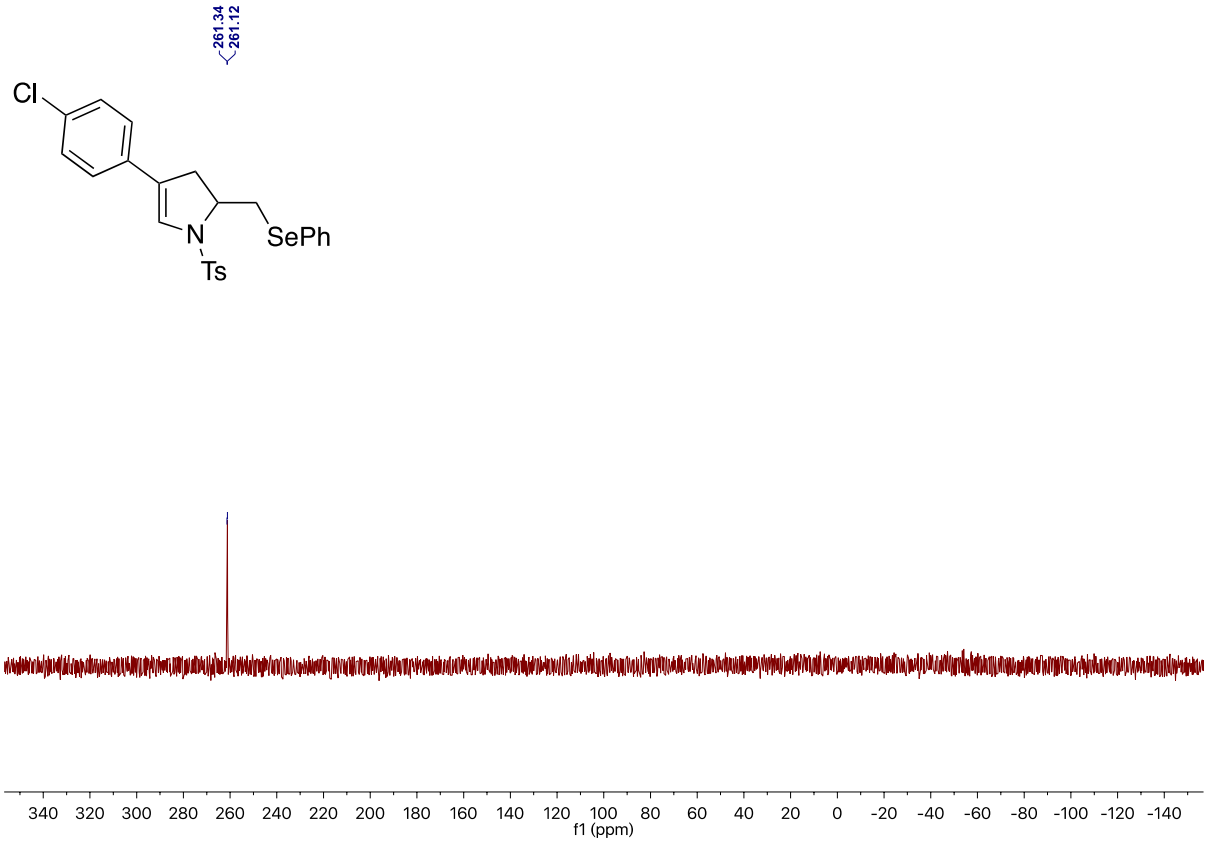
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

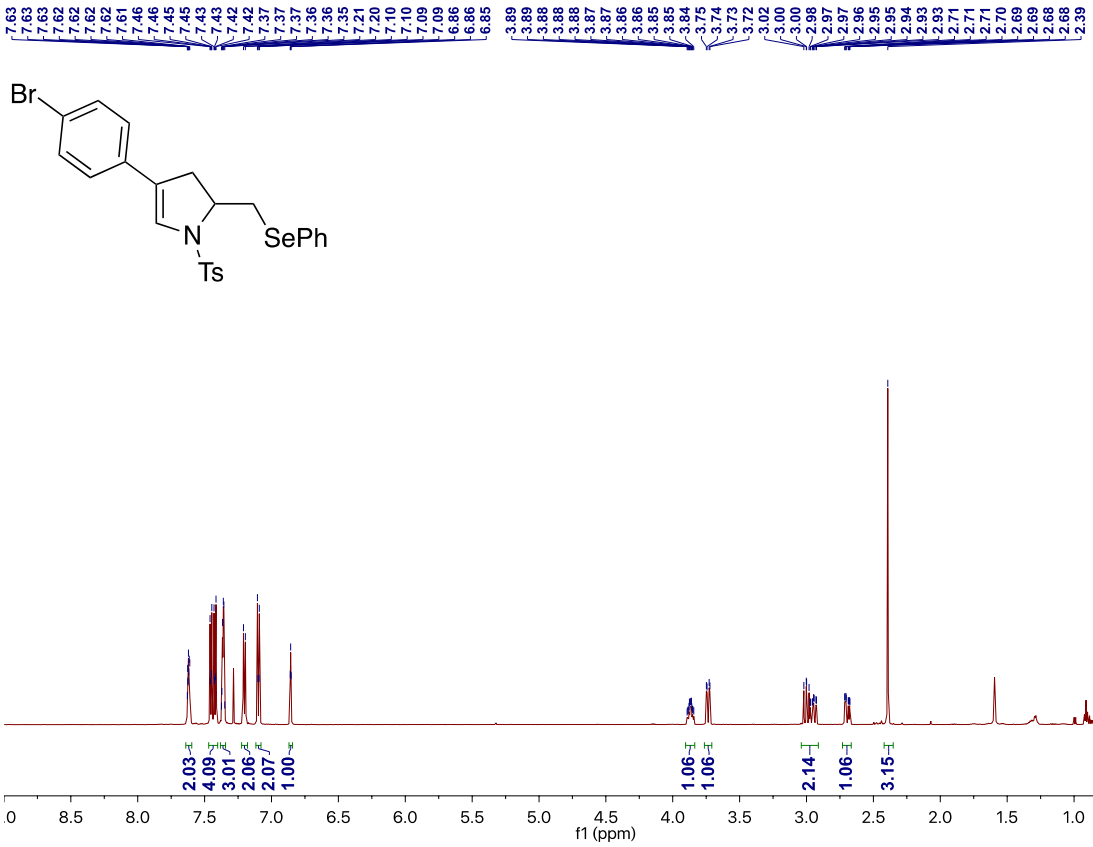


^{77}Se NMR (115 MHz, Chloroform-*d*)

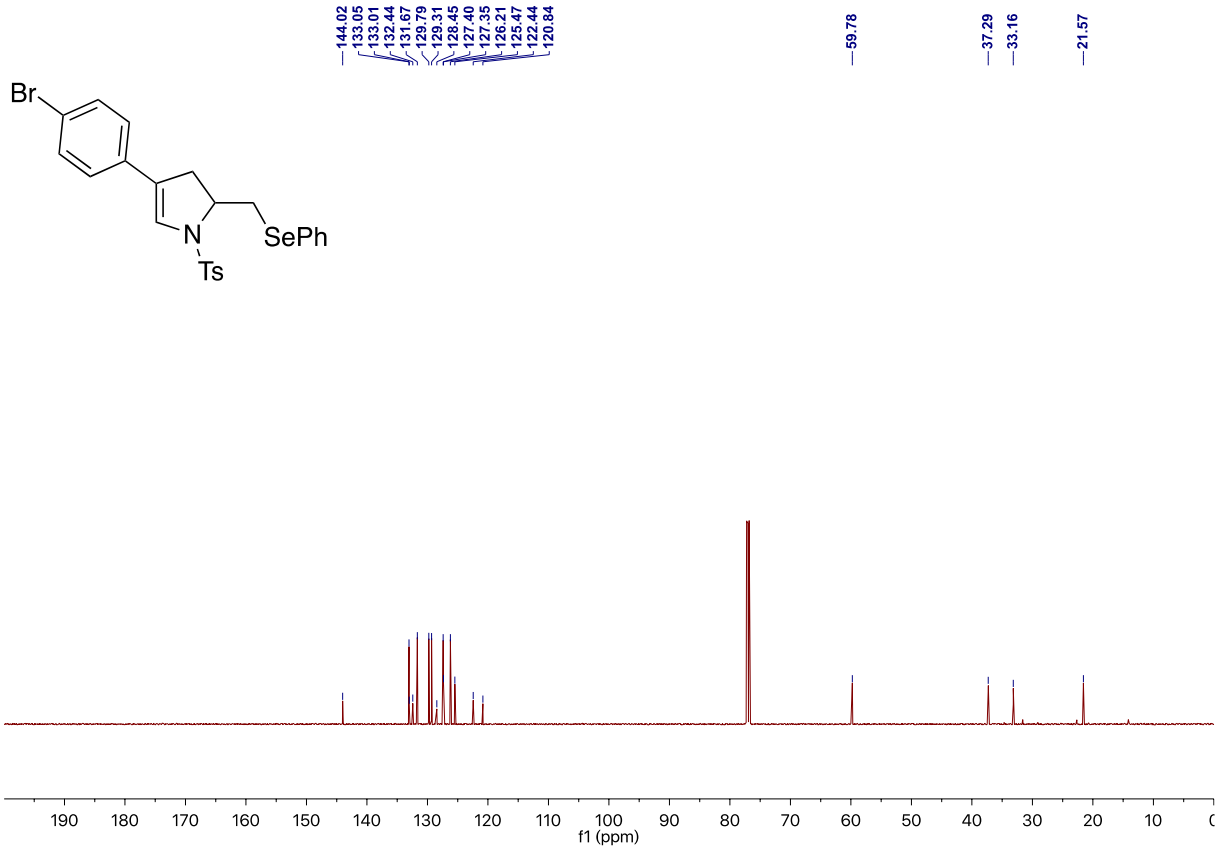


4-(4-bromophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9l)

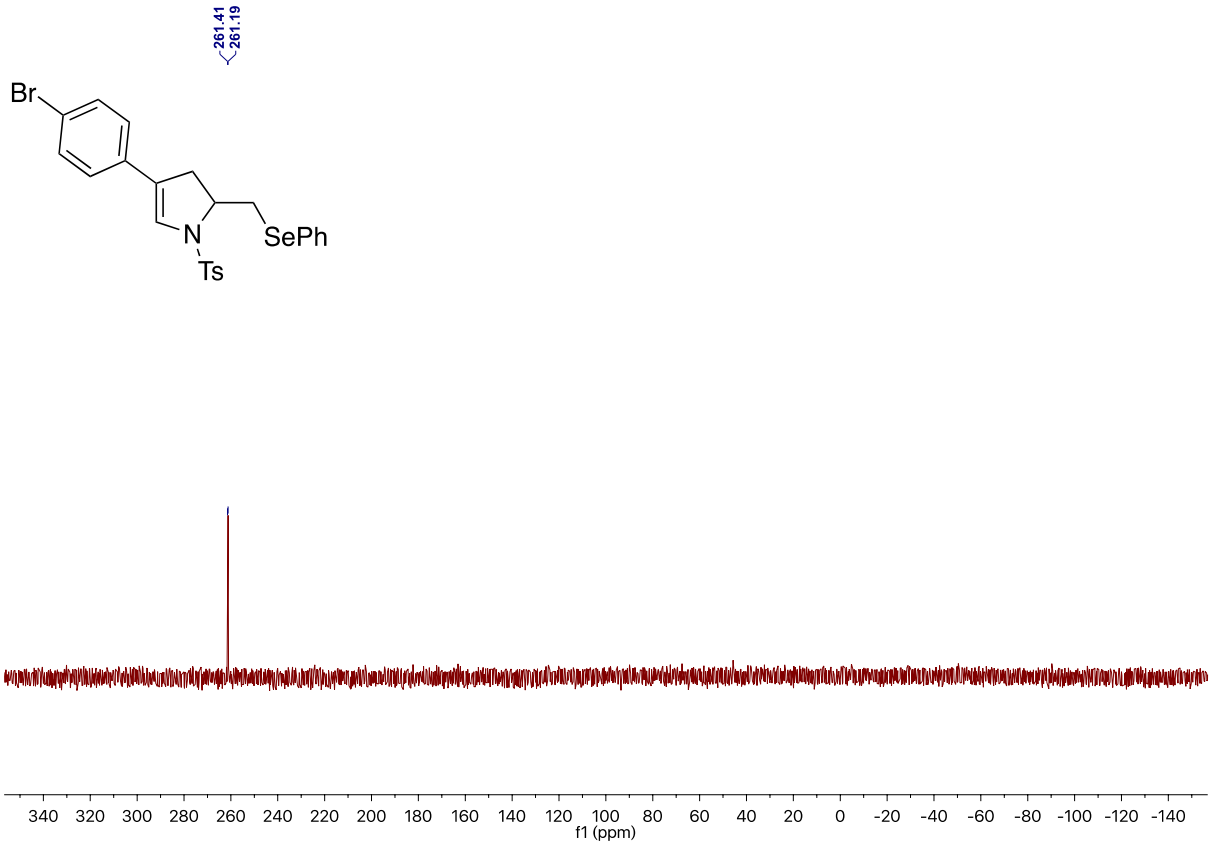
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

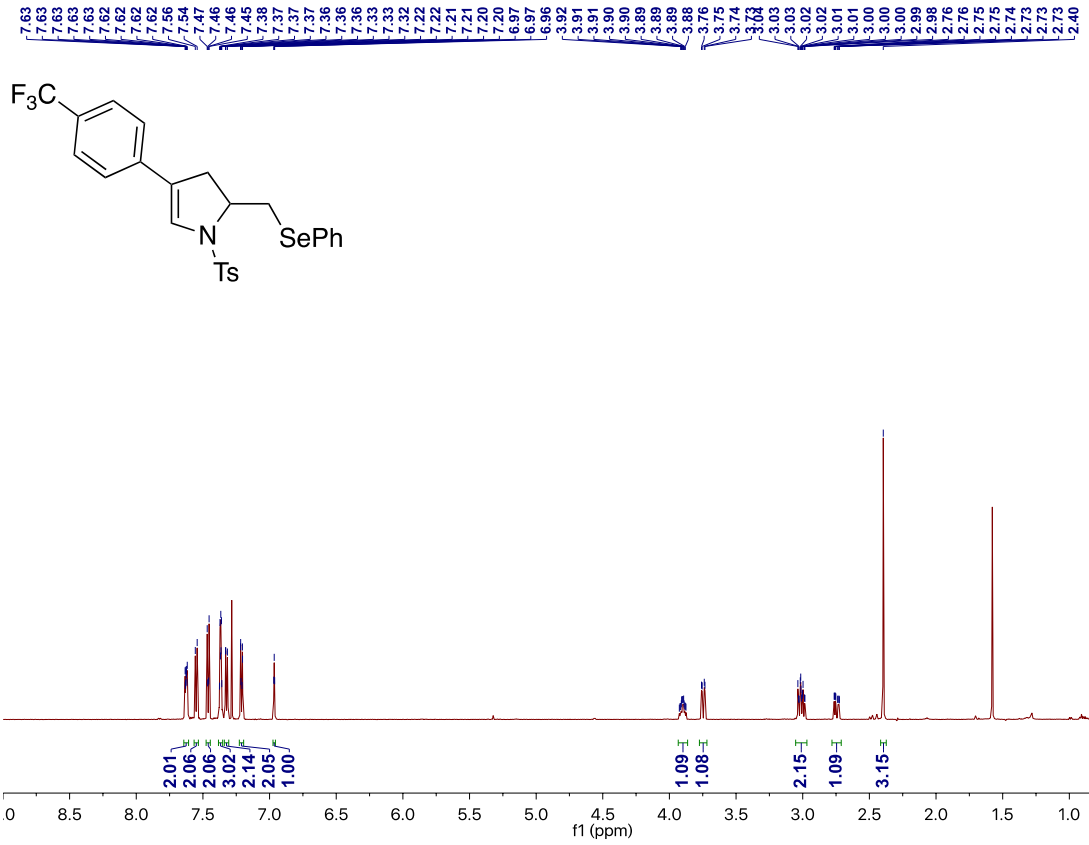


^{77}Se NMR (115 MHz, Chloroform-*d*)

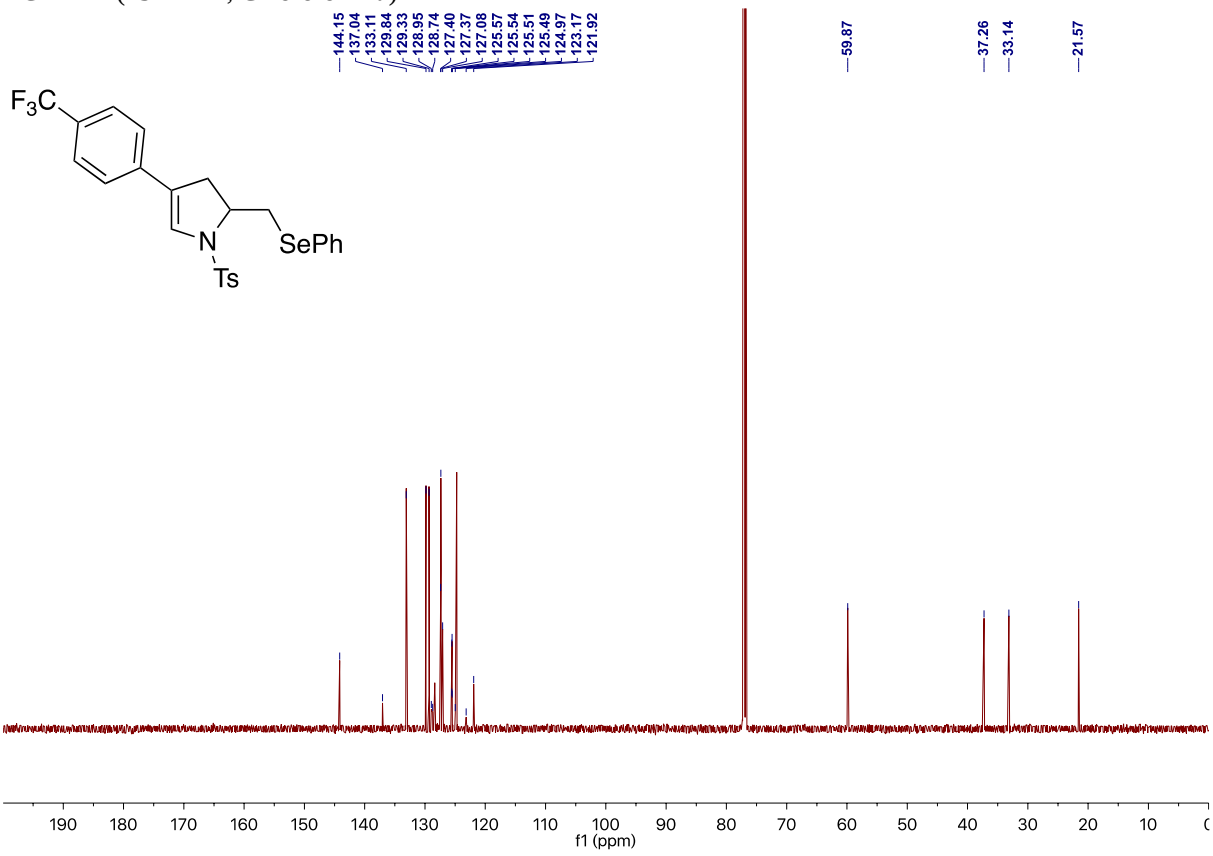


2-((phenylselanyl)methyl)-1-tosyl-4-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1*H*-pyrrole (9m)

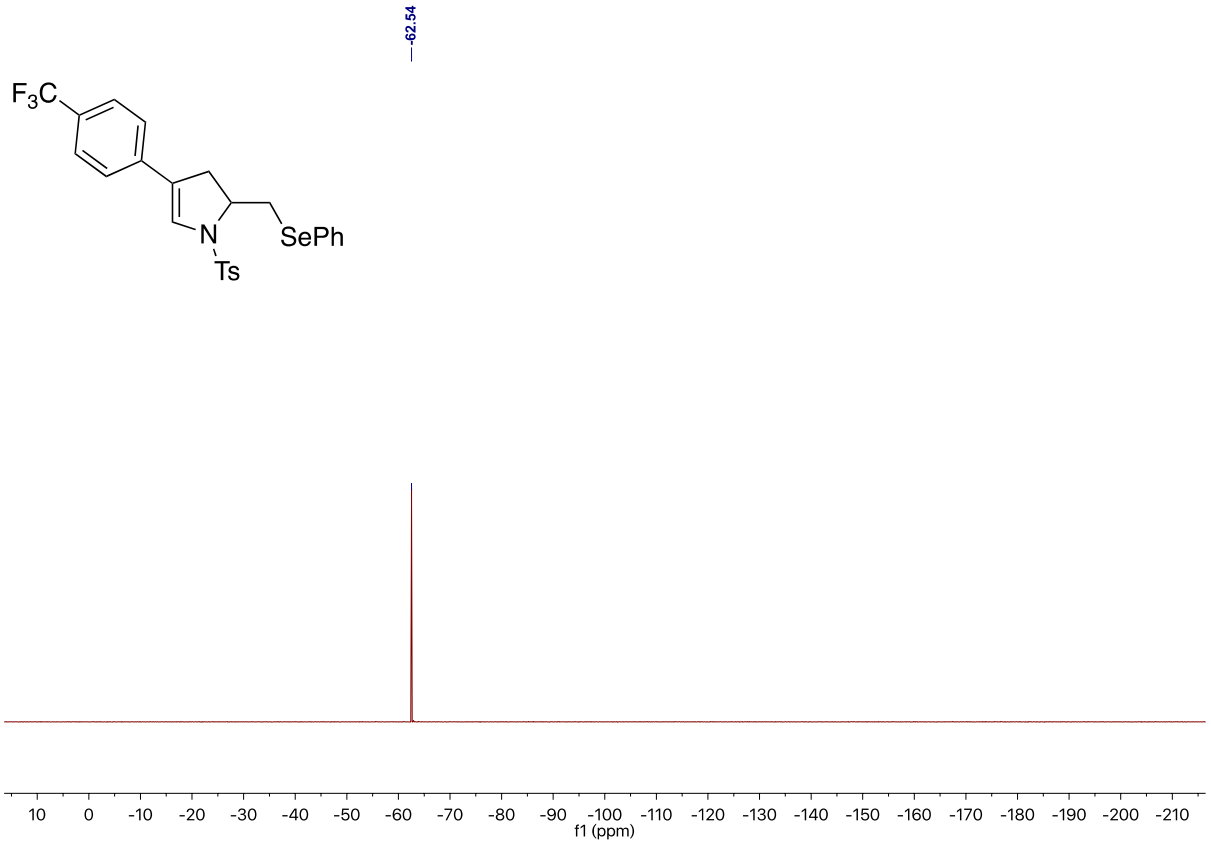
^{1}H NMR (600 MHz, Chloroform-*d*)



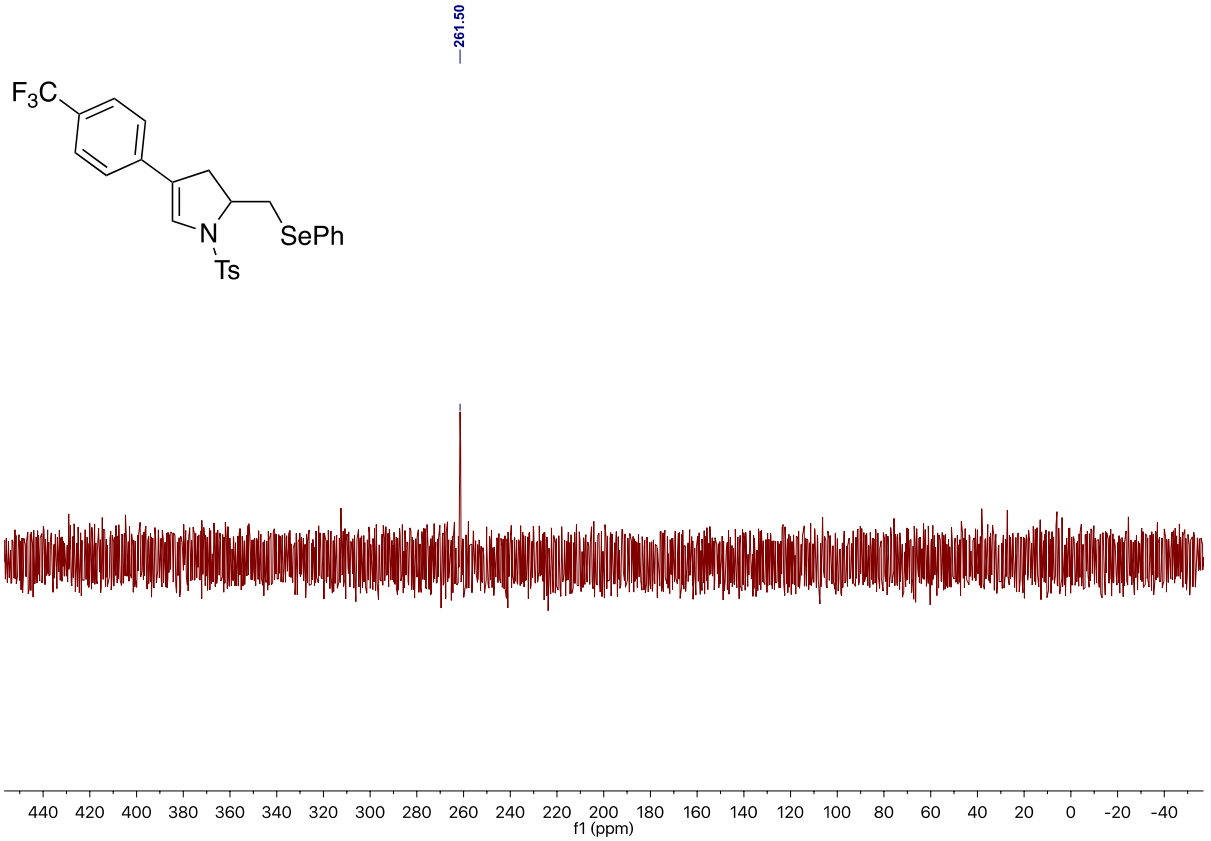
^{13}C NMR (151 MHz, Chloroform-*d*)



