Supplementary Information (SI) for ChemComm.
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Supplementary Information

# Visible Light-Induced *Ipso*-Chalcogenation of Aryl/Alkenyl Boronic Acids Assisted by a Chalcogen-Radical Transfer (ChRT) Strategy

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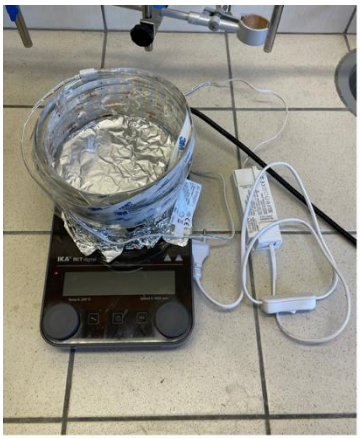
# 1. General Information

Unless otherwise noted, all air and moisture sensitive catalytic reactions were carried out in oven-dried glassware, microwave tubes or vials. All reagents including chalcogenides, boronic acids, solvents were obtained from Aldrich chemical co., Alfa Aesar, Fluorochem, TCI Europe and were used as received unless otherwise stated. 1,1,1,3,3,3-hexafluoropropan-2-ol (HFIP) was purchased from Fluorochem and stored under argon atmosphere over molecular sieves (4 Å), if necessary. Analytical thin layer chromatography (TLC) was performed on silica gel 60 $F_{254}$ aluminium plates (Merck). TLC plates were visualized by exposure to short-wave ultraviolet light (254 nm). Chromatography was carried out on Merck silica gel 60 (40-63 µm). Preparative thin layer chromatography (PTLC) was performed on silica gel 60 $F_{254}$ glass plates (20 × 20 cm from Merck). $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra were recorded on Agilent Mercury 400 MHz spectrometers at 298 K using $CDCl_3$ as solvent. $^{77}Se$ and $^{125}Te$ NMR spectra were recorded on Bruker Avance III HD 500 MHz spectrometer at 298 K using $CDCl_3$ as solvent. Chemical shifts are given in ppm relative to the residual solvent peak ($^{1}H$ NMR: $CDCl_3$ δ 7.26; $^{13}C$ NMR: $CDCl_3$ δ 77.16). Shift values are reported in ppm and all coupling constants (J) are printed in Hertz (Hz) with their multiplicity: s (singlet), br (broad signal), d (doublet), t (triplet), q (quartet), p (pentet), m (multiplet or unresolved). High resolution mass spectra (HRMS) measurements were performed at the core facility of the Faculty of Chemistry, University of Warsaw on a Nexera X3 system coupled with an LCMS-9030 quadrupole time-of-flight mass spectrometer (Shimadzu Corporation, Kyoto, Japan) with electron spray ionization (ESI, unless otherwise stated). Yields refer to isolated compounds, estimated to be >95% pure as determined by $^{1}H$-NMR. Photocatalytic reactions were performed in transparent reaction vials (3 to 50 mL, with a small magnetic stirrer kept inside) which were held on a designed vial stand at the centre of a stirring plate. Reaction temperature were measured using direct contact digital thermometer from Benetech (model no. GM1312). NMR spectra and HR-MS measurements were collected employing facilities available at the University of Warsaw (Department of Chemistry).

## 2. Standard photocatalytic reaction setup



(a) Designed photochemical reactor with LED stripes

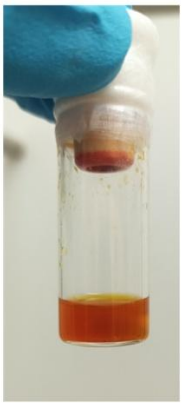
(b) Reaction vial stand & Digital thermometer

(c) Reaction vial & precision seal rubber septa

(d) Top view of photochemical reactor under white LEDs

(e) Reaction vial charged with reagents & degassed by sparging with argon

(f) Reaction vial under irradiation (front view & top view)



(h) Reaction vial after irradiation

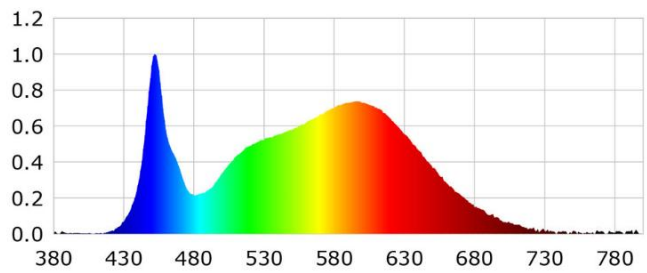
(i) Designed vial stand inside the photoreactor for multiple reactions

(j) Multiple reactions at a time

**Figure S1.** Standard photocatalytic reaction setup.

The photoreactor was constructed using the white LED tape (4000 K ± 100 K; 620 lm·m$^{-1}$ from Inspire-Cutflexi, France, with power adapter, model no: SMD-5M-4K) and a borosilicate glass crystallizer (h = 5 cm, ø = 10 cm). Walls of the crystallizer were covered with aluminium foil. The distance between the LEDs and reaction vials was ~2 cm.

**Table S1.** Emission spectrum of a white LED tape used for the construction of a photoreactor and some of its technical details.

| | |
|---|---|
|   | |
| Energy consumption in on-mode (kWh/1000 h) | 2 |
| Useful luminous flux (Φuse), indicating if it refers to the flux in a sphere (360˚), in a wide cone (120˚) or in a narrow cone (90˚), expressed in Lm | 500 (360) |
| On-mode power (Pon), expressed in W and rounded to the first decimal | 2.1 |
| Colour rendering index, rounded to the nearest integer, or the range of CRI-values | 80 |

| | |
|---|---|
| that can be set | |
| Chromaticity coordinates (x and y) | 0.380;0.380 |

## 3. Overview of substrates and products

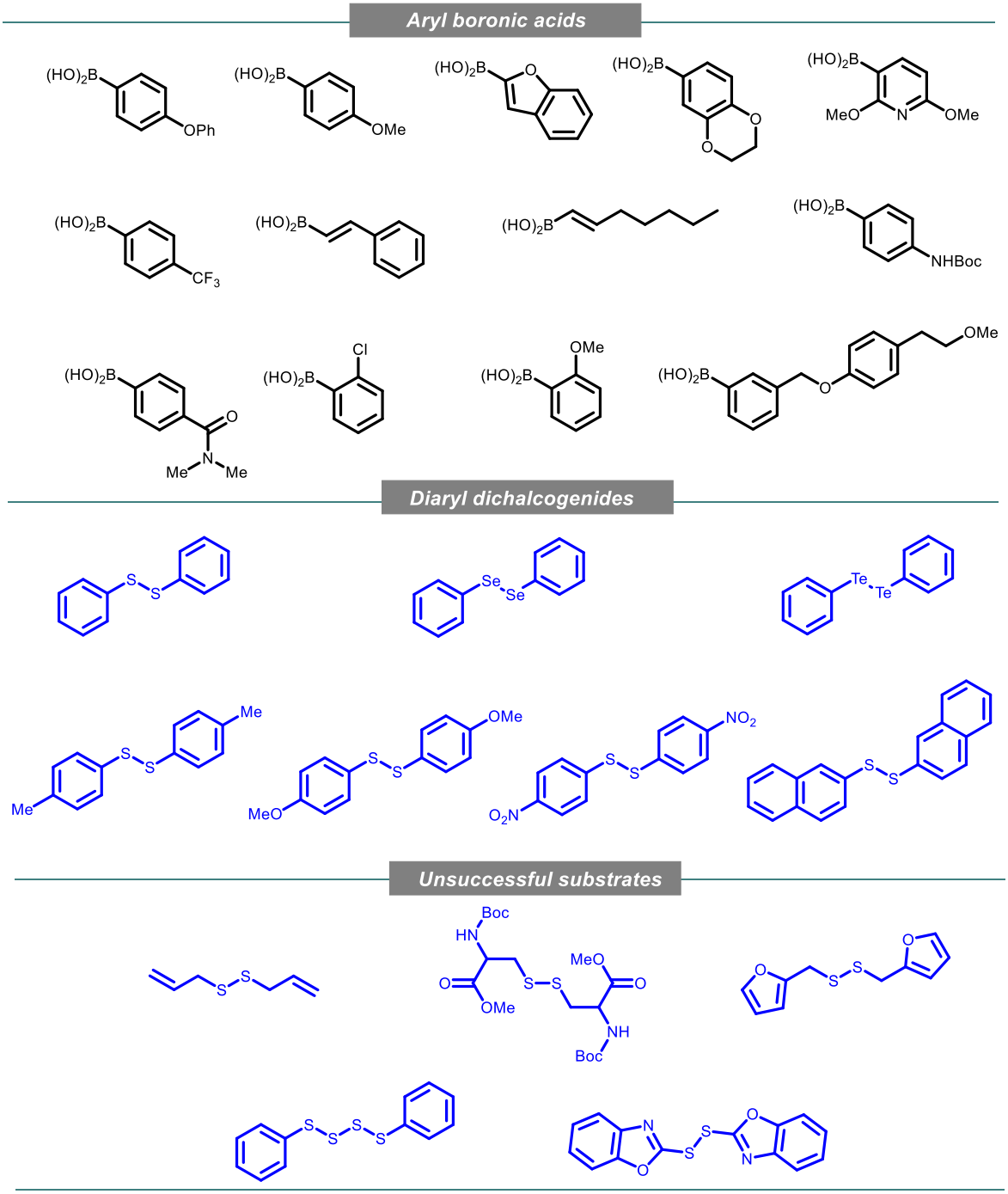



**Figure S2.** Overview of aryl boronic acids and diaryl dichalcogenides used in our work.

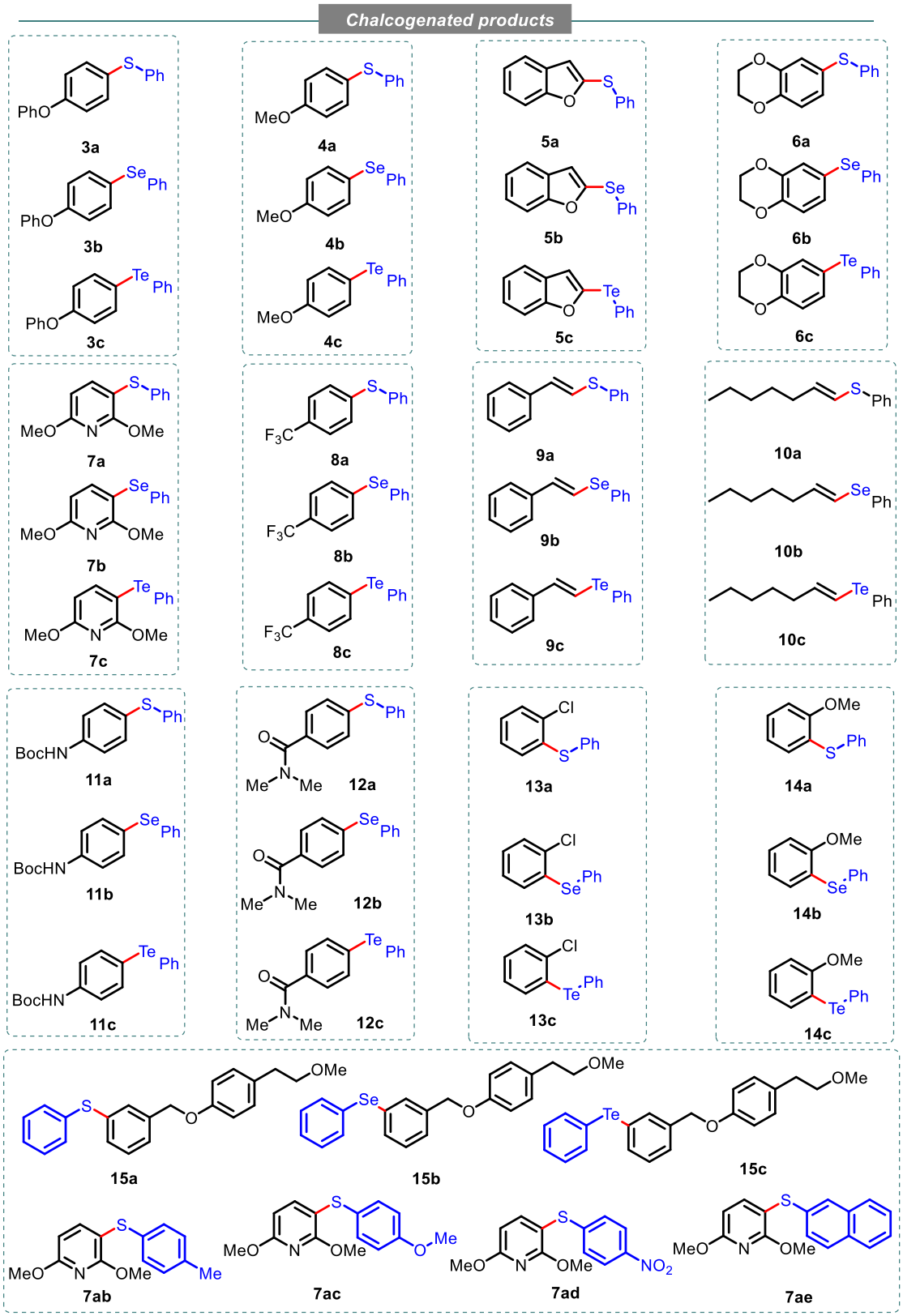
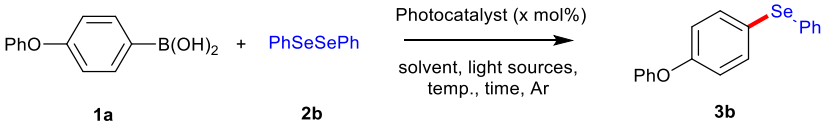



**Figure S3.** Overview of chalcogenated products.

# 4. Optimization studies

The reaction was initially optimized using 4-phenoxyphenylboronic acid (**1a**) and diphenyl diselenide (**2b**) as model substrates. Our optimization primarily focused on finding a suitable photocatalyst, light sources and an appropriate solvent. A brief summary of optimization results are presented in **Tables S2** and **S3**.

**Table S2.** Optimization of the *ipso*-chalcogenation of aryl boronic acid with PhSeSePh (**2b**).



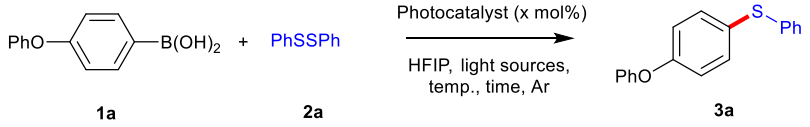

**1a** **2b** **3b**

| Entry | Photocatalyst (x mol %) | Solvent (mL) | Light Source | Temp. (°C) | Time (h) | Yield of 3 (%)[b] |
|---|---|---|---|---|---|---|
| 1 | Fluorescein (2.0) | HFIP (0.5) | White LED tape | 43 | 14 | 42 |
| 2 | *fac*-Ir(ppy)$_3$ (2.0) | HFIP (0.5) | White LED tape | 43 | 14 | 16 |
| 3 | Ir[dF(CF$_3$)ppy]$_2$(dtbpy)PF$_6$ (2.0) | HFIP (0.5) | White LED tape | 43 | 14 | 56 |
| 4 | Ru(bpy)$_3$(PF$_6$)$_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 14 | 86 |
| 5 | **Eosin Y-H$_2$ (2.0)** | **HFIP (0.5)** | **White LED tape** | 43 | **14** | **88 (84%[c])** |
| 6 | Eosin Y-H$_2$ (2.0) | MeCN (0.5) | White LED tape | 43 | 14 | 21 |
| 7 | Eosin Y-H$_2$ (2.0) | acetone (0.5) | White LED tape | 43 | 14 | 15 |
| 8 | Eosin Y-H$_2$ (2.0) | DMSO (0.5) | White LED tape | 43 | 14 | NR |
| 9 | Eosin Y-H$_2$ (2.0) | THF (0.5) | White LED tape | 43 | 14 | 14 |
| 10 | Eosin Y-H$_2$ (2.0) | MeOH (0.5) | White LED stripe | 43 | 14 | <5 |
| 11 | Eosin Y-H$_2$ (2.0) | EtOH (0.5) | White LED stripe | 43 | 14 | <5 |
| 12 | Eosin Y-H$_2$ (2.0) | *i*-PrOH (0.5) | White LED stripe | 43 | 14 | 11 |
| 13 | Eosin Y-H$_2$ (2.0) | TFE (0.5) | White LED stripe | 43 | 14 | 18 |
| 14 | Eosin Y-H$_2$ (2.0) | PFTB (0.5) | White LED stripe | 43 | 14 | 41 |
| 15[d] | Eosin Y-H$_2$ (2.0) | HFIP (0.5) | White LED tape | 31 | 14 | 29 |
| 16 | Eosin Y-H$_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 6 | 27 |
| 17 | Eosin Y-H$_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 10 | 53 |
| 18[e] | Eosin Y-H$_2$ (2.0) | HFIP (0.5) | Green LED Kessil lamp (525 nm) | 43 | 14 | 80 |
| 19[f] | Eosin Y-H$_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 14 | 61 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 20 | No photocatalyst | HFIP (0.5) | White LED tape | 43 | 14 | 12 |
| 21 | Eosin Y-$H_2$ (2.0) | HFIP (0.5) | dark | 43 | 14 | NR |
| 22 | No photocatalyst | HFIP (0.5) | dark | 43 | 14 | NR |
| 23 | No photocatalyst | HFIP (0.5) | dark | 60 | 14 | NR |

[a] Standard conditions: **1a** (0.2 mmol), **2b** (0.24 mmol), photocatalyst (2 mol%), solvent (0.4 M) were used under argon atmosphere with visible light irradiation using white light LED tape (4 W per 1 meter) mounted inside of a borosilicate glass crystallizer (temperature inside a vial was measured to be in the range of 41-43 °C). [b] Yield was determined by $^1$H NMR analysis using 1,3,5-trimethoxybenzene as the internal standard. [c] Isolated yield. [d] A fan was used (mounted ~10 cm above the reaction vial) to cool down the reactor (temperature inside a vial was measured to be ~31 ºC). [e] Reaction setup covered with aluminium foil to maintain the temperature of the reaction mixture. [f] Under air. TFE = trifluoroethanol. PFTB = Perfluoro-*tert*-butanol. NR = no reaction.

**Table S3.** Optimization of the *ipso*-chalcogenation of aryl boronic acid with PhSSPh (**2a**).




**1a** **2a** **3a**

| **Entry** | **Photocatalyst (x mol %)** | **Solvent (mL)** | **Light Source** | **Temp. (ºC)** | **Time (h)** | **Yield of 3 (%)[b]** |
|---|---|---|---|---|---|---|
| 1 | $Ru(bpy)_3(PF_6)_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 24 | 61 |
| 2 | Eosin Y-$Na_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 24 | 67 |
| 3 | Eosin Y-$H_2$ (2.0) | HFIP (0.5) | White LED tape | 43 | 24 | 69 (66%[c]) |
| 4[d] | Eosin Y-$H_2$ (2.0) | HFIP (0.5) | Green LED Kessil lamp (525 nm) | 43 | 24 | 63 |
| 5 | **Eosin Y-$H_2$ (3.0)** | **HFIP (0.5)** | **White LED tape** | **43** | **24** | **72 (69%[c])** |
| 6 | Eosin Y-$H_2$ (5.0) | HFIP (0.5) | White LED tape | 43 | 24 | 65 |

[a] Standard conditions: **1a** (0.2 mmol), **2a** (0.24 mmol), photocatalyst (2 mol%), solvent (0.4 M) were used under under argon atmosphere with visible light irradiation using white light LED tape (4 W per 1 meter) mounted inside of a borosilicate glass crystallizer (temperature inside a vial was measured to be in the range of 41-43 °C). [b] Yield was determined by $^1$H NMR analysis using 1,3,5-trimethoxybenzene as the internal standard. [c] Isolated yield. [d] Reaction setup covered with aluminium foil to maintain the temperature of the reaction mixture.

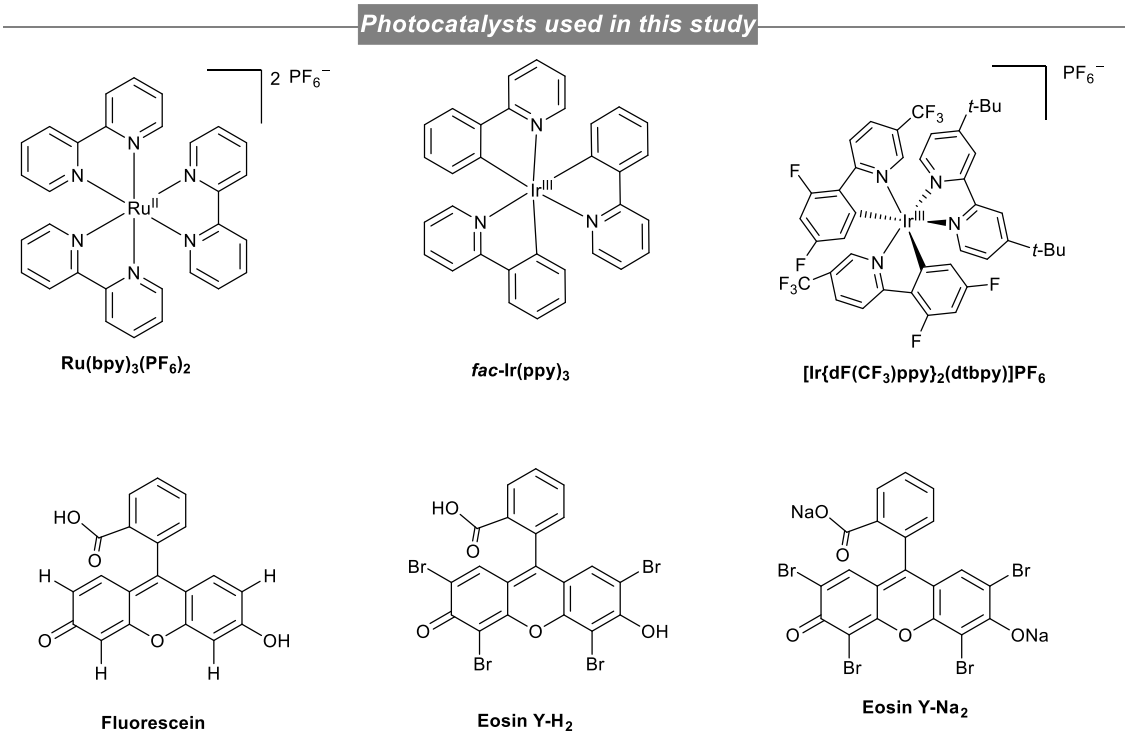
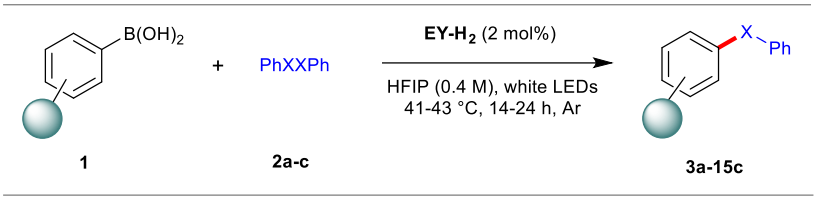



**Figure S4.** Photocatalysts used in this study.

# 5. Experimental section

## 5.1 General experimental procedure




An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with eosin Y (**EY-$H_2$**) (2.59 mg, 0.004 mmol) and 0.5 mL of HFIP. Then aryl boronic acids (0.20 mmol, 1) and diphenyl dichalcogenide (0.24 mmol) was added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by bubbling with argon for 3 minutes with an outlet needle. The reaction vial was placed under white light irradiation in the photoreactor and illuminated with stirring (850 rpm) at 41-43 °C for 14 h or 24 h. The reaction mixture was then allowed to cool to ambient temperature, diluted with 2-3 mL of DCM. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel to give the corresponding chalcogenated product.

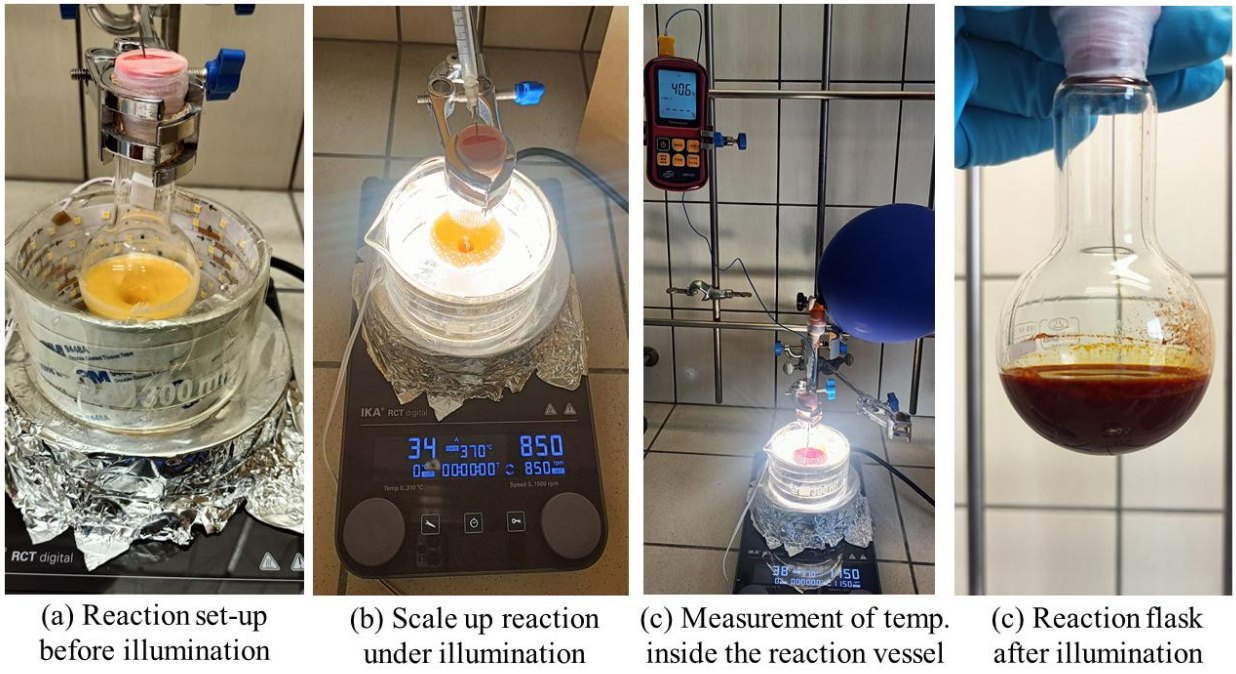
***Note 1:*** The reaction vial carefully should be sealed with precision seal rubber septa and properly parafilmed to avoid the solvent evaporation.

***Note 2:*** The temperature of the reaction vessel was measured using direct contact digital thermometer where a sensor was placed inside the reaction vial.

***Note 3:*** For all reactions with PhSSPh (**2a**), 3 mol% of **EY-$H_2$** were used.

## 5.2 Scale-up reaction

### 5.2.1 Experimental set-up

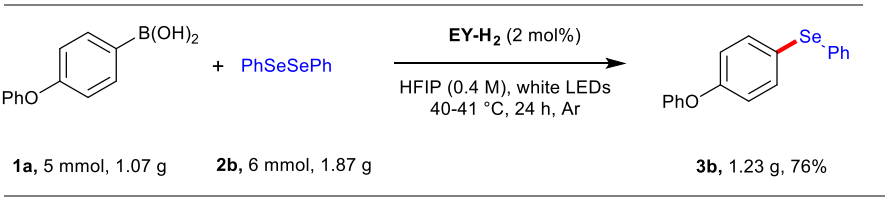


(a) Reaction set-up before illumination | (b) Scale up reaction under illumination | (c) Measurement of temp. inside the reaction vessel | (c) Reaction flask after illumination

**Figure S5.** Experimental set-up for scale-up reaction.

The scale up reaction was performed under illumination in the photoreactor with vigorous stirring (1150 rpm) for 24 h. Using a contact thermometer, the temperature inside the reaction vessel was measured to be between 40-41 ºC (Figure S5).

### 5.2.2 General procedure for the scale up reaction

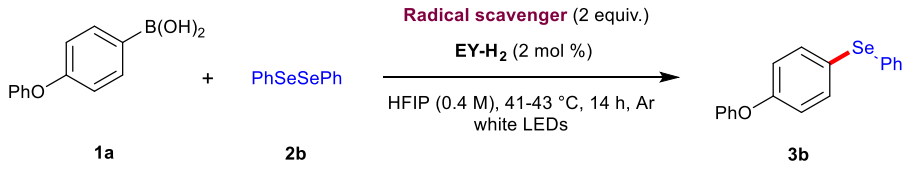



An oven-dried 50 mL round bottom flask with a magnetic stirring bar was charged with eosin Y-$H_2$ (64.78 mg, 0.1 mmol) and 12.5 mL of HFIP. Then 4-phenoxyphenylboronic acid (1.07 g, 5.0

mmol) and diphenyl diselenide (1.87 g, 6.0 mmol) were added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by bubbling with argon for 5 minutes with an outlet needle. The reaction vial was placed under white light irradiation in the photoreactor and illuminated with vigorous stirring at 40-41 °C for 24 h. The reaction mixture was then allowed to cool to ambient temperature, diluted with 10 mL of DCM. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel using 0-1% ethyl acetate in hexane to afford **3b** in 76% yield (1.23 g).

# 6. Mechanistic Investigations

## 6.1 Inhibition by radical trapping reagents

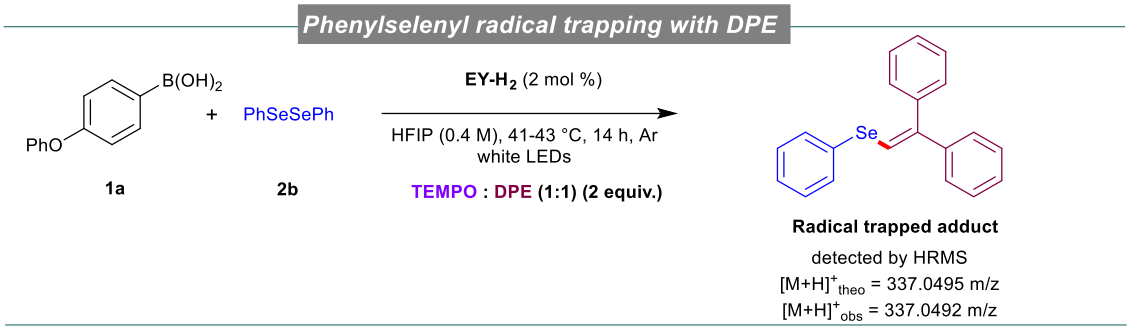



**1a** **2b** **3b**

| Radical scavenger | Yield of 3b / % |
|---|---|
| TEMPO | n.d. |
| BHT | n.d. |
| DPE | n.d. |

**Procedure:** An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with eosin Y-$H_2$ (2.59 mg, 0.004 mmol), 4-phenoxyphenylboronic acid (42.8 mg, 0.20 mmol) and diphenyl diselenide (75 mg, 0.24 mmol) followed by 0.5 mL of HFIP. Then, 2,2,6,6-tetramethyl-1-piperidine-1-oxyl (TEMPO) (62.5 mg, 0.4 mmol, 2.0 equiv) or 3,5-di-tertbutyl-4-hydroxytolune (BHT) (88.14 mg, 0.4 mmol, 2.0 equiv) or 1,1-diphenylethylene (DPE) (72.1 mg, 0.4 mmol, 2.0 equiv) were added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by sparging with argon for 3 minutes with an outlet needle. The reaction vial was placed under white light irradiation in the photoreactor and illuminated with vigorous stirring (850 rpm) at 41-43 °C for 14 h. The corresponding chalcogenated product **3b** was not detected (n.d.) based on thin layer chromatography (TLC) and $^1$H NMR analysis.

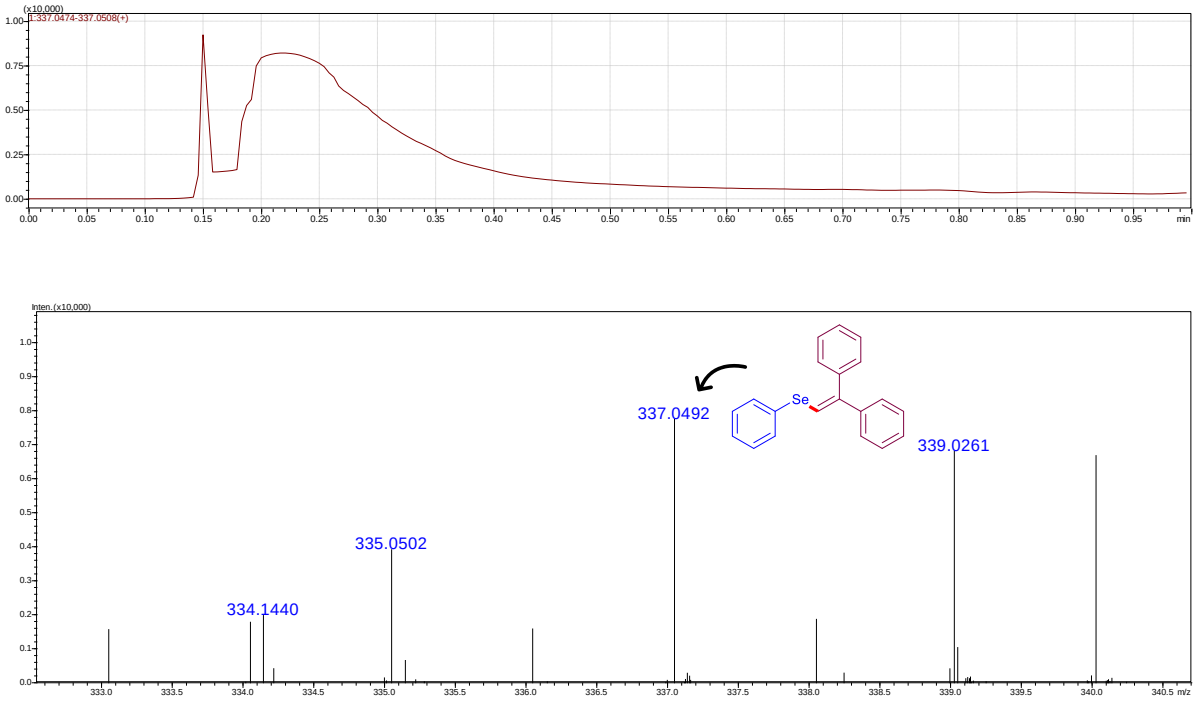
## 6.2 Radical-trapping experiment



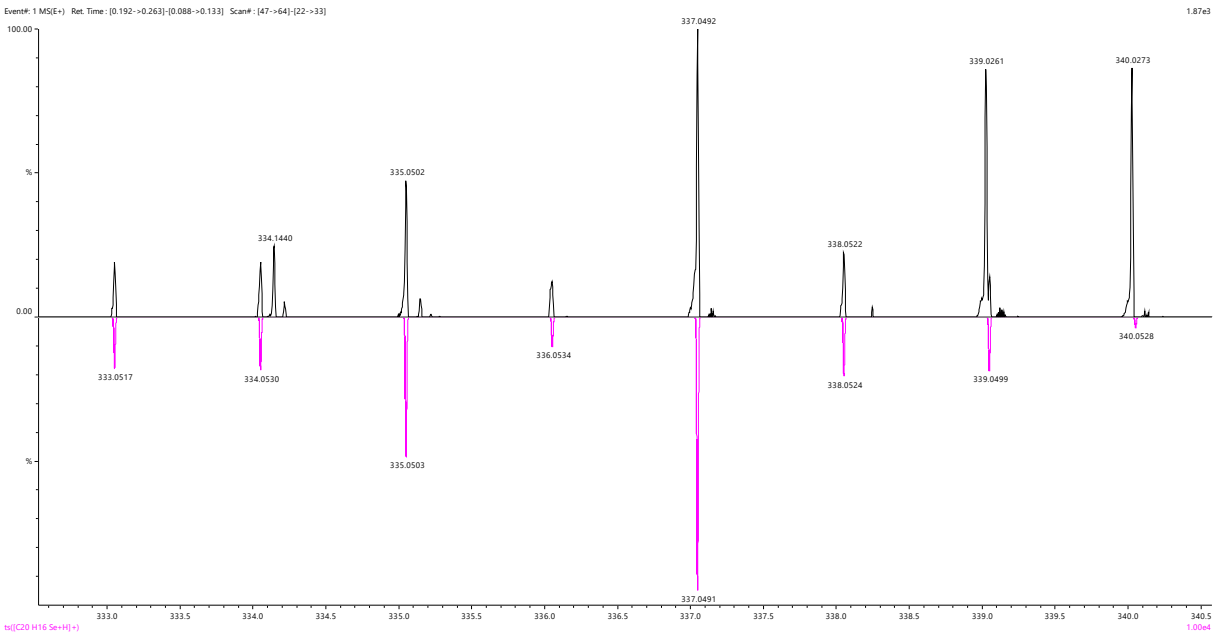

**Procedure:** An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with eosin Y-$H_2$ (2.59 mg, 0.004 mmol), 4-phenoxyphenylboronic acid (42.8 mg, 0.20 mmol), diphenyl diselenide (75 mg, 0.24 mmol) and 2,2,6,6-tetramethyl-1-piperidine-1-oxyl (TEMPO) (62.5 mg, 0.4 mmol, 2.0 equiv) and the resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degaased with argon. Then 1,1-diphenylethylene (DPE) (72.1 mg, 0.4 mmol, 2.0 equiv) was added followed by 0.5 mL of HFIP and again degassed by bubbling with argon for 2 minutes with an outlet needle. The reaction vial was placed under white LED (5 meter 20 W tapes mounted inside of a borosilicate glass crystallizer, base covered with aluminium foil) and irradiated (~2 cm away from the LED tapes) with vigorous stirring (850 rpm) at 41-43 °C for 14 h. The reaction mixture was then allowed to cool to ambient temperature, diluted with 2 mL of DCM. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to HRMS analysis. The corresponding adduct of phenylselenyl radical trapping, (2,2-diphenylvinyl)(phenyl)selane was confirmed by HR-MS (positive mode ESI) $[M+H]^+$ calcd 337.0495, found 337.0492 (**Figure S6**).

**HR-MS analysis:**

**XIC 337.0491 *m/z* ± 5 ppm**




## Isotopic Distribution 337.0492 *m/z*




## Formula predictor 337.0492 *m/z*

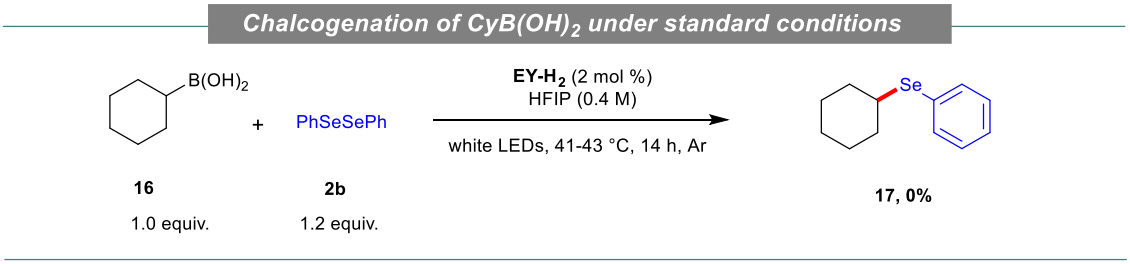
| # | Score | Pred. (M) | Pred. m/z | Meas. m/z | Diff. (mDa) | Formula (M) | Ion | Diff. (ppm) | Iso Score | DBE |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 76.83 | 336.04172 | 337.04900 | 337.04917 | 0.17 | C20 H16 Se | [M+H]+ | 0.508 | 74.25 | 13.0 |

**Figure S6.** HR-MS analysis of radical-trapping experiment with 1,1-diphenylethylene (DPE).

## 6.3 Control experiments

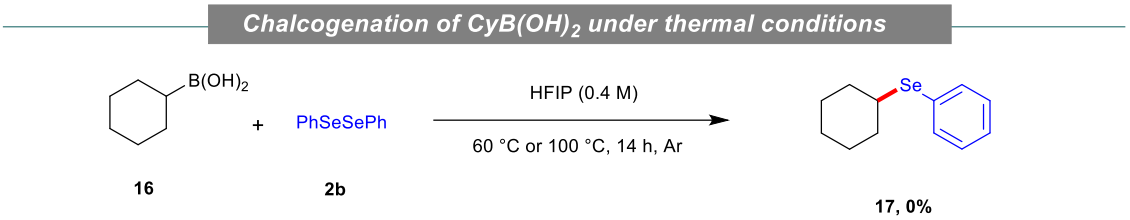
### 6.3.1 Chalcogenation of cyclohexylboronic acid

To get more information about the mechanism of this protocol, some control experiments were carried out. First, we check the efficiency of the transformation with cyclohexylboronic acid under standard conditions. To our surprise, the reaction with cyclohexylboronic acid under either standard or thermal (60 °C/100 °C) conditions did not provide the desired product and gave evidence that an *ipso*-attack requires the presence of a π-system in the boronic acid.




**Comment:** Unlike alkyl boronic acids, their aryl counterparts are amenable to accept PhSe$^{\bullet}$ through reorganization of a π-system to form an intermediate where electrons are partially delocalized (structure **IV** in Scheme 3D). Such an intermediate then can undergo an elimination process through a carbon-boron bond cleavage along with aromatic system restoration that is possibly the main thermodynamic driving force.

**Procedure:** An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with eosin Y-$H_2$ (2.59 mg, 0.004 mmol) and 0.5 mL of HFIP. Then cyclohexylboronic acid (25.6 mg, 0.20 mmol) and diphenyl diselenide (75 mg, 0.24 mmol) were added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by sparging with argon for 3 minutes with an outlet needle. The reaction vial placed under white light irradiation in the photoreactor and illuminated with vigorous stirring (850 rpm) at 41-43 °C for 14 h. The corresponding chalcogenated product **17** was not observed based on thin layer chromatography (TLC) and $^1$H NMR analysis.

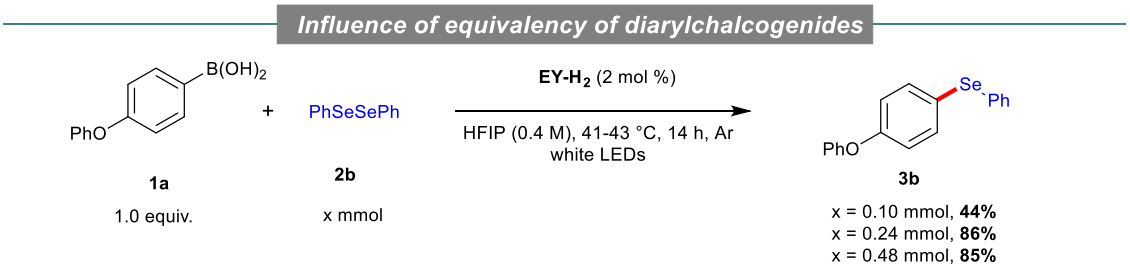



**Procedure:** An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with eosin Y-$H_2$ (2.59 mg, 0.004 mmol) and 0.5 mL of HFIP. Then cyclohexylboronic acid (25.6 mg, 0.20 mmol) and diphenyl diselenide (75 mg, 0.24 mmol) were added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by sparging with argon for 3 minutes with an outlet needle. The reaction vial was placed under an oil-bath with vigorous stirring (850 rpm) at 60 °C for 14 h. The corresponding chalcogenated product **17** was not observed based on thin layer chromatography (TLC) and $^1$H NMR analysis.

***Note***: The above reaction also performed at 100 °C for 14 h and the corresponding chalcogenated product **17** was not observed based on thin layer chromatography (TLC) and $^1$H NMR analysis.

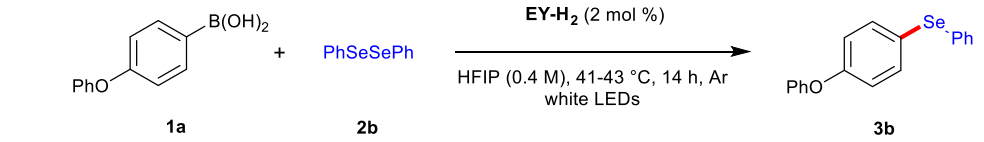
6.3.2 Influence of the amount of diphenyl diselenide

To gain a deeper insight into possible reaction course, we investigate the influence of the amount of the diphenyl dichalcogenides on the reaction efficiency. The optimal amount was found to be 0.24 mmol versus 0.20 mmol of aryl boronic acid. Moreover, larger excess of diphenyl diselenides (0.48 mmol) gave almost same yield of corresponding chalcogenated product **3b**. Finally, applying 0.1 mmol of diphenyl diselenide (i.e., 0.20 mmol of phenylselenyl radical) afforded the corresponding product **3b** in only 44% yield. This study suggested that every second equivalent of phenylselenyl radical (PhSe$^{\bullet}$) is essential for trapping a B(OH)$_2$-based leaving group.



## 6.4 Chalcogenation of aryl boronic acids: an NMR study

We performed a NMR study to capture the chemical transformation of aryl boronic acid and diphenyl diselenide to chalcogenated product with time under optimized reaction conditions.




**Procedure:** An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with eosin Y-$H_2$ (2.59 mg, 0.004 mmol) and 0.5 mL of HFIP. Then 4-phenoxyphenylboronic acid (42.8 mg, 0.20 mmol) and diphenyl diselenide (75 mg, 0.24 mmol) were added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by sparging with argon for 3 minutes with an outlet needle. The reaction vial placed under white light irradiation in the photoreactor and illuminated with vigorous stirring (850 rpm) at 41-43 °C for 14 h. After 2 h, 0.1 ml reaction aliquot was taken out by a syringe and concentrated by rotary evaporation followed by high vacuum and crude mixture subjected to $^1$HNMR analysis. The same procedure was followed to analyse the reaction mixture after 14 h (Figure S7).

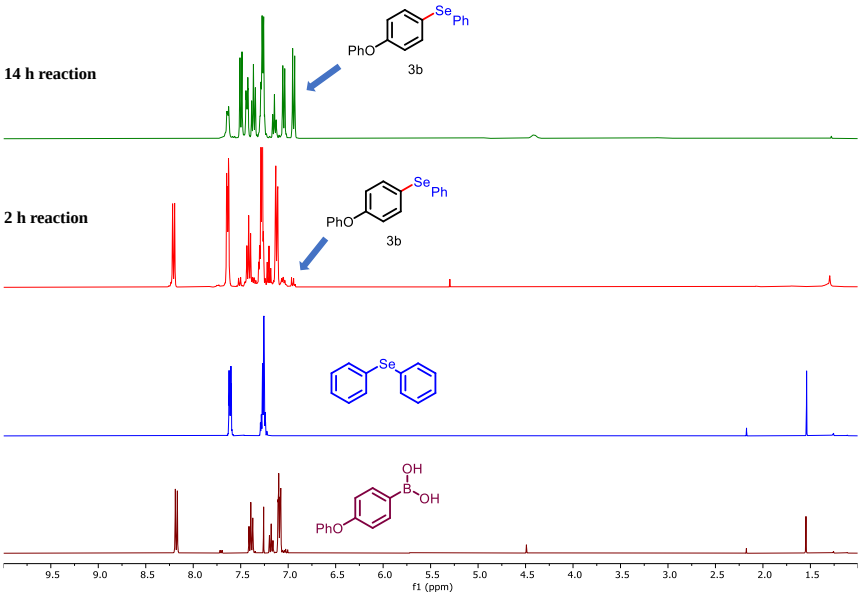
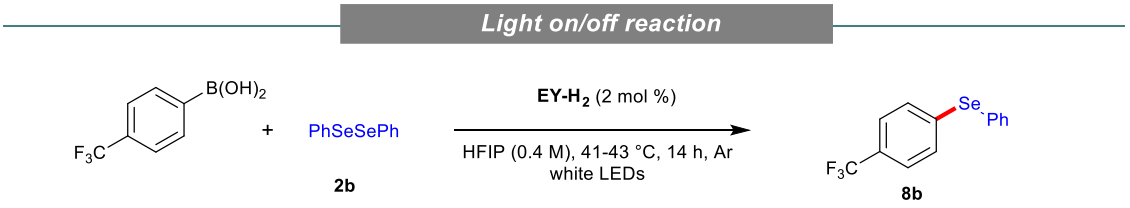



**Figure S7.** NMR study of the *ipso*-chalcogenation.

## 6.5 Light on/off experiment




**Procedure:** An oven-dried 3 mL reaction vial with a magnetic stirring bar was charged with **EY-$H_2$** (3.23 mg, 0.005 mmol) and 0.6 mL of HFIP. Then 4-(trifluoromethyl)phenylboronic acid (47.5 mg, 0.25 mmol) and diphenyl diselenide (93.6 mg, 0.30 mmol) were added. The resulting mixture was carefully sealed with precision seal rubber septa, parafilmed and degassed by bubbling with argon for 3 minutes with an outlet needle. The reaction vial placed under white light irradiation in the photoreactor and illuminated with vigorous stirring (850 rpm) at 41-43 °C where the reaction was placed in light and dark in every alternative 1 hour. After every time interval of 1 hour, a 0.1 mL reaction aliquot was taken out by a syringe and diluted with 0.5 mL of DCM and concentrated by rotary evaporation followed by high vacuum. The crude mixtures subjected to NMR analysis and the yield was determined by $^{19}$F-NMR spectroscopy using 1-fluoronaphthalene (0.10 mmol, 12.9 µL) as the internal standard (Figure S8 and Table S4).

**Table S4.** $^{19}$F NMR yields of 8b obtained during light on/off experiment.

| Entry | Time (h) | Irradiation | NMR Yield (%) |
|---|---|---|---|
| 1 | 1 | ON | 15 |
| 2 | 2 | OFF | 15 |
| 3 | 3 | ON | 18 |
| 4 | 4 | OFF | 18 |
| 5 | 5 | ON | 21 |
| 6 | 6 | OFF | 21 |

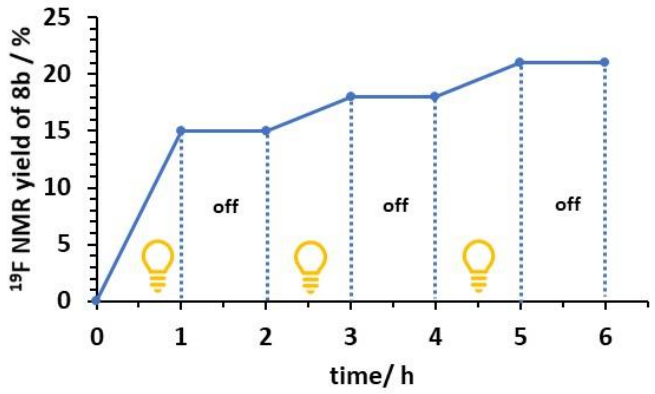



**Figure S8.** Light on/off experiment.

## 6.6 Luminescence quenching studies

**General:** Fluorescence measurements were carried out on an Edinburgh FS5 spectrometer equipped with a 450 W xenon arc lamp, double excitation and single emission monochromators (dwell time = 0.2 s; excitation bandwidth = 3 nm; excitation bandwidth = 3 nm). The excitation wavelength was fixed at 450 nm for all the experiments.

**Procedure:** A 5 mM solution of the quencher substrate in degassed HFIP was prepared and 50 μL of this stock solution was added to the solution (2.5 mL) of **EY-H$_2$** (1 μM degassed HFIP). The addition of the quencher was repeated six times (100 μL). After each addition, the solution was mixed, and the emission spectra of the excited catalyst was acquired from 500 nm to 700 nm (the excitation wavelength was fixed at 450 nm). The results shown in Figure S13 indicate that PhSeSePh quenched the excited-state emission of **EY-H$_2$** more effectively than PhB(OH)$_2$. The Stern-Volmer plot shows a linear correlation between the amounts of substrates and the ratio $I_0/I$, following the relationship: $I_0/I = 1 + K_{SV}[Q]$ (Q = Quencher) (Figure S21).

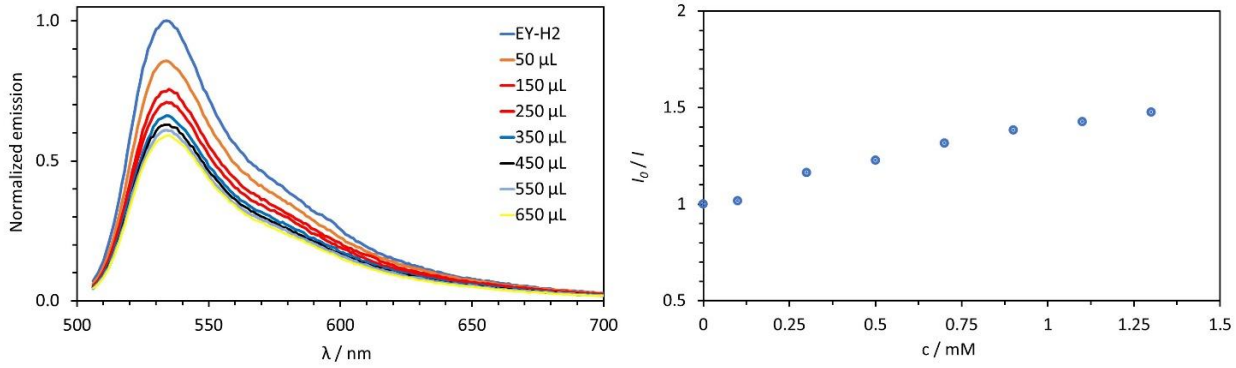



**Figure S9.** Stern-Volmer quenching studies of the excited **EY-H$_2$*** (1 µM) with PhB(OH)$_2$.

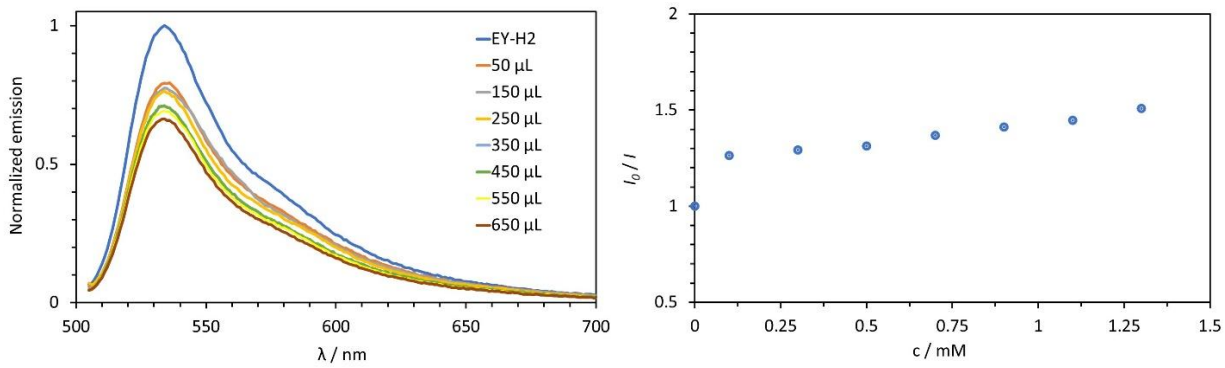



**Figure S10.** Stern-Volmer quenching studies of the excited **EY-H$_2$*** (1 µM) with PhSSPh (**2a**).

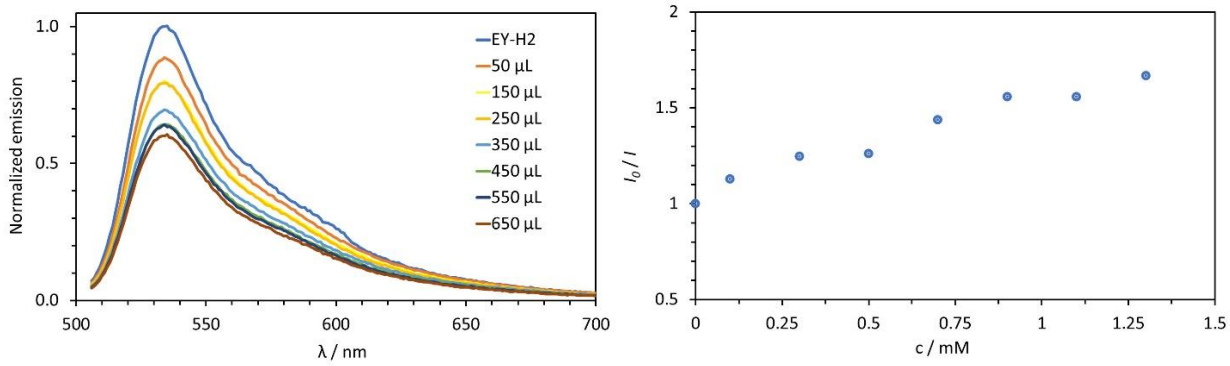



**Figure S11.** Stern-Volmer quenching studies of the excited **EY-H$_2$*** (1 µM) with PhSeSePh (**2b**).

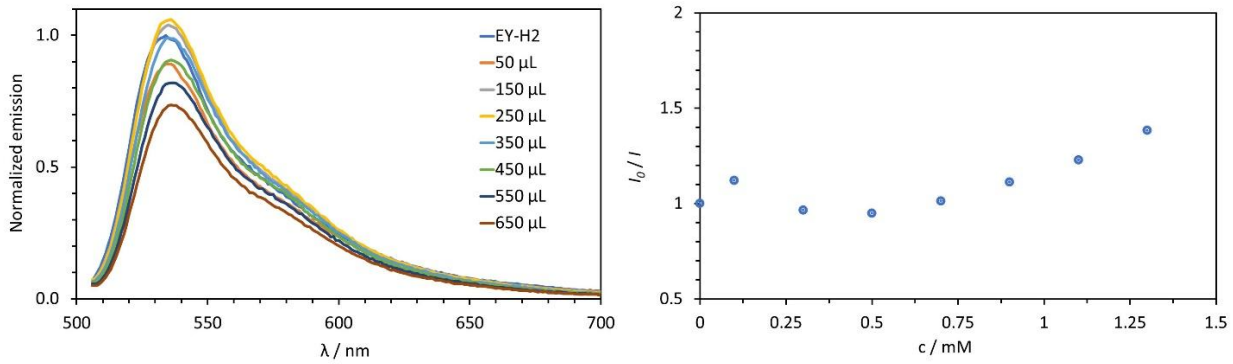



**Figure S12.** Stern-Volmer quenching studies of the excited **EY-H$_2$*** (1 µM) with PhTeTePh (**2c**).

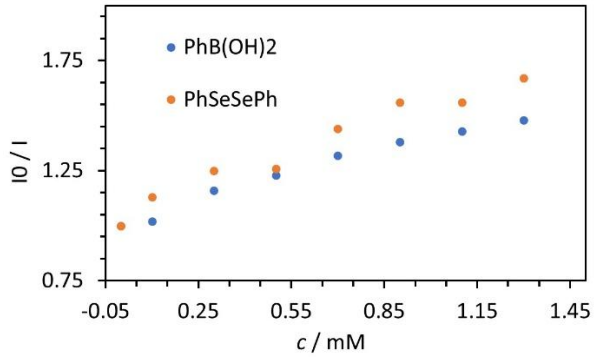
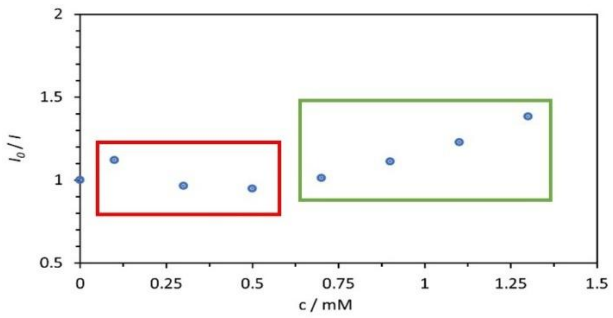
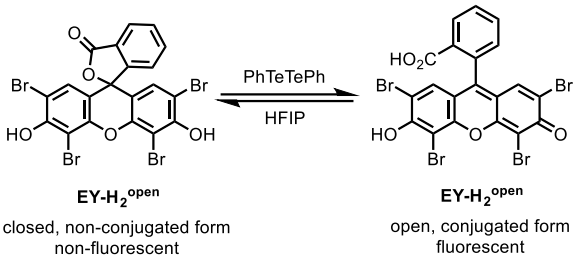



**Figure S13.** Comparison of quenching dynamics for PhB(OH)$_2$ and PhSeSePh (**2b**) at 4 mM concentrations.

**Comment to Figure S12:** In general, solutions of Eosin Y consist of a closed (**EY-H$_2$$^{closed}$**) and an open form (**EY-H$_2$$^{open}$**) (please, see Figure below), which remain in an equilibrium. It seems that initially, when a solution of PhTeTePh (quencher) is added to the solution of **EY-H$_2$**, counterintuitively the fluorescence response increases (a negative slope, a red rectangle in Figure below). It suggests that intermolecular interactions between PhTeTePh and **EY-H$_2$$^{closed}$** cause the shift of the equilibrium toward the open form (an increase in the emission intensity) and this effect prevails the quenching phenomenon at this stage. When adding 350-650 uL of the PhTeTePh solution, the quenching process starts to prevail over the other thus one can notice a positive slope (a green rectangle in Figure below). To sum up, the overall quenching effect in this case cannot be directly compared with that noted for PhB(OH)$_2$, where the quenching is rather balanced in the full range of **EY-H$_2$**/quencher ratios.

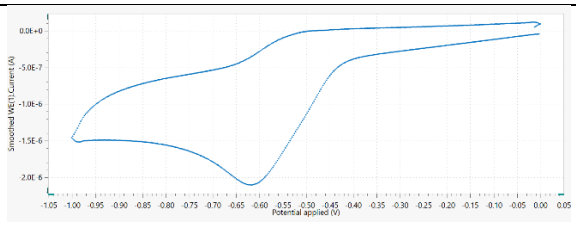
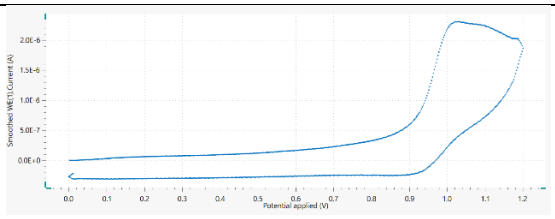


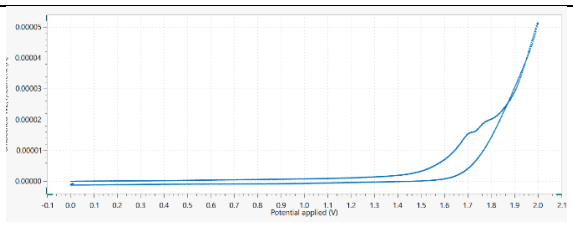
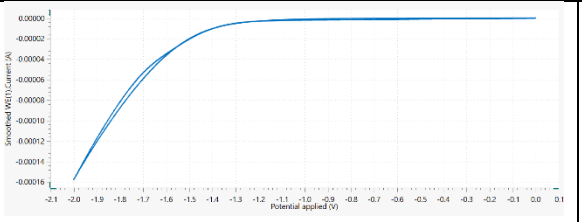
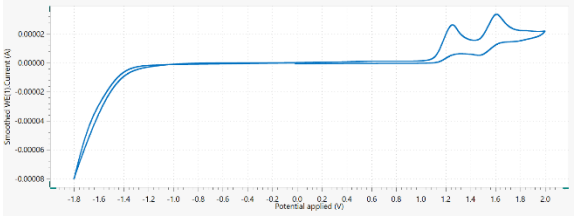
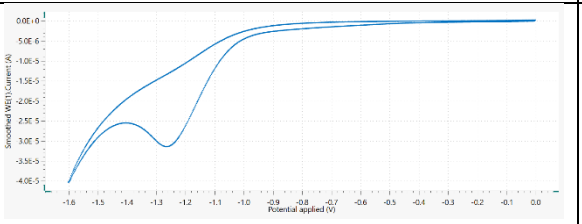
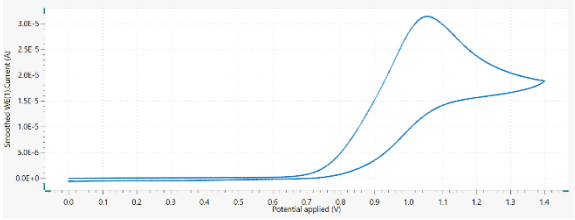
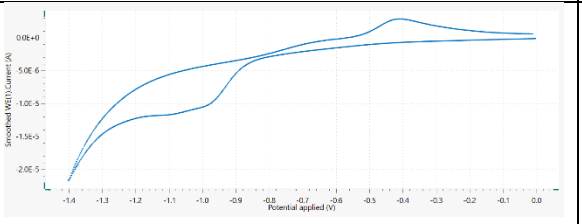
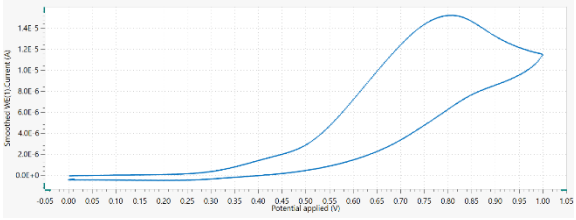
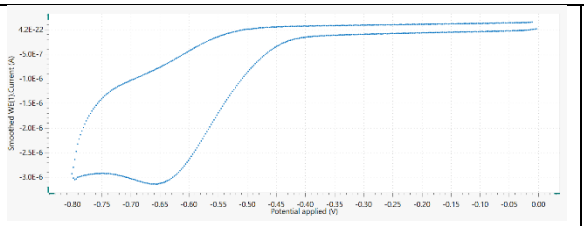
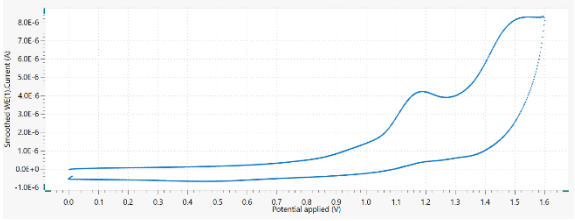
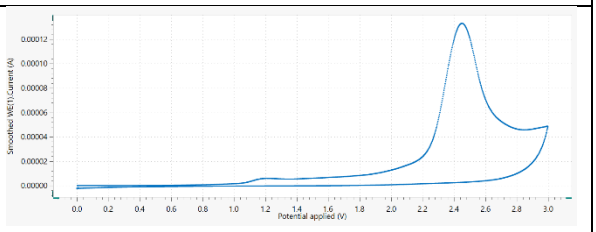




## 6.7 Cyclic voltammetry (CV) studies

**General:** Cyclic voltammetry measurements were conducted with a Metrohm Autolab PGSTAT204 potentiostat and Nova 2.1 software. For all experiments, a glassy carbon working electrode (disk, diameter: 3 mm), a platinum wire counter electrode and a Ag/AgCl/$KCl_{sat}$ reference electrode were used. *n*-$Bu_4NPF_6$ (100 mM) as conducting salt served as electrolyte for the measurements. The voltammograms were recorded under inert atmosphere in acetonitrile (MeCN) or 1,1,1,3,3,3-hexafluoroisopropan-2-ol (HFIP) at a scan rate of 100 mV/s. The samples were measured with an analyte concentration of 4 mM (1 mM for **EY-H$_2$**) and degassed with nitrogen prior to measurement.

