# Supporting information

## Recyclable iodine-catalyzed radical selenylative annulation of 2-alkynyl biaryls with diselenides in water: a green approach to selanyl polycyclic aromatic hydrocarbons and polycyclic heteroaromatics

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## 1. General reagent information

All reagents and solvents were purchased from Sigma-Aldrich, TCI, Finar and other local chemical companies. Flash column chromatography was performed using silica gel (100-200 mesh)

### 1.1. General analytical information

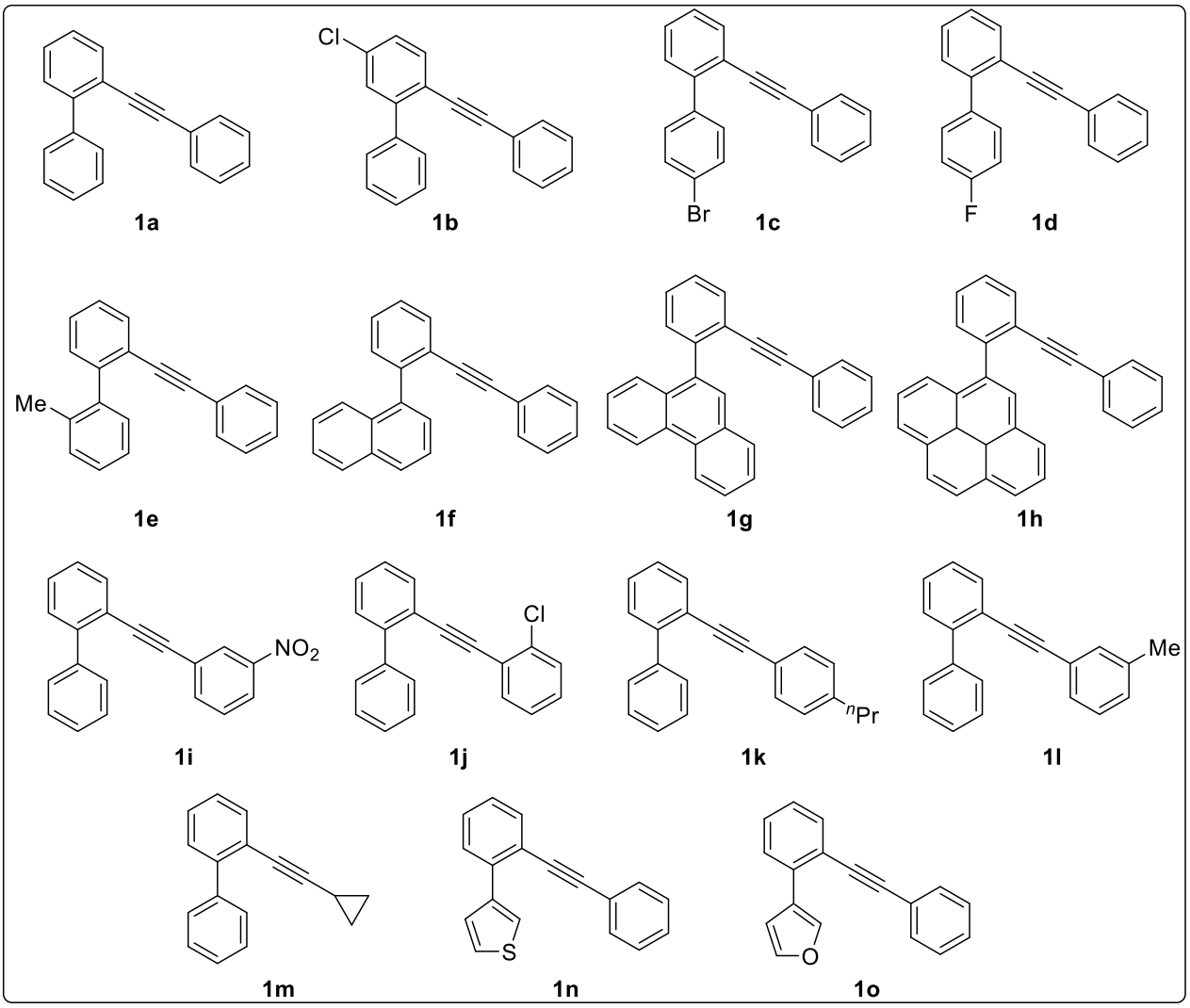
The starting materials such as 2-(phenylethynyl)-1,1'-biaryls and products such as 9-selanyl phenanthrenes and polycyclic heteroaromatics were characterized by $^{1}H$, $^{13}C$, $^{77}Se$ and $^{19}F$ NMR spectra which were recorded on a Bruker 400 MHz instrument (400 MHz for $^{1}H$ NMR, 100 MHz for $^{13}C$ NMR, 76 MHz for $^{77}Se$ NMR and 377 MHz for $^{19}F$ NMR). Copies of $^{1}H$, $^{13}C$, $^{77}Se$ and $^{19}F$ NMR spectra can be found at the end of the Supporting Information. $^{1}H$ NMR experiments are reported in units, parts per million (ppm), and were measured relative to residual chloroform (7.26 ppm) in the deuterated solvent. $^{13}C$ NMR spectra are reported in ppm relative to deuterochloroform (77.00 ppm) and all were obtained with $^{1}H$ decoupling. Coupling constants were reported in Hz. Reactions were monitored by thin layer chromatography (TLC) and $^{1}H$ NMR of the crude reaction mixture using 1,3,5-trimethoxybenzene as the internal standard. Mass spectral data were obtained on a high resolution mass spectrometer, Agilent MassHunter Qualitative Analysis B.06.00 and also in LCMS-8040 (Shimadzu). Melting points of unknown compounds were recorded on a KRUSS Optronic M3000 apparatus. Single Crystal X-ray data were recorded on Rigaku Oxford Diffraction (XtalLab).

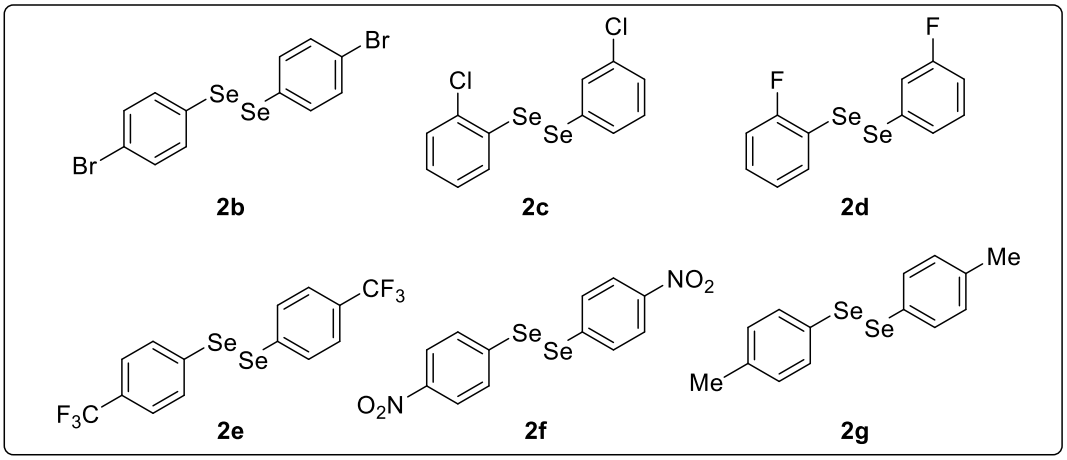
### 1.2. General computational information

All the Density Functional Theory (DFT) calculations were performed using Gaussian 09[1] package with M06-2X exchange-correlation functional[2] along with LANL2DZ basis set[3] Vibrational frequency calculations were performed to confirm local minima and transition states. To incorporate the entropic effects, the thermochemistry was computed at room temperature (T=298.15 K) and standard atmospheric pressure (P=1 atm). Solvent effects were incorporated using an implicit solvation scheme with water as the implicit solvent using the self-consistent reaction field within the conducting polarizable continuum model (CPCM).[4]

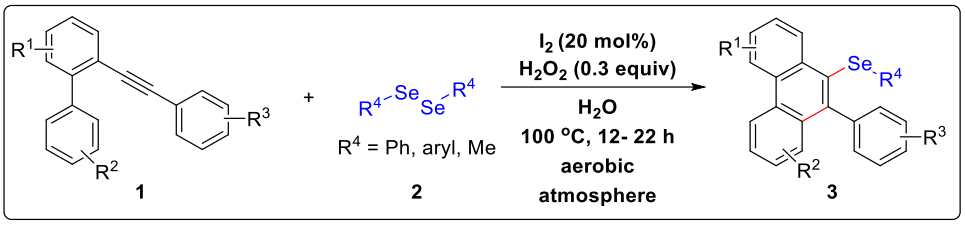
## 2. Synthesis of 2-alkynyl biaryls (1a-1o) and diaryl diselenides (2b-2g).

All starting materials (1a,[5] 1b,[5] 1c,[5] 1d,5 1e,[5] 1f,[5] 1g,[5] 1h,[5] 1i,[5] 1j,[5] 1l,[5] 1m,[5] 1n,[5] 1o,[5] 2b,[6] 2c,[6] 2d,[6] 2e,[6] 2f,[6] 2g[6]) which are as shown below were synthesized by following a literature protocol and characterized by $^{1}H$ and $^{13}C$ NMR.[5,6]

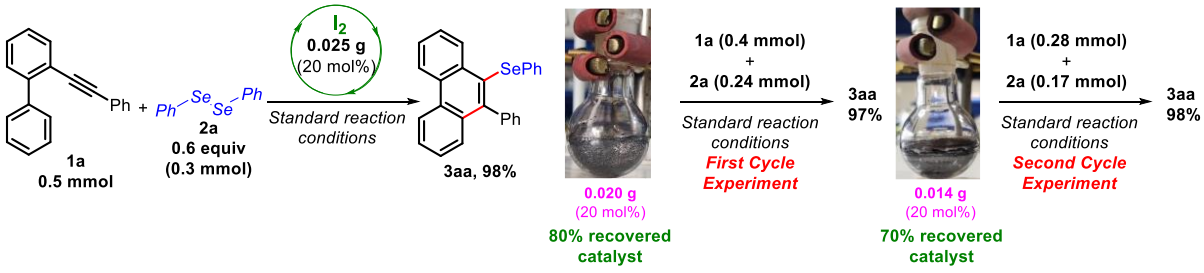


## 3. General experimental procedure for the synthesis of 9-selenylphenanthrenes (3aa-3ah and 3ba−3ma) and selenyl polycyclic heteroaromatics (3na and 3oa).



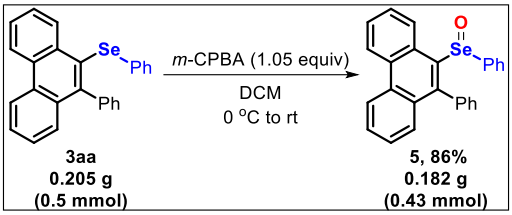

**Representative experimental procedure for the synthesis of phenyl(10-phenylphenanthren-9-yl)selane (3aa):** 2-(phenylethynyl)-1,1'-biphenyl **1a** (0.127 g, 0.5 mmol, 1 equiv), 1,2-diphenyldiselane **2a** (0.094 g, 0.3 mmol, 0.6 equiv) and $I_2$ (0.0254 g, 0.1 mmol) were taken in a round-bottomed flask (RBF) and $H_2O$ (0.3 mL) was added to it. Then 30% aqueous $H_2O_2$ (v/v) (0.012 mL, 0.15 mmol, 0.3 equiv) was added to the RBF and the reaction mixture was stirred in an oil bath at 100 $^oC$ under aerobic atmosphere. The progress of the reaction was monitored by TLC. The solution was then transferred to a separating funnel for extraction. The reaction mixture was extracted with ethyl acetate twice (2 X 20 mL) and the combined organic layer was washed with water (3 X 10 mL). The solvent was evaporated under reduced pressure and iodine was recovered from the reaction mixture first by column chromatography using pentane as eluent. The column chromatography process was further continued to afford the pure product, phenyl(10-phenylphenanthren-9-yl)selane **3aa** (0.202 g, 0.495 mmol) in 98% yield using hexane as eluent.




**3.1. Gram-scale synthesis of phenyl(10-phenylphenanthren-9-yl)selane (3aa):** 2-(Phenylethynyl)-1,1'-biphenyl **1a** (1.017 g, 4 mmol, 1 equiv), 1,2-diphenyldiselane **2a** (0.749 g, 2.4 mmol, 0.6 equiv) and $I_2$ (0.203 g, 0.8 mmol) were taken in a RBF and $H_2O$ (2.4 mL) was added to it. Then 30% aqueous $H_2O_2$ (v/v) (0.096 mL, 1.2 mmol, 0.3 equiv) was added to the RBF and the reaction mixture was stirred in an oil bath at 100 $^oC$ under aerobic

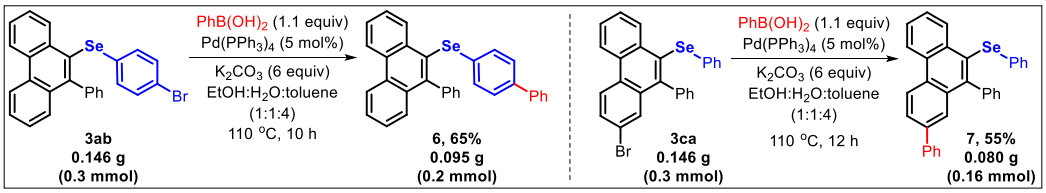
atmosphere. The progress of the reaction was monitored by TLC. The solution was then transferred to a separating funnel for extraction. The reaction mixture was extracted with ethyl acetate twice (2 X 20 mL) and the combined organic layer was washed with water (3 X 10 mL). The solvent was evaporated under reduced pressure and iodine was recovered from the reaction mixture first by column chromatography using pentane as eluent. The column chromatography process was further continued to afford the pure product, phenyl(10-phenylphenanthren-9-yl)selane **3aa** (1.32 g, 3.224 mmol) in 80.6% yield.

## 4. Experimental procedure for the synthesis of 9-phenyl-10-(phenylseleninyl)phenanthrene.[7]




3-Chloroperoxybenzoic acid, *m*-CPBA (purity: 65-70%) (0.140 g, 0.525 mmol) was added to a solution of phenyl(10-phenylphenanthren-9-yl)selane **3aa** (0.205 g, 0.5 mmol) dissolved in dichloromethane (2.5 mL) at 0 °C. The reaction mixture was cooled at 0 °C. Then, the reaction mixture was stirred vigorously for 2 h. After the completion of the reaction the solvent was evaporated under reduced pressure. The crude reaction mixture was extracted with dichloromethane thrice (3 x 10 mL). The combined organic layer was washed with water (3 x 10 mL) and evaporated under reduced pressure. The crude product was purified by flash column chromatography through silica gel to afford the 9-phenyl-10-(phenylseleninyl)phenanthrene ***5*** in (0.182 g, 0.43 mmol) in 86% yield.

## 4.1. Experimental procedure of Suzuki coupling reaction of 4-bromophenyl)(10-phenylphenanthren-9-yl)selane 3ab and (2-bromo-10-phenylphenanthren-9-yl)(phenyl)selane 3ca.[8]



**Representative experimental procedure for the Suzuki reaction with 3ab**: 4-Bromophenyl)(10-phenylphenanthren-9-yl)selane **3ab** (0.146 g, 0.3 mmol, 1 equiv), phenyl boronic acid (0.040 g, 0.33 mmol), $Pd(PPh_3)_4$ (0.017 g, 0.015 mmol), $K_2CO_3$ (0.248 g, 1.8 mmol) and solvent (0.96 mL, EtOH : $H_2O$ : PhMe = 1:1:4.4) were taken in a 25 mL round-bottom flask (RBF). The reaction mixture was refluxed at 110 $^oC$ and the progress of the reaction was monitored by thin layer chromatography. The mixture was cooled to room temperature and extracted with ethyl acetate (30x3 mL) three times. The combined organic layer was further washed with brine (30 mL) and subsequently dried over anhydrous $Na_2SO_4$. Finally the solvent was evaporated under reduced pressure to get the crude product which was purified by flash column chromatography on silica gel to afford [1,1'-biphenyl]-4-yl(10-phenylphenanthren-9-yl)selane **6** (0.0958 g, 0.2 mmol) in 65% yield.

## 5. X-ray crystal structure of 3ba, 3ea, 3la

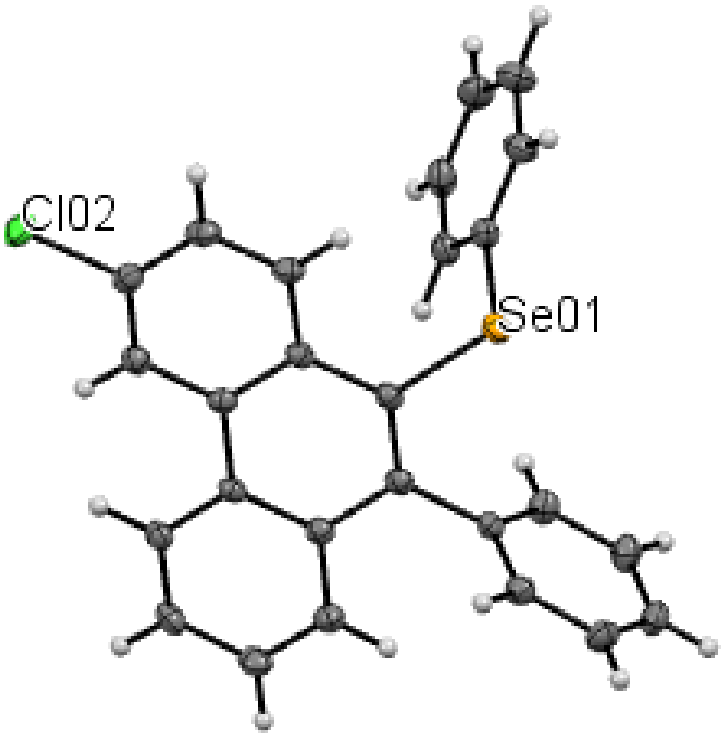



**Figure *S1***. X-ray crystal structure of **3ba** (thermal ellipsoids shown at 50% probability) including hetero-atom numbering.

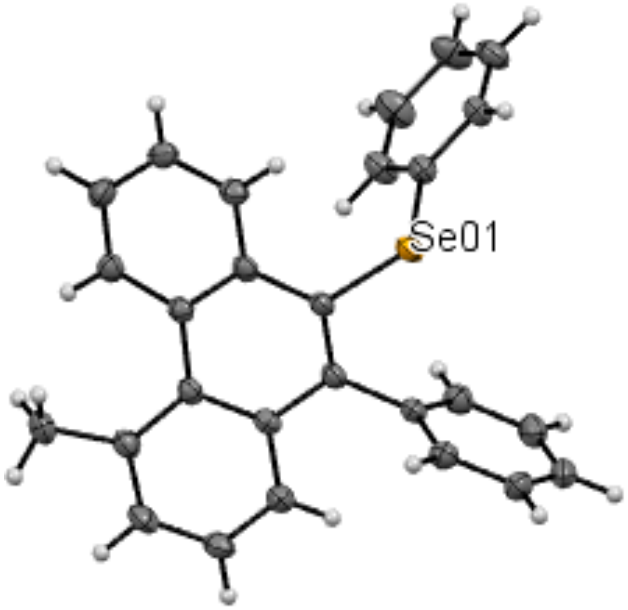



**Figure *S2*.** X-ray crystal structure of **3ea** (thermal ellipsoids shown at 50% probability) including hetero-atom numbering.