^{19}F NMR (565 MHz, Chloroform-*d*)

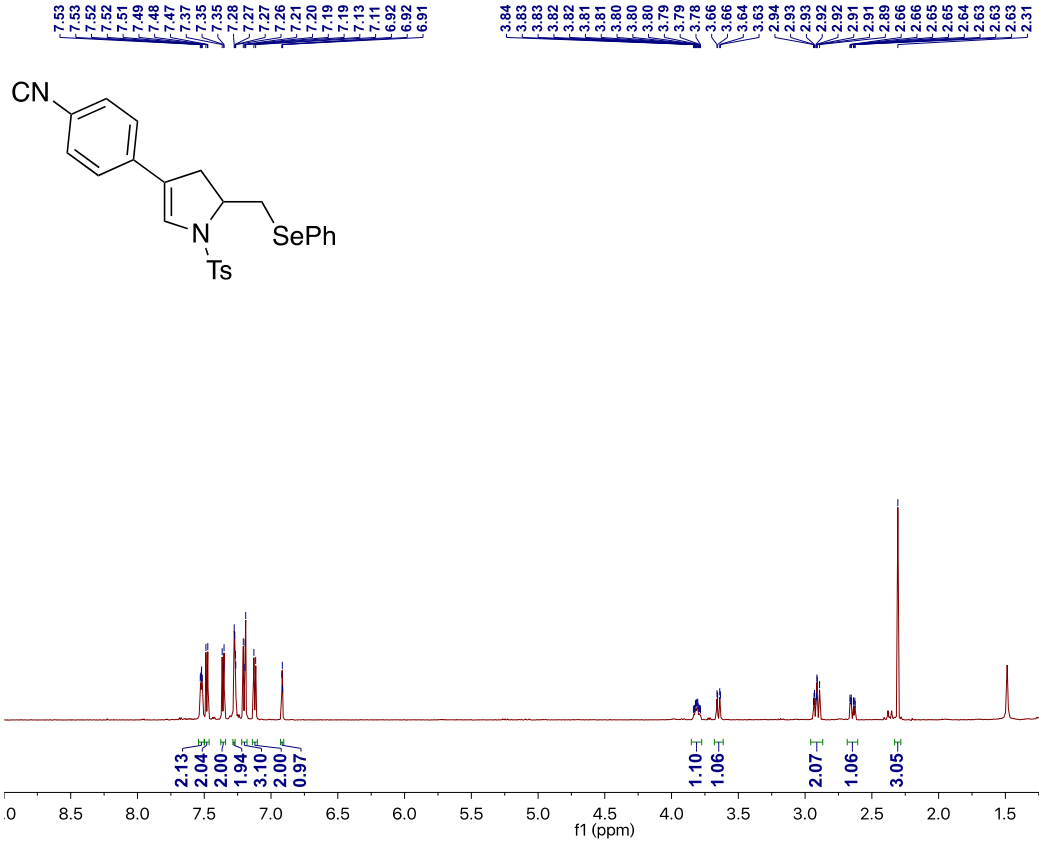


^{77}Se NMR (115 MHz, Chloroform-*d*)

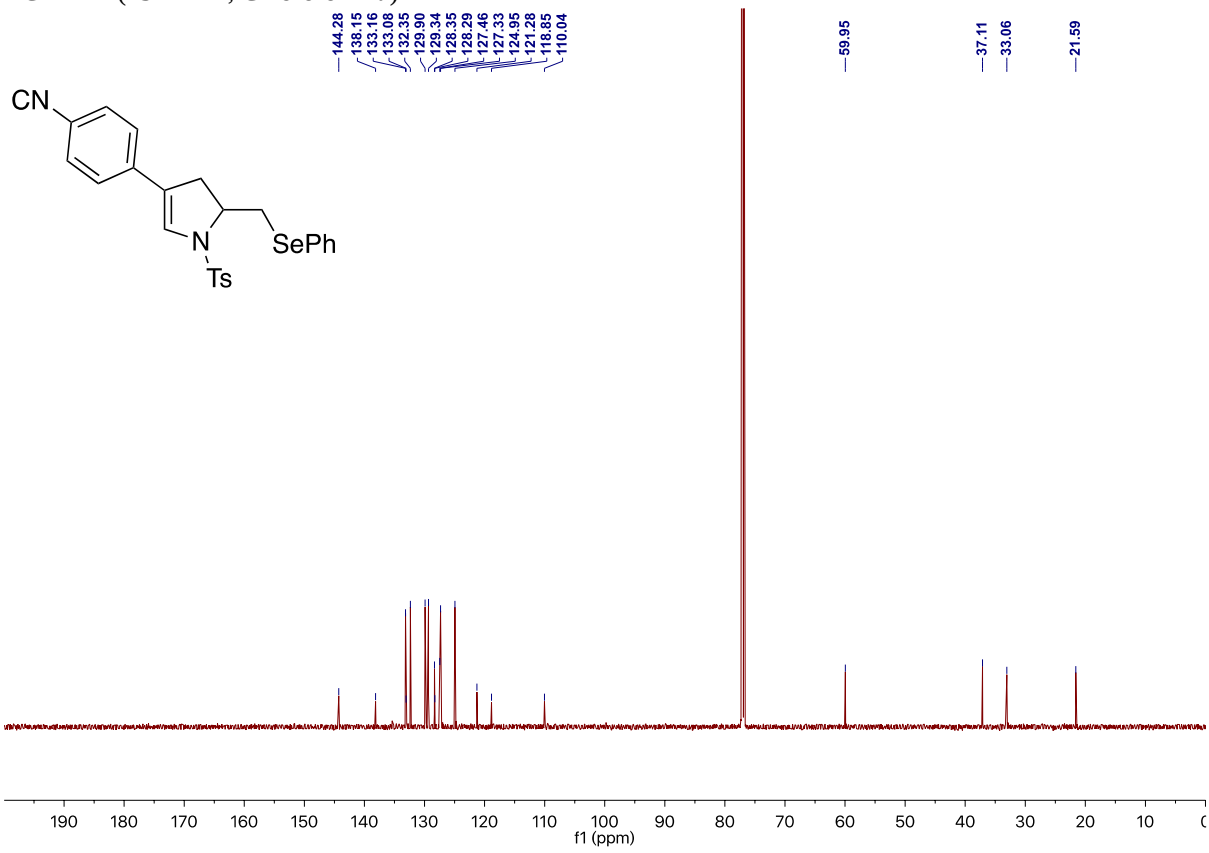


4-(4-isocyanophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9n)

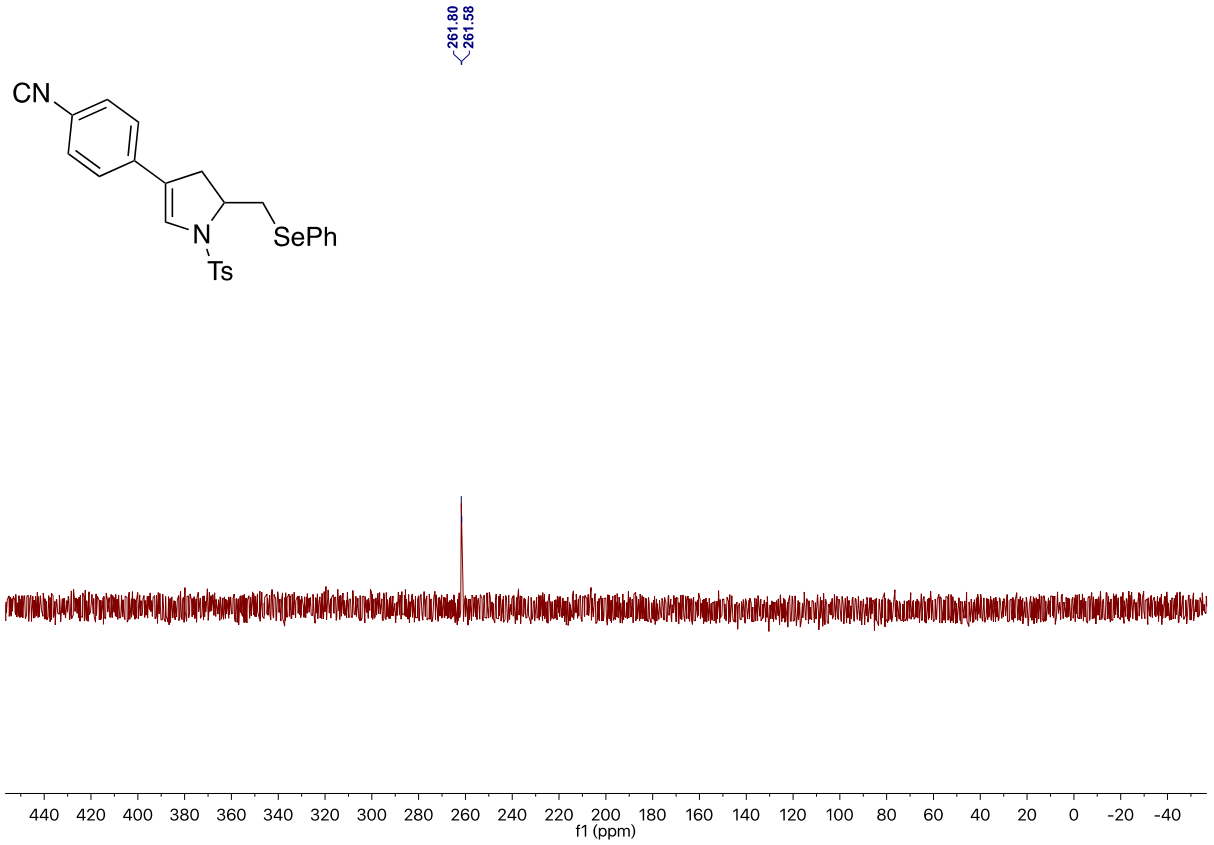
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

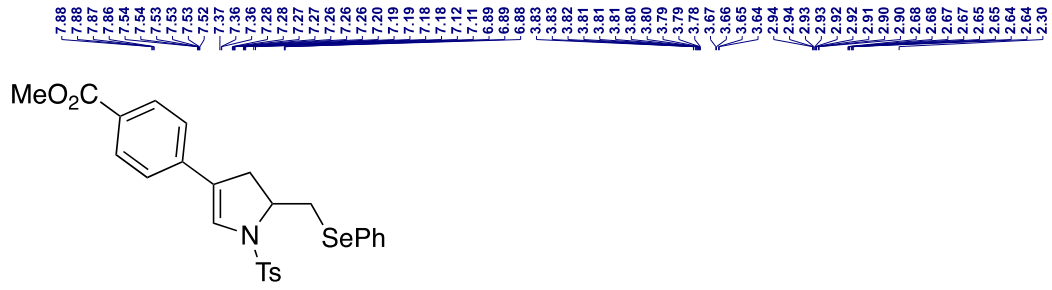


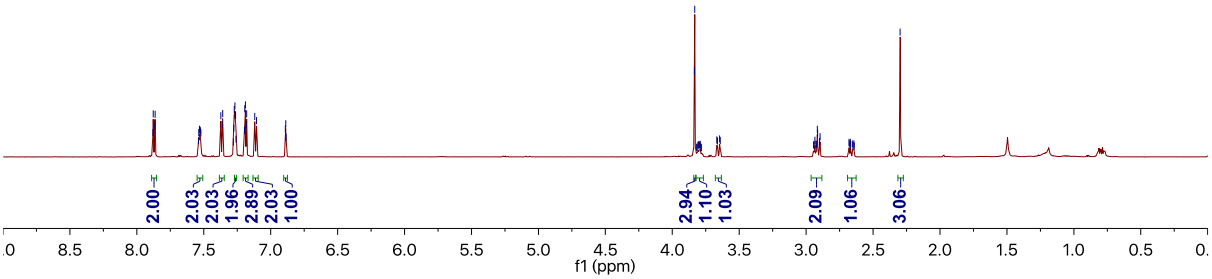
^{77}Se NMR (115 MHz, Chloroform-*d*)



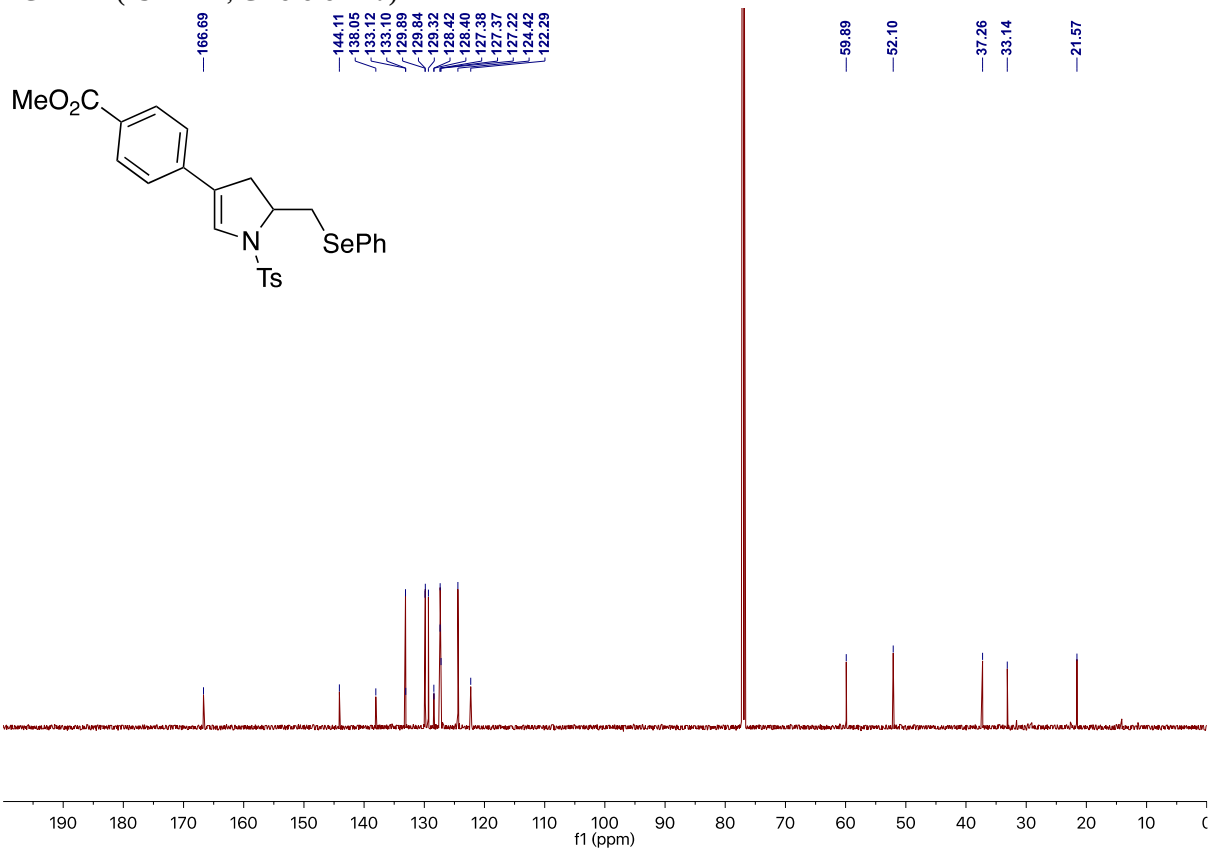
methyl 4-(5-((phenylselanyl)methyl)-1-tosyl-4,5-dihydro-1*H*-pyrrol-3-yl)benzoate (9o)

^{1}H NMR (600 MHz, Chloroform-*d*)

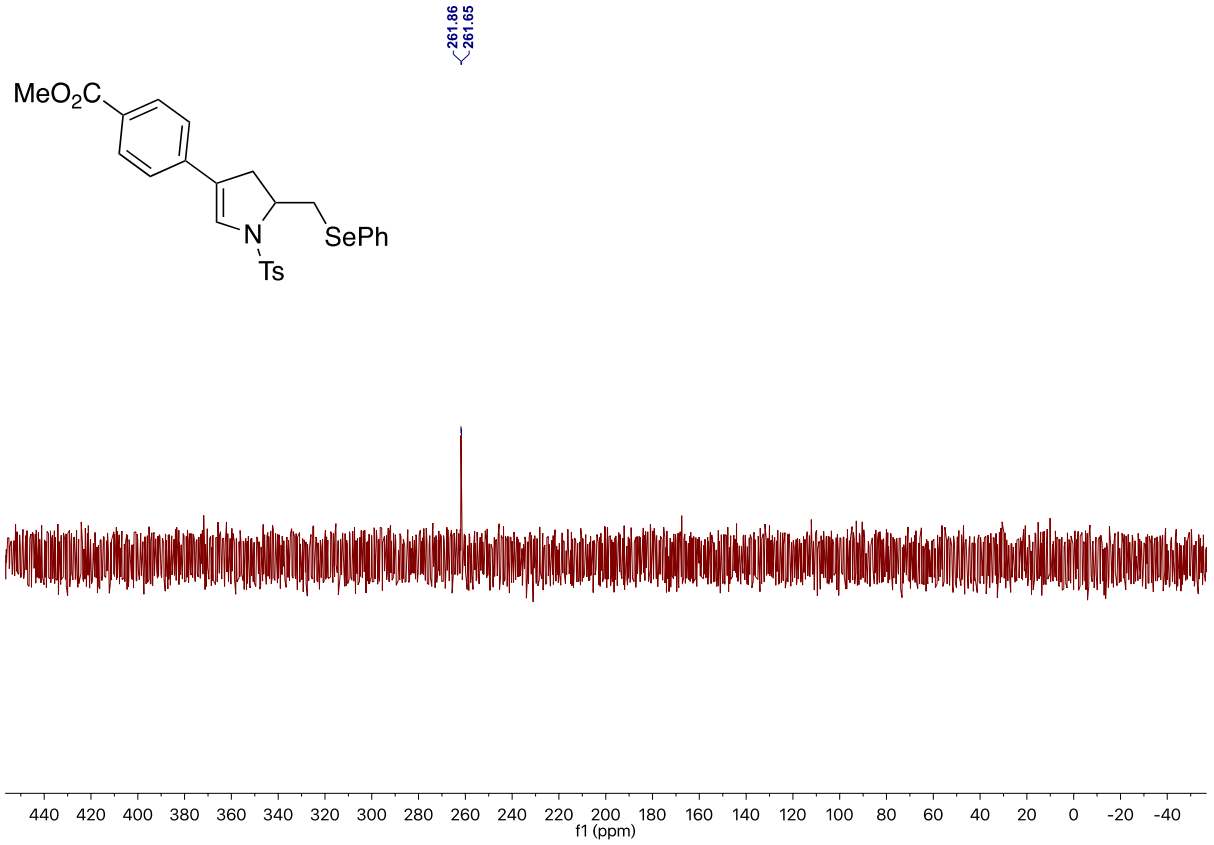




^{13}C NMR (151 MHz, Chloroform-*d*)

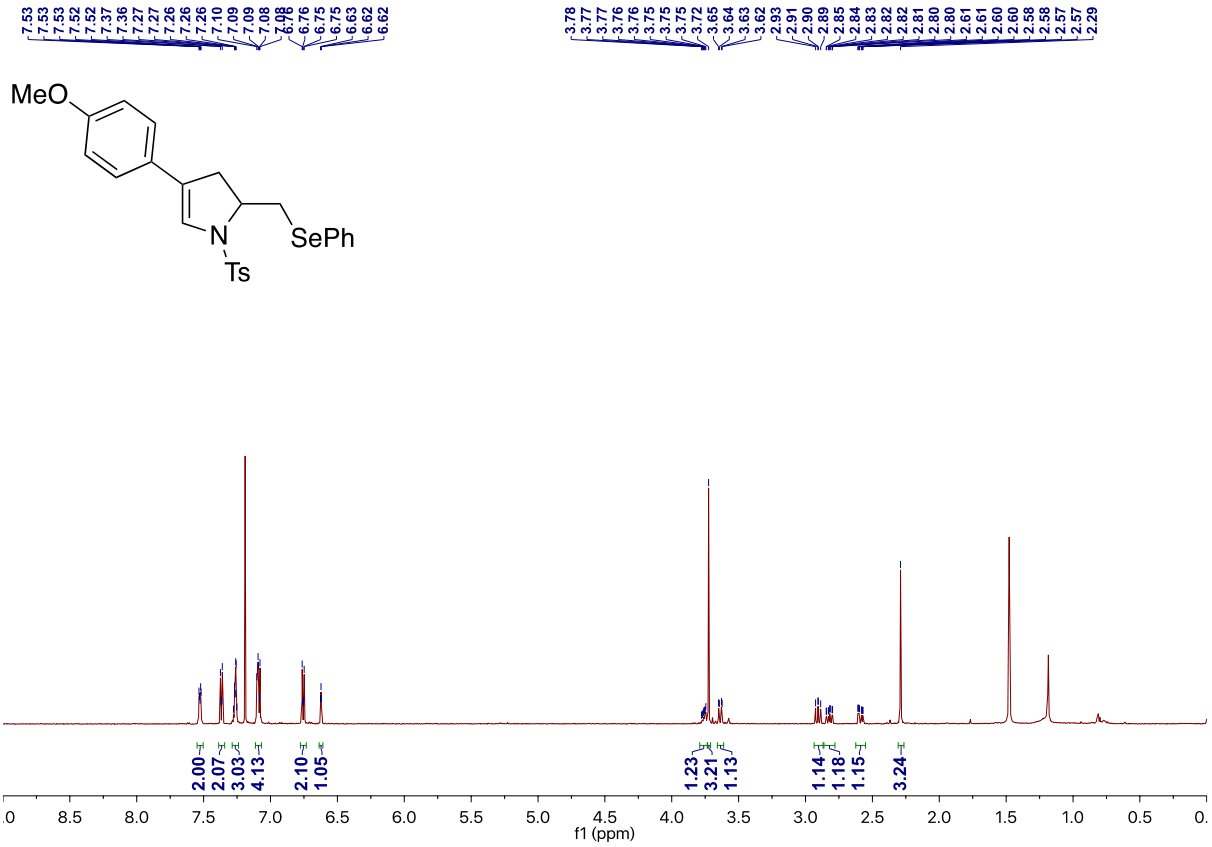


^{77}Se NMR (115 MHz, Chloroform-*d*)

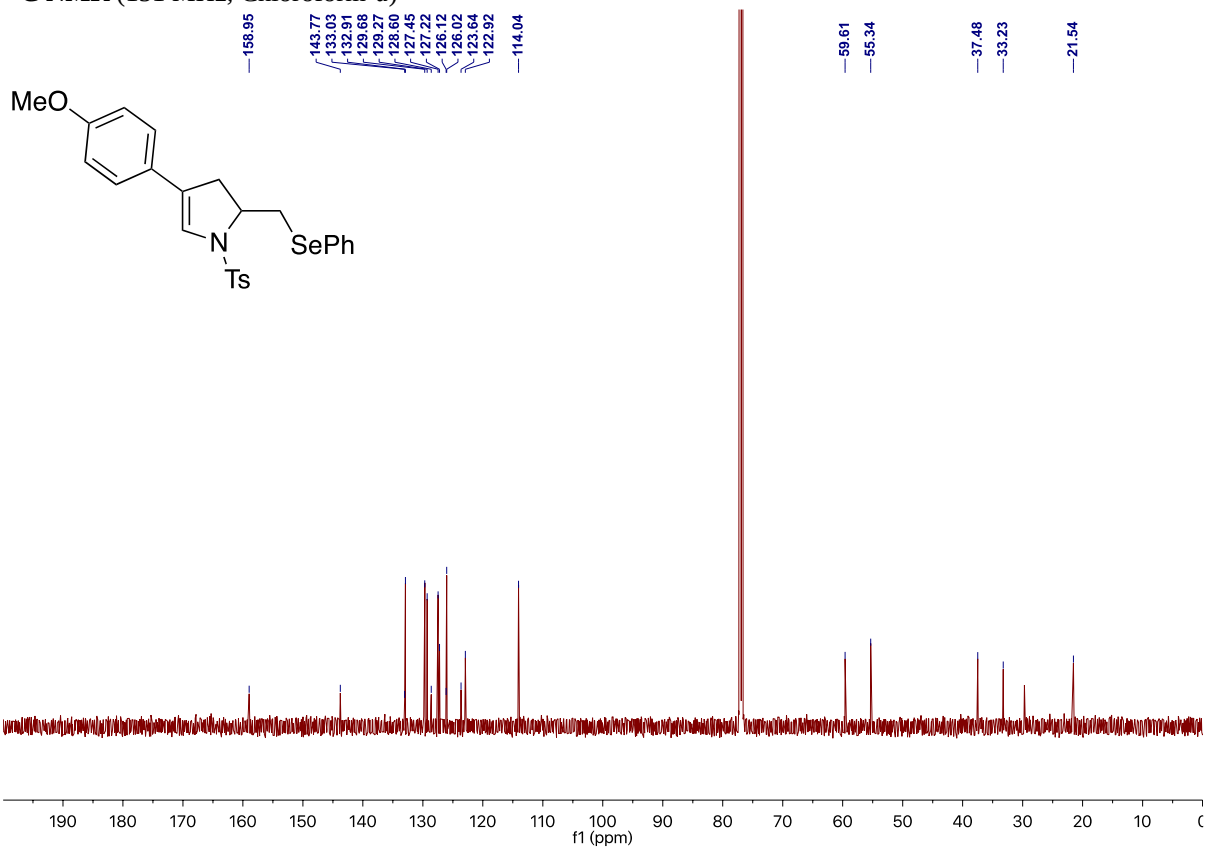


4-(4-methoxyphenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9p)