**Table S5.** CV traces of **EY-H$_2$**, $PhB(OH)_2$, PhSSPh (**2a**), PhSeSePh (**2b**) and PhTeTePh (**2c**) measured in MeCN or HFIP (potentials are given vs Ag/AgCl/$KCl_{sat}$).

| | Reduction | Oxidation |
|---|---|---|
| | HFIP | |
| **EY-H$_2$** |  |  |

| | | |
|---|---|---|
| $PhB(OH)_2$ | |  |
| PhSSPh (**2a**) |  |  |
| PhSeSePh (**2b**) |  |  |
| PhTeTePh (**2c**) |  |  |
| MeCN | | |
| **EY-$H_2$** |  |  |
| $PhB(OH)_2$ | |  |

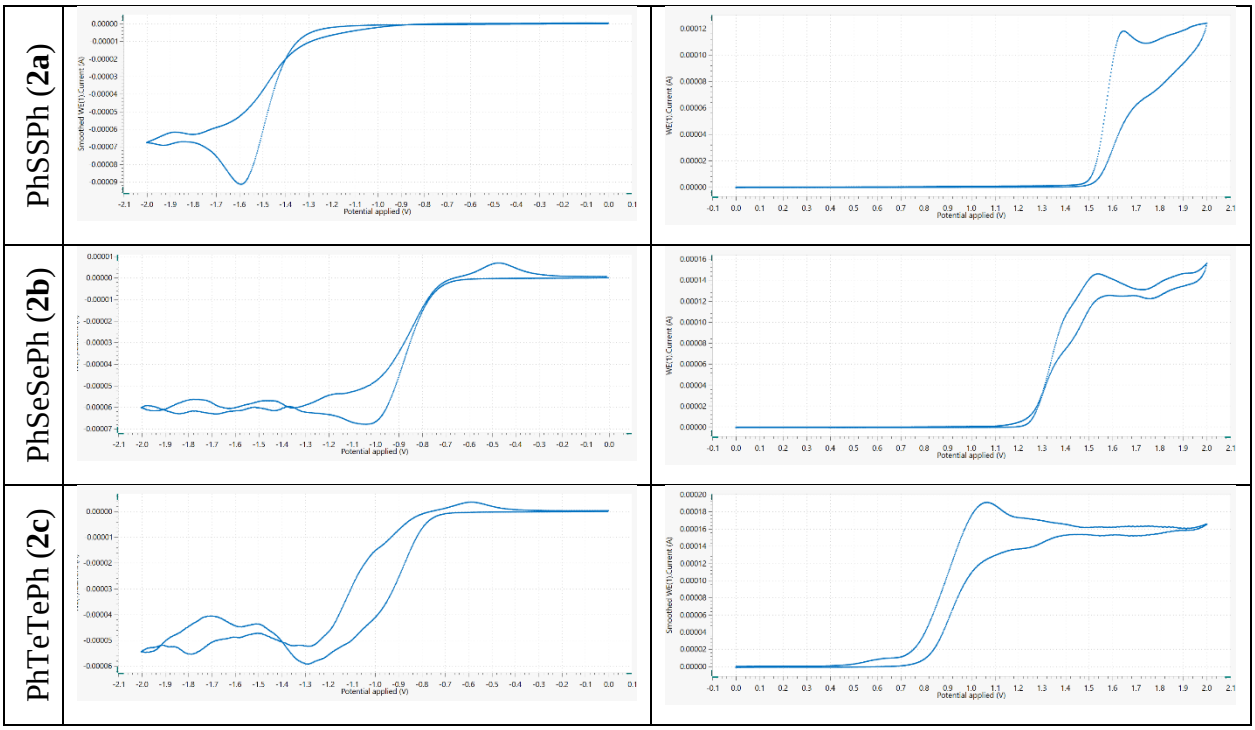



**Table S6.** Redox potentials determined from CV traces for **EY-H$_2$** (1 mM) and PhB(OH)$_2$, PhSSPh (**2a**), PhSeSePh (**2b**) and PhTeTePh (**2c**) (4 mM) in MeCN or HFIP (potentials are given vs. Fc/Fc$^+$).

| vs Fc/Fc$^+$ | **MeCN** | | **HFIP** | |
|---|---|---|---|---|
| | $E_{p,c}$ / V | $E_{p,a}$ / V | $E_{p,c}$ / V | $E_{p,a}$ / V |
| **EY-H$_2$** | -1.12 | 0.73 | -0.55 | 0.90 |
| PhB(OH)$_2$ | - | 2.00 | - | 1.66 |
| **2a** | -1.92 | 1.12 | - | 1.21 |
| **2b** | -1.31 | 0.90 | -1.18 | 0.85 |
| **2c** | -1.37 | 0.44 | -0.96 | 0.56 |

The free energy of a photoinduced electron transfer can be determined using the Gibbs energy of photoinduced electron transfer equation:

$$\Delta G_{et}\ (\text{eV}) = -\ [E_{p,c}(\text{A/A}^{\bullet-}) - E_{p,a}(\text{D/D}^{\bullet+})] - E_{PC*} + \Delta E \qquad \textbf{(1)}$$

where $E_{p,c}(A/A^{\bullet-})$ is the reduction potential of an electron acceptor ($A$), $E_{p,a}(D^{\bullet+}/D)$ is the oxidation potential of an electron donor ($D$), $E_{PC*}$ is the energy of the singlet or triplet excited state of a

photocatalyst, $\Delta E$ = < 0.1 eV, and is often neglected in photophysical estimations. For **EY-H$_2$**, the excitation energy of $^3$EY* is 1.91 eV.

**Table S7.** $\Delta G_{et}$ values calculated for a photoinduced electron transfer between **EY-H$_2$**$^*$ and the respective dichalcogenides according to the equation **(1)** based on electrochemical properties summarized in Table S5.

| $\Delta G_{et}$ (eV) | ***via* [PhSeSePh]$^{\bullet+}$** | | ***via* [PhSeSePh]$^{\bullet-}$** | |
|---|---|---|---|---|
| | **MeCN** | **HFIP** | **MeCN** | **HFIP** |
| **2a** | 0.33 | -0.15 | 0.74 | - |
| **2b** | 0.11 | -0.51 | 0.13 | 0.17 |
| **2c** | -0.35 | -0.80 | 0.19 | -0.05 |

## 7. Computational Studies

**General:** All the calculations were carried out using DFT (Density Functional Theory) with the Gaussian 09 program package. For geometry optimizations, the 6-31G(d,p) basis set was used for the C, N, O, H elements. On the basis of these optimized geometries, single-point calculations were carried out with the 6-311+G(2d,2p) basis set for SMD solvation model ($\varepsilon$ = 16.7) at 298 K, using HFIP as a solvent. To learn more about the reactant, we used the NBO tool in Gaussian 09. The stationary points were confirmed as transition states by analytical frequency calculations at the same basis set level as the geometry optimizations. The reported energies are Gibbs free energies, which include zero-point vibrational corrections, thermal corrections, and entropy corrections at 298 K. The latter are calculated as single-point corrections on the optimized structures with the same basis set combination used for the geometry optimizations. On the basis of the optimized geometries, all energies were also corrected with single-point dispersion effects using the DFT method.

A plausible mechanistic pathway is illustrated in Scheme 3D. The reaction is proposed to initiate via a single-electron transfer (SET) from diphenyl diselenide to the photoexcited eosin Y species,

**[EY–H₂]***. This step generates a radical cation intermediate (**I**), which subsequently undergoes Se–Se bond cleavage to produce a phenylselenyl radical (**II**) and a phenylselenyl cation (**III**).

The radical (**II**) then adds to the aryl boronic acid (**1a**), forming a new radical intermediate (**IV**). Meanwhile, the cation (**III**) is reduced by the eosin radical anion **[EY–H₂]•⁻**, regenerating the ground-state photocatalyst **[EY–H₂]** and producing an additional equivalent of the phenylselenyl radical (**II**), thereby closing the photoredox catalytic cycle. The newly generated radical (**II**) further reacts with intermediate (**IV**) to afford intermediate (**V**), which ultimately furnishes the desired chalcogenated product along with byproduct **VI**.

The addition of phenylselenyl (**II**) to aryl boronic acid (**1b**) to form intermediate (**IV**) requires +8.27 kcal mol⁻¹. Further reaction of intermediate (**IV**) with another phenylselenyl radical (**II**) forms intermediate (**V**) with an additional energy cost of +5.21 kcal mol⁻¹, followed by a final exergonic step (-32.84 kcal mol⁻¹) leading to the desired product.

During the addition of the phenylselenyl (**II**) to aryl boronic acid (**1b**), the transition state involves partial bond formation and redistribution of electron density around the boron center. HFIP molecules can stabilize this by hydrogen bonding to the hydroxyl groups, effectively lowering the energy of the transition state and facilitating the formation of intermediate (**IV**). A similar stabilization effect is expected in the subsequent step leading to intermediate (**V**), where the second radical addition also benefits from the HFIP-assisted hydrogen-bonding environment.

In contrast, path B proceeds via a reductive SET process, in which diphenyl diselenide forms a radical anion intermediate (**I**), while **[EY–H₂]*** is oxidized to the eosin radical cation **[EY–H₂]•⁺**. This initial step is highly unfavorable, with a free energy increase of +17.99 kcal mol⁻¹, indicating a thermodynamically uphill process (Figure S15A).

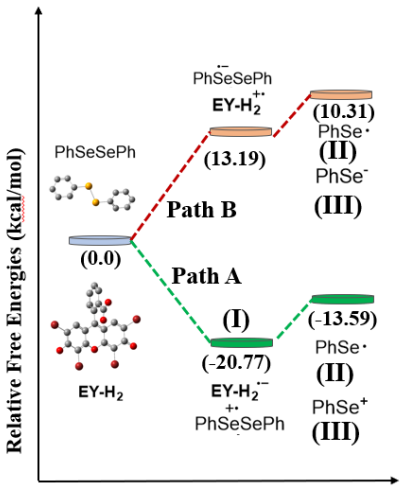
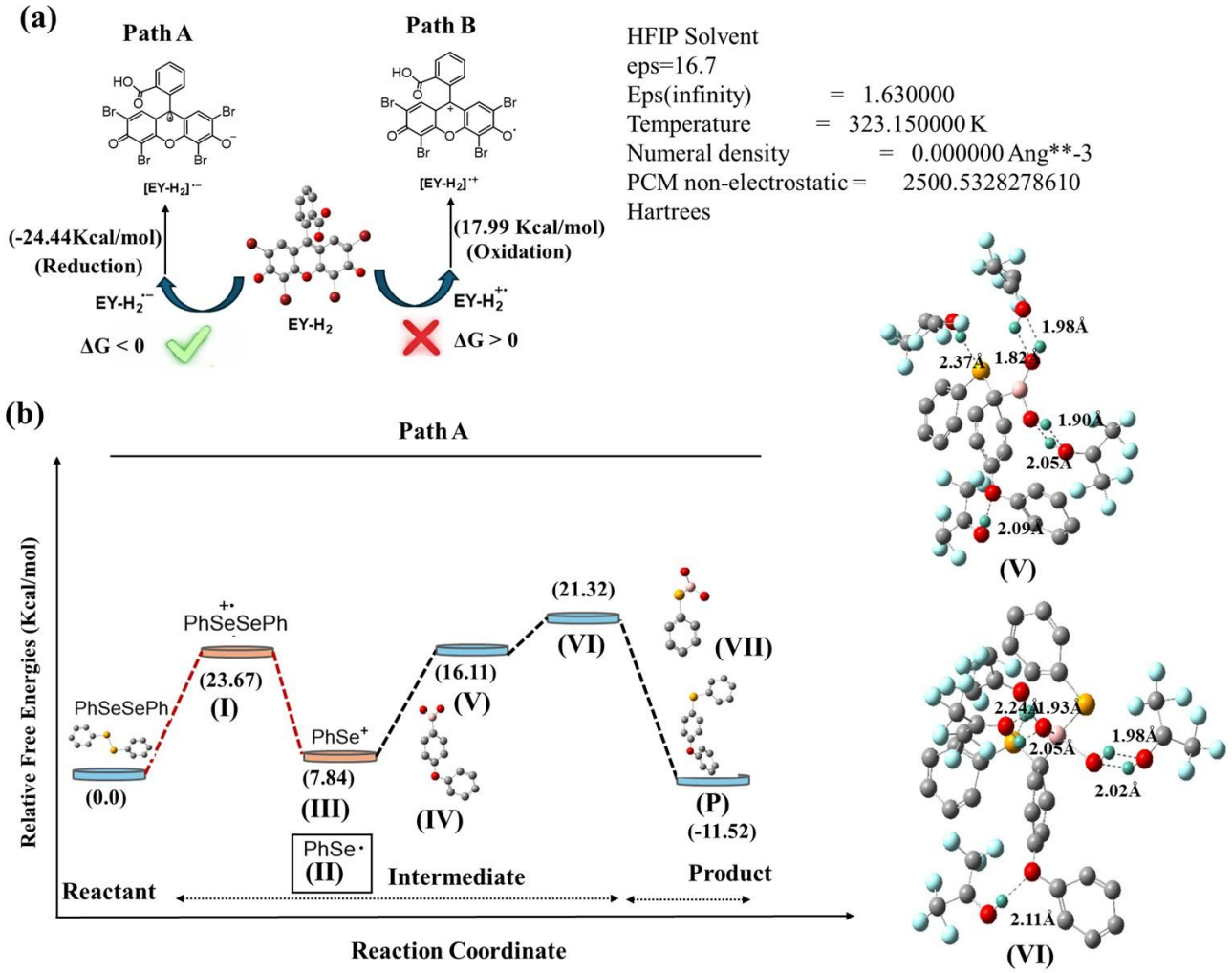



**Figure S14.** Free energy profiles (ΔG, kcal mol⁻¹) for the proposed first step of *ipso*-chalcogenation calculated at the B3LYP/LANL2DZ/6-311G(d,p) level with the SMD solvation model (ε = 16.7) at 298 K. Energies refer to the respective pairs of charged species.



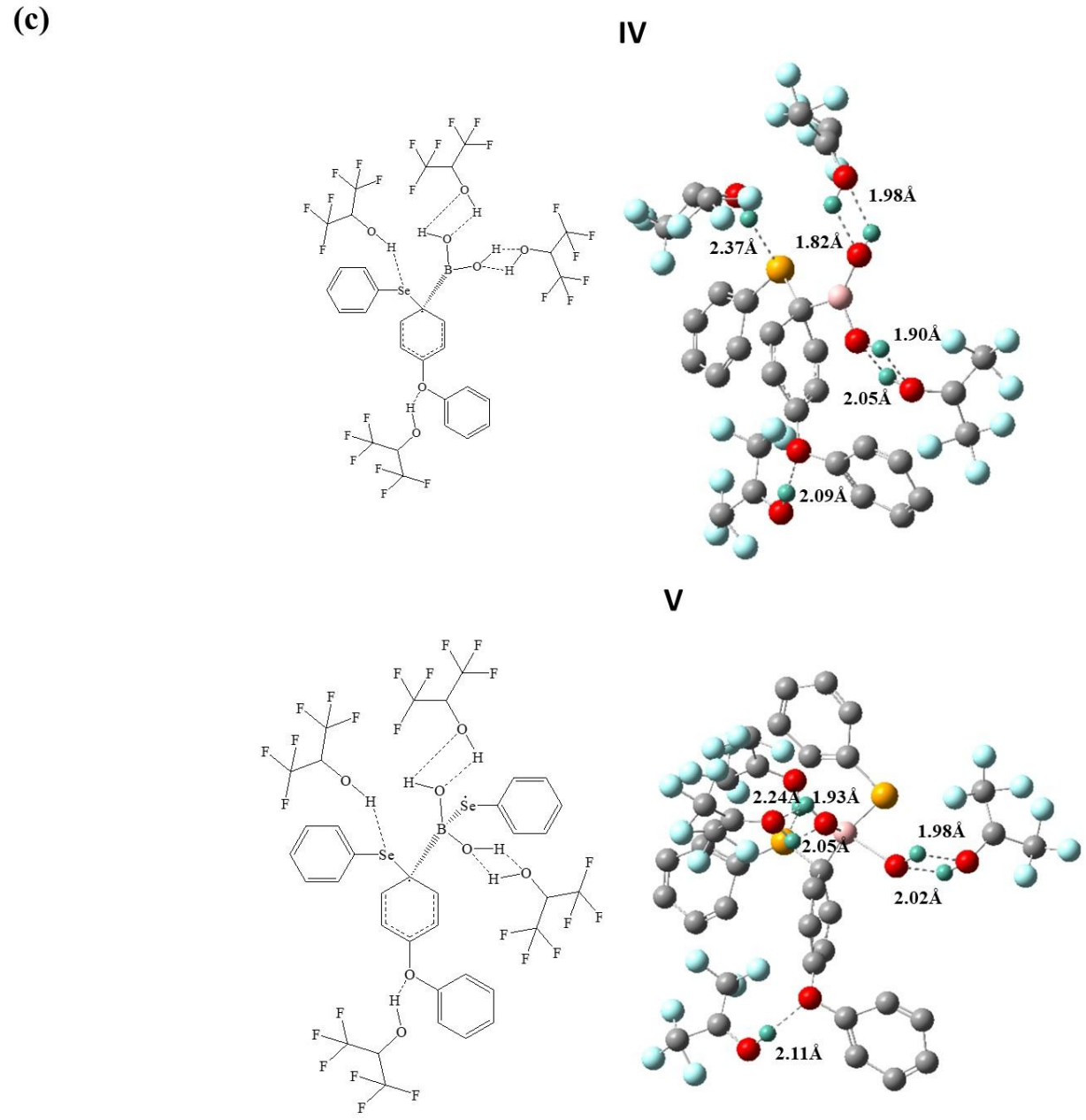



**Figure S15.** Free energy profiles (ΔG, kcal $mol^{-1}$) for the proposed first step of *ipso*-chalcogenation calculated at the B3LYP/LANL2DZ/6-311G(d,p) level with the SMD solvation model (ε = 16.7) at 298 K.

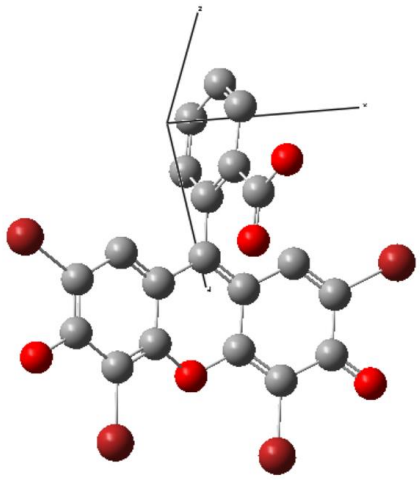
**Table S7.** The absolute energies and thermal correction to Gibbs free energy (a.u.).

| **Compound** | **Thermal correction to Gibbs free energy (353.15 K)** | **Absolute energies B3LYP/ 6-311+G(2d,2p)** |
|---|---|---|

| | | |
|---|---|---|
| EY-$H_2$ | 0.169908 | -1195.373466 |
| EY-$H_2^{\cdot+}$ | 0.169664 | -1195.334518 |
| EY-$H_2^{\cdot-}$ | 0.167860 | -1195.402134 |
| PhSeSePh | 0.137883 | -481.457481 |
| $[PhSeSePh]^{\bullet+}$ (**I**) | 0.142950 | -481.424825 |
| $[PhSeSePh]^{\bullet-}$ (**I**) | 0.133721 | -481.474456 |
| **II** | 0.056647 | -240.725575 |
| $PhSe^+$ (**III**) | 0.059157 | -240.697331 |
| $PhSe^-$ (**III**) | 0.069946 | -240.738301 |
| 4-PhO-$C_6H_4$-$B(OH)_2$ (**1a**) | 0.166826 | -714.302545 |
| **IV** | 0.588032 | -1655.280431 |
| **V** | 0.654820 | -1896.438441 |
| **VI** | 0.085904 | -417.297155 |
| Product **(3b)** | 0.216315 | -778.501688 |

**Cartesian coordinates for the optimized structures**

**EY-$H_2$**



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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.942205 | 1.584518 | -4.440545 |
| 2 | 6 | 0 | -2.052071 | 2.631238 | -5.294516 |
| 3 | 6 | 0 | -1.286351 | 3.938418 | -5.013574 |
| 4 | 6 | 0 | -0.502941 | 4.043032 | -3.911945 |
| 5 | 6 | 0 | -0.316685 | 2.827502 | -2.996287 |
| 6 | 6 | 0 | -1.017149 | 1.689160 | -3.214717 |
| 7 | 8 | 0 | 0.127089 | 5.297569 | -3.608180 |
| 8 | 6 | 0 | 1.247402 | 5.216830 | -2.701698 |
| 9 | 6 | 0 | 1.464152 | 4.012061 | -1.752542 |
| 10 | 6 | 0 | 0.682897 | 2.916298 | -1.846052 |
| 11 | 6 | 0 | 2.128275 | 6.248198 | -2.674940 |
| 12 | 6 | 0 | 3.279986 | 6.262177 | -1.652944 |
| 13 | 6 | 0 | 3.438675 | 5.102610 | -0.654452 |
| 14 | 6 | 0 | 2.589604 | 4.049397 | -0.701963 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 35 | 0 | -2.929286 | -0.019071 | -4.760346 |
| 16 | 8 | 0 | -2.881657 | 2.523728 | -6.454313 |
| 17 | 35 | 0 | -1.449652 | 5.416425 | -6.212293 |
| 18 | 35 | 0 | 1.932208 | 7.696630 | -3.904452 |
| 19 | 8 | 0 | 4.090128 | 7.224885 | -1.632096 |
| 20 | 35 | 0 | 4.835840 | 5.146244 | 0.647134 |
| 21 | 8 | 0 | 3.571907 | -0.235112 | -2.506983 |
| 22 | 6 | 0 | 0.815782 | 1.767053 | -0.829599 |
| 23 | 6 | 0 | 2.590753 | 0.785394 | -2.304981 |
| 24 | 6 | 0 | 1.746213 | 0.797501 | -1.017267 |
| 25 | 6 | 0 | 1.961125 | -0.291862 | 0.049928 |
| 26 | 6 | 0 | 1.241191 | -0.268778 | 1.196015 |
| 27 | 6 | 0 | 0.221099 | 0.857142 | 1.437537 |
| 28 | 6 | 0 | 0.033990 | 1.815711 | 0.498108 |
| 29 | 8 | 0 | 2.417448 | 1.673546 | -3.179465 |
| 30 | 1 | 0 | -0.923121 | 0.863221 | -2.541008 |
| 31 | 1 | 0 | 2.704206 | 3.239138 | -0.012581 |
| 32 | 1 | 0 | -2.903290 | 1.610240 | -6.748714 |
| 33 | 1 | 0 | 3.666074 | -0.406957 | -3.446771 |
| 34 | 1 | 0 | 2.680606 | -1.066673 | -0.114133 |
| 35 | 1 | 0 | 1.382946 | -1.030944 | 1.933517 |
| 36 | 1 | 0 | -0.340117 | 0.884011 | 2.348148 |
| 37 | 1 | 0 | -0.660526 | 2.609488 | 0.678292 |

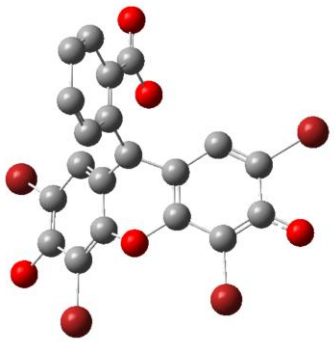
---

Rotational constants (GHZ): 0.1016672 0.0653756 0.0426956

Standard basis: LANL2DZ (5D, 7F)

There are 273 symmetry adapted cartesian basis functions of A symmetry.

**EY-$H_2^{\bullet-}$**



Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06 EigMax=2.50D+02
EigMin=1.00D-04

Number of steps in this run= 209 maximum allowed number of steps= 222.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.011393 | -0.360612 | -1.045556 |
| 2 | 6 | 0 | -3.313805 | -1.544598 | -0.432021 |
| 3 | 6 | 0 | -2.268408 | -2.254336 | 0.464585 |
| 4 | 6 | 0 | -1.054363 | -1.682986 | 0.632144 |
| 5 | 6 | 0 | -0.787198 | -0.315124 | 0.035046 |
| 6 | 6 | 0 | -1.642250 | 0.305639 | -0.797726 |
| 7 | 8 | 0 | 0.060658 | -2.332585 | 1.348066 |
| 8 | 6 | 0 | 1.353323 | -2.067102 | 0.665907 |
| 9 | 6 | 0 | 1.593872 | -0.841938 | 0.130746 |
| 10 | 6 | 0 | 2.424376 | -3.160816 | 0.517901 |
| 11 | 6 | 0 | 3.536623 | -2.915121 | -0.229443 |
| 12 | 6 | 0 | 3.724994 | -1.548839 | -0.934955 |
| 13 | 6 | 0 | 2.805130 | -0.565392 | -0.766504 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 35 | 0 | -4.284130 | 0.469920 | -2.202473 |
| 15 | 8 | 0 | -4.602199 | -2.134700 | -0.623651 |
| 16 | 35 | 0 | -2.682833 | -3.917294 | 1.307748 |
| 17 | 35 | 0 | 2.189951 | -4.857075 | 1.363980 |
| 18 | 8 | 0 | 4.445568 | -3.837673 | -0.356324 |
| 19 | 35 | 0 | 5.255767 | -1.245956 | -2.036361 |
| 20 | 8 | 0 | 0.159200 | -1.200209 | 2.591254 |
| 21 | 6 | 0 | 0.779098 | 1.398368 | 1.379864 |
| 22 | 6 | 0 | 0.380515 | -0.039659 | 3.396888 |
| 23 | 6 | 0 | 0.704091 | 1.310272 | 2.730116 |
| 24 | 6 | 0 | 0.942427 | 2.560095 | 3.597721 |
| 25 | 6 | 0 | 1.227171 | 3.748035 | 3.010961 |
| 26 | 6 | 0 | 1.312409 | 3.848143 | 1.476584 |
| 27 | 6 | 0 | 1.102673 | 2.748299 | 0.713092 |
| 28 | 8 | 0 | 0.310864 | -0.121462 | 4.650693 |
| 29 | 1 | 0 | -1.384954 | 1.233025 | -1.265332 |
| 30 | 1 | 0 | 2.927065 | 0.384813 | -1.243097 |
| 31 | 1 | 0 | -4.938537 | -1.894444 | -1.490112 |
| 32 | 1 | 0 | -0.211873 | -0.936926 | 1.745922 |
| 33 | 1 | 0 | 0.883201 | 2.490539 | 4.663814 |
| 34 | 1 | 0 | 1.392765 | 4.616419 | 3.613777 |
| 35 | 1 | 0 | 1.537227 | 4.786083 | 1.013307 |
| 36 | 1 | 0 | 1.161895 | 2.817855 | -0.353002 |
| 37 | 6 | 0 | 0.540759 | 0.148545 | 0.512259 |

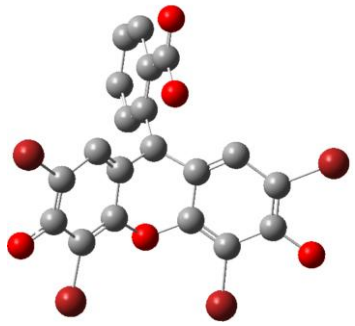
---

Rotational constants (GHZ): 0.0936571 0.0605031 0.0523942

Standard basis: LANL2DZ (5D, 7F)

There are 273 symmetry adapted cartesian basis functions of A symmetry.

**EY-$H_2^{\bullet+}$**



Symbolic Z-matrix:
Charge = 1 Multiplicity = 2

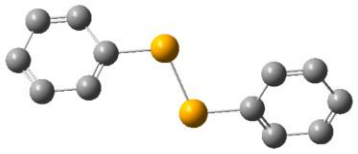
| | | | |
|---|---|---|---|
| C | -0.60967 | 5.28507 | 2.87208 |
| C | 0.55194 | 5.97252 | 2.66488 |
| C | 1.91883 | 5.25 | 2.74905 |
| C | 1.95112 | 3.92651 | 3.02872 |
| C | 0.63268 | 3.15815 | 3.14077 |
| C | -0.56868 | 3.76602 | 3.13314 |
| O | 3.21585 | 3.19647 | 3.2613 |
| C | 3.06558 | 2.22175 | 4.36308 |
| C | 4.03535 | 2.01242 | 5.28319 |
| C | 3.74646 | 1.08594 | 6.48971 |
| C | 2.52701 | 0.48699 | 6.62768 |
| C | 1.44628 | 0.68378 | 5.5457 |
| Br | -2.28397 | 6.20334 | 2.83241 |
| O | 0.50589 | 7.37171 | 2.37325 |
| Br | 3.5418 | 6.21923 | 2.47579 |
| Br | 5.73658 | 2.86193 | 5.10367 |
| O | 4.72008 | 0.86962 | 7.42895 |
| Br | 2.16262 | -0.59847 | 8.15643 |
| O | -1.22032 | 1.30263 | 4.54685 |
| C | 0.48294 | 0.62393 | 2.25718 |
| C | -1.61237 | 0.30525 | 3.60005 |
| C | -0.69547 | -0.02801 | 2.40848 |
| C | -1.11767 | -1.10212 | 1.38886 |
| C | -0.31079 | -1.39539 | 0.34028 |
| C | 1.02831 | -0.65455 | 0.16834 |
| C | 1.39985 | 0.29066 | 1.06562 |
| O | -2.7066 | -0.30012 | 3.74055 |
| H | -1.46856 | 3.21028 | 3.29523 |
| H | 0.48595 | 0.22053 | 5.63541 |
| H | -0.26397 | 7.76116 | 2.79425 |
| H | -0.71832 | 0.89213 | 5.25473 |
| H | -2.04808 | -1.61686 | 1.50832 |
| H | -0.60414 | -2.14168 | -0.36817 |
| H | 1.66537 | -0.8861 | -0.65956 |
| H | 2.33026 | 0.8054 | 0.94615 |

```
 C                     0.90515   1.69803   3.27681
 C                     1.75089   1.44766   4.47962


 ---------------------------------------------------------------------
------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
------
      1             6             0        -0.609665     5.285075
2.872082
      2             6             0         0.551940     5.972518
2.664885
      3             6             0         1.918830     5.249999
2.749051
      4             6             0         1.951119     3.926512
3.028719
      5             6             0         0.632683     3.158151
3.140766
      6             6             0        -0.568683     3.766018
3.133135
      7             8             0         3.215849     3.196473
3.261300
      8             6             0         3.065581     2.221749
4.363084
      9             6             0         4.035350     2.012415
5.283193
     10             6             0         3.746460     1.085939
6.489713
     11             6             0         2.527008     0.486992
6.627680
     12             6             0         1.446285     0.683778
5.545702
     13            35             0        -2.283975     6.203342
2.832410
     14             8             0         0.505885     7.371706
2.373251
     15            35             0         3.541796     6.219233
2.475794
     16            35             0         5.736581     2.861935
5.103669
     17             8             0         4.720085     0.869620
7.428947
     18            35             0         2.162616    -0.598474
8.156431
```

```
     19           8           0       -1.220320     1.302633
4.546852
     20           6           0        0.482945     0.623926
2.257182
     21           6           0       -1.612365     0.305252
3.600051
     22           6           0       -0.695465    -0.028012
2.408485
     23           6           0       -1.117667    -1.102117
1.388855
     24           6           0       -0.310794    -1.395390
0.340278
     25           6           0        1.028307    -0.654550
0.168342
     26           6           0        1.399845     0.290662
1.065617
     27           8           0       -2.706604    -0.300119
3.740546
     28           1           0       -1.468563     3.210282
3.295228
     29           1           0        0.485946     0.220527
5.635415
     30           1           0       -0.263975     7.761162
2.794250
     31           1           0       -0.718325     0.892133
5.254730
     32           1           0       -2.048081    -1.616858
1.508318
     33           1           0       -0.604142    -2.141684    -
0.368166
     34           1           0        1.665375    -0.886104    -
0.659564
     35           1           0        2.330260     0.805401
0.946155
     36           6           0        0.905147     1.698030
3.276813
     37           6           0        1.750889     1.447662
4.479617
 -------------------------------------------------------------
------
Stoichiometry    C20H8Br4O5(1+,2)
 Framework group  C1[X(C20H8Br4O5)]
 Deg. of freedom   105
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
```

PhSeSePh **(2b)**



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.930605 | 1.246304 | 0.000000 |
| 2 | 6 | 0 | -5.340172 | -0.045525 | 0.000000 |
| 3 | 6 | 0 | -4.301567 | -1.182582 | 0.000000 |
| 4 | 6 | 0 | -2.978027 | -0.891364 | 0.000000 |
| 5 | 6 | 0 | -2.512609 | 0.576624 | 0.000000 |
| 6 | 6 | 0 | -3.426582 | 1.577234 | 0.000000 |
| 7 | 34 | 0 | -0.617931 | 0.993510 | 0.000000 |

| | | | | |
|---|---|---|---|---|
| 8 | 34 | 0 | 0.617931 | -0.993510 |
| | | 0.000000 | | |
| 9 | 6 | 0 | 2.512609 | -0.576623 |
| | | 0.000000 | | |
| 10 | 6 | 0 | 3.426582 | -1.577234 |
| | | 0.000000 | | |
| 11 | 6 | 0 | 4.930605 | -1.246303 |
| | | 0.000000 | | |
| 12 | 6 | 0 | 5.340173 | 0.045525 |
| | | 0.000000 | | |
| 13 | 6 | 0 | 4.301567 | 1.182582 |
| | | 0.000000 | | |
| 14 | 6 | 0 | 2.978027 | 0.891364 |
| | | 0.000000 | | |
| 15 | 1 | 0 | -5.652234 | 2.036337 |
| | | 0.000000 | | |
| 16 | 1 | 0 | -6.385175 | -0.275457 |
| | | 0.000000 | | |
| 17 | 1 | 0 | -4.624941 | -2.202547 |
| | | 0.000000 | | |
| 18 | 1 | 0 | -2.256398 | -1.681397 |
| | | 0.000000 | | |
| 19 | 1 | 0 | -3.103207 | 2.597199 |
| | | 0.000000 | | |
| 20 | 1 | 0 | 3.103208 | -2.597199 |
| | | 0.000000 | | |
| 21 | 1 | 0 | 5.652234 | -2.036337 |
| | | 0.000000 | | |
| 22 | 1 | 0 | 6.385176 | 0.275457 |
| | | 0.000000 | | |

| | | | | |
|---|---|---|---|---|
| 23 | 1 | 0 | 4.624942 | 2.202548 |
| | | 0.000000 | | |
| 24 | 1 | 0 | 2.256398 | 1.681397 |
| | | 0.000000 | | |

---

Stoichiometry C12H10Se2

Framework group C2H[SGH(C12H10Se2)]

Deg. of freedom 23

Full point group C2H NOp 4

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.276724 | -4.547600 | 0.000000 |
| 2 | 6 | 0 | -1.103087 | -5.225200 | 0.000000 |
| 3 | 6 | 0 | 0.230593 | -4.455200 | 0.000000 |
| 4 | 6 | 0 | 0.230593 | -3.100000 | 0.000000 |
| 5 | 6 | 0 | -1.103087 | -2.330000 | 0.000000 |

| | | | | |
|---|---|---|---|---|
| 6 | 6 | 0 | -2.276724 | -3.007600 |
| | | 0.000000 | | |
| 7 | 34 | 0 | -1.103087 | -0.390000 |
| | | 0.000000 | | |
| 8 | 34 | 0 | 1.103087 | 0.390000 |
| | | 0.000000 | | |
| 9 | 6 | 0 | 1.103087 | 2.330000 |
| | | 0.000000 | | |
| 10 | 6 | 0 | 2.276724 | 3.007600 |
| | | 0.000000 | | |
| 11 | 6 | 0 | 2.276724 | 4.547600 |
| | | 0.000000 | | |
| 12 | 6 | 0 | 1.103087 | 5.225200 |
| | | 0.000000 | | |
| 13 | 6 | 0 | -0.230593 | 4.455200 |
| | | 0.000000 | | |
| 14 | 6 | 0 | -0.230593 | 3.100000 |
| | | 0.000000 | | |
| 15 | 1 | 0 | -3.203371 | -5.082600 |
| | | 0.000000 | | |
| 16 | 1 | 0 | -1.103087 | -6.295200 |
| | | 0.000000 | | |
| 17 | 1 | 0 | 1.157240 | -4.990200 |
| | | 0.000000 | | |
| 18 | 1 | 0 | 1.157240 | -2.565000 |
| | | 0.000000 | | |
| 19 | 1 | 0 | -3.203371 | -2.472600 |
| | | 0.000000 | | |
| 20 | 1 | 0 | 3.203371 | 2.472600 |
| | | 0.000000 | | |

| | | | | |
|---|---|---|---|---|
| 21 | 1 | 0 | 3.203371 | 5.082600 |
| | | 0.000000 | | |
| 22 | 1 | 0 | 1.103087 | 6.295200 |
| | | 0.000000 | | |
| 23 | 1 | 0 | -1.157240 | 4.990200 |
| | | 0.000000 | | |
| 24 | 1 | 0 | -1.157240 | 2.565000 |
| | | 0.000000 | | |

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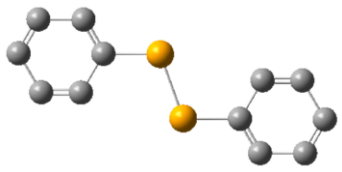
Rotational constants (GHZ): 1.5276242
0.1899434 0.1689378

Standard basis: LANL2DZ (5D, 7F)

There are 58 symmetry adapted cartesian basis functions of AG symmetry.

There are 14 symmetry adapted cartesian basis functions of BG symmetry.

## [PhSeSePh]$^{\bullet+}$ (**I**)



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.930605 | 1.246303 | 0.000000 |
| 2 | 6 | 0 | -5.340172 | -0.045525 | 0.000000 |
| 3 | 6 | 0 | -4.301567 | -1.182582 | 0.000000 |
| 4 | 6 | 0 | -2.978027 | -0.891364 | 0.000000 |
| 5 | 6 | 0 | -2.512609 | 0.576624 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -3.426582 | 1.577234 | 0.000000 |
| 7 | 34 | 0 | -0.617931 | 0.993510 | 0.000000 |
| 8 | 34 | 0 | 0.617931 | -0.993510 | 0.000000 |
| 9 | 6 | 0 | 2.512609 | -0.576623 | 0.000000 |
| 10 | 6 | 0 | 3.426582 | -1.577234 | 0.000000 |
| 11 | 6 | 0 | 4.930605 | -1.246303 | 0.000000 |
| 12 | 6 | 0 | 5.340173 | 0.045525 | 0.000000 |
| 13 | 6 | 0 | 4.301567 | 1.182582 | 0.000000 |
| 14 | 6 | 0 | 2.978027 | 0.891364 | 0.000000 |
| 15 | 1 | 0 | -5.652233 | 2.036337 | 0.000000 |
| 16 | 1 | 0 | -6.385175 | -0.275457 | 0.000000 |
| 17 | 1 | 0 | -4.624941 | -2.202547 | 0.000000 |
| 18 | 1 | 0 | -2.256398 | -1.681397 | 0.000000 |
| 19 | 1 | 0 | -3.103207 | 2.597199 | 0.000000 |
| 20 | 1 | 0 | 3.103208 | -2.597199 | 0.000000 |
| 21 | 1 | 0 | 5.652234 | -2.036337 | 0.000000 |
| 22 | 1 | 0 | 6.385176 | 0.275457 | 0.000000 |
| 23 | 1 | 0 | 4.624942 | 2.202547 | 0.000000 |
| 24 | 1 | 0 | 2.256398 | 1.681397 | 0.000000 |

---

Stoichiometry C12H10Se2(1+,2)

Framework group C2H[SGH(C12H10Se2)]

Deg. of freedom 23

Full point group C2H NOp 4

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.276724 | 4.547600 | 0.000000 |
| 2 | 6 | 0 | 1.103087 | 5.225200 | 0.000000 |
| 3 | 6 | 0 | -0.230593 | 4.455200 | 0.000000 |
| 4 | 6 | 0 | -0.230593 | 3.100000 | 0.000000 |
| 5 | 6 | 0 | 1.103087 | 2.330000 | 0.000000 |
| 6 | 6 | 0 | 2.276724 | 3.007600 | 0.000000 |
| 7 | 34 | 0 | 1.103087 | 0.390000 | 0.000000 |
| 8 | 34 | 0 | -1.103087 | -0.390000 | 0.000000 |
| 9 | 6 | 0 | -1.103087 | -2.330000 | 0.000000 |
| 10 | 6 | 0 | -2.276724 | -3.007600 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 6 | 0 | -2.276724 | -4.547600 | 0.000000 |
| 12 | 6 | 0 | -1.103087 | -5.225200 | 0.000000 |
| 13 | 6 | 0 | 0.230593 | -4.455200 | 0.000000 |
| 14 | 6 | 0 | 0.230593 | -3.100000 | 0.000000 |
| 15 | 1 | 0 | 3.203371 | 5.082600 | 0.000000 |
| 16 | 1 | 0 | 1.103087 | 6.295200 | 0.000000 |
| 17 | 1 | 0 | -1.157240 | 4.990200 | 0.000000 |
| 18 | 1 | 0 | -1.157240 | 2.565000 | 0.000000 |
| 19 | 1 | 0 | 3.203371 | 2.472600 | 0.000000 |
| 20 | 1 | 0 | -3.203371 | -2.472600 | 0.000000 |
| 21 | 1 | 0 | -3.203371 | -5.082600 | 0.000000 |
| 22 | 1 | 0 | -1.103087 | -6.295200 | 0.000000 |
| 23 | 1 | 0 | 1.157240 | -4.990200 | 0.000000 |
| 24 | 1 | 0 | 1.157240 | -2.565000 | 0.000000 |

---

Rotational constants (GHZ): 1.5276242 0.1899434 0.1689378

Standard basis: LANL2DZ (5D, 7F)

There are 58 symmetry adapted cartesian basis functions of AG symmetry.

[PhSeSePh]$^{\bullet-}$ (**I**)

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.930605 | 1.246304 | 0.000000 |
| 2 | 6 | 0 | -5.340172 | -0.045525 | 0.000000 |
| 3 | 6 | 0 | -4.301567 | -1.182582 | 0.000000 |
| 4 | 6 | 0 | -2.978027 | -0.891364 | 0.000000 |
| 5 | 6 | 0 | -2.512609 | 0.576624 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -3.426582 | 1.577234 | 0.000000 |
| 7 | 6 | 0 | 2.512609 | -0.576623 | 0.000000 |
| 8 | 6 | 0 | 3.426582 | -1.577234 | 0.000000 |
| 9 | 6 | 0 | 4.930605 | -1.246303 | 0.000000 |
| 10 | 6 | 0 | 5.340173 | 0.045525 | 0.000000 |
| 11 | 6 | 0 | 4.301567 | 1.182582 | 0.000000 |
| 12 | 6 | 0 | 2.978027 | 0.891364 | 0.000000 |
| 13 | 1 | 0 | -5.652234 | 2.036337 | 0.000000 |
| 14 | 1 | 0 | -6.385175 | -0.275457 | 0.000000 |
| 15 | 1 | 0 | -4.624942 | -2.202547 | 0.000000 |
| 16 | 1 | 0 | -2.256398 | -1.681397 | 0.000000 |
| 17 | 1 | 0 | -3.103208 | 2.597199 | 0.000000 |
| 18 | 1 | 0 | 3.103208 | -2.597199 | 0.000000 |
| 19 | 1 | 0 | 5.652234 | -2.036337 | 0.000000 |
| 20 | 1 | 0 | 6.385176 | 0.275457 | 0.000000 |
| 21 | 1 | 0 | 4.624942 | 2.202548 | 0.000000 |
| 22 | 1 | 0 | 2.256398 | 1.681397 | 0.000000 |
| 23 | 34 | 0 | -0.617931 | 0.993510 | 0.000000 |
| 24 | 34 | 0 | 0.617931 | -0.993510 | 0.000000 |

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Stoichiometry C12H10Se2(1-,2)

Framework group C2H[SGH(C12H10Se2)]

Deg. of freedom 23

Full point group C2H NOp 4

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

---

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.276724 | -4.547600 | 0.000000 |
| 2 | 6 | 0 | 1.103087 | -5.225200 | 0.000000 |
| 3 | 6 | 0 | -0.230593 | -4.455200 | 0.000000 |
| 4 | 6 | 0 | -0.230593 | -3.100000 | 0.000000 |
| 5 | 6 | 0 | 1.103087 | -2.330000 | 0.000000 |
| 6 | 6 | 0 | 2.276724 | -3.007600 | 0.000000 |
| 7 | 6 | 0 | -1.103087 | 2.330000 | -0.000000 |
| 8 | 6 | 0 | -2.276724 | 3.007600 | -0.000000 |
| 9 | 6 | 0 | -2.276724 | 4.547600 | -0.000000 |
| 10 | 6 | 0 | -1.103087 | 5.225200 | -0.000000 |
| 11 | 6 | 0 | 0.230593 | 4.455200 | -0.000000 |
| 12 | 6 | 0 | 0.230593 | 3.100000 | -0.000000 |
| 13 | 1 | 0 | 3.203371 | -5.082600 | 0.000000 |
| 14 | 1 | 0 | 1.103087 | -6.295200 | 0.000000 |
| 15 | 1 | 0 | -1.157240 | -4.990200 | 0.000000 |
| 16 | 1 | 0 | -1.157240 | -2.565000 | 0.000000 |
| 17 | 1 | 0 | 3.203371 | -2.472600 | 0.000000 |
| 18 | 1 | 0 | -3.203371 | 2.472600 | -0.000000 |
| 19 | 1 | 0 | -3.203371 | 5.082600 | -0.000000 |
| 20 | 1 | 0 | -1.103087 | 6.295200 | -0.000000 |
| 21 | 1 | 0 | 1.157240 | 4.990200 | -0.000000 |
| 22 | 1 | 0 | 1.157240 | 2.565000 | -0.000000 |
| 23 | 34 | 0 | 1.103087 | -0.390000 | 0.000000 |
| 24 | 34 | 0 | -1.103087 | 0.390000 | -0.000000 |

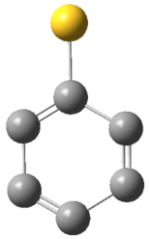
---

Rotational constants (GHZ): 1.5276242 0.1899434 0.1689378

Standard basis: LANL2DZ (5D, 7F)

There are 58 symmetry adapted cartesian basis functions of AG symmetry.

**Phenyl selenyl radical (II)**



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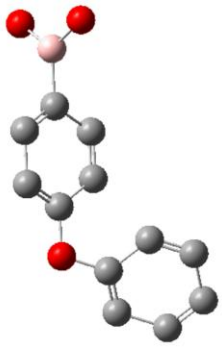
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.810805 | 0.381571 | 0.000000 |
| 2 | 6 | 0 | -1.569342 | -0.951944 | 0.000000 |
| 3 | 6 | 0 | -0.119809 | -1.471995 | 0.000000 |
| 4 | 6 | 0 | 0.914318 | -0.596125 | 0.000000 |
| 5 | 6 | 0 | 0.639929 | 0.919233 | 0.000000 |
| 6 | 6 | 0 | -0.635661 | 1.376878 | 0.000000 |
| 7 | 34 | 0 | 2.120305 | 2.173061 | 0.000000 |
| 8 | 1 | 0 | -2.817948 | 0.742905 | 0.000000 |
| 9 | 1 | 0 | -2.385839 | -1.643489 | 0.000000 |
| 10 | 1 | 0 | 0.070838 | -2.524874 | 0.000000 |
| 11 | 1 | 0 | 1.921461 | -0.957459 | 0.000000 |
| 12 | 1 | 0 | -0.826308 | 2.429757 | 0.000000 |

---

Distance matrix (angstroms):

1 2 3 4 5

**4-PhO-$C_6H_4$-$B(OH)_2$ (1a)**



---

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -1.29393 | 1.47494 | -0.95975 |
| C | -1.27473 | 0.12183 | -0.88704 |
| C | -1.05214 | -0.57334 | 0.46898 |
| C | -0.87546 | 0.16803 | 1.58958 |
| C | -0.89728 | 1.70566 | 1.50695 |
| C | -1.09315 | 2.3174 | 0.31365 |
| B | -1.11652 | 3.96486 | 0.22512 |
| O | -2.44407 | 4.72641 | 0.39621 |
| O | 0.18921 | 4.74094 | -0.02859 |
| O | -1.03189 | -2.00113 | 0.54571 |
| C | -0.54496 | -2.53787 | -0.68706 |
| C | -0.9696 | -3.75269 | -1.11187 |
| C | -0.44521 | -4.33072 | -2.43947 |
| C | 0.44089 | -3.62456 | -3.18293 |
| C | 0.92343 | -2.24409 | -2.70019 |
| C | 0.46197 | -1.73542 | -1.53191 |
| H | -1.44858 | 1.95794 | -1.90192 |
| H | -1.41423 | -0.46352 | -1.7718 |
| H | -0.72081 | -0.31497 | 2.53175 |
| H | -0.75778 | 2.29101 | 2.39171 |
| H | -2.2708 | 5.58956 | 0.77903 |

| | | | |
|---|---|---|---|
| H | 0.13583 | 5.60283 | 0.3908 |
| H | -1.66922 | -4.31023 | -0.52487 |
| H | -0.78049 | -5.28988 | -2.77488 |
| H | 0.80524 | -4.02618 | -4.10535 |
| H | 1.62305 | -1.68654 | -3.2872 |
| H | 0.79725 | -0.77626 | -1.19649 |

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

26 H 0.000000

27 H 2.425200 0.000000

Stoichiometry C12H11BO3

Framework group C1[X(C12H11BO3)]

Deg. of freedom 75

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.332529 | -0.632515 | 0.742904 |
| 2 | 6 | 0 | -0.078330 | -0.122641 | 0.683050 |
| 3 | 6 | 0 | 0.185072 | 1.185854 | -0.085104 |
| 4 | 6 | 0 | -0.837331 | 1.827454 | -0.701227 |
| 5 | 6 | 0 | -2.262556 | 1.248051 | -0.633213 |
| 6 | 6 | 0 | -2.494350 | 0.096575 | 0.042763 |
| 7 | 5 | 0 | -4.021377 | -0.524215 | 0.115635 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 8 | 0 | -4.965207 | -0.114646 | 1.261513 |
| 9 | 8 | 0 | -4.502771 | -1.513187 | -0.962230 |
| 10 | 8 | 0 | 1.508495 | 1.723872 | -0.148260 |
| 11 | 6 | 0 | 2.459773 | 0.657846 | -0.088587 |
| 12 | 6 | 0 | 3.679909 | 0.868527 | 0.462273 |
| 13 | 6 | 0 | 4.704363 | -0.279500 | 0.526534 |
| 14 | 6 | 0 | 4.385745 | -1.500444 | 0.032222 |
| 15 | 6 | 0 | 2.999226 | -1.739856 | -0.593753 |
| 16 | 6 | 0 | 2.097707 | -0.729592 | -0.650303 |
| 17 | 1 | 0 | -1.515542 | -1.541664 | 1.276622 |
| 18 | 1 | 0 | 0.728910 | -0.629218 | 1.169510 |
| 19 | 1 | 0 | -0.654318 | 2.736604 | -1.234942 |
| 20 | 1 | 0 | -3.069796 | 1.754628 | -1.119671 |
| 21 | 1 | 0 | -5.874039 | -0.144728 | 0.953747 |
| 22 | 1 | 0 | -5.451405 | -1.422896 | -1.078598 |
| 23 | 1 | 0 | 3.931474 | 1.832525 | 0.852558 |
| 24 | 1 | 0 | 5.667723 | -0.113156 | 0.961466 |
| 25 | 1 | 0 | 5.097542 | -2.298099 | 0.076868 |
| 26 | 1 | 0 | 2.747660 | -2.703855 | -0.984036 |
| 27 | 1 | 0 | 1.134347 | -0.895935 | -1.085237 |

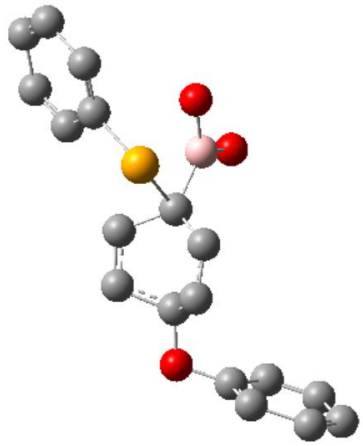
---

Rotational constants (GHZ): 1.3436169 0.2253284 0.2073439

Standard basis: LANL2DZ (5D, 7F)

There are 166 symmetry adapted cartesian basis functions of A symmetry.

**IV**



Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.51698 | -0.19543 | 0.86628 |
| C | -0.1828 | -1.42361 | 0.40543 |
| C | 1.2196 | -1.40185 | -0.18497 |
| C | 2.16852 | -1.19086 | 0.98541 |
| C | 2.01741 | 0.05448 | 1.49355 |
| B | 0.63019 | 2.37772 | 0.73023 |
| O | 0.47195 | 3.33746 | 1.92415 |
| O | 0.70718 | 2.93718 | -0.70249 |
| O | 1.52339 | -2.57436 | -0.94511 |
| C | 2.85053 | -2.47289 | -1.46791 |
| C | 3.89949 | -2.94227 | -0.74963 |
| C | 5.32871 | -2.833 | -1.31265 |
| C | 5.53746 | -2.26746 | -2.52639 |
| C | 4.34546 | -1.73408 | -3.34261 |
| C | 3.08775 | -1.83023 | -2.84716 |
| Se | 0.1719 | 1.17559 | 2.79855 |
| C | -1.56004 | 2.04898 | 2.76451 |
| C | -1.88304 | 2.95096 | 3.72298 |
| C | -3.25788 | 3.64426 | 3.69595 |

| | | | |
|---|---|---|---|
| C | -4.14475 | 3.35238 | 2.71369 |
| C | -3.77771 | 2.32741 | 1.62452 |
| C | -2.56785 | 1.7173 | 1.6483 |
| H | -1.51136 | 0.08654 | 1.14302 |
| H | -0.80814 | -2.2897 | 0.46655 |
| H | 1.29171 | -0.54483 | -0.82153 |
| H | 2.84421 | -1.92786 | 1.36644 |
| H | 2.69875 | 0.50107 | 2.18725 |
| H | 0.88798 | 4.17743 | 1.71684 |
| H | 1.10295 | 3.8116 | -0.68373 |
| H | 3.73467 | -3.3888 | 0.20867 |
| H | 6.15692 | -3.2036 | -0.74553 |
| H | 6.53049 | -2.19154 | -2.91757 |
| H | 4.51028 | -1.28755 | -4.30092 |
| H | 2.25954 | -1.45963 | -3.41428 |
| H | -1.1828 | 3.1814 | 4.49853 |
| H | -3.5129 | 4.35642 | 4.45272 |
| H | -5.1 | 3.83409 | 2.69491 |
| H | -4.47795 | 2.09696 | 0.84897 |
| H | -2.31283 | 1.00515 | 0.89153 |
| C | 0.71726 | 0.75001 | 0.98608 |

Stoichiometry C18H17BO3Se

Framework group C1[X(C18H17BO3Se)]

Deg. of freedom 114

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

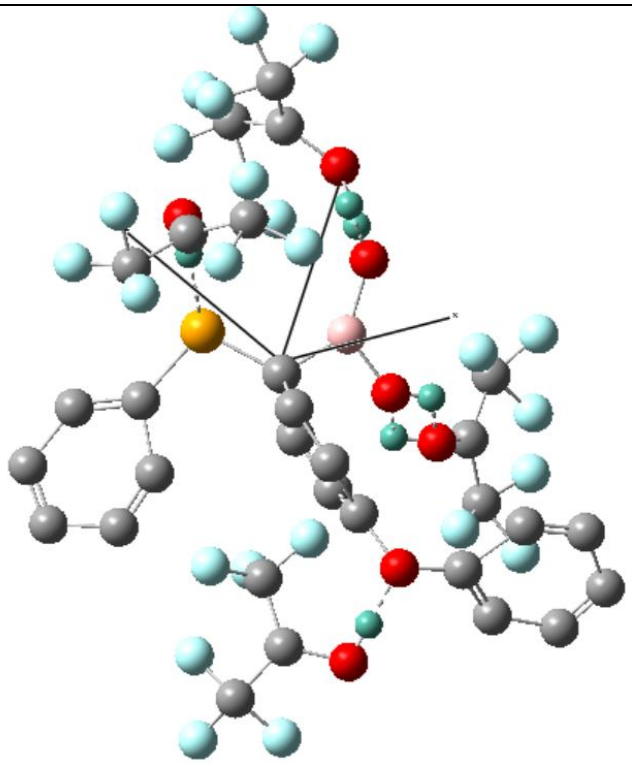
Largest concise Abelian subgroup C1 NOp 1

Rotational constants (GHZ): 0.5903946 0.1019859 0.1014550

Standard basis: LANL2DZ (5D, 7F)

There are 240 symmetry adapted cartesian basis functions of A  symmetry.