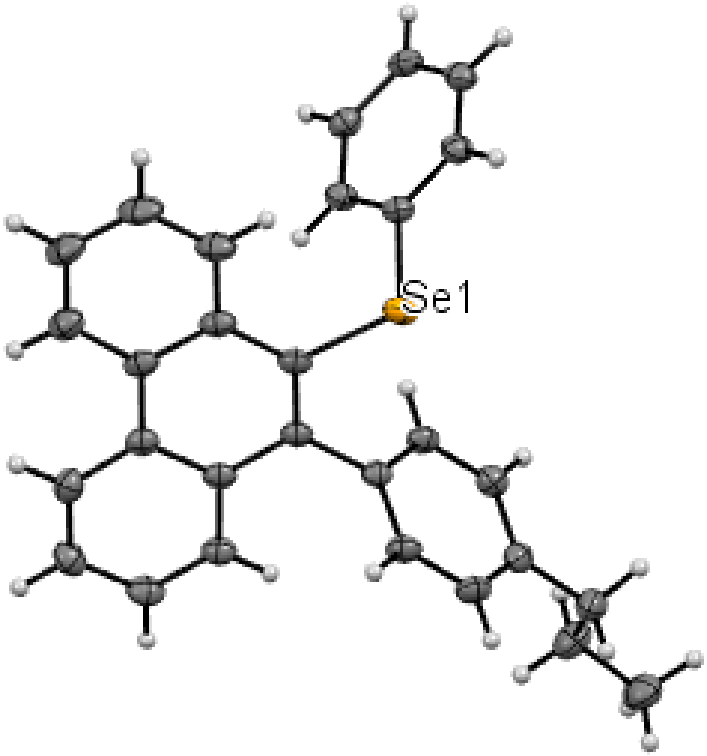



**Figure *S3*.** X-ray crystal structure of **3la** (thermal ellipsoids shown at 50% probability) including hetero-atom numbering.

## 5.1. Table-*S1*. Selected crystal data for compounds 3ba, 3ea, 3la

| | **3ba** | **3ea** | **3la** |
|---|---|---|---|
| ***Empirical formula*** | $C_{26}H_{17}ClSe$ | $C_{27}H_{20}Se$ | $C_{29}H_{24}Se$ |
| ***Formula weight*** | 443.80 | 423.419 | 451.47 |
| ***Temperature/K*** | 100 | 100 | 100 |
| ***Crystal system*** | monoclinic | monoclinic | triclinic |
| ***Space group*** | P 1 21/c 1 | P 1 21/c 1 | P -1 |
| ***a/Å*** | 15.3921(2) | 11.2182(3) | 9.9628(2) |
| ***b/Å*** | 10.18330(10) | 10.3531(3) | 10.1107(2) |
| ***c/Å*** | 13.1358(2) | 17.3831(5) | 12.9334(2) |
| ***α (°)*** | 90 | 90 | 71.458(2) |
| ***β (°)*** | 107.7750(10) | 100.258(3) | 73.161(2) |
| ***γ(°)*** | 90 | 90 | 63.999(2) |
| ***Volume/Å$^3$*** | 1960.65(4) | 1986.66(10) | 1092.75(4) |
| ***Z*** | 4 | 4 | 2 |
| ***μ/mm$^{-1}$*** | 3.894 | 2.605 | 2.402 |
| ***$D_x$ [g cm$^{-3}$]*** | 1.503 | 1.416 | 1.372 |
| ***F(000)*** | 896 | 862.989 | 463.6 |
| ***2Θ range for data collection (°)*** | 5.5900-79.1990 | 4.0480-79.2670 | 5.0300-79.4120 |
| ***Index ranges*** | -19≤ h ≤ 19, -<br>-12 ≤ k ≤ 12, -<br>-16 ≤ l ≤ 13 | -13≤ h ≤ 14, -<br>-11 ≤ k ≤ 12, -<br>-16 ≤ l ≤ 21 | -12≤ h ≤ 9, -<br>-12 ≤ k ≤ 12, -<br>-16 ≤ l ≤ 16 |
| ***Reflections measured*** | 7962 | 5183 | 12419 |
| ***Unique reflections*** | 4133 | 4136 | 4610 |
| ***Parameters /restraints/*** | 321/0 | 254/0 | 285/0 |
| ***Goodness-of-fit on F2*** | 1.149 | 1.085 | 1.027 |
| ***$R_1$ [I ≥ 2σ(I)]*** | 0.075 | 0.100 | 0.0309 |
| ***$wR_2$ (all data)*** | 0.0882( 4133) | 0.1256 (4136) | 0.0814( 4610) |
| ***Largest diff. peak/hole/e Å$^{-3}$*** | 0.548/-0.523 | 0.6378/-0.9648 | 0.5256/-0.6478 |
| ***CCDC*** | ***2176784*** | ***2176838*** | ***2170363*** |

## 6. *Table S2.* Calculation of EcoScale score for the $I_2$-catalyzed synthetic process to synthesize phenyl(10-phenylphenanthren-9-yl)selane (3aa) from 2-(phenylethynyl)-1,1'-biphenyl (1a) and diphenyl diselenide (2a)

**EcoScale Calculation:**

**EcoScale = 100 - Sum of individual penalties**
**Score on EcoScale: > 75, Excellent; >50, acceptable; <50, Inadequate**

| Parameters | Penalty Points |
|---|---|
| **1.** Yield: (100 - % of yield)/2 = (100 - 98)/2 = 1 | **1** |
| **2.** Price of reaction components (To obtain 10 mmol of end product, **3aa**) | |
| **A. Calculation of Penalty Points :** | |
| **a.** 2-(Phenylethynyl)-1,1'-biphenyl = 10.2 mmol = 2.59 g = USD 13.84 | |
| [ Synthesis cost : Required Chemicals : | |
| i) [1,1'-biphenyl]-2-amine = 2.54 g = USD 7.39 | |
| **ii)** HCl = 7.8 mL= USD 0.25 | |
| **iii)** $NaNO_2$ = 1.26 g = USD 0.056 | |
| i**v)** KI = 3.75 g = USD 1.192 | |
| **v)** Bis(triphenyl phosphine)Pd(II) dichloride= 0.089 g = USD 1.70 | |
| **vi)** CuI = 0.024 g = USD 0.008 | |
| **vii)** Phenyl acetylene = 1.68 mL = USD 2.35 | |
| **viii)** Triethylamine = 33.15 mL = USD 0.343 | |
| **b.** 1,2-diphenyldiselane = 6.12 mmol = 1.92 g = USD 7.68 | |
| **c.** Iodine (As catalyst) = 2.02 mmol = 0.517 g = USD 0.152 | |
| **d.** Hydrogen Peroxide (30% aqueous solution) = 0.24 mL = USD 0.063 | |
| Total cost of synthesis of **3aa** = (13.30 + 7.68 + 0.152 + 0.063) = USD 21.195<br>Thus expensive, since \$10<(total cost of synthesis of 10 mmol of **3aa**) < \$50: | **3** |
| **3.** Safety | |
| 1,2-diphenyldiselane (T) | **5** |
| Iodine (T) | **5** |
| **4.** Technical Setup | |
| Common Setup | **0** |
| **5.** Temperature/ Time | |
| 100 °C, 12 h (Heating, > 1h) | **3** |
| **6.** Work up and purification : | |
| **a.** Adding solvent | **0** |
| **b.** Liquid-Liquid extraction | **3** |
| **c.** Classical Chromatography | **10** |
| **Total penalty points:** | **30** |

**B. EcoScale calculation:**

**EcoScale score: (100 - 30) = 70 (>50; it is an acceptable synthesis)**

## 7. *In situ* detection of phenylselenyl iodide PhSeI by LC-MS

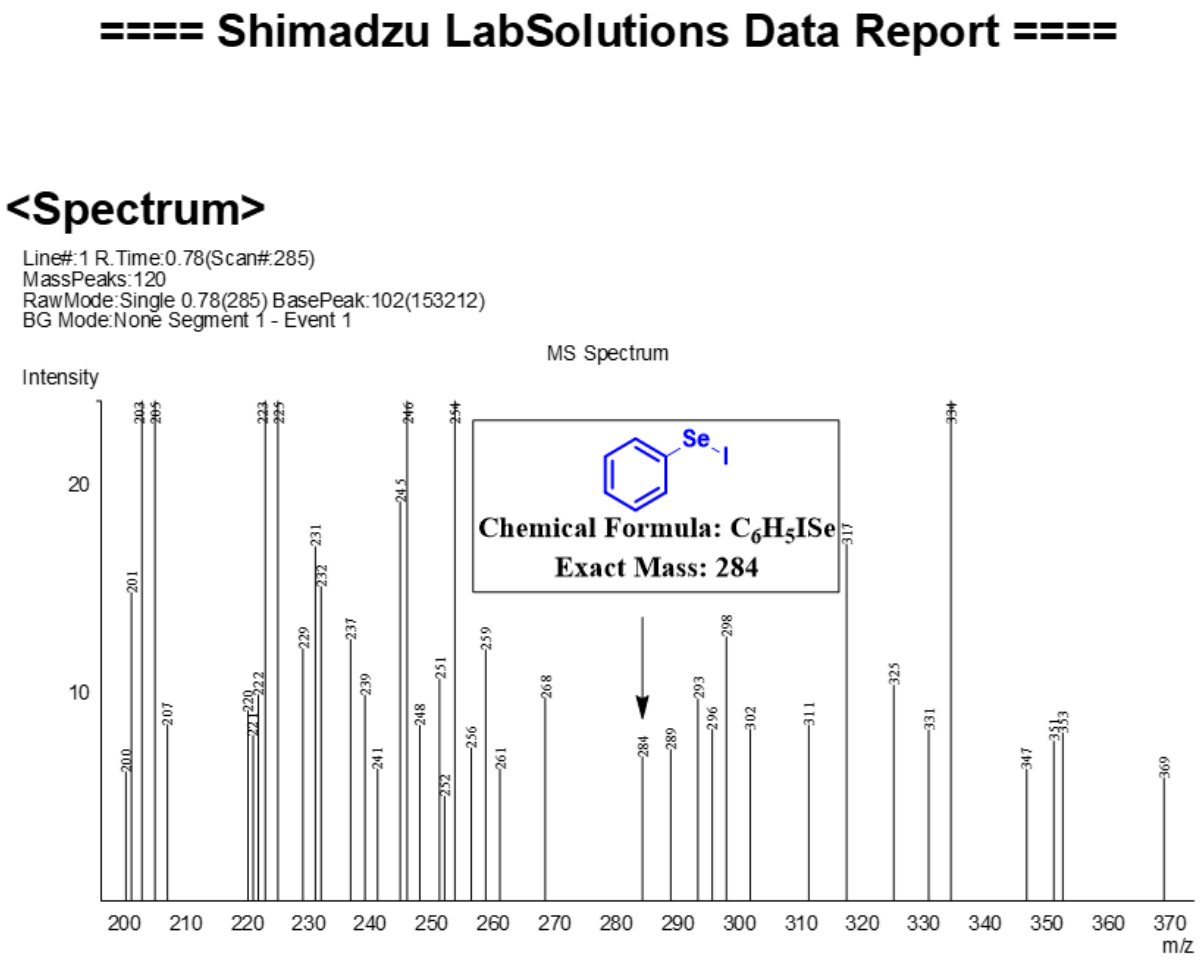



**Figure *S4*.** Mass spectrum of the reaction mixture of diphenyl diselenide and $I_2$

## 8. Calculation of the bond dissociation energies (BDE) for PhSe-X (X = Cl, Br, and I)

The bond dissociation energies (BDE) for PhSe-X (X=Cl, Br, and I) were calculated using the following equation:

$$BDE_X = E_{PhSe^{\bullet}} + E_{X^{\bullet}} - E_{PhSeX}$$

where, $E_{PhSeX}$ represents Gibb's free energy for PhSeX (X= Cl, Br, I), $E_{PhSe^{\bullet}}$ represents Gibb's free energy for PhSe$^{\bullet}$ radical, and $E_{X^{\bullet}}$ is Gibb's free energy for halogen radical.

## 8.1. Table *S3*. The bond dissociation energies (kcal/mol) of the Se-X bond (X = Cl, Br, I) at the M06-2X/LanL2DZ level of theory in water as an implicit solvent

| System | Bond dissociation energy (Se-X bond, X=Cl, Br, I ) |
|---|---|
| PhSeCl | 47.53 |
| PhSeBr | 39.57 |
| PhSeI | 34.40 |

## 9. *In situ* detection of (2,2-diphenylvinyl)(phenyl)selane by LC-MS

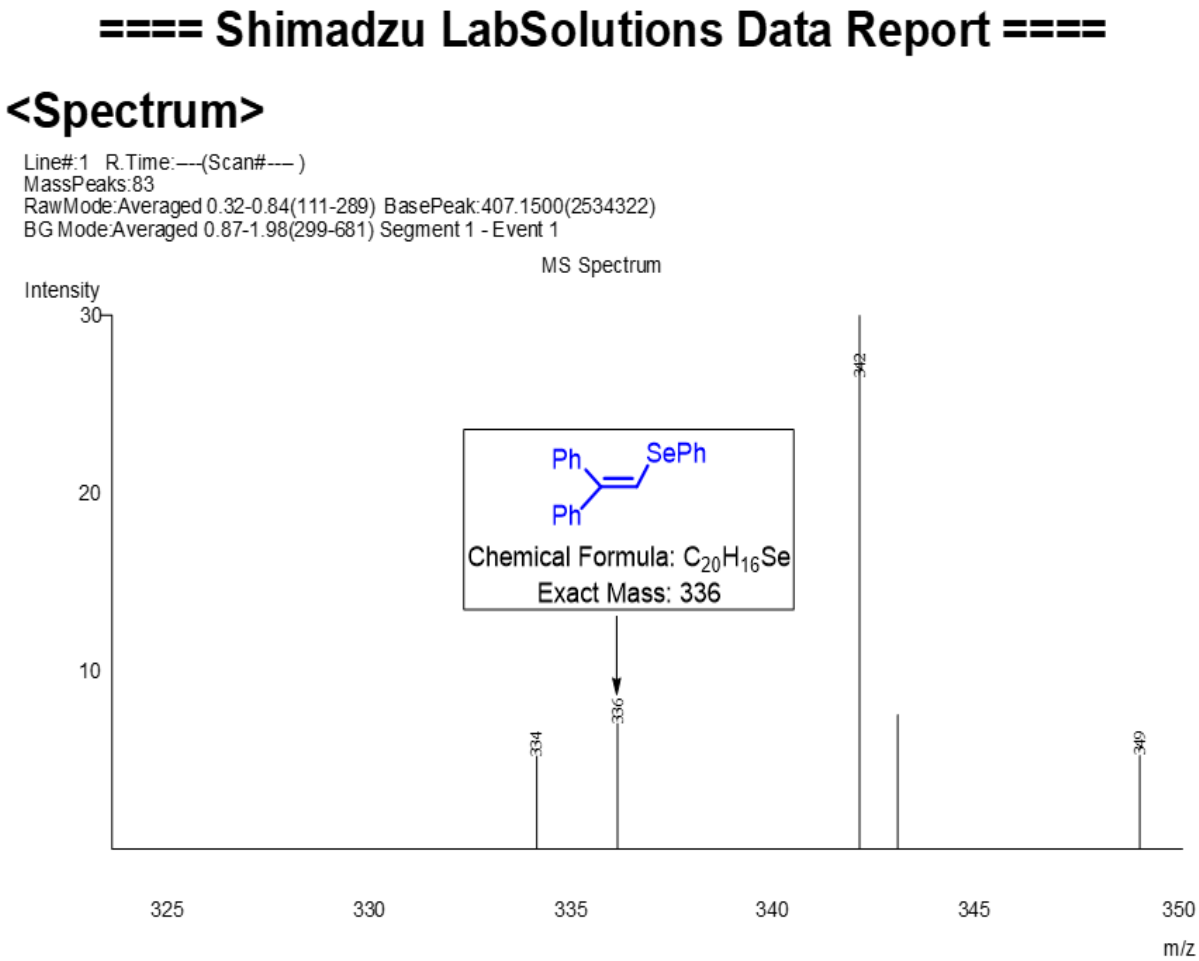



**Figure *S5***. Mass spectrum of the reaction mixture of **1a** and diphenyl diselenide **2a** in the presence of radical quencher, ethene-1,1-diyldibenzene under standard reaction

## 10. Free energy barrier for the initial step for the polar pathway

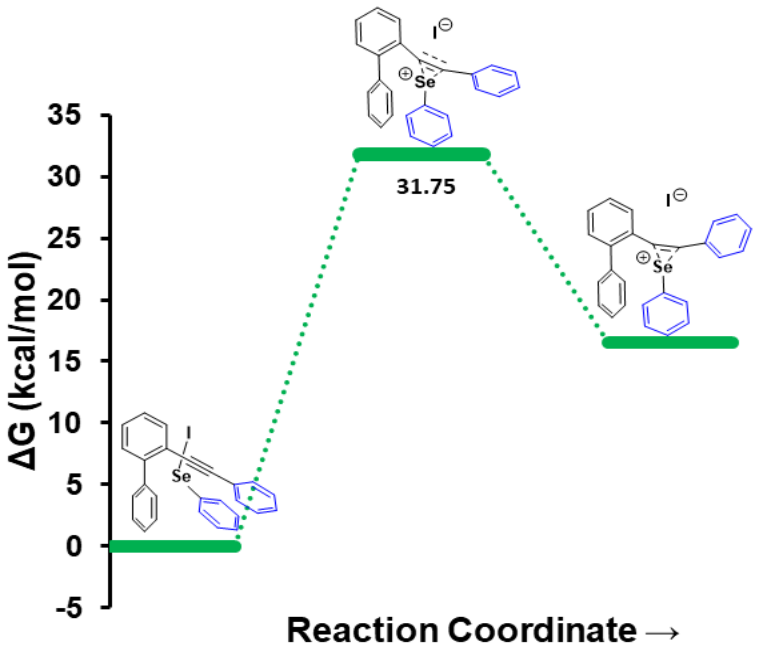
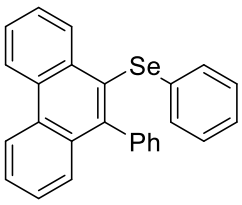
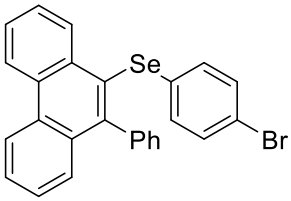



**Figure *S6*.** Free energy profile for the initial step of for the conversion of **1a** and PhSeI to **3aa** through the polar pathway in water

## 11. Analytical data of all synthesized products (3aa - 3ah, 3ba - 3oa and 5, 6, 7)

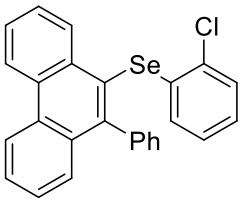



**Phenyl(10-phenylphenanthren-9-yl)selane (3aa):**[9] Yellow solid (0.201 g, 98%); eluent hexane; mp = 82−84 °C; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.85 – 8.74 (m, 3H), 7.72 (m, 2H), 7.62 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.50 – 7.46 (m, 3H), 7.33 – 7.27 (m, 2H), 7.10 (d, *J* = 1.5 Hz, 5H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 146.81, 141.95, 134.23, 132.42, 132.13, 131.07, 130.70, 130.62, 129.65, 129.13, 128.90, 127.94, 127.61, 127.57, 127.43, 127.29, 127.02, 126.72, 125.47, 122.68, 122.55 (Overlapping peaks are present). **$^{77}$Se NMR (76 MHz, DMSO-$d_6$)** δ 318.29 (s).

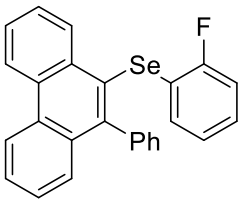



**4-Bromophenyl)(10-phenylphenanthren-9-yl)selane (3ab):** Yellow solid (0.185 g, 76%); eluent hexane; mp = 127−129 °C; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.61 (t, *J* = 7.4 Hz, 2H), 8.50 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.43 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.37 – 7.27 (m, 5H), 7.10 – 7.06 (m, 2H), 7.02 – 6.96 (m, 2H), 6.78 – 6.70 (m, 2H). **$^{13}$C NMR**

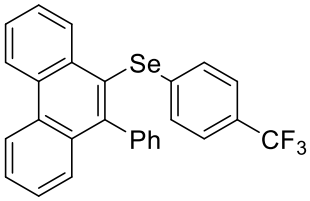
**(100 MHz, $CDCl_3$)** δ 146.99, 141.75, 133.18, 132.11, 132.02, 131.88, 131.09, 130.74, 130.59, 130.31, 129.54, 128.91, 127.99, 127.68, 127.61, 127.40, 127.14, 126.81, 122.78, 122.55, 119.35 55 (Overlapping peaks are present).**$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 323.21 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}BrSe$ [M]: 487.9679; found: 487.9665.