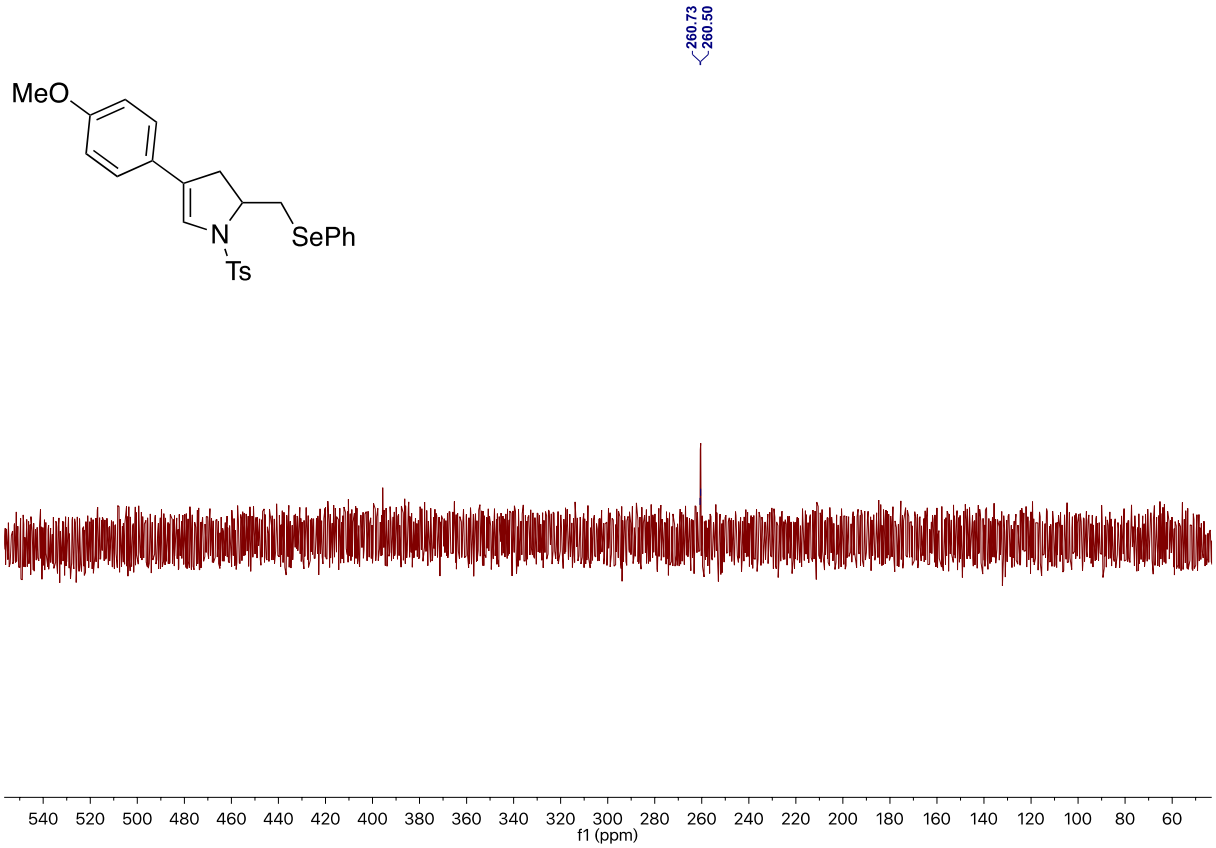
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

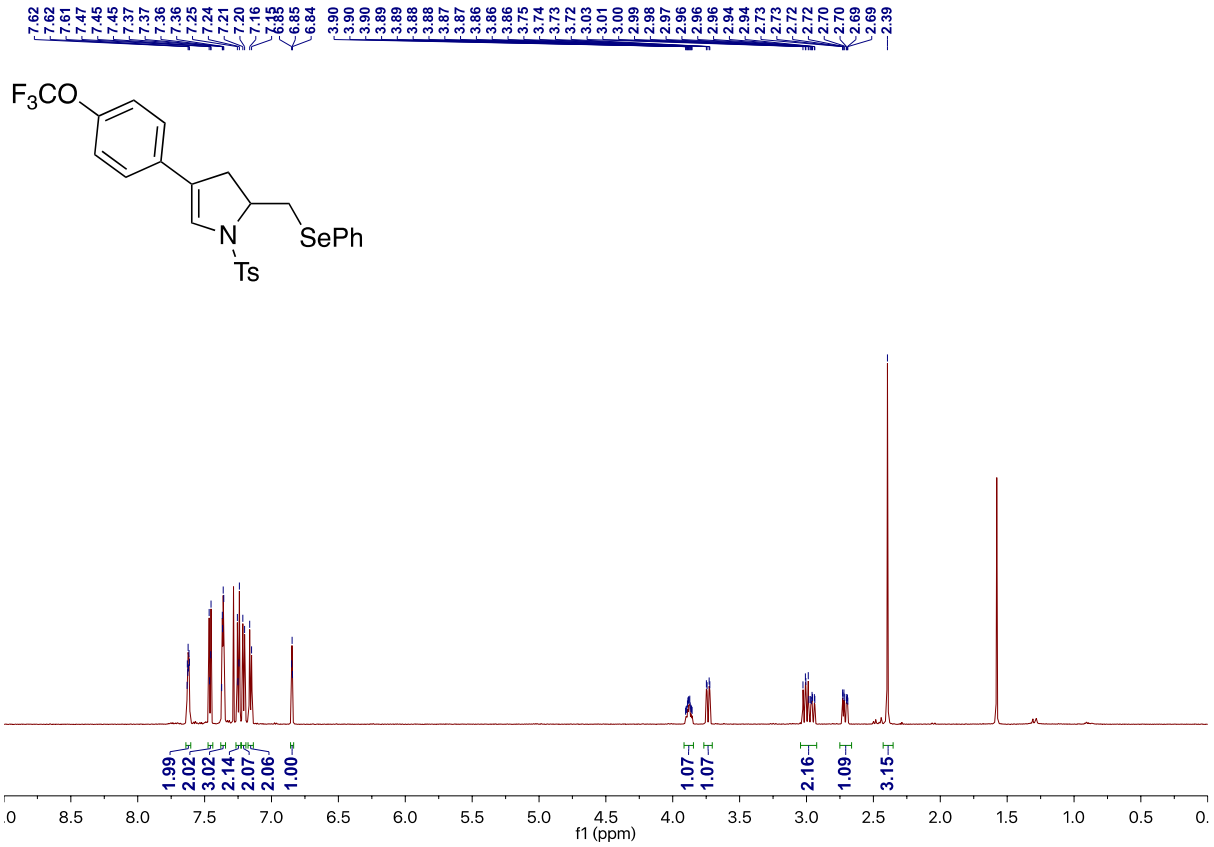


^{77}Se NMR (115 MHz, Chloroform-*d*)

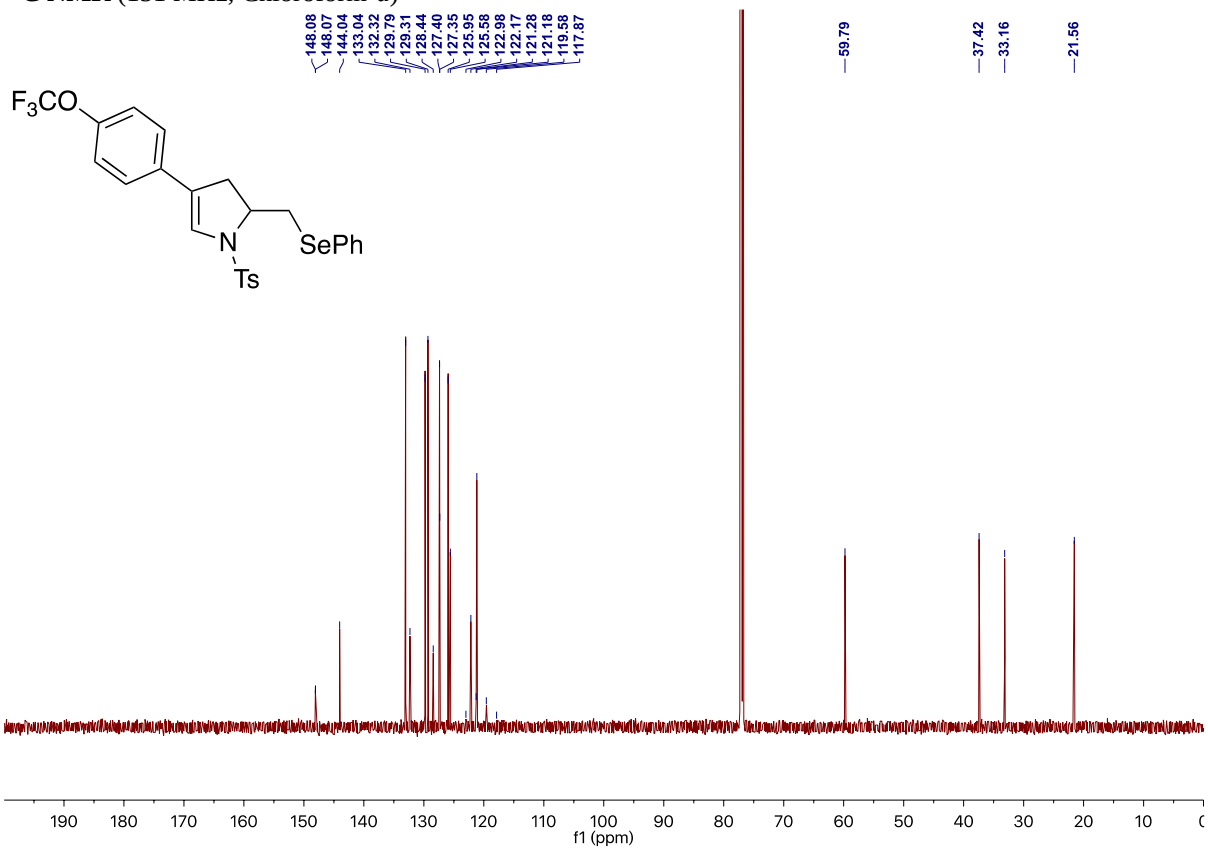


2-((phenylselanyl)methyl)-1-tosyl-4-(4-(trifluoromethoxy)phenyl)-2,3-dihydro-1*H*-pyrrole (9q)

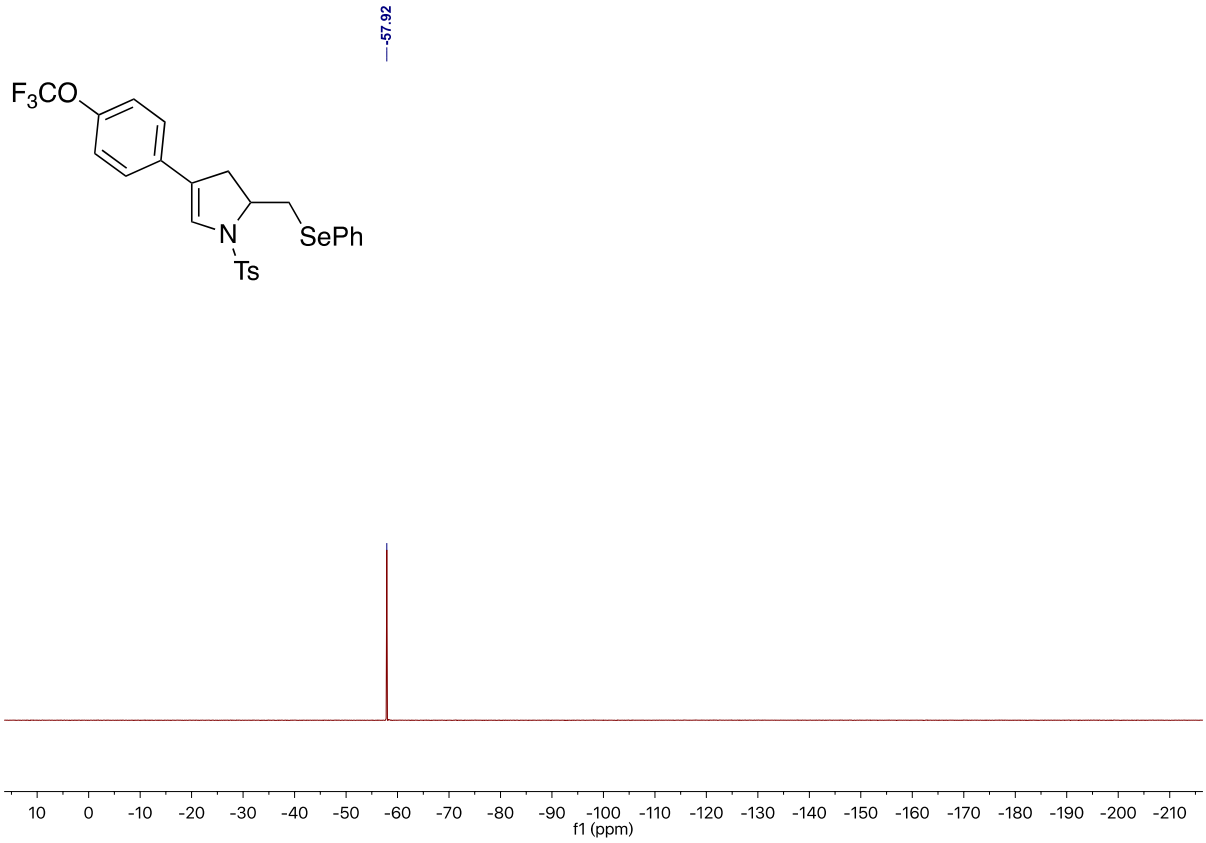
^{1}H NMR (600 MHz, Chloroform-*d*)



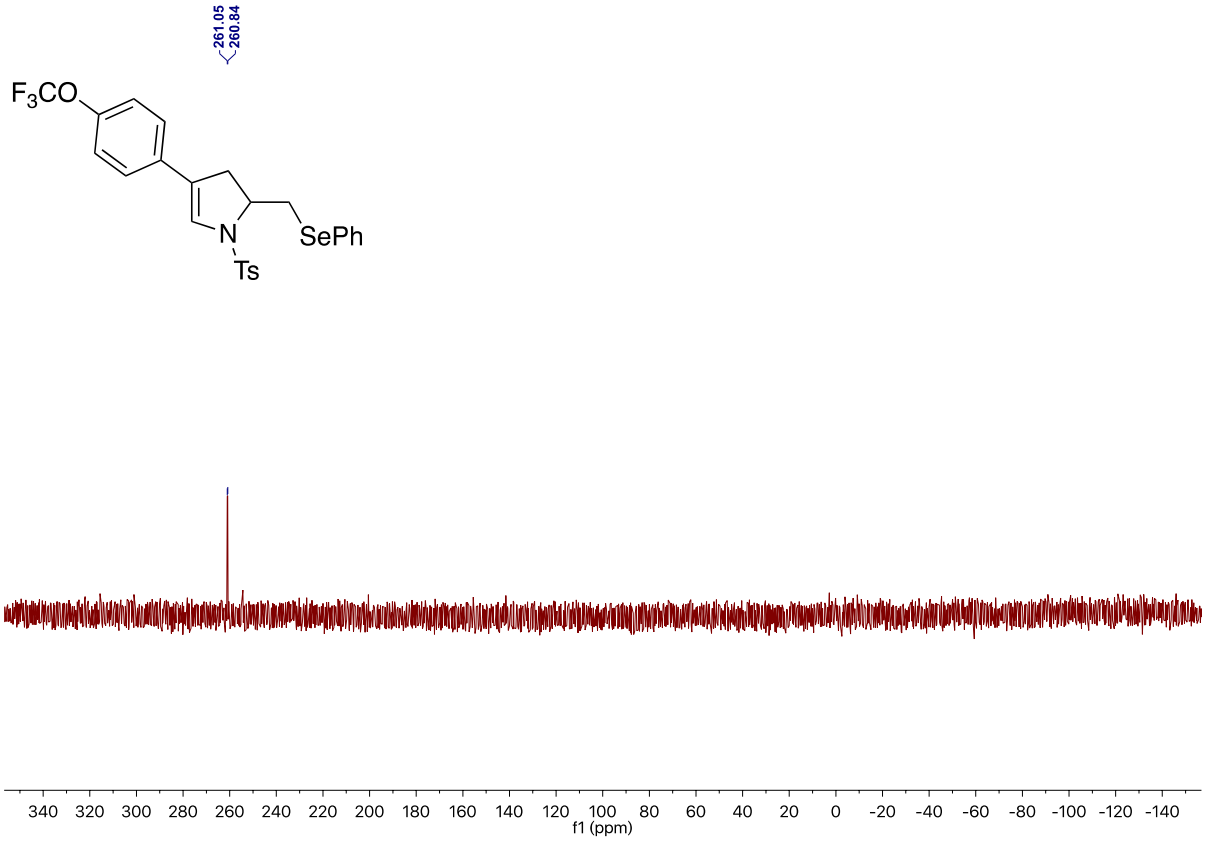
^{13}C NMR (151 MHz, Chloroform-*d*)



^{19}F NMR (565 MHz, Chloroform-*d*)

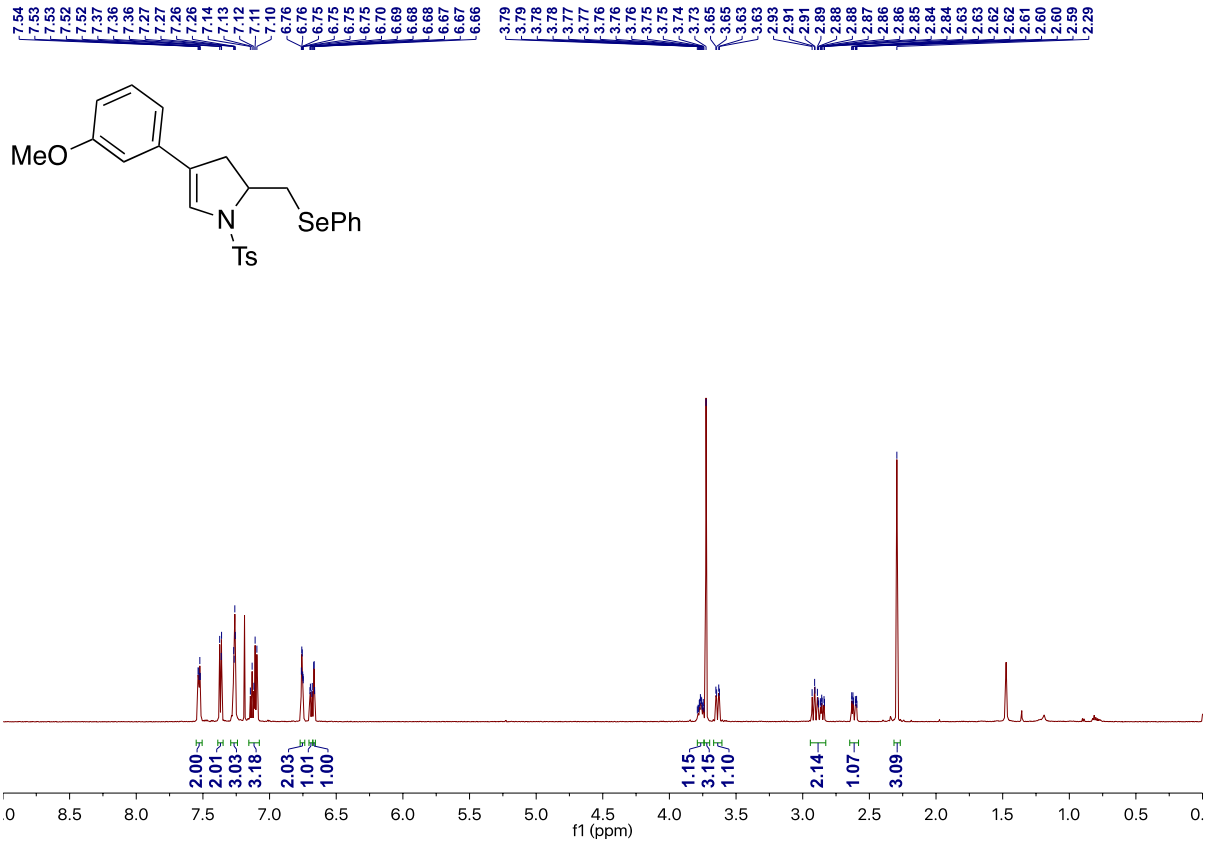


^{77}Se NMR (115 MHz, Chloroform-*d*)

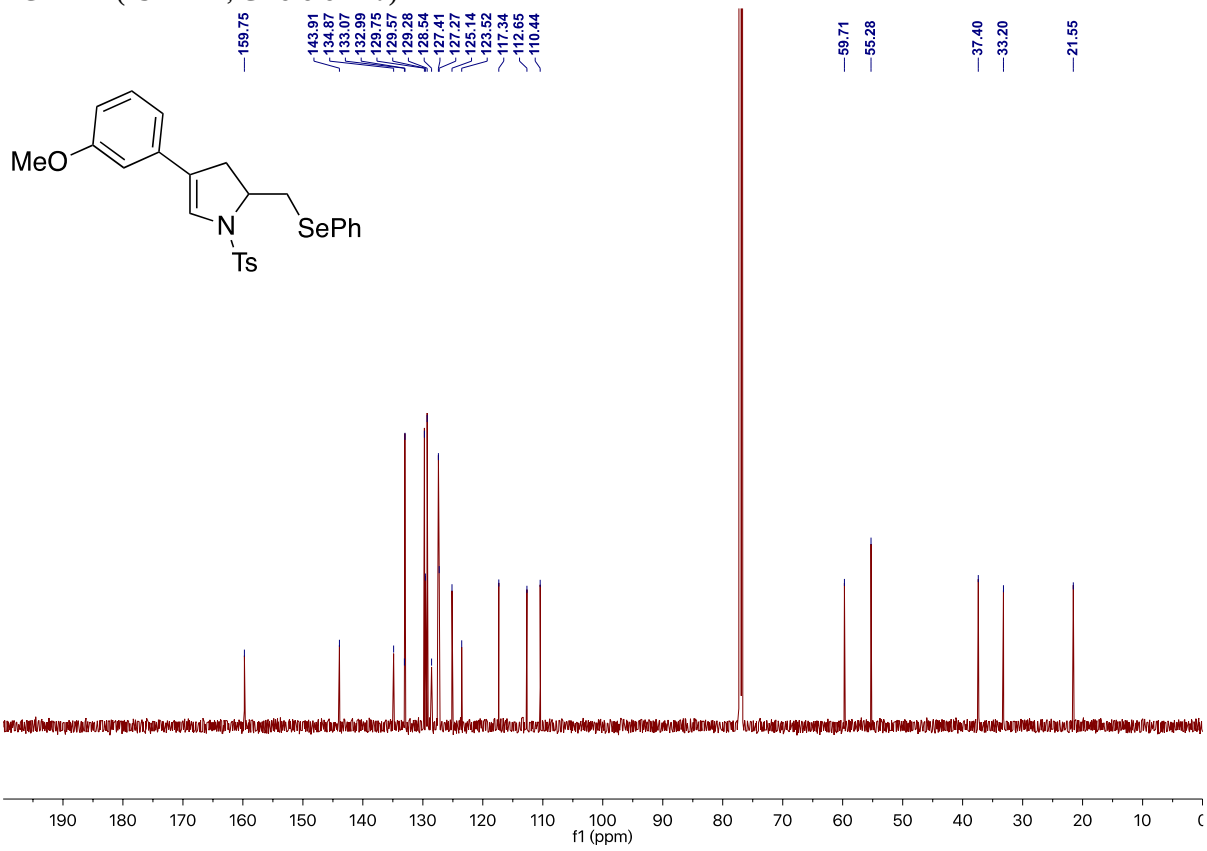


4-(3-methoxyphenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9r)

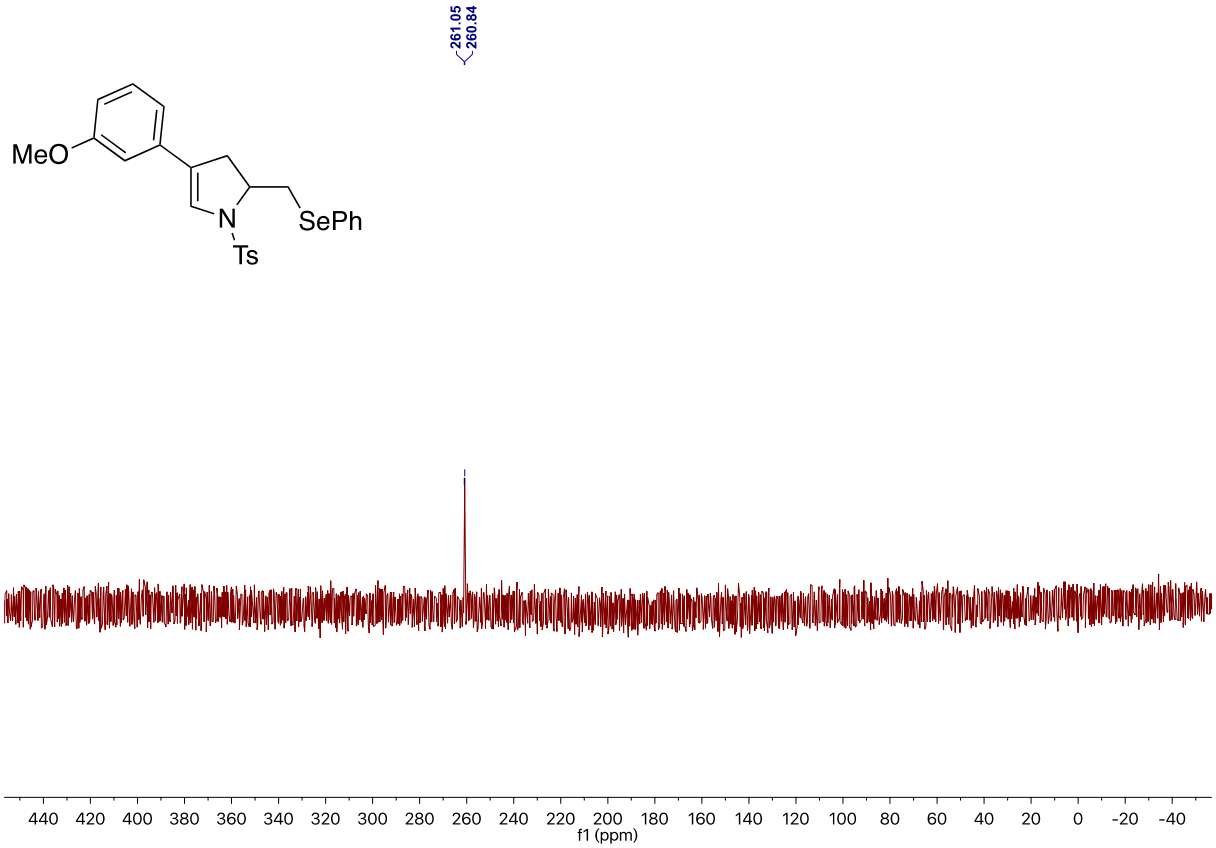
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