# IV



| | | | |
|---|---|---|---|
| C | -1.10801 | 0.19735 | 2.27333 |
| C | -0.58493 | -0.65477 | 3.29231 |
| C | 0.66149 | -1.1762 | 3.65993 |
| C | 1.14213 | -0.42454 | 2.60852 |
| C | 0.54676 | 0.37725 | 1.62284 |
| C | -0.73505 | 0.89352 | 0.91531 |
| B | 0.37521 | 2.0474 | 0.54652 |
| O | 0.07896 | 2.87388 | -0.74834 |
| O | 1.60882 | 1.11334 | 0.49214 |
| O | 1.19945 | -2.07925 | 4.70155 |
| C | 2.48437 | -1.69242 | 5.22019 |
| C | 3.08111 | -1.88604 | 6.49609 |
| C | 4.44342 | -1.53551 | 7.15462 |

| | | | |
|---|---|---|---|
| C | 5.37331 | -0.91665 | 6.46975 |
| C | 4.96287 | -0.6049 | 5.06806 |
| C | 3.73873 | -0.95941 | 4.59639 |
| Se | -2.14977 | 2.21731 | 1.17457 |
| C | -3.86209 | 1.39708 | 0.66542 |
| C | -5.13645 | 1.4227 | 1.2583 |
| C | -6.5293 | 0.82494 | 0.94156 |
| C | -6.7214 | 0.08 | -0.11928 |
| C | -5.48247 | -0.11018 | -0.93086 |
| C | -4.30474 | 0.45986 | -0.55038 |
| Se | 0.59154 | 3.37251 | 2.11204 |
| C | 2.48215 | 3.71233 | 2.38983 |
| C | 3.64191 | 3.60368 | 1.60064 |
| C | 5.16595 | 3.71704 | 1.89629 |
| C | 5.60624 | 4.03909 | 3.09491 |
| C | 4.51109 | 4.3077 | 4.06653 |
| C | 3.21821 | 4.17185 | 3.70434 |
| C | -1.3786 | -1.92149 | 5.59078 |
| C | -1.54946 | -1.09954 | 4.29947 |
| C | -2.61109 | -2.53456 | 6.28328 |
| O | -0.07119 | -2.1413 | 6.13614 |
| F | -2.24421 | -3.64327 | 6.95942 |
| F | -3.1274 | -1.62972 | 7.14853 |
| F | -3.54259 | -2.85132 | 5.36238 |
| F | -0.2983 | -0.68032 | 4.58215 |
| F | -2.80558 | -0.93458 | 4.77201 |
| F | -1.70782 | 0.18204 | 3.90099 |
| H | 0.56521 | -2.11014 | 5.41785 |
| C | -2.15885 | 4.69787 | -0.91593 |
| C | -2.39833 | 6.24301 | -1.09088 |
| C | -3.24383 | 3.84538 | -0.28664 |

| | | | |
|---|---|---|---|
| O | -0.99249 | 3.93783 | -1.31347 |
| F | -2.58892 | 2.85423 | -0.93622 |
| F | -4.33307 | 3.12988 | -0.61955 |
| F | -4.04149 | 4.89016 | -0.56897 |
| F | -1.49245 | 6.14751 | -2.08004 |
| F | -3.68725 | 5.8949 | -0.84945 |
| F | -2.96875 | 7.13649 | -1.93415 |
| H | -0.19739 | 3.81481 | -0.75165 |
| C | 3.6382 | -0.37477 | 0.55913 |
| C | 2.75504 | -1.4789 | 1.2338 |
| C | 5.08321 | -0.71057 | 0.22939 |
| O | 3.1557 | 0.95137 | 0.23741 |
| F | 4.94705 | 0.32005 | -0.62777 |
| F | 5.81934 | -1.23662 | -0.767 |
| F | 4.65711 | -1.98517 | 0.36508 |
| F | 1.72026 | -0.74218 | 0.79143 |
| F | 3.70284 | -2.30812 | 0.74025 |
| F | 1.92794 | -2.50899 | 0.93057 |
| H | 2.51324 | 1.29832 | 0.80807 |
| H | 2.31125 | 1.04905 | -0.18047 |
| H | -0.80965 | 3.01345 | -1.09068 |

Stoichiometry C33H5BF18O6Se2

Framework group C1[X(C33H5BF18O6Se2)]

Deg. of freedom 189

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---

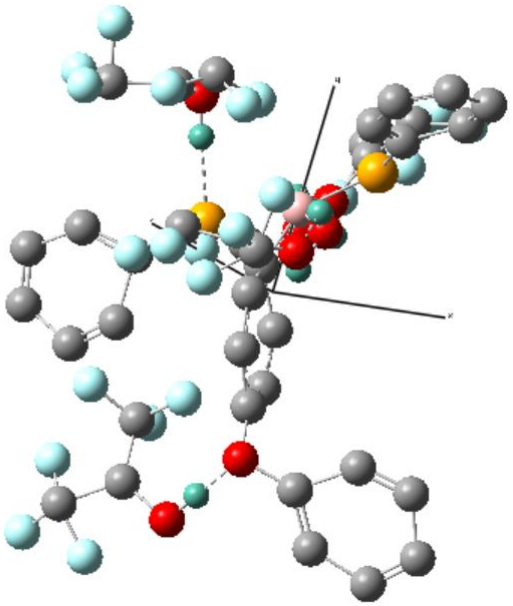
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.070255 | 1.369973 | 0.376301 |
| 2 | 6 | 0 | 1.261177 | 1.853065 | 0.197540 |
| 3 | 6 | 0 | 2.560281 | 1.332181 | 0.237499 |
| 4 | 6 | 0 | 1.931780 | 0.126778 | 0.468685 |
| 5 | 6 | 0 | 0.597583 | -0.263103 | 0.660560 |
| 6 | 6 | 0 | -0.890393 | 0.125487 | 0.872882 |
| 7 | 5 | 0 | -0.992434 | -1.413776 | 0.306866 |
| 8 | 8 | 0 | -2.296425 | -2.186126 | 0.694899 |
| 9 | 8 | 0 | 0.322202 | -1.935242 | 0.936965 |
| 10 | 8 | 0 | 3.941522 | 1.838282 | 0.076541 |
| 11 | 6 | 0 | 4.827784 | 0.941999 | -0.616898 |
| 12 | 6 | 0 | 5.963141 | 1.188522 | -1.436476 |
| 13 | 6 | 0 | 6.990288 | 0.317236 | -2.209927 |
| 14 | 6 | 0 | 6.914854 | -0.990298 | -2.172398 |
| 15 | 6 | 0 | 5.773357 | -1.490659 | -1.349597 |
| 16 | 6 | 0 | 4.932211 | -0.632588 | -0.714885 |
| 17 | 34 | 0 | -2.443166 | 0.700618 | -0.165966 |
| 18 | 6 | 0 | -3.361889 | 2.121649 | 0.834375 |
| 19 | 6 | 0 | -3.923383 | 3.347333 | 0.436152 |
| 20 | 6 | 0 | -4.661650 | 4.517474 | 1.131424 |
| 21 | 6 | 0 | -4.893263 | 4.501404 | 2.421125 |
| 22 | 6 | 0 | -4.370553 | 3.274339 | 3.092576 |
| 23 | 6 | 0 | -3.726971 | 2.308610 | 2.378476 |
| 24 | 34 | 0 | -0.822494 | -1.443611 | -1.748319 |
| 25 | 6 | 0 | 0.370603 | -2.886995 | -2.258426 |
| 26 | 6 | 0 | 0.806111 | -4.081572 | -1.655940 |
| 27 | 6 | 0 | 1.894130 | -5.137152 | -2.009365 |
| 28 | 6 | 0 | 2.596663 | -5.047283 | -3.119614 |

| | | | | | |
|---|---|---|---|---|---|
| 29 | 6 | 0 | 2.203820 | -3.888305 | -3.966959 |
| 30 | 6 | 0 | 1.248052 | -3.027387 | -3.558911 |
| 31 | 6 | 0 | 2.592066 | 4.121984 | -0.575910 |
| 32 | 6 | 0 | 1.375127 | 3.259306 | -0.192347 |
| 33 | 6 | 0 | 2.468364 | 5.657525 | -0.610909 |
| 34 | 8 | 0 | 3.849103 | 3.500771 | -0.874260 |
| 35 | 9 | 0 | 3.671791 | 6.213341 | -0.358275 |
| 36 | 9 | 0 | 2.045317 | 6.038800 | -1.839586 |
| 37 | 9 | 0 | 1.576362 | 6.065550 | 0.313179 |
| 38 | 9 | 0 | 2.103886 | 2.261521 | -0.734928 |
| 39 | 9 | 0 | 0.687317 | 4.350076 | -0.599152 |
| 40 | 9 | 0 | 0.349206 | 2.599128 | -0.773701 |
| 41 | 1 | 0 | 3.895460 | 2.668187 | -0.398273 |
| 42 | 6 | 0 | -4.886351 | -1.426092 | -0.343114 |
| 43 | 6 | 0 | -6.003912 | -2.040704 | -1.264381 |
| 44 | 6 | 0 | -4.808799 | 0.079008 | -0.174045 |
| 45 | 8 | 0 | -3.884437 | -2.139977 | 0.420192 |
| 46 | 9 | 0 | -4.138680 | -0.264236 | 0.951284 |
| 47 | 9 | 0 | -5.288250 | 1.067857 | 0.601529 |
| 48 | 9 | 0 | -6.065200 | 0.062668 | -0.652311 |
| 49 | 9 | 0 | -5.842432 | -3.145673 | -0.515284 |
| 50 | 9 | 0 | -6.538041 | -0.798740 | -1.150358 |
| 51 | 9 | 0 | -7.302869 | -2.423966 | -1.239908 |
| 52 | 1 | 0 | -3.011940 | -2.413496 | 0.063975 |
| 53 | 6 | 0 | 2.535010 | -2.741223 | 1.826475 |
| 54 | 6 | 0 | 2.910365 | -1.250188 | 2.126806 |
| 55 | 6 | 0 | 3.514718 | -3.827350 | 2.238834 |
| 56 | 8 | 0 | 1.308096 | -3.142260 | 1.171655 |
| 57 | 9 | 0 | 2.417918 | -4.606204 | 2.162209 |
| 58 | 9 | 0 | 3.803829 | -4.610157 | 3.294789 |
| 59 | 9 | 0 | 4.020844 | -2.856454 | 3.029900 |

| | | | | | |
|---|---|---|---|---|---|
| 60 | 9 | 0 | 1.592232 | -1.022683 | 1.985391 |
| 61 | 9 | 0 | 3.759570 | -1.813751 | 3.016047 |
| 62 | 9 | 0 | 2.796287 | -0.299136 | 3.085776 |
| 63 | 1 | 0 | 0.970989 | -2.549220 | 0.544399 |
| 64 | 1 | 0 | 0.488675 | -2.751765 | 1.442450 |
| 65 | 1 | 0 | -3.131216 | -1.745948 | 0.883811 |

---

## V



| | | | |
|---|---|---|---|
| C | -1.10801 | 0.19735 | 2.27333 |
| C | -0.58493 | -0.65477 | 3.29231 |

| | | | |
|---|---|---|---|
| C | 0.66149 | -1.1762 | 3.65993 |
| C | 1.14213 | -0.42454 | 2.60852 |
| C | 0.54676 | 0.37725 | 1.62284 |
| C | -0.73505 | 0.89352 | 0.91531 |
| B | 0.37521 | 2.0474 | 0.54652 |
| O | 0.07896 | 2.87388 | -0.74834 |
| O | 1.60882 | 1.11334 | 0.49214 |
| O | 1.19945 | -2.07925 | 4.70155 |
| C | 2.48437 | -1.69242 | 5.22019 |
| C | 3.08111 | -1.88604 | 6.49609 |
| C | 4.44342 | -1.53551 | 7.15462 |
| C | 5.37331 | -0.91665 | 6.46975 |
| C | 4.96287 | -0.6049 | 5.06806 |
| C | 3.73873 | -0.95941 | 4.59639 |
| Se | -2.14977 | 2.21731 | 1.17457 |
| C | -3.86209 | 1.39708 | 0.66542 |
| C | -5.13645 | 1.4227 | 1.2583 |
| C | -6.5293 | 0.82494 | 0.94156 |
| C | -6.7214 | 0.08 | -0.11928 |
| C | -5.48247 | -0.11018 | -0.93086 |
| C | -4.30474 | 0.45986 | -0.55038 |
| Se | 0.59154 | 3.37251 | 2.11204 |
| C | 2.48215 | 3.71233 | 2.38983 |
| C | 3.64191 | 3.60368 | 1.60064 |
| C | 5.16595 | 3.71704 | 1.89629 |
| C | 5.60624 | 4.03909 | 3.09491 |
| C | 4.51109 | 4.3077 | 4.06653 |
| C | 3.21821 | 4.17185 | 3.70434 |
| C | -1.3786 | -1.92149 | 5.59078 |
| C | -1.54946 | -1.09954 | 4.29947 |
| C | -2.61109 | -2.53456 | 6.28328 |

| | | | |
|---|---|---|---|
| O | -0.07119 | -2.1413 | 6.13614 |
| F | -2.24421 | -3.64327 | 6.95942 |
| F | -3.1274 | -1.62972 | 7.14853 |
| F | -3.54259 | -2.85132 | 5.36238 |
| F | -0.2983 | -0.68032 | 4.58215 |
| F | -2.80558 | -0.93458 | 4.77201 |
| F | -1.70782 | 0.18204 | 3.90099 |
| H | 0.56521 | -2.11014 | 5.41785 |
| C | -2.15885 | 4.69787 | -0.91593 |
| C | -2.39833 | 6.24301 | -1.09088 |
| C | -3.24383 | 3.84538 | -0.28664 |
| O | -0.99249 | 3.93783 | -1.31347 |
| F | -2.58892 | 2.85423 | -0.93622 |
| F | -4.33307 | 3.12988 | -0.61955 |
| F | -4.04149 | 4.89016 | -0.56897 |
| F | -1.49245 | 6.14751 | -2.08004 |
| F | -3.68725 | 5.8949 | -0.84945 |
| F | -2.96875 | 7.13649 | -1.93415 |
| H | -0.19739 | 3.81481 | -0.75165 |
| C | 3.6382 | -0.37477 | 0.55913 |
| C | 2.75504 | -1.4789 | 1.2338 |
| C | 5.08321 | -0.71057 | 0.22939 |
| O | 3.1557 | 0.95137 | 0.23741 |
| F | 4.94705 | 0.32005 | -0.62777 |
| F | 5.81934 | -1.23662 | -0.767 |
| F | 4.65711 | -1.98517 | 0.36508 |
| F | 1.72026 | -0.74218 | 0.79143 |
| F | 3.70284 | -2.30812 | 0.74025 |
| F | 1.92794 | -2.50899 | 0.93057 |
| H | 2.51324 | 1.29832 | 0.80807 |
| H | 2.31125 | 1.04905 | -0.18047 |

H -0.80965 3.01345 -1.09068

Stoichiometry C33H5BF18O6Se2

Framework group C1[X(C33H5BF18O6Se2)]

Deg. of freedom 189

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.070255 | 1.369973 | 0.376301 |
| 2 | 6 | 0 | 1.261177 | 1.853065 | 0.197540 |
| 3 | 6 | 0 | 2.560281 | 1.332181 | 0.237499 |
| 4 | 6 | 0 | 1.931780 | 0.126778 | 0.468685 |
| 5 | 6 | 0 | 0.597583 | -0.263103 | 0.660560 |
| 6 | 6 | 0 | -0.890393 | 0.125487 | 0.872882 |
| 7 | 5 | 0 | -0.992434 | -1.413776 | 0.306866 |
| 8 | 8 | 0 | -2.296425 | -2.186126 | 0.694899 |
| 9 | 8 | 0 | 0.322202 | -1.935242 | 0.936965 |
| 10 | 8 | 0 | 3.941522 | 1.838282 | 0.076541 |
| 11 | 6 | 0 | 4.827784 | 0.941999 | -0.616898 |
| 12 | 6 | 0 | 5.963141 | 1.188522 | -1.436476 |
| 13 | 6 | 0 | 6.990288 | 0.317236 | -2.209927 |
| 14 | 6 | 0 | 6.914854 | -0.990298 | -2.172398 |
| 15 | 6 | 0 | 5.773357 | -1.490659 | -1.349597 |
| 16 | 6 | 0 | 4.932211 | -0.632588 | -0.714885 |
| 17 | 34 | 0 | -2.443166 | 0.700618 | -0.165966 |
| 18 | 6 | 0 | -3.361889 | 2.121649 | 0.834375 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 6 | 0 | -3.923383 | 3.347333 | 0.436152 |
| 20 | 6 | 0 | -4.661650 | 4.517474 | 1.131424 |
| 21 | 6 | 0 | -4.893263 | 4.501404 | 2.421125 |
| 22 | 6 | 0 | -4.370553 | 3.274339 | 3.092576 |
| 23 | 6 | 0 | -3.726971 | 2.308610 | 2.378476 |
| 24 | 34 | 0 | -0.822494 | -1.443611 | -1.748319 |
| 25 | 6 | 0 | 0.370603 | -2.886995 | -2.258426 |
| 26 | 6 | 0 | 0.806111 | -4.081572 | -1.655940 |
| 27 | 6 | 0 | 1.894130 | -5.137152 | -2.009365 |
| 28 | 6 | 0 | 2.596663 | -5.047283 | -3.119614 |
| 29 | 6 | 0 | 2.203820 | -3.888305 | -3.966959 |
| 30 | 6 | 0 | 1.248052 | -3.027387 | -3.558911 |
| 31 | 6 | 0 | 2.592066 | 4.121984 | -0.575910 |
| 32 | 6 | 0 | 1.375127 | 3.259306 | -0.192347 |
| 33 | 6 | 0 | 2.468364 | 5.657525 | -0.610909 |
| 34 | 8 | 0 | 3.849103 | 3.500771 | -0.874260 |
| 35 | 9 | 0 | 3.671791 | 6.213341 | -0.358275 |
| 36 | 9 | 0 | 2.045317 | 6.038800 | -1.839586 |
| 37 | 9 | 0 | 1.576362 | 6.065550 | 0.313179 |
| 38 | 9 | 0 | 2.103886 | 2.261521 | -0.734928 |
| 39 | 9 | 0 | 0.687317 | 4.350076 | -0.599152 |
| 40 | 9 | 0 | 0.349206 | 2.599128 | -0.773701 |
| 41 | 1 | 0 | 3.895460 | 2.668187 | -0.398273 |
| 42 | 6 | 0 | -4.886351 | -1.426092 | -0.343114 |
| 43 | 6 | 0 | -6.003912 | -2.040704 | -1.264381 |
| 44 | 6 | 0 | -4.808799 | 0.079008 | -0.174045 |
| 45 | 8 | 0 | -3.884437 | -2.139977 | 0.420192 |
| 46 | 9 | 0 | -4.138680 | -0.264236 | 0.951284 |
| 47 | 9 | 0 | -5.288250 | 1.067857 | 0.601529 |
| 48 | 9 | 0 | -6.065200 | 0.062668 | -0.652311 |
| 49 | 9 | 0 | -5.842432 | -3.145673 | -0.515284 |

| | | | | | |
|---|---|---|---|---|---|
| 50 | 9 | 0 | -6.538041 | -0.798740 | -1.150358 |
| 51 | 9 | 0 | -7.302869 | -2.423966 | -1.239908 |
| 52 | 1 | 0 | -3.011940 | -2.413496 | 0.063975 |
| 53 | 6 | 0 | 2.535010 | -2.741223 | 1.826475 |
| 54 | 6 | 0 | 2.910365 | -1.250188 | 2.126806 |
| 55 | 6 | 0 | 3.514718 | -3.827350 | 2.238834 |
| 56 | 8 | 0 | 1.308096 | -3.142260 | 1.171655 |
| 57 | 9 | 0 | 2.417918 | -4.606204 | 2.162209 |
| 58 | 9 | 0 | 3.803829 | -4.610157 | 3.294789 |
| 59 | 9 | 0 | 4.020844 | -2.856454 | 3.029900 |
| 60 | 9 | 0 | 1.592232 | -1.022683 | 1.985391 |
| 61 | 9 | 0 | 3.759570 | -1.813751 | 3.016047 |
| 62 | 9 | 0 | 2.796287 | -0.299136 | 3.085776 |
| 63 | 1 | 0 | 0.970989 | -2.549220 | 0.544399 |
| 64 | 1 | 0 | 0.488675 | -2.751765 | 1.442450 |
| 65 | 1 | 0 | -3.131216 | -1.745948 | 0.883811 |

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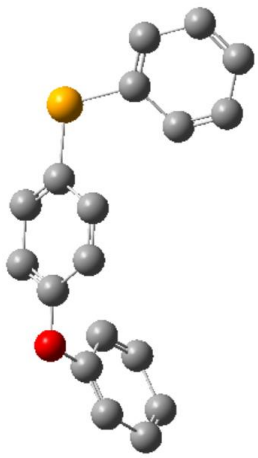
**3b**



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| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
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| 1 | 6 | 0 | -0.558701 | -0.626477 | -0.410155 |
| 2 | 6 | 0 | 0.479302 | -1.765385 | -0.385722 |
| 3 | 6 | 0 | 1.797922 | -1.488983 | -0.248955 |
| 4 | 6 | 0 | 2.248801 | -0.035213 | -0.053702 |
| 5 | 6 | 0 | 1.359751 | 0.975102 | -0.087930 |
| 6 | 6 | 0 | -0.137354 | 0.657022 | -0.284681 |
| 7 | 8 | 0 | 2.737858 | -2.556302 | -0.276287 |
| 8 | 6 | 0 | 3.152977 | -2.785188 | -1.611761 |
| 9 | 6 | 0 | 4.376314 | -3.301036 | -1.843716 |
| 10 | 6 | 0 | 4.829727 | -3.549965 | -3.280662 |
| 11 | 6 | 0 | 4.009199 | -3.238742 | -4.312654 |
| 12 | 6 | 0 | 2.610040 | -2.649316 | -4.042190 |
| 13 | 6 | 0 | 2.203862 | -2.451673 | -2.774601 |
| 14 | 34 | 0 | -1.421510 | 2.089783 | -0.369328 |
| 15 | 6 | 0 | -0.488446 | 3.642597 | -1.050928 |
| 16 | 6 | 0 | -0.947287 | 4.887875 | -0.757119 |
| 17 | 6 | 0 | -0.203584 | 6.125755 | -1.285649 |
| 18 | 6 | 0 | 0.901540 | 5.966785 | -2.056986 |
| 19 | 6 | 0 | 1.417665 | 4.551501 | -2.389099 |
| 20 | 6 | 0 | 0.767096 | 3.466964 | -1.918184 |
| 21 | 1 | 0 | -1.598901 | -0.840171 | -0.526725 |
| 22 | 1 | 0 | 0.155301 | -2.778280 | -0.484111 |
| 23 | 1 | 0 | 3.292580 | 0.162248 | 0.120033 |
| 24 | 1 | 0 | 1.683444 | 1.988170 | 0.005106 |
| 25 | 1 | 0 | 5.023755 | -3.537539 | -1.019243 |
| 26 | 1 | 0 | 5.792797 | -3.965328 | -3.463853 |
| 27 | 1 | 0 | 4.335975 | -3.399919 | -5.323758 |
| 28 | 1 | 0 | 1.961855 | -2.397091 | -4.856043 |
| 29 | 1 | 0 | 1.225423 | -2.060273 | -2.577834 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 1 | 0 | -1.824963 | 5.009518 | -0.158696 |
| 31 | 1 | 0 | -0.561621 | 7.107554 | -1.046949 |
| 32 | 1 | 0 | 1.421550 | 6.820367 | -2.436801 |
| 33 | 1 | 0 | 2.297435 | 4.423254 | -2.996998 |
| 34 | 1 | 0 | 1.131405 | 2.495107 | -2.147958 |

---

Rotational constants (GHZ): 0.5247252 0.1260914 0.1112130

Standard basis: LANL2DZ (5D, 7F)

There are 207 symmetry adapted cartesian basis functions of A symmetry.

There are 207 symmetry adapted basis functions of A symmetry.

207 basis functions, 543 primitive gaussians, 207 cartesian basis functions

68 alpha electrons 68 beta electrons

nuclear repulsion energy 1260.6617409484 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Using the following non-standard input for PCM:

eps=16.7 epsinf=1.626 HBondAcidity=0.77 HBondBasicity=0.00

SurfaceTensionAtInterface=13.19 CarbonAromaticity=0.0

--- end of non-standard input.

---

Polarizable Continuum Model (PCM)

==========

Model : PCM.

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 34.

Lebedev-Laikov grids with approx. 5.0 points / Ang**2.

Smoothing algorithm: York/Karplus (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : Generic,

Eps = 16.700000

Eps(infinity) = 1.626000

RSolv = 0.000000 Ang.

Molar volume = 0.000000 cm**3/mol

Thermal expansion coefficient = 0.000000 K**-1

Absolute temperature = 298.150000 K

Numeral density = 0.000000 Ang**-3

Hydrogen bond acidity = 0.770000

Hydrogen bond basicity = 0.000000

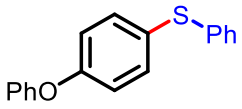
Surface tension at interface = 13.190000 (cal/mol)*Ang**-2

Carbon aromaticity = 0.000000

Electronegative halogenicity = 0.000000

## 8. Experimental and analytical data

**(4-Phenoxyphenyl)(phenyl)sulfane (3a)[1]**

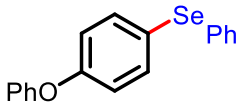



**3a**

The title compound **3a** was synthesized according to the general procedure (24 h) and was obtained

after purification by column chromatography on silica gel (hexane only) as colorless oil (69%, 38.4 mg); TLC $R_f$ = 0.6; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.32 (m, 4H), 7.28-7.24 (m, 4H), 7.21-7.16 (m, 1H), 7.12 (tt, *J* = 7.0, 1.2 Hz, 1H), 7.03 (dt, *J* = 7.7, 1.1 Hz, 2H), 6.97 – 6.94 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.48, 156.65, 137.36, 134.35, 129.98, 129.59, 129.20, 128.31, 126.53, 123.89, 119.43; HR-MS (ESI) *m/z* calcd for $C_{18}H_{14}OS$ $[M+H]^+$ : 279.0840; found: 279.0838.

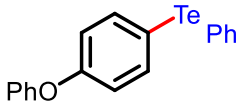
**(4-Phenoxyphenyl)(phenyl)selane (3b)[2]**




**3b**

The title compound **3b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as yellow liquid (84%, 54.6 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.48 (m, 2H), 7.45 – 7.43 (m, 2H), 7.37 – 7.33 (m, 2H), 7.28 – 7.21 (m, 3H), 7.16 – 7.11 (m, 1H), 7.06 – 7.03 (m, 2H), 6.96 – 6.92 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.53, 156.64, 135.79, 132.24, 131.99, 129.94, 129.37, 127.04, 123.82, 123.66, 119.58, 119.38; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 403.39; HR-MS (ESI) *m/z* calcd for $C_{18}H_{14}OSe$ $[M]^+$ : 326.0205; found: 326.0209.

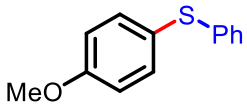
**(4-Phenoxyphenyl)(phenyl)tellane (3c)**




**3c**

The title compound **3c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as white solid (86%, 64.3 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.73 – 7.70 (m, 2H), 7.43 – 7.38 (m, 2H), 7.34 – 7.30 (m, 1H), 7.28 – 7.24 (m, 2H), 7.18 (tt, *J* = 7.0, 1.1 Hz, 1H), 7.10 – 7.06 (m, 2H), 6.94 – 6.90 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 158.04, 156.62, 140.67, 137.39, 129.99, 129.61, 127.79, 123.91, 119.90, 119.52, 115.36, 106.75; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 676.66; HR-MS (ESI) *m/z* calcd for $C_{18}H_{14}OTe$ $[M]^+$ : 376.0102; found: 376.0103.

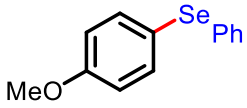
**(4-Methoxyphenyl)(phenyl)sulfane (4a)**[1]




**4a**

The title compound **4a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as colorless oil (58%, 25.0 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.45 (m, 2H), 7.30 – 7.25 (m, 2H), 7.23 – 7.16 (m, 3H), 6.96 – 6.92 (m, 2H), 3.86 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.95, 138.73, 135.49, 129.04, 128.30, 125.87, 124.40, 115.10, 55.47; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OS$ $[M+H]^+$ : 217.0682; found: 217. 0680; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OS$ $[M]^+$ : 216.0603; found: 216.0602.

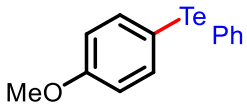
**(4-methoxyphenyl)(phenyl)selane (4b)**[3]




**4b**

The title compound **4b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow liquid (84%, 44.2 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.63-7.61 (m, 2H), 7.46 – 7.43 (m, 2H), 7.33 – 7.28 (m, 3H), 6.96 (dd, *J* = 8.7, 2.0 Hz, 2H), 3.89 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.87, 136.64, 133.31, 130.97, 129.24, 126.53, 120.00, 115.22, 55.37; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 397.54; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OSe$ $[M]^+$ : 264.0048; found: 264.0053.

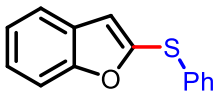
**(4-methoxyphenyl)(phenyl)tellane (4c)**[3]




**4c**

The title compound **4c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow solid (89%, 55.5 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.72 (m, 2H), 7.57 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.23 – 7.15 (m, 3H), 6.82 – 6.79 (m, 2H), 3.81 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 160.14, 141.34, 136.53, 129.49, 127.40, 116.05, 115.67, 103.33, 55.31; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 664.61; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OTe$ $[M]^+$ : 313.9945; found: 313.9947

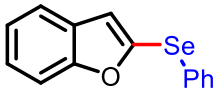
**2-(Phenylthio)benzofuran (5a)[4]**




**5a**

The title compound **5a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (hexane only) as colorless oil (68%, 30.7 mg); TLC $R_f$ = 0.6; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.62-7.59 (m, 1H), 7.51-7.49 (m, 1H), 7.39 – 7.25 (m, 7H), 7.08 (d, *J* = 1.0 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 156.92, 148.03, 134.38, 129.39, 129.20, 128.49, 127.65, 127.25, 125.33, 123.20, 121.07, 114.52, 111.54; HR-MS (ESI) *m/z* calcd for $C_{14}H_{10}OS$ $[M+H]^+$ : 227.2525; found: 227.2527.

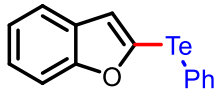
**2-(Phenylselanyl)benzofuran (5b)[3]**




**5b**

The title compound **5b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as yellow liquid (84%, 45.8 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.3 Hz, 1H), 7.73 – 7.67 (m, 3H), 7.53 – 7.42 (m, 5H), 7.26 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.63, 143.72, 131.71, 129.97, 129.57, 128.66, 127.65, 124.97, 123.10, 120.81, 116.03, 111.42; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 330.81; HR-MS (ESI) *m/z* calcd for $C_{14}H_{10}OSe$ $[M]^+$ : 273.9892; found: 273.9891.

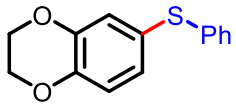
**2-(Phenyltellanyl)benzofuran (5c)[3]**




**5c**

The title compound **5c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as white solid (92%, 59.2 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 6.8 Hz, 2H), 7.60 (d, *J* = 6.9 Hz, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.34 – 7.24 (m, 6H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.24, 137.25, 129.77, 129.04, 128.25, 127.08, 124.94, 122.94, 122.49, 120.64, 114.22, 111.33; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 557.40; HR-MS (ESI) *m/z* calcd for $C_{14}H_{10}OTe$ $[M]^+$ : 323.9789; found: 323.9792.

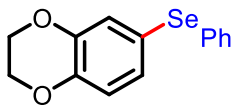
**6-(Phenylthio)-2,3-dihydrobenzo[*b*][1,4]dioxine (6a)[5]**




**6a**

The title compound **6a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (5% ethyl acetate in hexane) as colorless liquid (60%, 29.3 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 4H), 7.21 – 7.16 (m, 1H), 7.01 (d, *J* = 2.2 Hz, 1H), 6.96 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 4.28 – 4.24 (m, 4H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 144.05, 143.87, 137.82, 129.14, 129.09, 126.57, 126.25, 125.89, 122.11, 118.19, 64.45, 64.34; HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}O_2S$ $[M+H]^+$ : 245.0636; found: 245.0640.

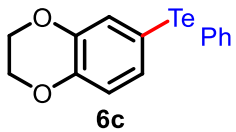
**6-(phenylselanyl)-2,3-dihydrobenzo[*b*][1,4]dioxine (6b)[5]**




**6b**

The title compound **6b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2% ethyl acetate in hexane) as yellow liquid (82%, 47.7 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.41 (m, 2H), 7.24 (dd, *J* = 3.6, 2.4 Hz, 3H), 7.12 (d, *J* = 2.0 Hz, 1H), 7.08 – 7.05 (m, 1H), 6.83 (dd, *J* = 8.3, 2.9 Hz, 1H), 4.24 (d, *J* = 5.9 Hz, 4H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 144.07, 143.84, 132.59, 131.62, 129.26, 127.84, 126.81, 123.46, 121.01, 118.26, 64.35, 64.28; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 408.58; HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}O_2Se$ $[M+Na]^+$ : 264.9738; found: 264.9735.

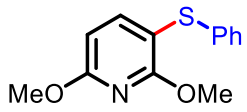
**6-(phenyltellanyl)-2,3-dihydrobenzo[*b*][1,4]dioxine (6c)**




**6c**

The title compound **6c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2% ethyl acetate in hexane) as yellow oil (86%, 58.4 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.63 (m, 2H), 7.32 (d, *J* = 1.9 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.22 – 7.18 (m, 2H), 6.75 (d, *J* = 8.2 Hz, 1H), 4.24 (d, *J* = 1.2 Hz, 4H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 144.29, 144.24, 137.10, 132.64, 129.49, 128.16, 127.58, 118.66, 115.60, 103.84, 64.42, 64.31; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 687.74; HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}O_2Te$ $[M]^+$ : 341.9895; found: 341.9900.

**2,6-Dimethoxy-3-(phenylthio)pyridine (7aa)[6]**

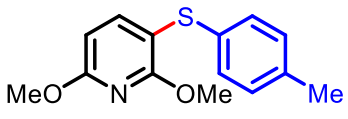



**7aa**

The title compound **7aa** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as pale yellow oil (64%, 31.6 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.1 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.17 – 7.13 (m, 3H), 6.34 (d, *J* = 8.1 Hz, 1H), 3.97 (s, 3 H), 3.96 (s, 3 H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.74, 162.42, 147.30, 137.10, 129.02, 128.03, 125.89,

105.18, 102.34, 54.21, 53.91; HR-MS (ESI) *m/z* calcd for $C_{13}H_{13}NO_2S$ $[M+H]^+$ : 248.0746; found: 248.0741.

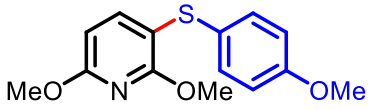
**2,6-Dimethoxy-3-(*p*-tolylthio)pyridine (7ab)**




**7ab**

The title compound **7ab** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as colorless oil (66%, 34.5 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.1 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 9.4 Hz, 2H), 6.30 (d, *J* = 8.1 Hz, 1H), 3.97 (s, 3H), 3.93 (s, 3H), 2.30 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.31, 161.80, 146.15, 136.30, 132.80, 129.90, 129.32, 128.67, 106.64, 102.16, 54.18, 53.89, 21.14; HR-MS (ESI) *m/z* calcd for $C_{14}H_{15}NO_2S$ $[M+H]^+$ : 262.0896; found: 262.0897.

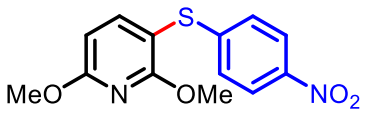
**2,6-Dimethoxy-3-((4-methoxyphenyl)thio)pyridine (7ac)**




**7ac**

The title compound **7ac** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as colorless oil (48%, 26.6 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 8.9 Hz, 2H), 6.83 (d, *J* = 9.0 Hz, 2H), 6.25 (d, *J* = 8.1 Hz, 1H), 3.97 (s, 3H), 3.91 (s, 3H), 3.78 (s, 3H); 13C NMR (101 MHz, $CDCl_3$) δ 162.70, 160.75, 159.16, 144.21, 132.87, 125.79, 114.86, 108.69, 101.93, 55.43, 54.06, 53.82; HR-MS (ESI) *m/z* calcd for $C_{14}H_{15}NO_3S$ $[M+H]^+$ : 278.0851; found: 278.0852.

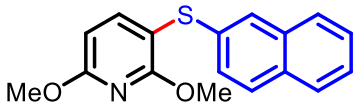
**2,6-Dimethoxy-3-((4-nitrophenyl)thio)pyridine (7ad)**




**7ad**

The title compound **7ad** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as pale yellow solid (53%, 31.0 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.9 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.08 (d, *J* = 9.0 Hz, 2H), 6.42 (d, *J* = 8.1 Hz, 1H), 3.99 (s, 3H), 3.94 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 165.05, 163.39, 148.90, 148.41, 145.23, 125.48, 124.07, 103.21, 100.95, 54.42, 54.10; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}N_2O4S$ $[M+H]^+$ : 293.0596; found: 293.0594.

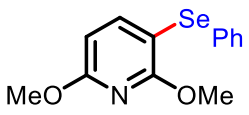
**2,6-Dimethoxy-3-(naphthalen-2-ylthio)pyridine (7ae)**




**7ae**

The title compound **7ae** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as colorless oil (59%, 35.0 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.2 Hz, 1H), 7.71 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.57 (s, 1H), 7.46 – 7.39 (m, 2H), 7.29 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.36 (d, *J* = 8.1 Hz, 1H), 3.97 (d, *J* = 2.7 Hz, 6H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.77, 162.41, 147.24, 134.53, 133.90, 131.87, 128.63, 127.83, 127.23, 126.59, 126.47, 126.20, 125.68, 105.24, 102.41, 54.25, 53.94; HR-MS (ESI) *m/z* calcd for $C_{17}H_{15}NO_2S$ $[M+H]^+$ : 298.0896; found: 298.0899.

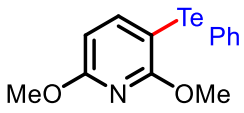
**2,6-Dimethoxy-3-(phenylselenyl)pyridine (7b)[7]**




**7b**

The title compound **7b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow liquid (80%, 47.0 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.1 Hz, 1H), 7.41 – 7.39 (m, 2H), 7.24 (dd, *J* = 5.0, 2.3 Hz, 3H), 6.25 (d, *J* = 8.1 Hz, 1H), 3.96 (s, 3H), 3.92 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.42, 161.29, 146.34, 132.34, 130.73, 129.35, 127.17, 102.40, 54.17, 53.81; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 627.32; HR-MS (ESI) *m/z* calcd for $C_{13}H_{13}NO_2Se$ $[M+H]^+$ : 296.0185; found: 296.0188.

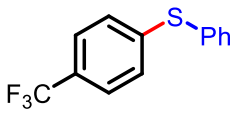
**2,6-Dimethoxy-3-(phenyltellanyl)pyridine (7c)[7]**




**7c**

The title compound **7c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow liquid (90%, 61.7 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.3 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.24 (t, *J* = 7.3 Hz, 2H), 6.20 (d, *J* = 8.0 Hz, 1H), 3.96 (s, 3H), 3.90 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.98, 161.98, 147.95, 139.37, 129.67, 128.33, 113.16, 103.16, 86.61, 54.22, 53.70; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 561.50; HR-MS (ESI) *m/z* calcd for $C_{13}H_{13}NO_2Te$ $[M+H]^+$ : 346.0082; found: 346.0085.

**Phenyl(4-(trifluoromethyl)phenyl)sulfane (8a)[1]**

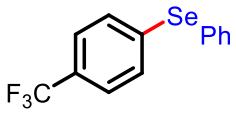



**8a**

The title compound **8a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (hexane only) as colorless oil (41%, 20.8 mg); TLC $R_f$ = 0.7; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.48 (m, 4H), 7.43 – 7.38 (m, 3H), 7.28 (d, *J* = 8.1 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 143.00, 142.98, 133.68, 132.63, 129.82, 128.79, 128.42, 128.33, 128.00, 126.01, 125.95 (q, J = 3.8 Hz), 125.59, 122.89; $^{19}$F NMR (376

MHz, $CDCl_3$) δ -62.48; HR-MS (ESI) *m/z* calcd for $C_{13}H_9F_3S$ $[M+H]^+$ : 255.0450; found: 255.0447.

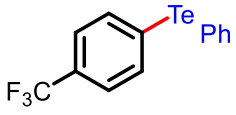
**Phenyl(4-(trifluoromethyl)phenyl)selane (8b)[3]**




**8b**

The title compound **8b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as yellow oil (65%, 39.0 mg); TLC $R_f$ = 0.6; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.59 (m, 2H), 7.50 – 7.44 (m, 4H), 7.40-7.35 (m, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 137.96, 134.99, 131.13, 129.86, 128.67, 126.08, 126.05, 126.0 (q, J = 3.7 Hz); $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -62.57 (d, *J* = 4.5 Hz); $^{77}Se$ NMR (95 MHz, $CDCl_3$) δ 422.96; HR-MS (ESI) *m/z* calcd for $C_{13}H_9F_3Se$ $[M]^+$ : 301.9816; found: 301.9818.

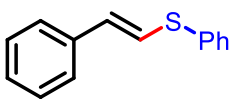
**Phenyl(4-(trifluoromethyl)phenyl)tellane (8c)[3]**




**8c**

The title compound **8c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as yellow liquid (72%, 50.3 mg); TLC $R_f$ = 0.6; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.68 (d, *J* = 8.5 Hz, 2H), 7.44 – 7.37 (m, 3H), 7.33 – 7.28 (m, 2H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 139.55, 138.15, 136.53, 129.98, 128.84, 126.00 (q, *J* = 3.8 Hz), 122.87, 121.19, 121.18, 113.47; $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -62.82; $^{125}Te$ NMR (158 MHz, $CDCl_3$) δ 708.64; HR-MS (ESI) *m/z* calcd for $C_{13}H_9F_3Te$ $[M]^+$ : 351.9713; found: 351.9714.

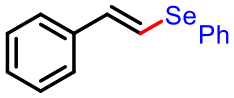
**(*E*)-phenyl(styryl)sulfane (9a)[8]**




**9a**

The title compound **9a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (hexane only) as yellow oil (52%, 22.0 mg); TLC $R_f$ = 0.6; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.0 Hz, 2H), 7.32 (t, *J* = 8.7 Hz, 6H), 7.28 – 7.20 (m, 3H), 6.88 (d, *J* = 15.5 Hz, 1H), 6.73 (d, *J* = 15.5 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.66, 135.37, 131.95, 129.97, 129.30, 128.83, 127.73, 127.09, 126.17, 123.53; HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}S$ $[M+H]^+$ : 213.0736; found: 213.0740.

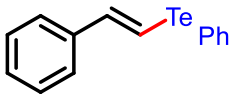
**(*E*)-phenyl(styryl)selane (9b)[8]**




**9b**

The title compound **9b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as colorless oil (83%, 43.0 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.48 (m, 2H), 7.28 – 7.22 (m, 7H), 7.19 – 7.16 (m, 1H), 7.12 (d, *J* = 15.8 Hz, 1H), 6.82 (d, *J* = 15.7 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 137.07, 135.20, 132.61, 130.26, 129.43, 128.75, 127.73, 127.72, 127.49, 126.16, 126.15, 119.53; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 384.62; HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}Se$ $[M+H]^+$ : 261.0178; found: 261.0179.

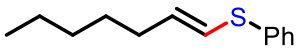
**(*E*)-phenyl(styryl)tellane (9c)[9]**




**9c**

The title compound **9c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as pale yellow oil (88%, 54.0 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.77 (m, 2H), 7.58 (d, *J* = 16.6 Hz, 1H), 7.35 – 7.25 (m, 8H), 7.14 (d, *J* = 16.6 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 143.36, 138.12, 137.95, 129.63, 128.70, 128.04, 127.98, 127.57, 126.23, 113.57, 109.27, 101.62; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 604.51; HR-MS (ESI) *m/z* calcd for $C_{14}H_{12}Te$ $[M]^+$ : 309.9996; found: 310.0000.

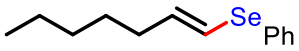
**(*E*)-hept-1-en-1-yl(phenyl)sulfane (10a)**[10]



**10a**

The title compound **10a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (hexane only) as yellow liquid (43%, 17.7 mg); TLC $R_f$ = 0.6; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.29 (m, 4H), 7.22 – 7.17 (m, 1H), 6.23 – 6.13 (m, 1H), 6.06 – 5.82 (m, 1H), 2.27 (q, *J* = 6.6 Hz, 1H), 2.18 (q, *J* = 6.8 Hz, 1H), 1.49 – 1.42 (m, 2H), 1.37 – 1.31 (m, 4H), 0.92 (t, *J* = 6.4 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 137.98, 136.84, 136.70, 133.88, 129.06, 129.04, 128.85, 128.48, 126.20, 126.10, 122.65, 120.74, 33.19, 31.55, 31.44, 29.23, 28.82, 22.61, 14.19; HR-MS (ESI) *m/z* calcd for $C_{13}H_{18}S$ $[M]^+$ : 206.1123; found: 206.1112.

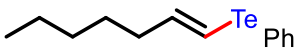
**(*E*)-hept-1-en-1-yl(phenyl)selane (10b)**[11]



**10b**

The title compound **10b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as yellow oil (45%, 22.7 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.1 Hz, 2H), 7.30 – 7.22 (m, 3H), 6.41 (d, *J* = 14.0 Hz, 1H), 6.17 – 6.09 (m, 1H), 2.20 – 2.15 (m, 2H), 1.45 (p, *J* = 7.4 Hz, 2H), 1.33 (q, *J* = 3.7 Hz, 4H), 0.92 (t, *J* = 6.5 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 140.81, 135.54, 131.39, 129.21, 126.71, 116.02, 34.38, 31.40, 28.65, 22.58, 14.16; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 360.84; HR-MS (ESI) *m/z* calcd for $C_{13}H_{18}Se$ $[M]^+$ : 254.0569; found: 254.0571.

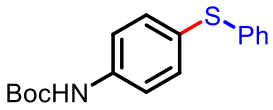
**(*E*)-hept-1-en-1-yl(phenyl)tellane (10c)**[11]



**10c**

The title compound **10c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (hexane only) as pale yellow oil (48%, 29.0 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.69 (m, 2H), 7.33 – 7.23 (m, 3H), 6.77 (dt, *J* = 15.9, 1.4 Hz, 1H), 6.42 (dt, *J* = 16.0, 6.8 Hz, 1H), 2.27 – 2.21 (m, 2H), 1.51 – 1.44 (m, 2H), 1.40 – 1.30 (m, 4H), 0.94 (t, J = 6.8 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 149.35, 136.92, 129.41, 127.46, 114.29, 98.12, 36.86, 31.40, 28.53, 22.60, 14.17; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 565.00; HR-MS (ESI) *m/z* calcd for $C_{13}H_{18}Te$ $[M]^+$ : 304.0466; found: 304.0471.

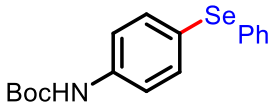
***tert*-Butyl (4-(phenylthio)phenyl)carbamate (11a)[12]**




**11a**

The title compound **11a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (10-15% ethyl acetate in hexane) as yellow solid (41%, 24.7 mg); TLC $R_f$ = 0.3; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 4H), 7.25 – 7.19 (m, 4H), 7.19 – 7.13 (m, 1H), 6.63 (s, 1H), 1.52 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 152.69, 138.45, 137.75, 134.00, 129.11, 129.10, 127.70, 126.25, 119.35, 80.94, 28.41; HR-MS (ESI) *m/z* calcd for $C_{17}H_{19}NO_2S$ $[M+H]^+$ : 302.1213; found: 302.1209.

***tert*-Butyl (4-(phenylselanyl)phenyl)carbamate (11b)**

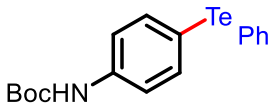



**11b**

The title compound **11b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (10-15% ethyl acetate in hexane) as yellow oil (52%, 36.2 mg); TLC $R_f$ = 0.2; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.46 (m, 2H), 7.38 – 7.35 (m, 2H), 7.32 (d, *J* = 8.7 Hz, 2H), 7.25 – 7.20 (m, 3H), 6.59 (s, 1H), 1.52 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 152.69, 138.49, 135.47, 132.65, 131.55, 129.31, 126.82, 123.23, 119.47,

80.93, 28.42; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 402.96; HR-MS (ESI) *m/z* calcd for $C_{17}H_{19}NO_2Se$ $[M+Na]^+$ : 372.0479; found: 372. 0474.

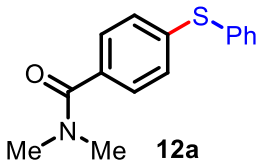
***tert*-Butyl (4-(phenyltellanyl)phenyl)carbamate (11c)**




**11c**

The title compound **11c** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (10-15% ethyl acetate in hexane) as dark brown liquid (60%, 47.6 mg); TLC $R_f$ = 0.2; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.6 Hz, 2H), 7.59 (d, *J* = 6.2 Hz, 2H), 7.30 – 7.16 (m, 5H), 6.54 (s, 1H), 1.52 (s, 8H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 152.65, 140.27, 138.81, 136.89, 129.52, 129.09, 127.55, 123.15, 119.68, 115.67, 106.51, 80.96, 28.43; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 673.81; HR-MS (ESI) *m/z* calcd for $C_{17}H_{19}NO_2Te$ $[M+Na]^+$ : 422.0376; found: 422.0375.

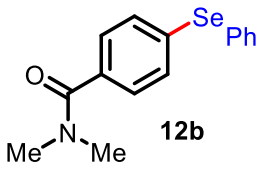
***N,N*-dimethyl-4-(phenylthio)benzamide (12a)**




**12a**

The title compound **12a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (50% ethyl acetate in hexane) as colorless oil (44%, 22.6 mg); TLC $R_f$ = 0.2; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.1 Hz, 3H), 7.31 – 7.20 (m, 6H), 3.03 (s, 3H), 2.92 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.84, 138.77, 134.20, 133.84, 132.26, 129.40, 129.35, 129.21, 128.24, 127.86, 127.82, 126.93, 39.48, 35.29; HR-MS (ESI) *m/z* calcd for $C_{15}H_{15}NOS$ $[M+H]^+$ : 258.0947; found: 258.0949.

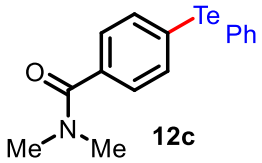
***N,N* -dimethyl-4-(phenylselanyl)benzamide (12b)[13]**




**12b**

The title compound **12b** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (50% ethyl acetate in hexane) as yellow liquid (53%, 32.2 mg); TLC $R_f$ = 0.1; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.37 (m, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.18-7.16 (m, 5H), 2.95 (s, 3H), 2.83 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.80, 134.71, 133.77, 133.76, 131.57, 129.39, 129.35, 128.18, 127.86, 127.82, 126.88, 39.42, 35.21; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 416.94; HR-MS (ESI) *m/z* calcd for $C_{15}H_{15}NOSe$ $[M+H]^+$ : 306.0390; found: 306.0394.

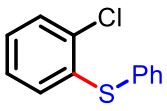
***N,N*-dimethyl-4-(phenyltellanyl)benzamide (12c)[13]**




**12c**

The title compound **12c** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (50% ethyl acetate in hexane) as pale yellow oil (67%, 47.2 mg); TLC $R_f$ = 0.1; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.66 – 7.62 (m, 2H), 7.39 (d, *J* = 2.1 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.24 – 7.21 (m, 3H), 3.07 (s, 3H), 2.95 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.11, 138.72, 137.08, 135.61, 129.73, 129.55, 128.39, 128.33, 128.05, 127.09, 117.24, 114.02, 39.63, 35.41; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 697.21; HR-MS (ESI) *m/z* calcd for $C_{15}H_{15}NOTe$ $[M+H]^+$ : 356.0294; found: 356.0297.

**(2-Chlorophenyl)(phenyl)sulfane (13a)[6]**

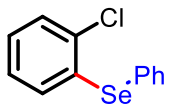



**13a**

The title compound **13a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (1-2% ethyl acetate in hexane)

as pale yellow oil (42%, 18.5 mg); TLC $R_f$ = 0.6; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 8.0, 1.8 Hz, 2H), 7.42 – 7.35 (m, 4H), 7.16 – 7.09 (m, 2H), 7.01 – 6.99 (m, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.63, 133.36, 132.81, 130.22, 129.86, 129.70, 129.18, 128.43, 127.61, 127.36, 127.32, 127.27; HR-MS (ESI) *m/z* calcd for $C_{12}H_9ClS$ $[M+H]^+$ : 221.0194; found: 221.0190.

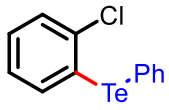
**(2-Chlorophenyl)(phenyl)selane (13b)[14]**




**13b**

The title compound **13b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (1-2% ethyl acetate in hexane) as yellow liquid (57%, 30.5 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.64 (m, 2H), 7.45 – 7.35 (m, 4H), 7.13 (td, *J* = 7.6, 1.7 Hz, 1H), 7.05 (td, *J* = 7.5, 1.4 Hz, 1H), 6.96 (dd, *J* = 7.9, 1.7 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.14, 133.95, 133.56, 130.74, 129.88, 129.49, 128.95, 127.99, 127.39, 127.38; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 409.00; HR-MS (ESI) *m/z* calcd for $C_{12}H_9ClSe$ $[M]^+$ : 267.9550; found: 267.9551.

**(2-Chlorophenyl)(phenyl)tellane (13c)[15]**




**13c**

The title compound **13c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (1-2% ethyl acetate in hexane) as pale yellow liquid (63%, 39.8 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.0 Hz, 2H), 7.49 – 7.45 (m, 1H), 7.38 – 7.31 (m, 3H), 7.12 (td, *J* = 8.6, 4.8 Hz, 1H), 6.97 (t, *J* = 3.9 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 141.37, 136.58, 134.43, 130.10, 129.31, 128.84, 128.15, 127.53, 120.70, 113.43; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 666.82; HR-MS (ESI) *m/z* calcd for $C_{12}H_9ClTe$ $[M]^+$ : 317.9439; found: 317.9444.

**(2-Methoxyphenyl)(phenyl)sulfane (14a)[1]**


**14a**

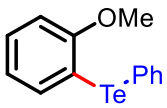
The title compound **14a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as pale yellow oil (46%, 19.8 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.30 (m, 4H), 7.28 – 7.23 (m, 2H), 7.10 (dd, *J* = 7.7, 1.7 Hz, 1H), 6.93 – 6.86 (m, 2H), 3.88 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.42, 134.60, 131.72, 131.58, 129.25, 128.45, 127.17, 124.18, 121.35, 110.97, 55.99; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OS$ $[M+H]^+$ : 217.0684; found: 217.0690.

**(2-Methoxyphenyl)(phenyl)selane (14b)[16]**


**14b**

The title compound **14b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow liquid (59%, 31.0 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 2H), 7.37 – 7.32 (m, 3H), 7.20 (ddd, *J* = 8.1, 7.3, 1.6 Hz, 1H), 6.97 (dd, *J* = 7.7, 1.7 Hz, 1H), 6.87 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.80 (td, *J* = 7.5, 1.2 Hz, 1H), 3.90 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 156.74, 135.57, 130.93, 129.57, 128.39, 128.22, 127.83, 122.03, 121.75, 110.52, 55.99. $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 356.03; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OSe$ $[M]^+$ : 264.0048; found: 264.0052.

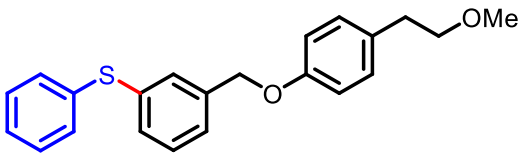
**(2-Methoxyphenyl)phenyl)tellane (14c)[15]**




**14c**

The title compound **14c** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow solid (66%, 41.0 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 6.7 Hz, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.22 – 7.16 (m, 1H), 6.97 (d, *J* = 9.2 Hz, 1H), 6.81 (d, *J* = 8.2 Hz, 1H), 6.76 (t, *J* = 8.1 Hz, 1H), 3.89 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 158.17, 141.30, 133.66, 129.75, 128.76, 128.22, 122.51, 112.16, 109.77, 107.85, 56.01; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 580.68; HR-MS (ESI) *m/z* calcd for $C_{13}H_{12}OTe$ $[M]^+$ : 313.9945; found: 313.9950.

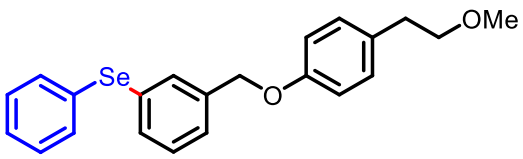
**(3-((4-(2-Methoxyethyl)phenoxy)methyl)phenyl)(phenyl)sulfane (15a)**




**15a**

The title compound **15a** was synthesized according to the general procedure (24 h) and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as colorless liquid (65%, 45.5 mg); TLC $R_f$ = 0.5; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.43 (s, 1H), 7.38 (d, *J* = 6.8 Hz, 2H), 7.35 – 7.27 (m, 6H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 5.00 (s, 2H), 3.62 – 3.57 (m, 2H), 3.38 (s, 3H), 2.86 (t, *J* = 7.1 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.17, 138.47, 136.45, 135.42, 131.54, 131.39, 130.26, 129.90, 129.64, 129.47, 129.34, 127.32, 126.08, 114.88, 73.92, 69.61, 58.76, 35.41; HR-MS (ESI) *m/z* calcd for $C_{22}H_{22}O_2S$ $[M+H]^+$ : 351.1413; found: 351.1415.

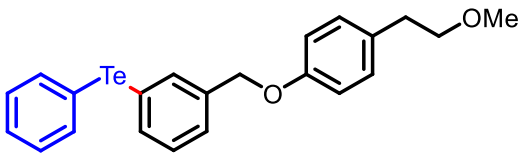
**(3-((4-(2-Methoxyethyl)phenoxy)methyl)phenyl)(phenyl)selane (15b)**




**15b**

The title compound **15b** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as yellow oil (78%, 62.0 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.52-7.49 (m, 2H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.7 Hz, 1H), 7.32 – 7.28 (m, 4H), 7.17 – 7.15 (m, 2H), 6.91 – 6.89 (m, 2H), 5.00 (s, 2H), 3.60 (t, *J* = 7.1 Hz, 2H), 3.38 (s, 3H), 2.86 (t, *J* = 7.1 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.16, 138.52, 133.29, 132.32, 131.67, 131.51, 130.89, 129.89, 129.56, 129.47, 127.55, 126.43, 114.86, 73.91, 69.57, 58.75, 35.40; $^{77}$Se NMR (95 MHz, $CDCl_3$) δ 414.72; HR-MS (ESI) *m/z* calcd for $C_{22}H_{22}O_2Se$ $[M+H]^+$ : 399.0857; found: 399.0850.

**(3-((4-(2-Methoxyethyl)phenoxy)methyl)phenyl)(phenyl)tellane (15c)**




**15c**

The title compound **15c** was synthesized according to the general procedure and was obtained after purification by column chromatography on silica gel (2-5% ethyl acetate in hexane) as colorless oil (86%, 76.7 mg); TLC $R_f$ = 0.4; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.71 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 6.9 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.23 (td, *J* = 7.6, 1.8 Hz, 3H), 7.15 – 7.13 (m, 2H), 6.89 – 6.87 (m, 2H), 4.98 (s, 2H), 3.58 (t, *J* = 7.1 Hz, 2H), 3.37 (s, 3H), 2.84 (t, *J* = 7.1 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.22, 138.55, 138.21, 137.42, 136.77, 131.53, 129.91, 129.71, 129.66, 128.04, 127.07, 115.08, 114.89, 114.61, 73.95, 69.60, 58.78, 35.43; $^{125}$Te NMR (158 MHz, $CDCl_3$) δ 693.55; HR-MS (ESI) *m/z* calcd for $C_{22}H_{22}O_2Te$ $[M+Na]^+$: 471.0580; found: 471.0576.