**(2-Chlorophenyl)(10-phenylphenanthren-9-yl)selane (3ac):** Yellow solid (0.160 g, 72%); eluent hexane; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.84 (t, *J* = 8.8 Hz, 2H), 8.70 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.75 (ddd, *J* = 15.7, 7.7, 1.3 Hz, 2H), 7.67 – 7.60 (m, 2H), 7.58 – 7.53 (m, 1H), 7.52 – 7.47 (m, 3H), 7.33 (ddd, *J* = 6.0, 3.4, 1.5 Hz, 3H), 7.03 (td, *J* = 7.7, 1.5 Hz, 1H), 6.85 (td, *J* = 7.8, 1.3 Hz, 1H), 6.70 (dd, *J* = 8.0, 1.5 Hz, 1H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 147.63, 141.55, 134.67, 132.31, 132.12, 132.09, 131.21, 130.70, 130.27, 129.45, 129.25, 129.07, 128.97, 127.98, 127.76, 127.69, 127.44, 127.19, 127.04, 126.77, 126.71, 126.20, 122.74, 122.56. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 321.32 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}ClSe$ [M]: 444.0184; found: 444.0191.

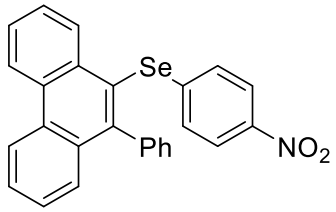



**(2-Fluorophenyl)(10-phenylphenanthren-9-yl)selane (3ad):** Yellow solid (0.151 g, 71%); eluent hexane; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.81 (d, *J* = 8.8 Hz, 2H), 8.65 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.74 – 7.68 (m, 2H), 7.61 – 7.57 (m, 1H), 7.51 – 7.49 (m, 2H), 7.47 – 7.43 (m, 3H), 7.27 (s, 1H), 7.25 – 7.24 (m, 1H), 7.05 (dtd, *J* = 6.4, 5.4, 2.7 Hz, 1H), 6.98 – 6.93 (m, 1H), 6.77 – 6.72 (m, 1H), 6.70 – 6.65 (m, 1H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 159.79 (d, $^{1}J_{C\text{-}F}$ = 241 Hz), 147.50, 141.68, 132.22 (d, $^{3}J_{C\text{-}F}$ = 18 Hz), 131.18, 130.72, 130.32, 129.50, 128.92, 128.01, 127.68, 127.63, 127.45, 127.28, 127.15, 127.08, 126.79, 125.81, 125.53, 124.68, 124.66, 122.67 (d, $^{3}J_{C\text{-}F}$ = 17 Hz), 120.96 (d, $^{2}J_{C\text{-}F}$ = 22 Hz), 115 (d, $^{2}J_{C\text{-}F}$ = 22 Hz). **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 321.26 (s). **$^{19}$F NMR (377 MHz, $CDCl_3$)** δ -106.16 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}FSe$ [M]: 428.0480; found: 428.0483.

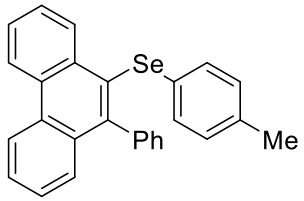



**(10-Phenylphenanthren-9-yl)(4-(trifluoromethyl)phenyl)selane (3ae):** Yellow solid (0.16 g, 67%); eluent hexane; mp = 190−192 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.78 – 8.73 (m, 2H), 8.58 (d, *J* = 8.2 Hz, 1H), 7.66 (m, 2H), 7.56 (dd, *J* = 11.2, 4.0 Hz, 1H), 7.48 – 7.38 (m, 5H), 7.26 – 7.18 (m, 4H), 7.07 (d, *J* = 8.2 Hz, 2H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 147.40, 141.71, 139.69, 132.07, 131.24, 130.82, 130.17, 129.45, 129.03, 128.61, 128.05,

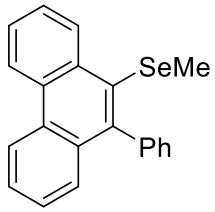
127.84, 127.82, 127.67, 127.52, 127.30, 126.91, 126.47, 125.61, 125.58, 122.89, 122.62, 120.10. **$^{77}$Se NMR (76 MHz, CDCl$_3$)** δ 333.47 (s). **$^{19}$F NMR (76 MHz, CDCl$_3$)** δ -62.44 (s). HRMS (ESI) m/z calcd for $C_{27}H_{17}F_3Se$ [M]: 478.0448; found: 478.0447.



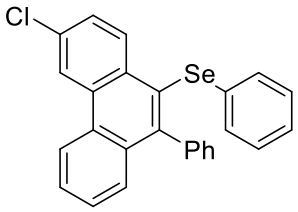

**(4-Nitrophenyl)(10-phenylphenanthren-9-yl)selane (3af):** Yellow solid (0.151 g, 66%); eluent hexane; mp = 170−172 °C; **$^1$H NMR (400 MHz, CDCl$_3$)** δ 8.74 (d, *J* = 4.0 Hz, 2H), 8.49 (d, *J* = 7.8 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 5.6 Hz, 2H), 7.58 – 7.53 (m, 1H), 7.44 (d, *J* = 26.3 Hz, 5H), 7.19 (s, 2H), 7.06 (d, *J* = 7.9 Hz, 2H). **$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 147.74, 145.61, 145.13, 141.50, 131.99, 131.79, 131.35, 130.93, 129.79, 129.29, 129.12, 128.39, 128.13, 128.09, 127.99, 127.71, 127.49, 127.05, 125.82, 123.79, 123.04, 122.68. **$^{77}$Se NMR (76 MHz, CDCl$_3$)** δ 350.20 (s). HRMS (ESI), m/z calcd for $C_{26}H_{18}NO_2Se$ [M + H]$^+$: 456.0497; found: 456.0499.



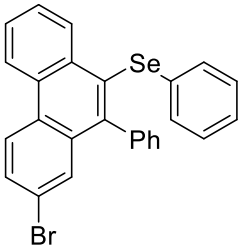

**(10-Phenylphenanthren-9-yl)(*p*-tolyl)selane (3ag):**[10] White solid (0.146 g, 69%); eluent hexane; mp = 110−112 °C; **$^1$H NMR (400 MHz, CDCl$_3$)** δ 8.85 – 8.74 (m, 3H), 7.71 (m, 2H), 7.61 (m, 1H), 7.57 – 7.44 (m, 5H), 7.36 – 7.28 (m, 2H), 7.01 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 2.24 (s, 3H). **$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 146.62, 142.03, 135.26, 132.45, 132.13, 131.02, 130.69, 130.32, 129.73, 129.28, 128.85, 127.93, 127.51, 127.34, 127.25, 126.94, 126.68, 122.65, 122.52, 20.8855 (Overlapping peaks are present).



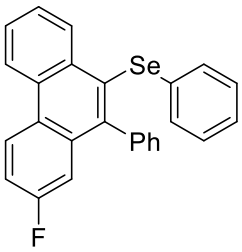

**Methyl(10-phenylphenanthren-9-yl)selane (3ah):** Yellow solid (0.129 g, 74%); eluent hexane; mp = 150−152 °C; **$^1$H NMR (400 MHz, CDCl$_3$)** δ 8.77 (d, *J* = 7.5 Hz, 1H), 8.66 (t, *J* = 7.7 Hz, 2H), 7.62 (dd, *J* = 6.3, 2.5 Hz, 2H), 7.56 – 7.53 (m, 1H), 7.44 – 7.42 (m, 2H), 7.36 – 7.33 (m, 2H), 7.23 (dd, *J* = 5.4, 1.5 Hz, 2H), 7.15 (d, *J* = 2.4 Hz, 1H), 1.96 (s, 3H). **$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 145.44, 142.42, 132.32, 131.92, 130.55, 130.35, 129.94, 129.37, 128.53, 128.01, 127.68, 127.43, 127.21, 126.99, 126.81, 126.64, 122.91, 122.44, 10.04. **$^{77}$Se NMR (76 MHz, CDCl$_3$)** δ 118.24 (s). Anal calcd for $C_{21}H_{16}Se$: C, 72.62; H, 4.64; found C, 72.26; H, 4.92.



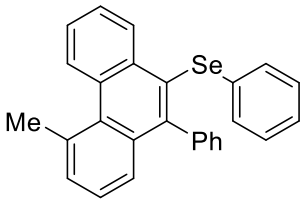

**(6-Chloro-10-phenylphenanthren-9-yl)(phenyl)selane (3ba):** Off White solid (0.120 g, 54%); eluent hexane; mp = 163−165 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.72 (d, *J* = 2.1 Hz, 1H), 8.69 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.9 Hz, 1H), 7.71 (m, 1H), 7.53 – 7.43 (m, 6H), 7.25 – 7.22 (m, 2H), 7.10 – 7.00 (m, 5H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 147.04, 141.63, 133.87, 133.28, 132.45, 132.36, 131.80, 130.86, 130.09, 129.61, 129.20, 129.03, 128.03, 127.93, 127.72, 127.47, 127.39, 127.14, 125.72, 122.63, 122.32 55 (Overlapping peaks are present). **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 325.10 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}ClSe$ [M]: 444.0184; found: 444.0190; the assignment is also supported by an X-ray crystallographic structure determination (**CCDC 2176784**).



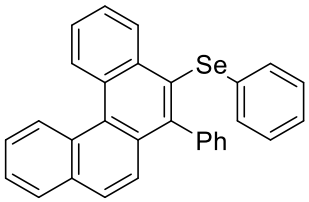

**(2-Bromo-10-phenylphenanthren-9-yl)(phenyl)selane (3ca):** Yellowish viscous solid (0.210 g, 86%); eluent hexane; mp = 190−192 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 9.03 – 8.89 (m, 2H), 8.85 – 8.75 (m, 1H), 7.95 – 7.82 (m, 3H), 7.81 – 7.77 (m, 1H), 7.66 (dd, *J* = 4.5, 2.2 Hz, 4H), 7.49 – 7.43 (m, 2H), 7.26 (s, 4H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 146.76, 145.53, 141.89, 141.06, 133.89, 133.44, 132.30, 130.84, 130.75, 130.45, 130.12, 129.56, 129.21, 128.93, 128.11, 127.59, 126.98, 126.68, 125.62, 124.31, 122.52, 121.01. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 328.34 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}BrSe$ $[M]^+$: 487.9679; found: 487.9707.



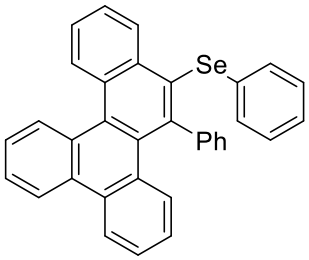

**(2-Fluoro-10-phenylphenanthren-9-yl)(phenyl)selane (3da):** Yellow solid (0.161 g, 75%); eluent hexane; mp = 140−142 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.79 – 8.75 (m, 1H), 8.74 – 8.71 (m, 1H), 8.68 (d, *J* = 8.1 Hz, 1H), 7.69 (m, 1H), 7.58 (m, 1H), 7.46 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.45 – 7.41 (m, 1H), 7.26 – 7.22 (m, 2H), 7.14 (dd, *J* = 10.8, 2.7 Hz, 1H), 7.07 (s, 5H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 161.18 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 145.98, 141.40, 133.97, 133.64 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 131.97, 130.79, 130.34, 129.56, 129.30, 129.23, 128.97, 128.16, 127.67, 127.58, 127.38, 125.66, 124.90 (d, $^{3}J_{C\text{-}F}$ = 9 Hz) 122.52, 116.3 (d, $^{2}J_{C\text{-}F}$ = 24 Hz), 113.27 (d, $^{2}J_{C\text{-}F}$ = 22 Hz) (Overlapping peaks are present). **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 327.35 (s). **$^{19}$F NMR (377 MHz, $CDCl_3$)** δ -113.38 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}FSe$ $[M]^+$: 428.0480; found: 428.0506.



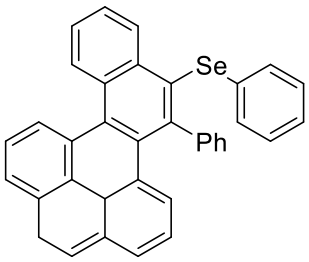

**(4-Methyl-10-phenylphenanthren-9-yl)(phenyl)selane (3ea):** Off White solid (0.176 g, 83%); eluent hexane; mp = 130−132 °C; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.79 (d, *J* = 8.0 Hz, 1H), 8.75 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.52 (m, 3H), 7.42 – 7.34 (m, 4H), 7.28 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.19 (dd, *J* = 6.4, 3.1 Hz, 2H), 7.05 – 6.94 (m, 5H), 3.11 (s, 3H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 147.13, 142.61, 134.85, 134.21, 133.58, 133.28, 132.00, 131.82, 131.29, 130.31, 129.65, 129.13, 128.87, 127.90, 127.74, 127.62, 127.30, 127.17, 126.81, 125.73, 125.55, 125.42, 27.22. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 324.16 (s). The assignment is supported by an X-ray crystallographic structure determination (**CCDC 2176838).**




**Phenyl(6-phenylbenzo[*c*]phenanthren-5-yl)selane (3fa):**[10] Off White solid (0.102 g, 44%); eluent hexane; mp = 122−124 °C; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 9.11 (t, *J* = 8.3 Hz, 2H), 8.84 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.81 – 7.58 (m, 6H), 7.47 (m, 4H), 7.28 (dd, *J* = 7.2, 2.2 Hz, 2H), 7.08 (s, 5H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 146.01, 141.94, 134.24, 133.65, 133.45, 130.51, 130.26, 130.02, 129.55, 129.44, 129.09, 128.93, 128.86, 128.57, 128.19, 127.98, 127.40, 127.12, 127.03, 126.56, 126.22, 126.18, 125.70, 125.60.

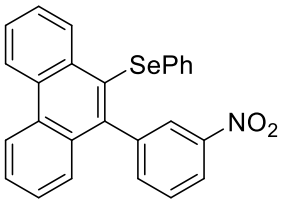



**Phenyl(5-phenylbenzo[*g*]chrysen-6-yl)selane (3ga):**[10] Off White solid (0.140 g, 55%); eluent hexane; mp = 210−212 °C; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.81 – 8.66 (m, 4H), 8.58 (d, *J* = 8.0 Hz, 1H), 7.71 (m, 2H), 7.63 – 7.53 (m, 3H), 7.50 – 7.34 (m, 6H), 7.06 (s, 6H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 144.55, 143.37, 134.51, 133.77, 131.40, 131.29, 130.67, 130.25, 130.09, 129.93, 129.84, 129.54, 129.27, 129.14, 128.90, 128.67, 128.10, 127.88, 127.57, 127.23, 126.95, 126.49, 126.21, 125.97, 125.70, 125.61, 123.54, 123.03.

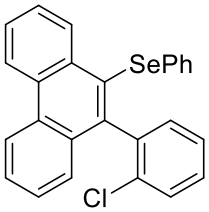



**Phenyl(14-phenyldibenzo[*ij*,*no*]tetraphen-13-yl)selane (3ha):**[10] Brown solid (0.182 g, 68%); eluent hexane; mp = 220−222 °C; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 9.37 (d, *J* = 9.3 Hz, 1H), 9.16 (d, *J* = 8.2 Hz, 1H), 8.87 (dd, *J* = 8.2, 1.1 Hz, 1H), 8.32 (d, *J* = 9.3 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.16 (d, *J* = 7.2 Hz, 1H), 8.13 (s, 1H), 8.05 (t, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.78 – 7.73 (m, 1H), 7.68 (dd, *J* = 11.1, 4.1 Hz, 1H), 7.58 – 7.52 (m, 3H), 7.40 – 7.36 (m, 2H), 7.15 (dd, *J* = 6.5, 3.3 Hz, 2H),

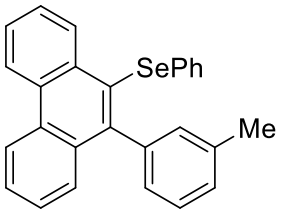
7.12 – 7.06 (m, 3H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 146.39, 142.01, 134.17, 133.06, 131.65, 130.95, 130.59, 130.22, 129.97, 129.55, 129.40, 128.98, 128.12, 128.03, 127.85, 127.57, 127.33, 127.19, 127.13, 126.75, 126.40, 126.26, 126.13, 125.65, 125.19, 124.97, 124.76, 124.33.



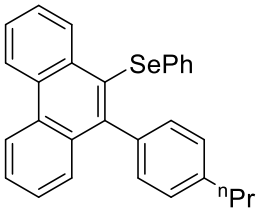

**(10-(3-Nitrophenyl)phenanthren-9-yl)(phenyl)selane (3ia):** Yellow crystal (0.107 g, 47%); eluent hexane; mp = 150−152 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.85 – 8.78 (m, 3H), 8.32 – 8.24 (m, 1H), 8.03 – 7.98 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 1.2 Hz, 1H), 7.60 – 7.49 (m, 5H), 7.33 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.06 – 7.04 (m, 2H), 6.98 (d, *J* = 1.6 Hz, 1H). **$^{13}$C NMR (100 MHz, $CDC_3$)** δ 147.84, 143.16, 136.07, 133.50, 131.40, 131.16, 130.82, 130.58, 129.53, 129.10, 128.89, 128.63, 127.93, 127.89, 127.83, 127.68, 127.11, 126.14, 125.04, 122.92, 122.83, 122.35. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 352.1 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}NO_2Se$ [M]: 455.0425; found: 455.0436.



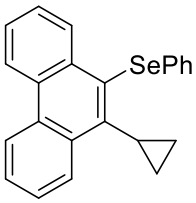

**(10-(2-Chlorophenyl)phenanthren-9-yl)(phenyl)selane (3ja) :**Yellow crystal (0.120 g, 54%); eluent hexane; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.84 (t, *J* = 8.8 Hz, 2H), 8.70 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.75 (m, 2H), 7.67 – 7.60 (m, 2H), 7.58 – 7.53 (m, 1H), 7.52 – 7.47 (m, 3H), 7.33 (ddd, *J* = 6.0, 3.4, 1.5 Hz, 3H), 7.03 (td, *J* = 7.7, 1.5 Hz, 1H), 6.85 (m, 1H), 6.70 (dd, *J* = 8.0, 1.5 Hz, 1H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 147.63, 141.55, 134.67, 132.31, 132.12, 132.09, 131.21, 130.70, 130.27, 129.45, 129.25, 129.07, 128.97, 127.98, 127.76, 127.69, 127.44, 127.19, 127.04, 126.77, 126.71, 126.20, 122.74, 122.56. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 322.65 (s). HRMS (ESI) m/z calcd for $C_{26}H_{17}ClSe$ [M]: 444.0184; found: 444.0191.



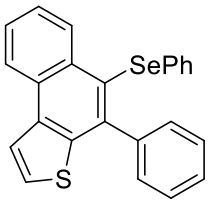

**Phenyl(10-(m-tolyl)phenanthren-9-yl)selane (3ka):** Yellow solid (0.180 g, 85%); eluent hexane; mp = 140−142 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.82 (t, *J* = 7.4 Hz, 3H), 7.73 (m, 2H), 7.68 – 7.59 (m, 2H), 7.57 – 7.51 (m, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.14 (ddd, *J* = 14.6, 6.8, 2.6 Hz, 7H), 2.43 (s, 3H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 146.91, 141.82, 137.39, 134.37, 132.48, 132.17, 131.02, 130.61, 130.40, 129.28, 128.92, 128.84, 127.99, 127.80, 127.63, 127.51, 127.36, 126.92, 126.67, 125.47, 122.66, 122.50, 21.50. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 323.31 (s). HRMS (ESI) m/z calcd for $C_{27}H_{20}Se$ [M]: 424.0730; found: 424.0728.