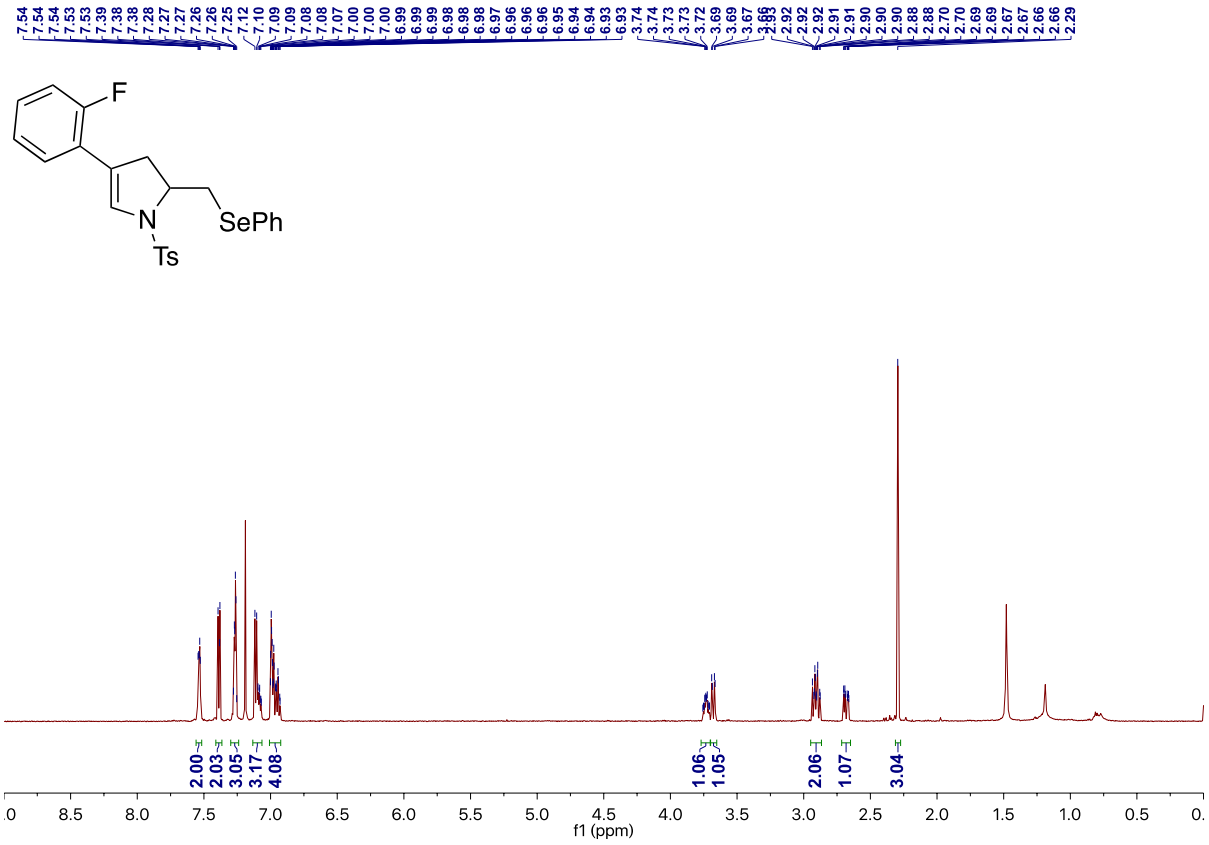


^{77}Se NMR (115 MHz, Chloroform-*d*)

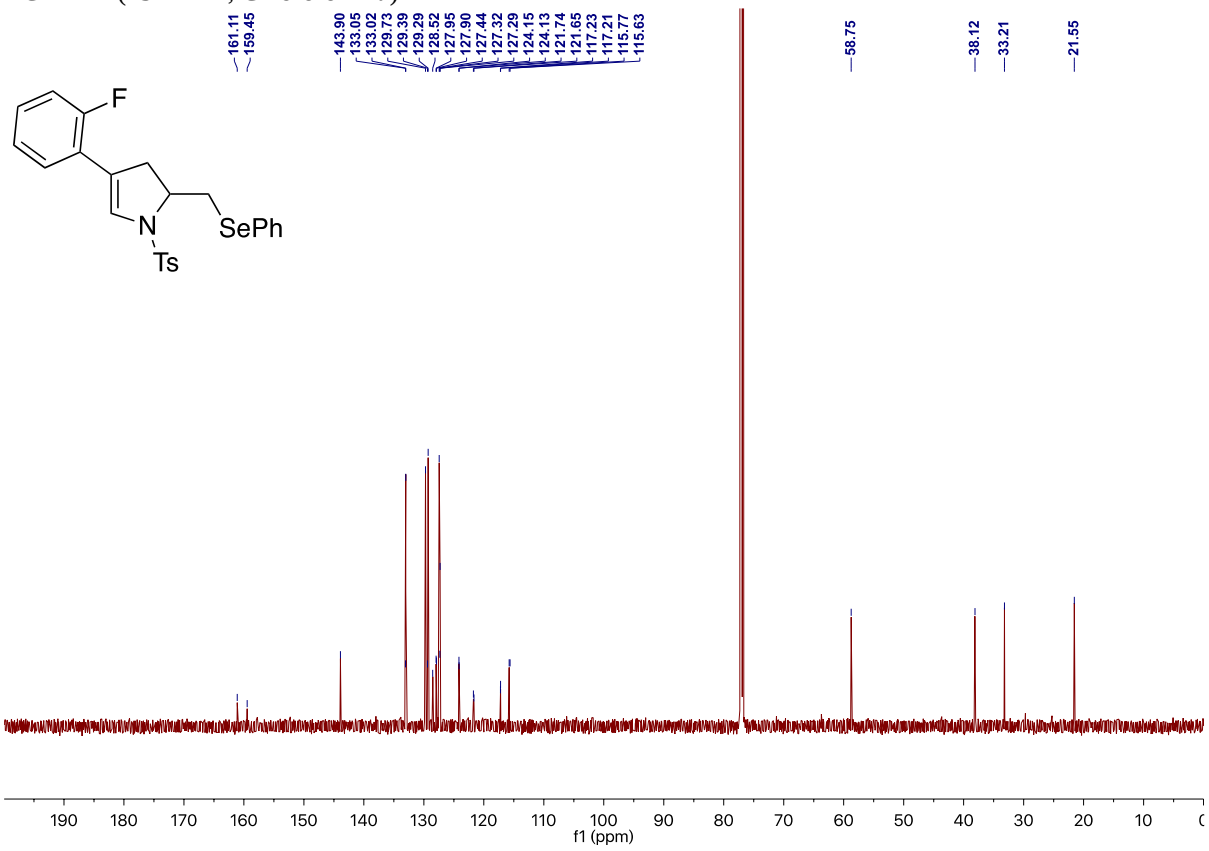


4-(2-fluorophenyl)-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9s)

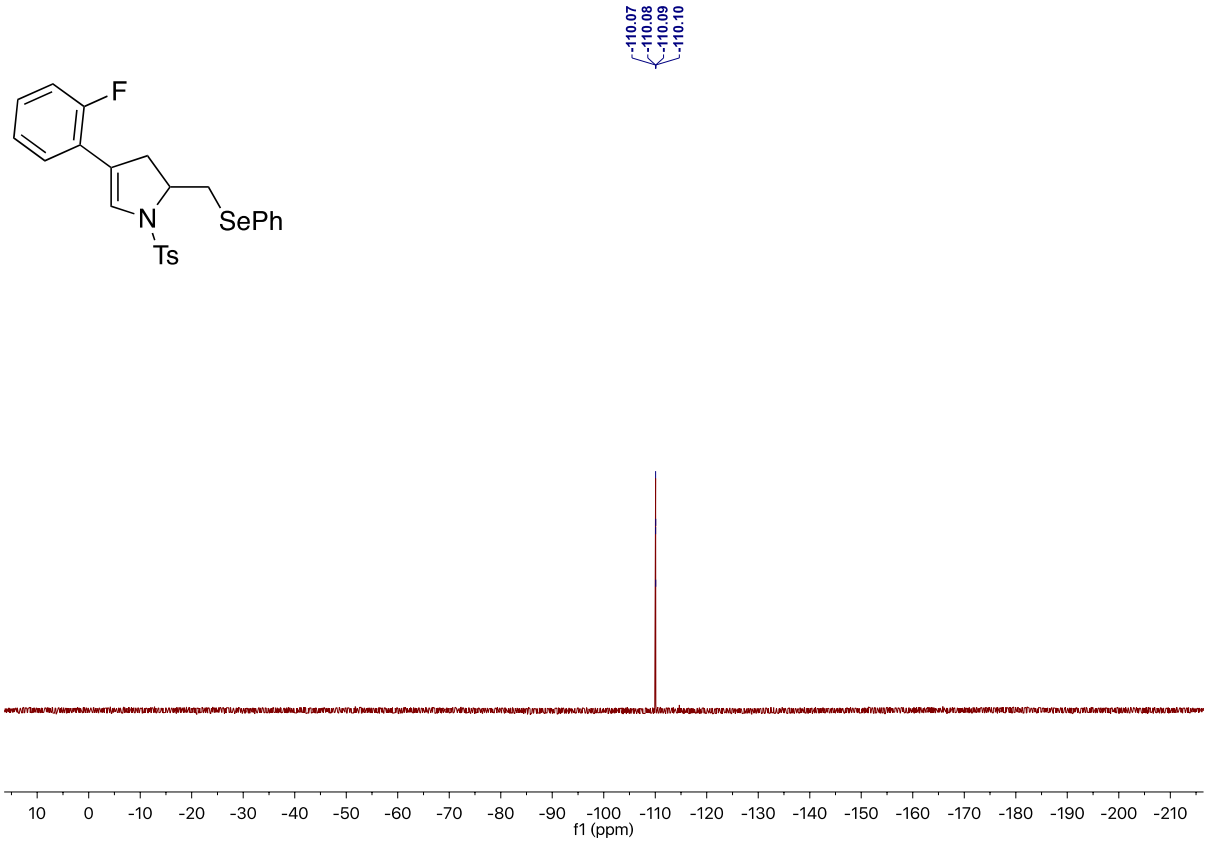
^{1}H NMR (600 MHz, Chloroform-*d*)



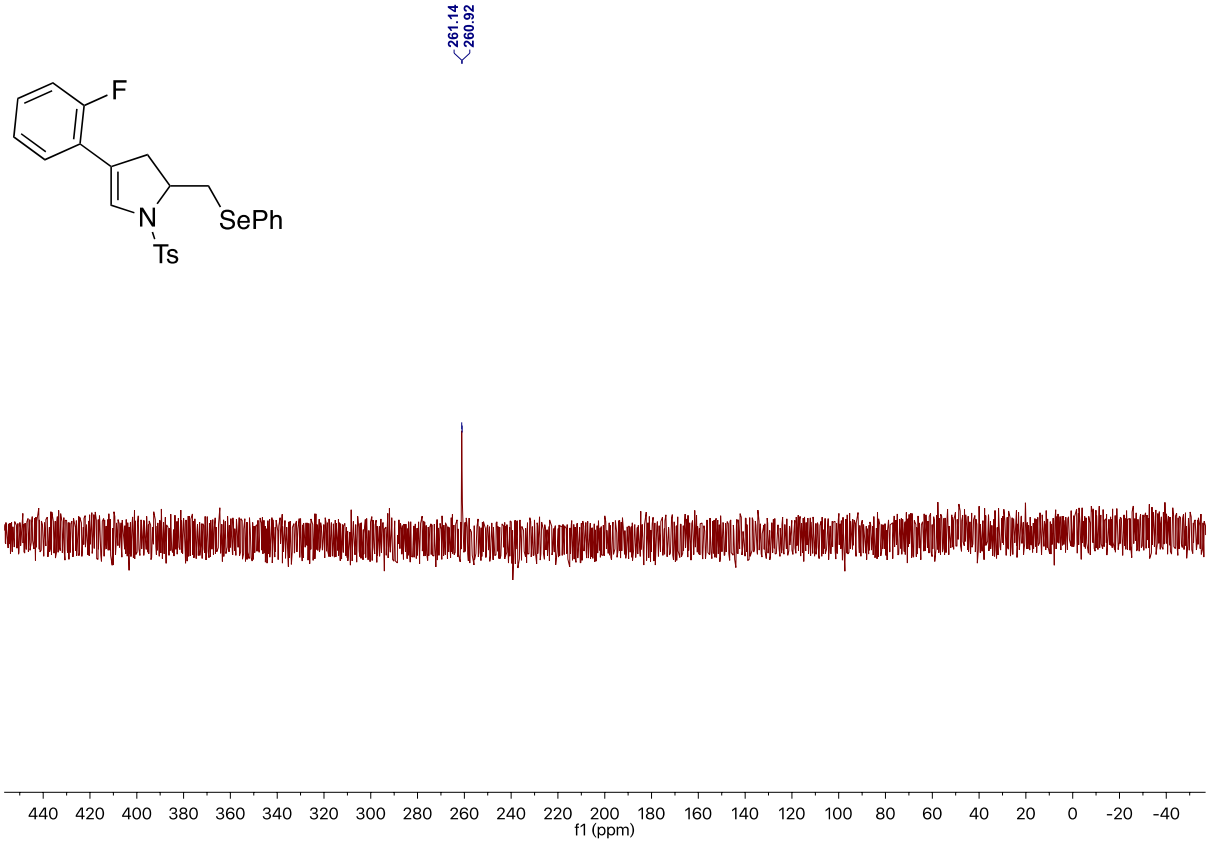
^{13}C NMR (151 MHz, Chloroform-*d*)



^{19}F NMR (565 MHz, Chloroform-*d*)

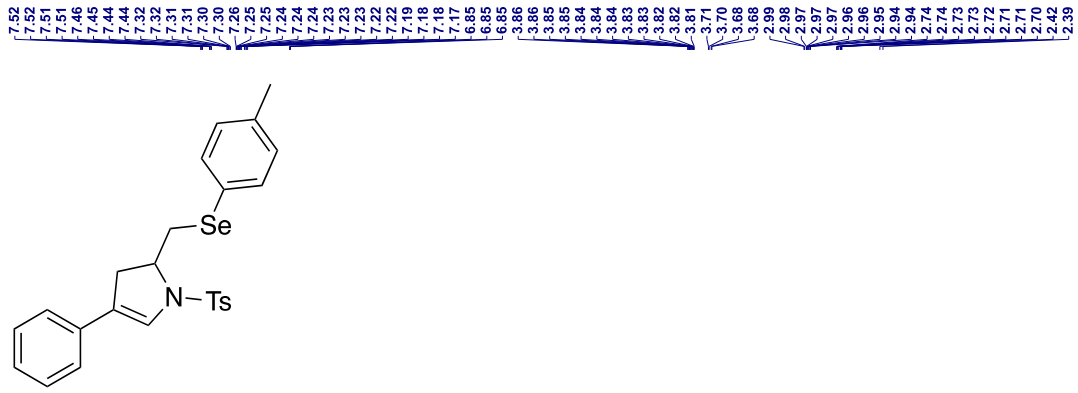


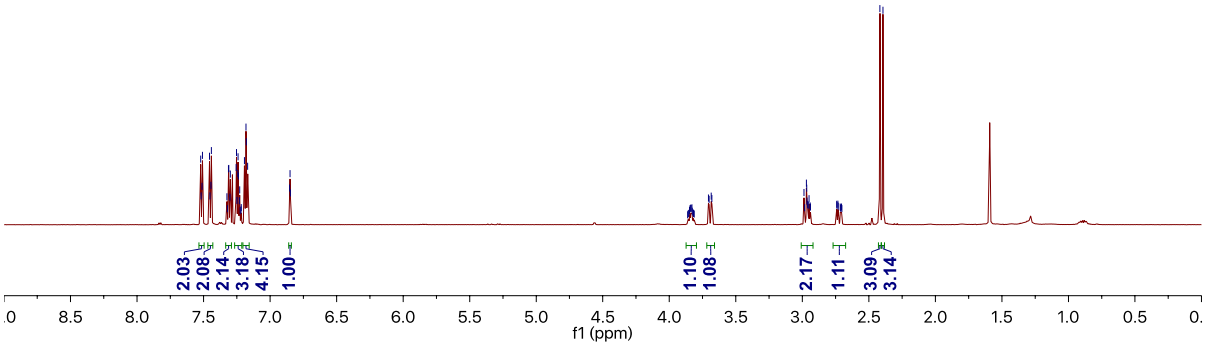
^{77}Se NMR (115 MHz, Chloroform-*d*)



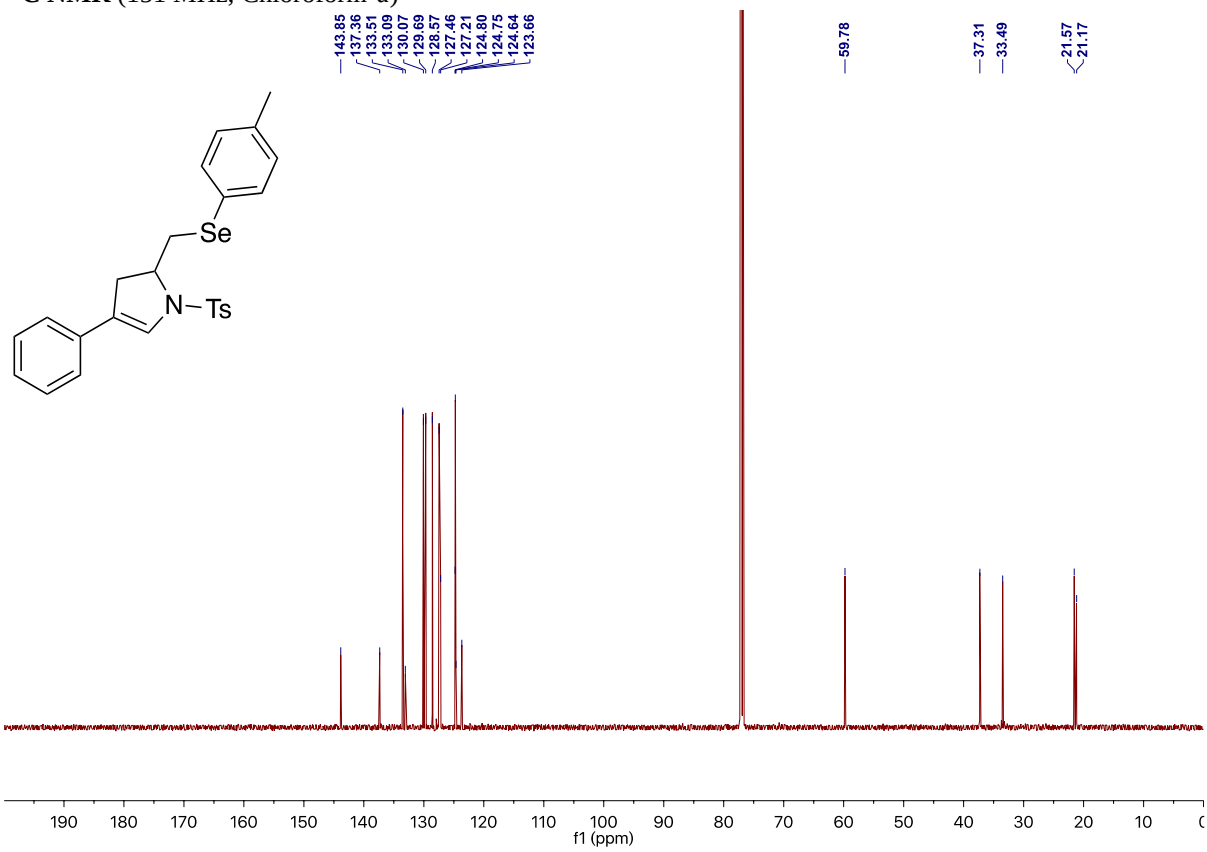
4-phenyl-2-((*p*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9t)

^{1}H NMR (600 MHz, Chloroform-*d*)

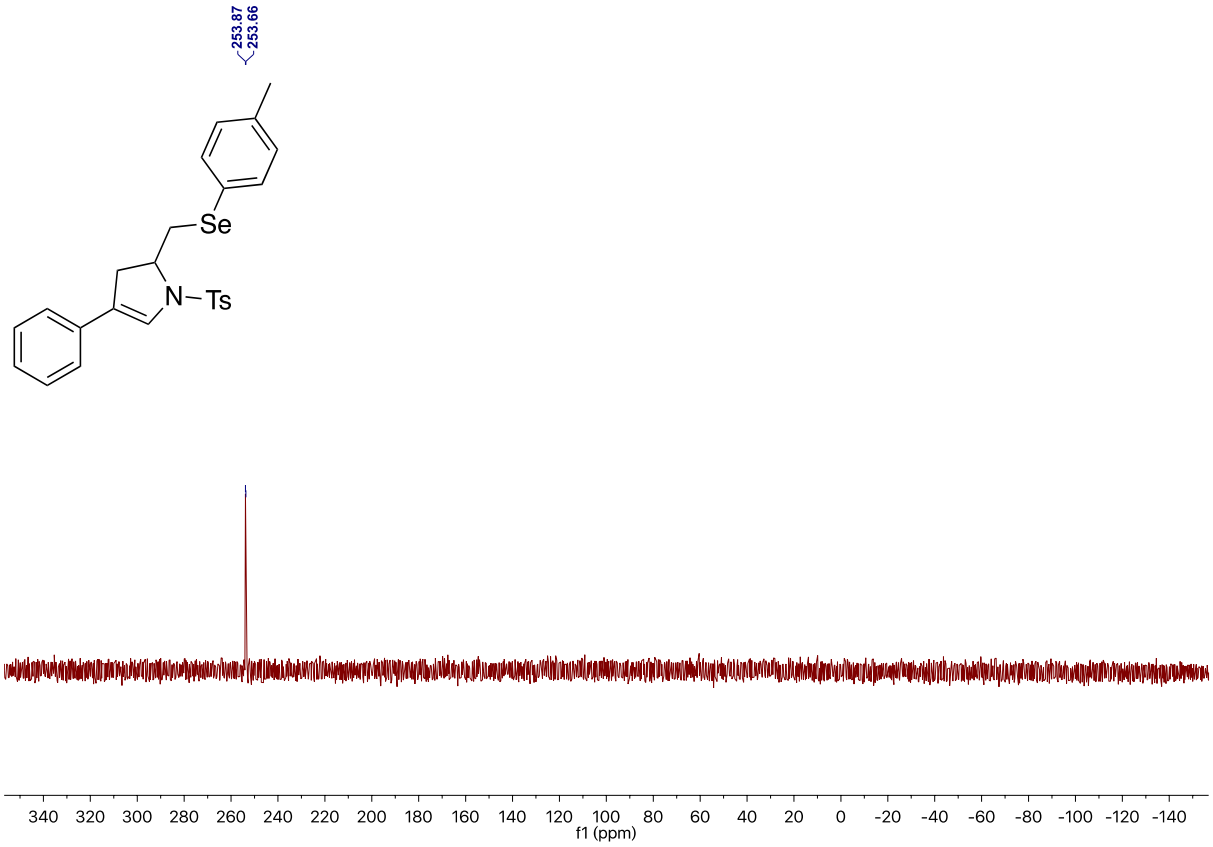




^{13}C NMR (151 MHz, Chloroform-*d*)