## 9. References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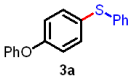
# 10. NMR spectra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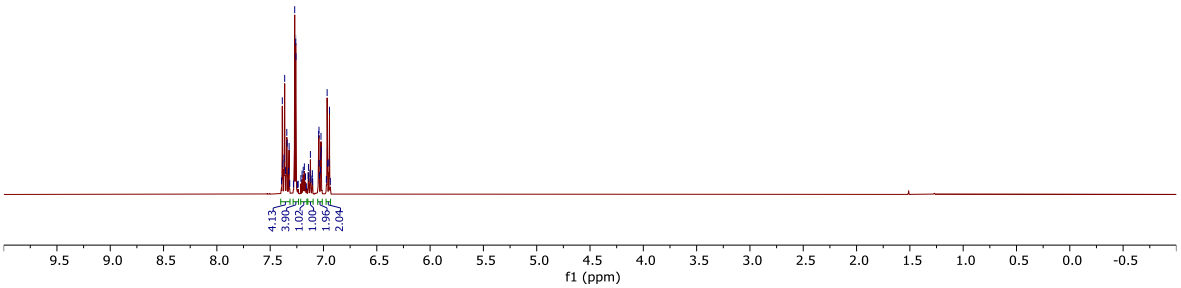



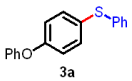


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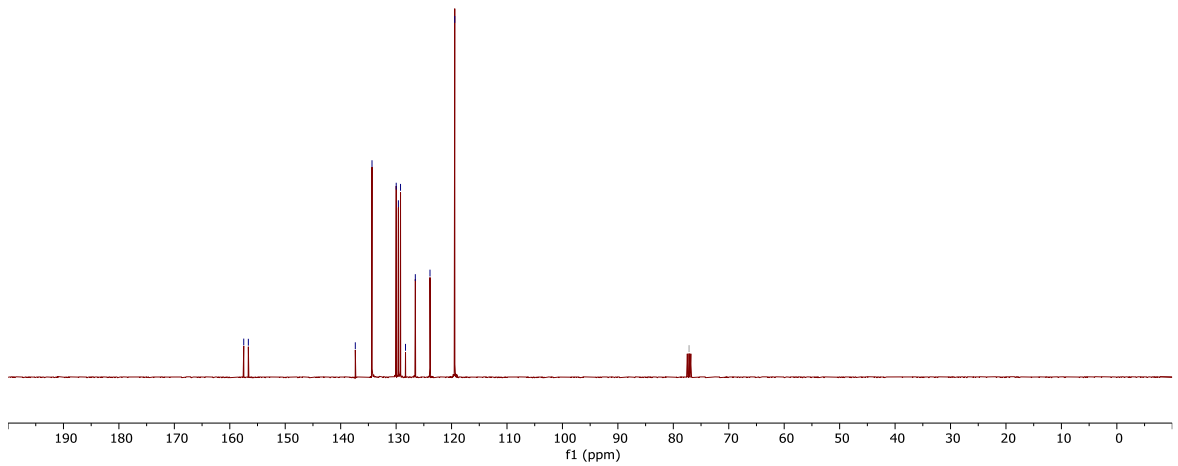

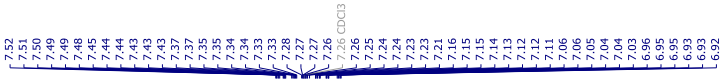
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7.50
7.49
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7.48
7.45
7.44
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7.43
7.43
7.43
7.37
7.37
7.35
7.35
7.34
7.34
7.33
7.33
7.28
7.27
7.27
7.26
CDCl3
7.26
7.25
7.24
7.24
7.23
7.23
7.21
7.16
7.15
7.15
7.14
7.13
7.12
7.12
7.11
7.06
7.06
7.05
7.04
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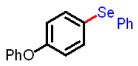
6.96
6.95
6.95
6.93
6.93
6.92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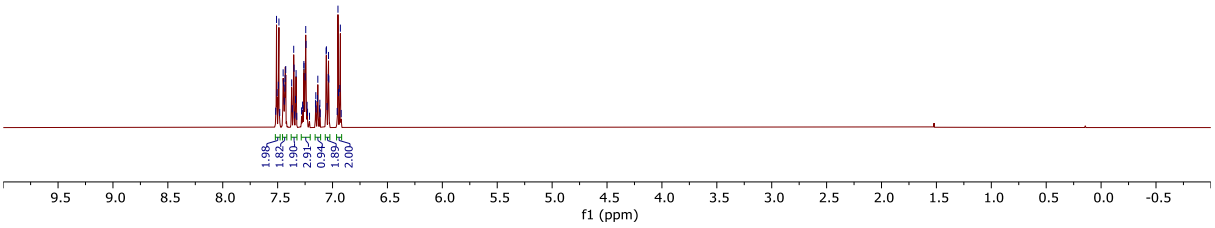
Ph
PhO

**3b**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1.89
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
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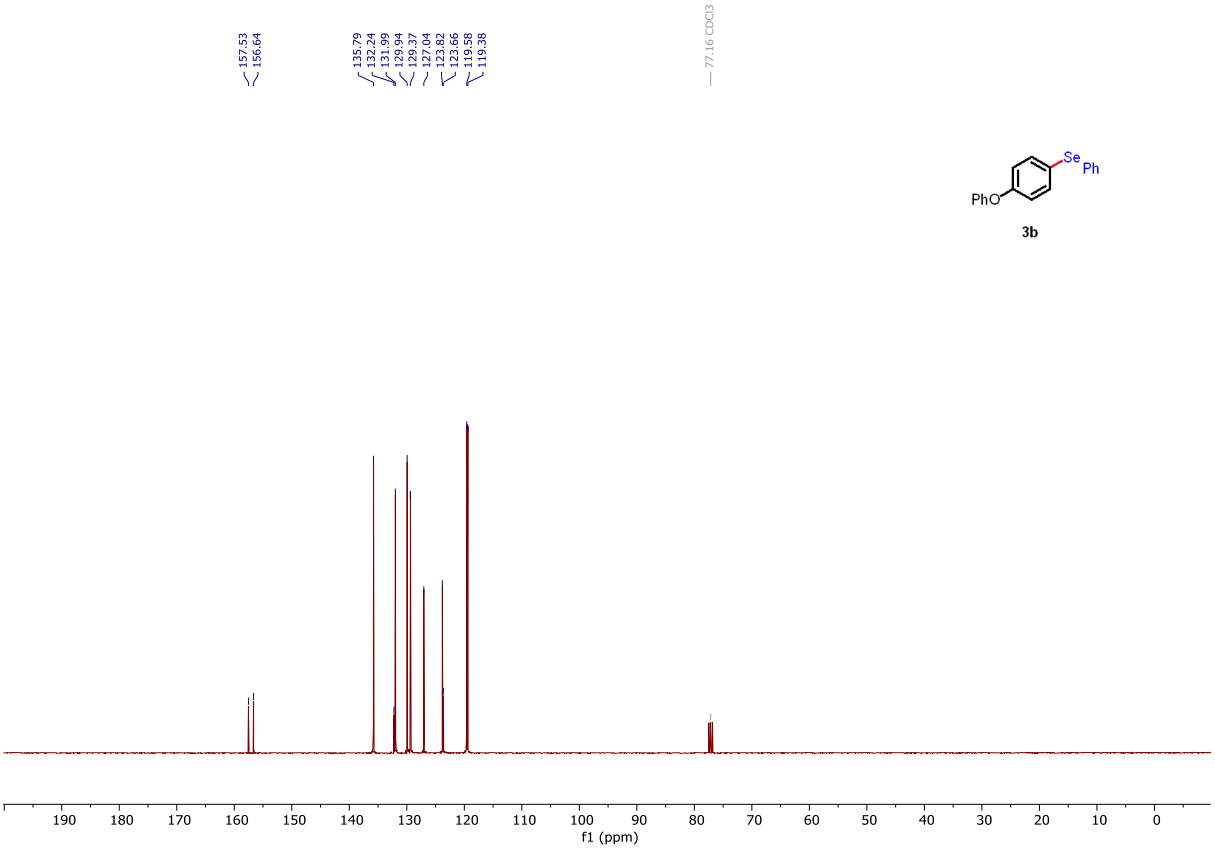
1.0
0.5
0.0
-0.5
f1 (ppm)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156.64
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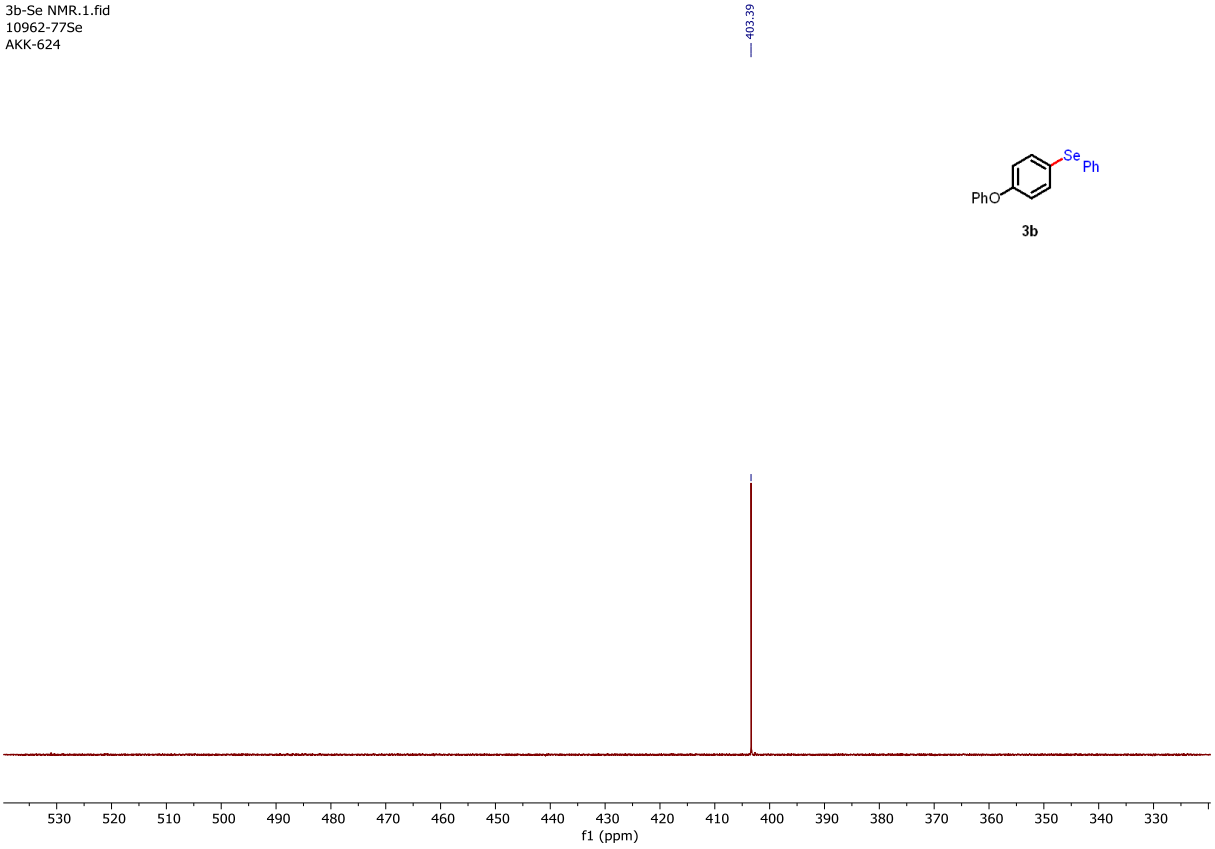
127.04
123.82
123.66
119.58
119.38
77.16 CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Se
Ph
PhO

**3b**

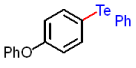
3b-Se NMR.1.fid
10962-77Se
AKK-624







**3b**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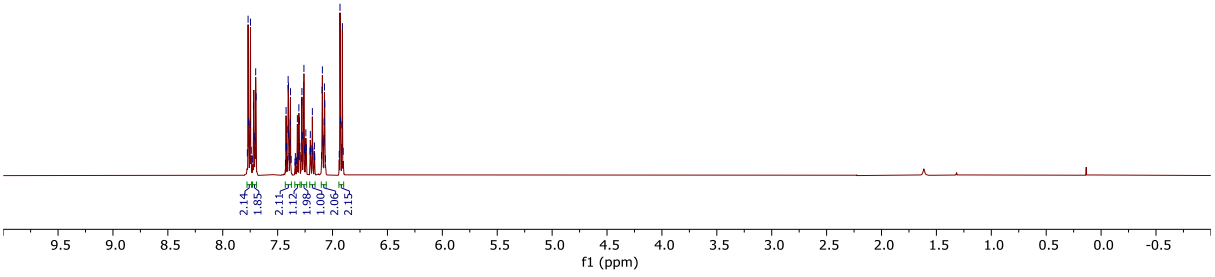

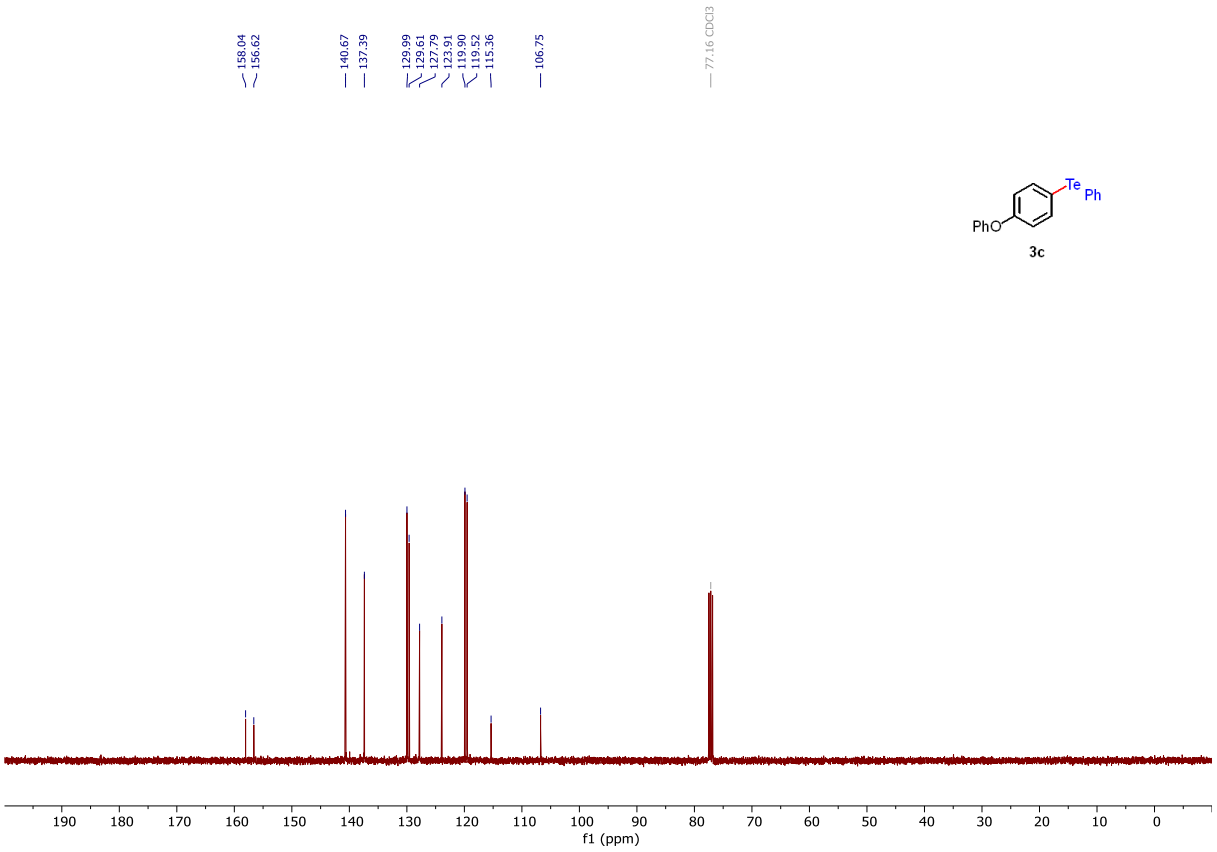


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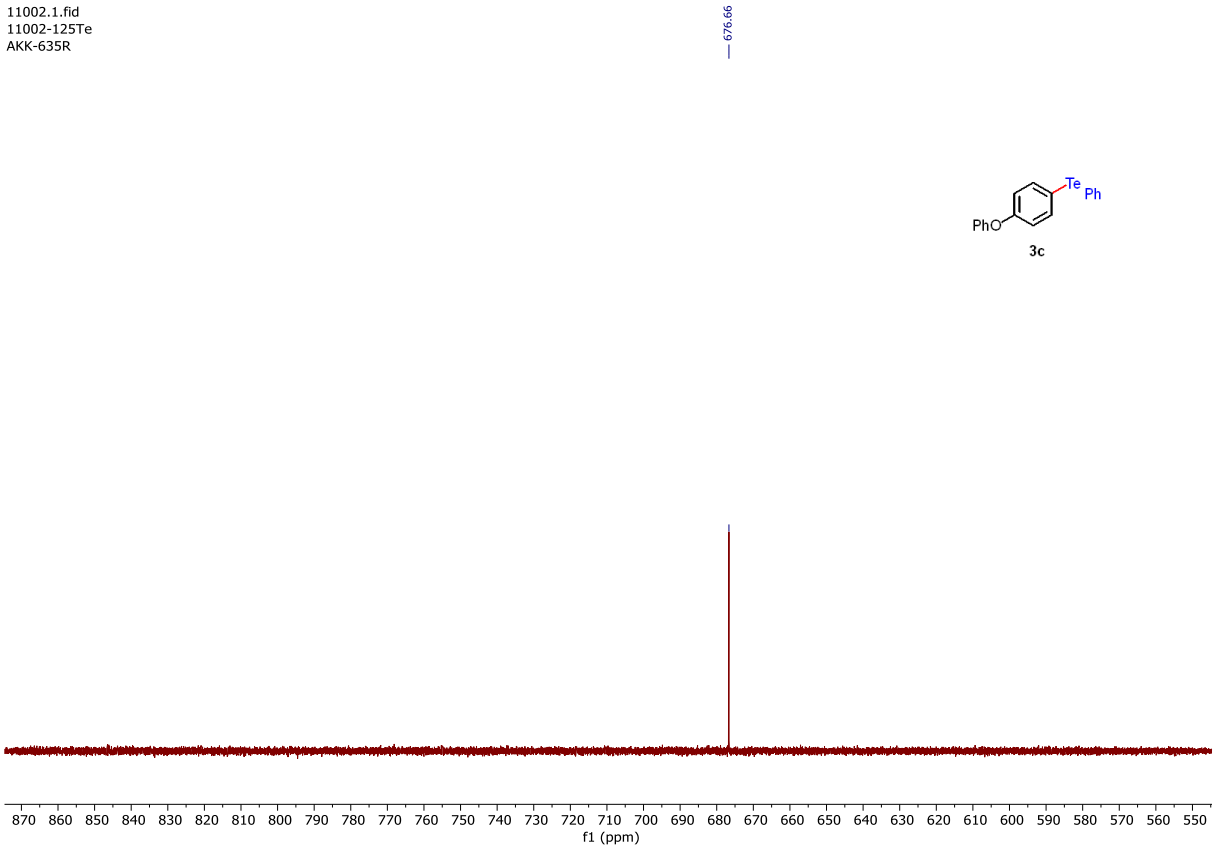

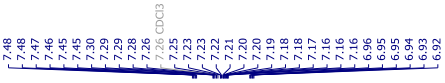
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7.45
7.30
7.29
7.29
7.28
7.26
7.26 CDCl3
7.25
7.23
7.23
7.22
7.21
7.20
7.20
7.19
7.18
7.18
7.17
7.16
7.16
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6.95
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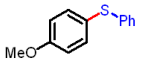
6.93
6.92


3.86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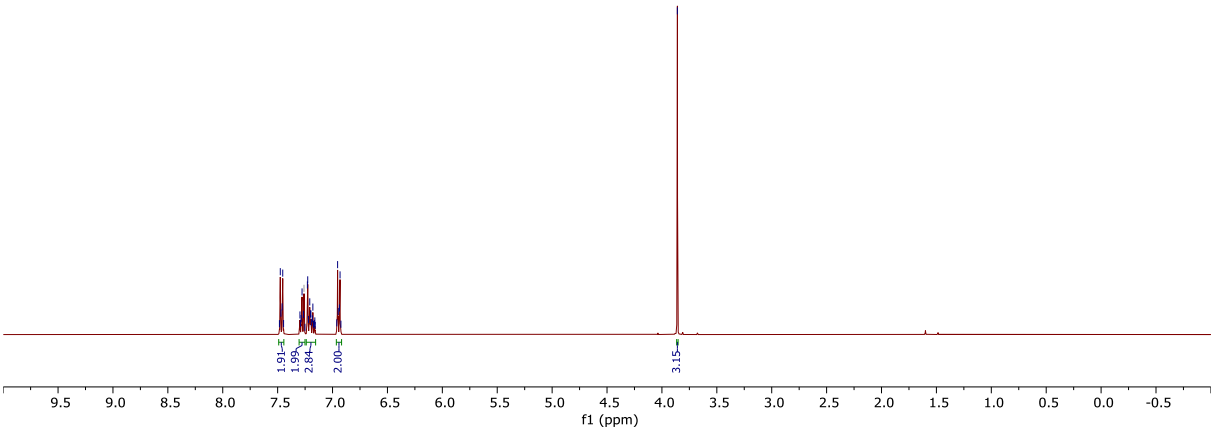
Ph
MeO

**4a**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8.5
8.0
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


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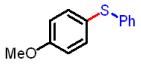
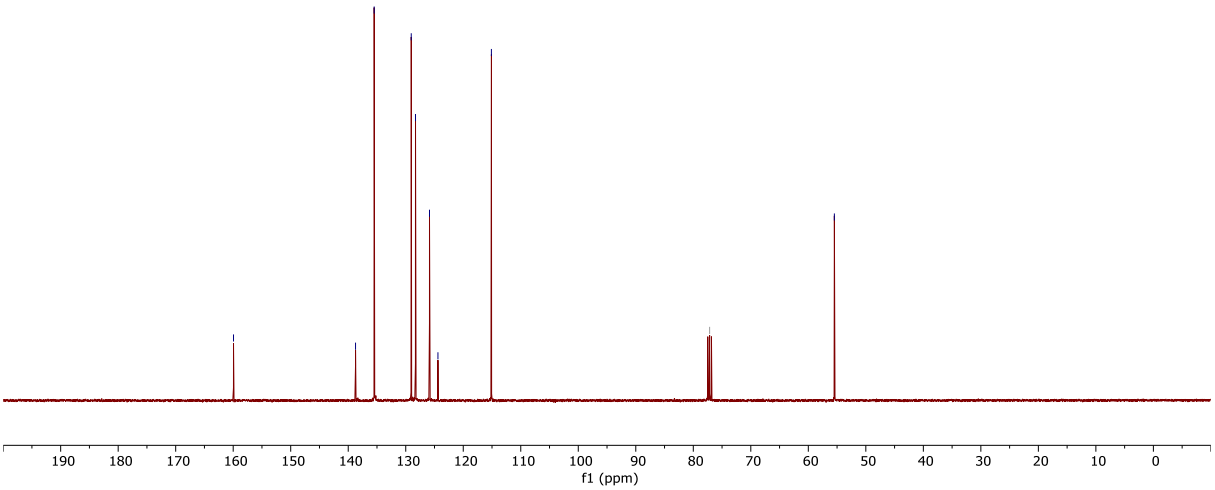
138.73
135.49
129.04
128.30
125.87
124.40
115.10
77.16 CDCl3
55.47


S
Ph
MeO

**4a**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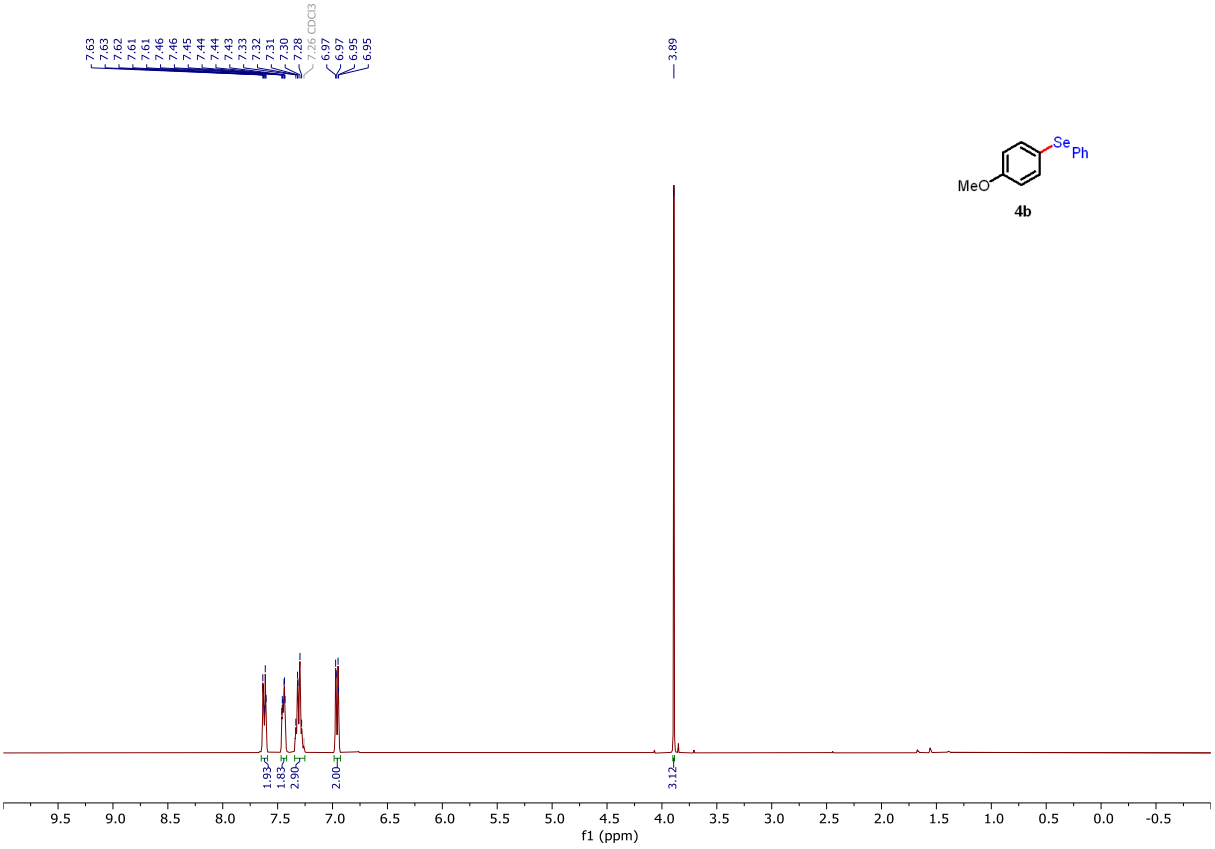
40
30
20
10
0
f1 (ppm)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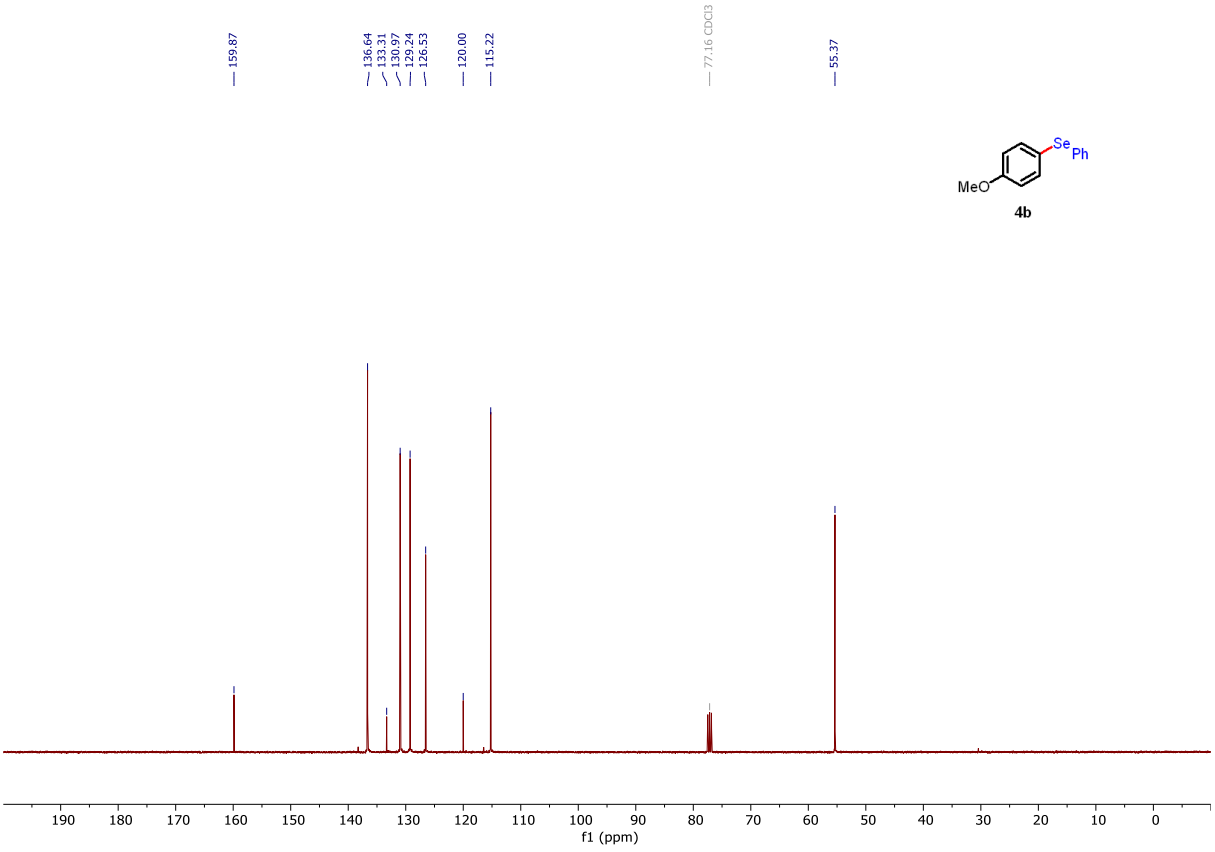
7.44
7.43
7.33
7.32
7.31
7.30
7.28
7.26 CDCl3
6.97
6.97
6.95
6.95
3.89
Se
Ph
MeO
4b
1.93
1.83
2.90
2.00
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.53
120.00
115.22
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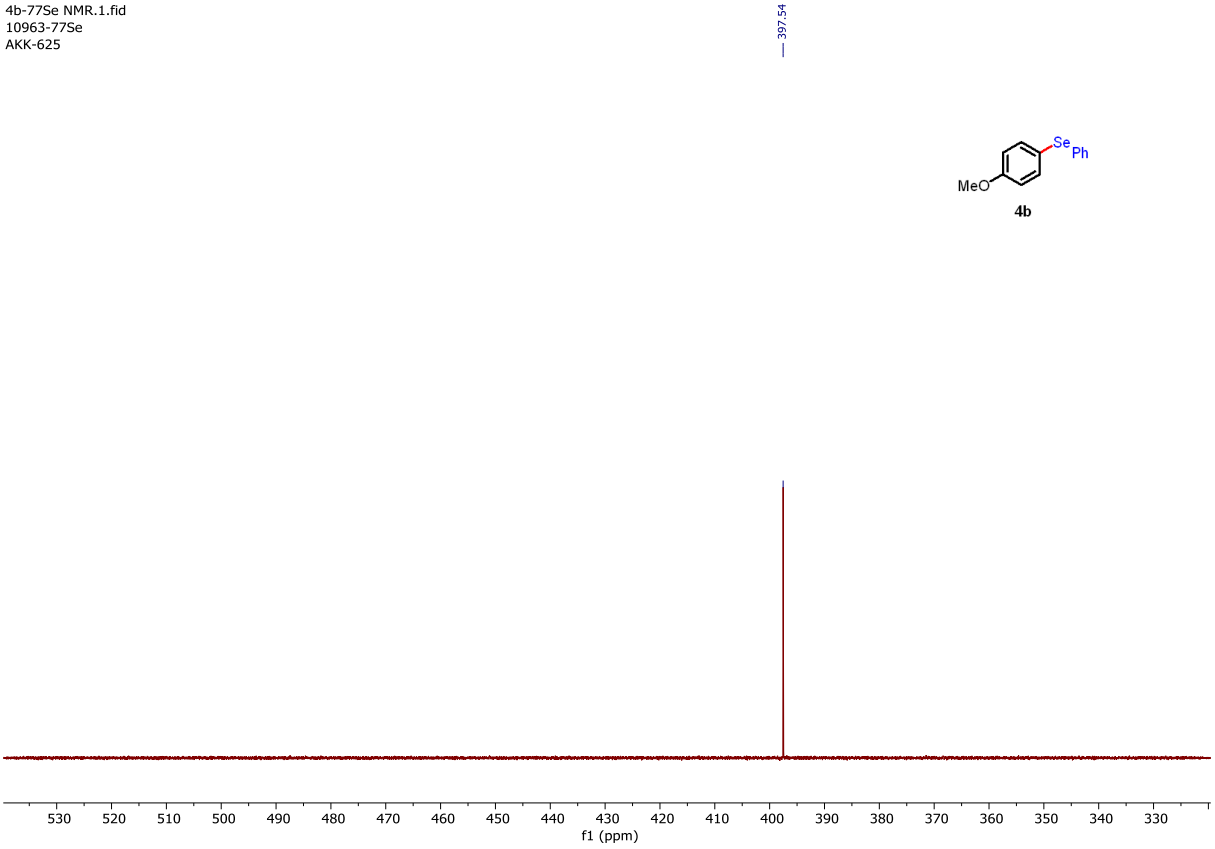
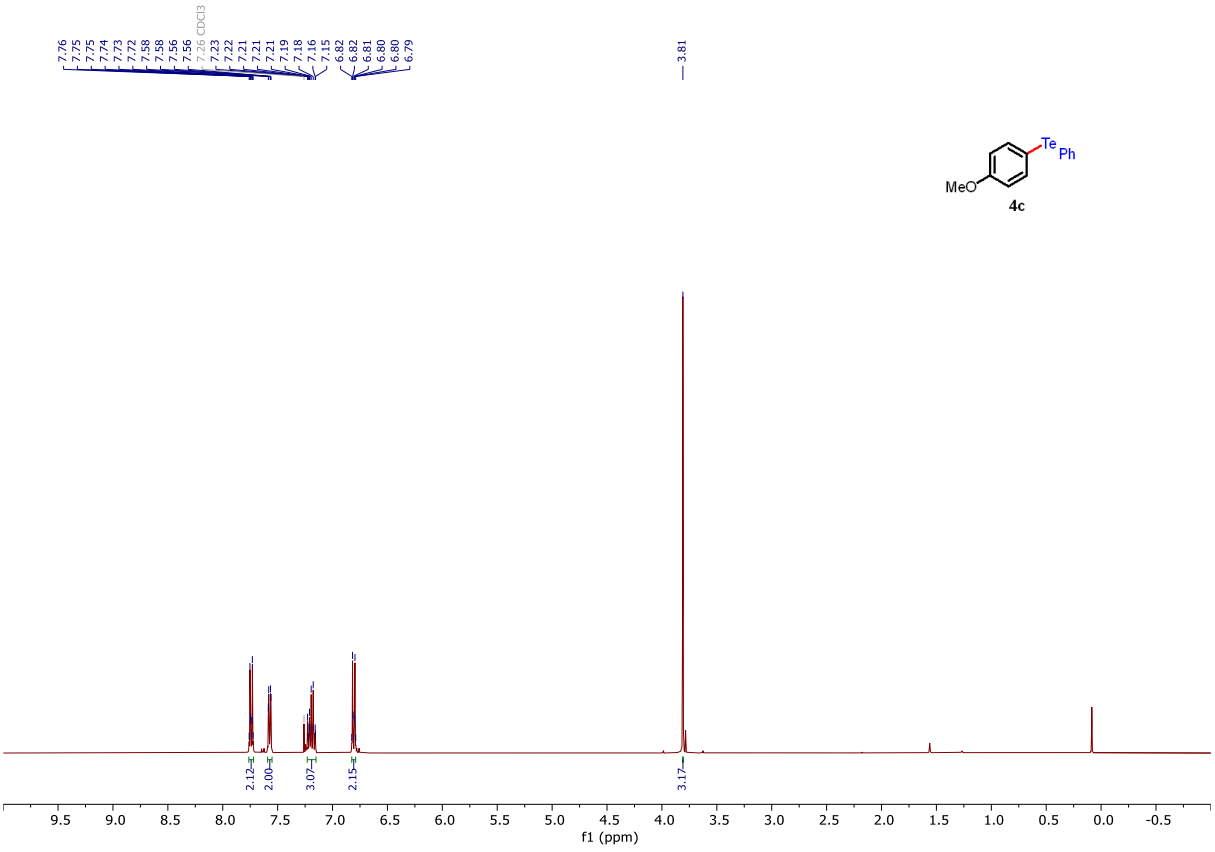
55.37
Se
Ph
MeO
4b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4b-77Se NMR.1.fid
10963-77Se
AKK-625




**4b**

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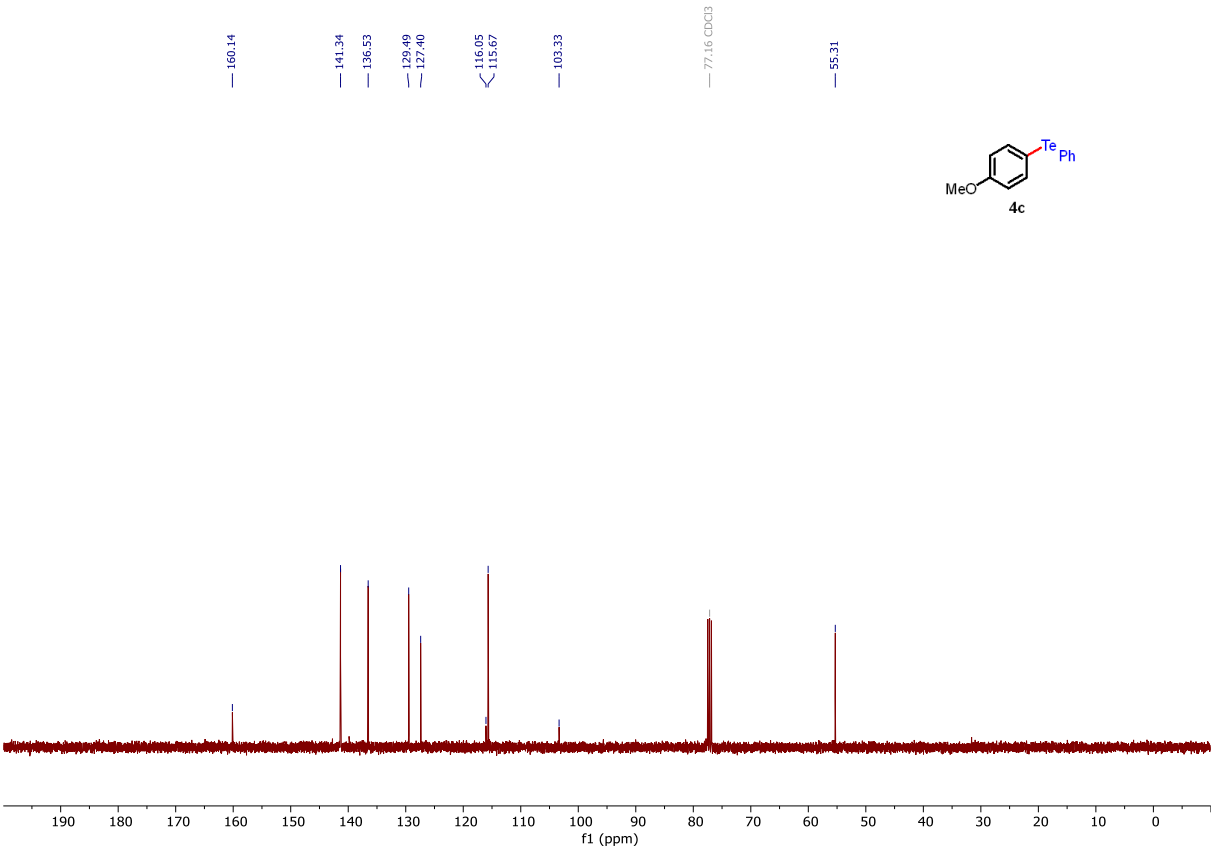


4c-125Te NMR.1.fid
11003-125Te
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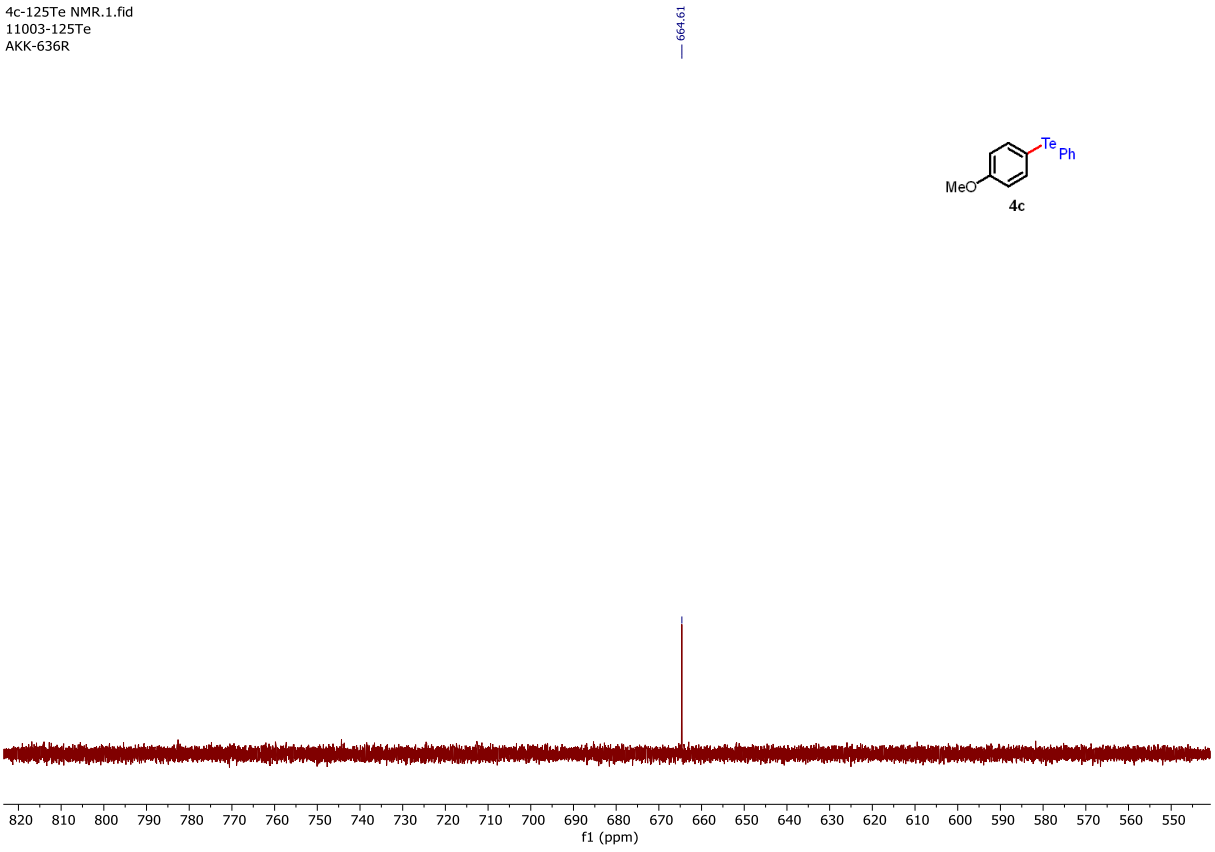
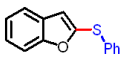
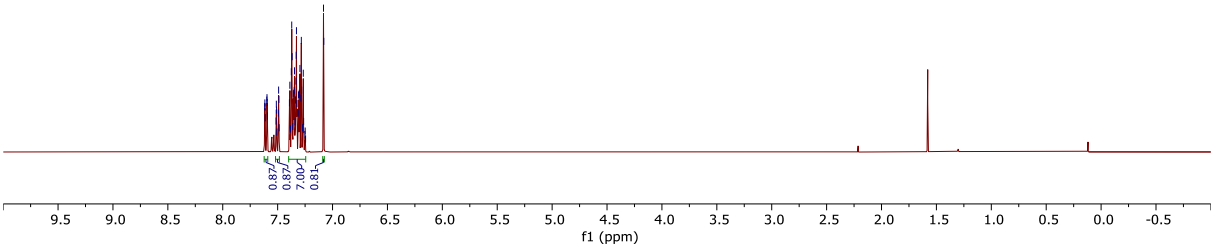



7.62 7.62 7.61 7.61 7.60 7.60 7.60 7.60 7.59 7.51 7.51 7.51 7.51 7.49 7.49 7.49 7.49 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.28 7.28 7.27 7.27 7.26 7.26 CDCl3 7.25 7.25 7.25 7.08 7.08


S
Ph

5a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0.87
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0.81
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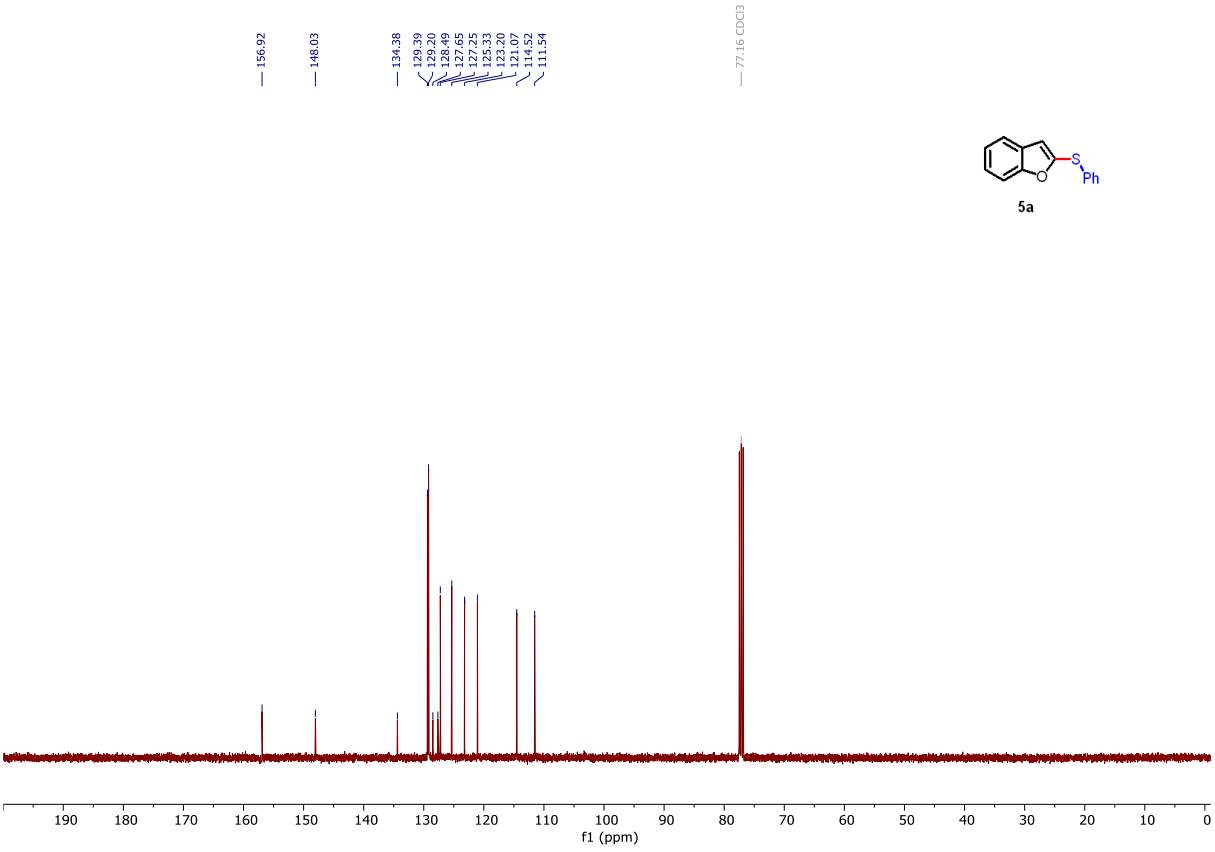
f1 (ppm)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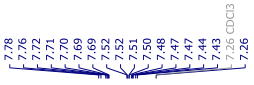
128.49
127.65
127.25
125.33
123.20
121.07
114.52
111.54
77.16 CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


S
Ph

5a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7.69
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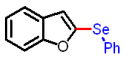
7.47
7.44
7.43
7.26 CDCl3
7.26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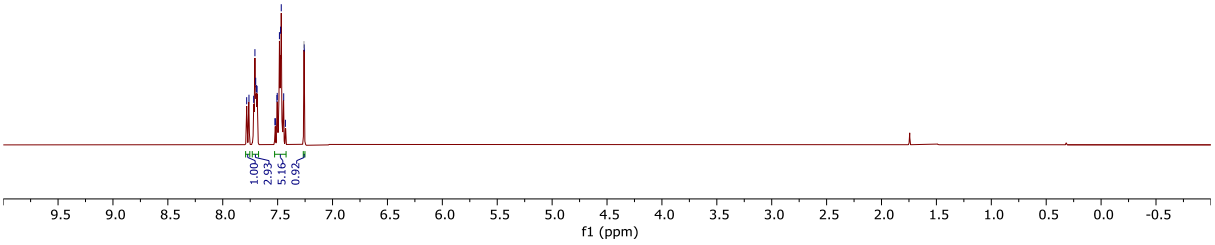
Ph

**5b**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2.93
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0.92
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


157.63
143.72
131.71
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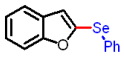
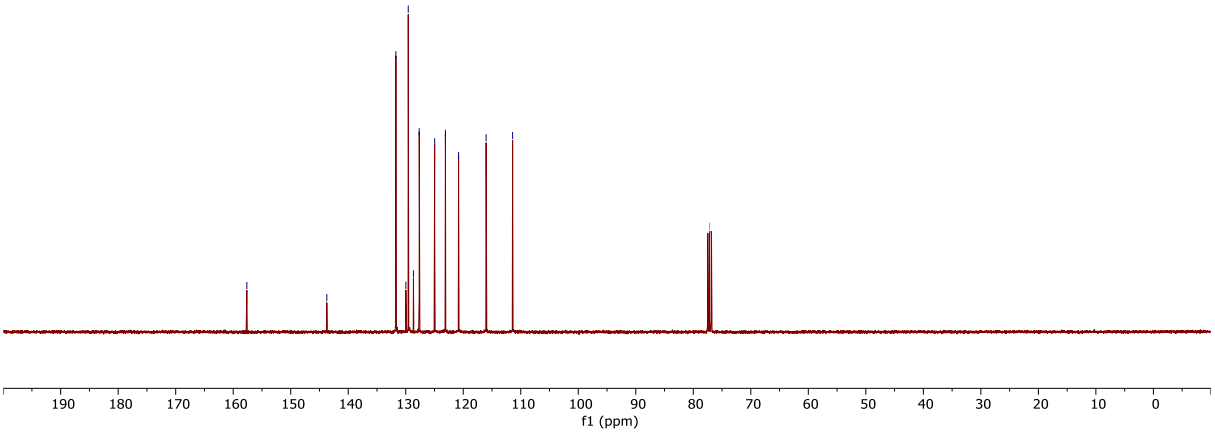
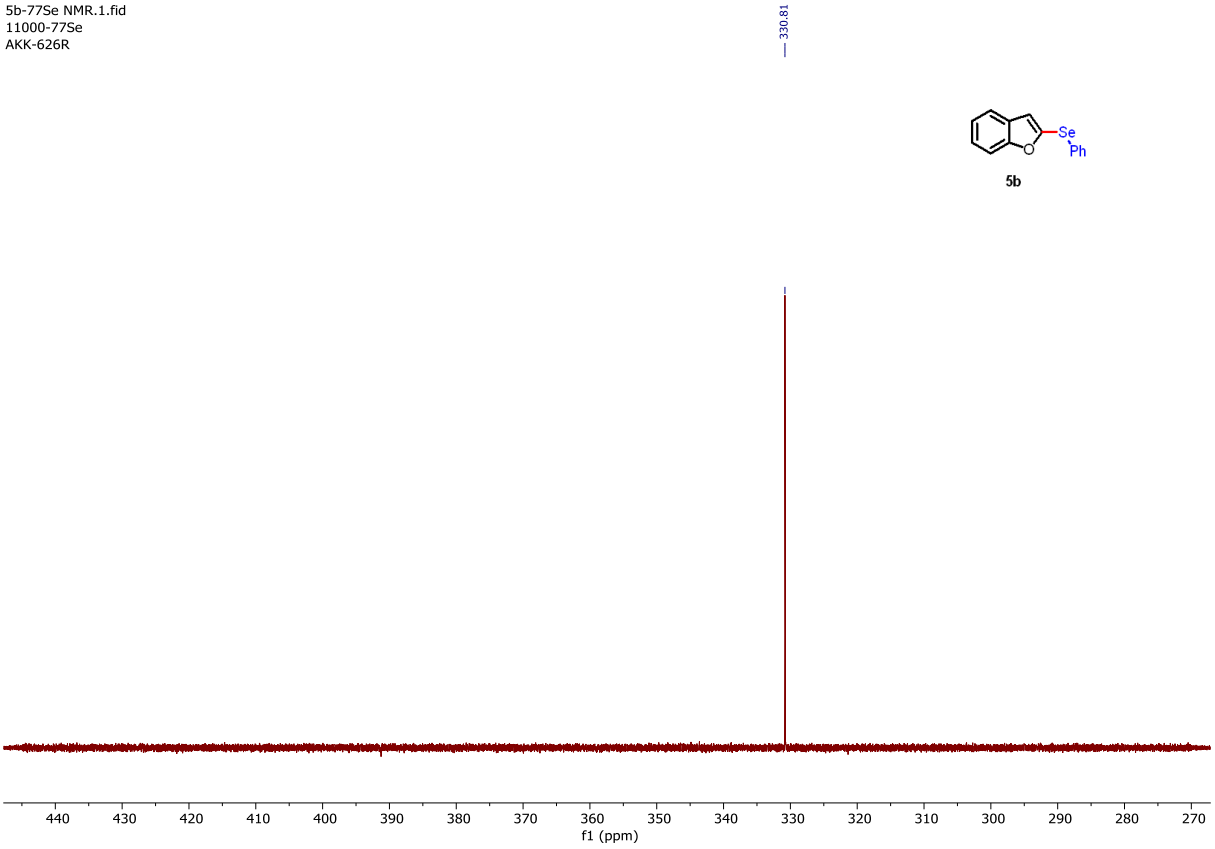
128.66
127.65
124.97
123.10
120.81
116.03
111.42
77.16 CDCl3

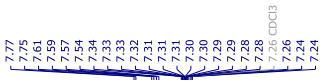

Se
Ph

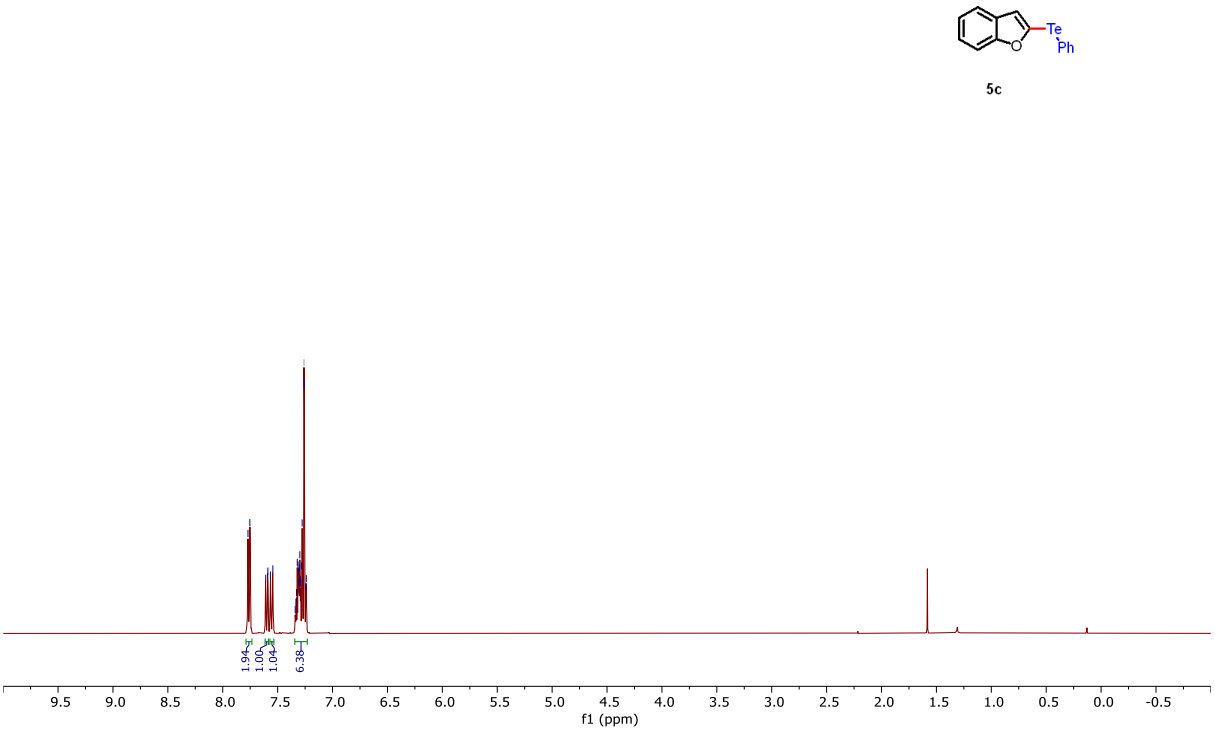
**5b**

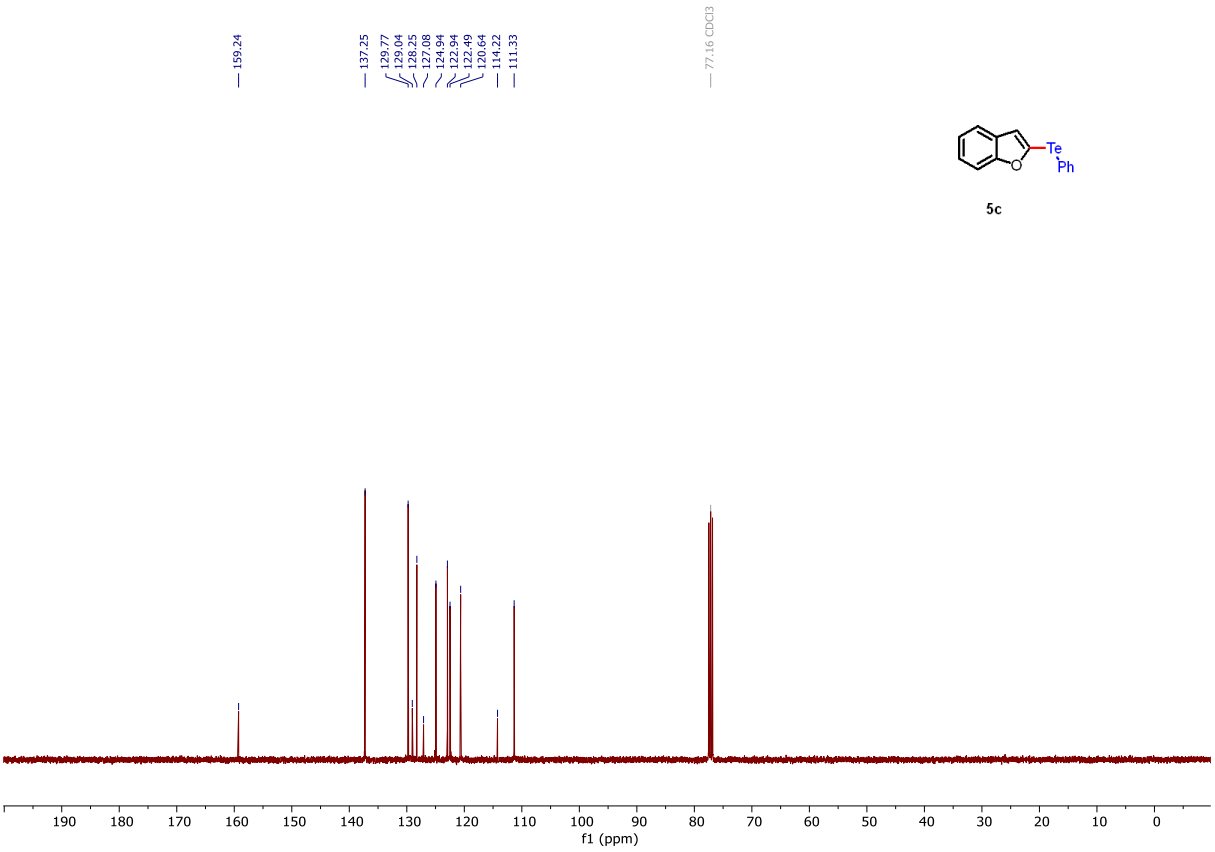

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

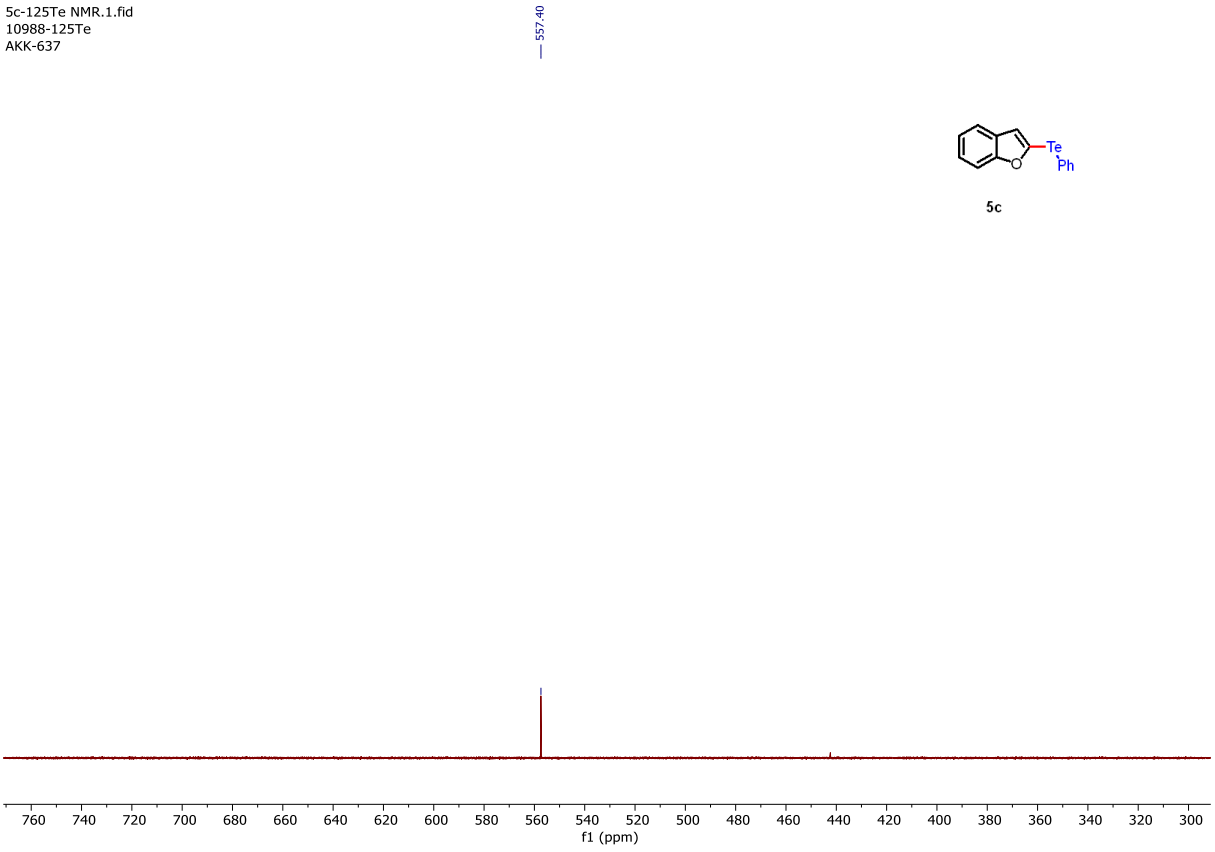
5b-77Se NMR.1.fid
11000-77Se
AKK-626R

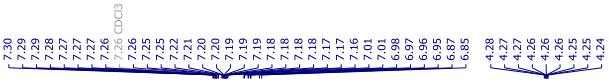


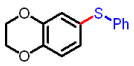



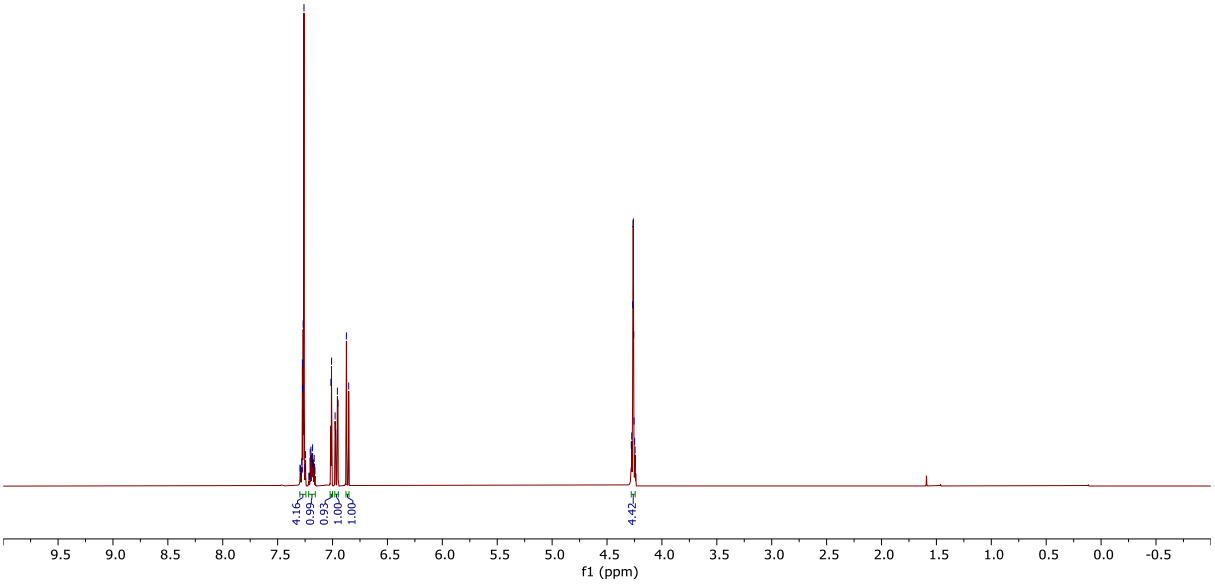

159.24
137.25
129.77
129.04
128.25
127.08
124.94
122.94
122.49
120.64
114.22
111.33
77.16 CDCl3
Te
Ph
5c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


5c-125Te NMR.1.fid
10988-125Te
AKK-637
557.40
Te
Ph
5c
760
740
720
700
680
660
640
620
600
580
560
540
520
500
480
460
440
420
400
380
360
340
320
300
f1 (ppm)

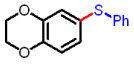

7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.26 CDCl3
7.26
7.25
7.25
7.22
7.21
7.20
7.20
7.19
7.19
7.19
7.18
7.18
7.18
7.18
7.17
7.17
7.16
7.01
7.01
6.98
6.97
6.96
6.95
6.87
6.85
4.28
4.27
4.27
4.26
4.26
4.26
4.25
4.25
4.24


S
Ph

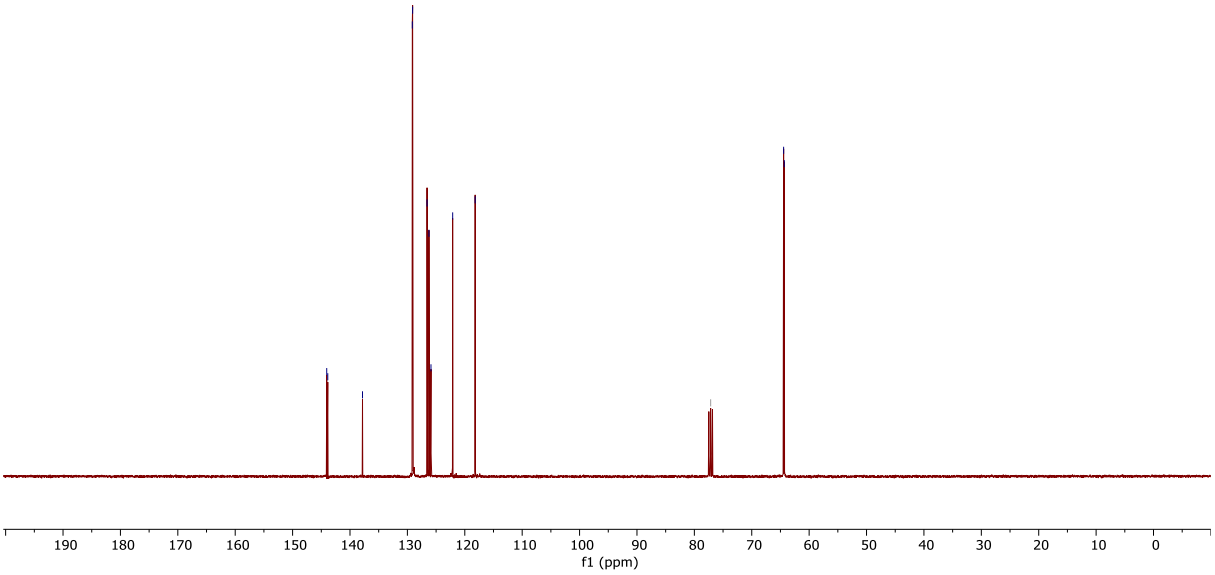
6a

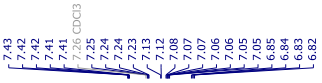

4.16
0.99
0.93
1.00
1.00
4.42
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


144.05
143.87
137.82
129.14
129.09
126.57
126.25
125.89
122.11
118.19
77.16 CDCl3
64.45
64.34

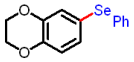

S
Ph

6a

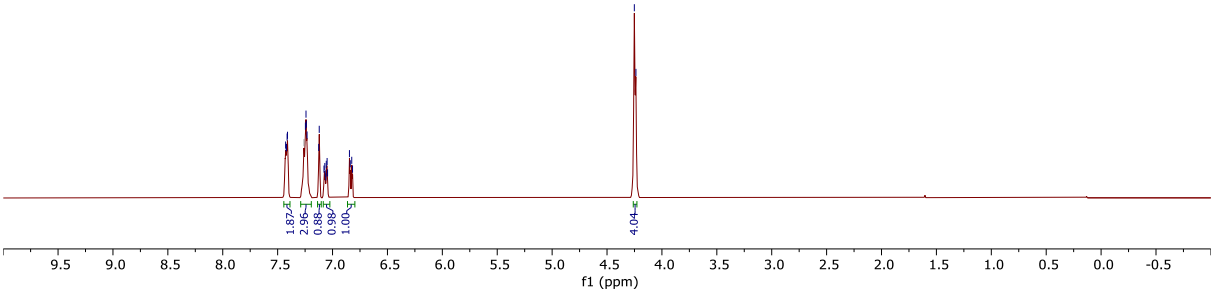

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.43
7.42
7.42
7.41
7.41
7.26 CDCl3
7.25
7.24
7.24
7.23
7.13
7.12
7.08
7.07
7.07
7.06
7.06
7.05
7.05
6.85
6.84
6.83
6.82