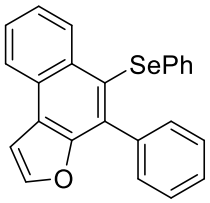

**Phenyl(10-(4-propylphenyl)phenanthren-9-yl)selane (3la) :**Reddish Brown solid (0.102 g, 45%); eluent hexane; mp = 125−127 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.67 (t, *J* = 8.6 Hz, 2H), 8.59 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.49 – 7.45 (m, 1H), 7.42 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.40 – 7.36 (m, 1H), 7.14 (d, *J* = 9.5 Hz, 3H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.95 (s, 4H), 2.63 – 2.58 (m, 2H), 1.66 (dd, *J* = 15.1, 7.5 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 146.93, 141.66, 139.17, 134.35, 132.48, 132.34, 131.06, 130.65, 129.51, 129.28, 128.98, 128.88, 127.98, 127.81, 127.50, 127.36, 126.91, 126.68, 125.47, 122.67, 122.51, 37.92, 24.43, 13.95. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 323.50 (s). HRMS (ESI) m/z calcd for $C_{29}H_{24}Se$ [M]: 452.1043; found: 452.1046; the assignment is supported by an X-ray crystallographic structure determination (CCDC **2170363**).



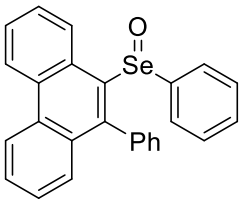

**(10-Cyclopropylphenanthren-9-yl)(phenyl)selane (3ma):** Brown Viscous liquid(0.101 g, 54%); eluent hexane; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.49 – 7.45 (m, 2H), 7.38 – 7.36 (m, 3H), 7.33 – 7.29 (m, 2H), 7.18 – 7.13 (m, 4H), 7.10 – 7.08 (m, 2H), 1.75 (ddd, *J* = 8.2, 5.2, 3.0 Hz, 1H), 0.75 – 0.67 (m, 2H), 0.64 – 0.57 (m, 1H), 0.43 – 0.35 (m, 1H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 143.49, 140.84, 140.44, 138.06, 134.34, 132.27, 130.95, 130.08, 129.57, 129.46, 129.37, 129.08, 128.85, 128.49, 128.43, 127.81, 127.18, 127.05, 126.43, 104.39, 24.23, 10.38, 9.41. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 410.69 (s). Anal calcd for $C_{23}H_{18}Se$: C, 73.99; H, 4.86; found C, 73.26; H, 4.49.



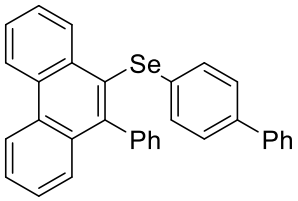

**4-Phenyl-5-(phenylselanyl)naphtho[2,1-*b*]thiophene (3na):** Yellow solid (0.160 g, 77%); eluent hexane; mp = 95−97 °C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.76 (d, *J* = 8.3 Hz, 1H), 8.42 (dd, *J* = 8.1, 0.6 Hz, 1H), 8.08 (d, *J* = 5.5 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.60 – 7.56 (m, 1H), 7.49 – 7.45 (m, 3H), 7.42 – 7.39 (m, 2H), 7.08 (s, 5H). **$^{13}$C NMR (100 MHz, $CDCl_3$)** δ 142.45, 141.77, 139.71, 137.00, 134.24, 132.82, 130.45, 129.10, 129.07, 128.89, 128.47, 128.10, 128.02, 126.78, 126.68, 126.56, 125.52, 123.91, 123.86, 122.24. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 306.69 (s). HRMS (ESI) m/z calcd for $C_{24}H_{16}SSe$ [M]: 416.0138; found: 416.0139.



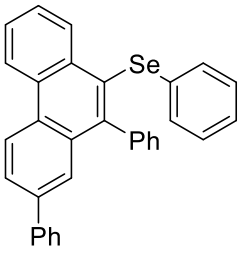

**4-Phenyl-5-(phenylselanyl)naphtho[2,1-*b*]furan (3oa):** Brown solid (0.080 g, 40%); eluent hexane; **$^{1}$H NMR (400 MHz, CDCl$_3$)** δ 8.73 (d, *J* = 8.4 Hz, 1H), 8.21 (dd, *J* = 8.1, 0.7 Hz, 1H), 7.77 (d, *J* = 2.1 Hz, 1H), 7.63 (dt, *J* = 4.2, 2.3 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.46 – 7.43 (m, 3H), 7.39 (ddd, *J* = 3.6, 2.4, 1.7 Hz, 2H), 7.36 (d, *J* = 2.1 Hz, 1H), 7.08 – 7.00 (m, 5H). **$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 150.75, 145.54, 137.38, 134.71, 134.38, 132.19, 131.50, 130.69, 130.05, 129.11, 128.94, 127.98, 127.79, 126.63, 126.01, 125.57, 124.53, 124.14, 123.76, 105.81. **$^{77}$Se NMR (76 MHz, CDCl$_3$)** δ 302.58 (s). HRMS (ESI) m/z calcd for $C_{24}H_{16}OSe$ [M]: 400.0366; found: 400.0359.




**9-Phenyl-10-(phenylseleninyl)phenanthrene (5):** Orange crystal (0.182 g, 86%); eluent hexane; mp = 172−175 °C; **$^{1}$H NMR (400 MHz, CDCl$_3$)** δ 8.99 (d, *J* = 8.2 Hz, 1H), 8.66 (dd, *J* = 14.6, 8.3 Hz, 2H), 7.71 – 7.64 (m, 3H), 7.62 – 7.57 (m, 2H), 7.53 (m, 5H), 7.46 – 7.40 (m, 2H), 7.32 (m, 3H). **$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 143.71, 141.87, 137.15, 135.40, 131.64, 131.23, 130.59, 130.36, 130.31, 130.15, 129.20, 129.08, 128.59, 128.35, 127.31, 127.23, 127.05, 126.59, 126.11, 122.65, 122.59 (Overlapping peaks are present). **$^{77}$Se NMR (76 MHz, CDCl$_3$)** δ 895.08 (s). HRMS (ESI) m/z calcd for $C_{26}H_{18}OSe$ [M]: 426.0523; found: 426.0656.




**[1,1'-biphenyl]-4-yl(10-phenylphenanthren-9-yl)selane (6):** Yellow liquid (0.095 g, 65%); eluent hexane; **$^{1}$H NMR (400 MHz, CDCl$_3$)** δ 8.86 – 8.76 (m, 3H), 7.72 (dd, *J* = 3.2, 1.8 Hz, 2H), 7.63 (d, *J* = 1.2 Hz, 1H), 7.54 – 7.53 (m, 1H), 7.52 – 7.47 (m, 6H), 7.40 (dd, *J* = 8.2, 6.8 Hz, 2H), 7.34 – 7.30 (m, 5H), 7.17 – 7.12 (m, 2H). **$^{13}$C NMR (100 MHz, CDCl$_3$)** δ 146.89, 141.94, 140.40, 138.37, 133.41, 132.43, 132.15, 131.10, 130.73, 130.62, 129.67, 129.44, 128.91, 128.69, 127.98, 127.66, 127.53, 127.50, 127.33, 127.09, 127.07, 126.76, 126.66, 122.73, 122.57(Overlapping peaks are present). **$^{77}$Se NMR (76 MHz, CDCl$_3$)** δ 319.82 (s). Anal calcd for $C_{32}H_{22}Se$: C, 79.17; H, 4.57; found C, 79.84; H, 4.06.

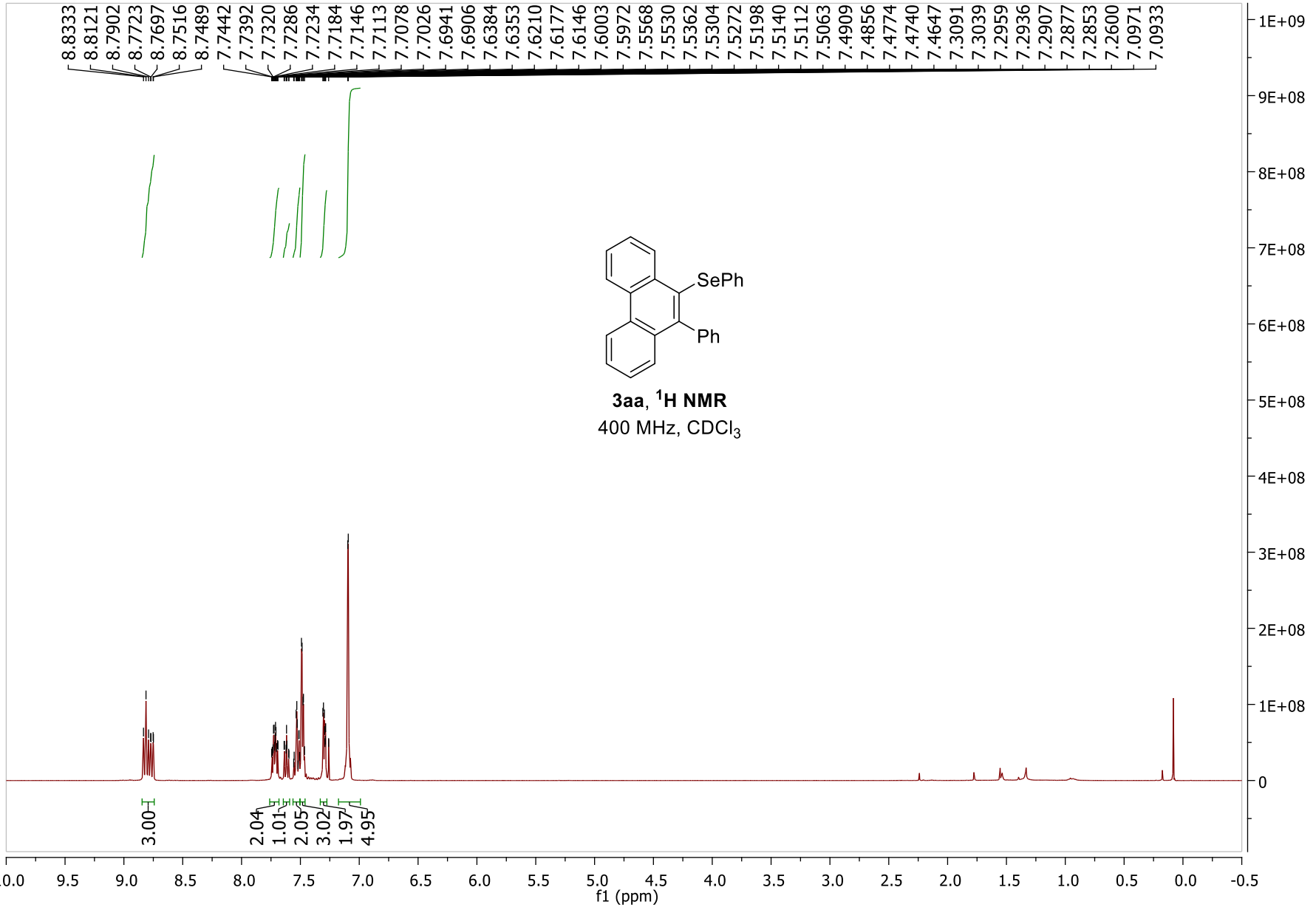



**(2,10-diphenylphenanthren-9-yl)(phenyl)selane (7):** Yellow solid (0.080 g, 55%); eluent hexane; mp = 73-75 $^{o}$C; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.76 (ddd, *J* = 18.5, 9.3, 4.8 Hz, 3H), 7.95 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.60 – 7.57 (m, 1H), 7.57 – 7.49 (m, 3H), 7.45 – 7.38 (m, 5H), 7.35 (dd, *J* = 4.9, 3.6 Hz, 1H), 7.28 (d, *J* = 2.4 Hz, 1H), 7.23 (s, 1H), 7.05 (d, *J* = 4.2 Hz, 4H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 144.05, 141.82, 140.65, 140.57, 139.36, 134.25, 132.53, 130.72, 130.58, 130.23, 130.23, 129.71, 129.22, 128.94, 128.85, 128.20, 128.04, 127.60, 127.45, 127.30, 127.15, 126.95, 126.68, 125.54, 123.20, 122.76. **$^{77}$Se NMR (76 MHz, $CDCl_3$)** δ 324.04 (s). Anal calcd for $C_{32}H_{22}Se$: C, 79.17; H, 4.57; found C, 79.95; H, 4.04.

## 12. References

1. G. W. T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria,, J. R. C. M. A. Robb, G. Scalmani, V. Barone, B. Mennucci,, H. N. G. A. Petersson, M. Caricato, X. Li, H. P. Hratchian, J. B. A. F. Izmaylov, G. Zheng, J. L. Sonnenberg, M. Hada,, K. T. M. Ehara, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, O. K. Y. Honda, H. Nakai, T. Vreven, J. A. Montgomery, Jr., F. O. J. E. Peralta, M. Bearpark, J. J. Heyd, E. Brothers, V. N. S. K. N. Kudin, T. Keith, R. Kobayashi, J. Normand, A. R. K. Raghavachari, J. C. Burant, S. S. Iyengar, J. Tomasi, N. R. M. Cossi, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, C. A. V. Bakken, J. Jaramillo, R. Gomperts, R. E. Stratmann, A. J. A. O. Yazyev, R. Cammi, C. Pomelli, J. W. Ochterski, K. M. R. L. Martin, V. G. Zakrzewski, G. A. Voth, J. J. D. P. Salvador, S. Dapprich, A. D. Daniels, J. B. F. O. Farkas, J. V. Ortiz, J. Cioslowski, and and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.
2. R. Peverati and D. G. Truhlar, The Journal of Physical Chemistry Letters, 2011, **2**, 2810-2817.
3. S. Chiodo, N. Russo and E. Sicilia, The Journal of chemical physics, 2006, **125**, 104107-104115.
4. V. Barone and M. Cossi, The Journal of Physical Chemistry A, 1998, **102**, 1995-2001.
5. N. Mukherjee and T. Chatterjee, *Green Chem.*, 2021, **23**, 10006−10013.
6. D. Singh, A. M. Deobald, L. R. S. Camargo, G. Tabarelli, O. E. D. Rodrigues and A. L. Braga, *Org. Lett.*, 2010, **12,** 3288–3291.