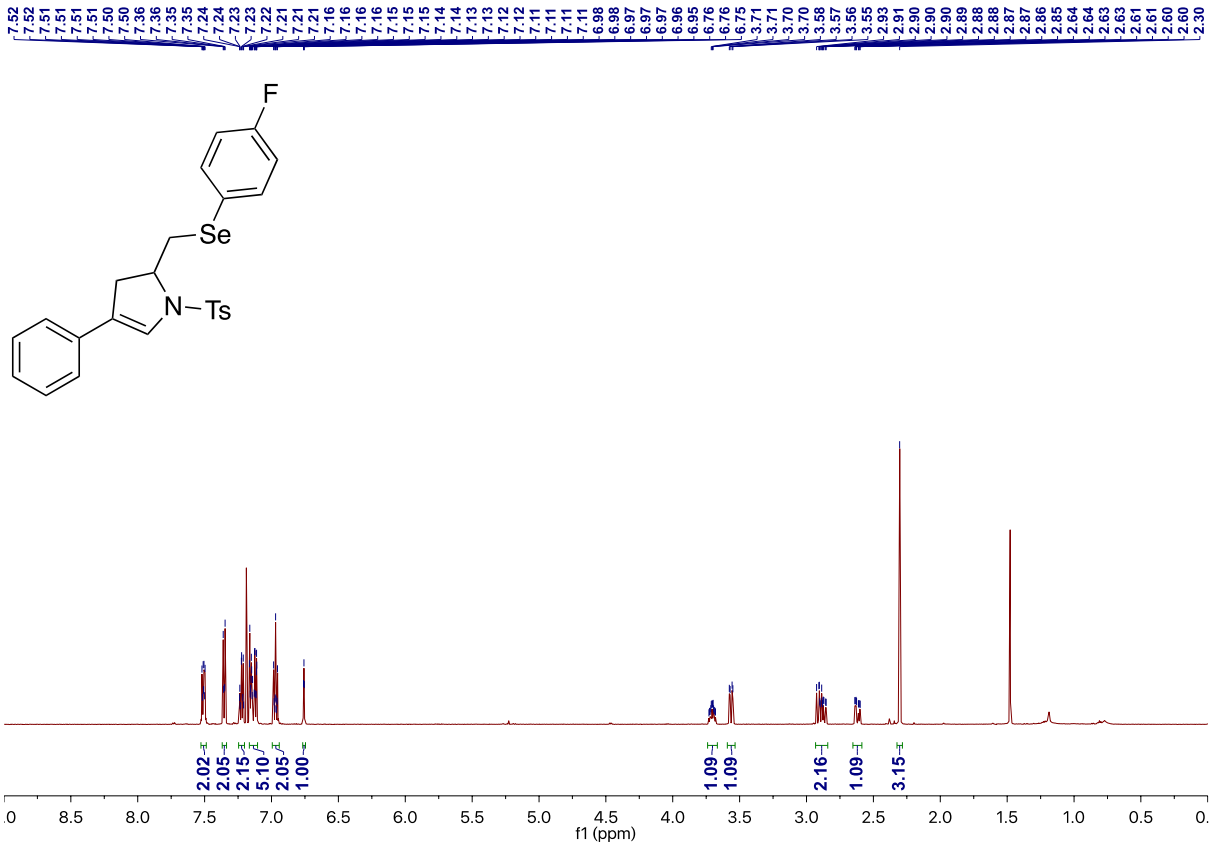


^{77}Se NMR (115 MHz, Chloroform-*d*)

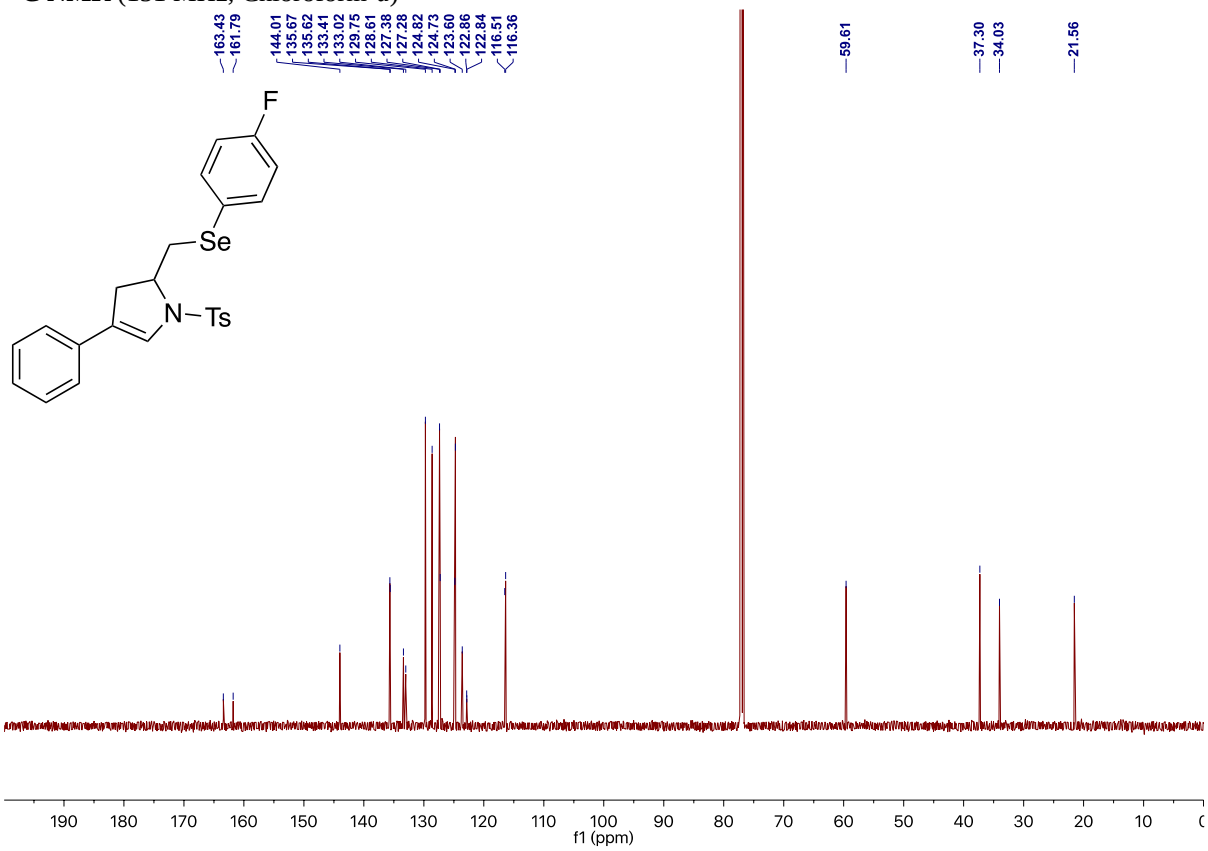


2-(((4-fluorophenyl)selanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (9u)

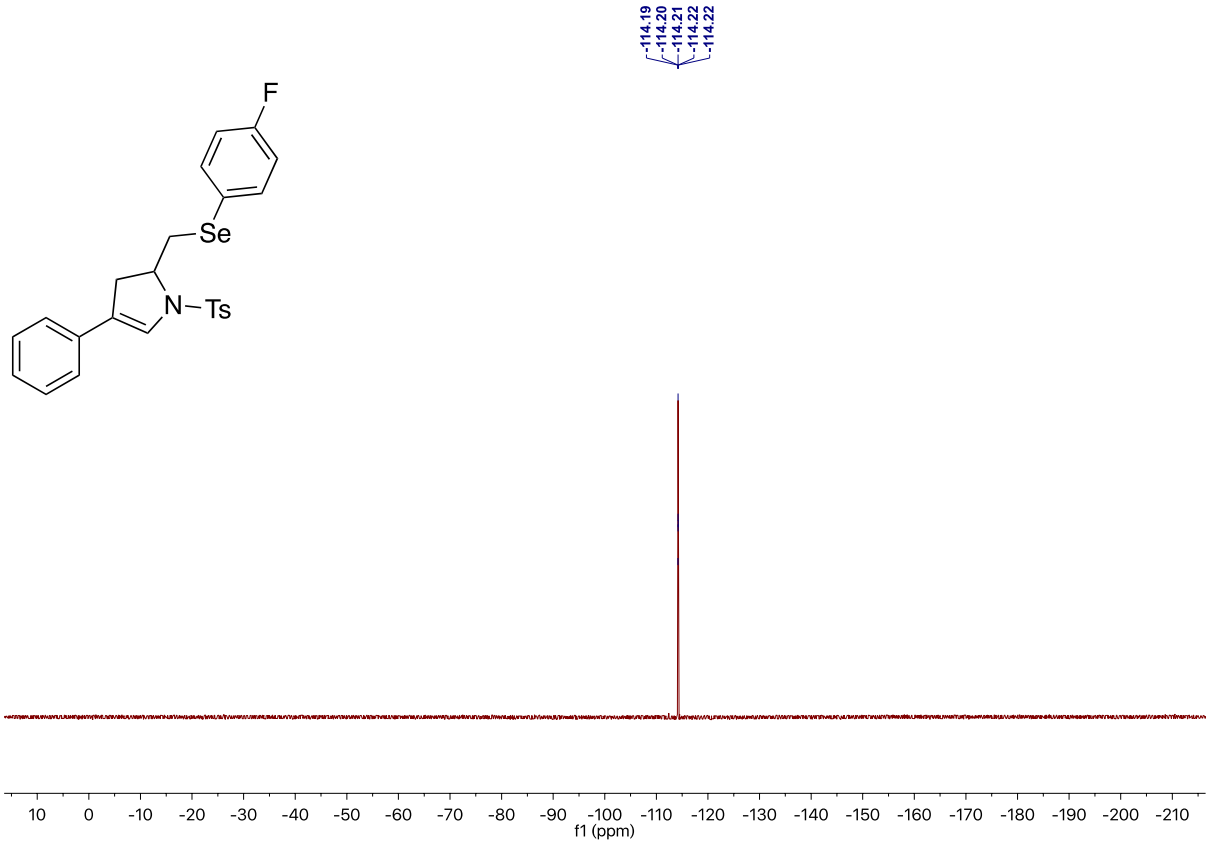
^{1}H NMR (600 MHz, Chloroform-*d*)



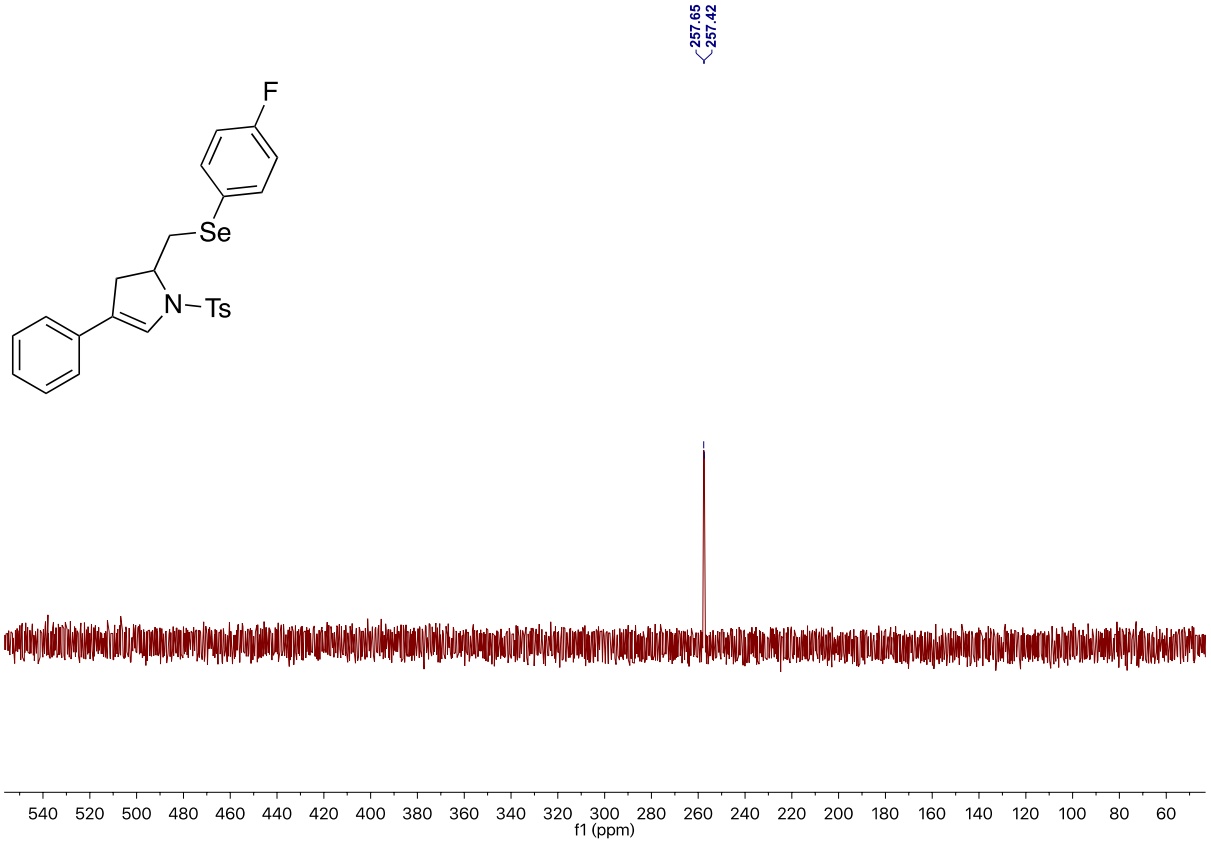
^{13}C NMR (151 MHz, Chloroform-*d*)



^{19}F NMR (565 MHz, Chloroform-*d*)

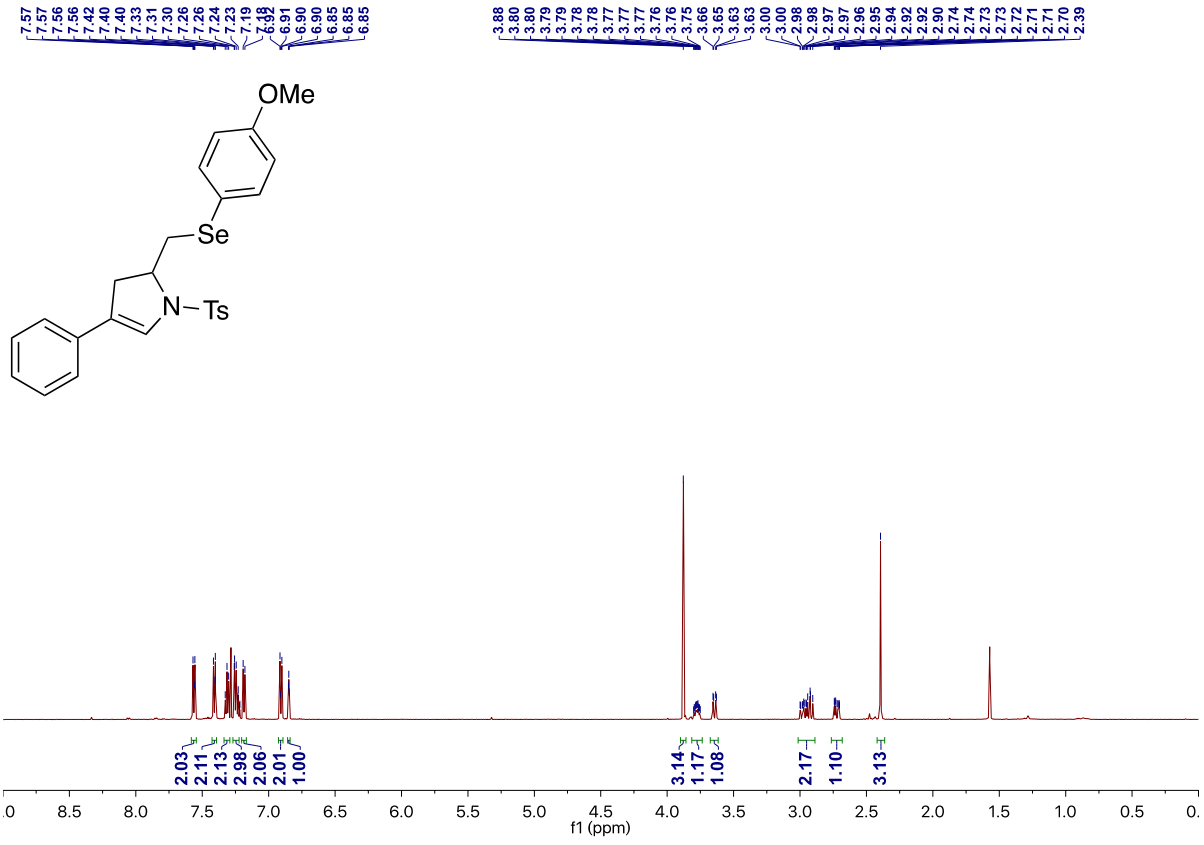


^{77}Se NMR (115 MHz, Chloroform-*d*)

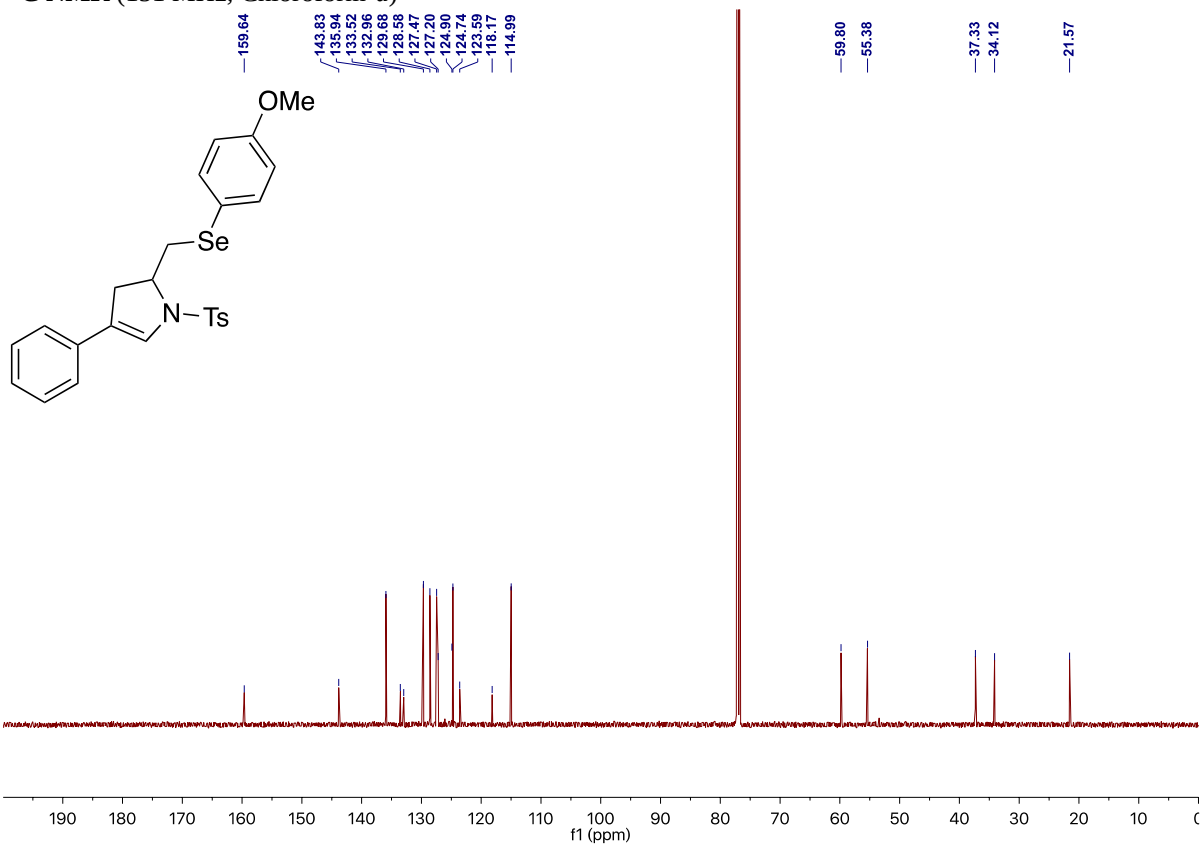


2-(((4-methoxyphenyl)selanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (9v)

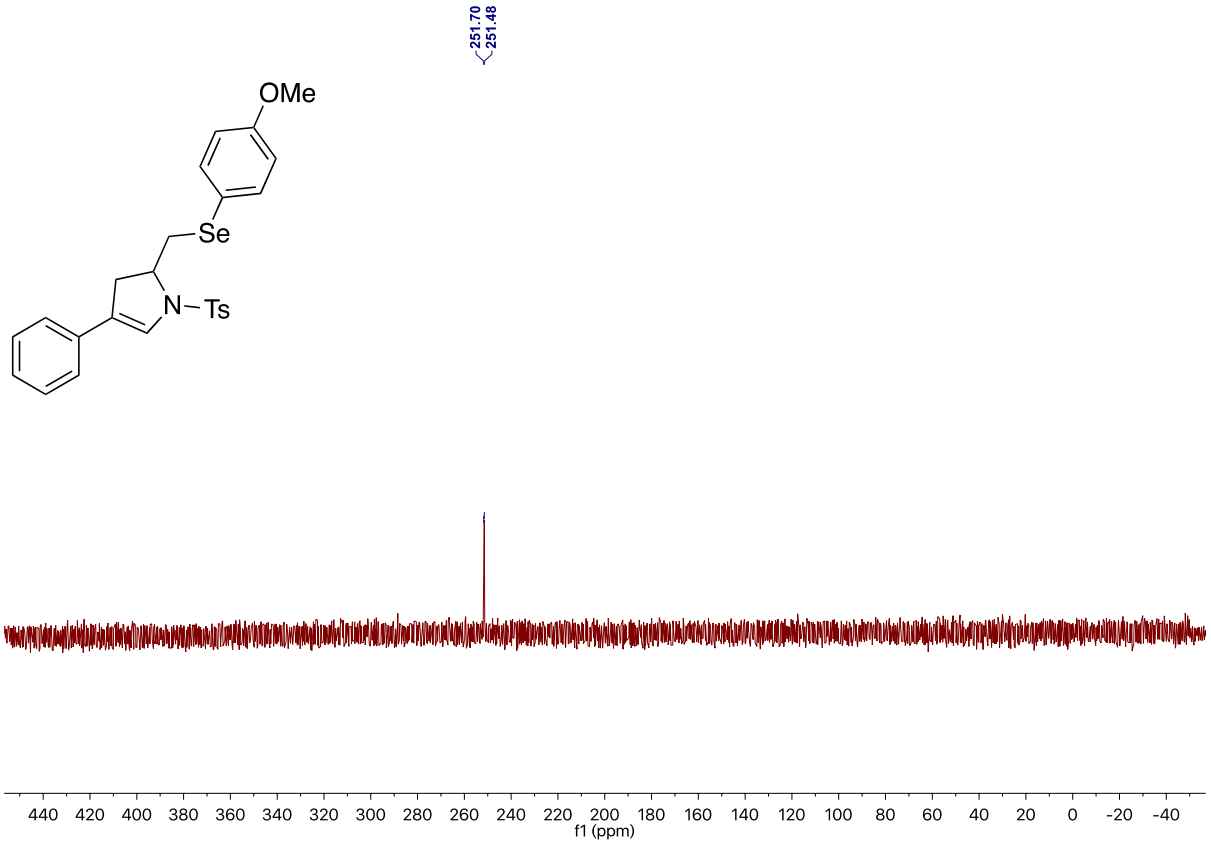
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

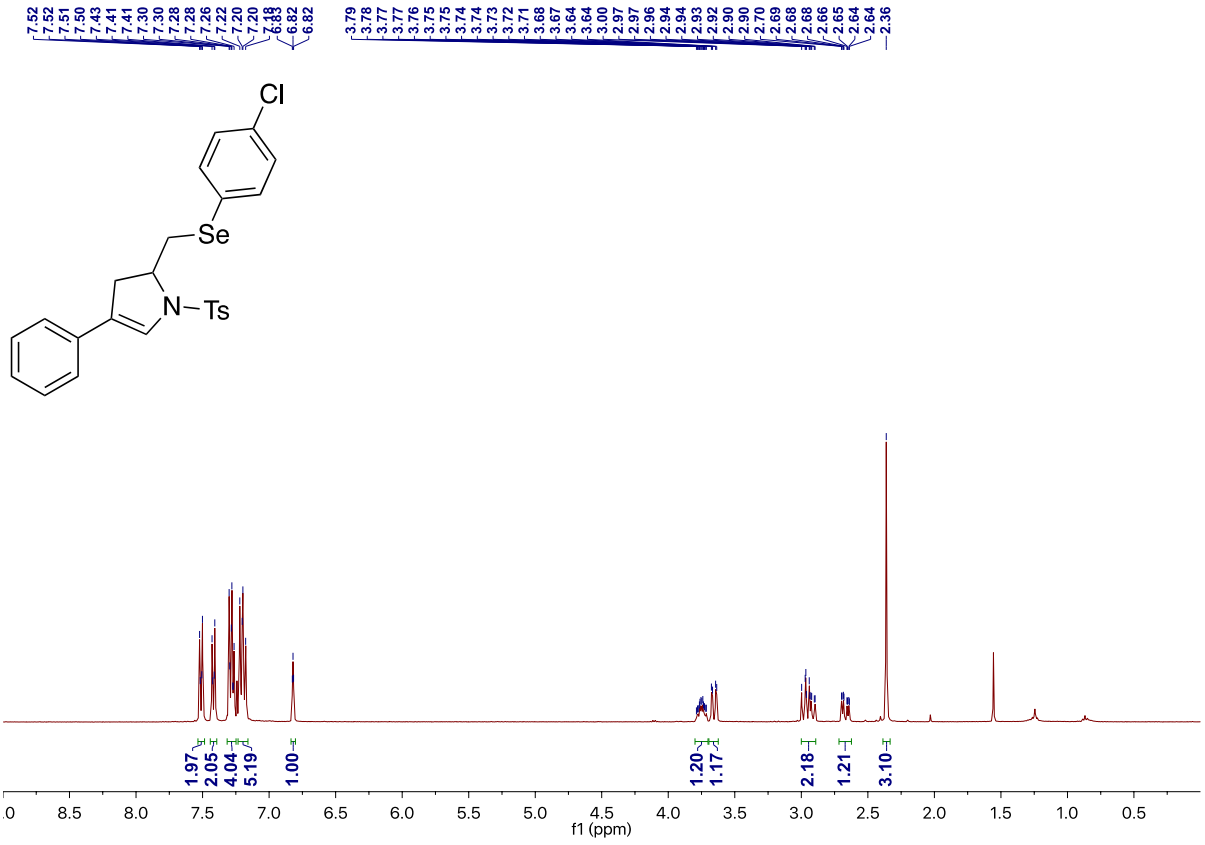


^{77}Se NMR (115 MHz, Chloroform-*d*)