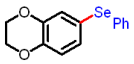

4.25
4.24


Se
Ph

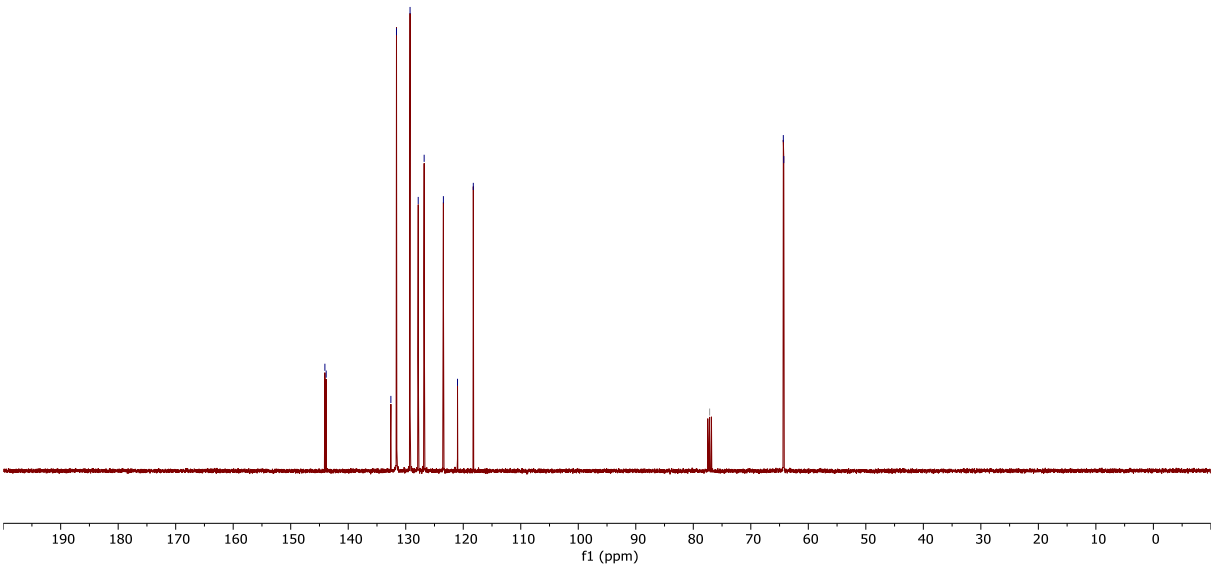
**6b**


1.87
2.96
0.88
0.98
1.00
4.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

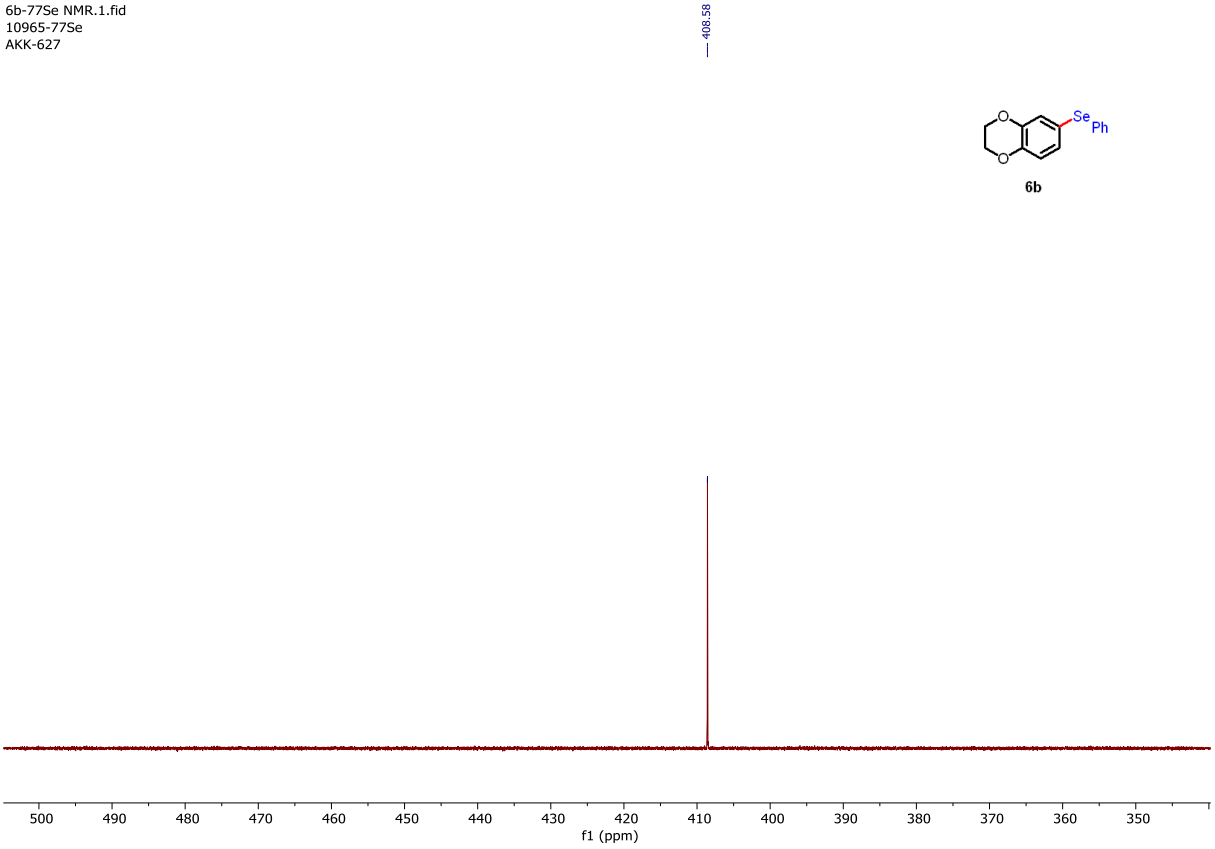

144.06
143.83
132.58
131.61
129.25
127.83
126.80
123.45
121.00
118.25
77.16 CDCl3
64.35
64.27


Se
Ph

**6b**


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

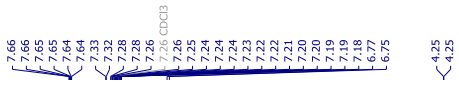
6b-77Se NMR.1.fid
10965-77Se
AKK-627

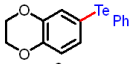




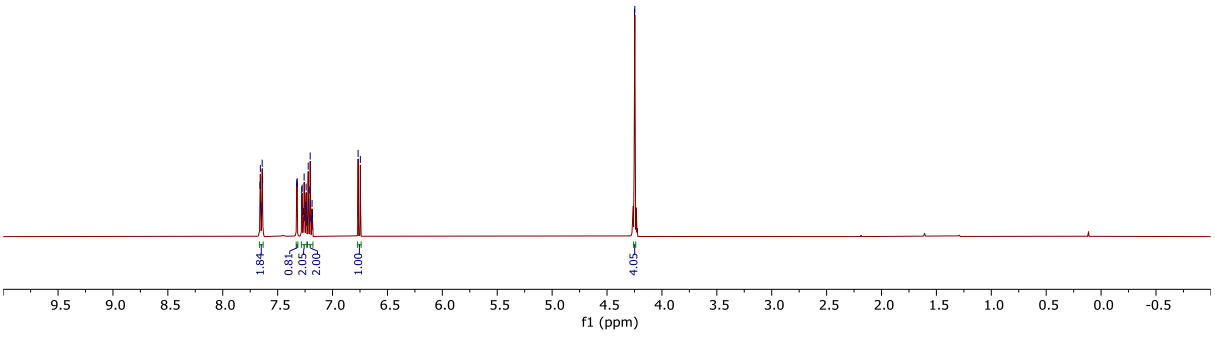


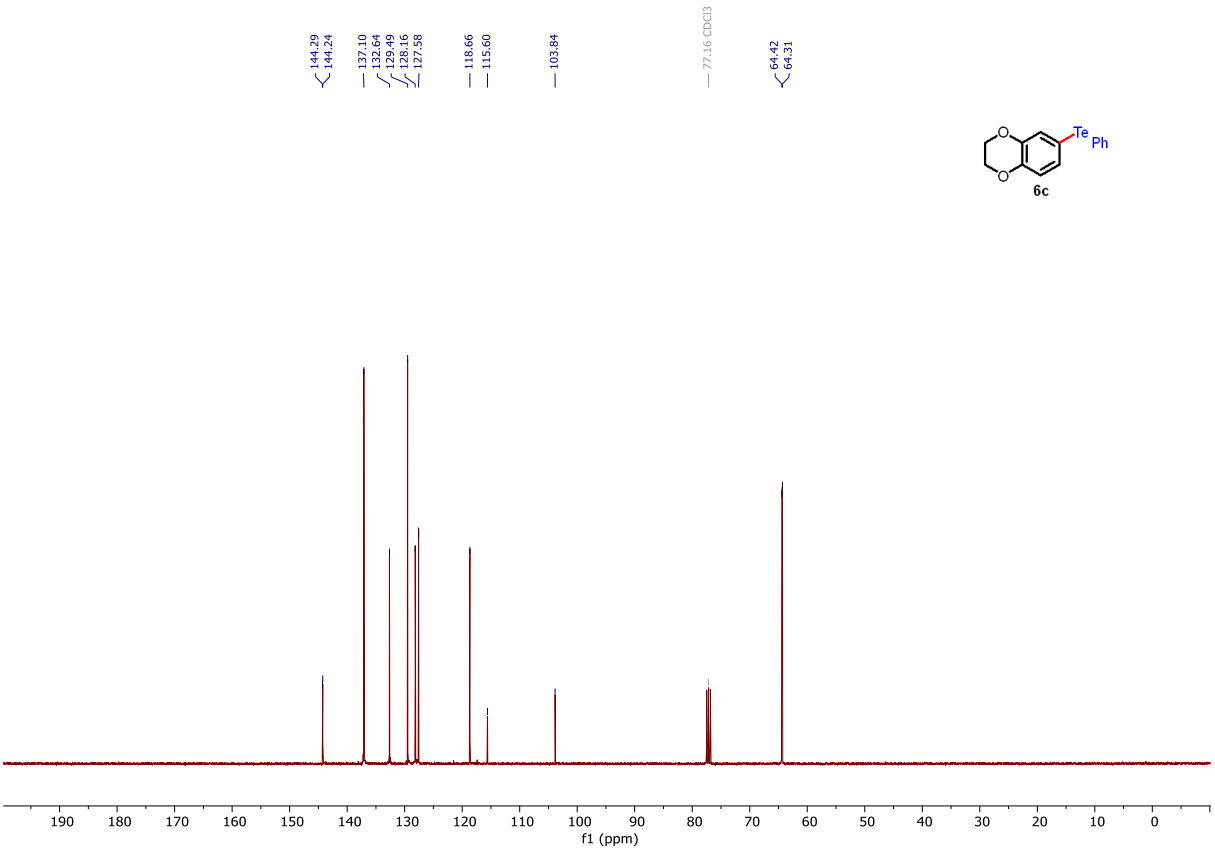
**6b**



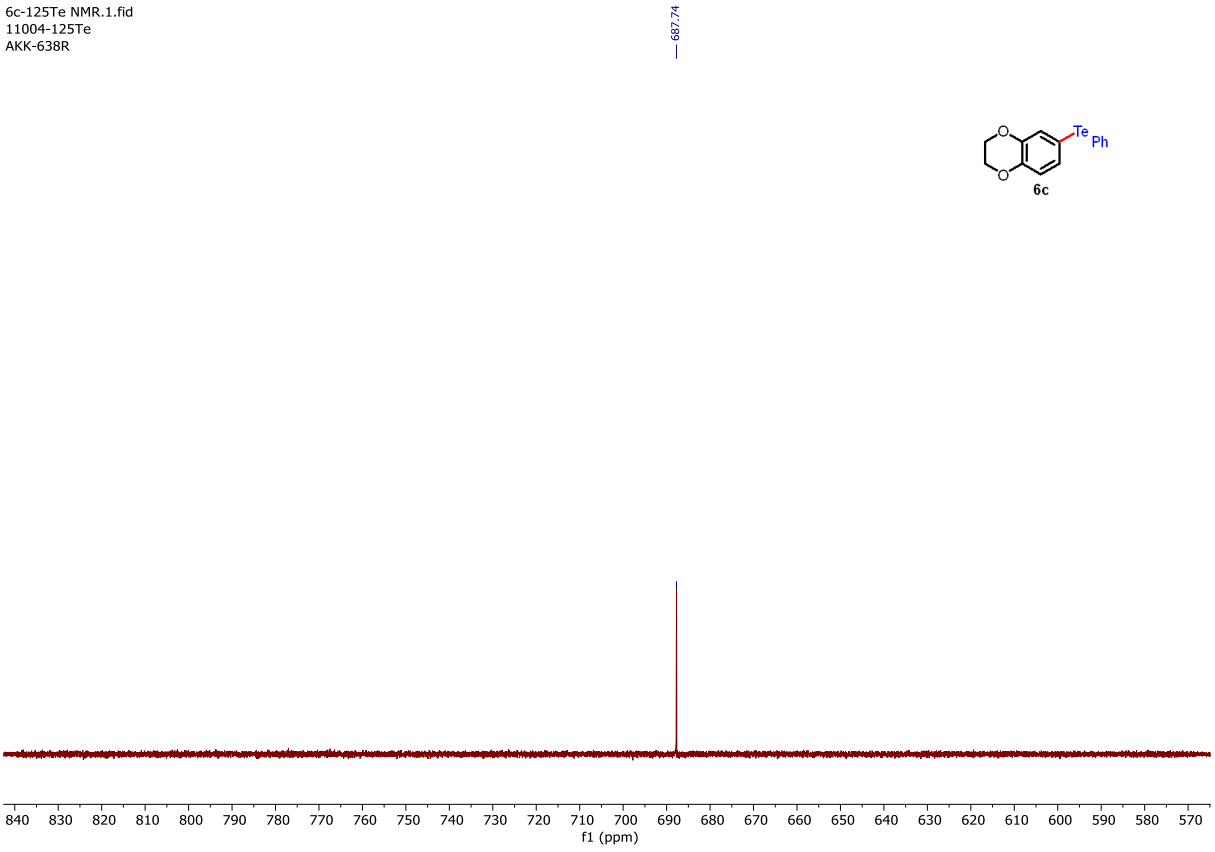



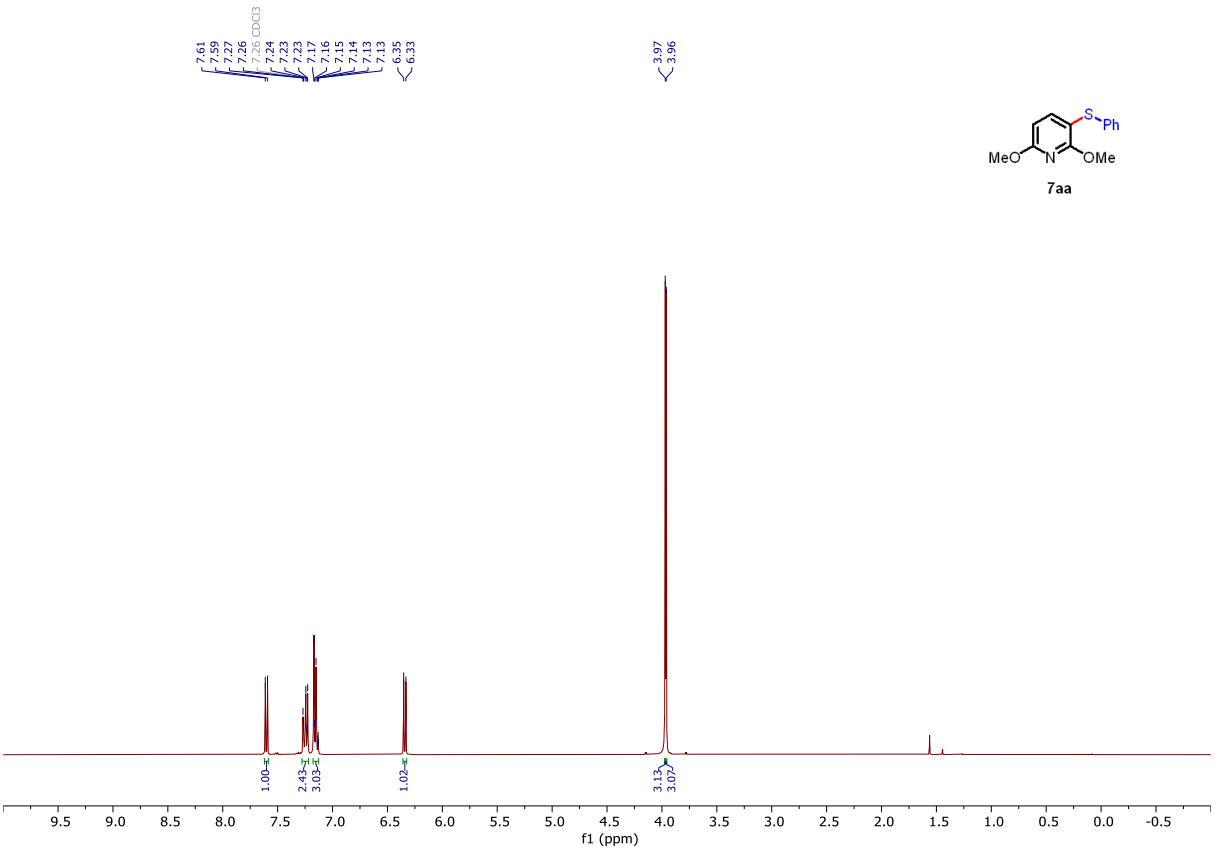

**6c**





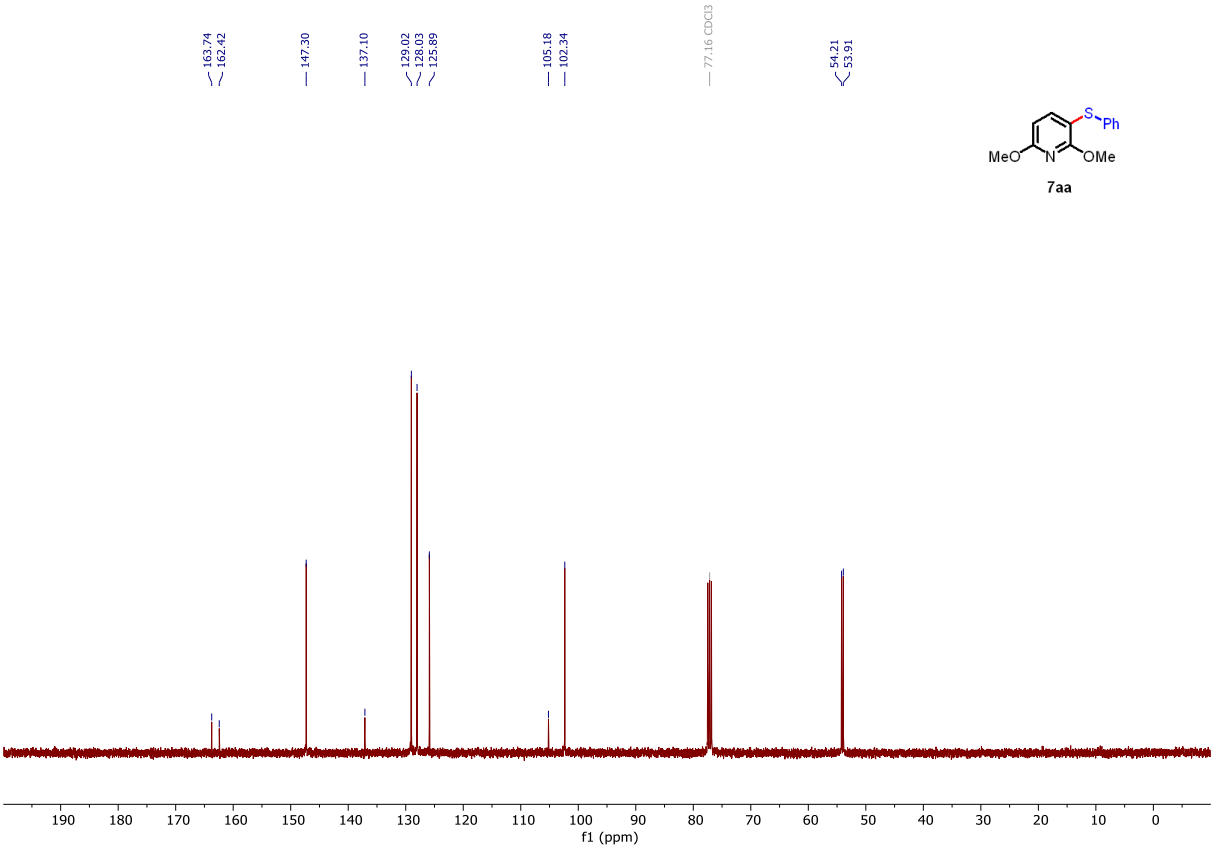

6c-125Te NMR.1.fid
11004-125Te
AKK-638R




7.61
7.59
7.27
7.26
7.26 CDCl3
7.24
7.23
7.23
7.17
7.16
7.15
7.14
7.13
7.13
6.35
6.33
3.97
3.96
1.00
2.43
3.03
1.02
3.13
3.07
f1 (ppm)

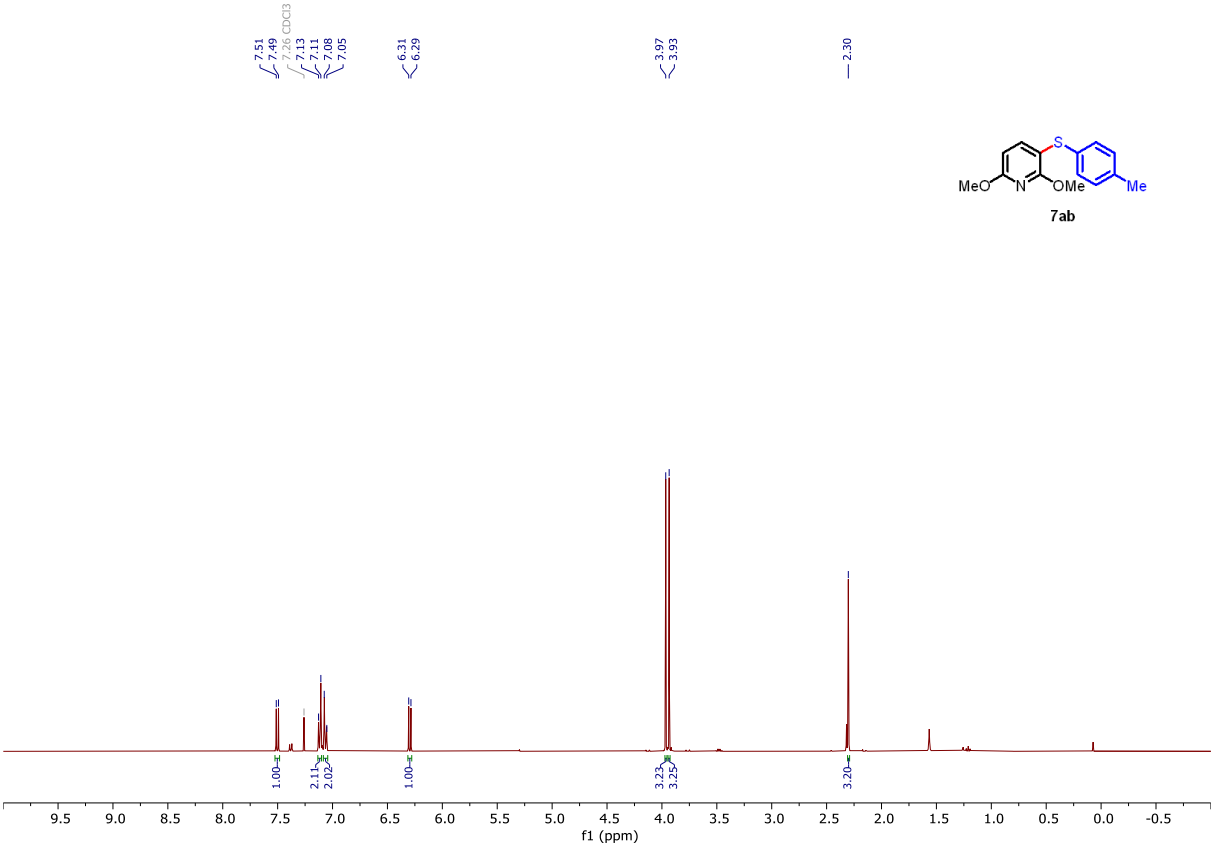

S
Ph
MeO
N
OMe

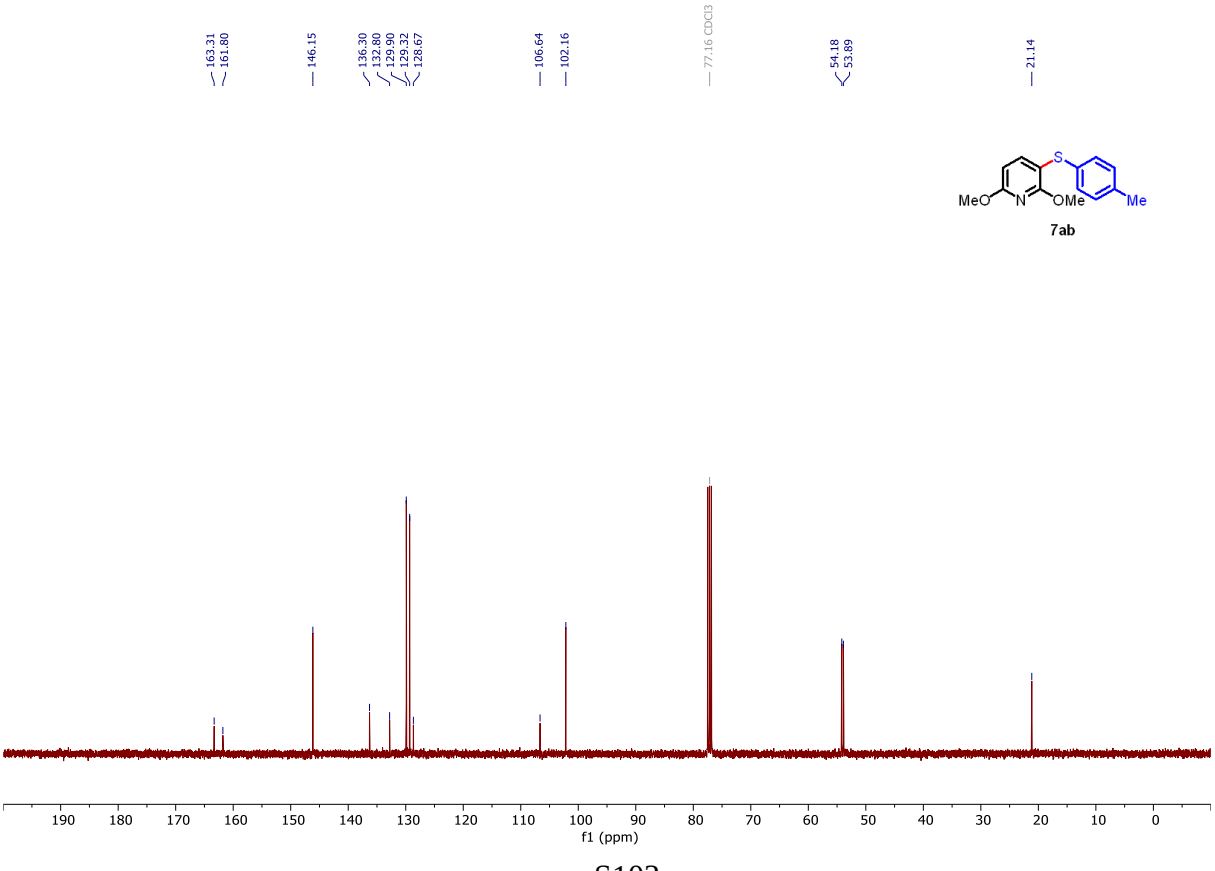
7aa

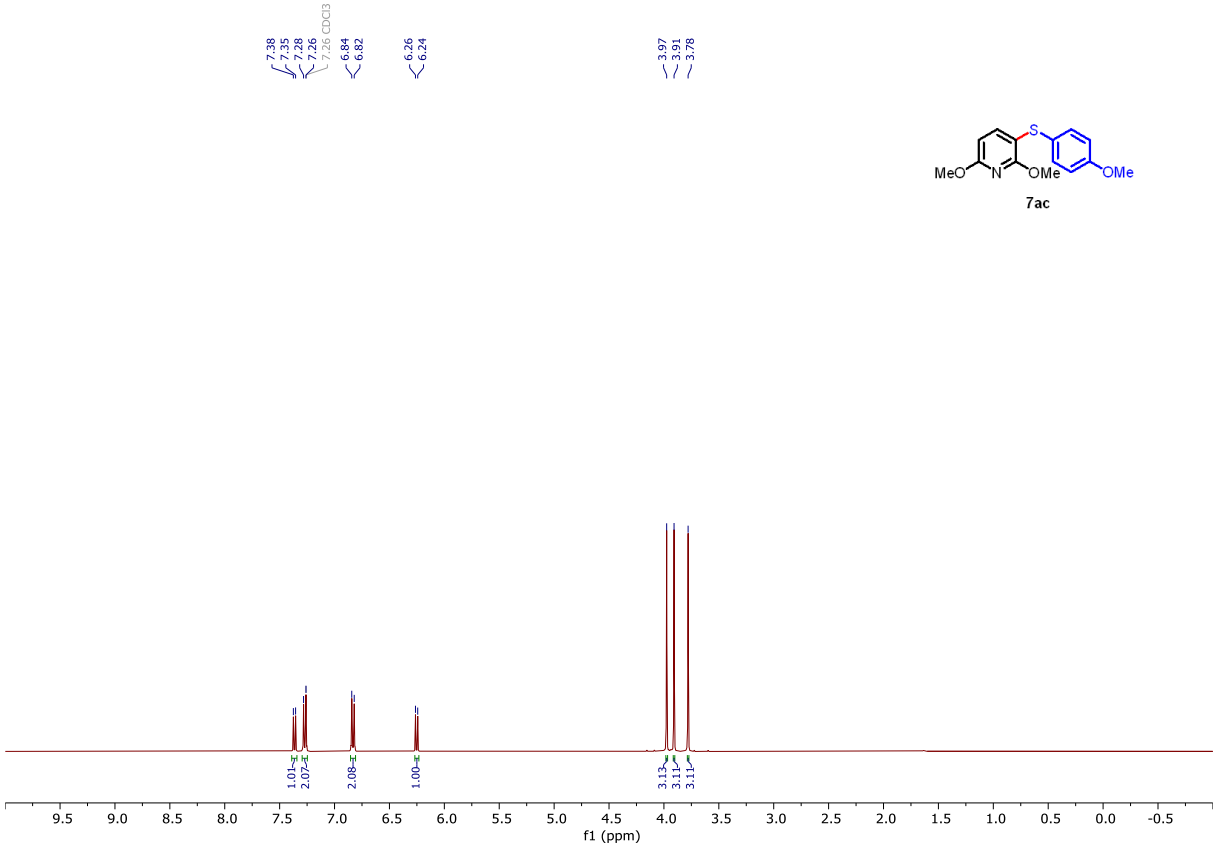

163.74
162.42
147.30
137.10
129.02
128.03
125.89
105.18
102.34
77.16 CDCl3
54.21
53.91
f1 (ppm)

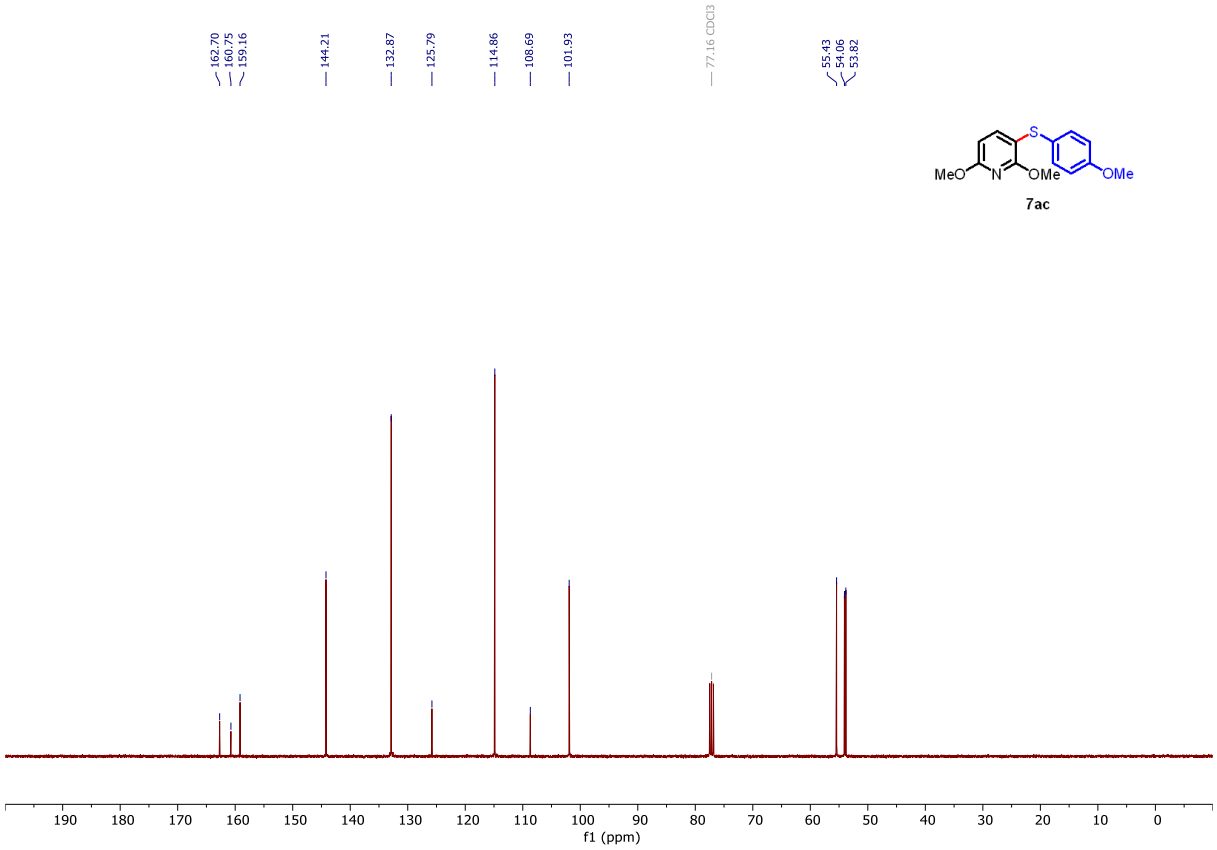

S
Ph
MeO
N
OMe

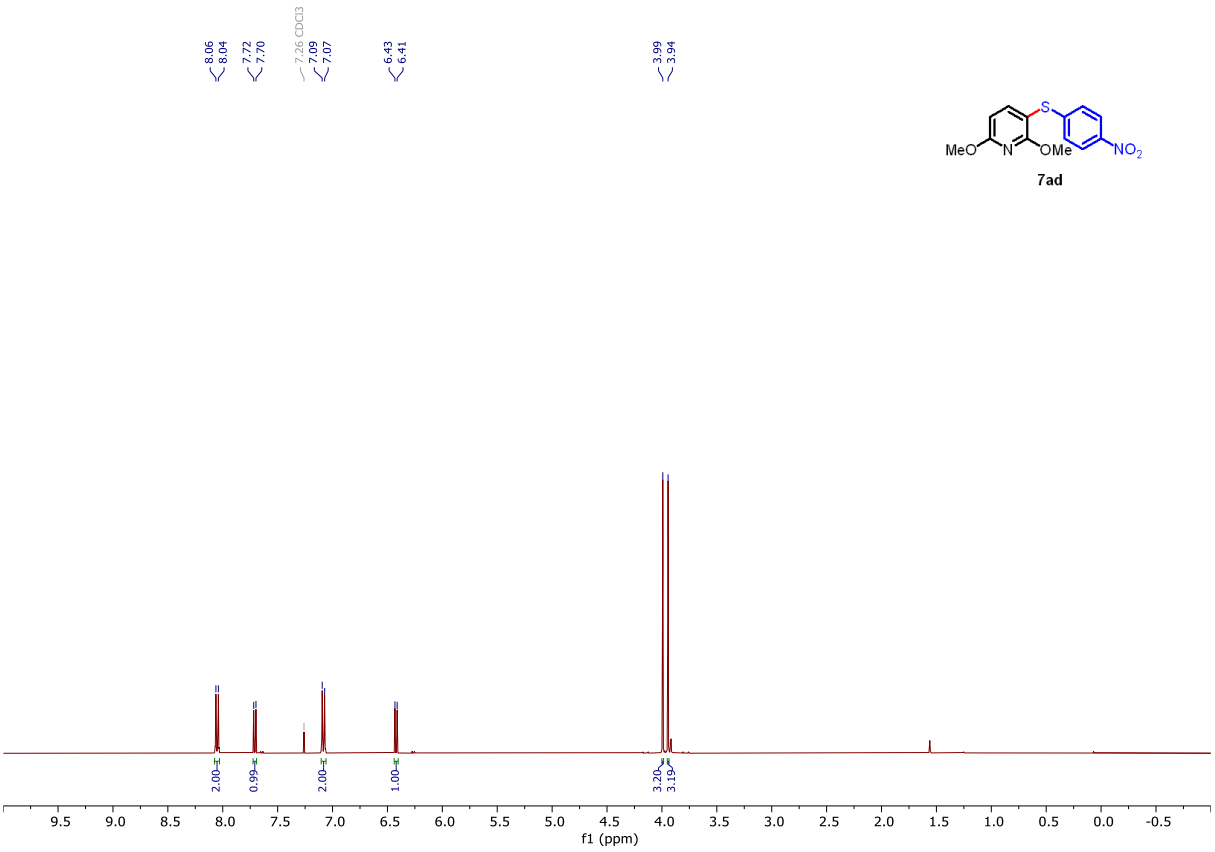
7aa

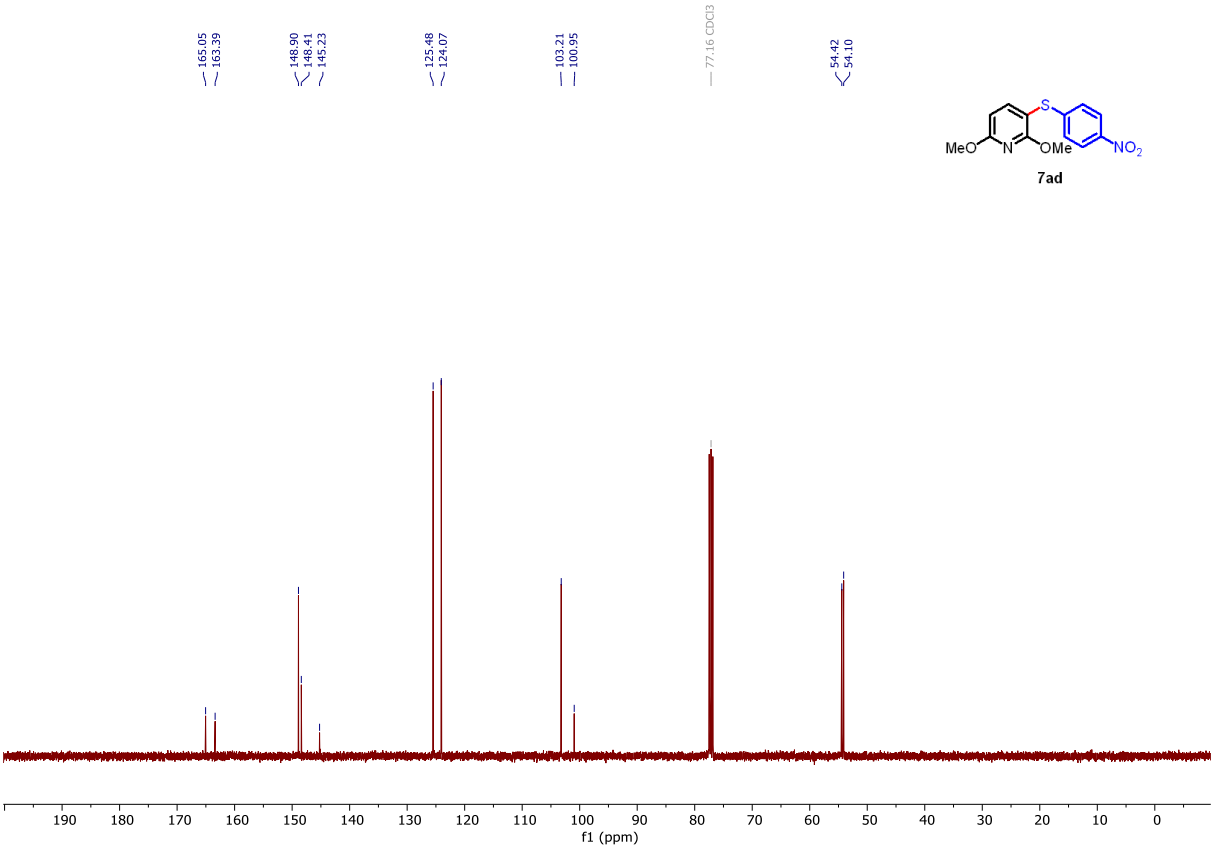

7.51
7.49
7.16 CDCl3
7.13
7.11
7.08
7.05
6.31
6.29
3.97
3.93
2.30
MeO
N
OMe
S
Me
7ab
1.00
2.11
2.02
1.00
3.23
3.25
3.20
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

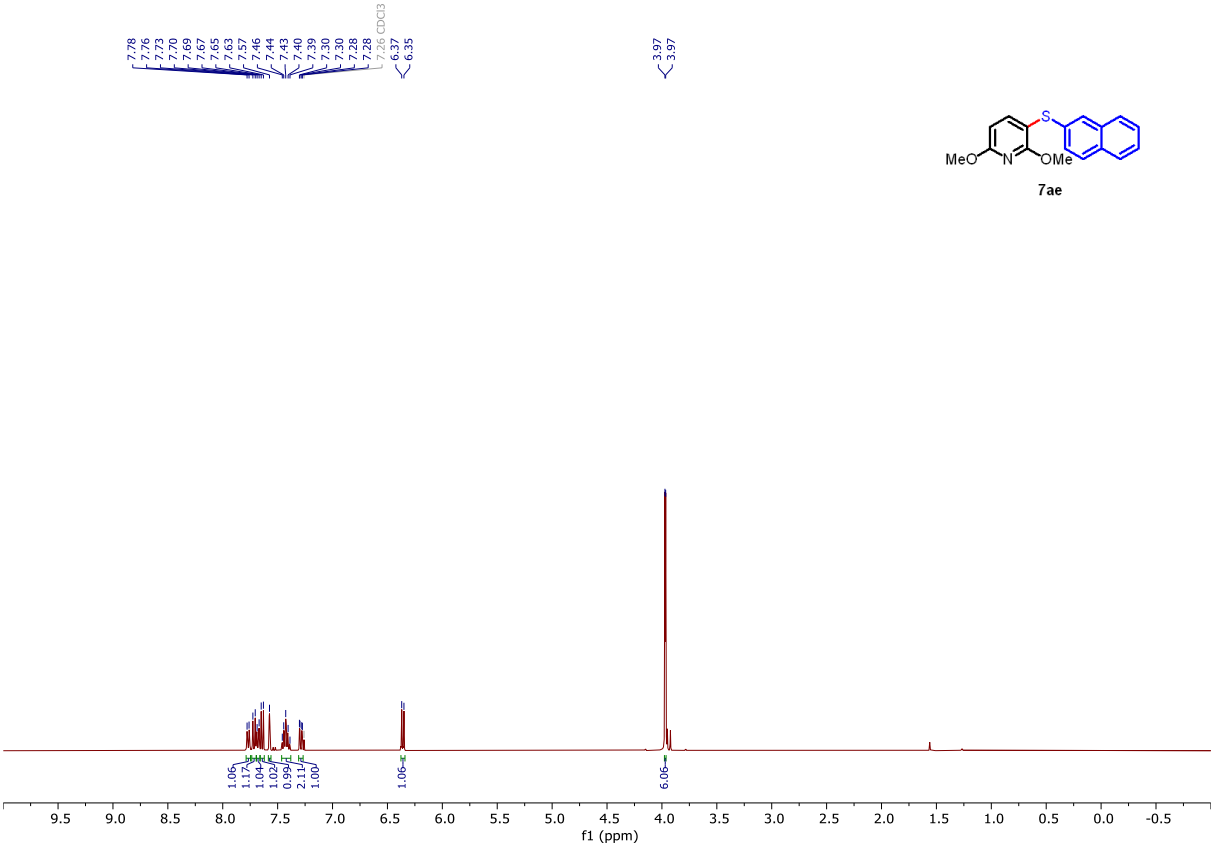

163.31
161.80
146.15
136.30
132.80
129.90
129.32
128.67
106.64
102.16
77.16 CDCl3
54.18
53.89
21.14
MeO
N
OMe
S
Me
7ab
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

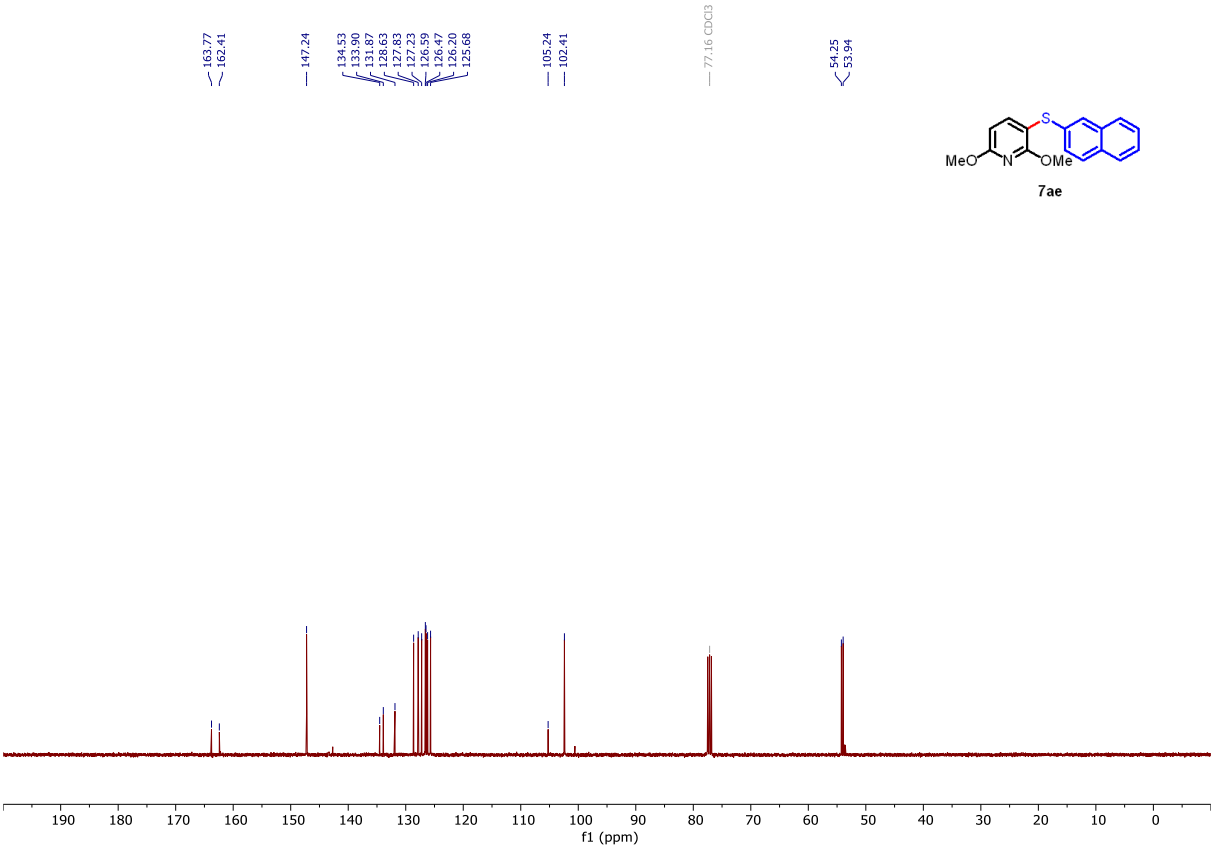

7.38
7.35
7.28
7.26
7.26 CDCl3
6.84
6.82
6.26
6.24
3.97
3.91
3.78
MeO
N
S
OMe
OMe
7ac
1.01
2.07
2.08
1.00
3.13
3.11
3.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

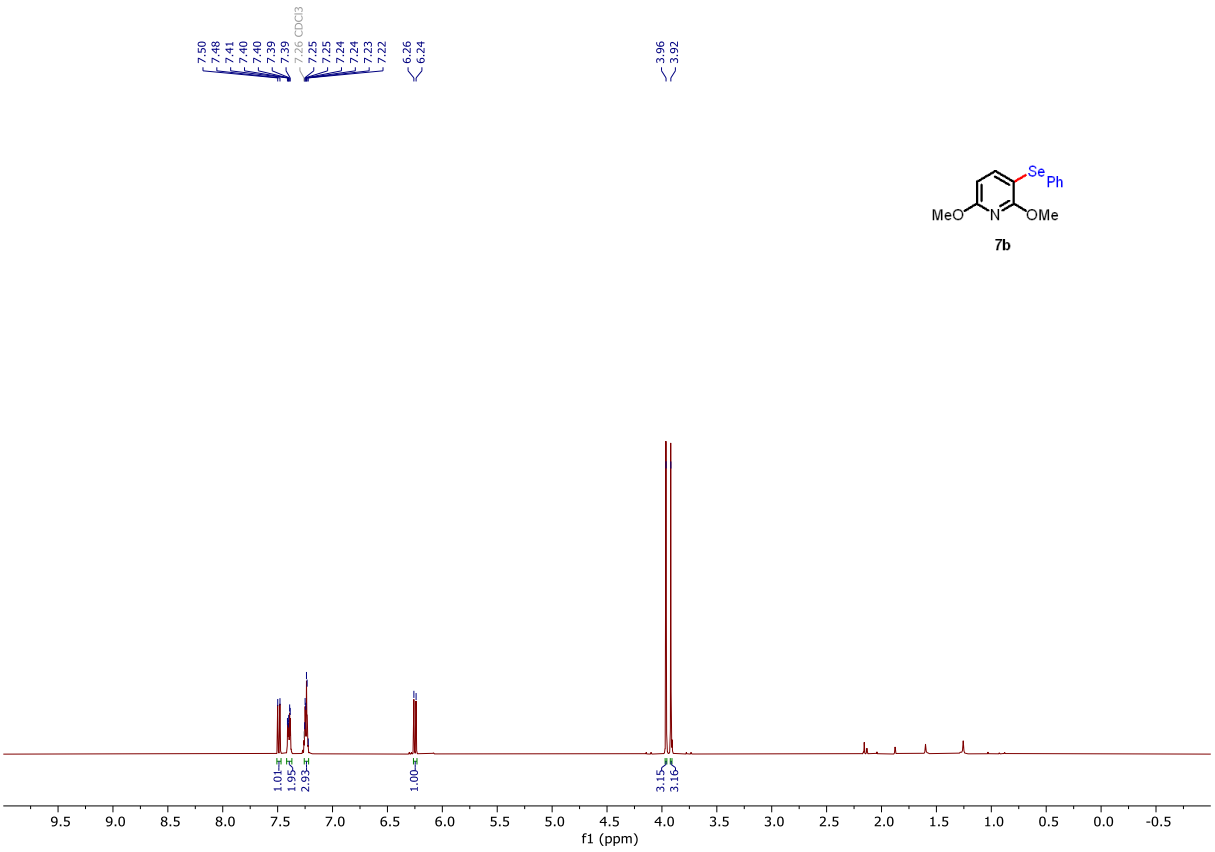

162.70
160.75
159.16
144.21
132.87
125.79
114.86
108.69
101.93
77.16 CDCl3
55.43
54.06
53.82
MeO
N
S
OMe
OMe
7ac
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

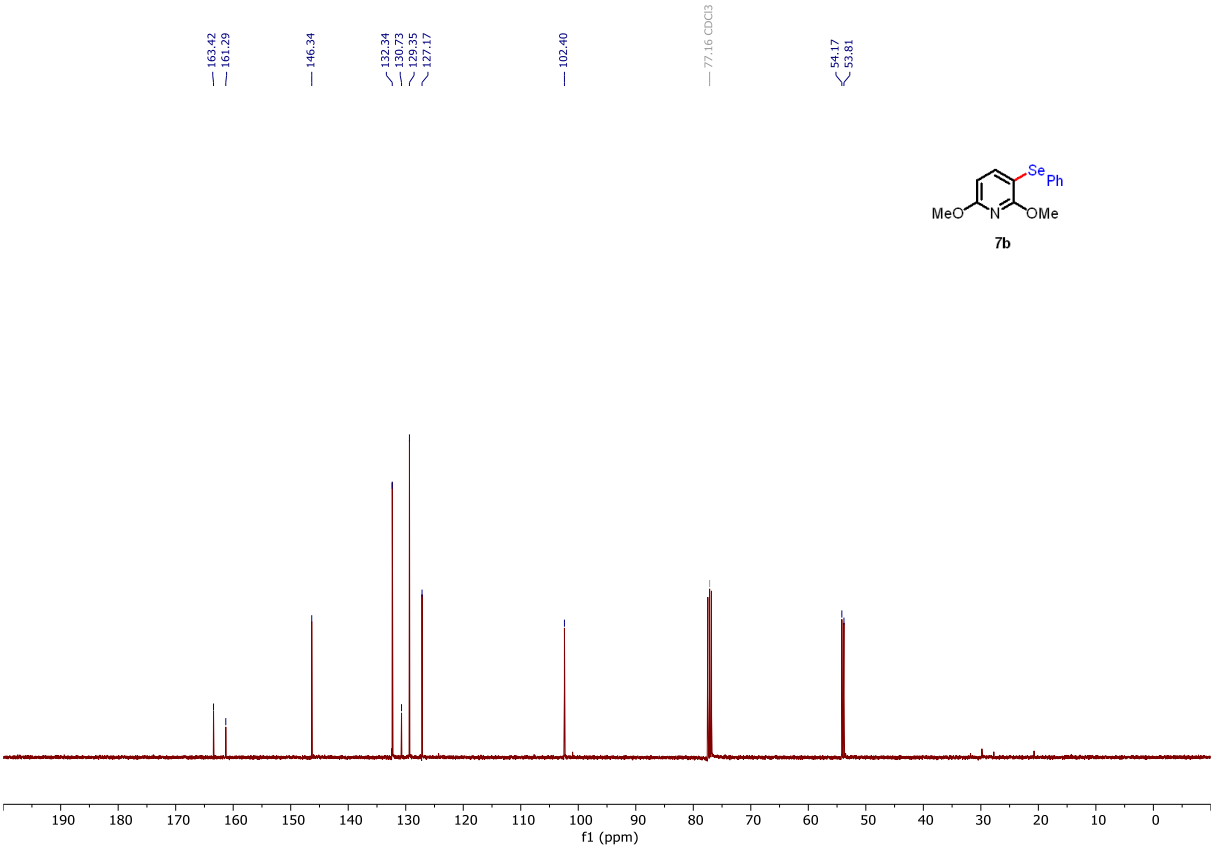

8.06
8.04
7.72
7.70
7.26 CDCl3
7.09
7.07
6.43
6.41
3.99
3.94
MeO
N
OMe
S
NO2
7ad
2.00
0.99
2.00
1.00
3.20
3.19
f1 (ppm)


165.05
163.39
148.90
148.41
145.23
125.48
124.07
103.21
100.95
77.16 CDCl3
54.42
54.10
MeO
N
OMe
S
NO2
7ad
f1 (ppm)

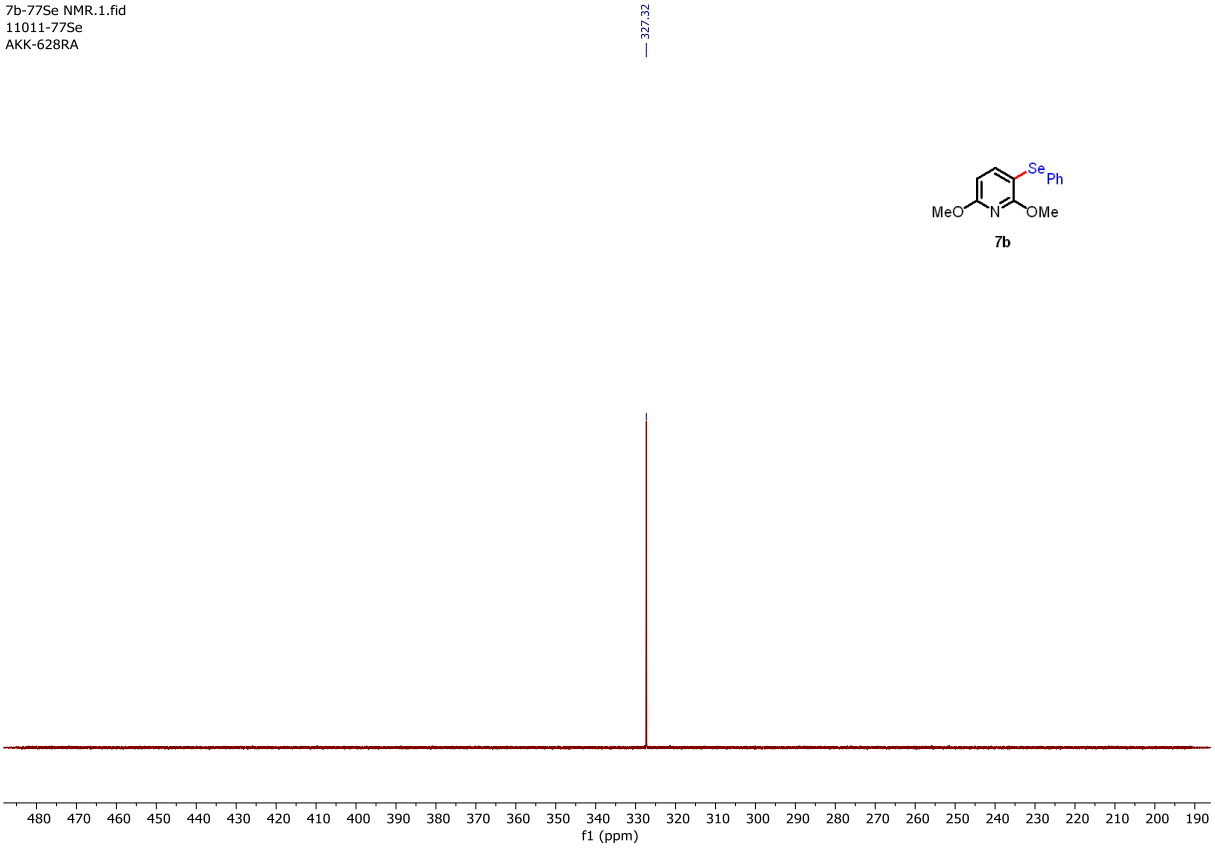

7.78
7.76
7.73
7.70
7.69
7.67
7.65
7.63
7.57
7.46
7.44
7.43
7.40
7.39
7.30
7.30
7.28
7.28
7.26 CDCl3
6.37
6.35
3.97
3.97
MeO
N
OMe
S
7ae
1.06
1.17
1.04
1.02
0.99
2.11
1.00
1.06
6.06
f1 (ppm)


163.77
162.41
147.24
134.53
133.90
131.87
128.63
127.83
127.23
126.59
126.47
126.20
125.68
105.24
102.41
77.16 CDCl3
54.25
53.94
MeO
N
OMe
S
7ae
f1 (ppm)

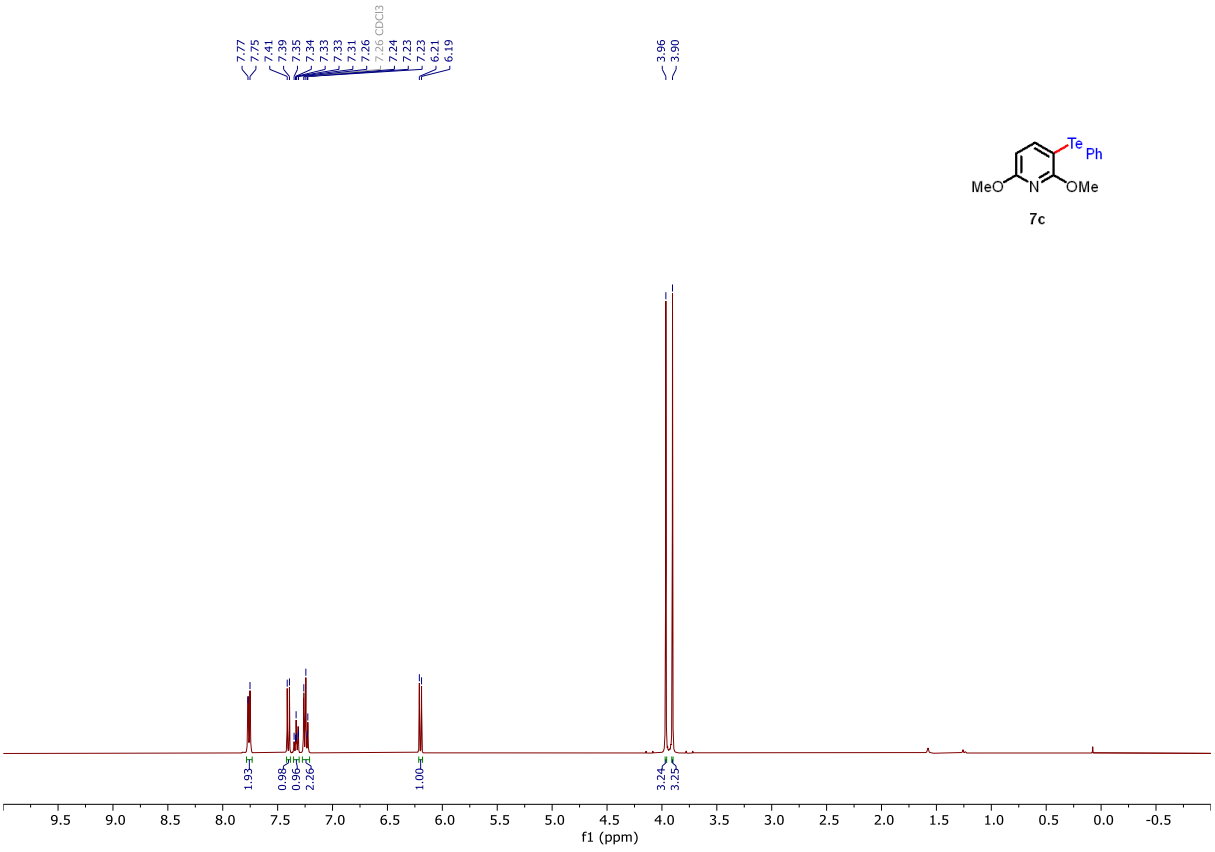

7.50
7.48
7.41
7.40
7.40
7.39
7.39
7.26 CDCl3
7.25
7.25
7.24
7.24
7.23
7.22
6.26
6.24
3.96
3.92
Se
Ph
MeO
N
OMe
7b
1.01
1.95
2.93
1.00
3.15
3.16
f1 (ppm)


163.42
161.29
146.34
132.34
130.73
129.55
127.17
102.40
77.16 CDCl3
54.17
53.81
Se
Ph
MeO
N
OMe
7b
f1 (ppm)