7. S. An, Z. Zhang and P. Li, *Eur. J. Org. Chem*., 2021, 3059-3070
8. N. Mukherjee and T. Chatterjee, *J. Org. Chem.*, 2021, **86**, 7881–7890
9. S. An, Z. Zhang, P. Li, *Eur. J. Org. Chem.* 2021, **21**, 3059–3070.
10. T. B. Grimaldi, G. Lutz, D. F. Back and G. Zeni, *Org. Biomol. Chem.* 2016, **14**, 10415-10426.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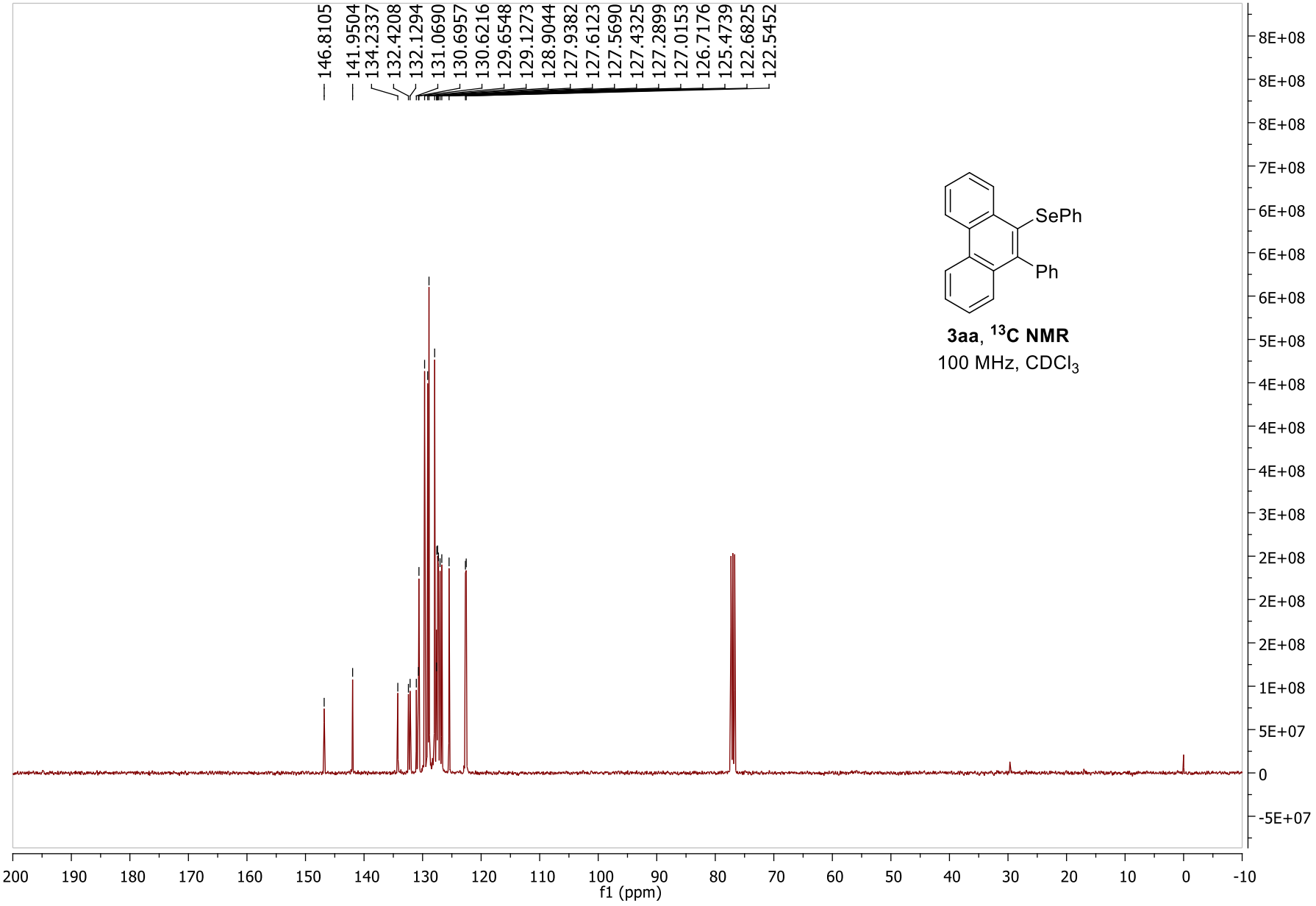
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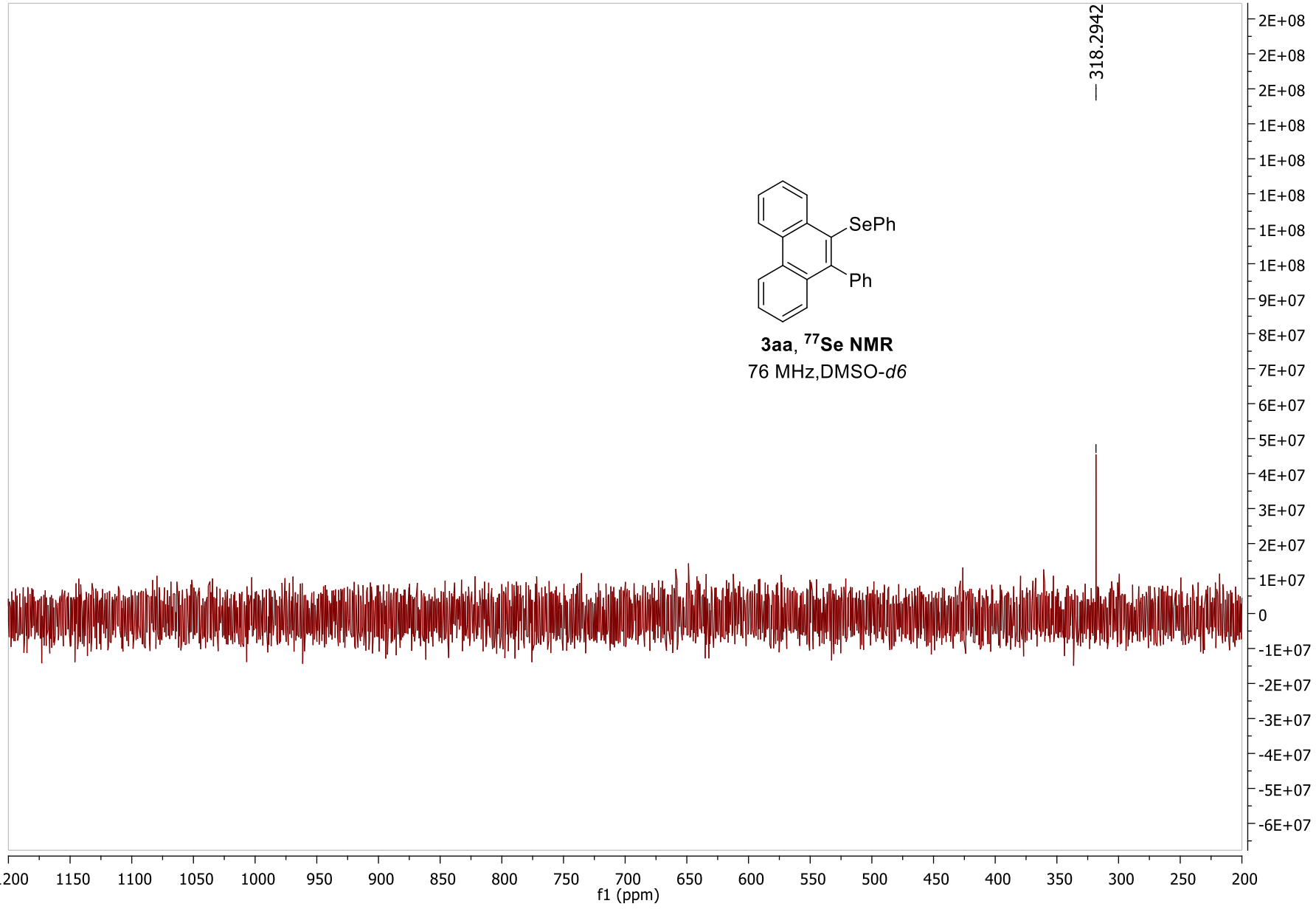
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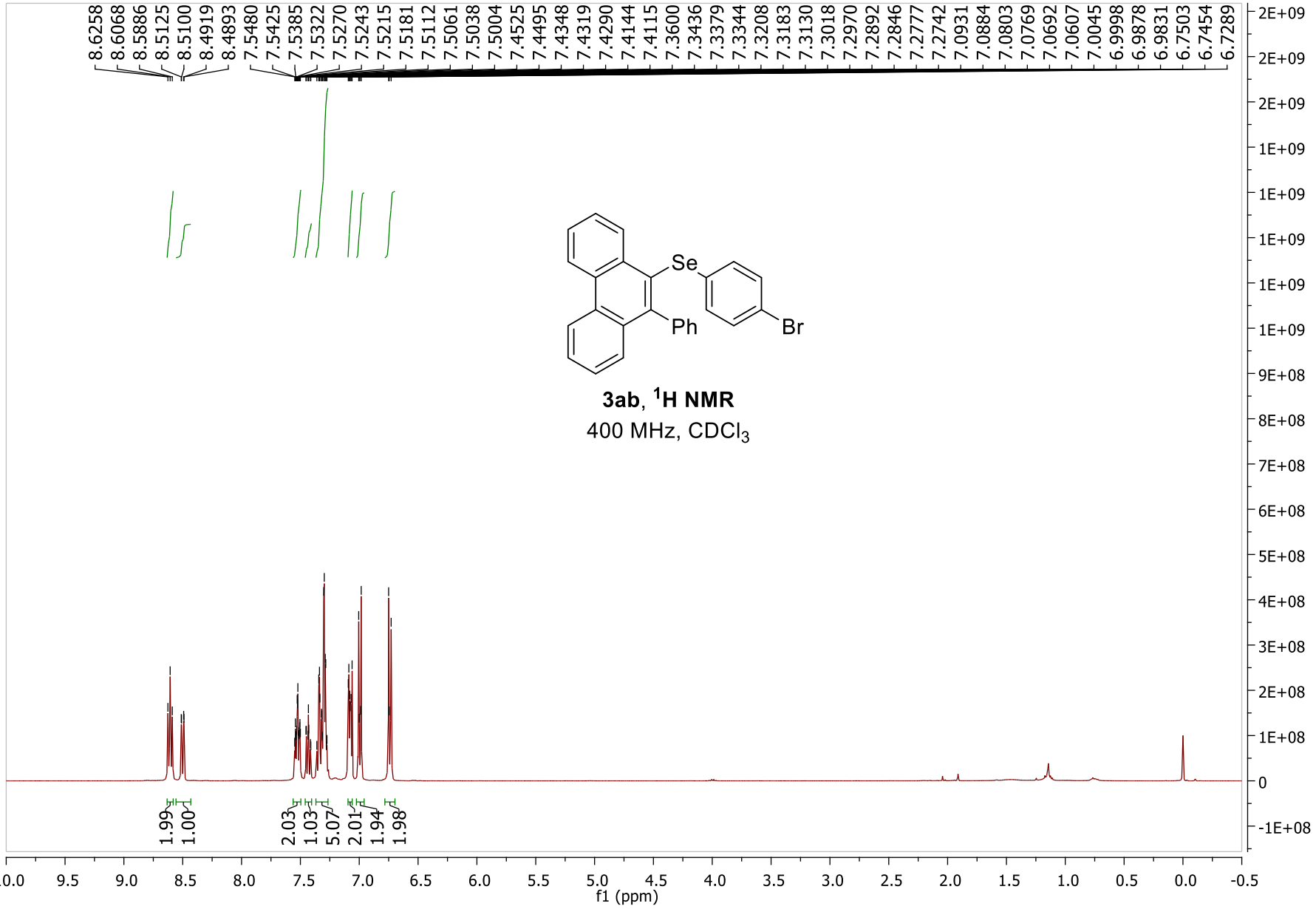
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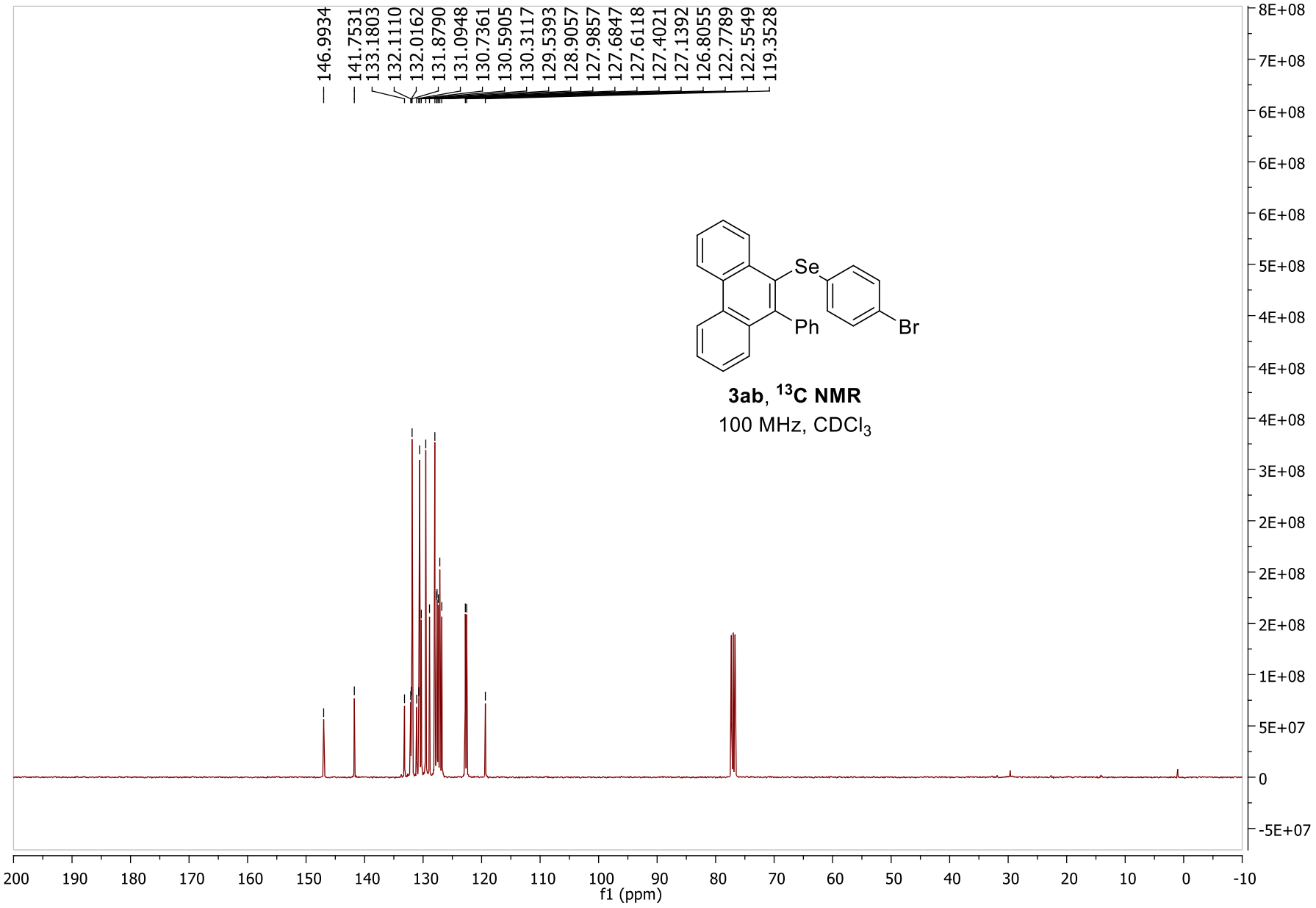
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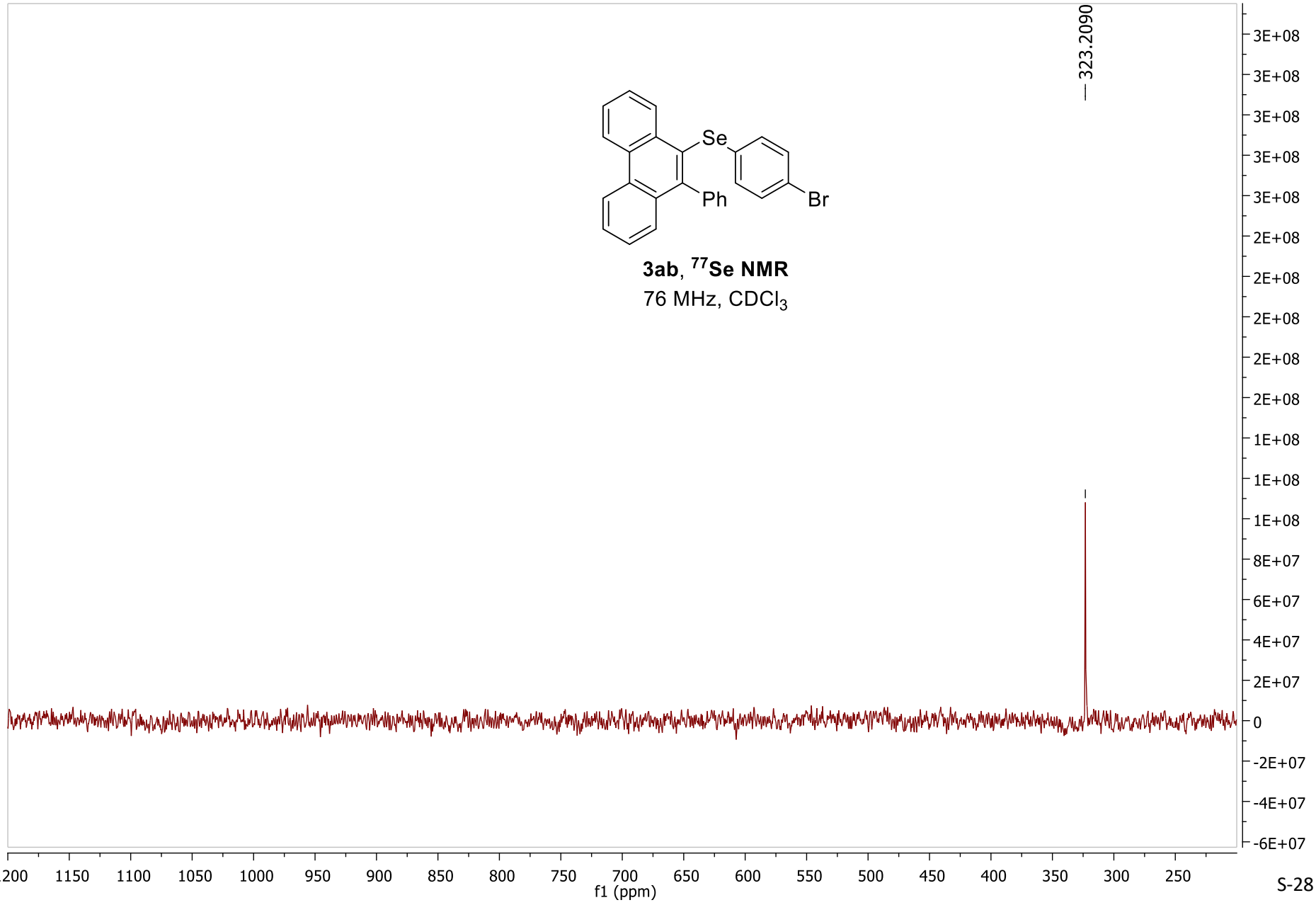
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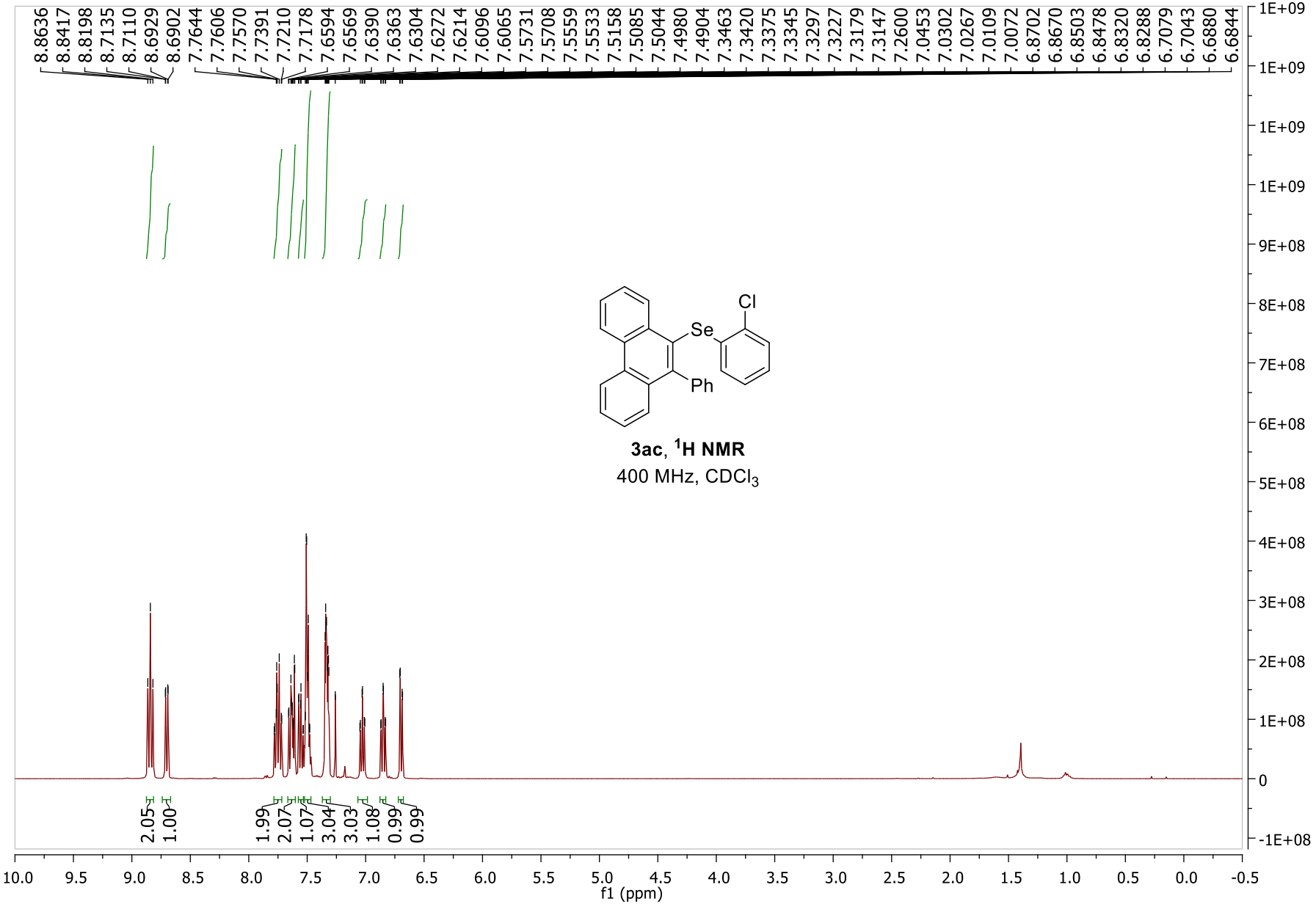
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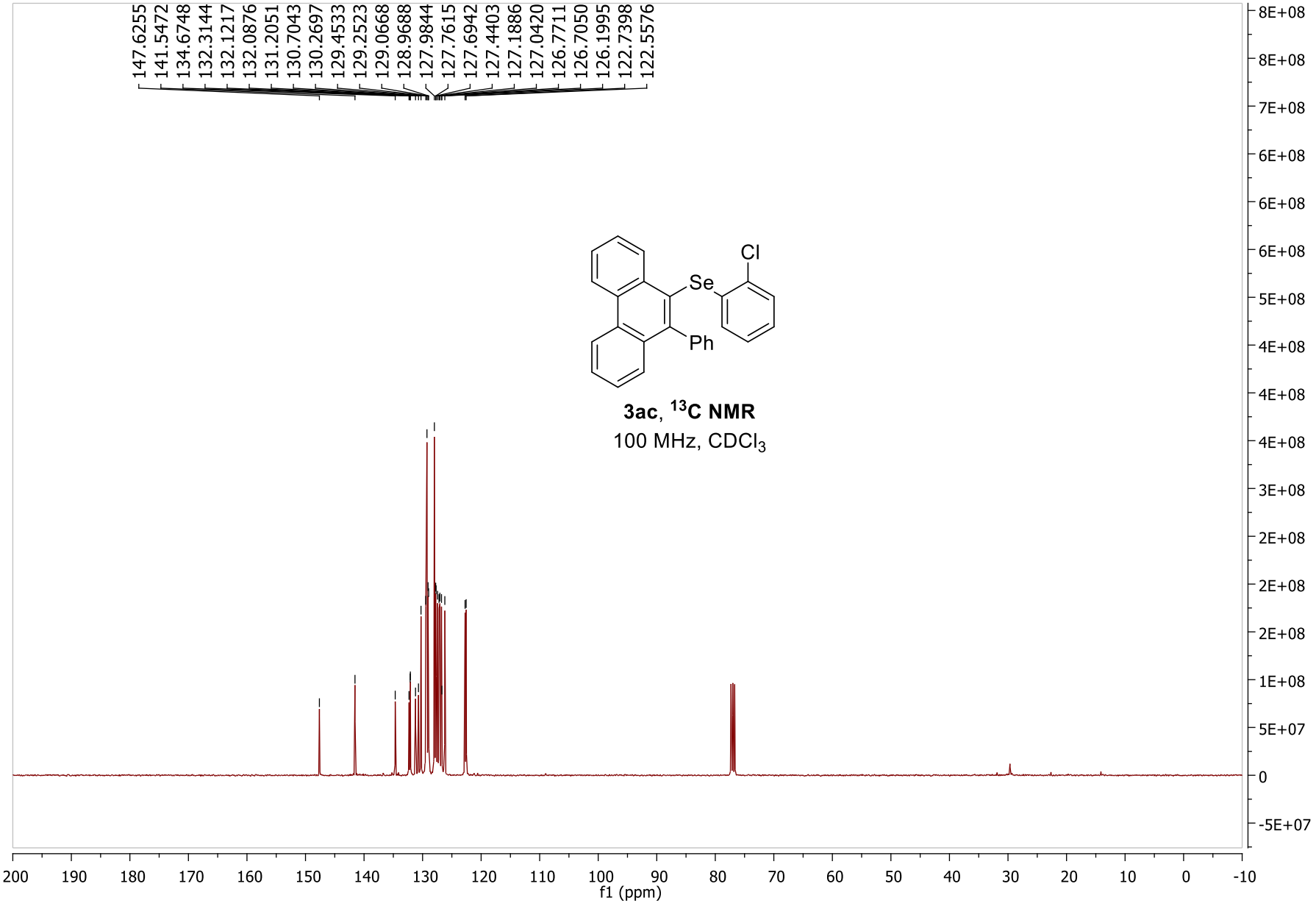
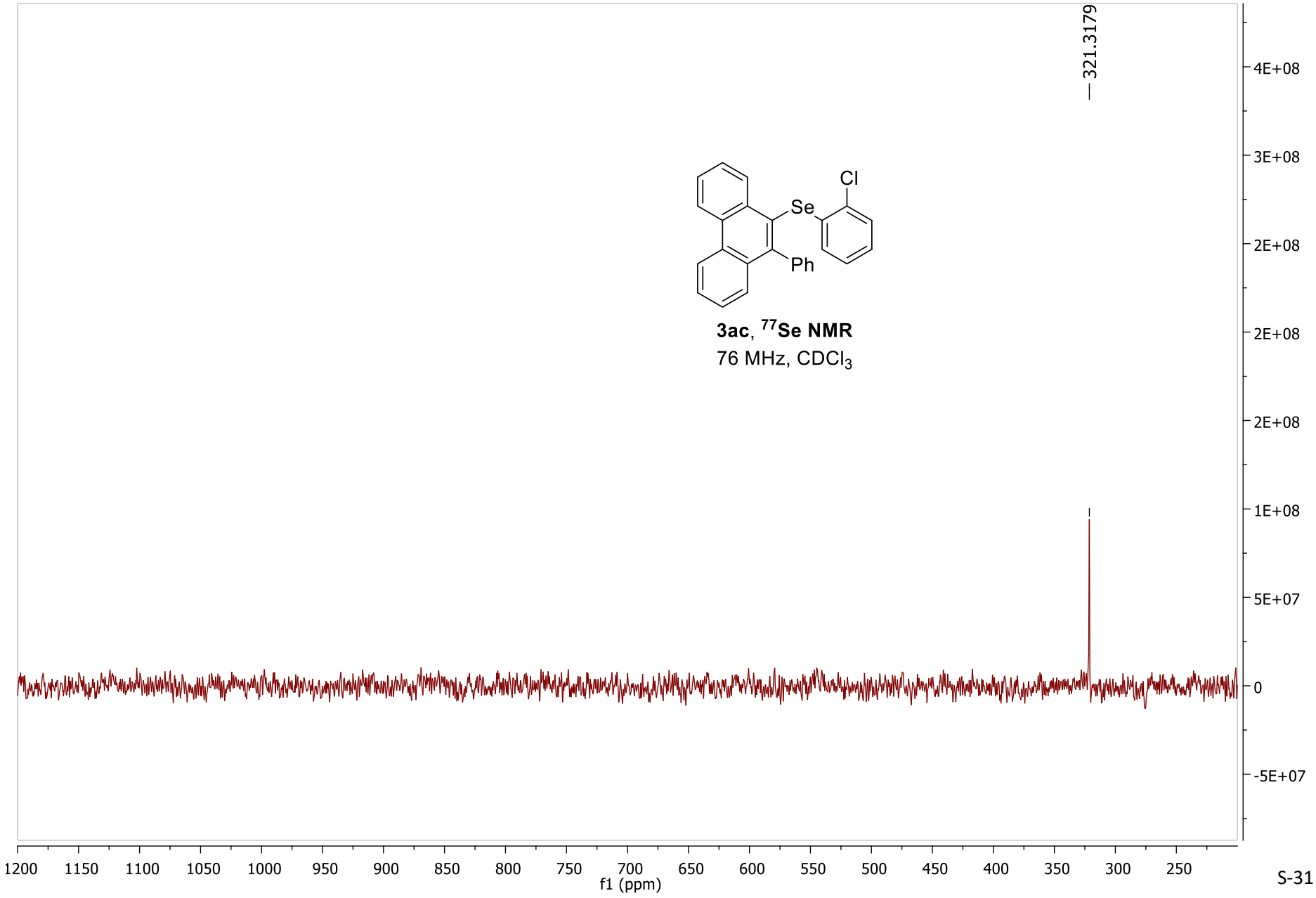
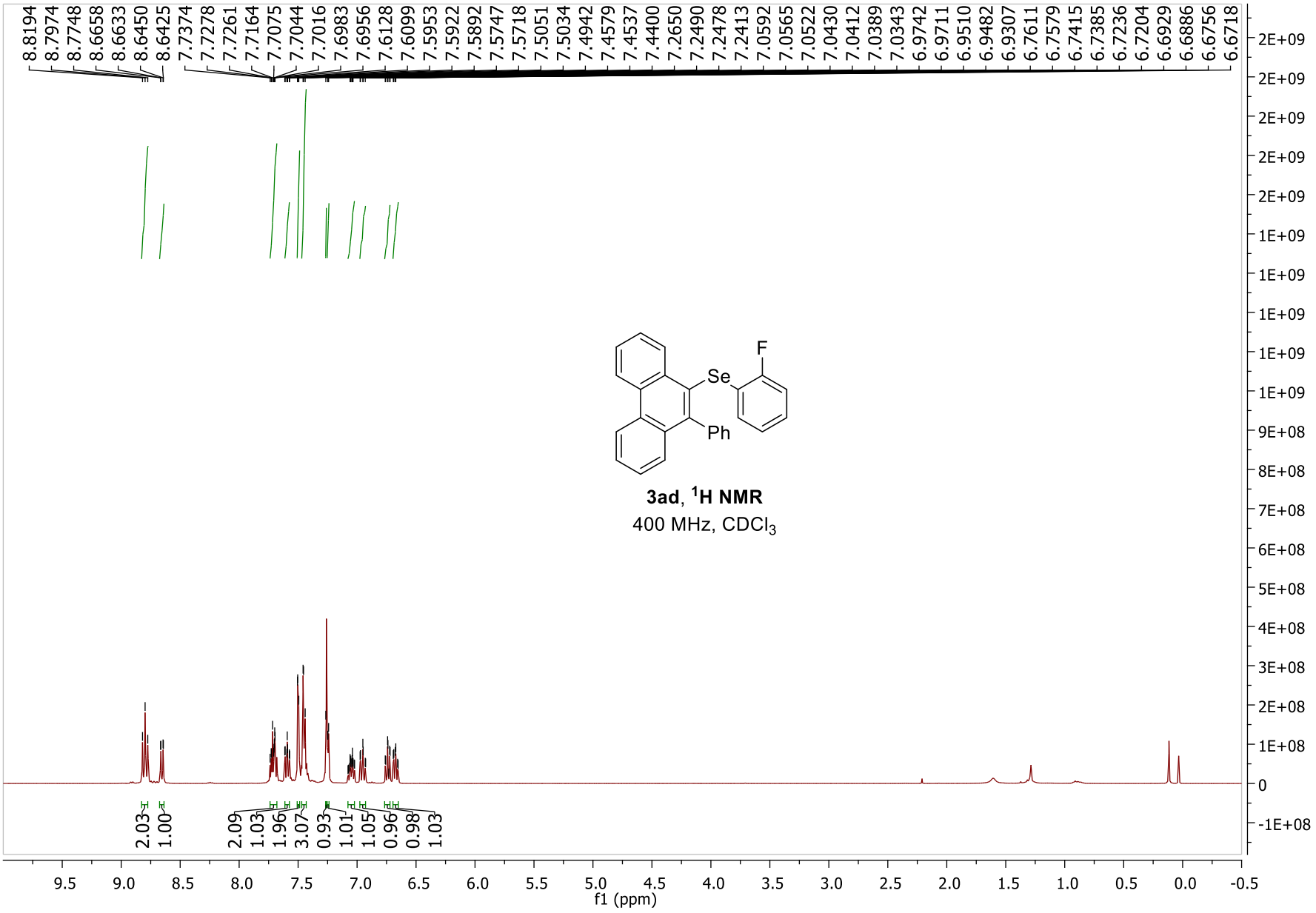
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