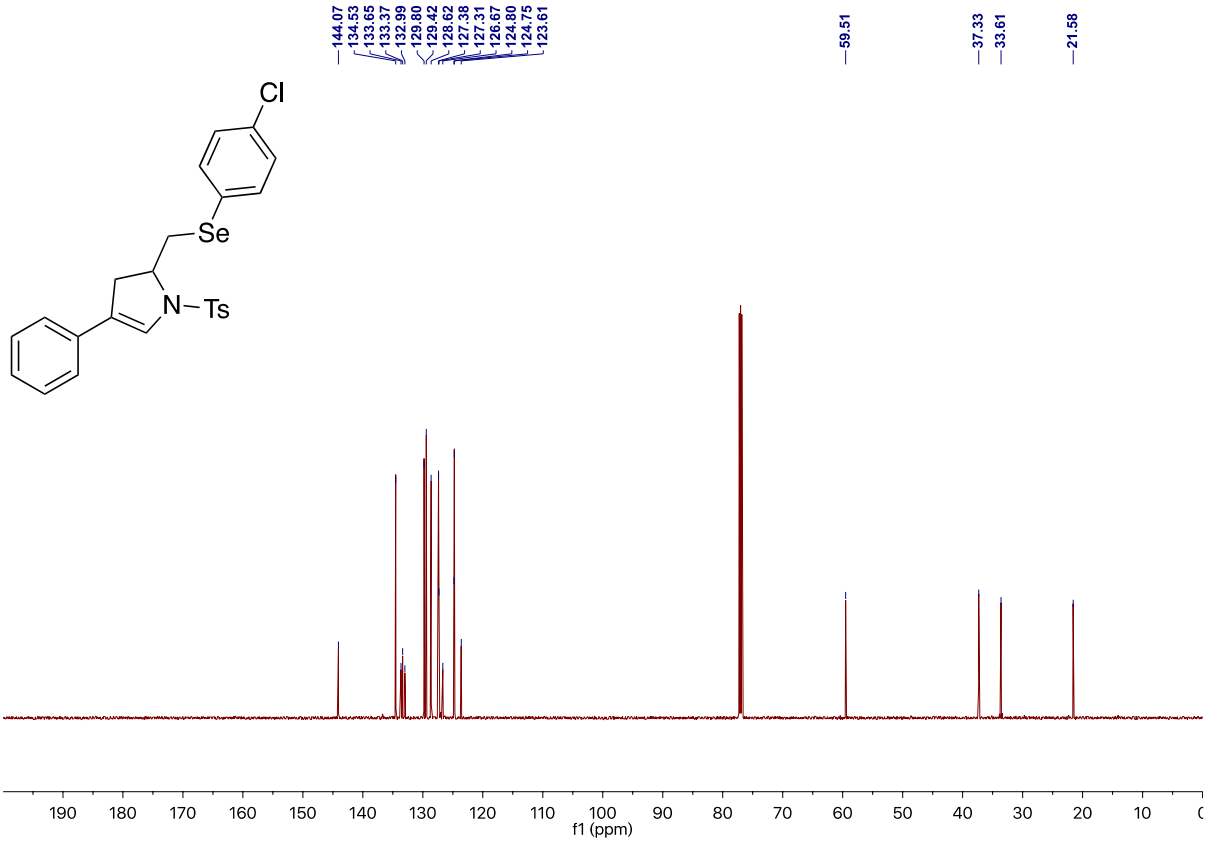


2-(((4-chlorophenyl)selanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (9w)

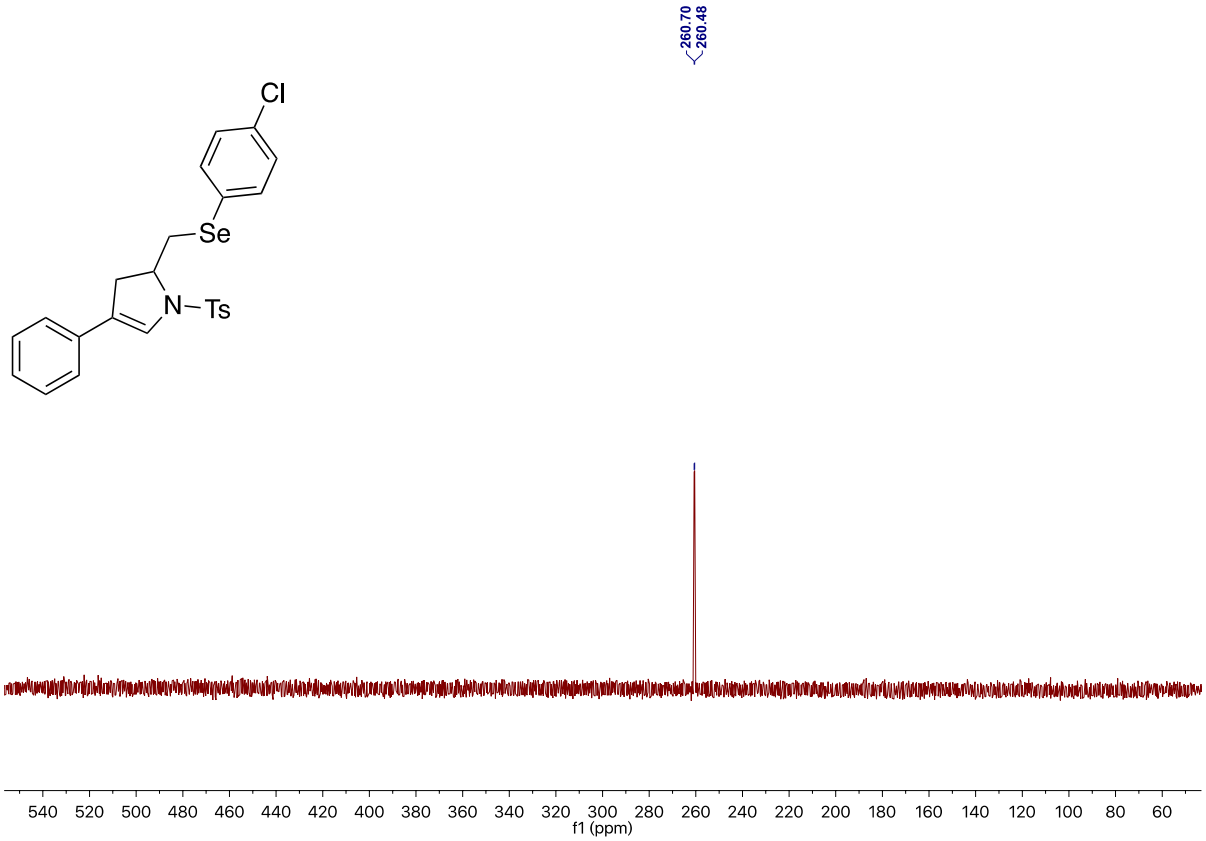
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

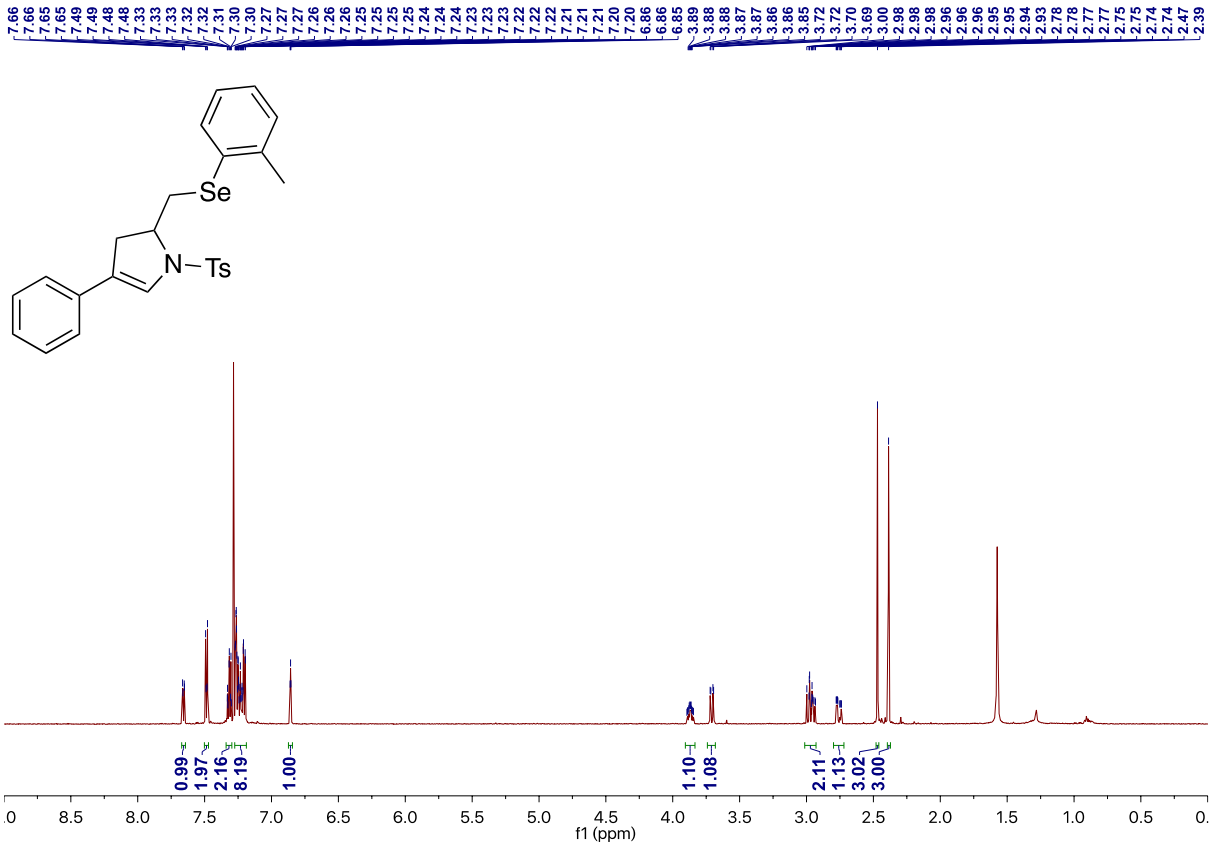


^{77}Se NMR (115 MHz, Chloroform-*d*)

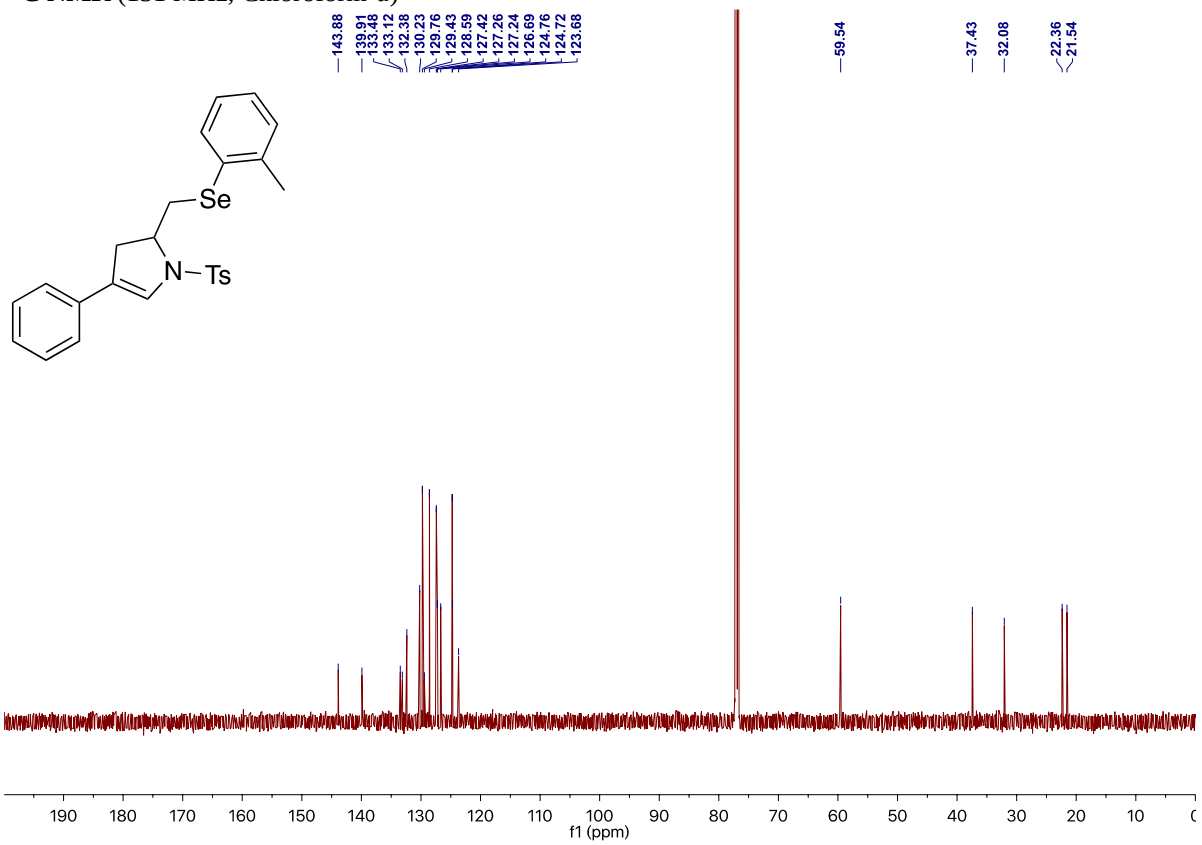


4-phenyl-2-((*o*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9x)

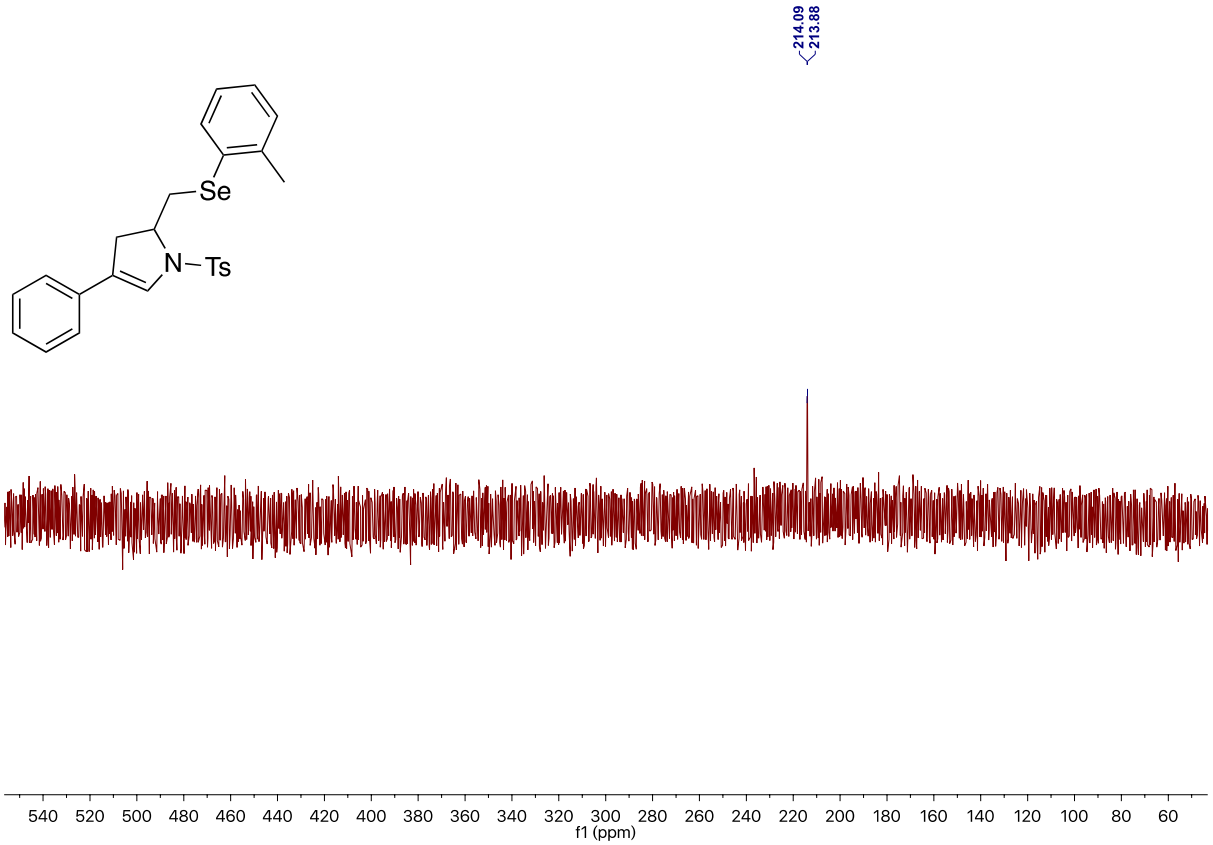
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

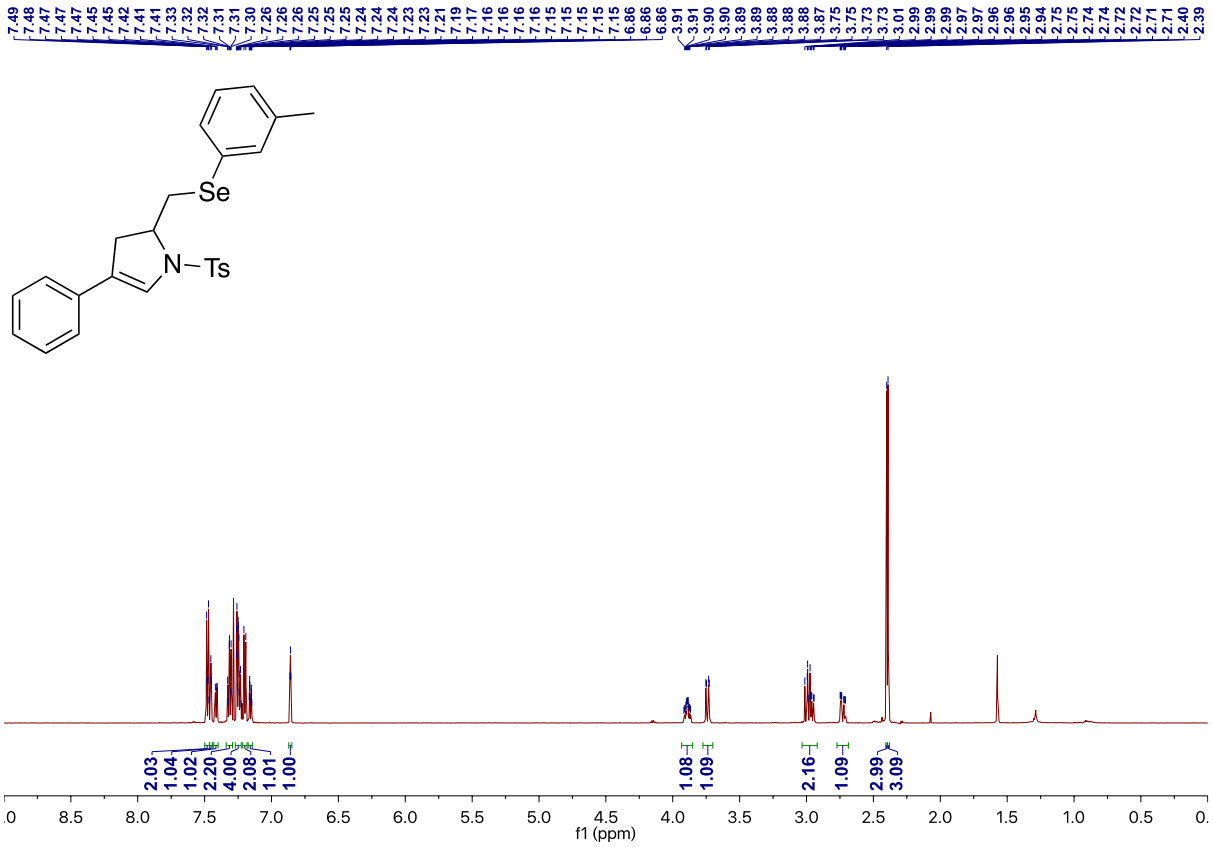


^{77}Se NMR (115 MHz, Chloroform-*d*)

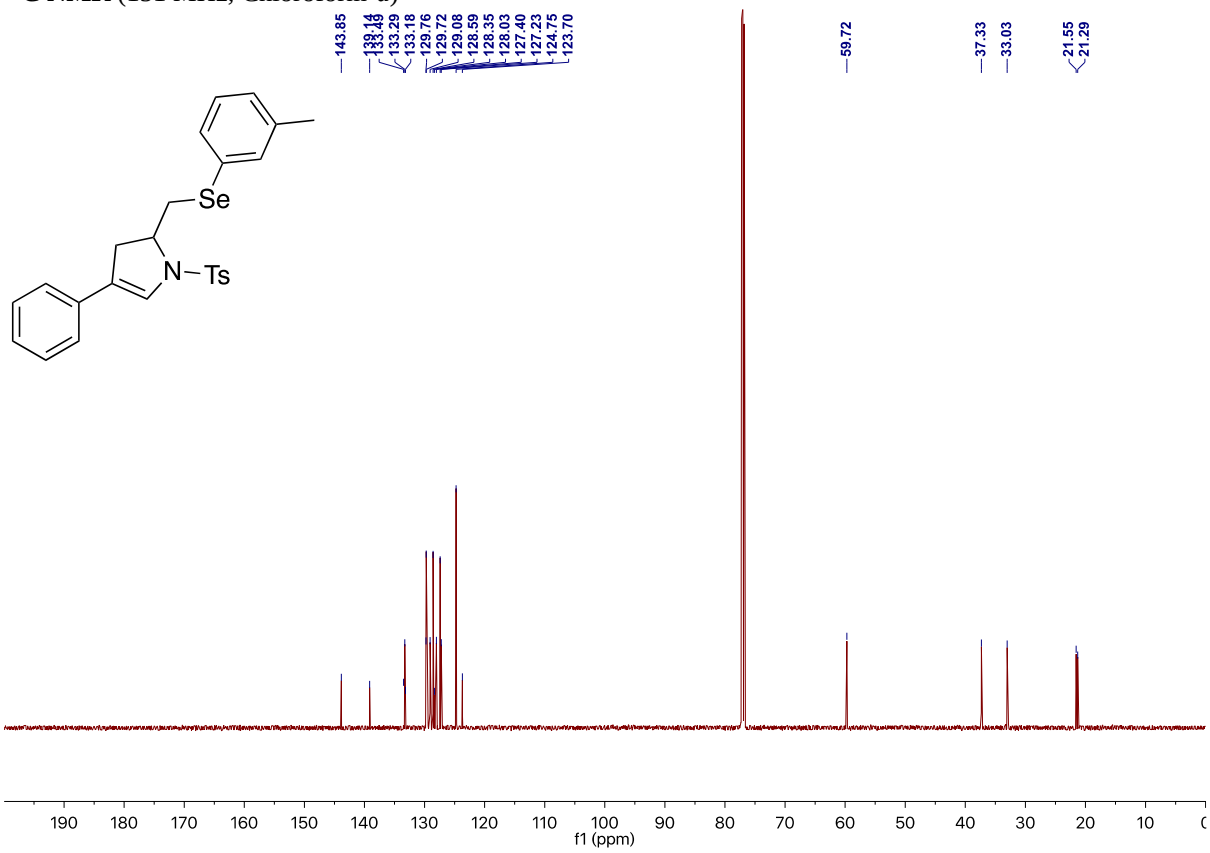


4-phenyl-2-((*m*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9y)

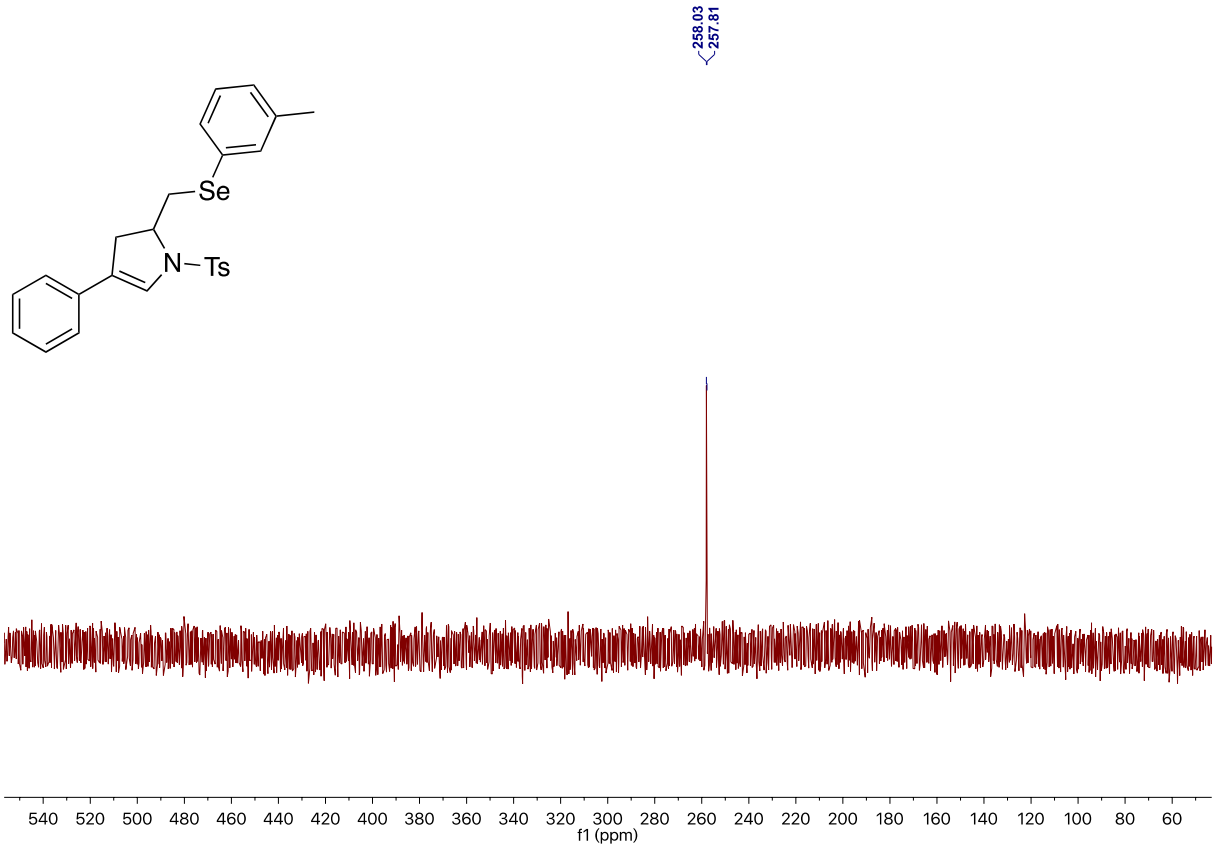
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