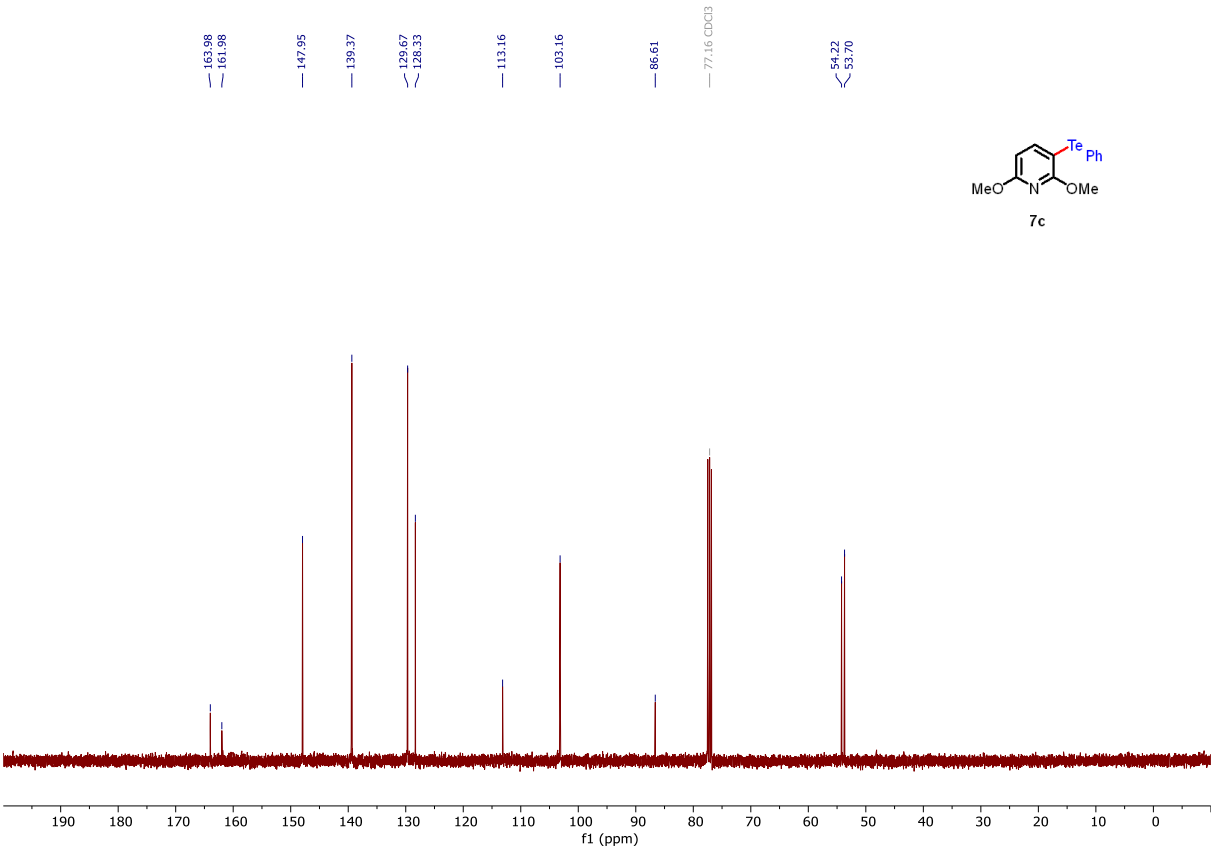
7b-77Se NMR.1.fid
11011-77Se
AKK-628RA



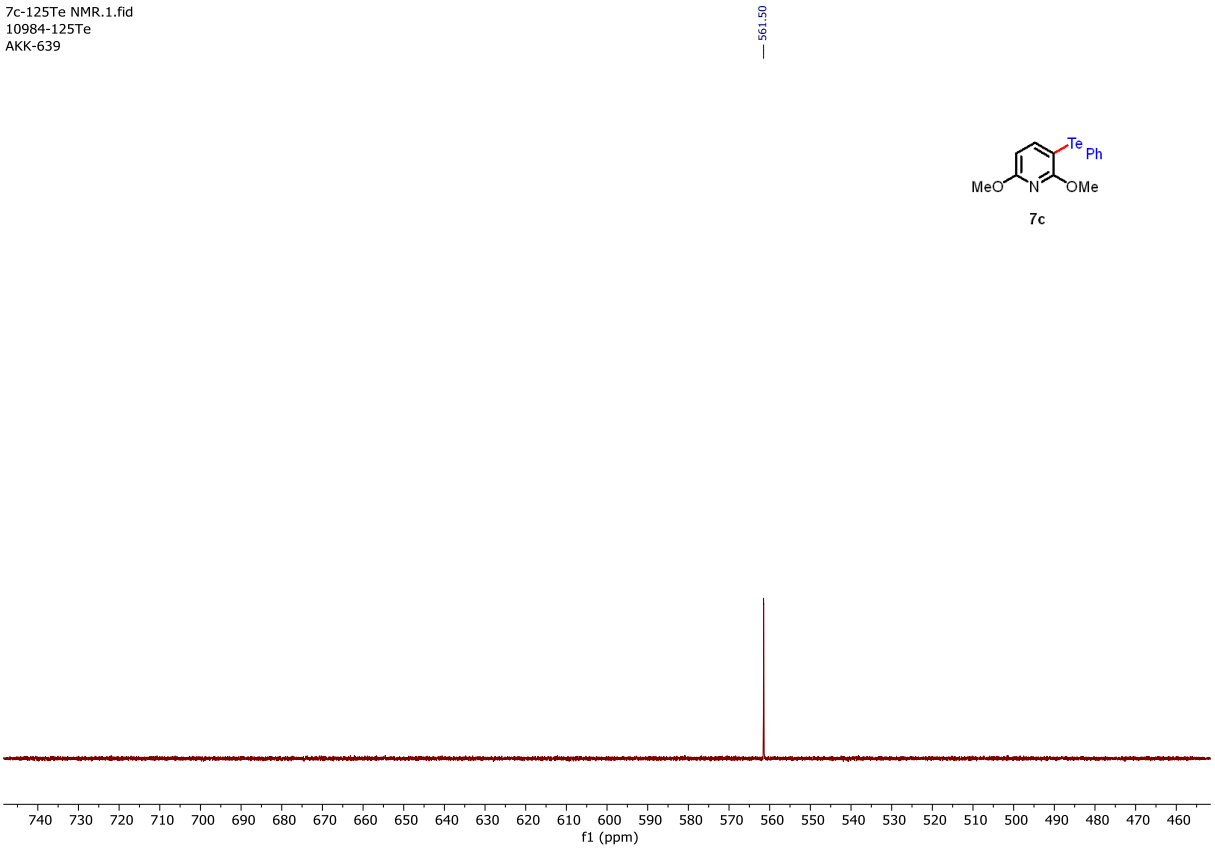

7b

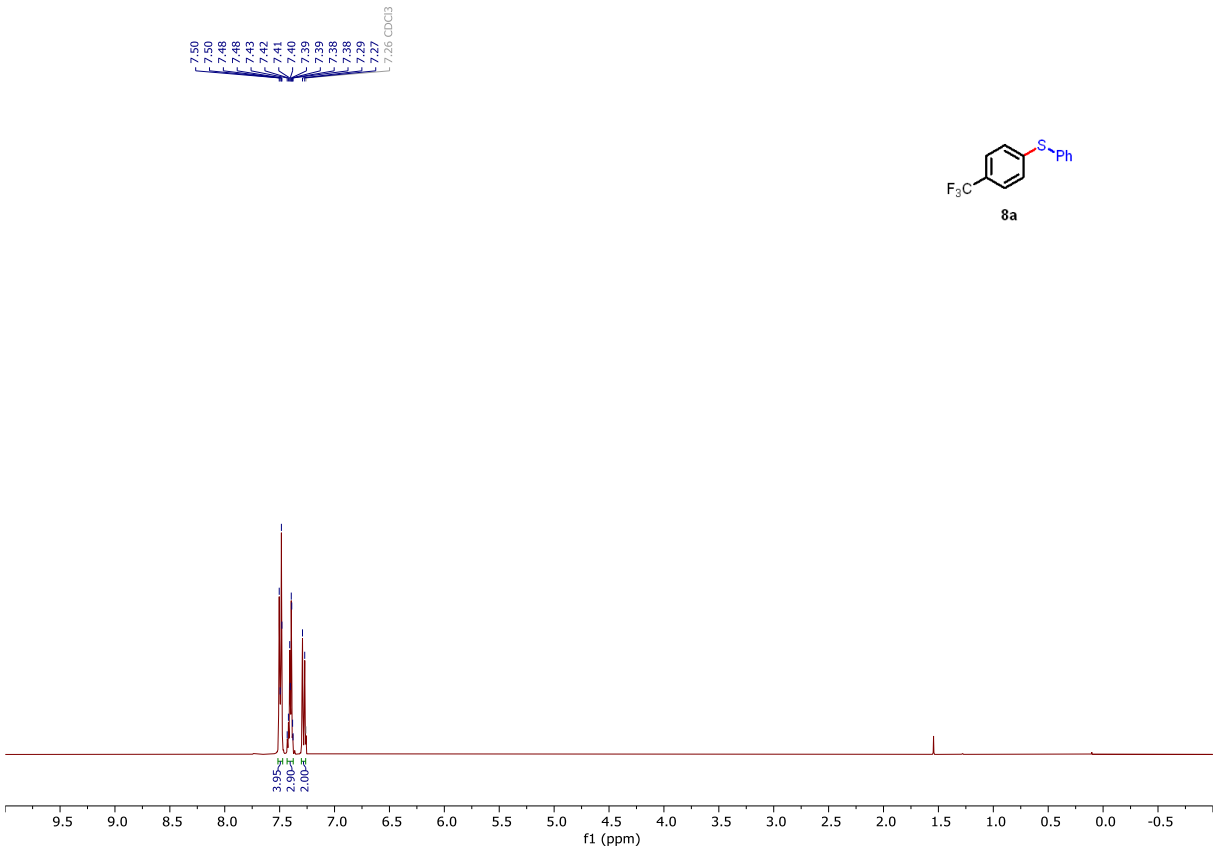


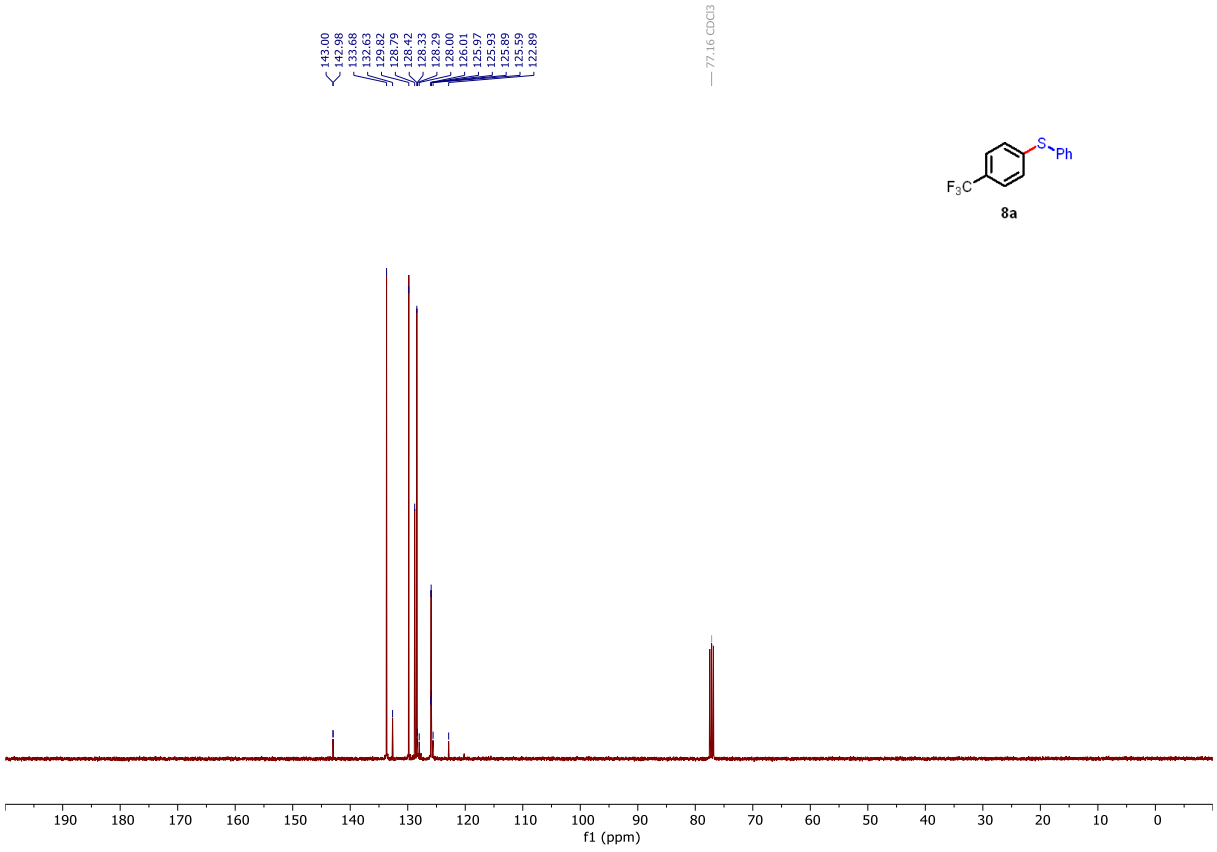

7c

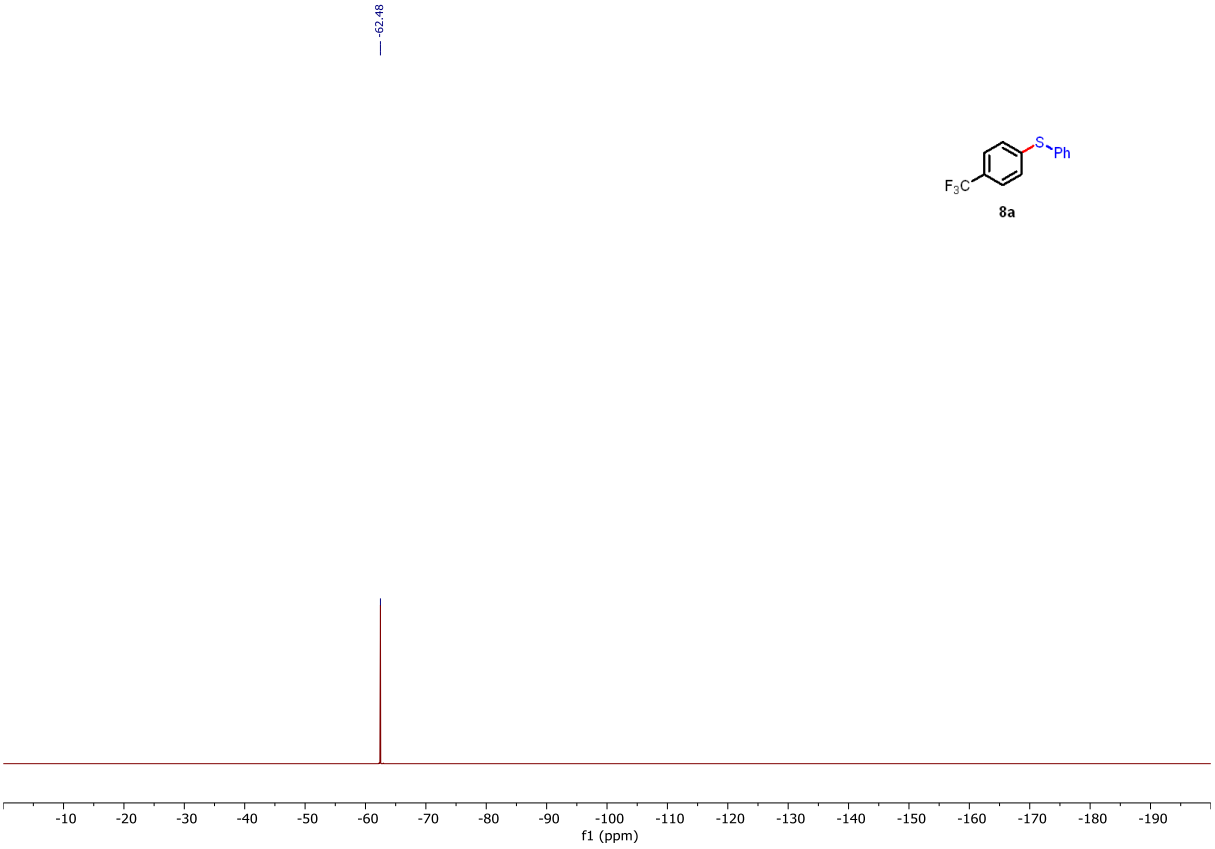


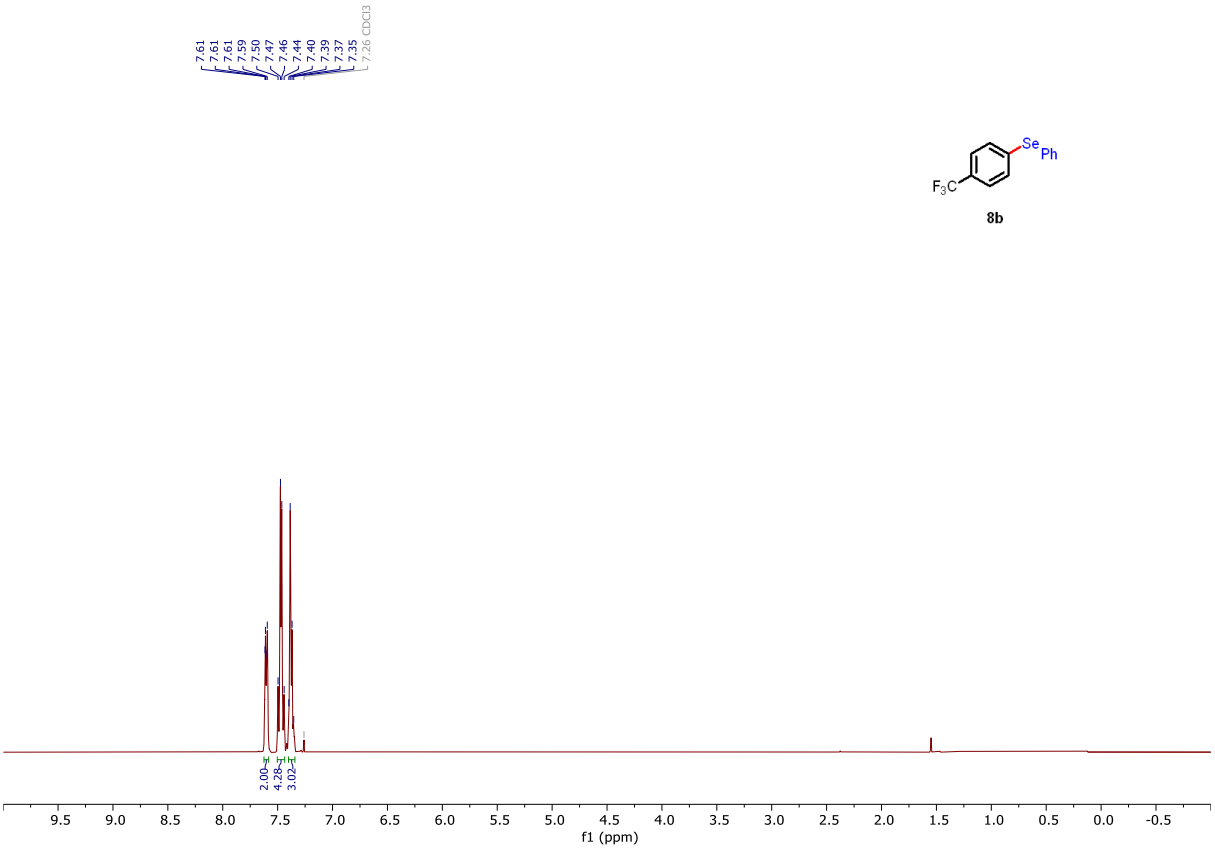

7c-125Te NMR.1.fid
10984-125Te
AKK-639

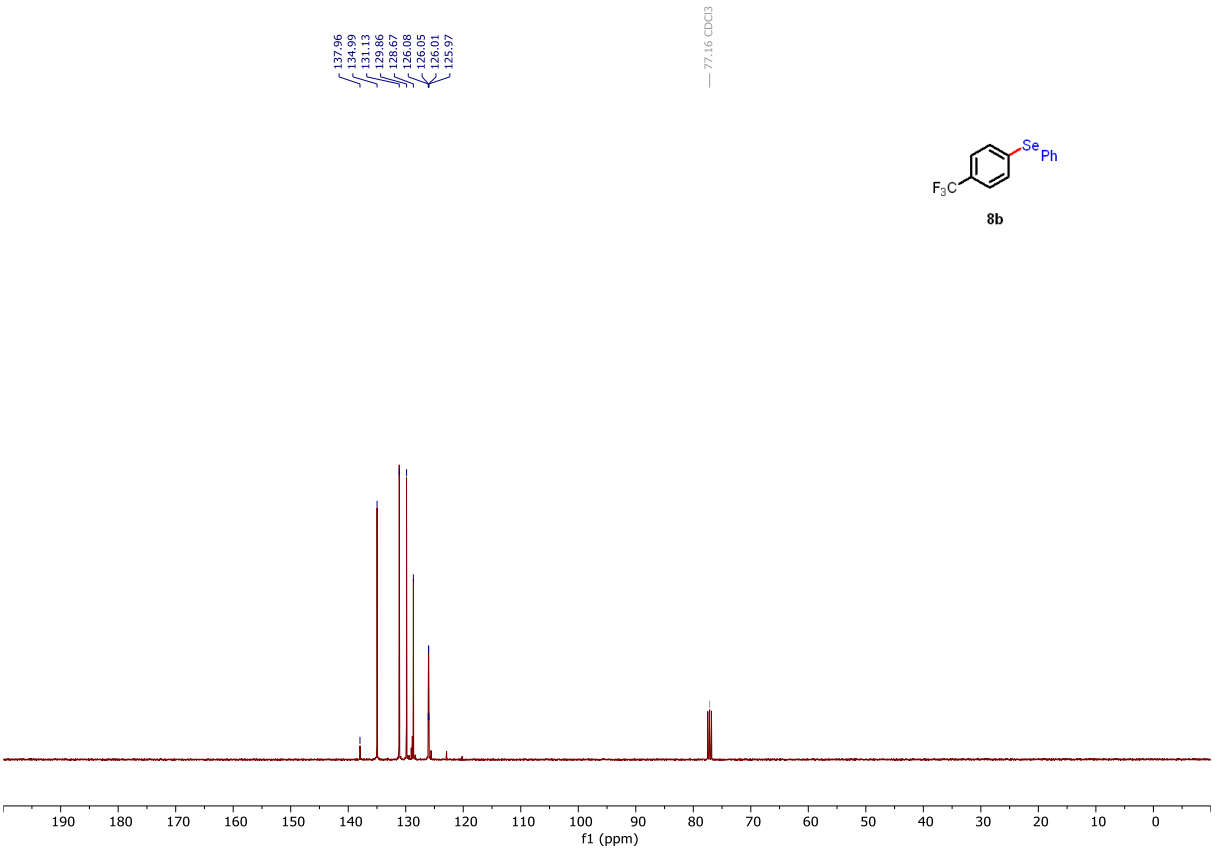


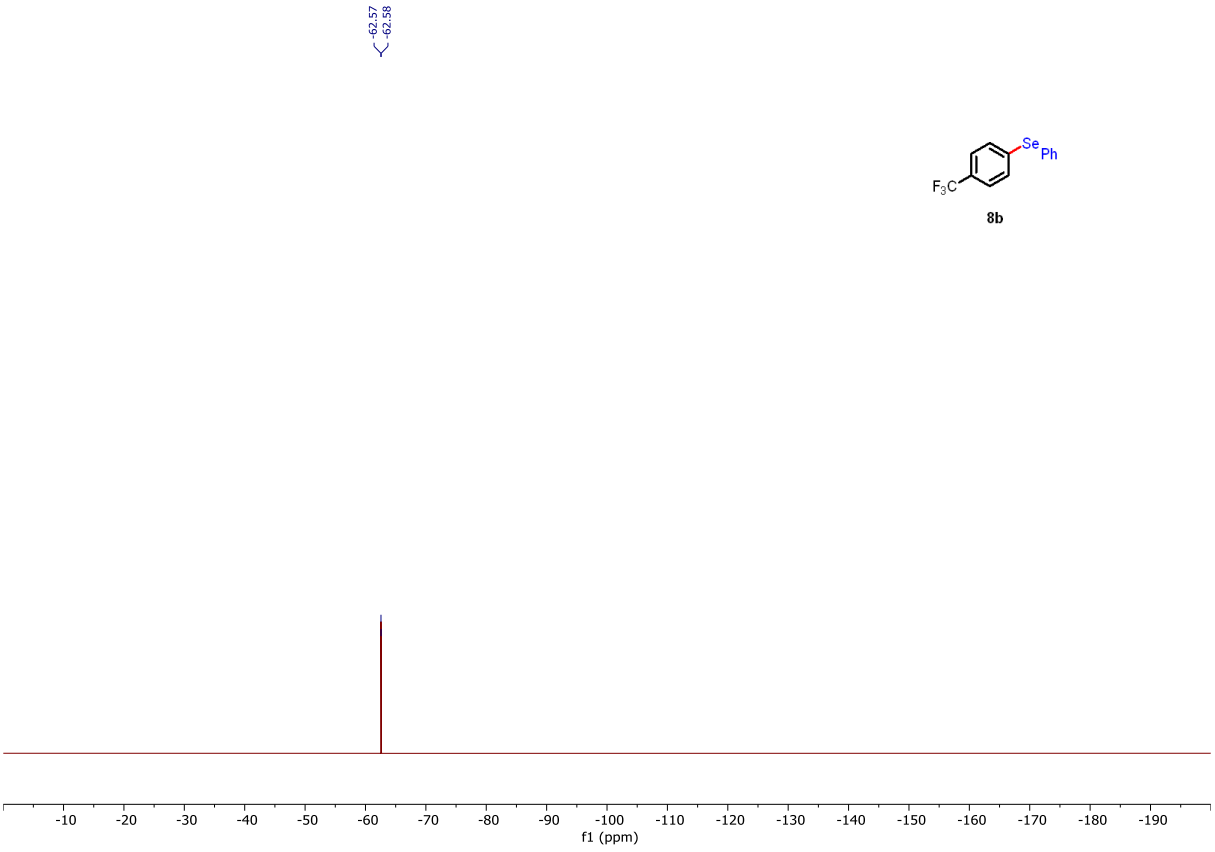

7.50
7.50
7.48
7.48
7.43
7.42
7.41
7.40
7.39
7.39
7.38
7.38
7.29
7.27
7.26 CDCl3
S
Ph
F3C
8a
3.95
2.90
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


143.00
142.98
133.68
132.63
129.82
128.79
128.42
128.33
128.29
128.00
126.01
125.97
125.93
125.89
125.59
122.89
77.16 CDCl3
S
Ph
F3C
8a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

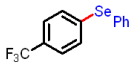

-62.48
S
Ph
F3C
8a
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)


7.61
7.61
7.61
7.59
7.50
7.47
7.46
7.44
7.40
7.39
7.37
7.35
7.26 CDCl3
Se
Ph
F3C
8b
2.00
4.28
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

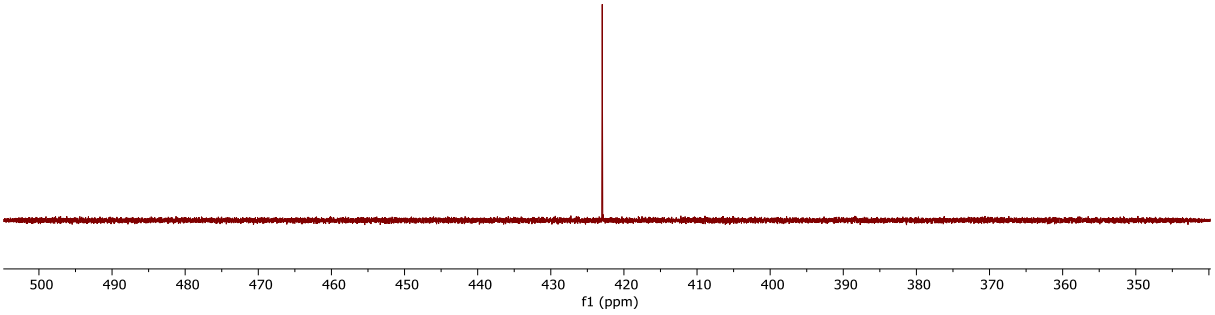

137.96
134.99
131.13
129.86
128.67
126.08
126.05
126.01
125.97
77.16 CDCl3
Se
Ph
F3C
8b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

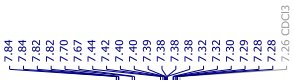

-62.57
-62.58
Se
Ph
F3C
8b
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

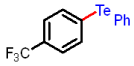
8b-77Se NMR.1.fid
10969-77Se
AKK-629



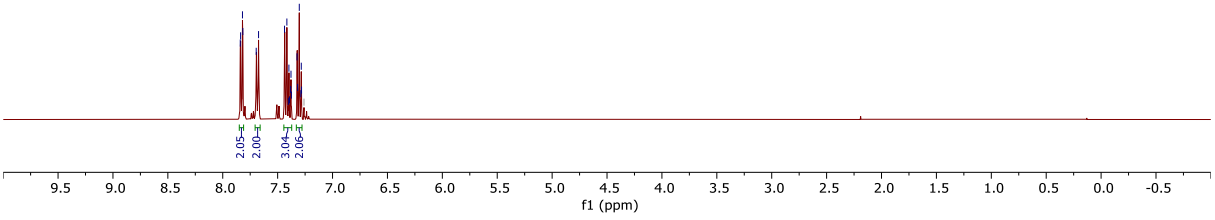

**8b**

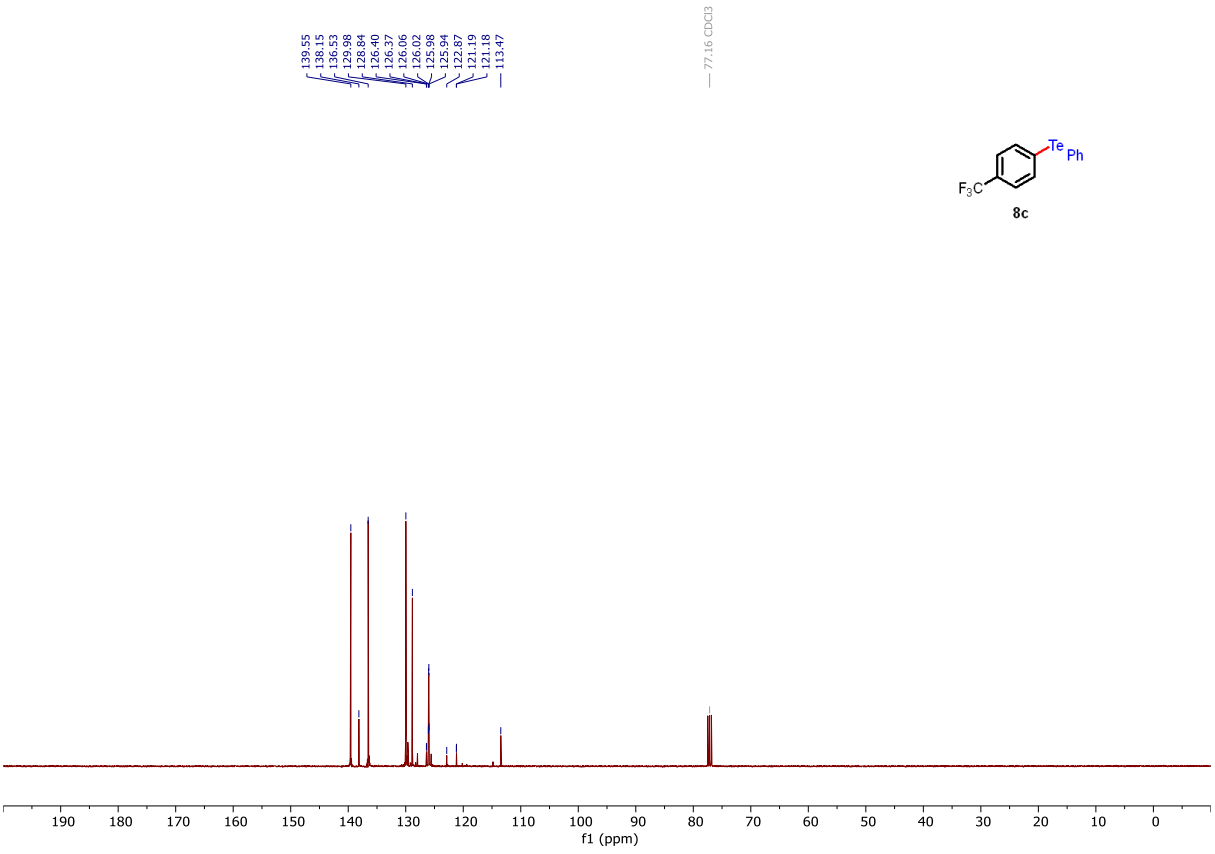


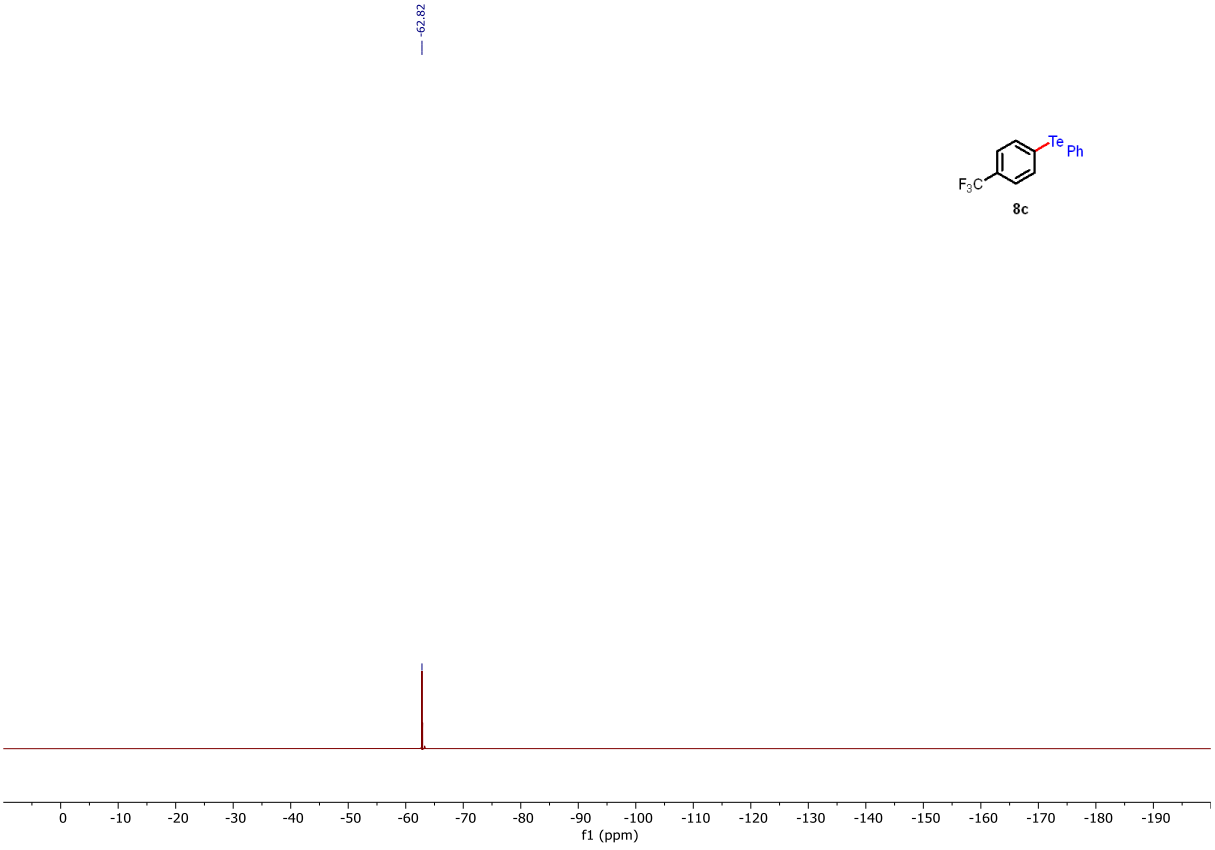




**8c**

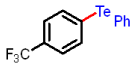



139.55
138.15
136.53
129.98
128.84
126.40
126.37
126.06
126.02
125.98
125.94
122.87
121.19
121.18
113.47
77.16 CDCl3
Te Ph
F3C
8c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

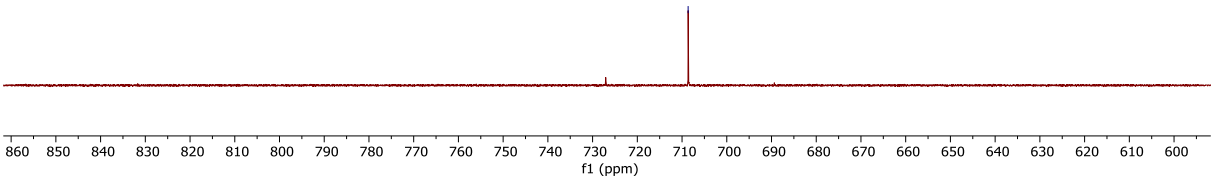

-62.82
Te Ph
F3C
8c
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

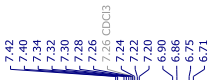
8c-125Te NMR.1.fid
11019-125Te
AKK-640R3

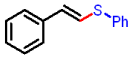
708.64



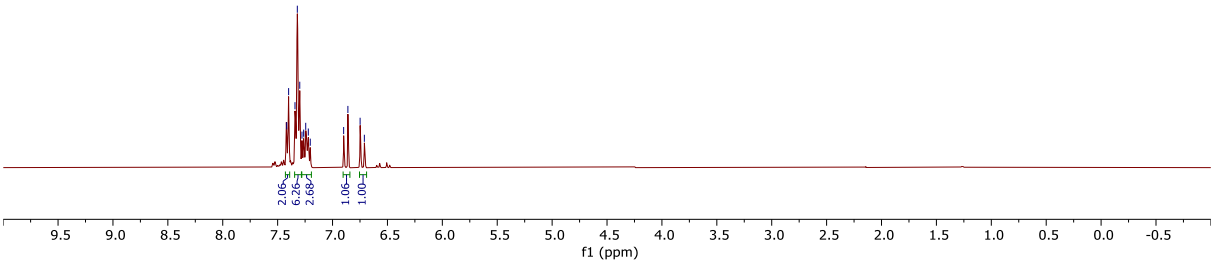

**8c**

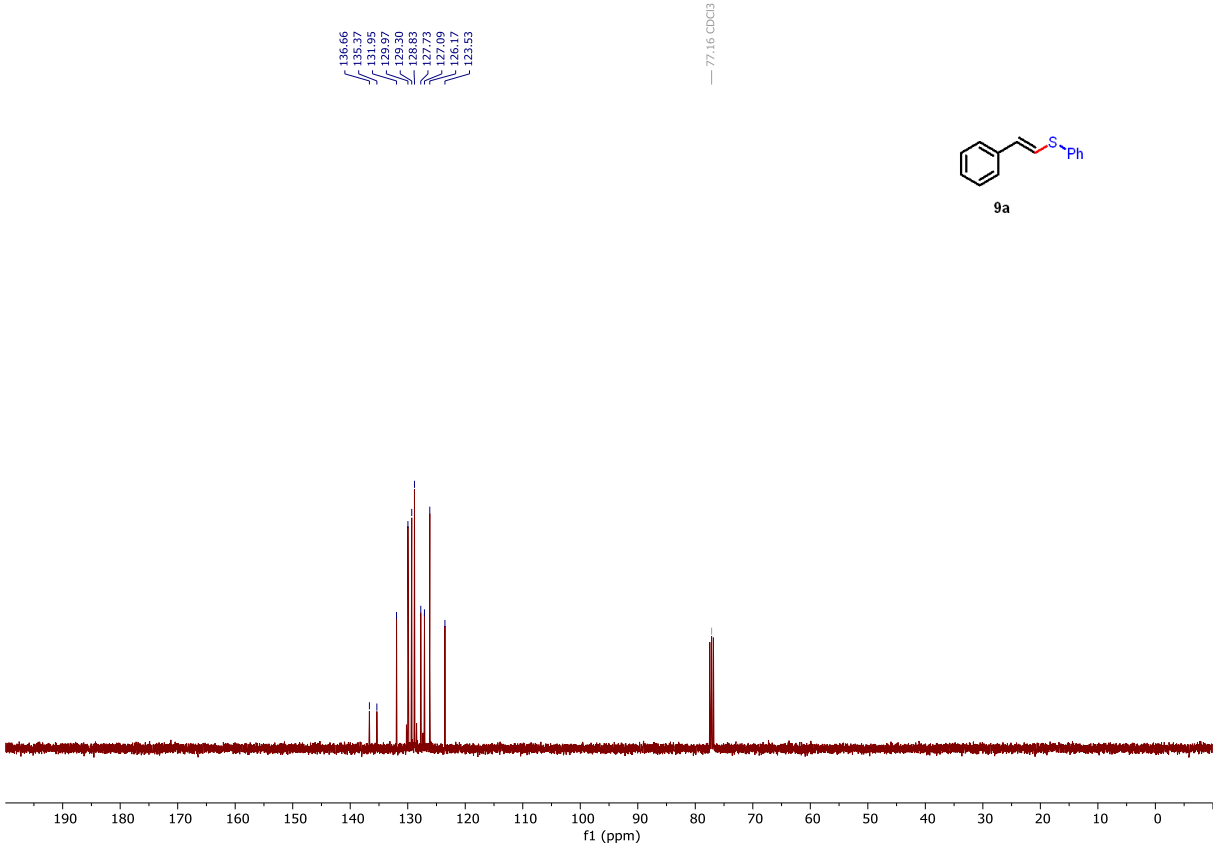


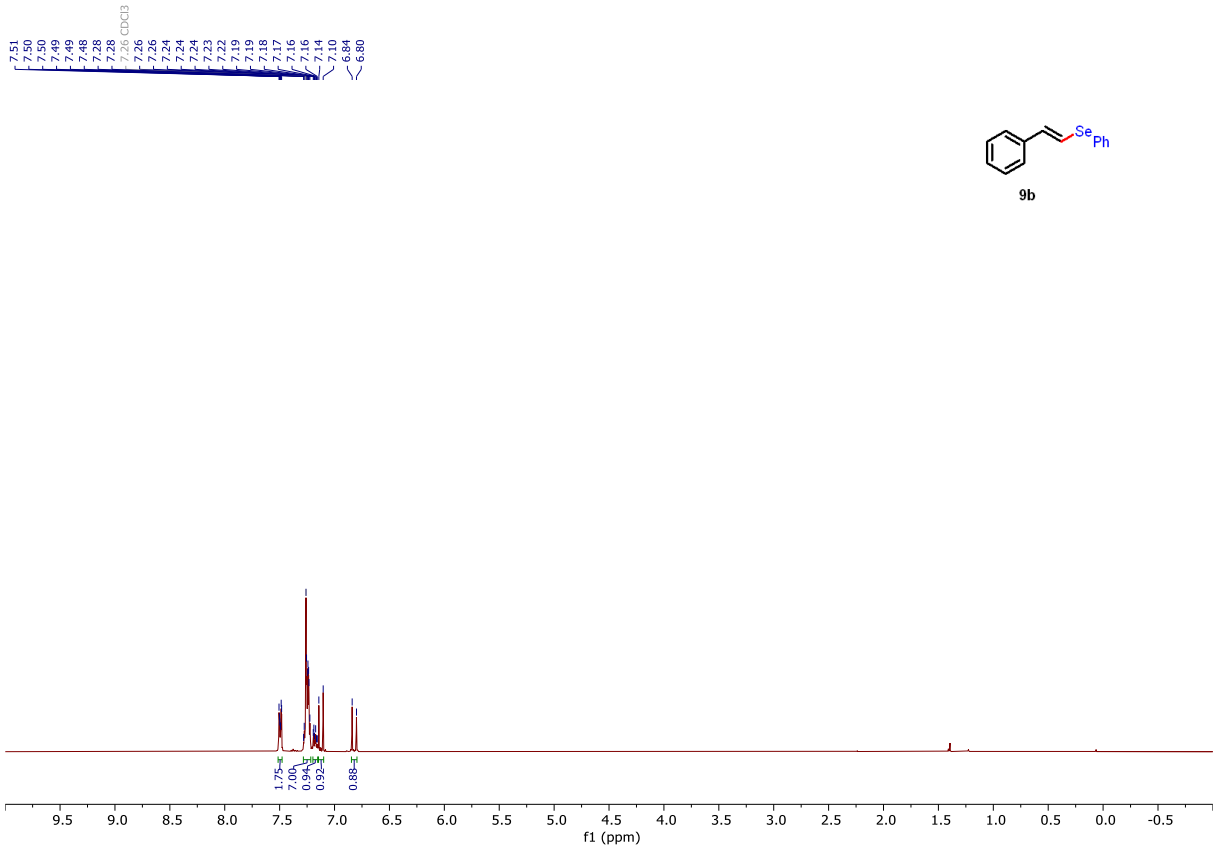



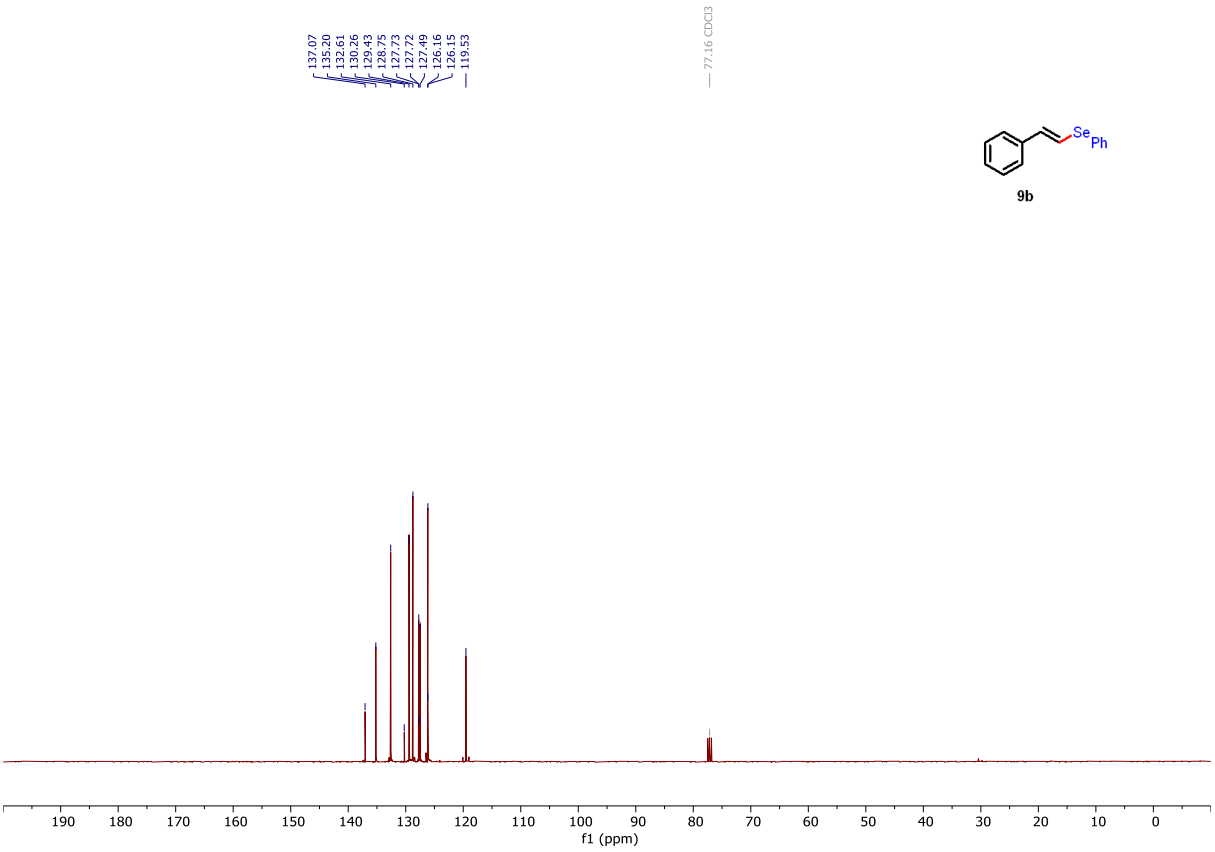




**9a**

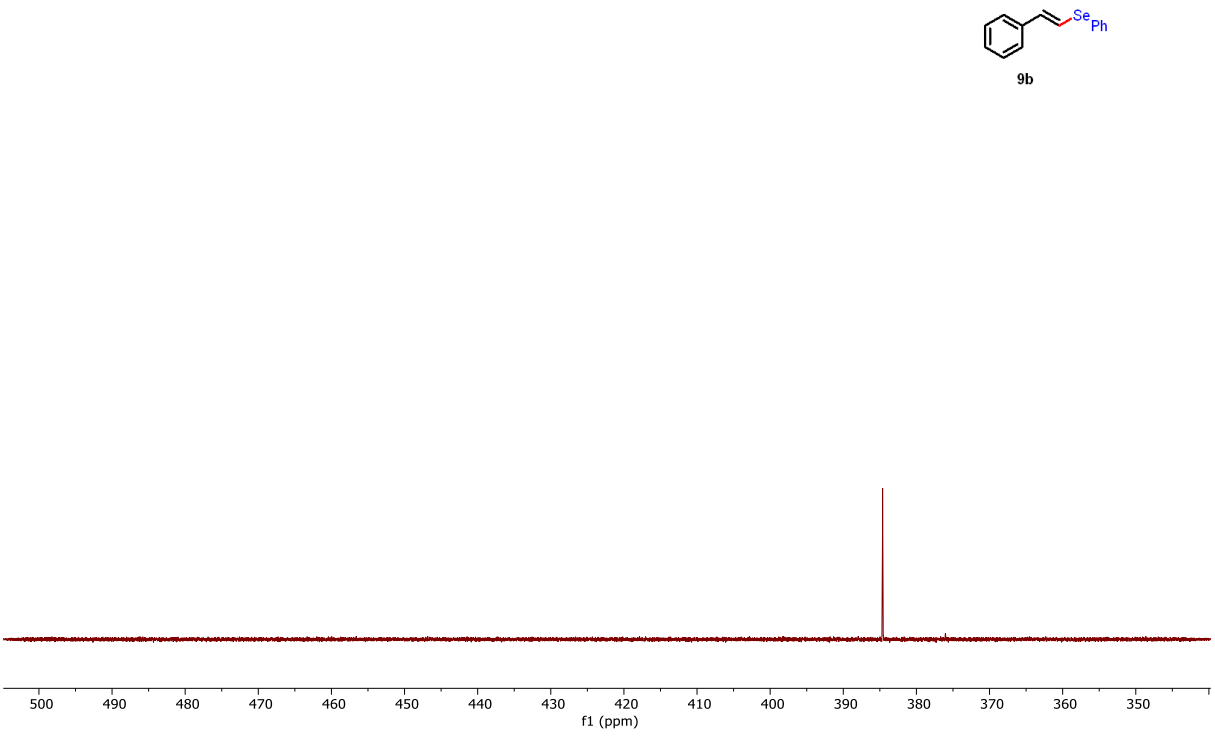


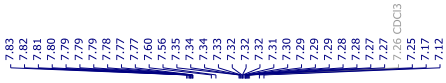

136.66
135.37
131.95
129.97
129.30
128.83
127.73
127.09
126.17
123.53
77.16 CDCl3
S
Ph
9a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.51
7.50
7.50
7.49
7.49
7.48
7.28
7.28
7.26 CDCl3
7.26
7.24
7.24
7.24
7.23
7.22
7.19
7.19
7.18
7.17
7.16
7.16
7.14
7.10
6.84
6.80
Se
Ph
9b
1.75
7.00
0.94
0.92
0.88
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)




9b-77Se NMR.1.fid
10970-77Se
AKK-630




7.83
7.82
7.81
7.80
7.79
7.79
7.79
7.79
7.78
7.77
7.77
7.60
7.56
7.35
7.34
7.34
7.33
7.32
7.32
7.32
7.31
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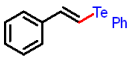
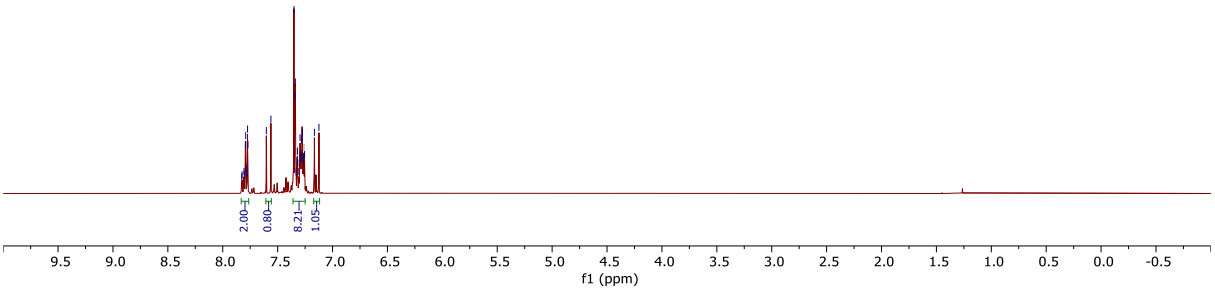
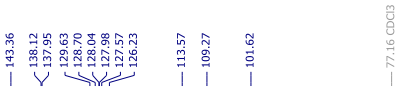
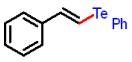
7.28
7.28
7.27
7.27
7.26 CDCl3
7.25
7.17
7.12


Te
Ph

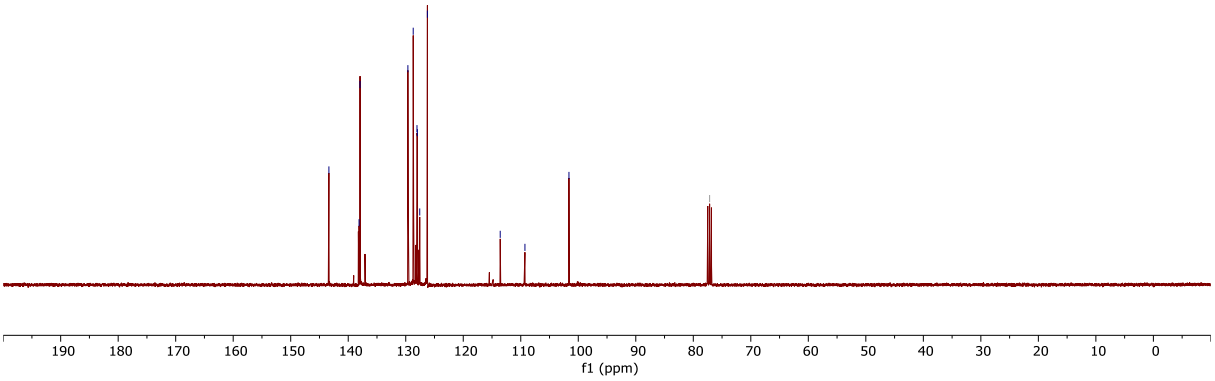
**9c**


2.00
0.80
8.21
1.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

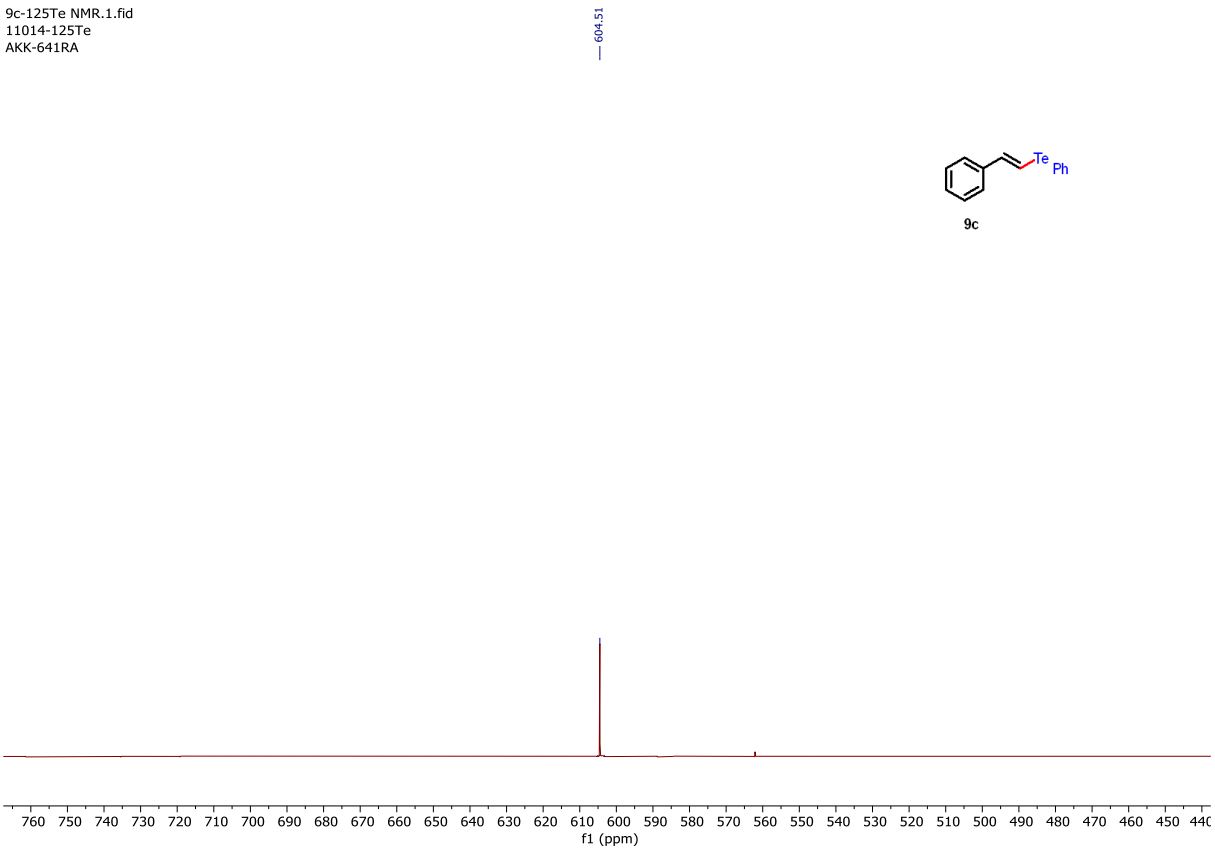

143.36
138.12
137.95
129.63
128.70
128.04
127.98
127.57
126.23
113.57
109.27
101.62
77.16 CDCl3


Te
Ph

**9c**


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

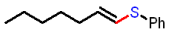
9c-125Te NMR.1.fid
11014-125Te
AKK-641RA



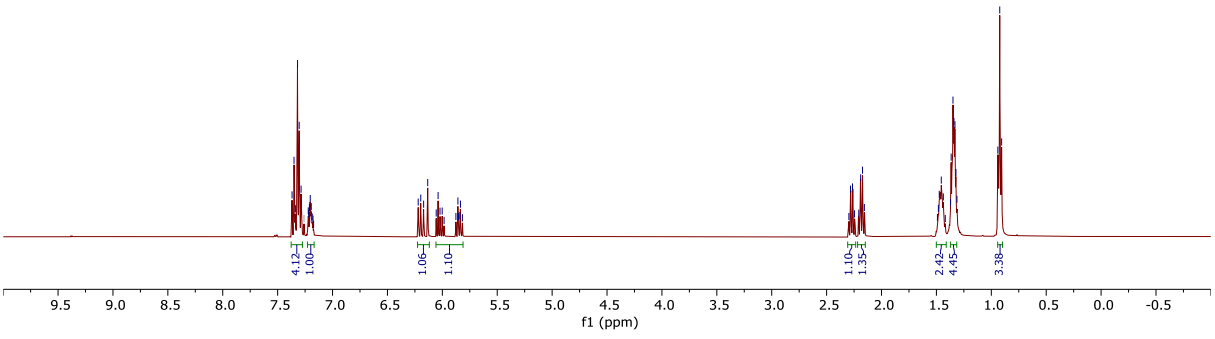


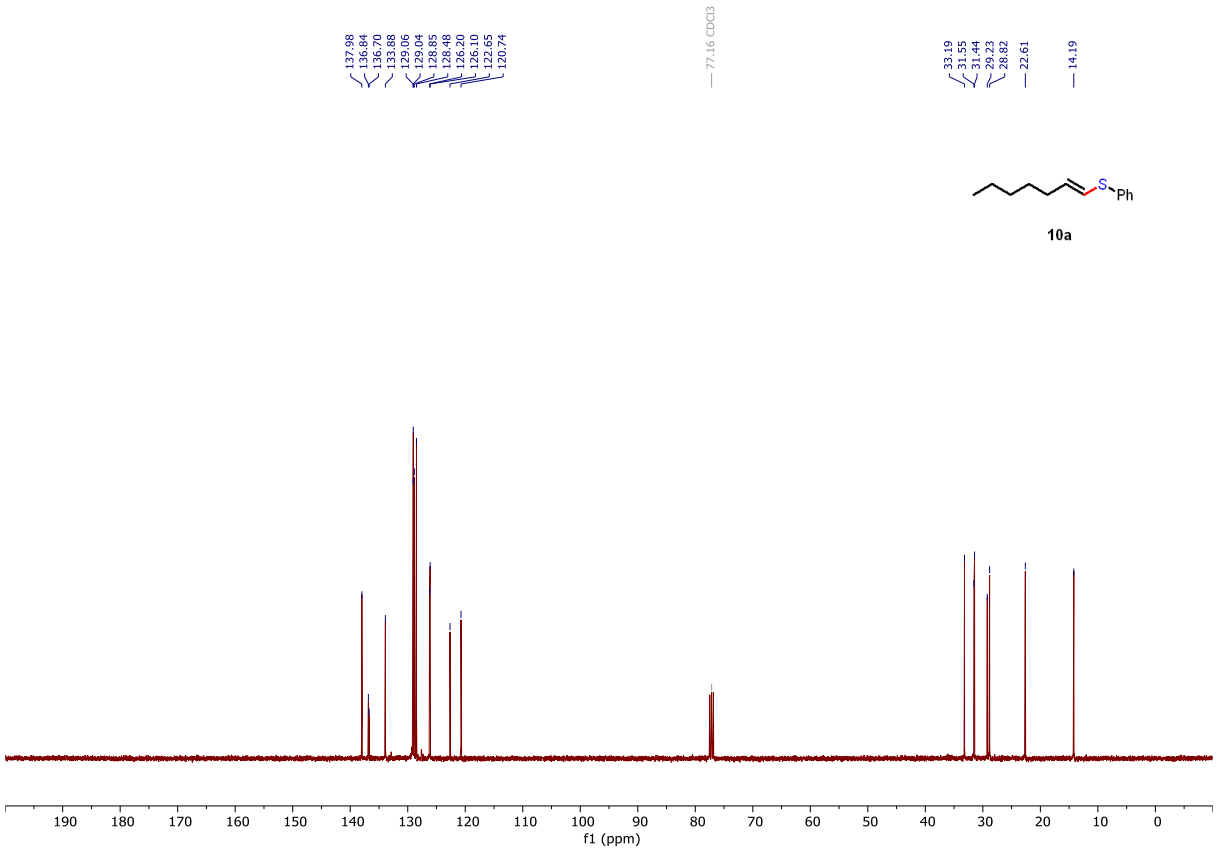


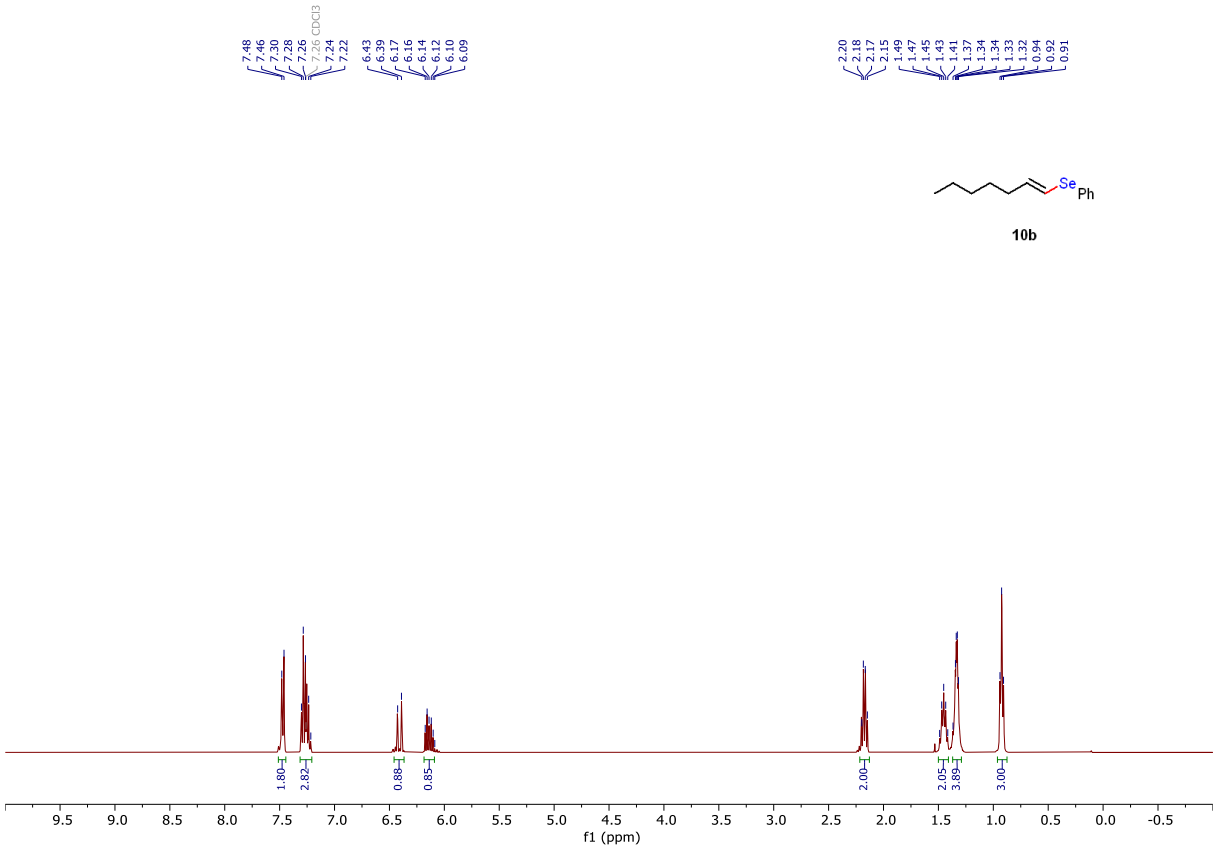
**9c**

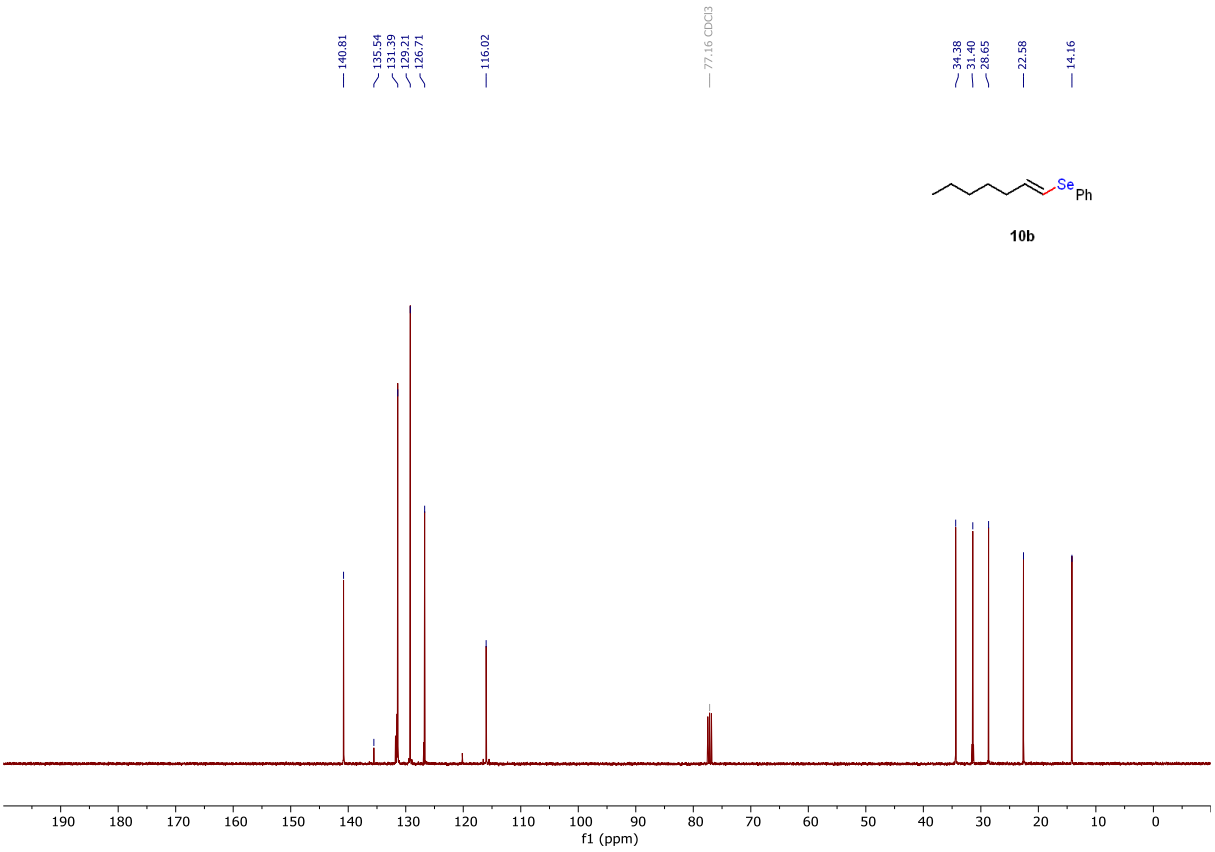




**10a**

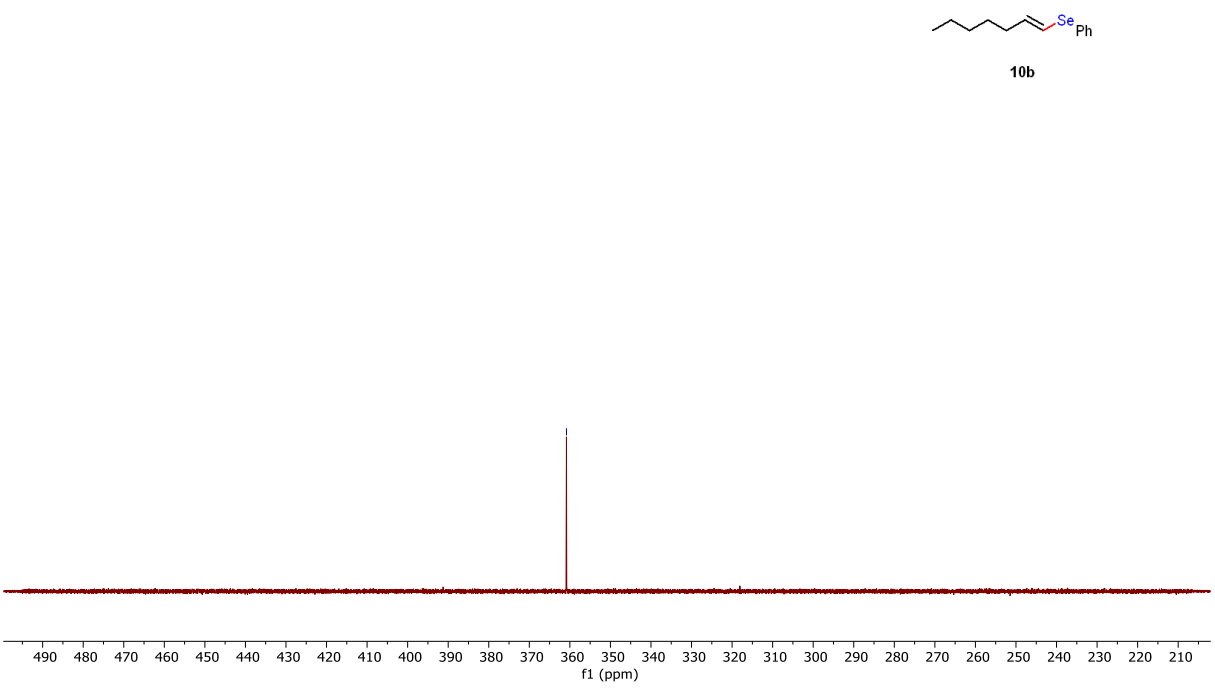



137.98
136.84
136.70
133.88
129.06
129.04
128.85
128.48
126.20
126.10
122.65
120.74
77.16 CDCl3
33.19
31.55
31.44
29.23
28.82
22.61
14.19
S
Ph
10a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