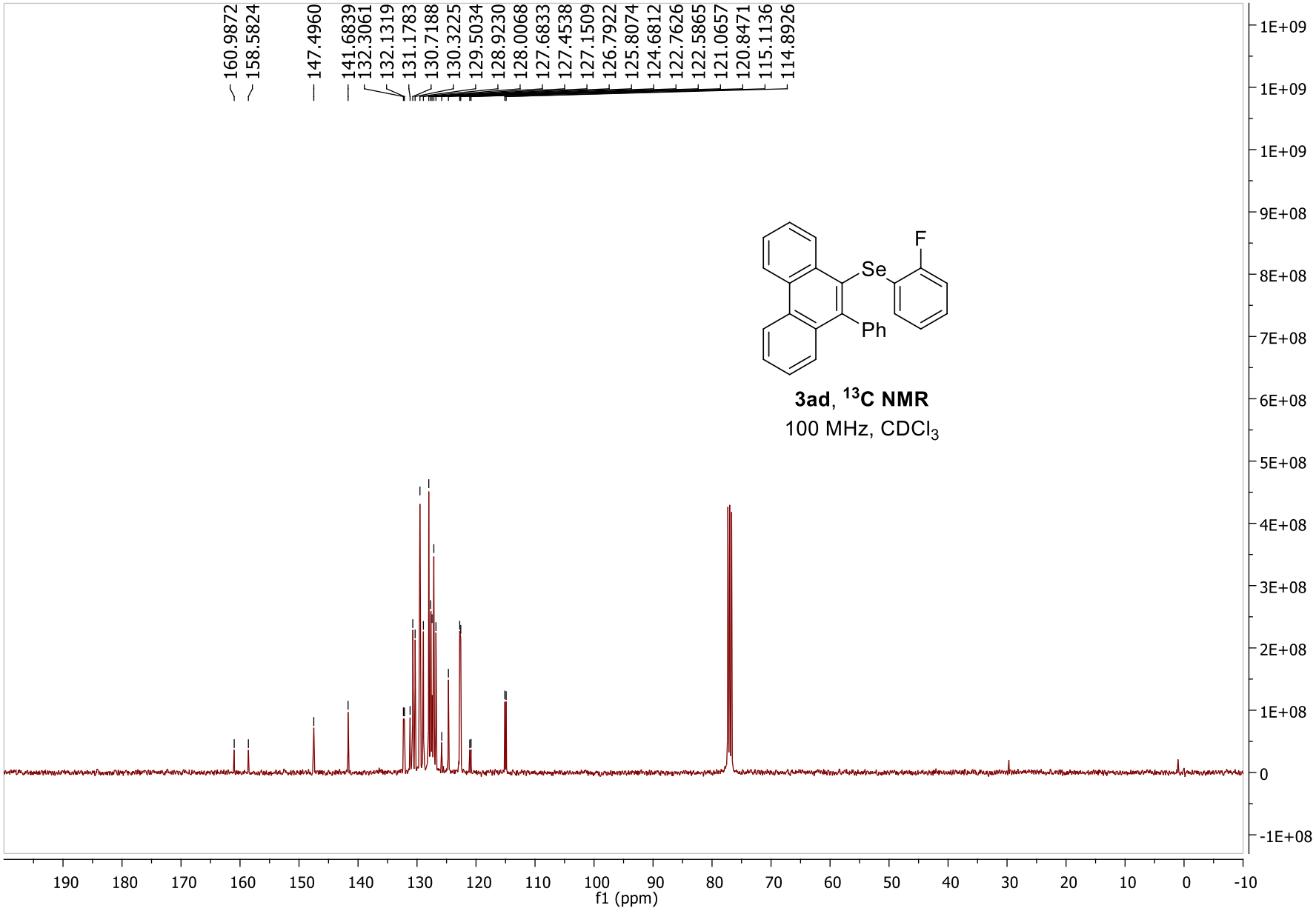

147.6255
141.5472
134.6748
132.3144
132.1217
132.0876
131.2051
130.7043
130.2697
129.4533
129.2523
129.0668
128.9688
127.9844
127.7615
127.6942
127.4403
127.1886
127.0420
126.7711
126.7050
126.1995
122.7398
122.5576
Cl
Se
Ph
3ac, 13C NMR
100 MHz, CDCl3
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

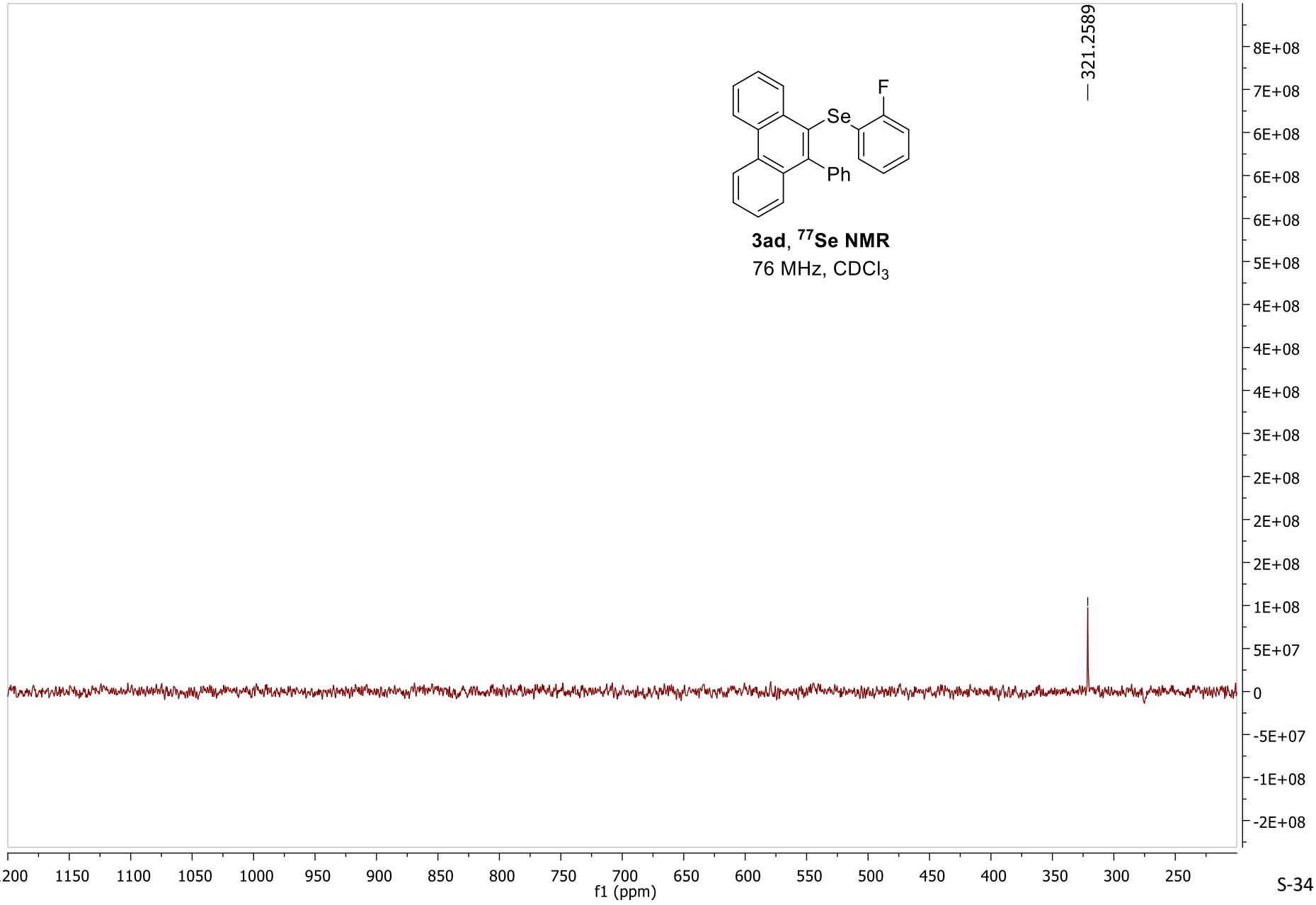

321.3179
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
Cl
Se
Ph
3ac, 77Se NMR
76 MHz, CDCl3
1200
1150
1100
1050
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
f1 (ppm)