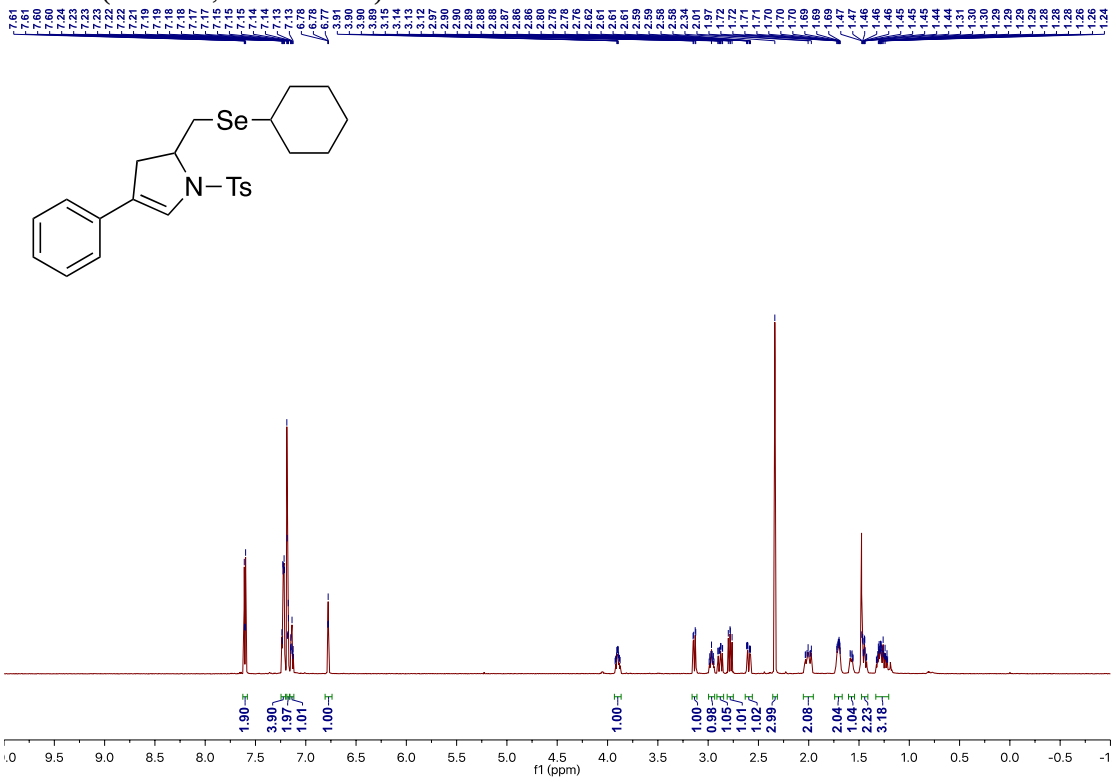


^{77}Se NMR (115 MHz, Chloroform-*d*)

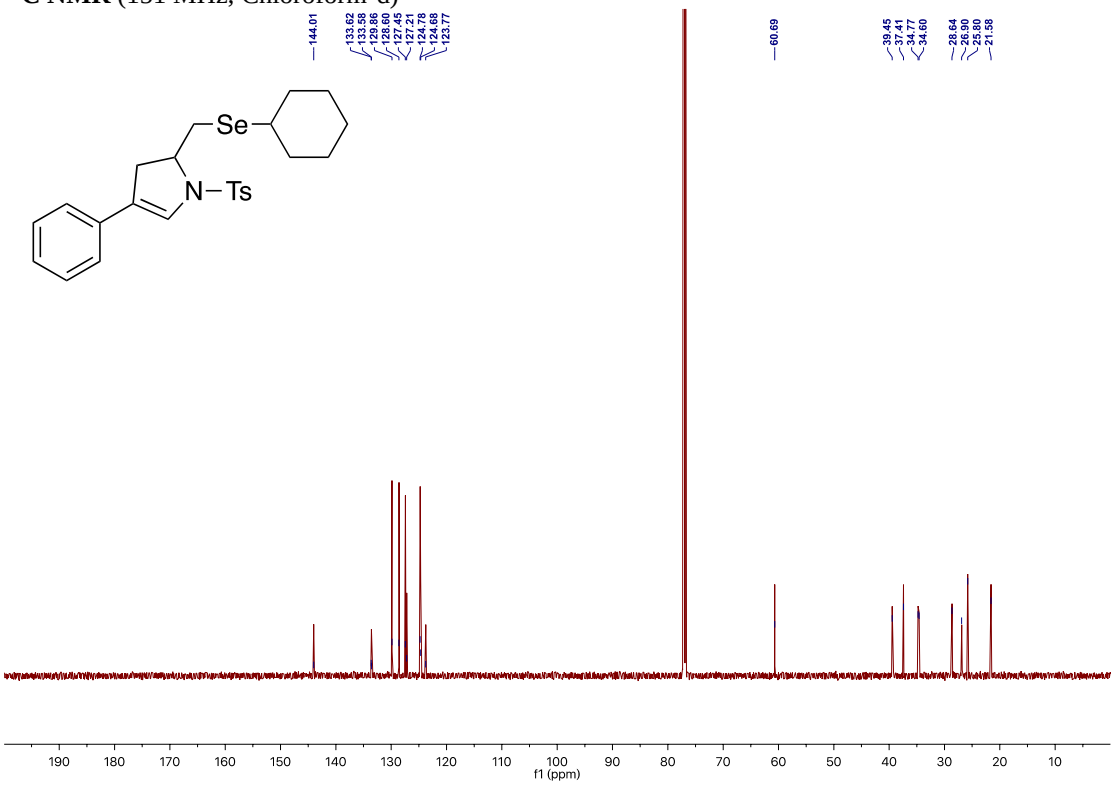


2-((cyclohexylselanyl)methyl)-4-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole (9z)

H NMR (600 MHz, Chloroform-*d*)

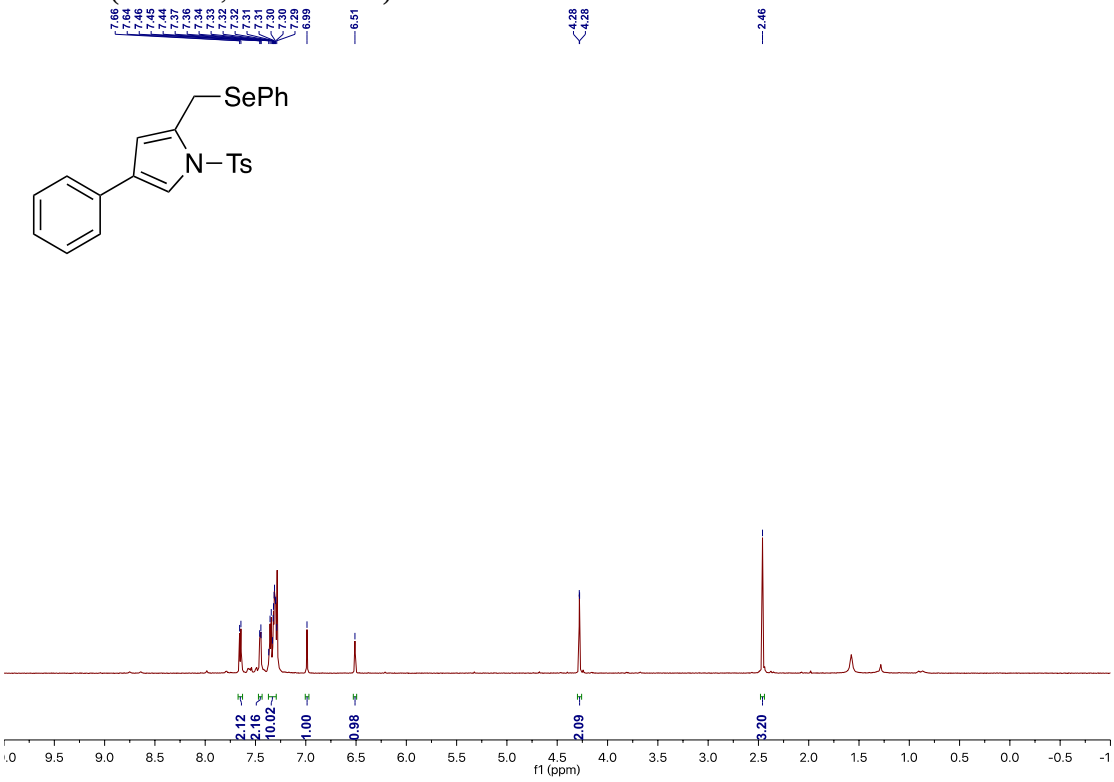


^{13}C NMR (151 MHz, Chloroform-d)

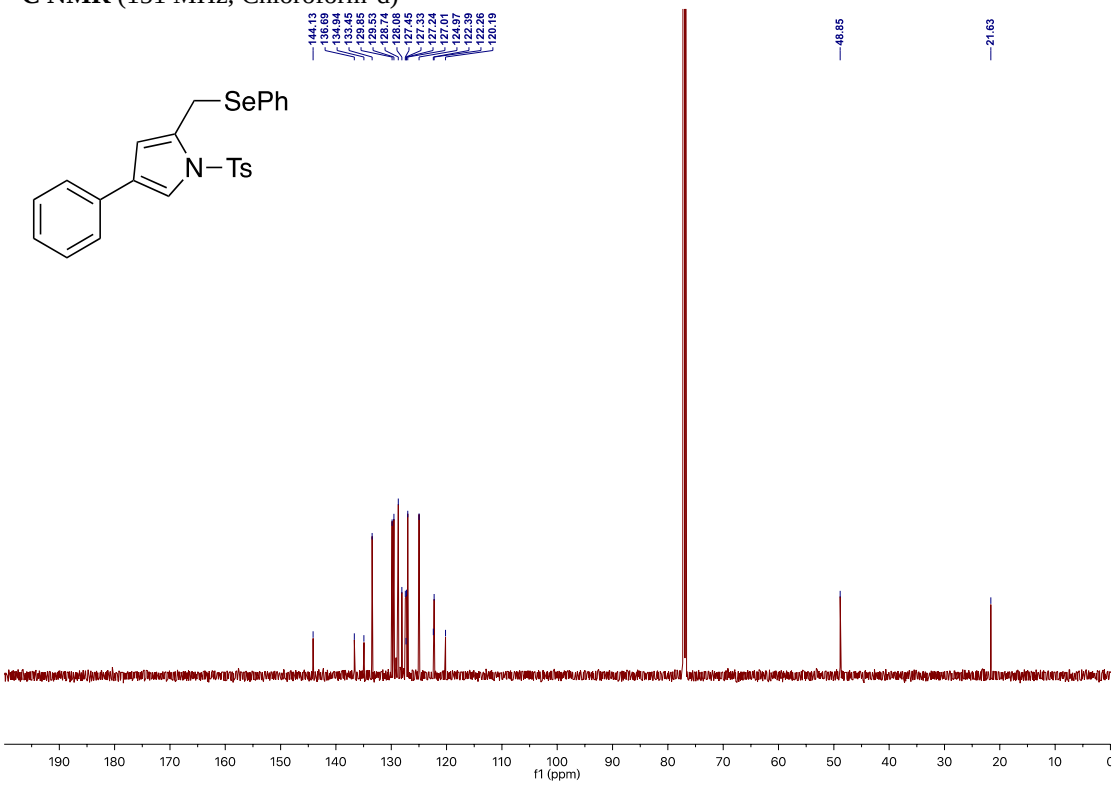


4-phenyl-2-((phenylselanyl)methyl)-1-tosyl-1*H*-pyrrole (9aa)

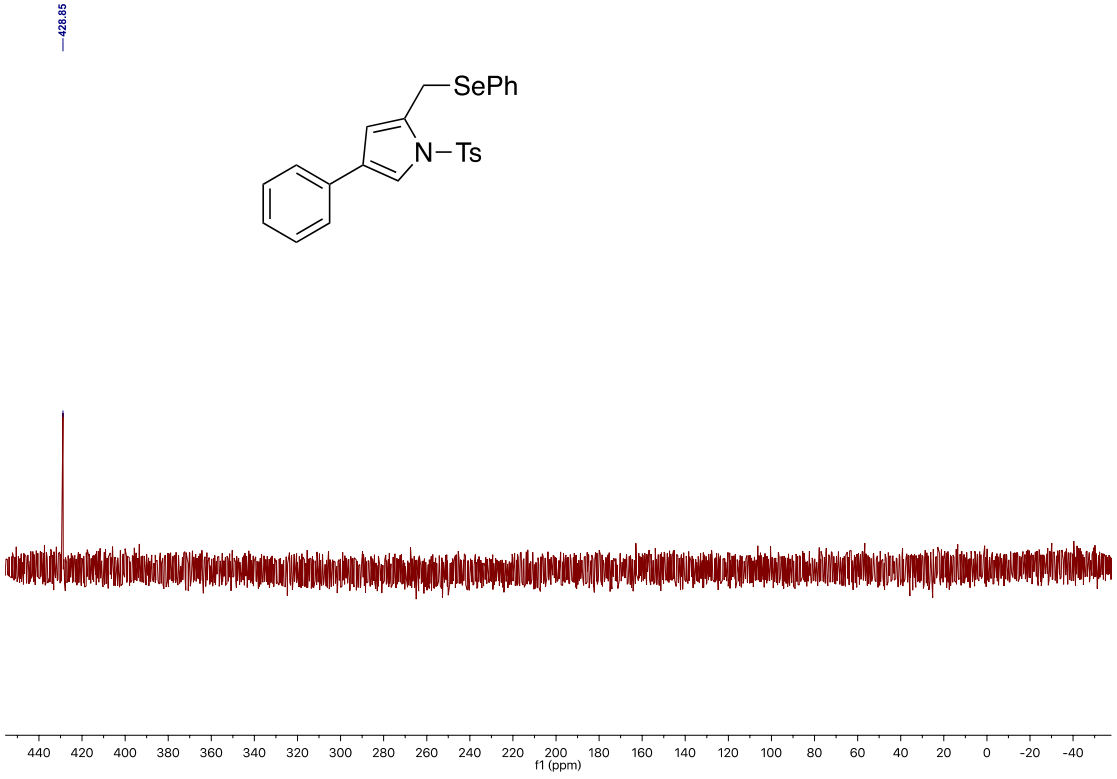
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

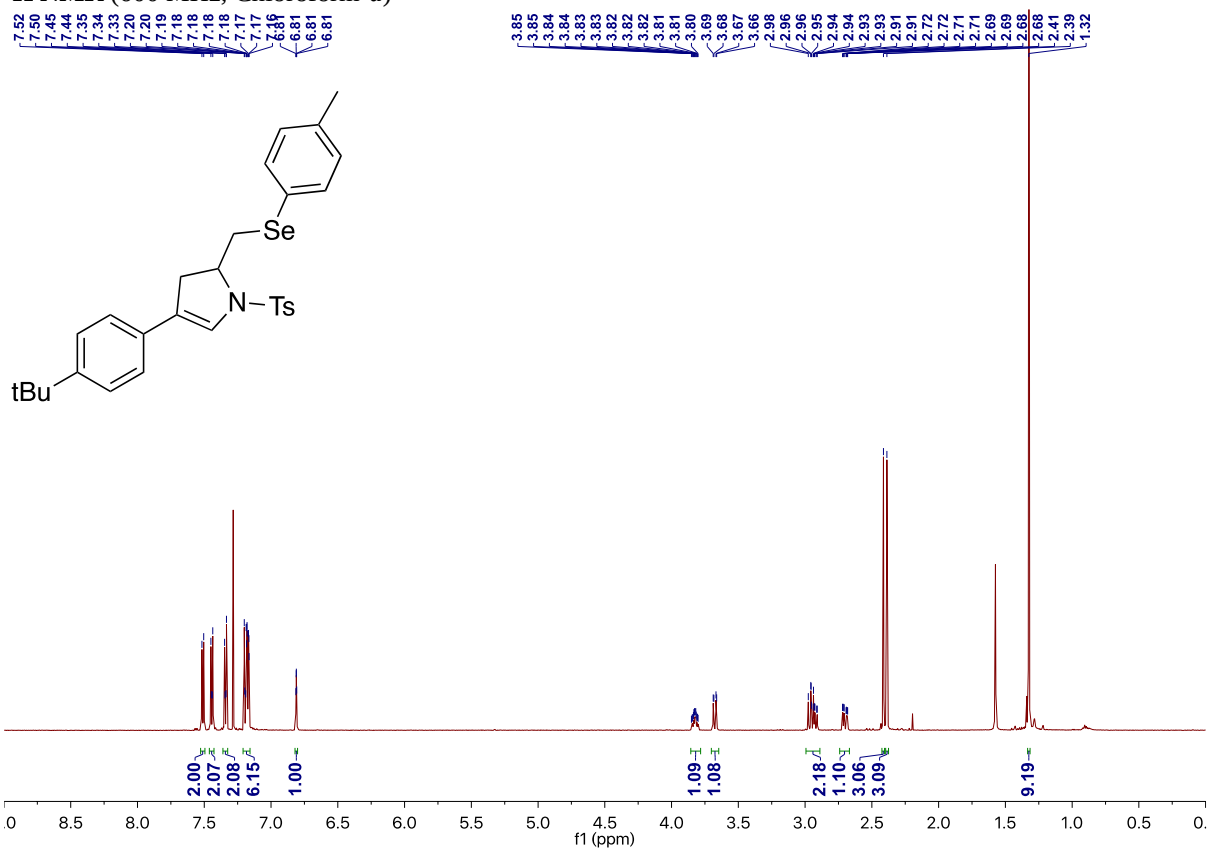


^{77}Se NMR (115 MHz, Chloroform-*d*)

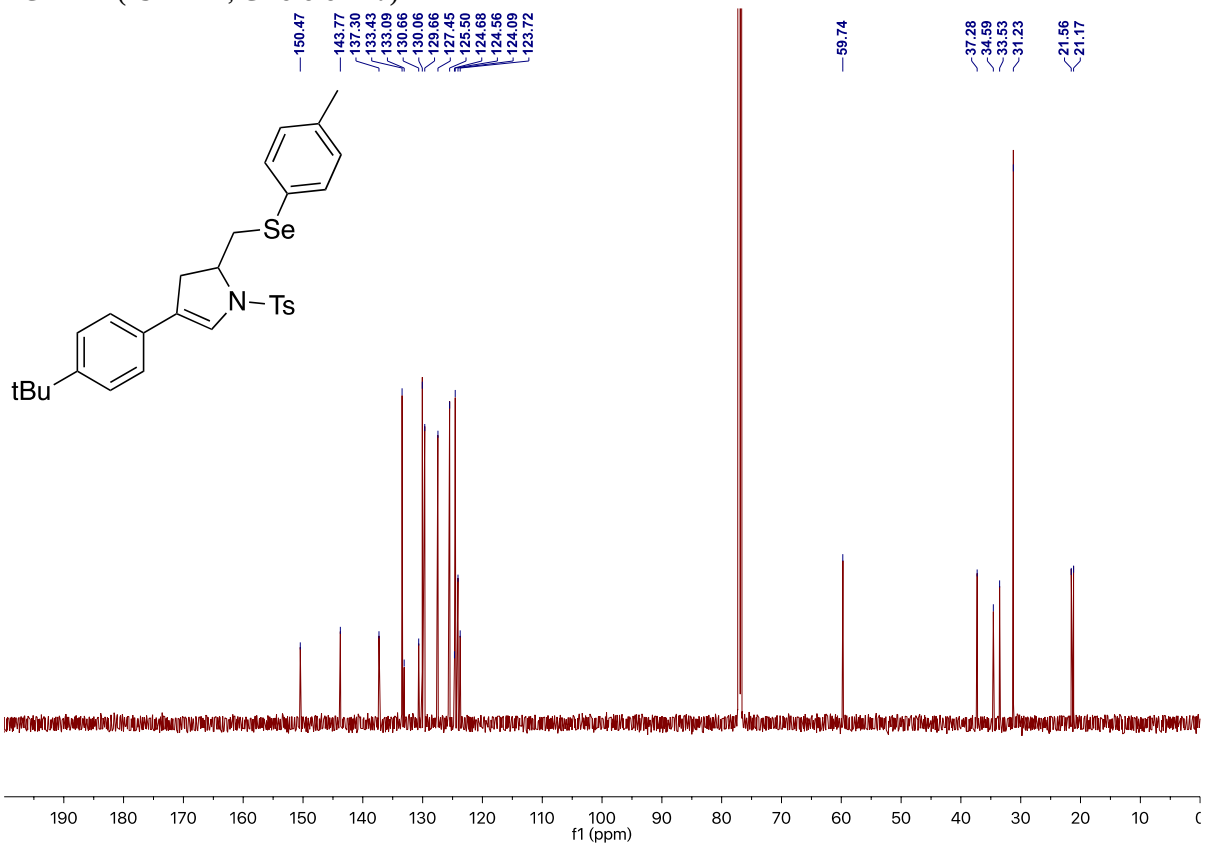


4-(4-(*tert*-butyl)phenyl)-2-((*p*-tolylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (9ab)

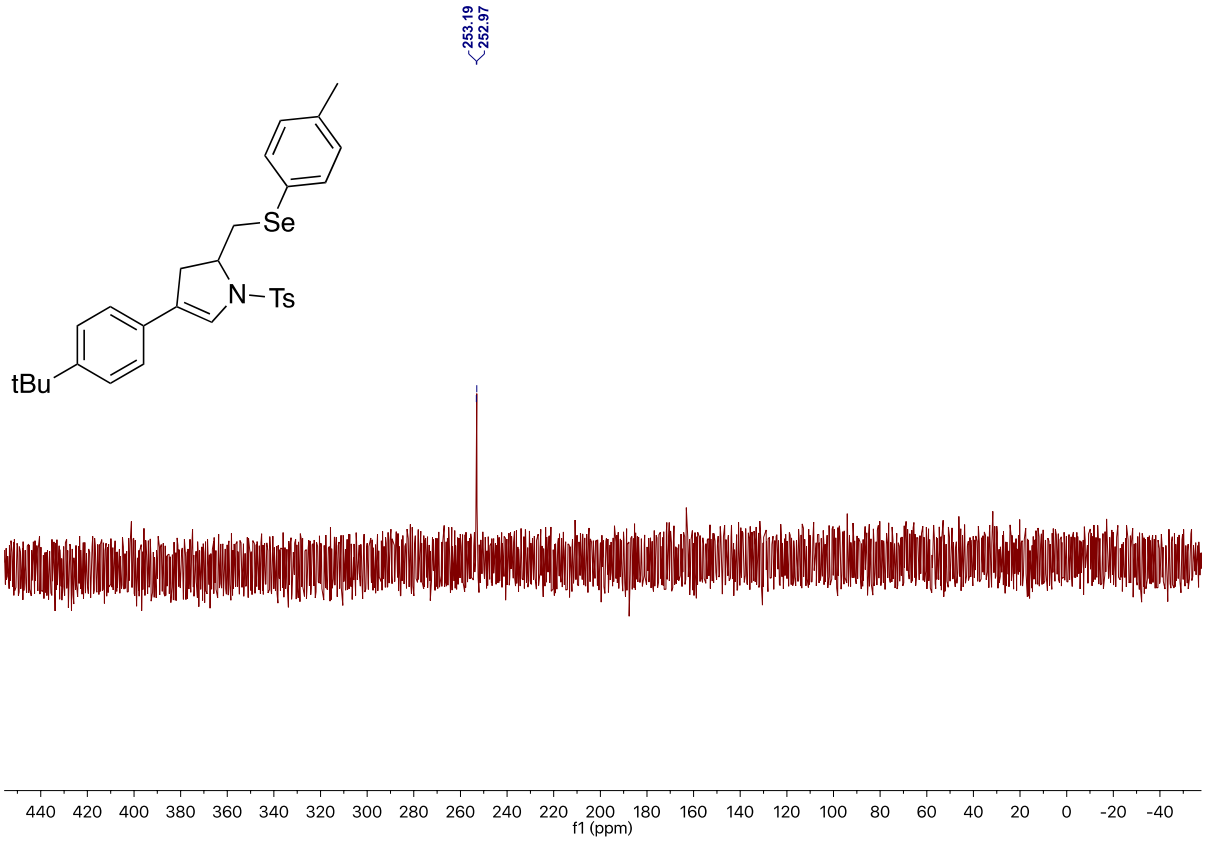
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