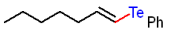

7.48
7.46
7.30
7.28
7.26
7.25 CDCl3
7.24
7.22
6.43
6.39
6.17
6.16
6.14
6.12
6.10
6.09
2.20
2.18
2.17
2.15
1.49
1.47
1.45
1.43
1.41
1.37
1.34
1.34
1.33
1.32
0.94
0.92
0.91
Se
Ph
10b
1.80
2.82
0.88
0.85
2.00
2.05
3.89
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



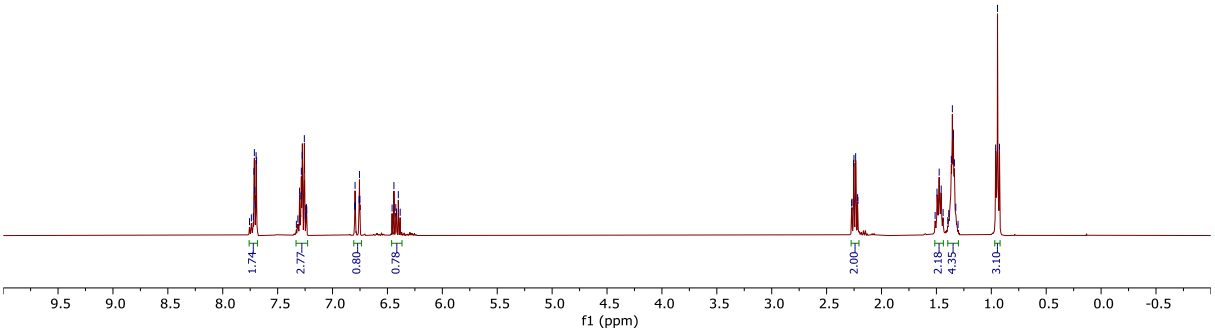

10b-77Se NMR.1.fid
11012-77Se
AKK-631RA

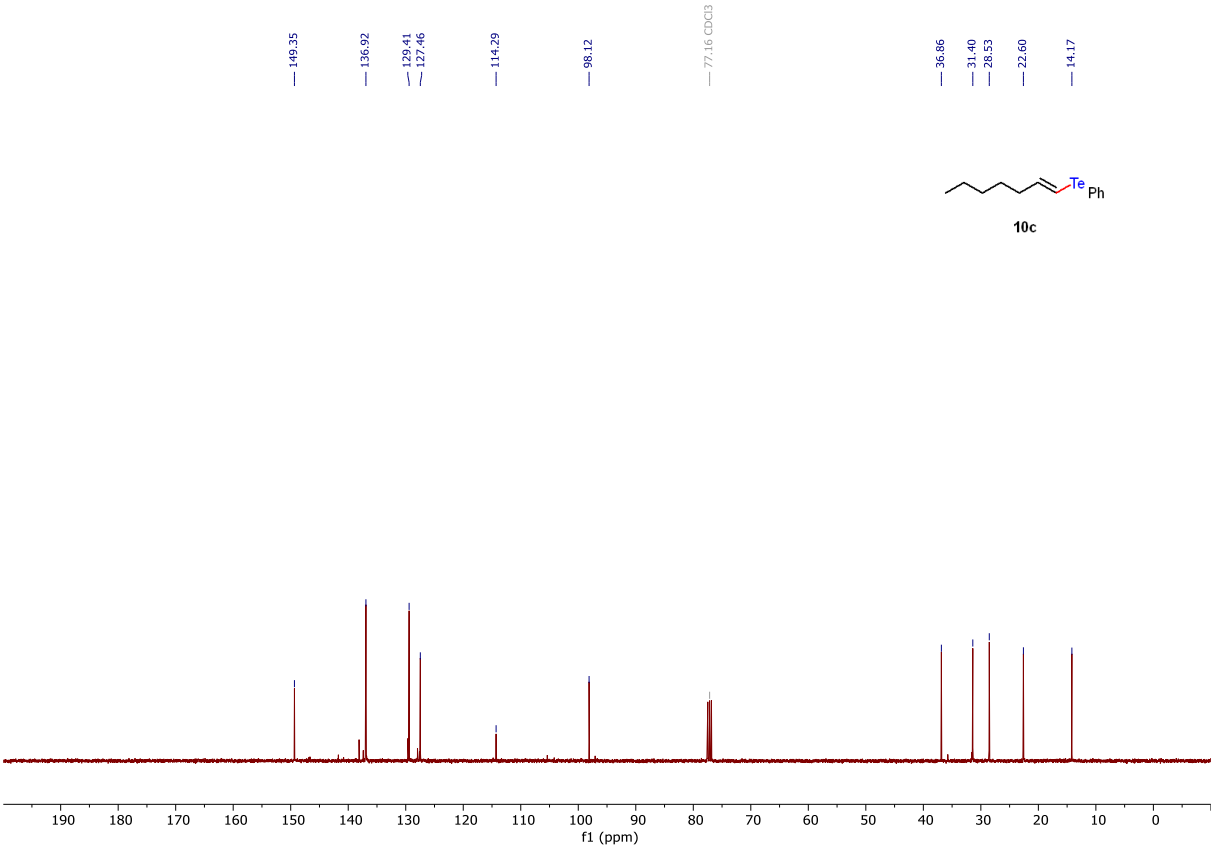



7.76
7.74
7.72
7.72
7.71
7.71
7.70
7.70
7.69
7.33
7.32
7.30
7.29
7.28
7.28
7.26 CDCl3
7.26
7.24
7.24
7.23
6.80
6.79
6.79
6.76
6.75
6.75
6.46
6.44
6.42
6.42
6.40
6.38
2.27
2.27
2.25
2.25
2.24
2.22
2.21
1.51
1.49
1.47
1.46
1.44
1.40
1.39
1.36
1.35
1.34
1.34
1.32
1.30
0.96
0.94
0.93


Te
Ph

**10c**


1.74
2.77
0.80
0.78
2.00
2.18
4.35
3.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

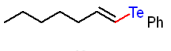

149.35
136.92
129.41
127.46
114.29
98.12
77.16 CDCl3
36.86
31.40
28.53
22.60
14.17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Te
Ph

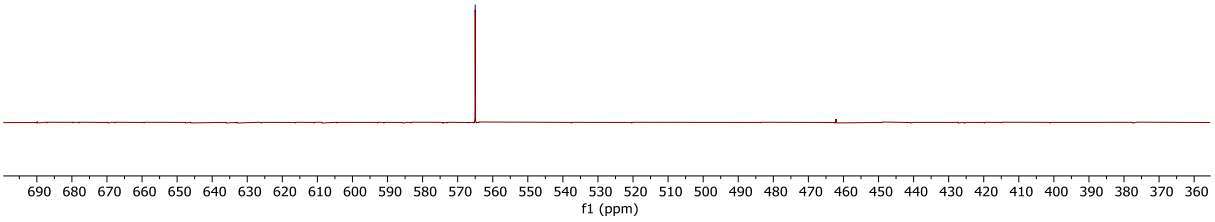
**10c**

10c-125Te NMR.1.fid
11015-125Te
AKK-642RA

565.00



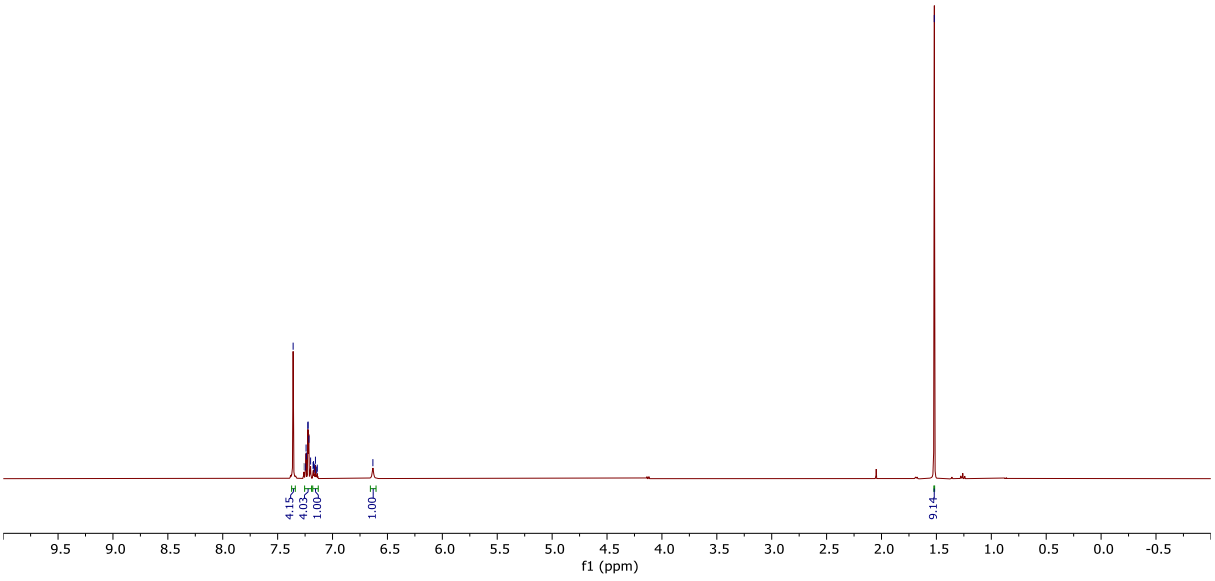

**10c**

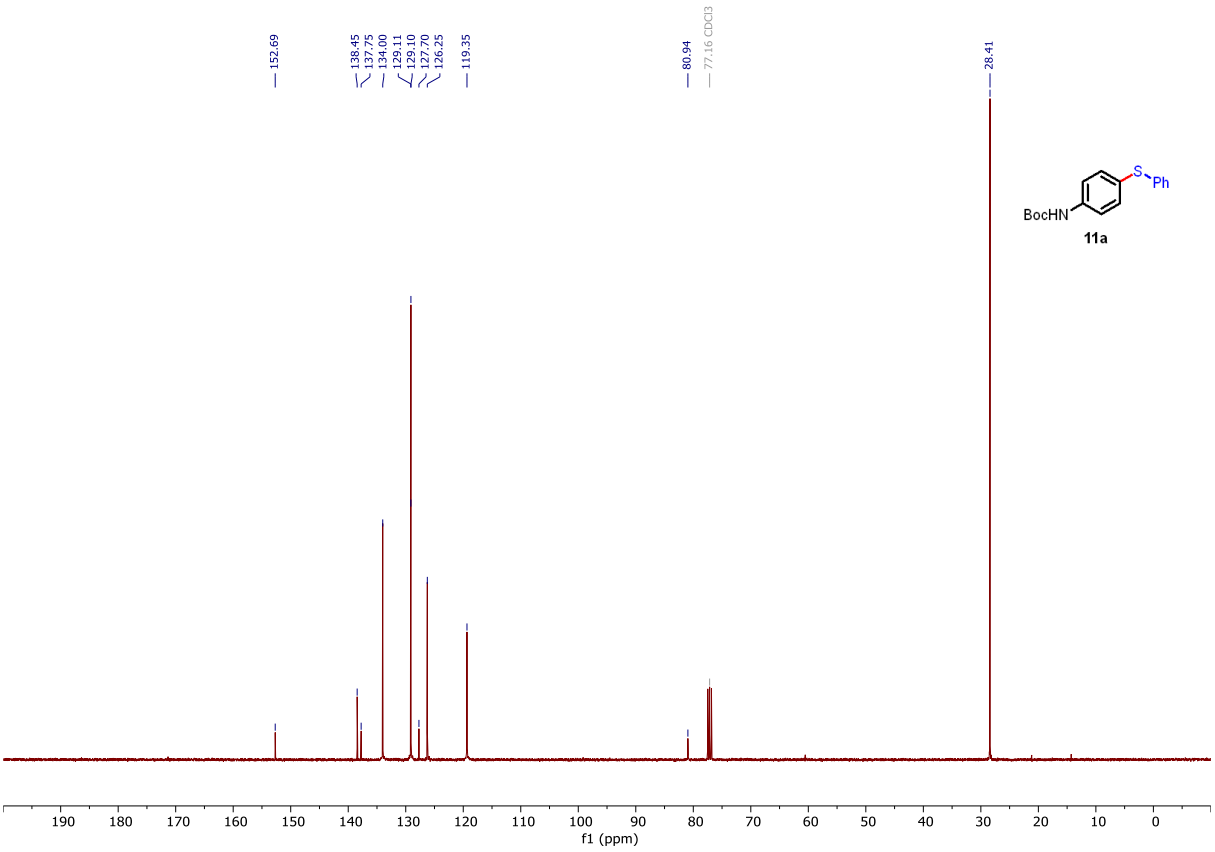


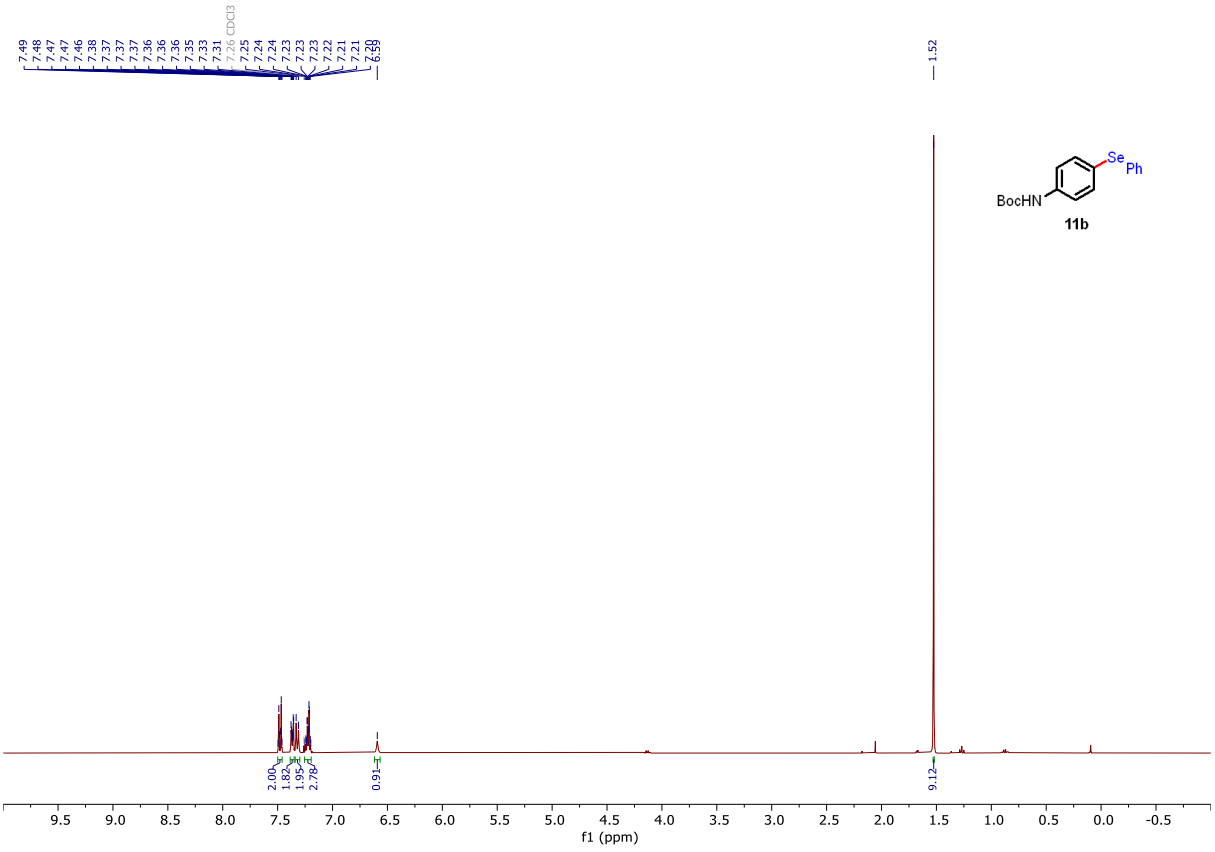

7.36
7.26 CDCl3
7.25
7.24
7.24
7.22
7.22
7.22
7.20
7.18
7.17
7.17
7.16
7.16
7.14
7.14
6.63

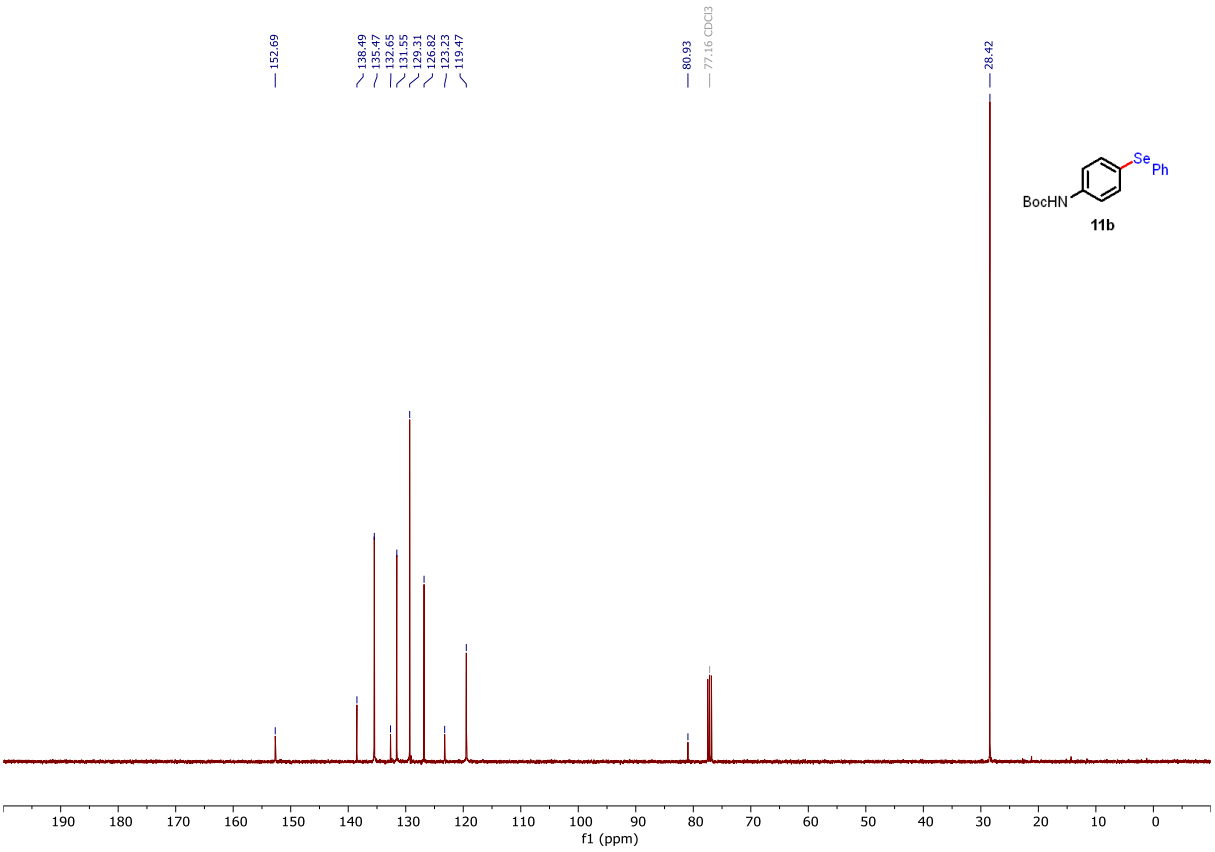
1.52


**11a**

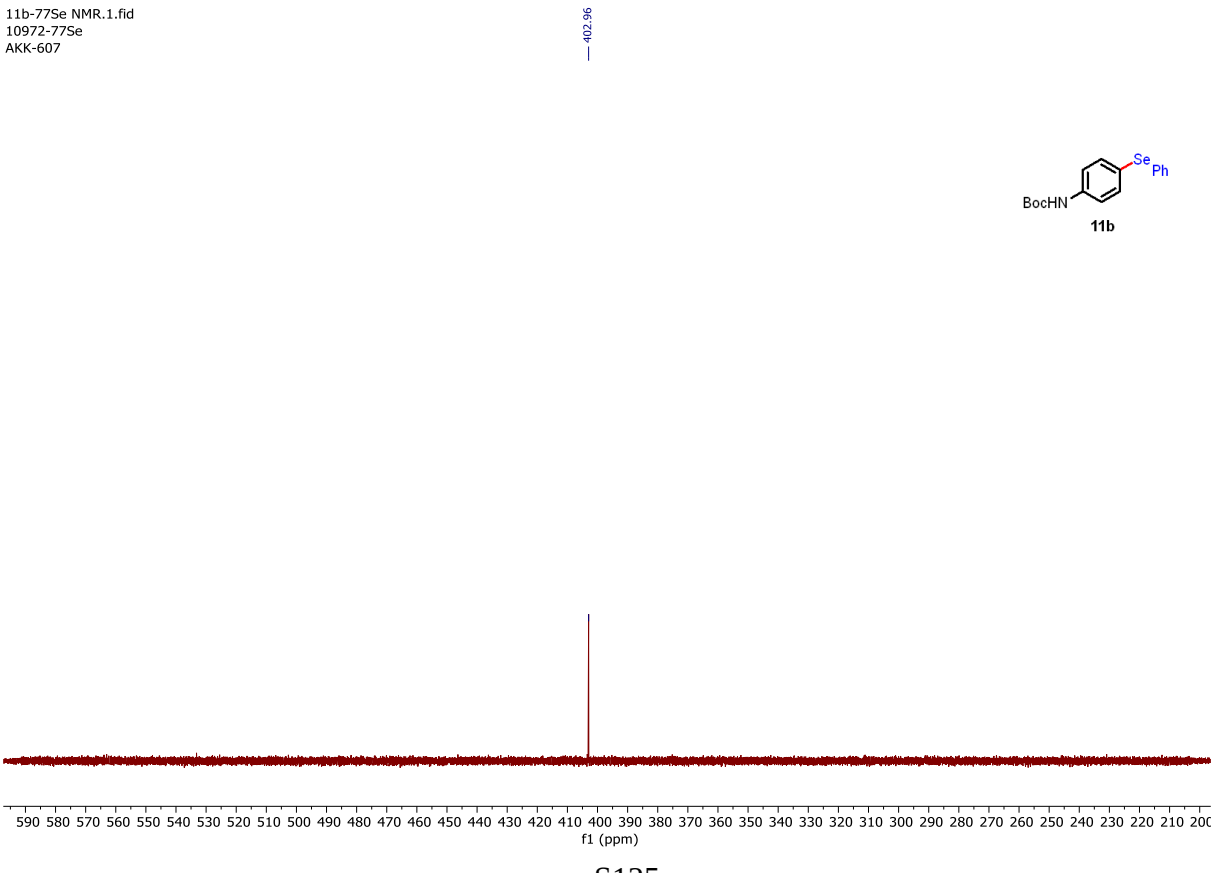


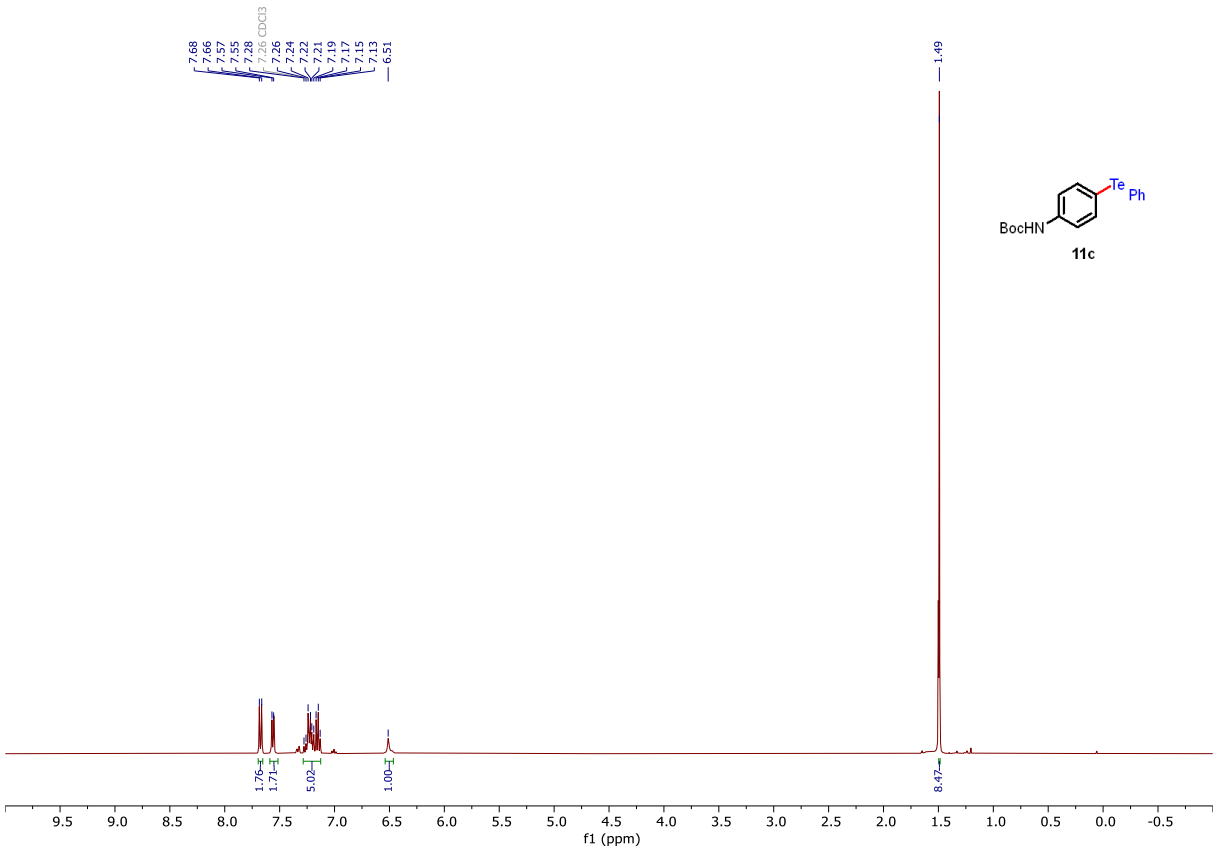

152.69
138.45
137.75
134.00
129.11
129.10
127.70
126.25
119.35
80.94
77.16 CDCl3
28.41
S
Ph
BocHN
11a
f1 (ppm)

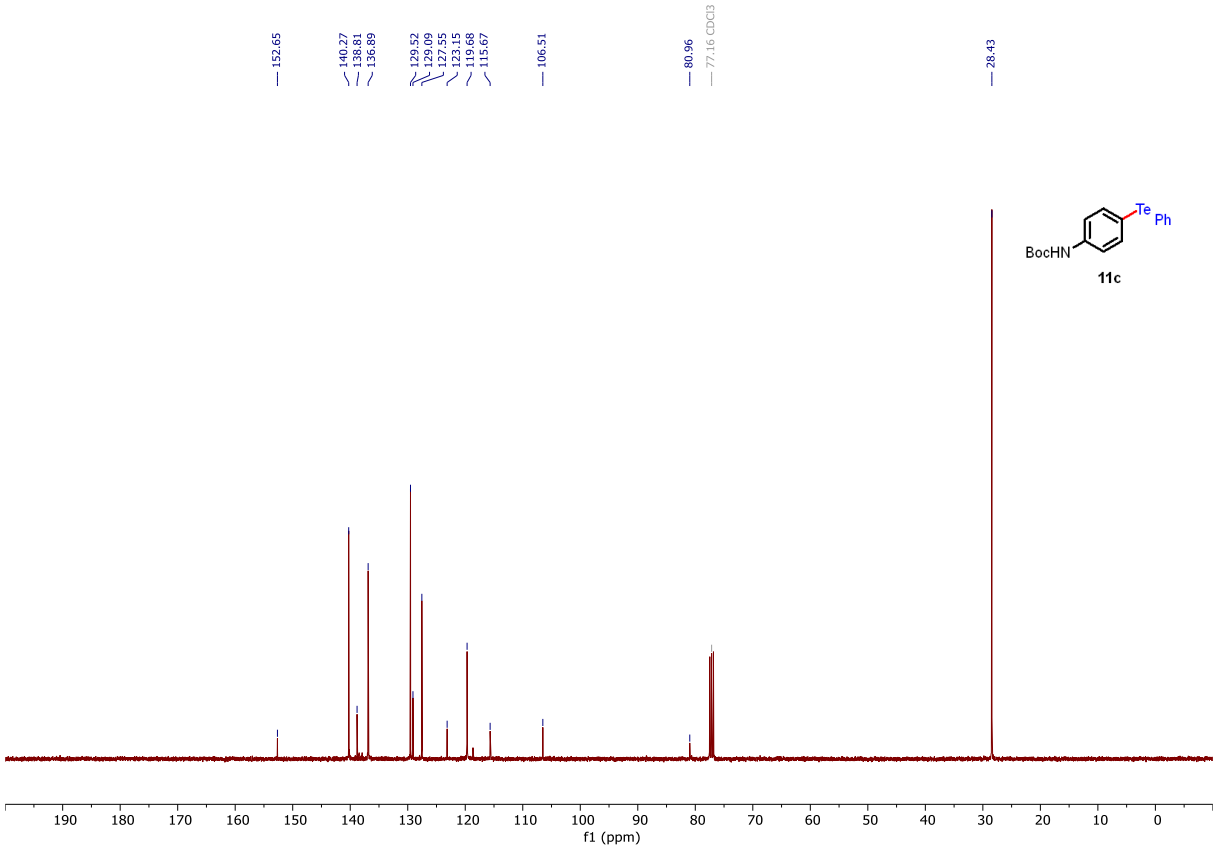

7.49
7.48
7.47
7.47
7.47
7.46
7.38
7.37
7.37
7.37
7.36
7.36
7.36
7.35
7.33
7.31
7.26 CDCl3
7.25
7.24
7.24
7.23
7.23
7.23
7.22
7.21
7.21
7.20
6.99
1.52
Se
Ph
BocHN
11b
2.00
1.82
1.95
2.78
0.91
9.12
f1 (ppm)




11b-77Se NMR.1.fid
10972-77Se
AKK-607

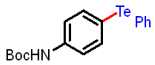



7.68
7.66
7.57
7.55
7.28
7.26 CDCl3
7.26
7.24
7.22
7.21
7.19
7.17
7.15
7.13
6.51
1.49
1.76
1.71
5.02
1.00
8.47
BocHN
Te
Ph
11c
f1 (ppm)

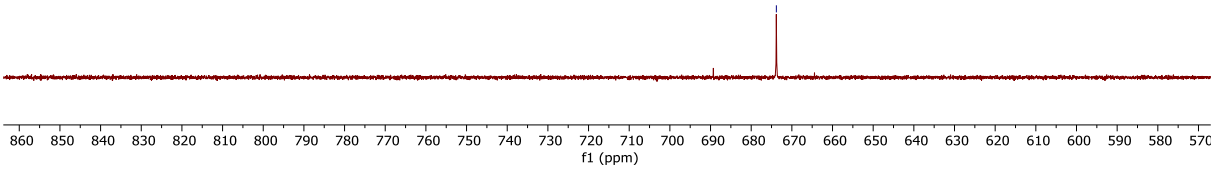

152.65
140.27
138.81
136.89
129.52
129.09
127.55
123.15
119.68
115.67
106.51
80.96
77.16 CDCl3
28.43
BocHN
Te
Ph
11c
f1 (ppm)

11c-125Te NMR.1.fid
10980-125Te
AKK-608

673.81

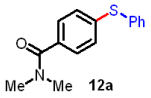



**11c**

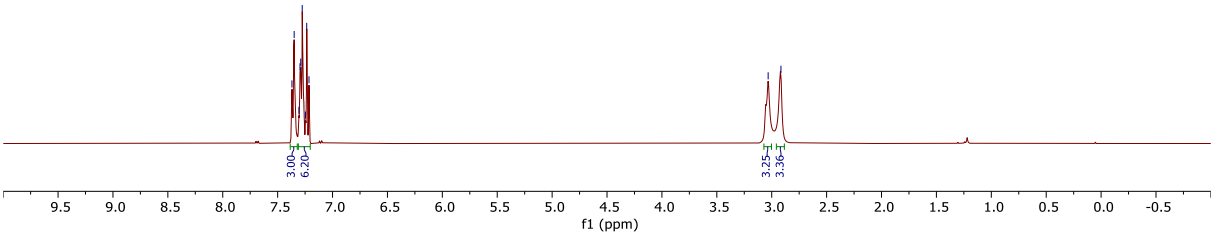


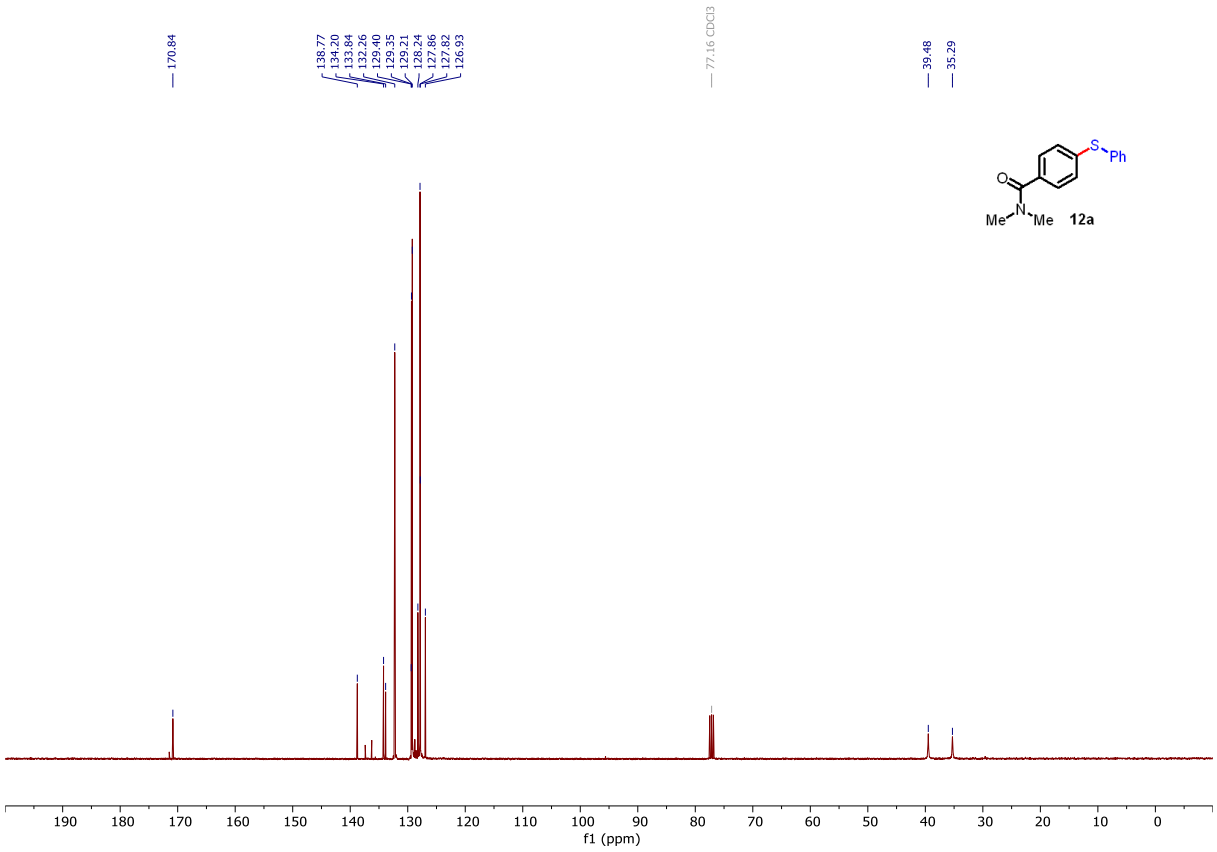

7.37
7.35
7.31
7.30
7.29
7.28
7.26 CDCl3
7.25
7.24
7.21

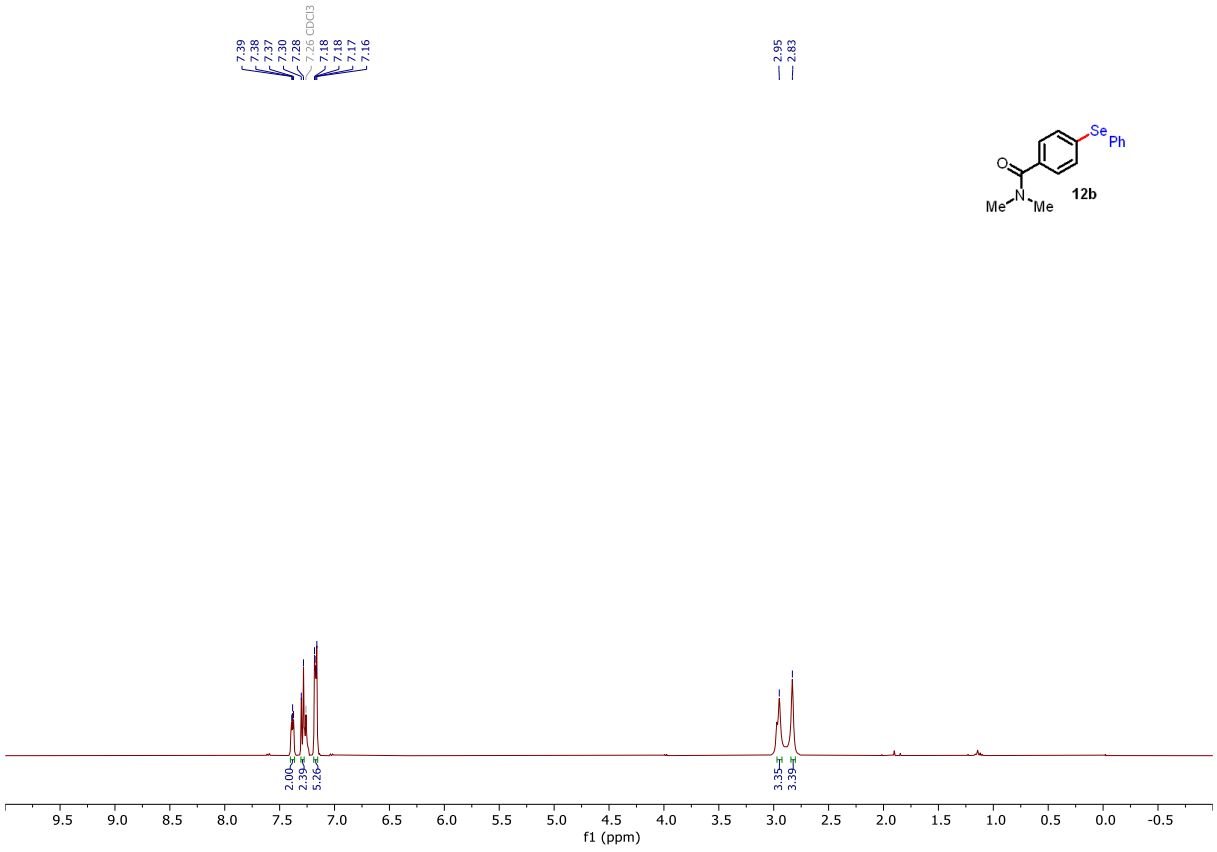
3.03
2.92

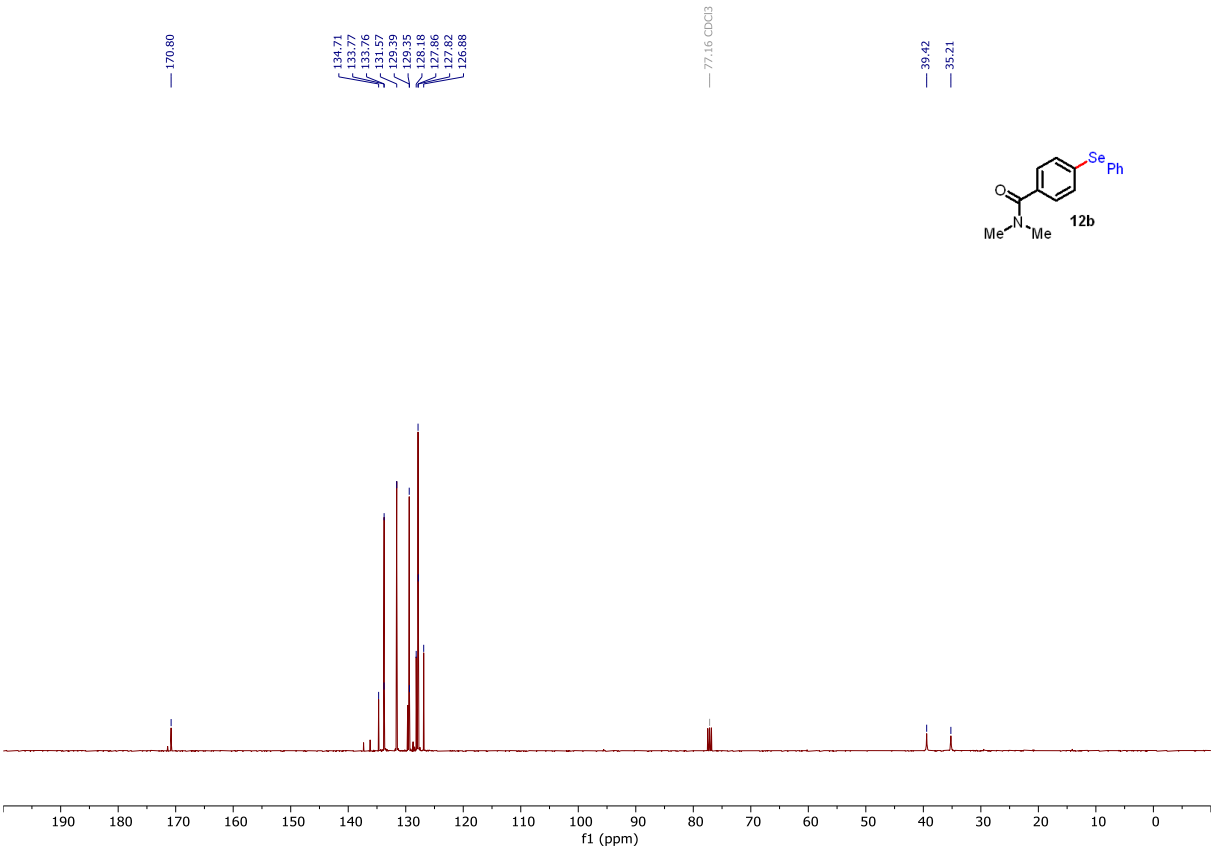



**12a**

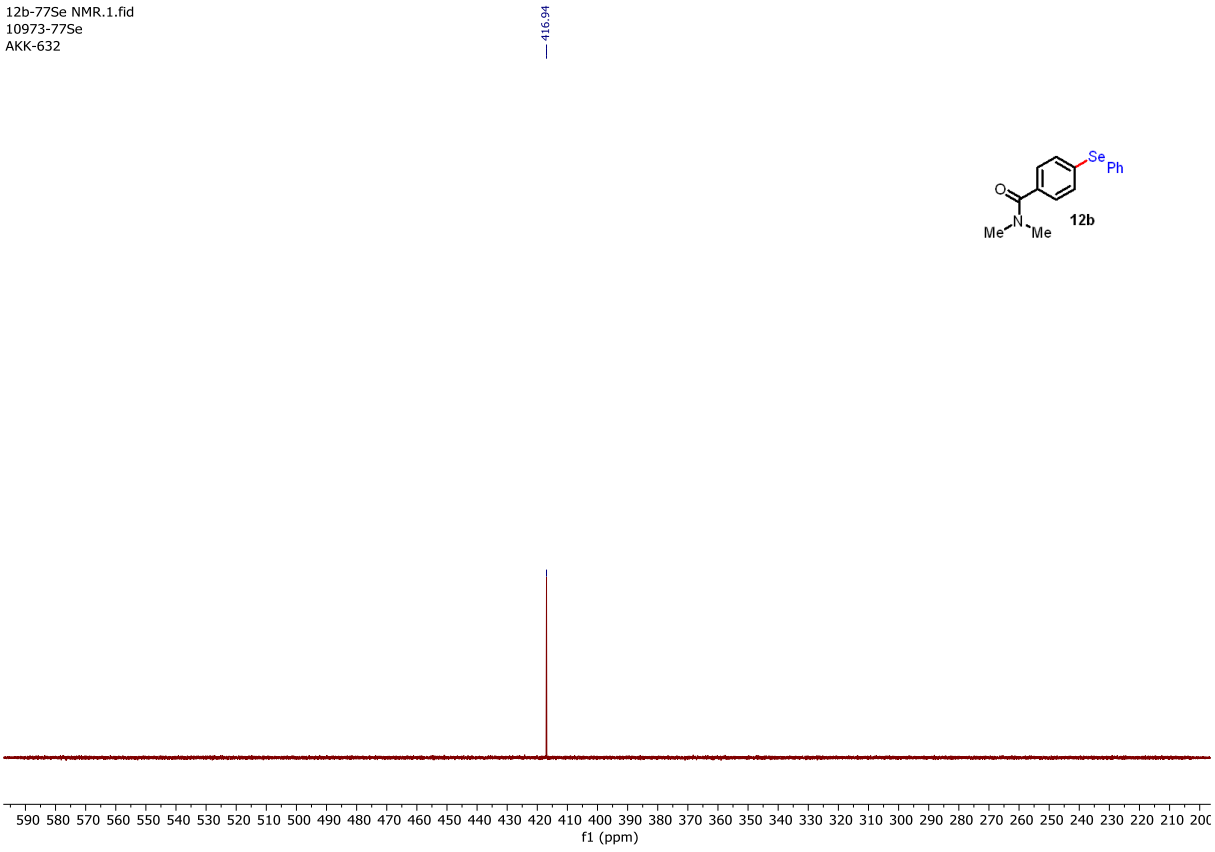



170.84
138.77
134.20
133.84
132.26
129.40
129.35
129.21
128.24
127.86
127.82
126.93
77.16 CDCl3
39.48
35.29
S
Ph
O
N
Me
Me
12a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.39
7.38
7.37
7.30
7.28
7.26 CDCl3
7.18
7.18
7.17
7.16
2.95
2.83
Se
Ph
O
N
Me
Me
12b
2.00
2.39
5.26
3.35
3.39
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

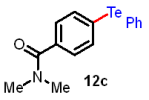


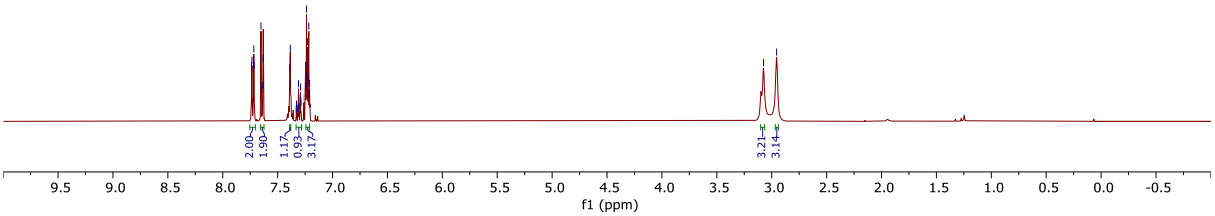

12b-77Se NMR.1.fid
10973-77Se
AKK-632




7.74
7.73
7.72
7.71
7.65
7.65
7.64
7.63
7.39
7.38
7.33
7.33
7.32
7.32
7.31
7.30
7.29
7.29
7.29
7.26 CDCl3
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.21
7.21


3.07
2.96

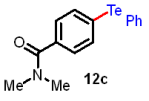

Te
Ph
O
N
Me
Me
12c

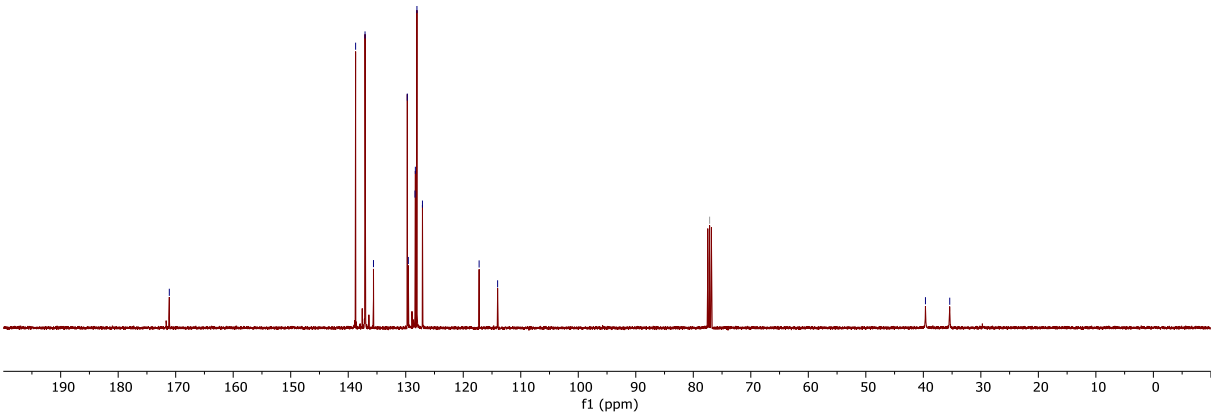

2.00
1.90
1.17
0.93
3.17
3.21
3.14
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


171.11
138.72
137.08
135.61
129.73
129.55
128.39
128.33
128.05
127.09
117.24
114.02


77.16 CDCl3

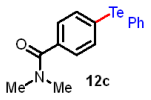

39.63
35.41


Te
Ph
O
N
Me
Me
12c

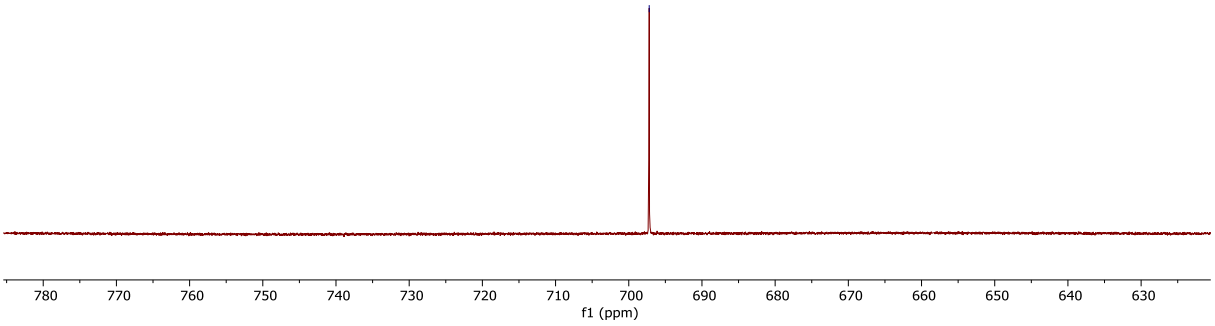

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

12c-125Te NMR.1.fid
11008-125Te
AKK-643R

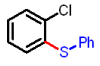
697.21



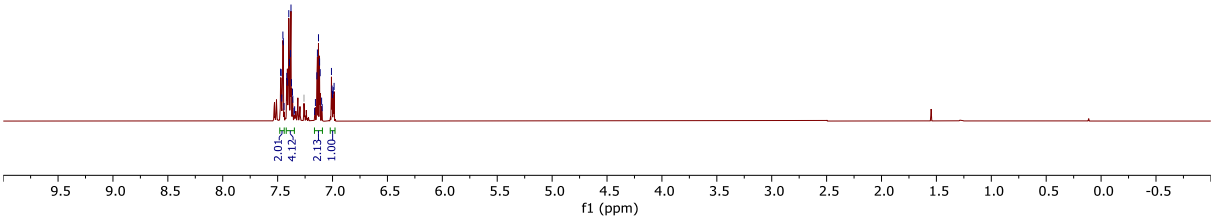

12c

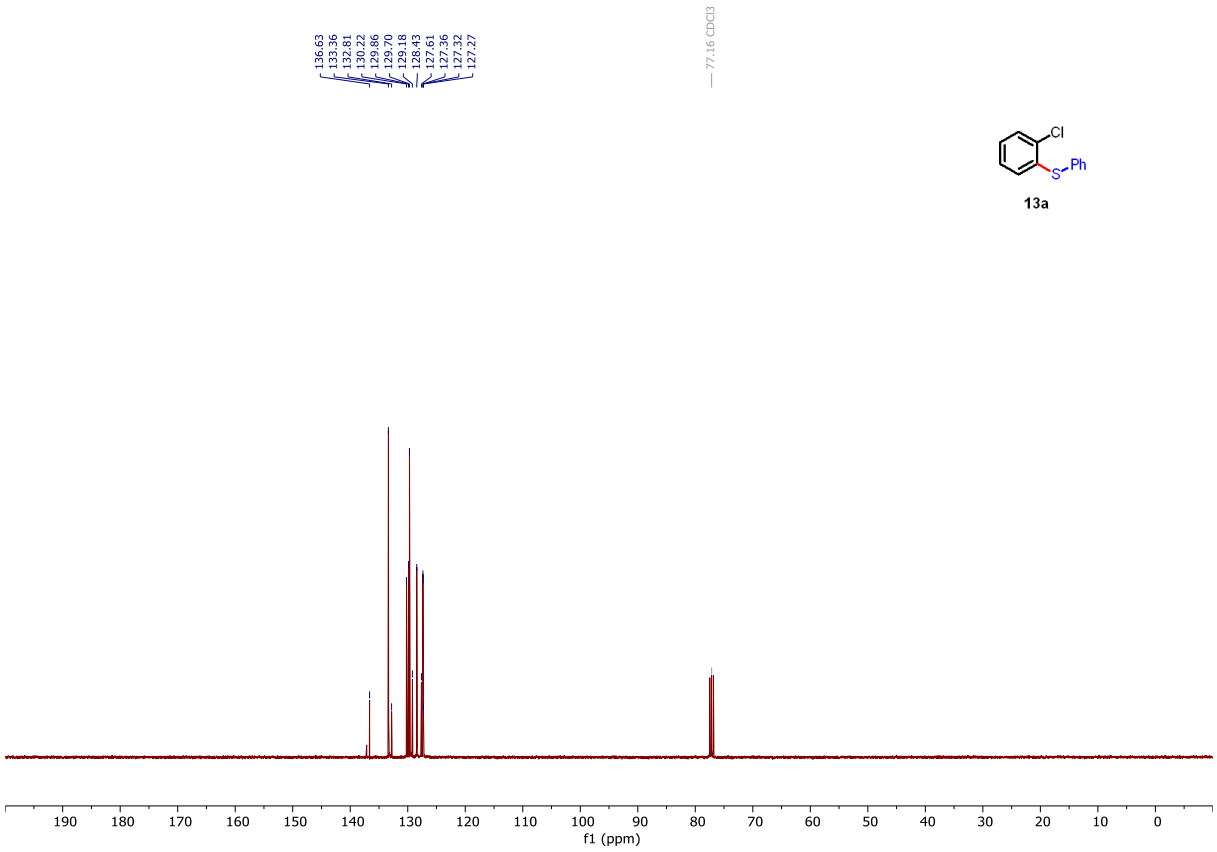


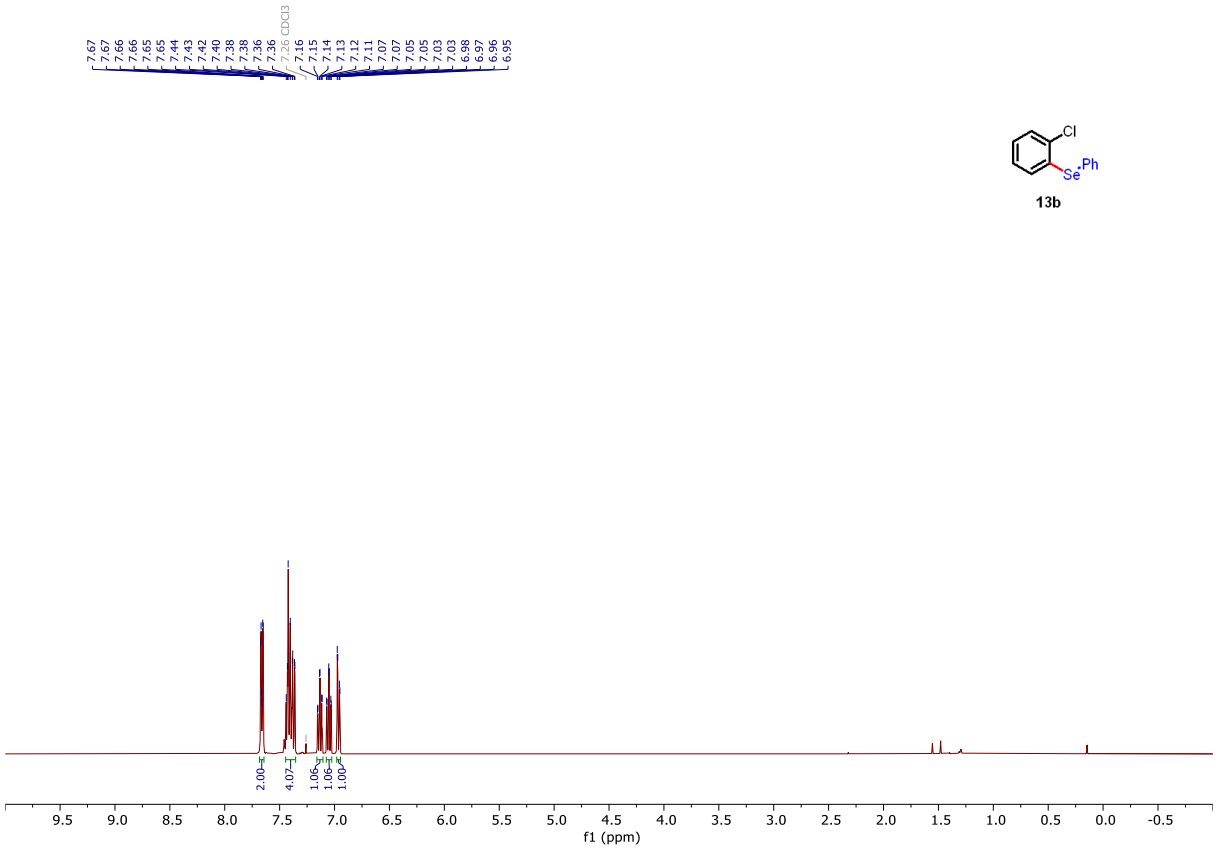


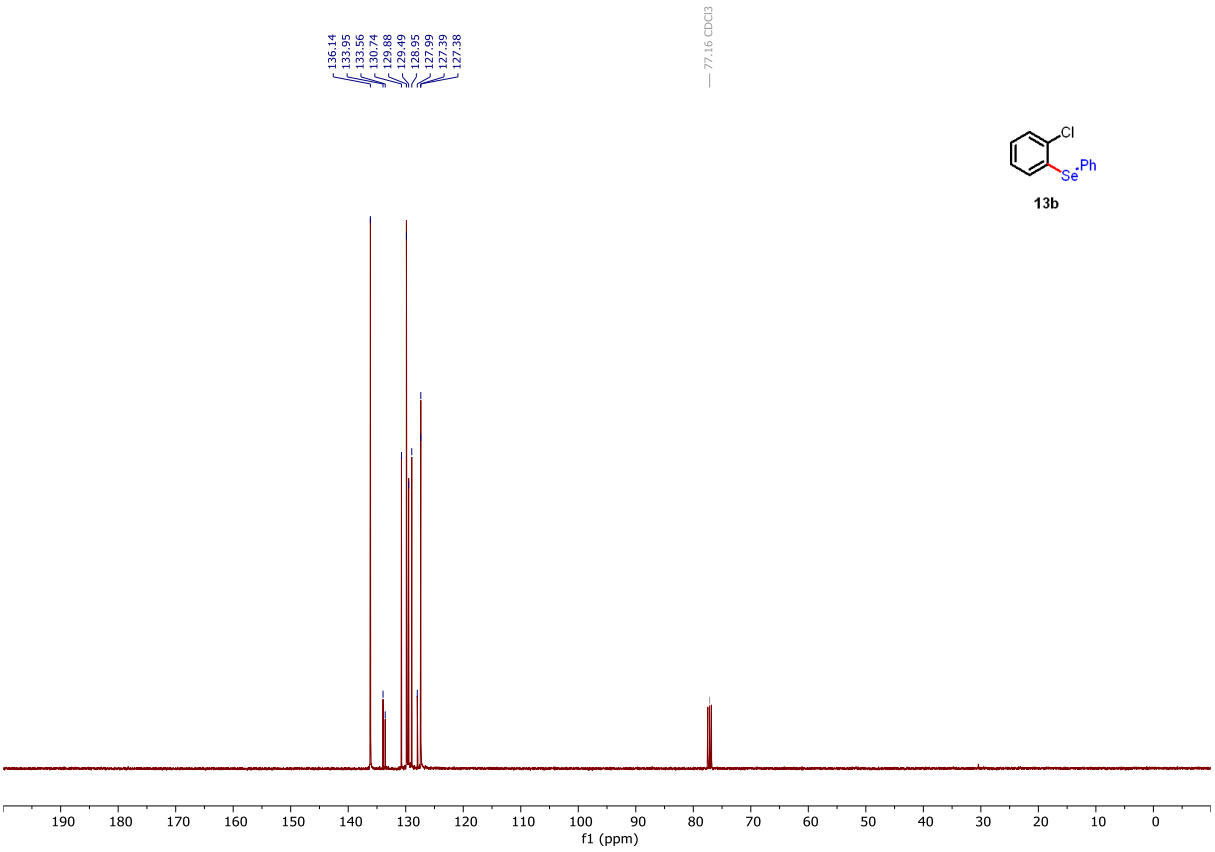



13a

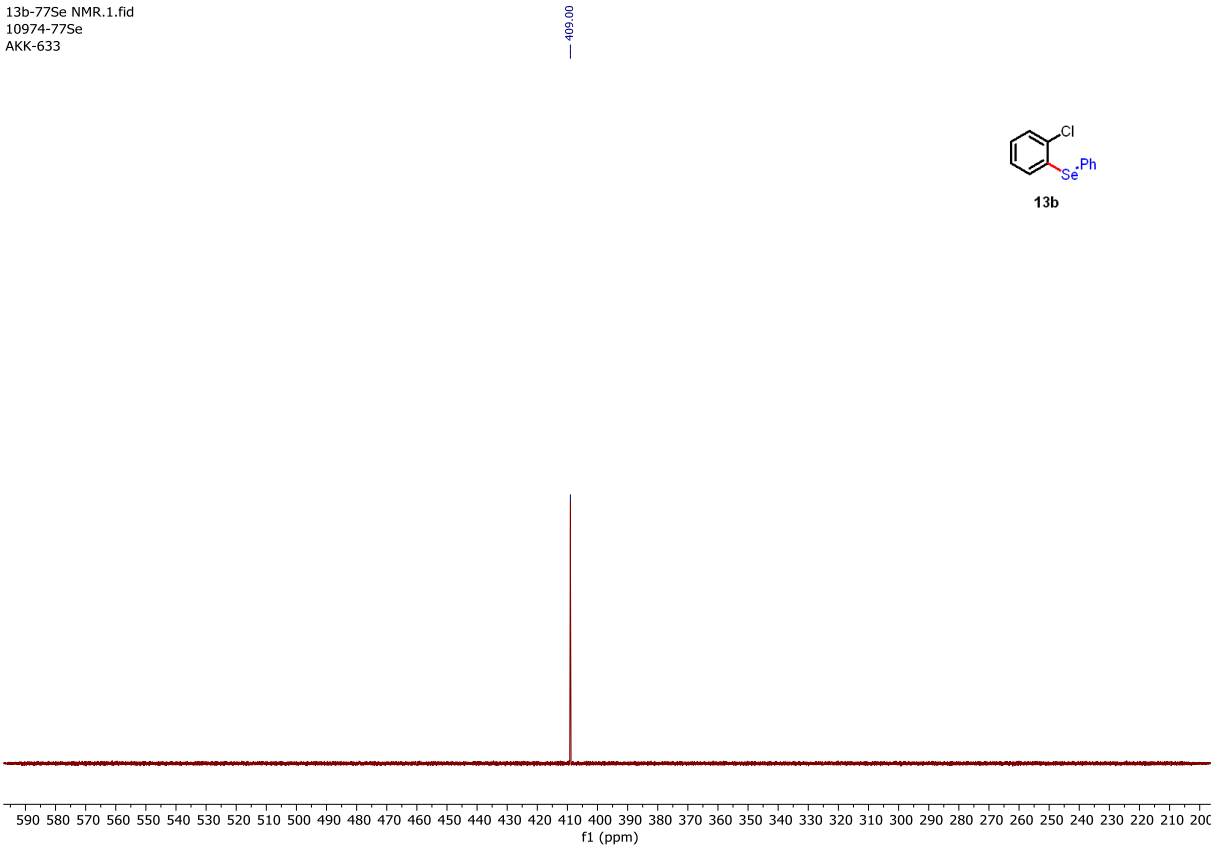


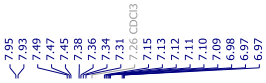

136.63
133.36
132.81
130.22
129.86
129.70
129.18
128.43
127.61
127.36
127.32
127.27
77.16 CDCl3
Cl
S
Ph
13a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.67
7.67
7.66
7.66
7.65
7.65
7.44
7.43
7.42
7.40
7.38
7.38
7.36
7.36
7.26 CDCl3
7.16
7.15
7.14
7.13
7.12
7.11
7.07
7.07
7.05
7.05
7.03
7.03
6.98
6.97
6.96
6.95
Cl
Se
Ph
13b
2.00
4.07
1.06
1.06
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