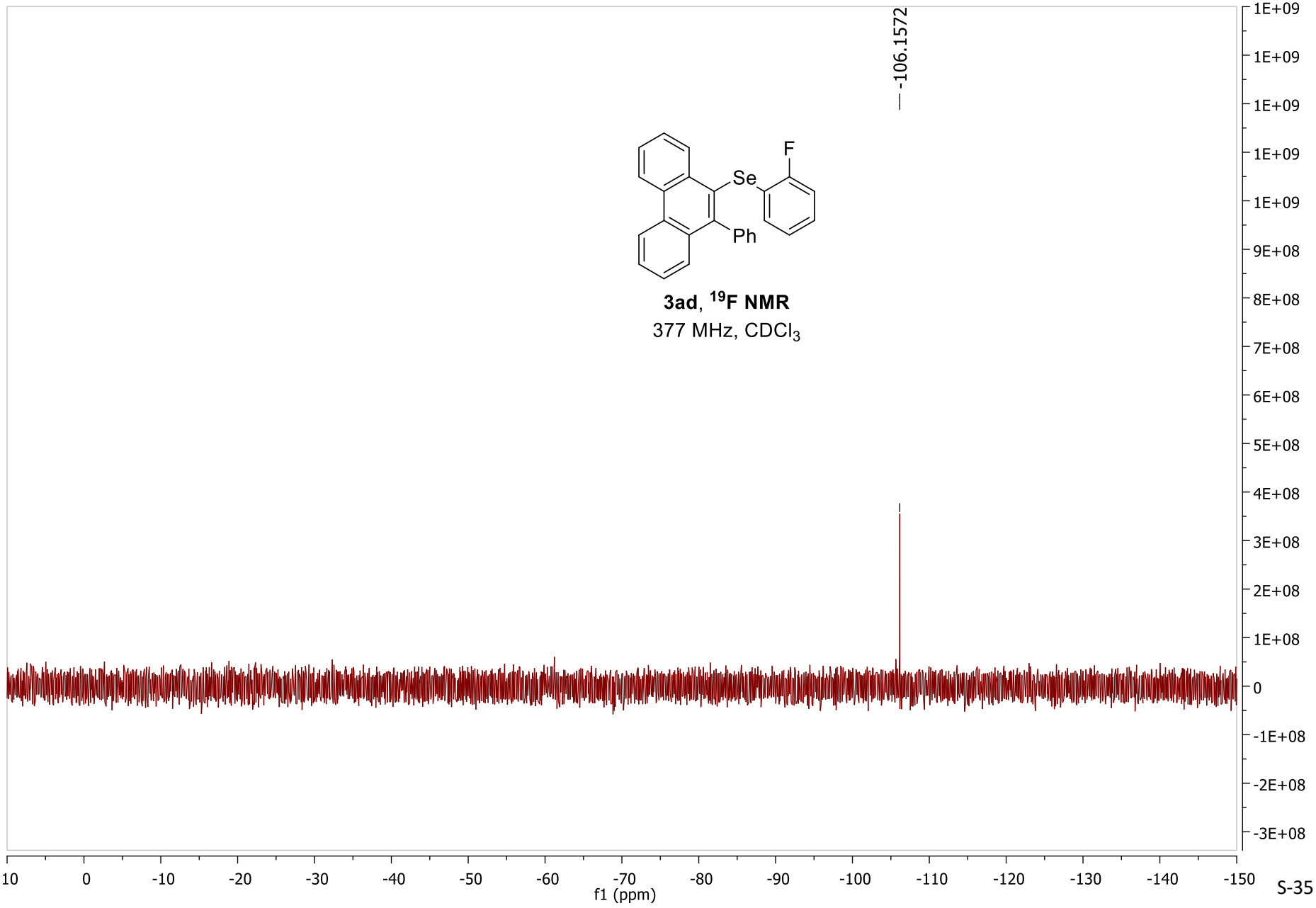


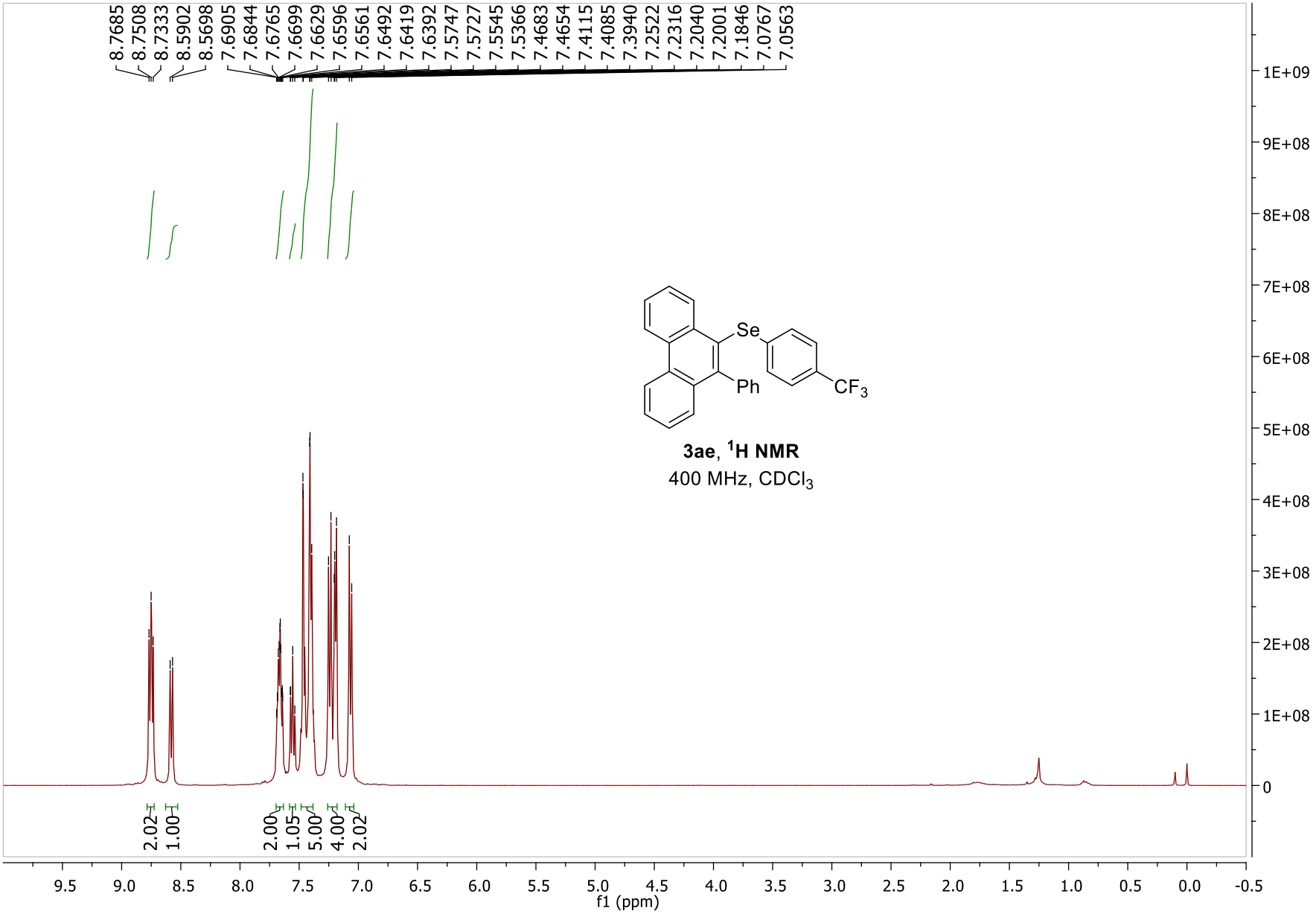

**3ad**, **$^{1}$H NMR**

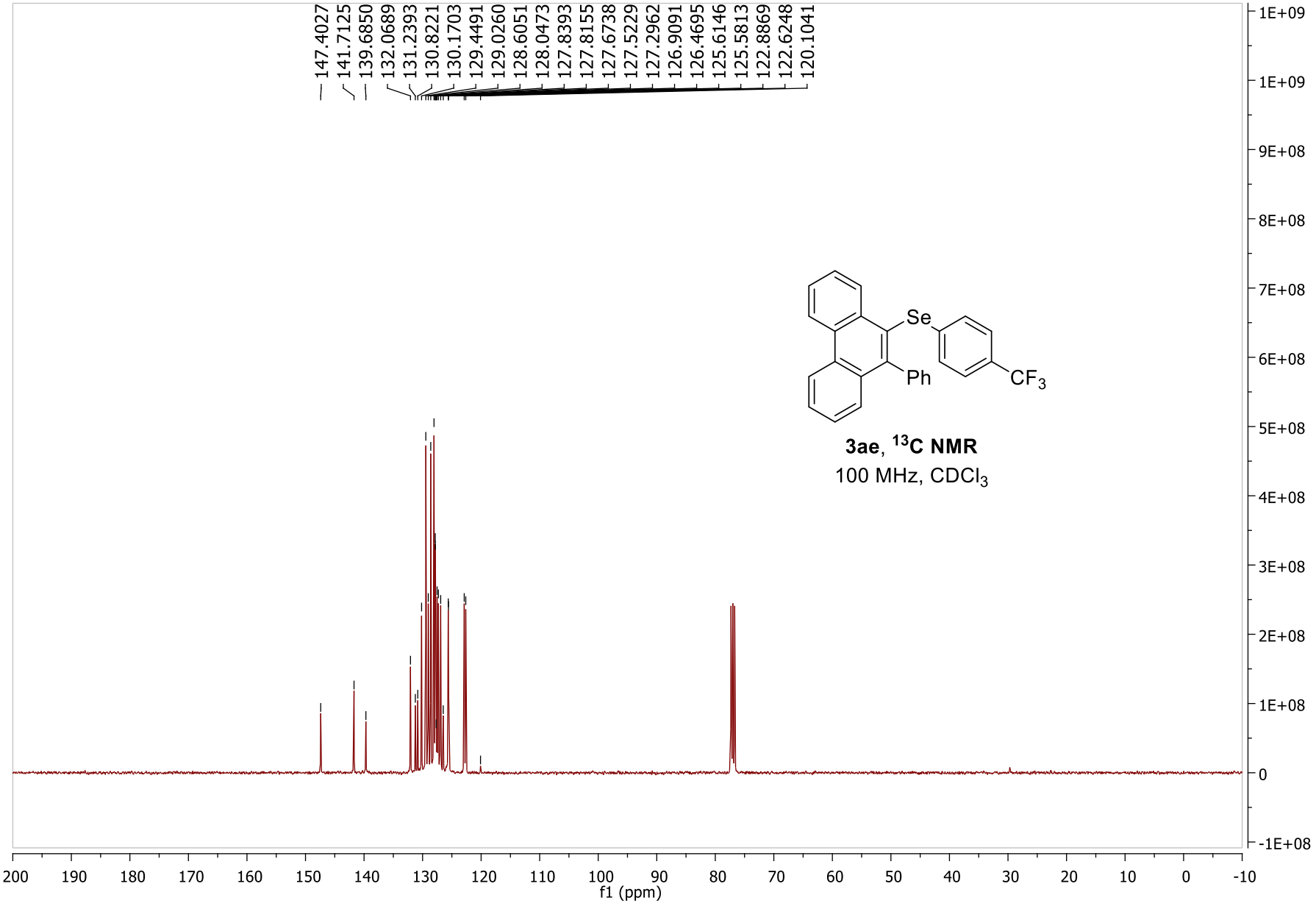
400 MHz, $CDCl_3$

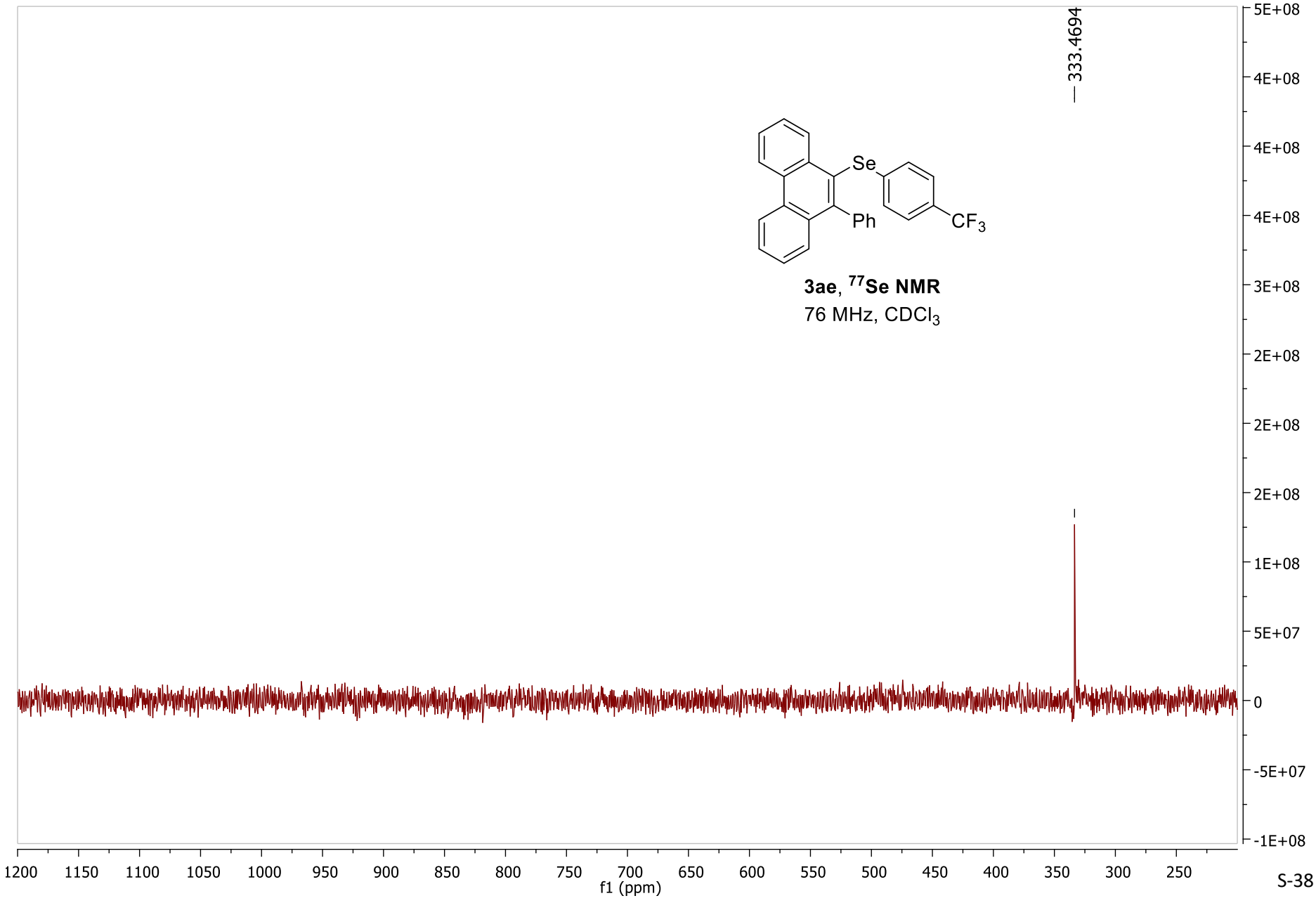

160.9872
158.5824
147.4960
141.6839
132.3061
132.1319
131.1783
130.7188
130.3225
129.5034
128.9230
128.0068
127.6833
127.4538
127.1509
126.7922
125.8074
124.6812
122.7626
122.5865
121.0657
120.8471
115.1136
114.8926
F
Se
Ph
3ad, 13C NMR
100 MHz, CDCl3
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

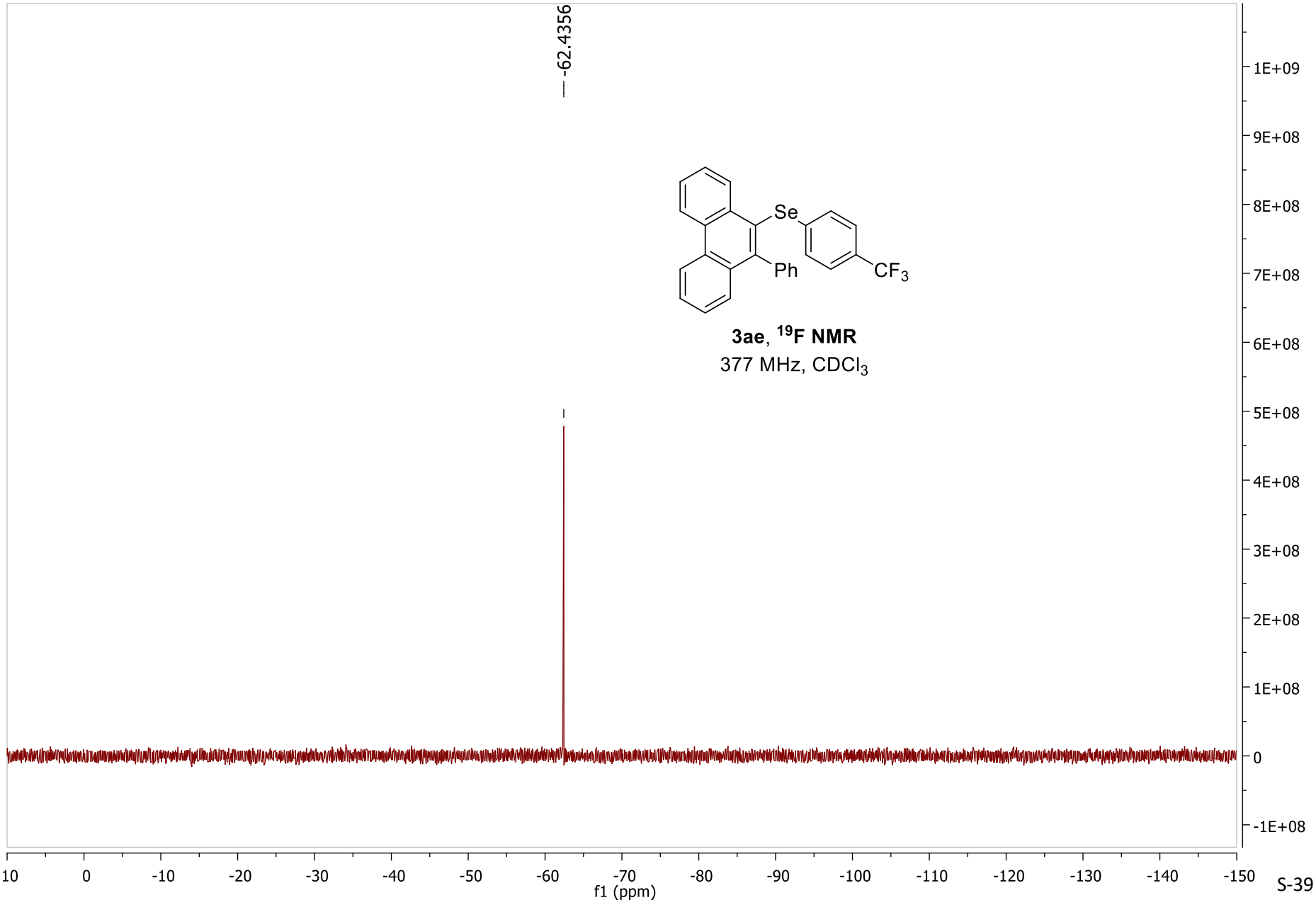

321.2589
F
Se
Ph
3ad, 77Se NMR
76 MHz, CDCl3
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


-106.1572
F
Se
Ph
3ad, 19F NMR
377 MHz, CDCl3
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
-2E+08
-3E+08
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)


8.7685
8.7508
8.7333
8.5902
8.5698
7.6905
7.6844
7.6765
7.6699
7.6629
7.6596
7.6561
7.6492
7.6419
7.6392
7.5747
7.5727
7.5545
7.5366
7.4683
7.4654
7.4115
7.4085
7.3940
7.2522
7.2316
7.2040
7.2001
7.1846
7.0767
7.0563
Se
Ph
CF3
3ae, 1H NMR
400 MHz, CDCl3
2.02
1.00
2.00
1.05
5.00
4.00
2.02
f1 (ppm)


147.4027
141.7125
139.6850
132.0689
131.2393
130.8221
130.1703
129.4491
129.0260
128.6051
128.0473
127.8393
127.8155
127.6738
127.5229
127.2962
126.9091
126.4695
125.6146
125.5813
122.8869
122.6248
120.1041
Se
Ph
CF3
3ae, 13C NMR
100 MHz, CDCl3
f1 (ppm)