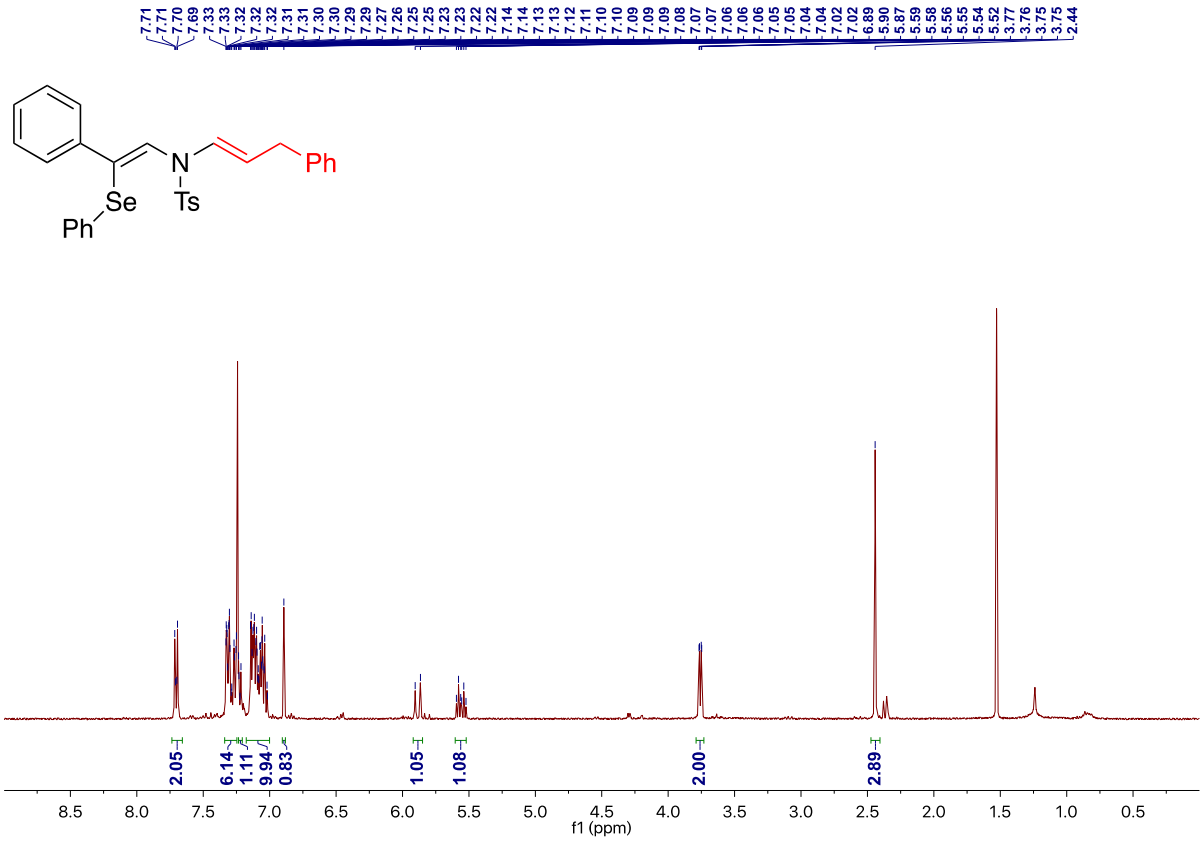


^{77}Se NMR (115 MHz, Chloroform-*d*)

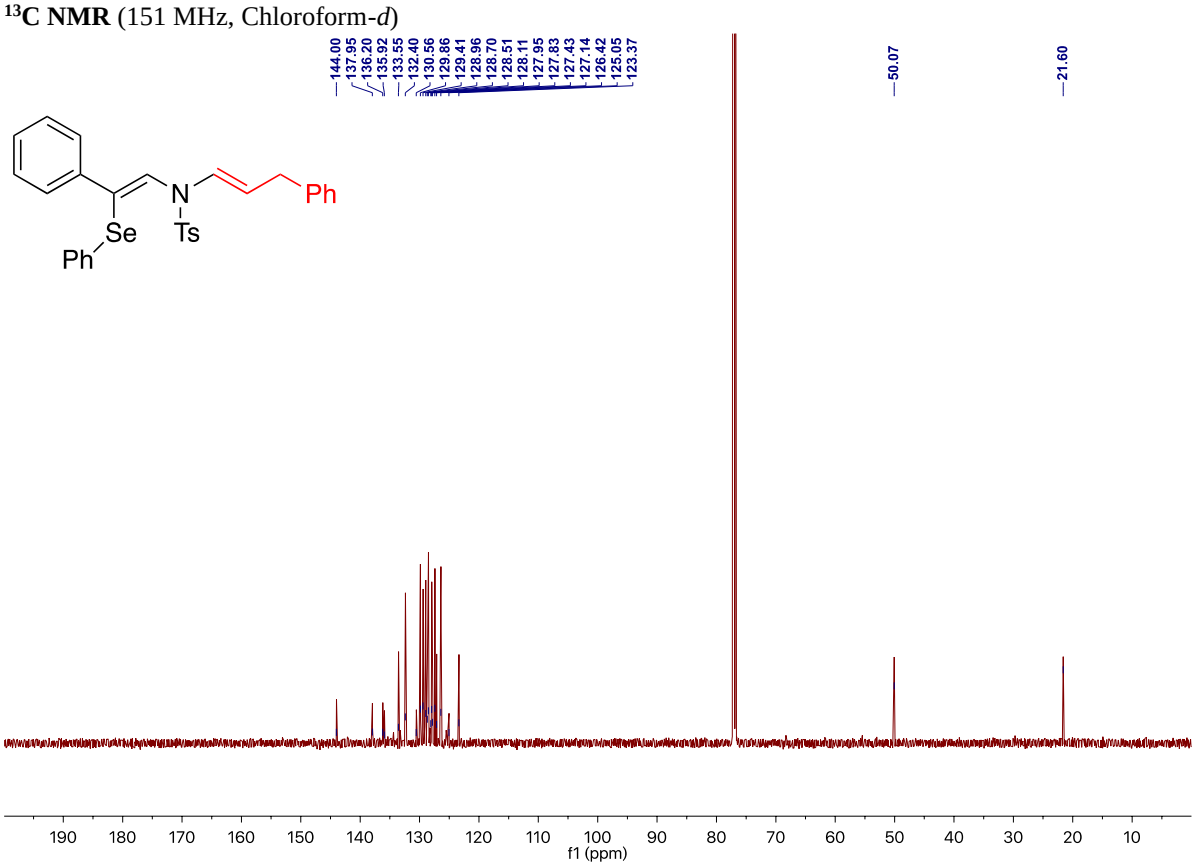


4-methyl-*N*-((*Z*)-2-phenyl-2-(phenylselanyl)vinyl)-*N*-((*E*)-3-phenylprop-1-en-1-yl)benzenesulfonamide (8a')

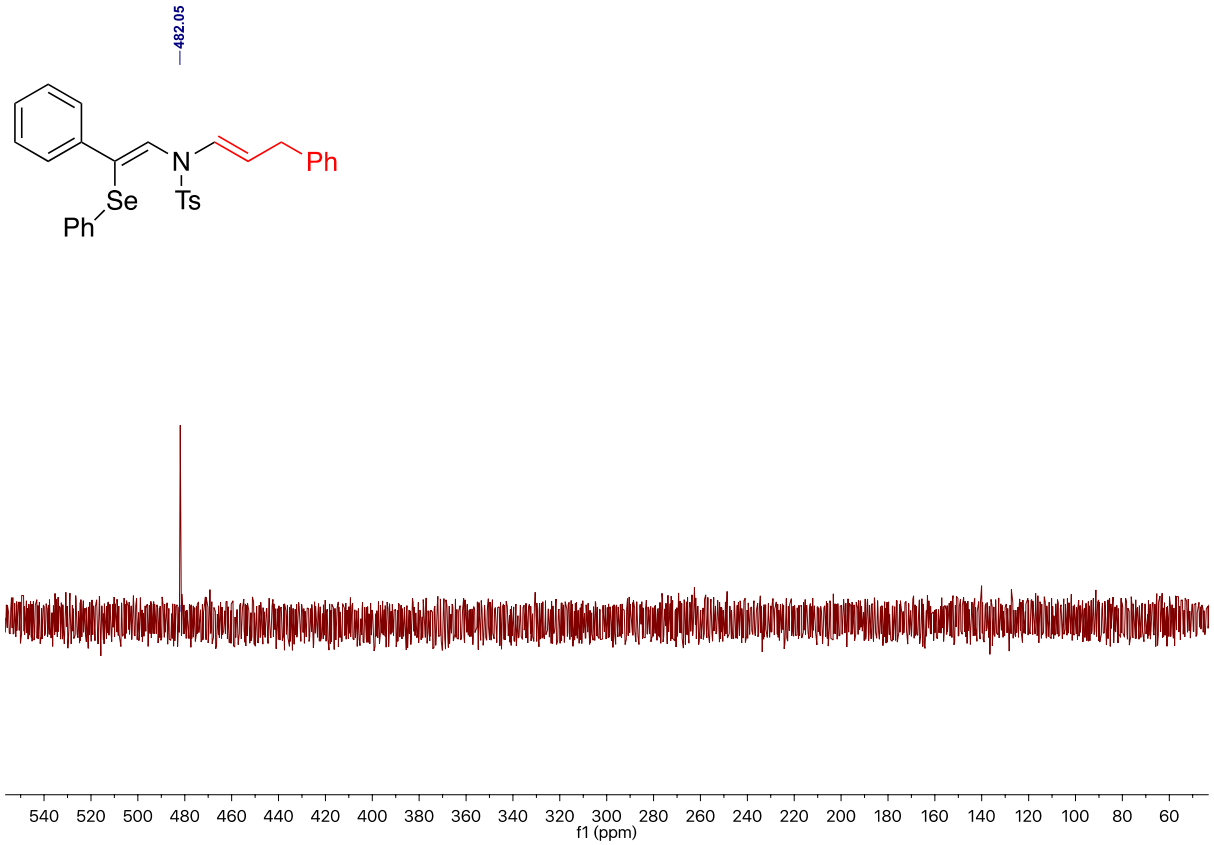
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

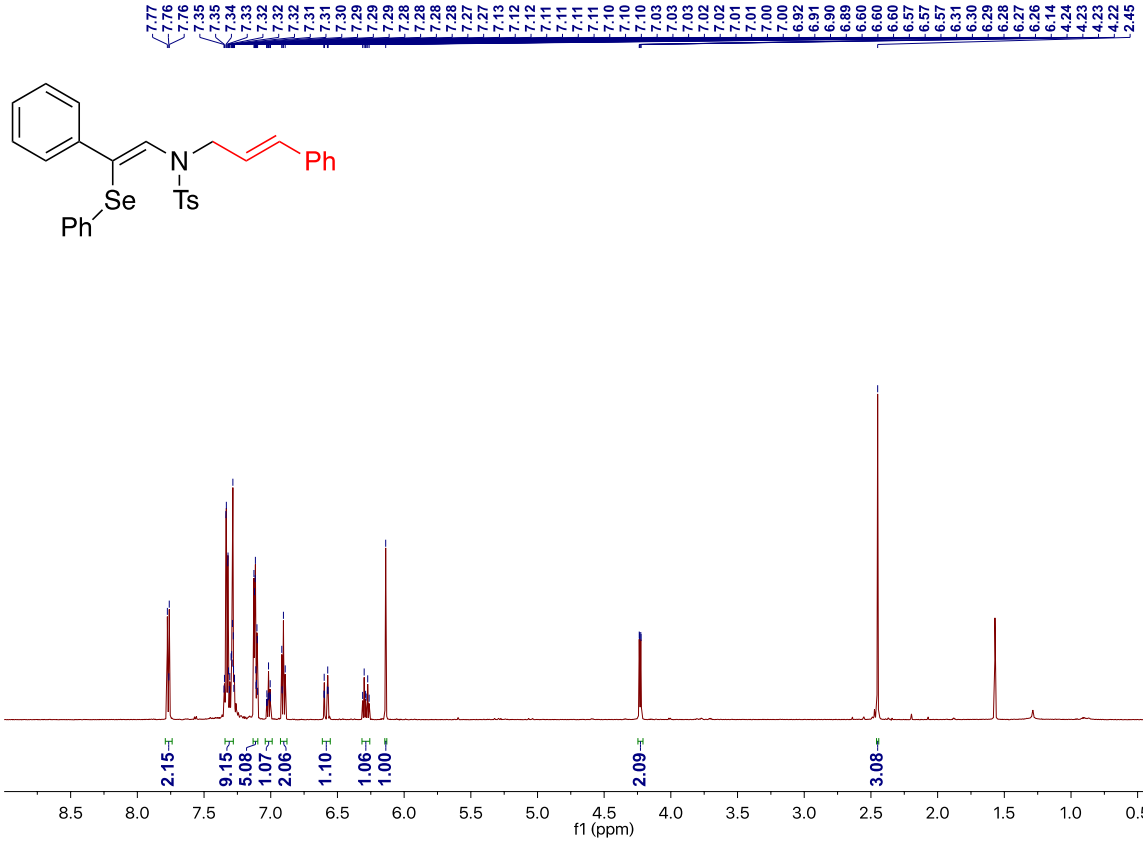


^{77}Se NMR (115 MHz, Chloroform-*d*)

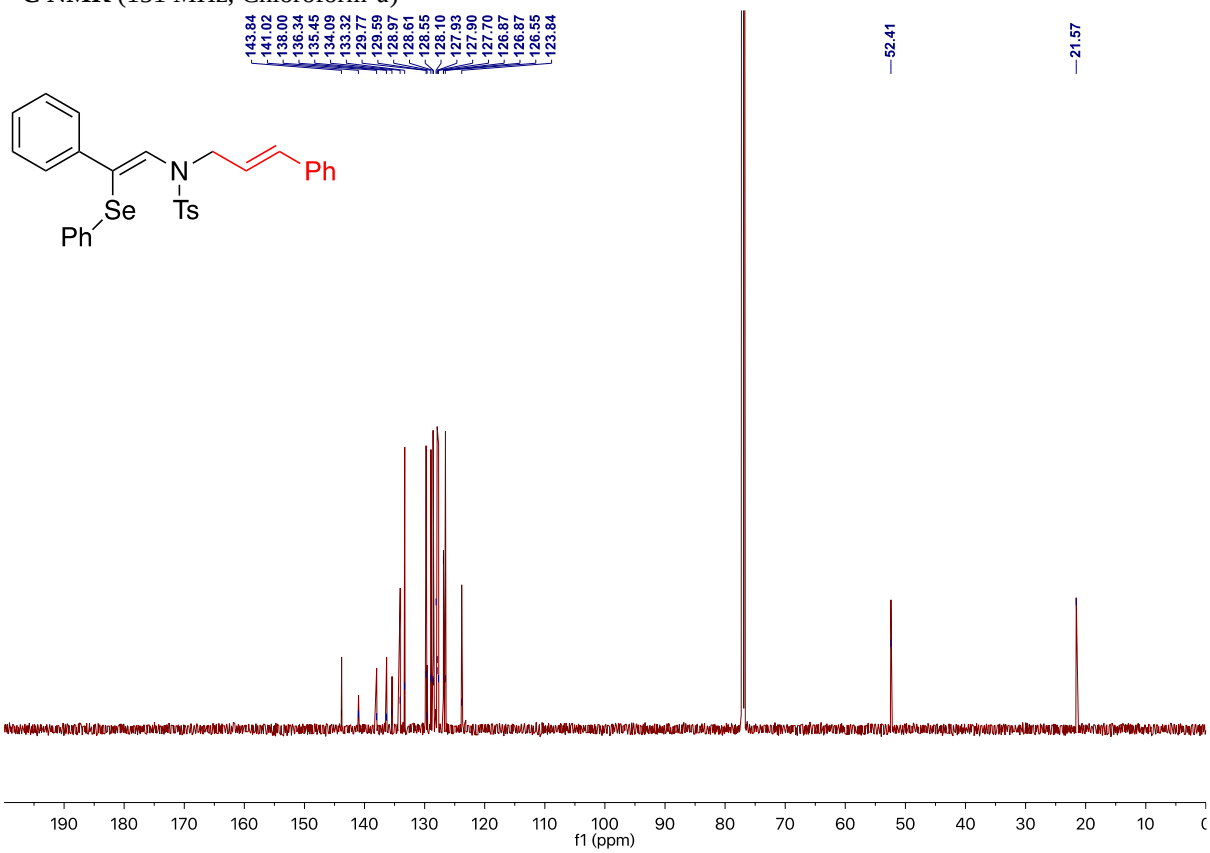


***N*-cinnamyl-4-methyl-*N*-((*Z*)-2-phenyl-2-(phenylselanyl)vinyl)benzenesulfonamide (8a)**

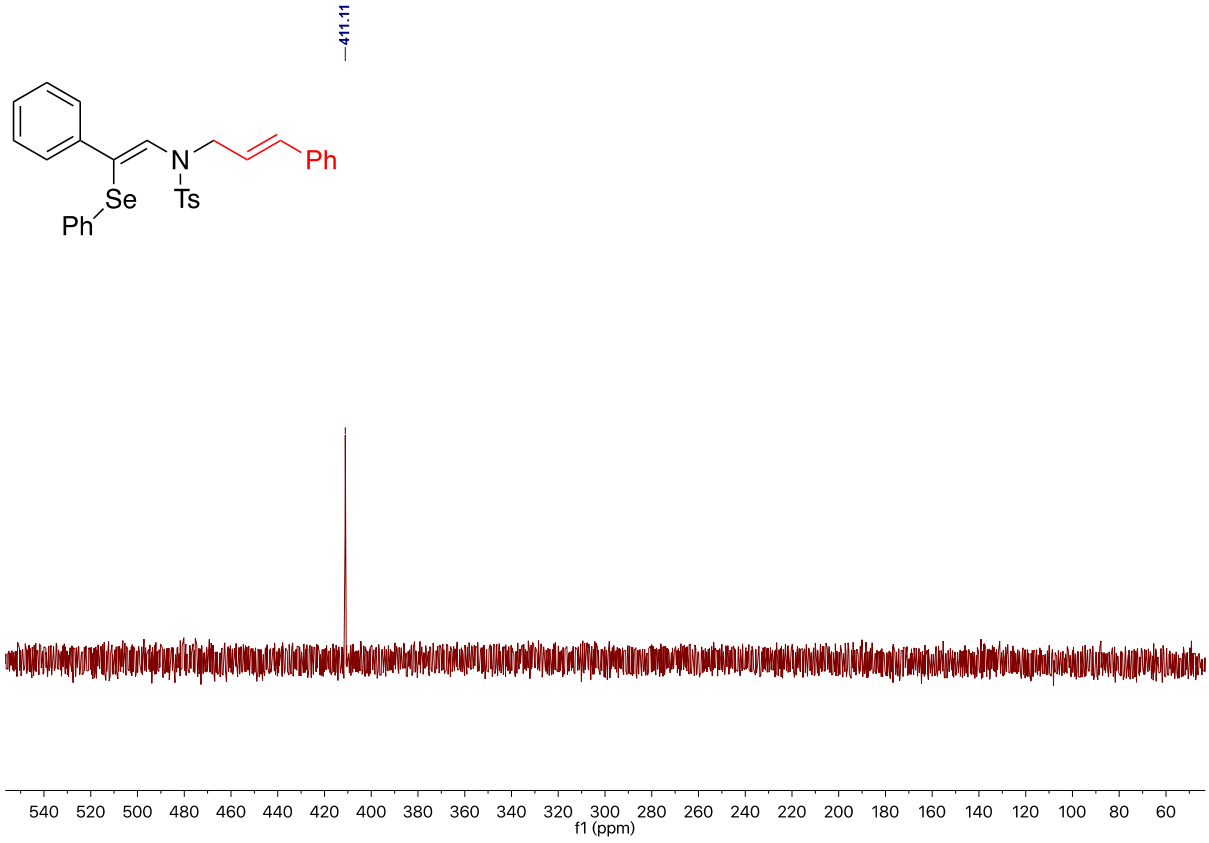
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

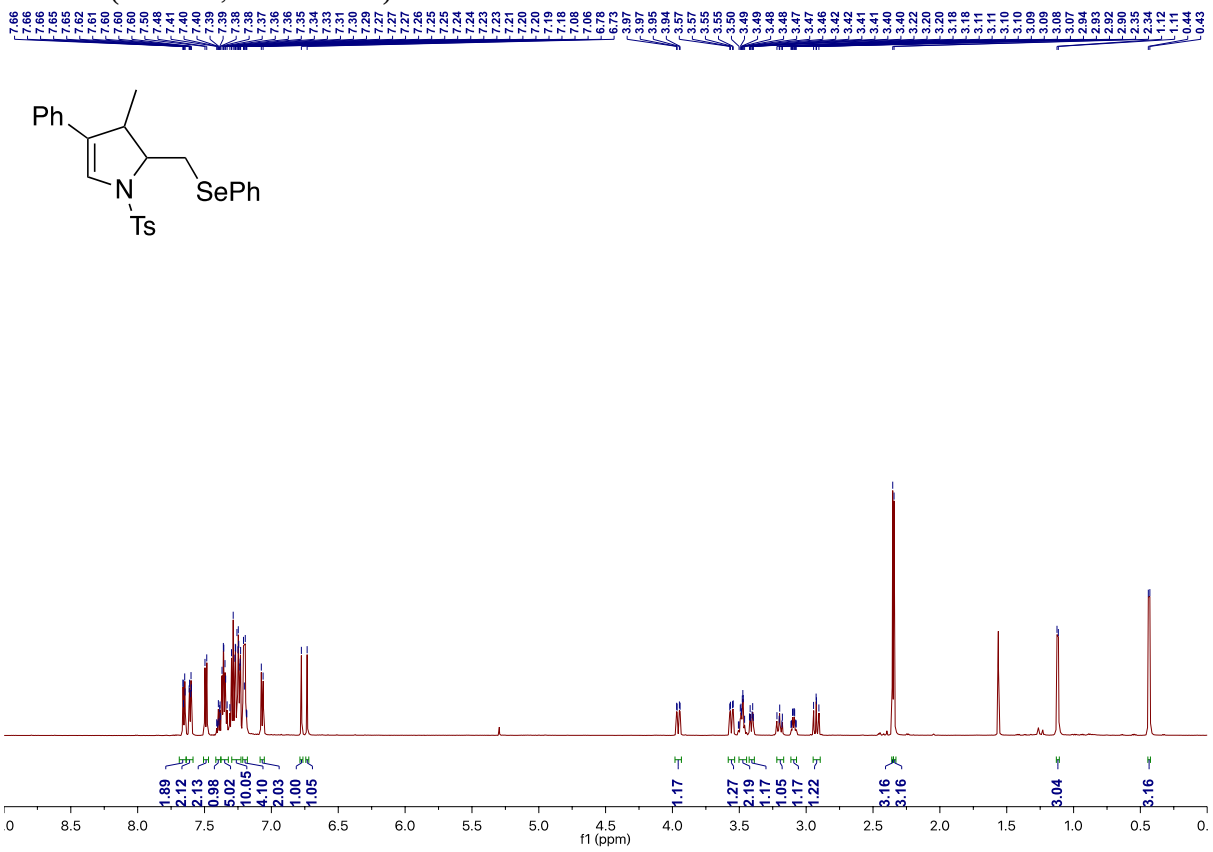


^{77}Se NMR (115 MHz, Chloroform-*d*)

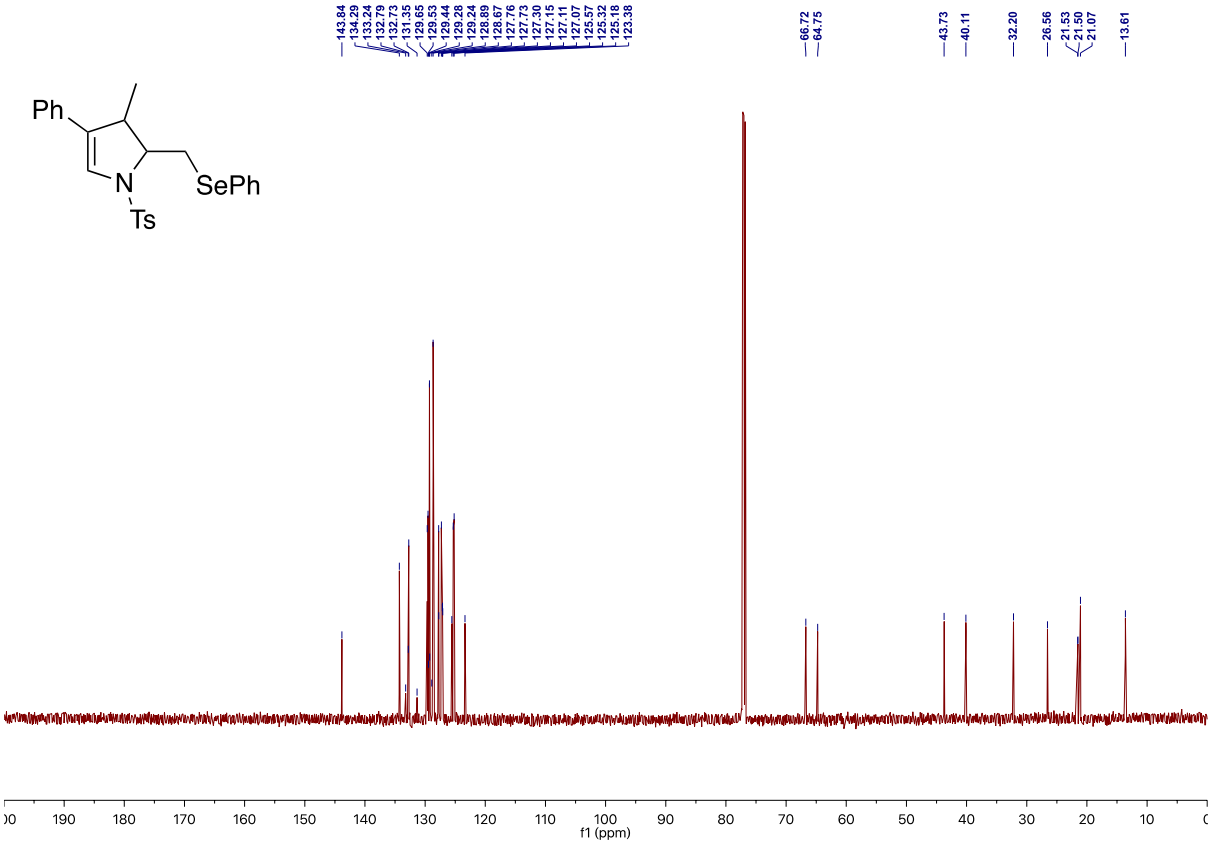


3-methyl-4-phenyl-2-((phenylselanyl)methyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (15, d.r.=1:1)

^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)



^{77}Se NMR (115 MHz, Chloroform-*d*)