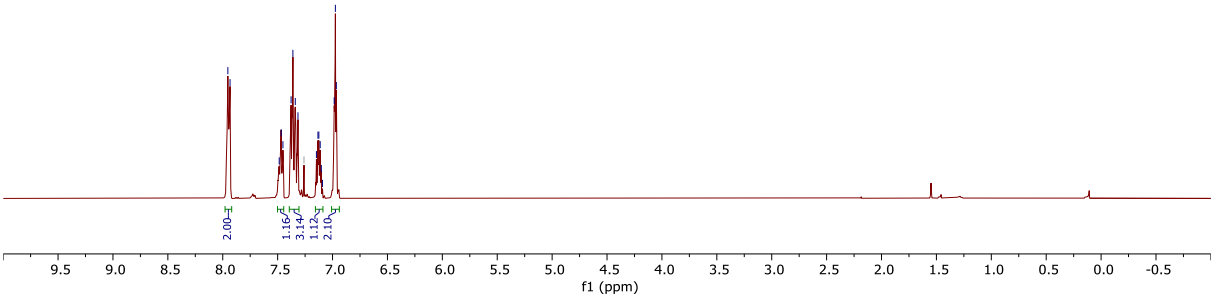

13b-77Se NMR.1.fid
10974-77Se
AKK-633




7.95
7.93
7.49
7.47
7.45
7.38
7.36
7.34
7.31
7.26 CDCl3
7.15
7.13
7.12
7.11
7.10
7.09
6.98
6.97
6.97


Cl
Te
Ph

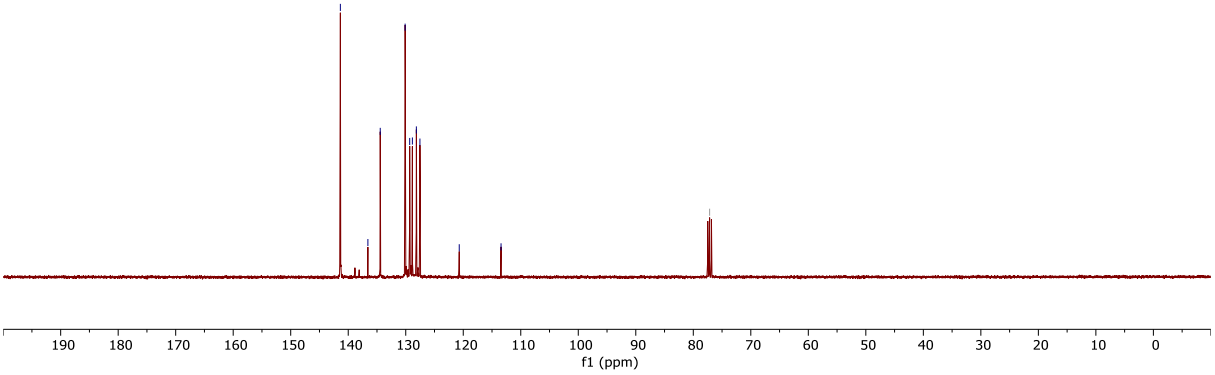
13c


2.00
1.16
3.14
1.12
2.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

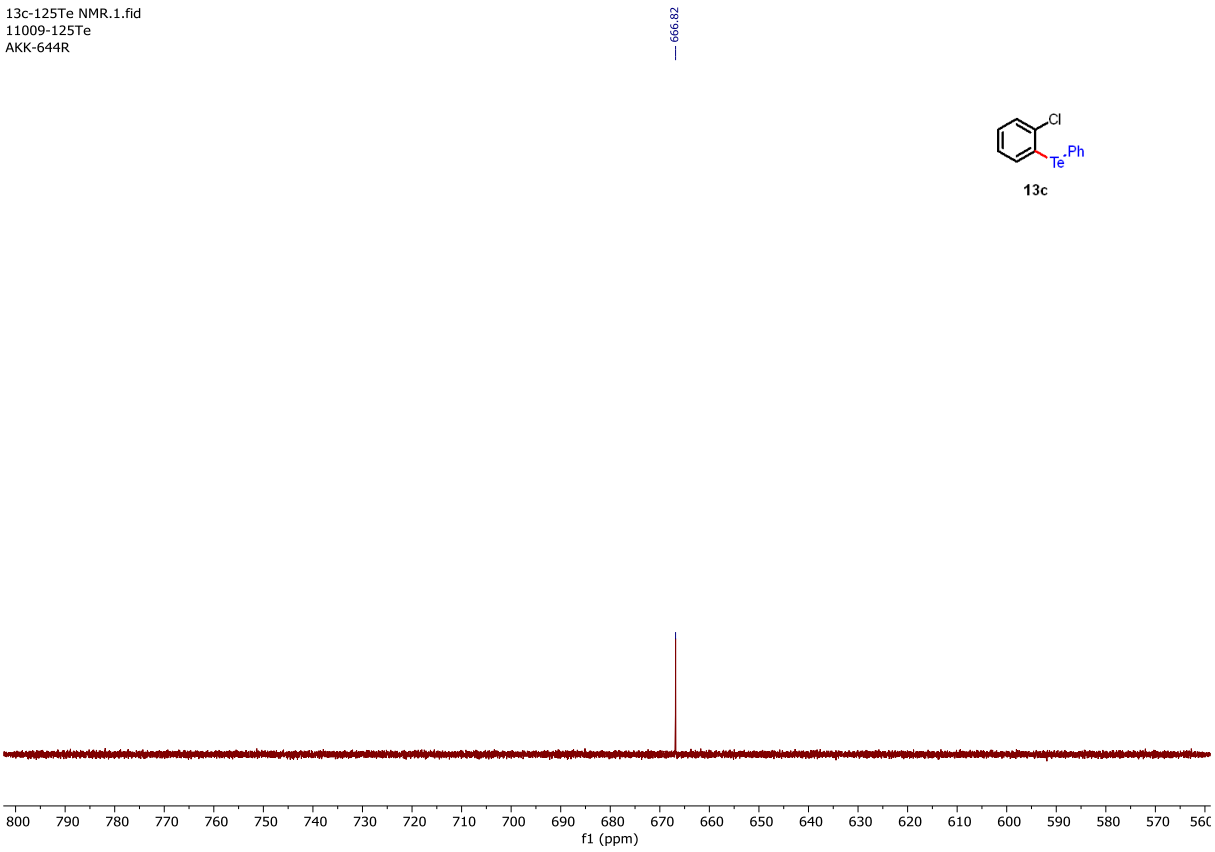

141.37
136.58
134.43
130.10
129.31
128.84
128.15
127.53
120.70
113.43
77.16 CDCl3


Cl
Te
Ph

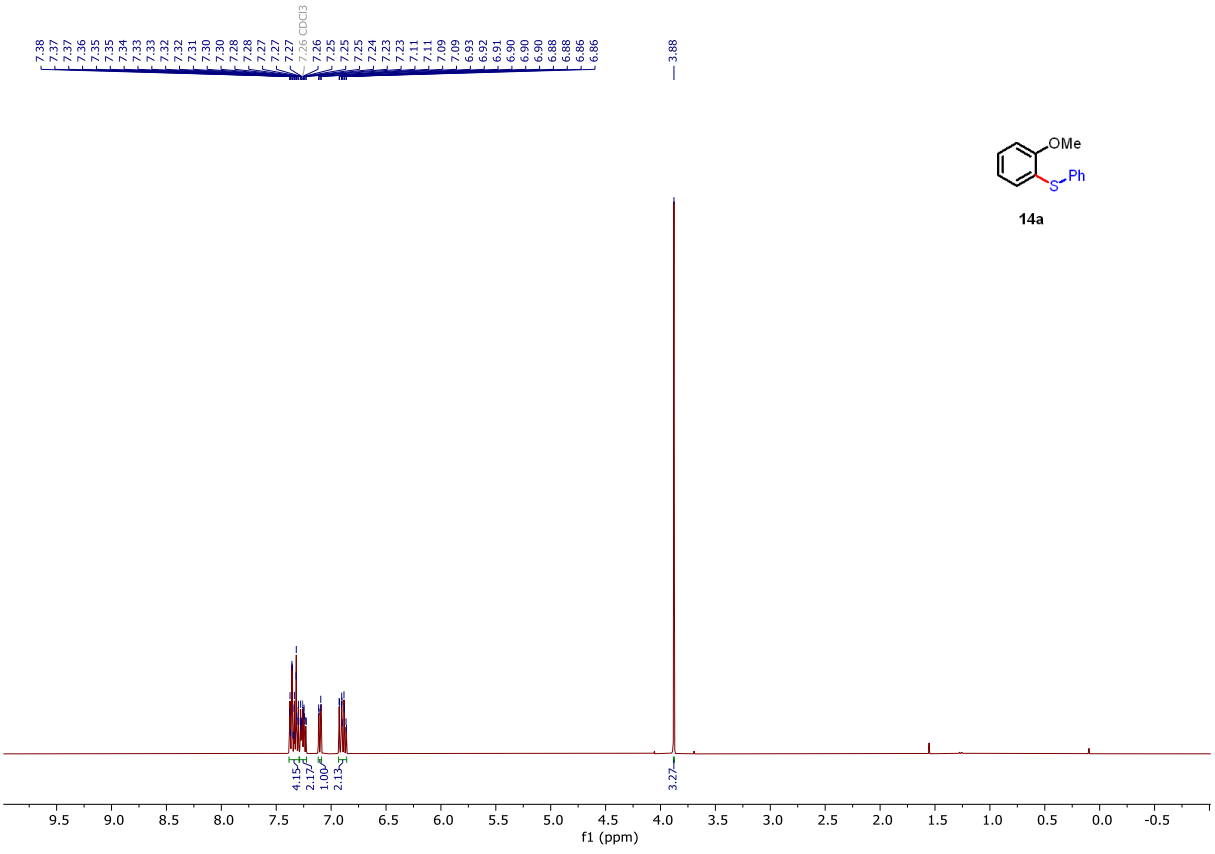
13c


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

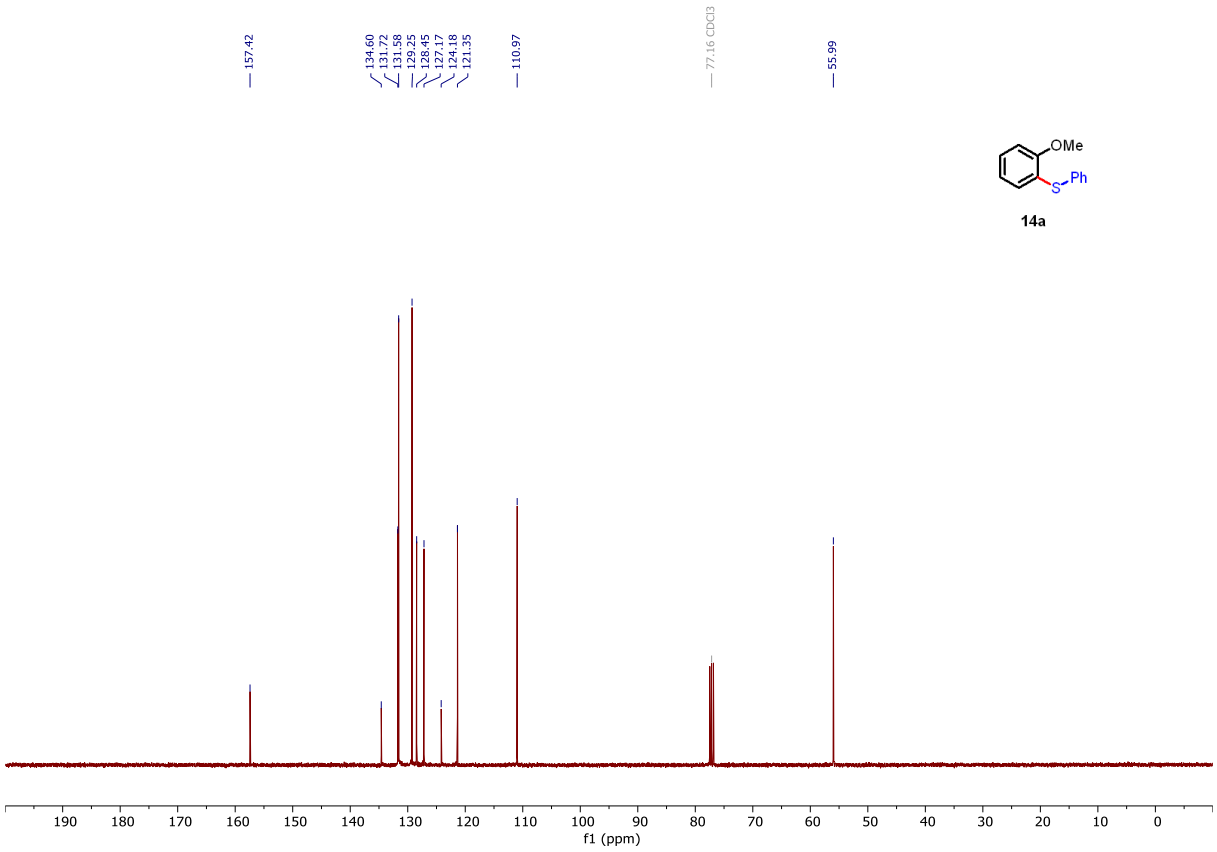
13c-125Te NMR.1.fid
11009-125Te
AKK-644R

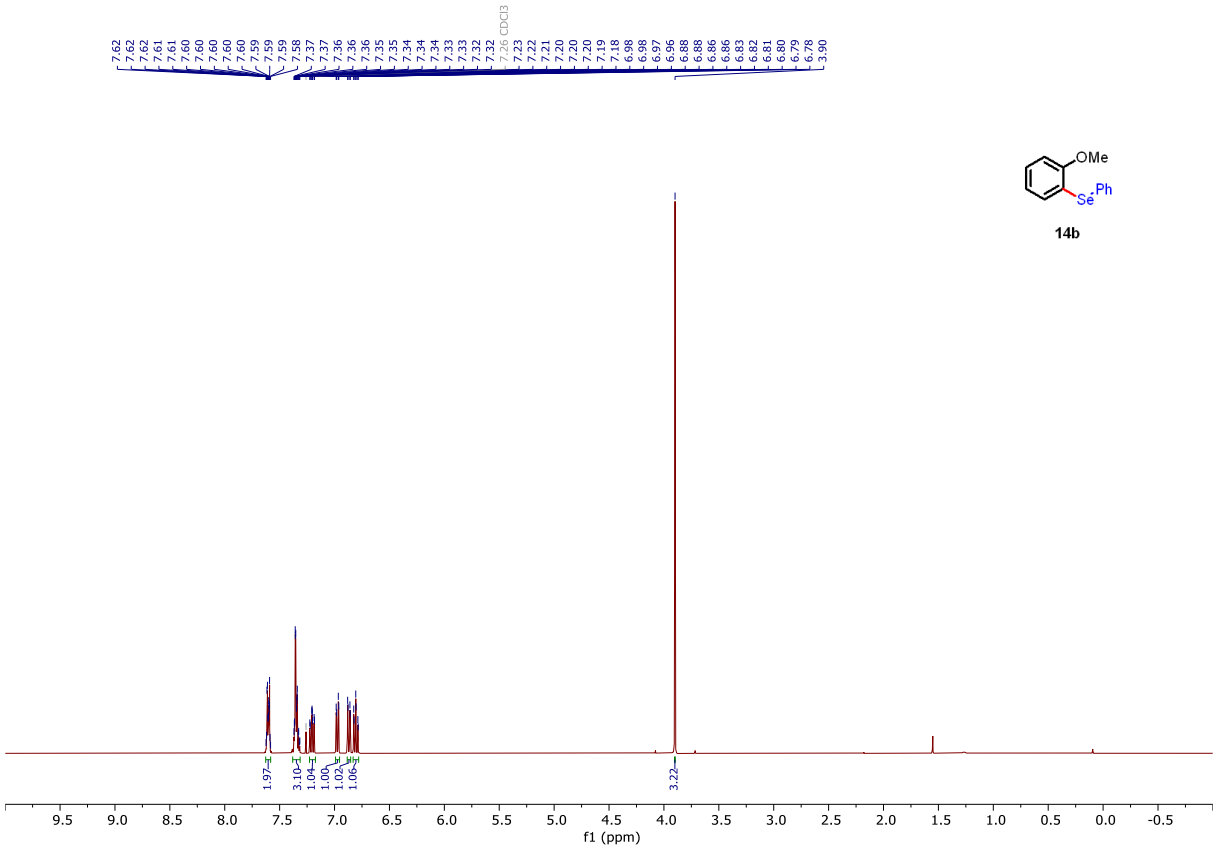


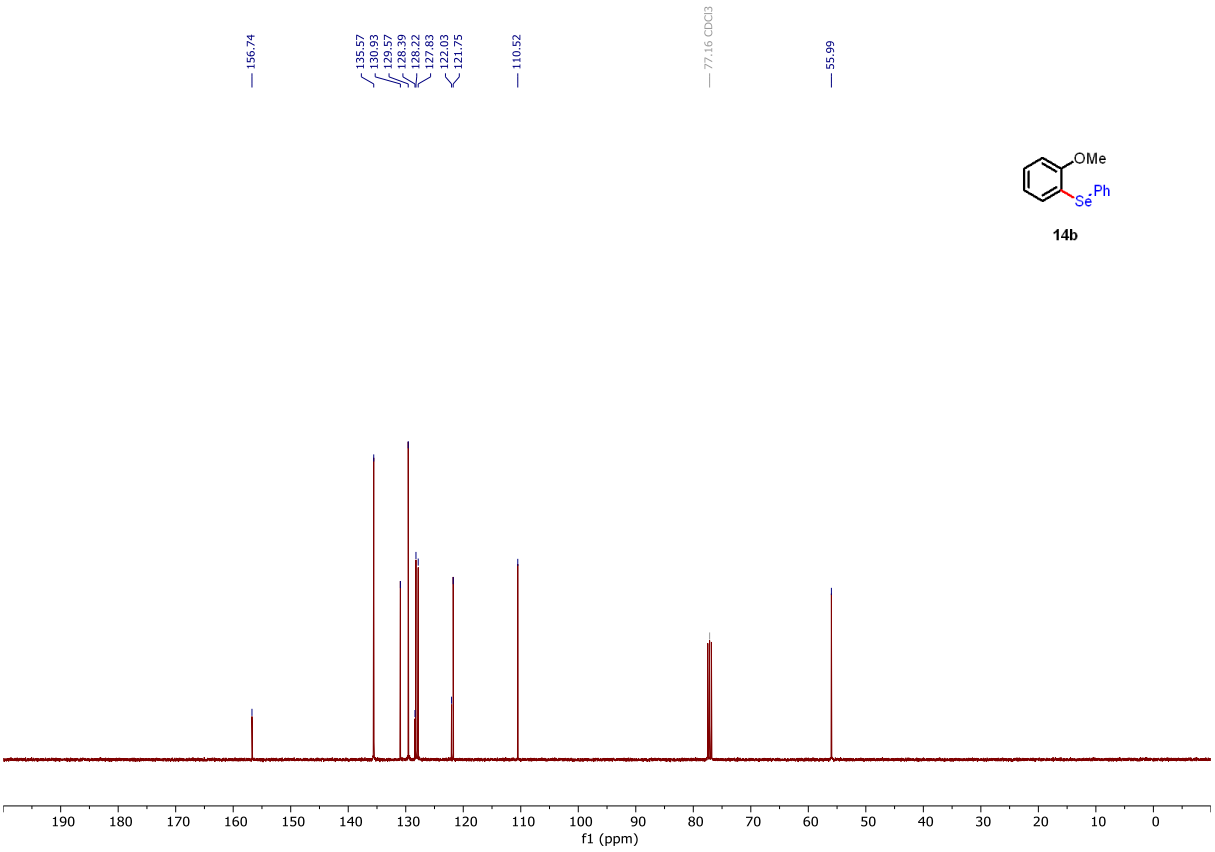

13c



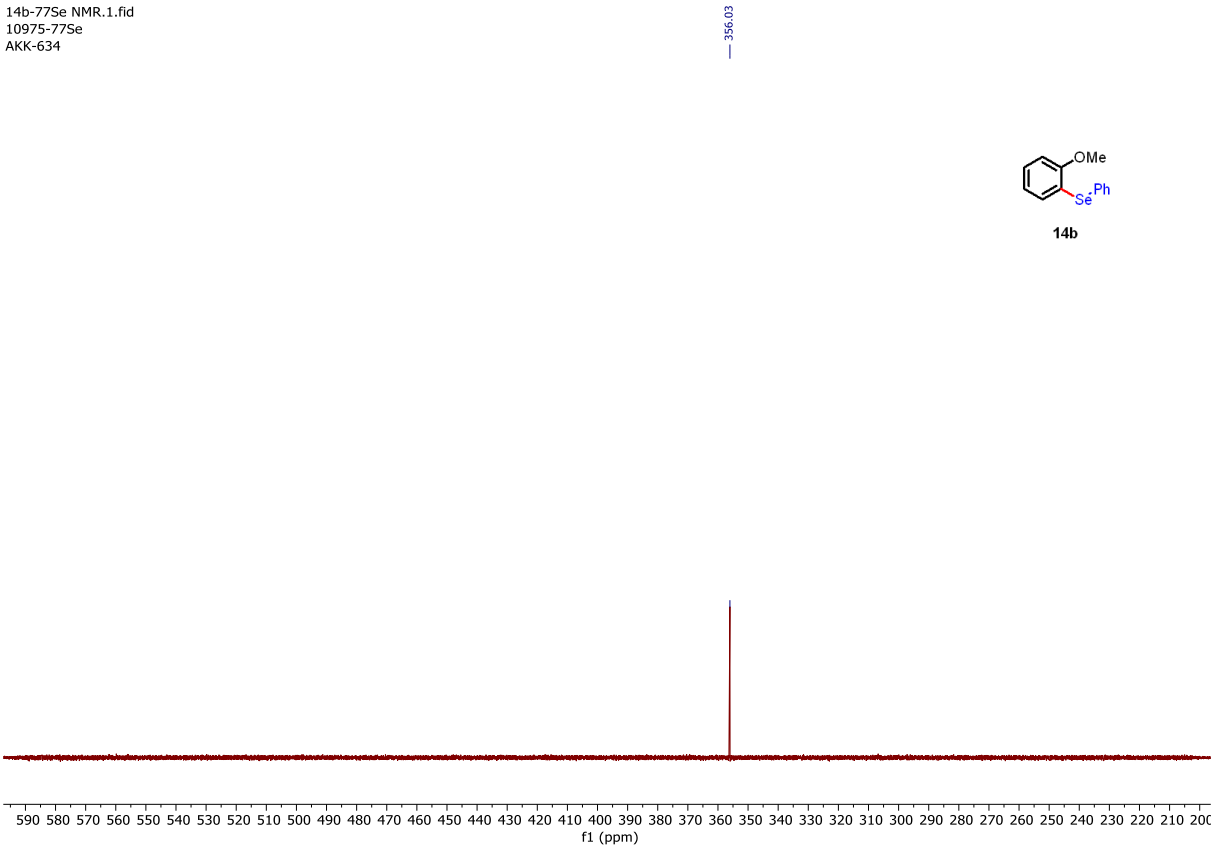

14a

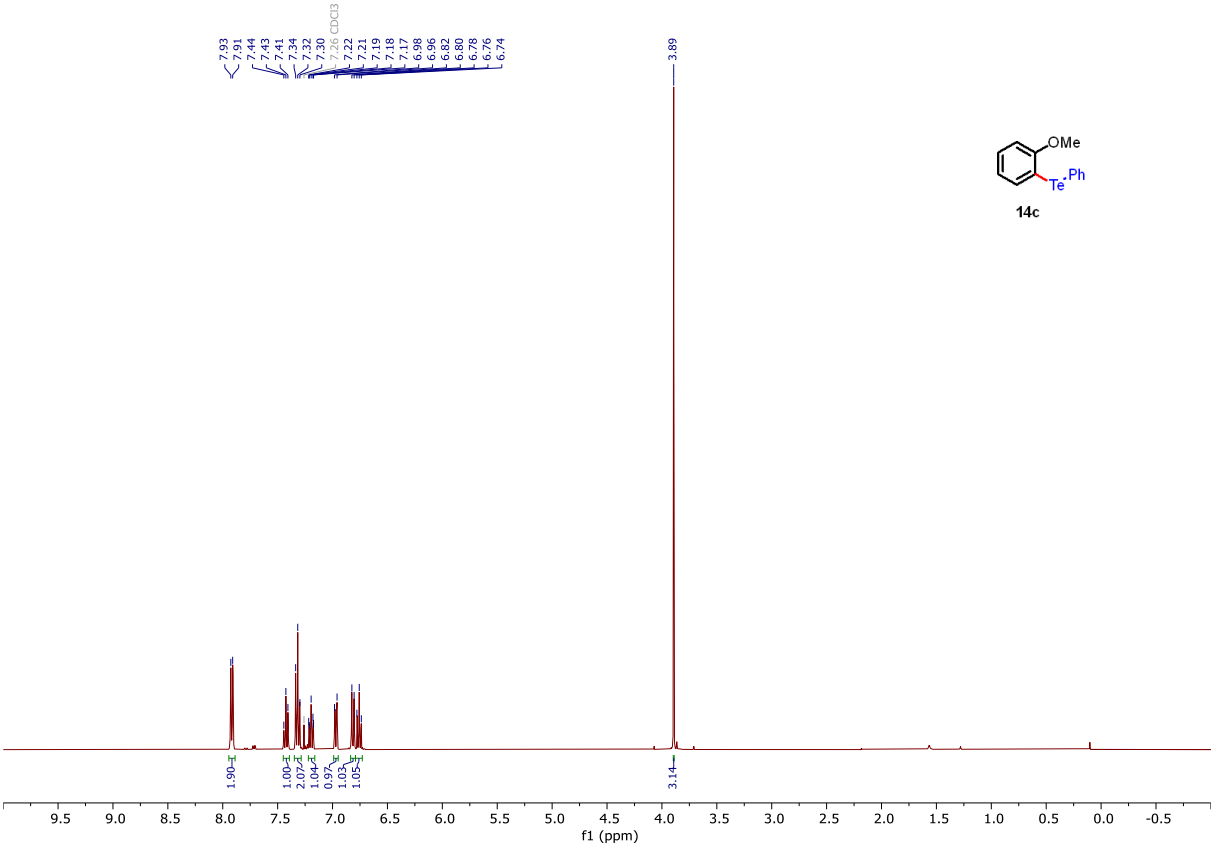

157.42
134.60
131.72
131.58
129.25
128.45
127.17
124.18
121.35
110.97
77.16 CDCl3
55.99
OMe
S
Ph
14a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

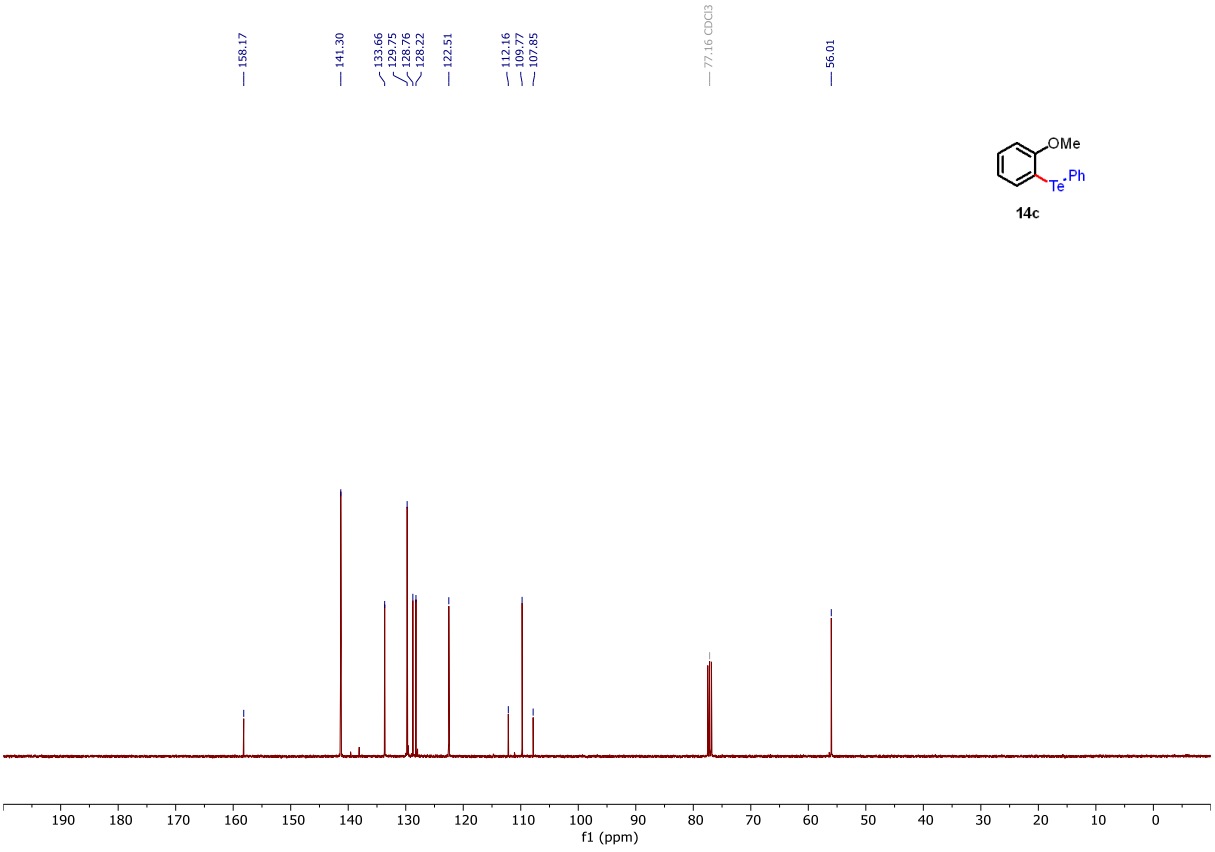

7.62 7.62 7.62 7.61 7.61 7.60 7.60 7.60 7.60 7.60 7.59 7.59 7.59 7.58 7.37 7.37 7.36 7.36 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.32
7.26 CDCl3
7.23 7.22 7.21 7.20 7.20 7.20 7.19 7.18 6.98 6.98 6.97 6.96 6.88 6.88 6.86 6.86 6.83 6.82 6.81 6.80 6.79 6.78 3.90
OMe
Se
Ph
14b
1.97 3.10 1.04 1.00 1.02 1.06 3.22
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



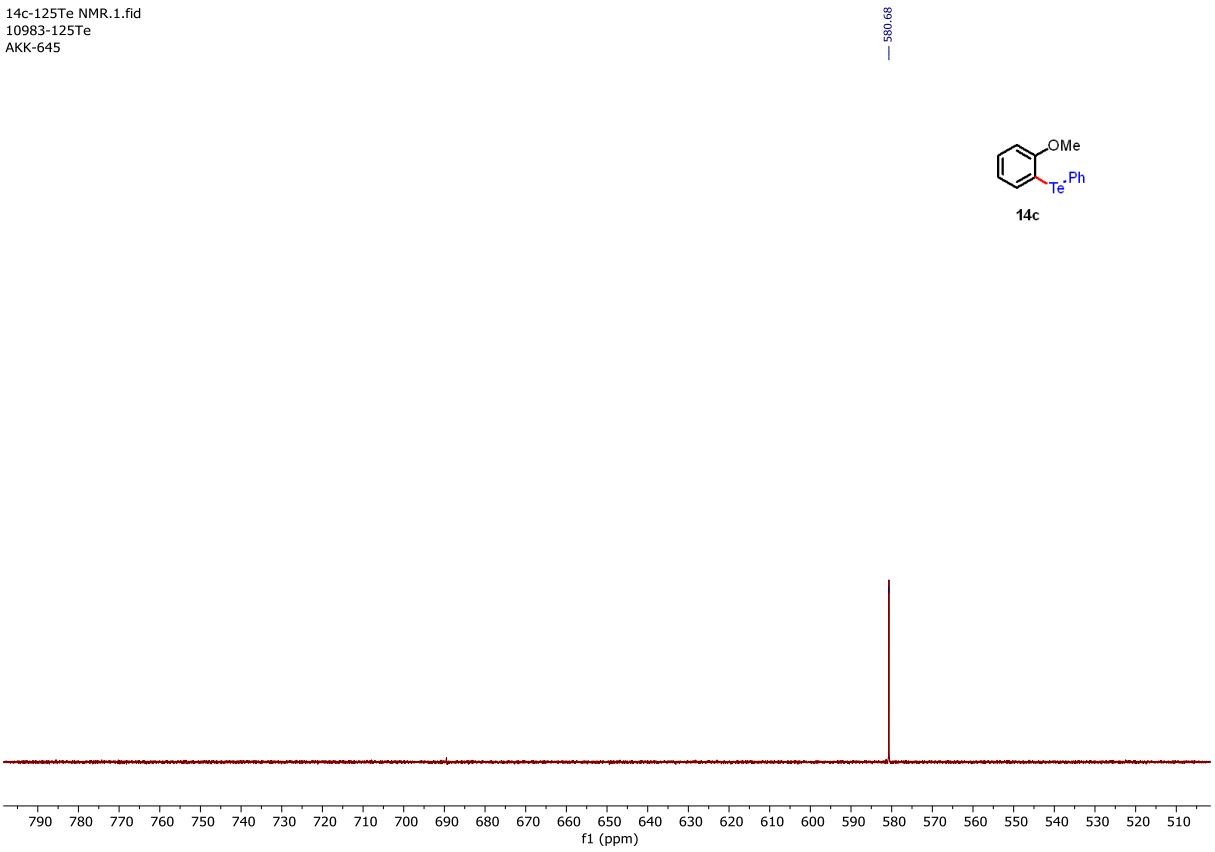

14b-77Se NMR.1.fid
10975-77Se
AKK-634

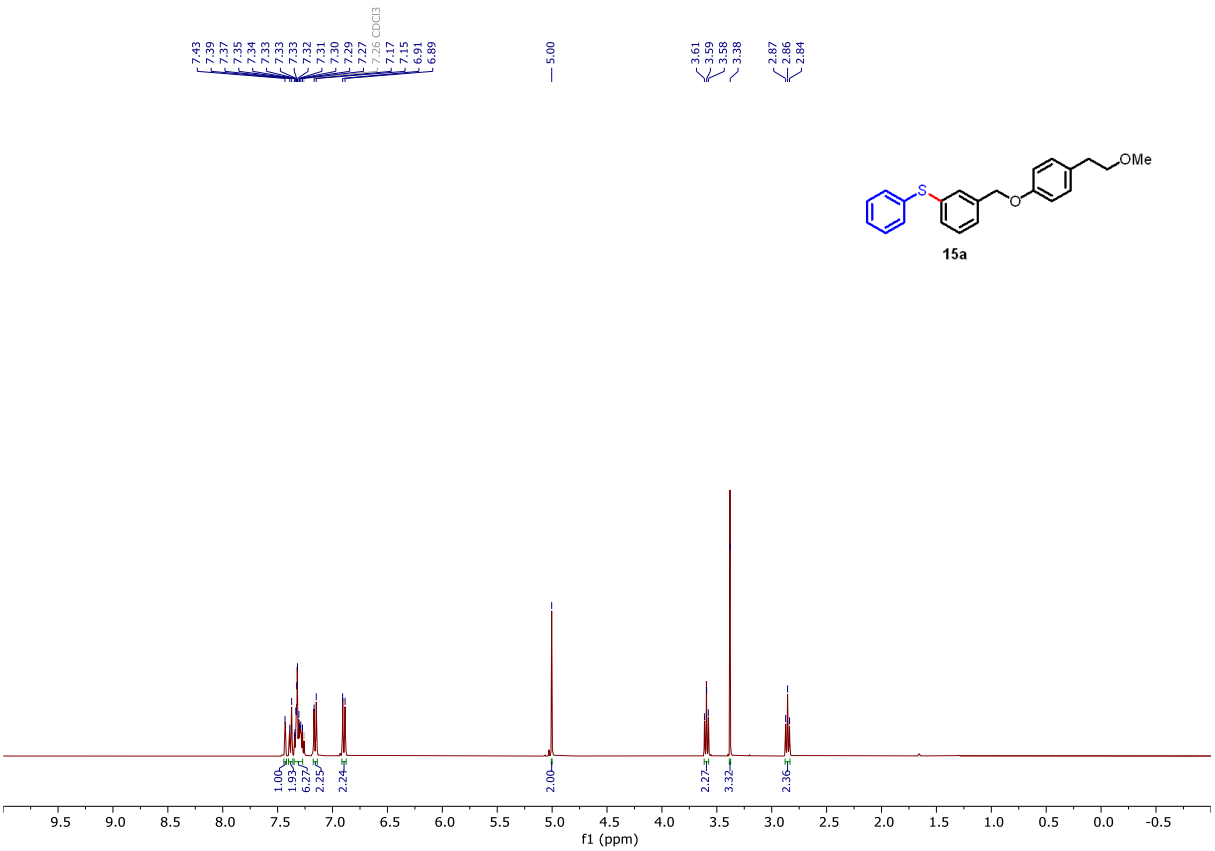


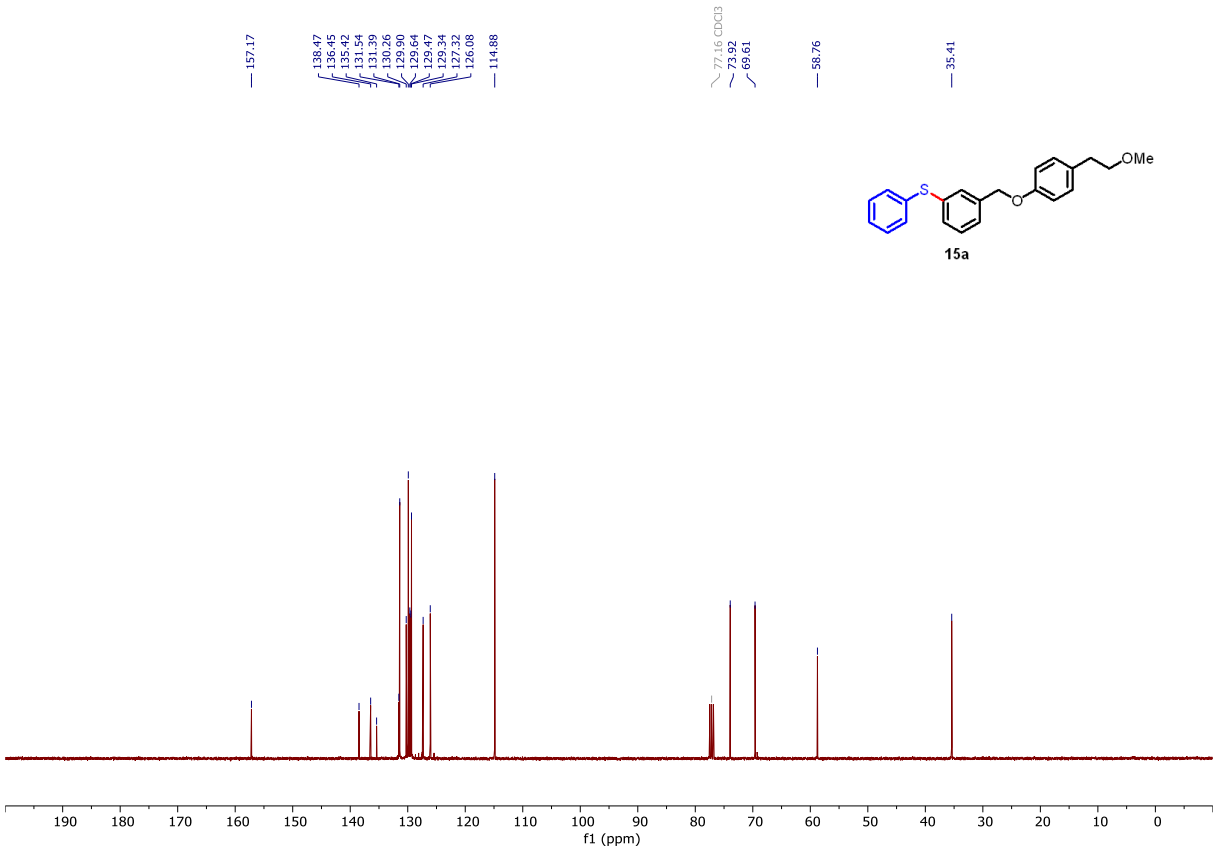

7.93
7.91
7.44
7.43
7.41
7.34
7.32
7.30
7.26 CDCl3
7.22
7.21
7.19
7.18
7.17
6.98
6.96
6.82
6.80
6.78
6.76
6.74
3.89
OMe
Ph
Te
14c
1.90
1.00
2.07
1.04
0.97
1.03
1.05
3.14
f1 (ppm)

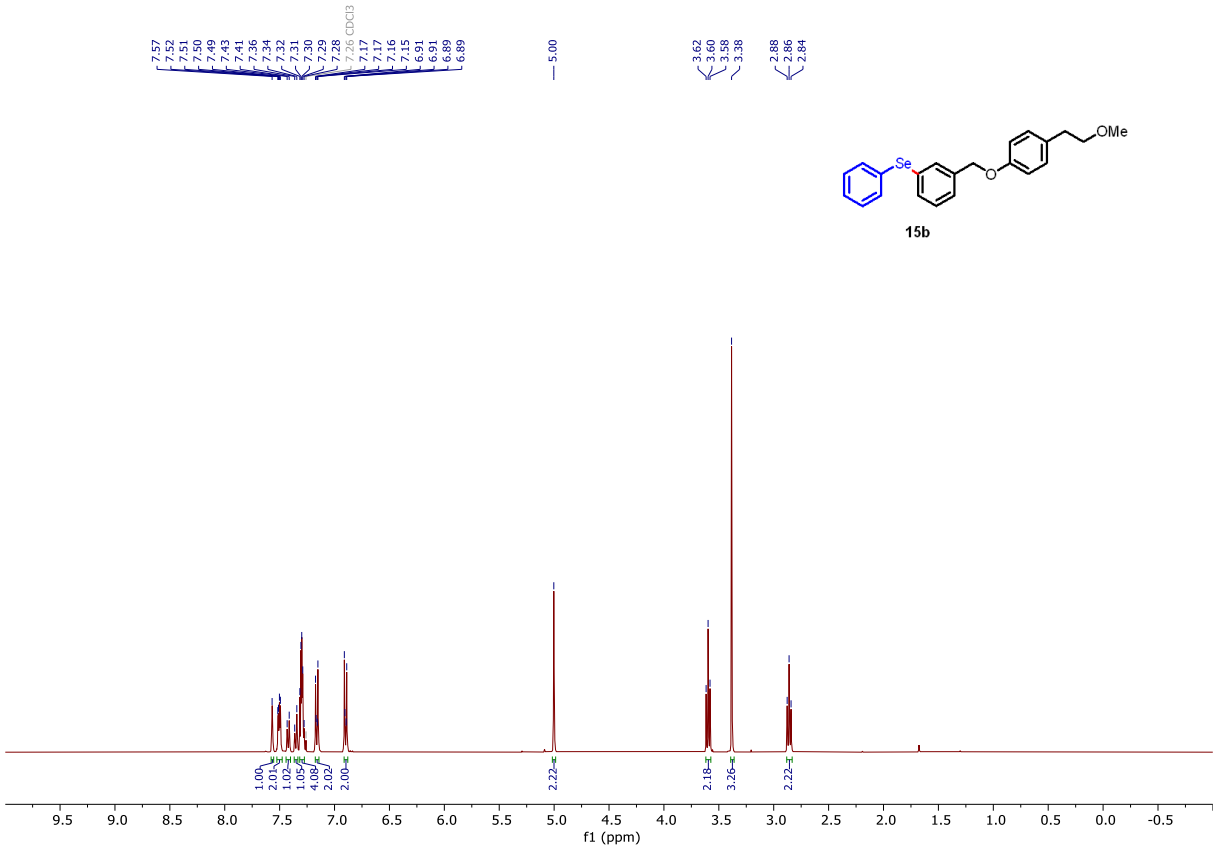

158.17
141.30
133.66
129.75
128.76
128.22
122.51
112.16
109.77
107.85
77.16 CDCl3
56.01
OMe
Ph
Te
14c
f1 (ppm)

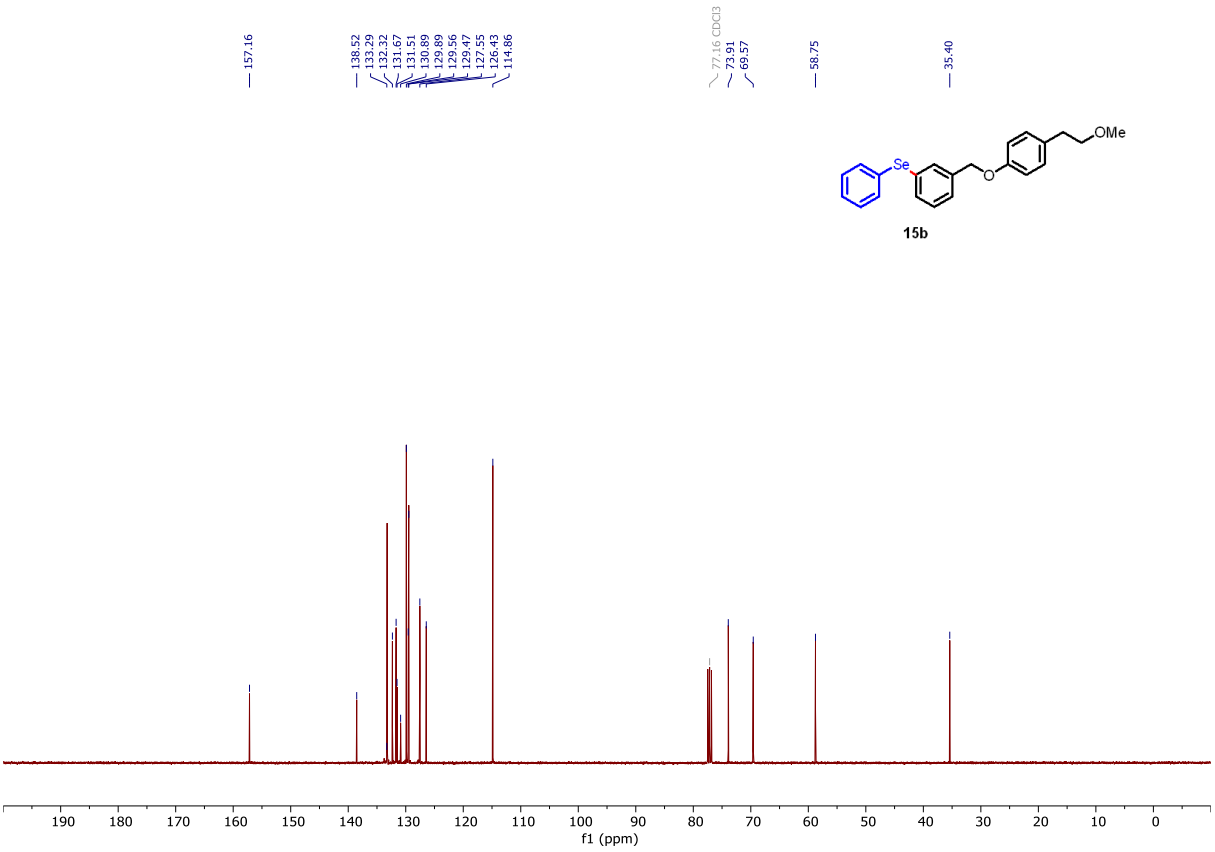
14c-125Te NMR.1.fid
10983-125Te
AKK-645

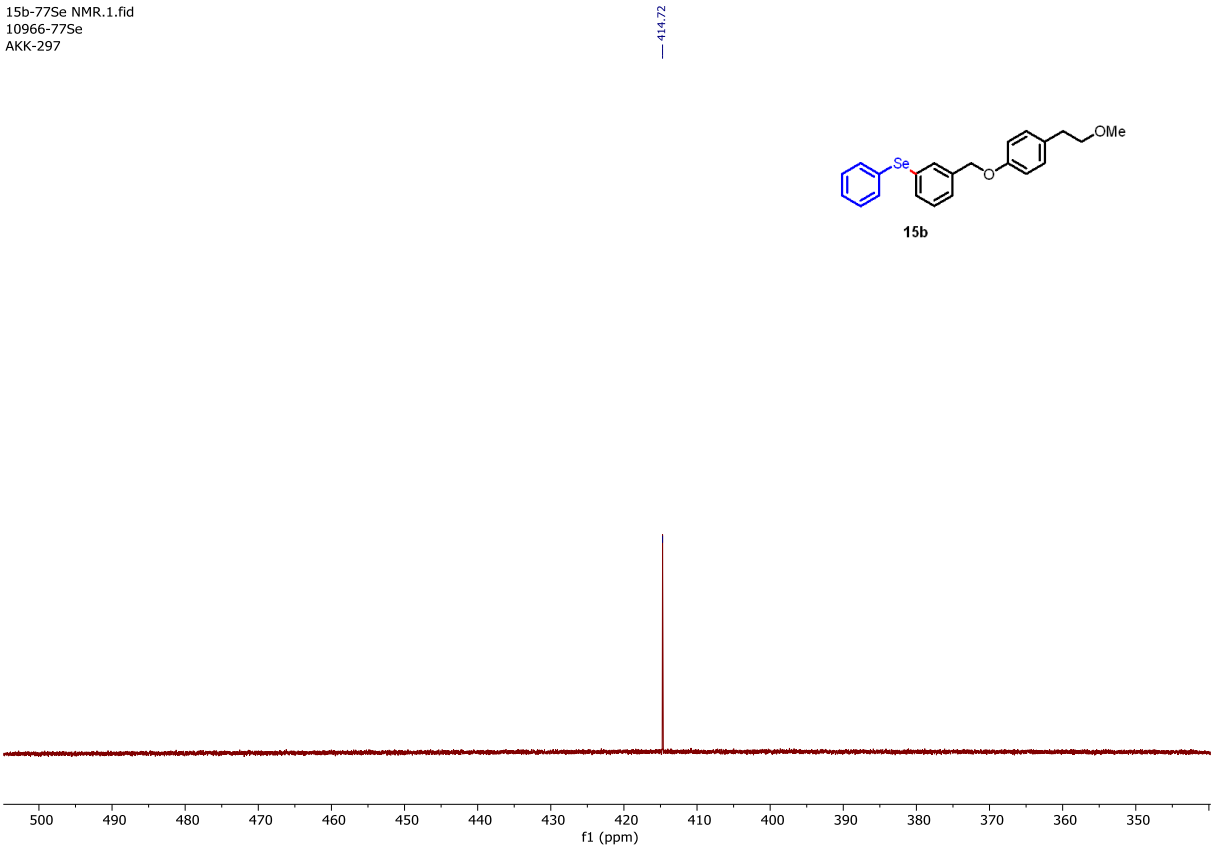


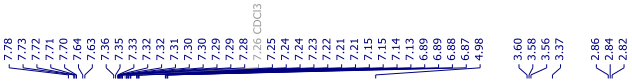




157.17
138.47
136.45
135.42
131.54
131.39
130.26
129.90
129.64
129.47
129.34
127.32
126.08
114.88
77.16 CDCl3
73.92
69.61
58.76
35.41
S
O
OMe
15a
f1 (ppm)


7.57
7.52
7.51
7.50
7.49
7.43
7.41
7.36
7.34
7.32
7.31
7.30
7.29
7.28
7.26 CDCl3
7.17
7.17
7.16
7.15
6.91
6.91
6.89
6.89
5.00
3.62
3.60
3.58
3.38
2.88
2.86
2.84
Se
O
OMe
15b
1.00
2.01
1.02
1.05
4.08
2.02
2.00
2.22
2.18
3.26
2.22
f1 (ppm)


157.16
138.52
133.29
132.32
131.67
131.51
130.89
129.56
129.47
127.55
126.43
114.86
77.16 CDCl3
73.91
69.57
58.75
35.40
Se
O
OMe
15b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


15b-77Se NMR.1.fid
10966-77Se
AKK-297
414.72
Se
O
OMe
15b
500 490 480 470 460 450 440 430 420 410 400 390 380 370 360 350
f1 (ppm)


7.78
7.73
7.72
7.71
7.70
7.64
7.63
7.36
7.35
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.26 CDCl3
7.25
7.24
7.24
7.23
7.22
7.21
7.21
7.15
7.15
7.14
7.13
6.89
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6.87
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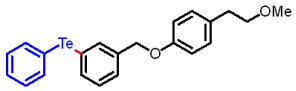
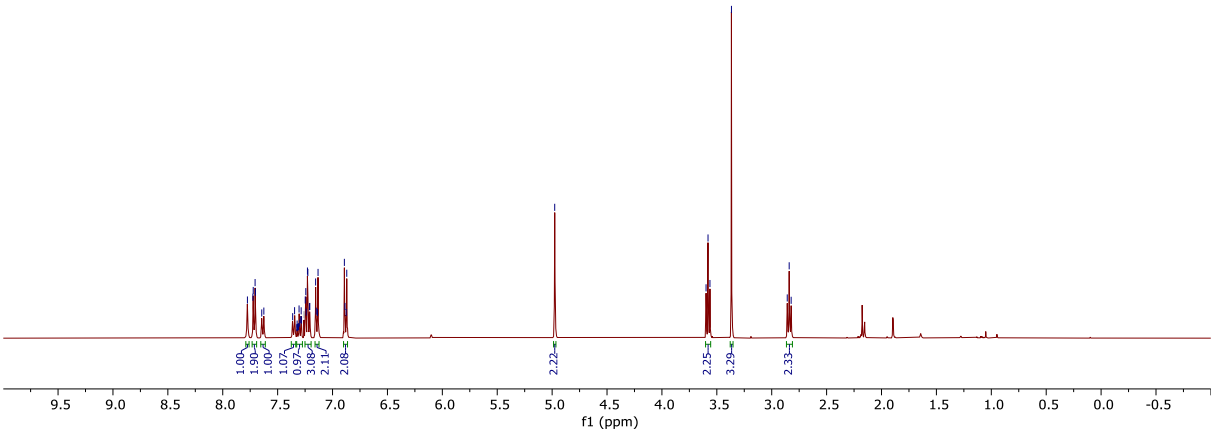
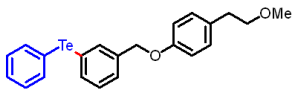
3.58
3.56
3.37
2.86
2.84
2.82


Te
O
OMe

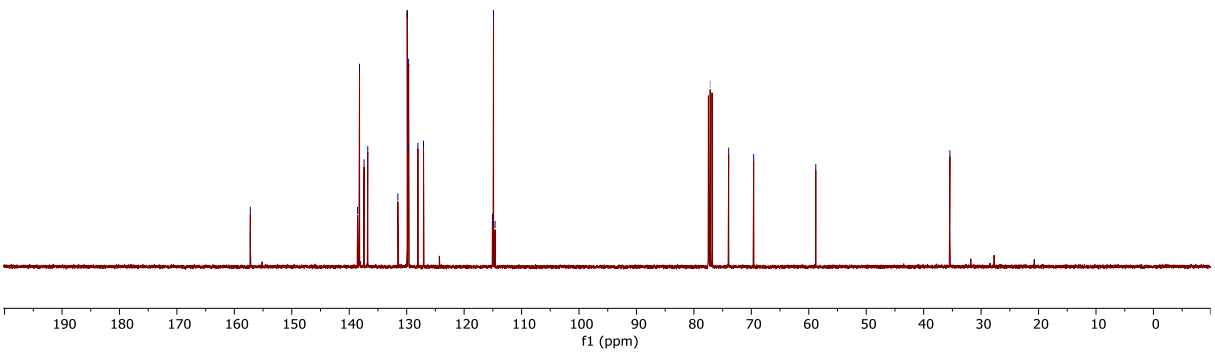
**15c**


1.00
1.90
1.00
1.07
0.97
3.08
2.11
2.08
2.22
2.25
3.29
2.33
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


157.22
138.55
138.21
137.42
136.77
131.53
129.91
129.71
129.66
128.04
127.07
115.08
114.89
114.61
77.16 CDCl3
73.95
69.60
58.78
35.43

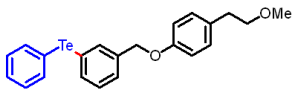

Te
O
OMe

**15c**


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

15c-125Te NMR.1.fid
10967-125Te
AKK-267

693.55




**15c**