333.4694
Se
Ph
CF3
3ae, 77Se NMR
76 MHz, CDCl3
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


-62.4356
Se
Ph
CF3
3ae, 19F NMR
377 MHz, CDCl3
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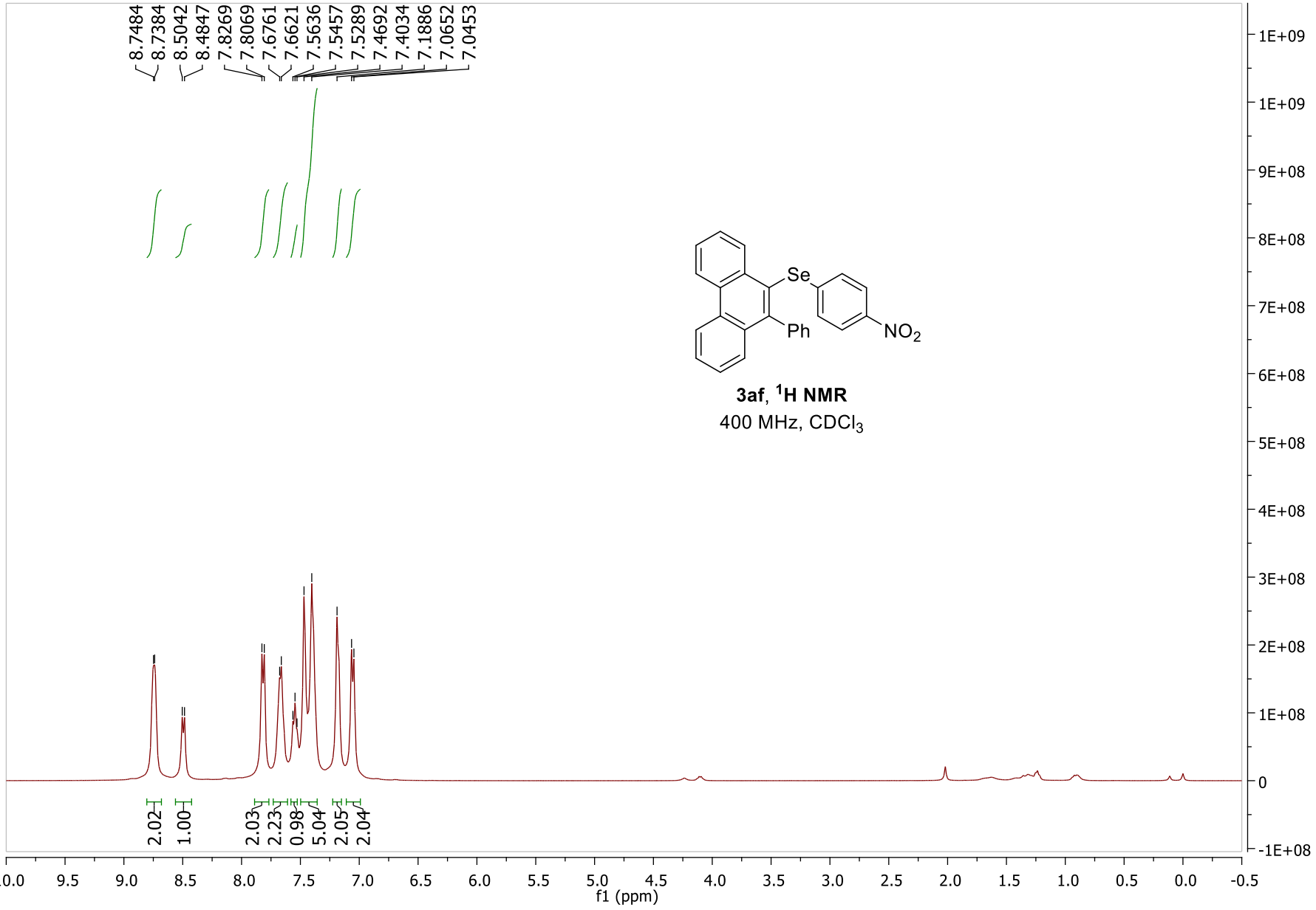
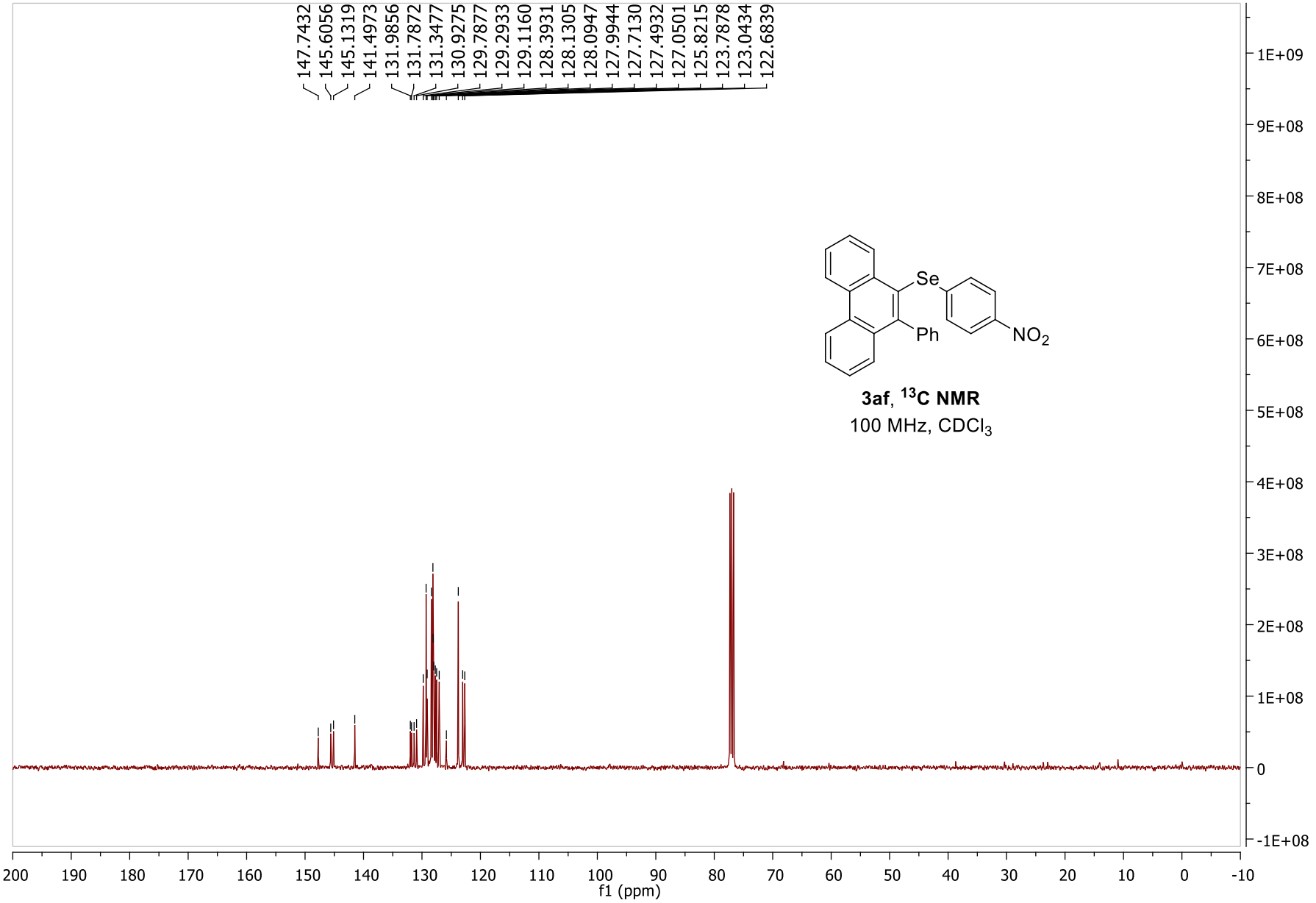
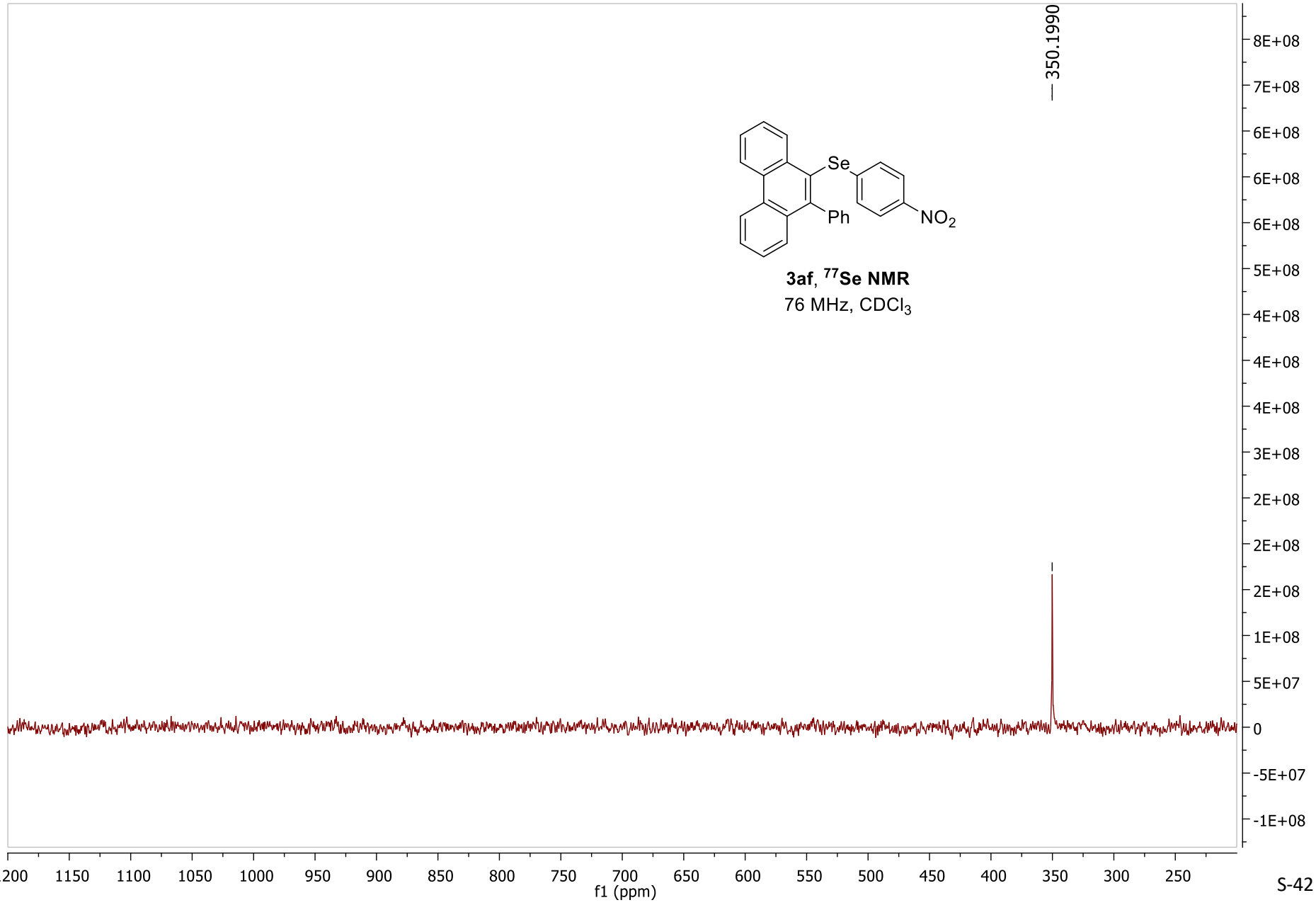
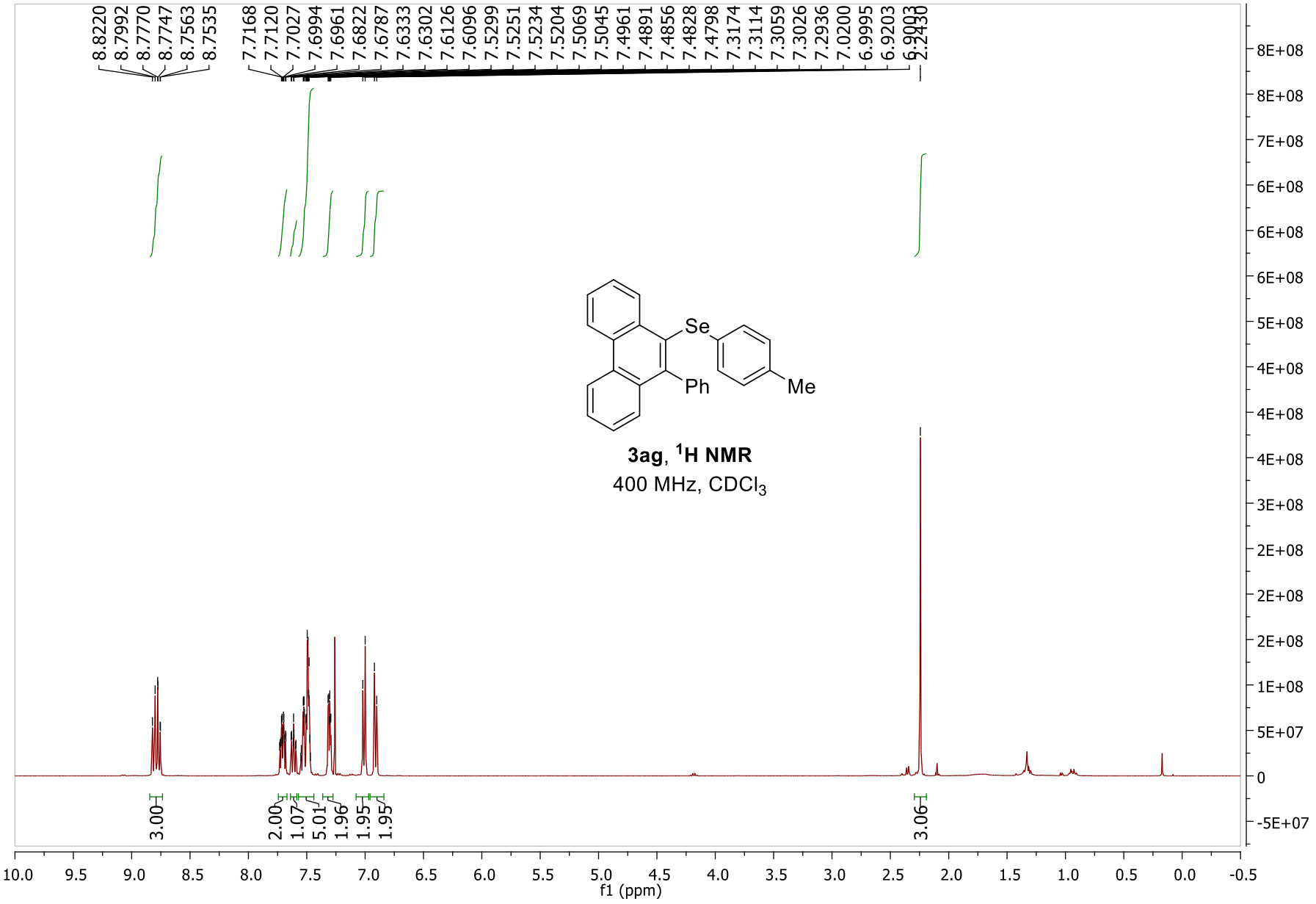
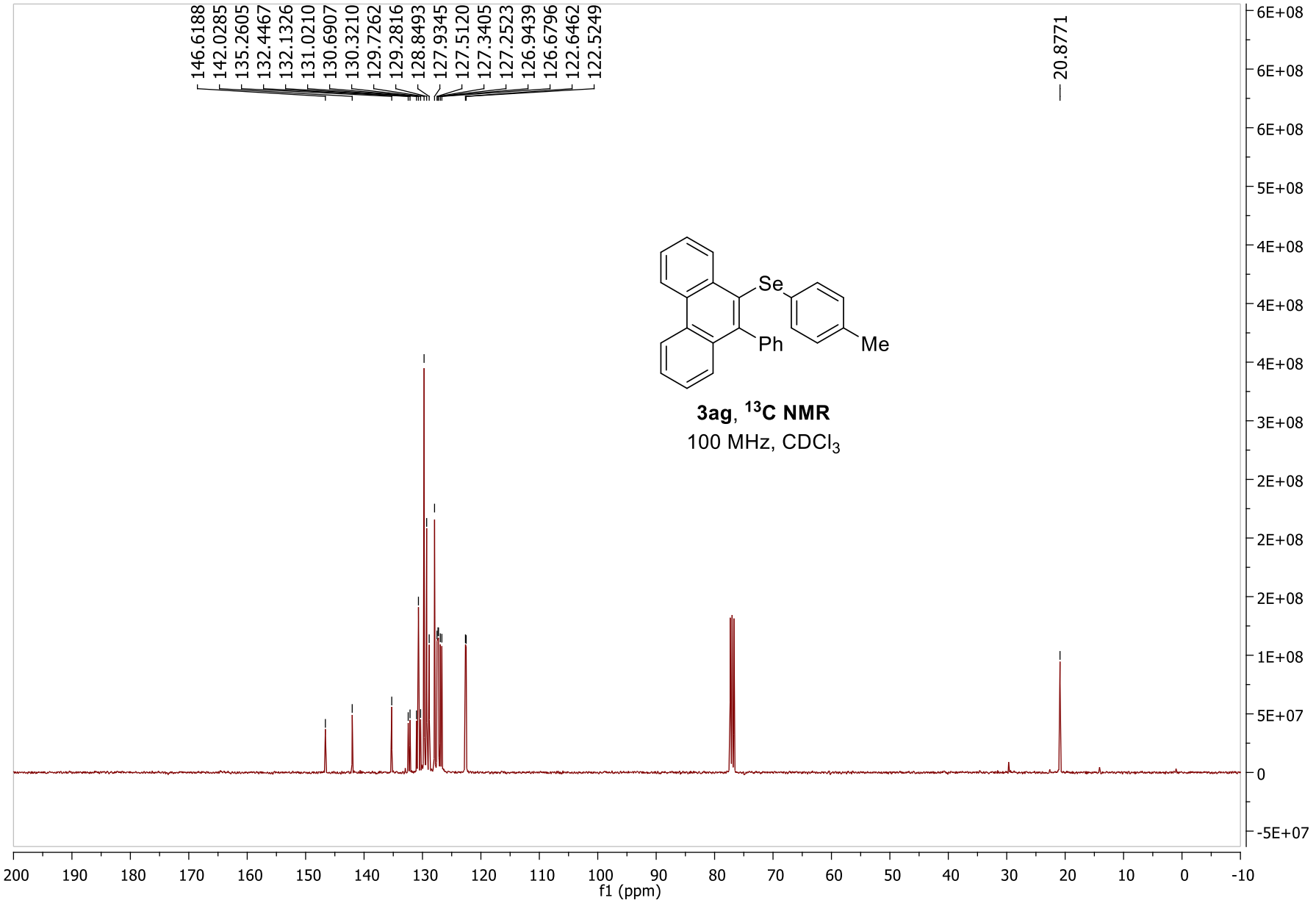
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

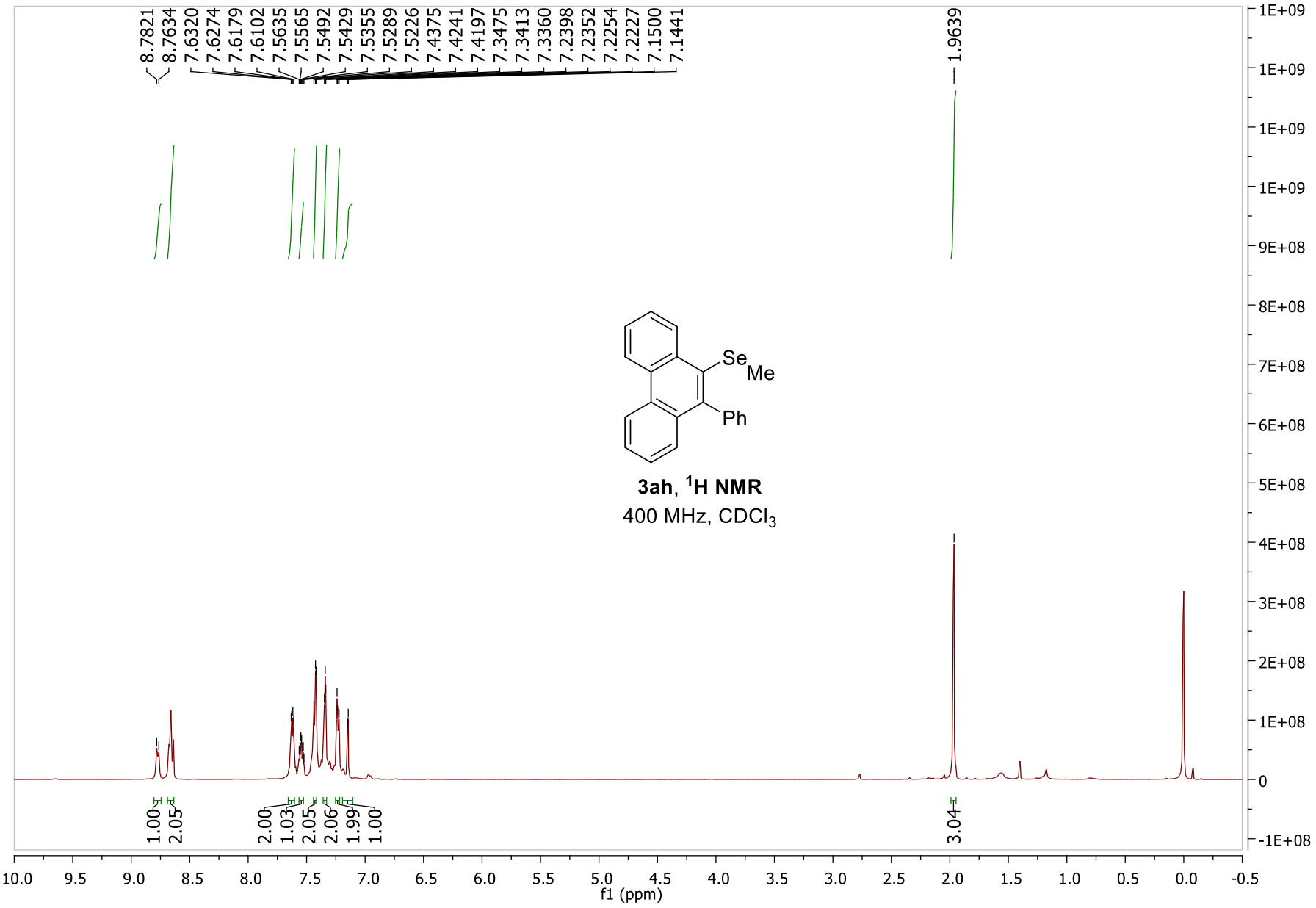

8.7484
8.7384
8.5042
8.4847
7.8269
7.8069
7.6761
7.6621
7.5636
7.5457
7.5289
7.4692
7.4034
7.1886
7.0652
7.0453
Se
Ph
NO2
3af, 1H NMR
400 MHz, CDCl3
2.02
1.00
2.03
2.23
0.98
5.04
2.05
2.04
f1 (ppm)

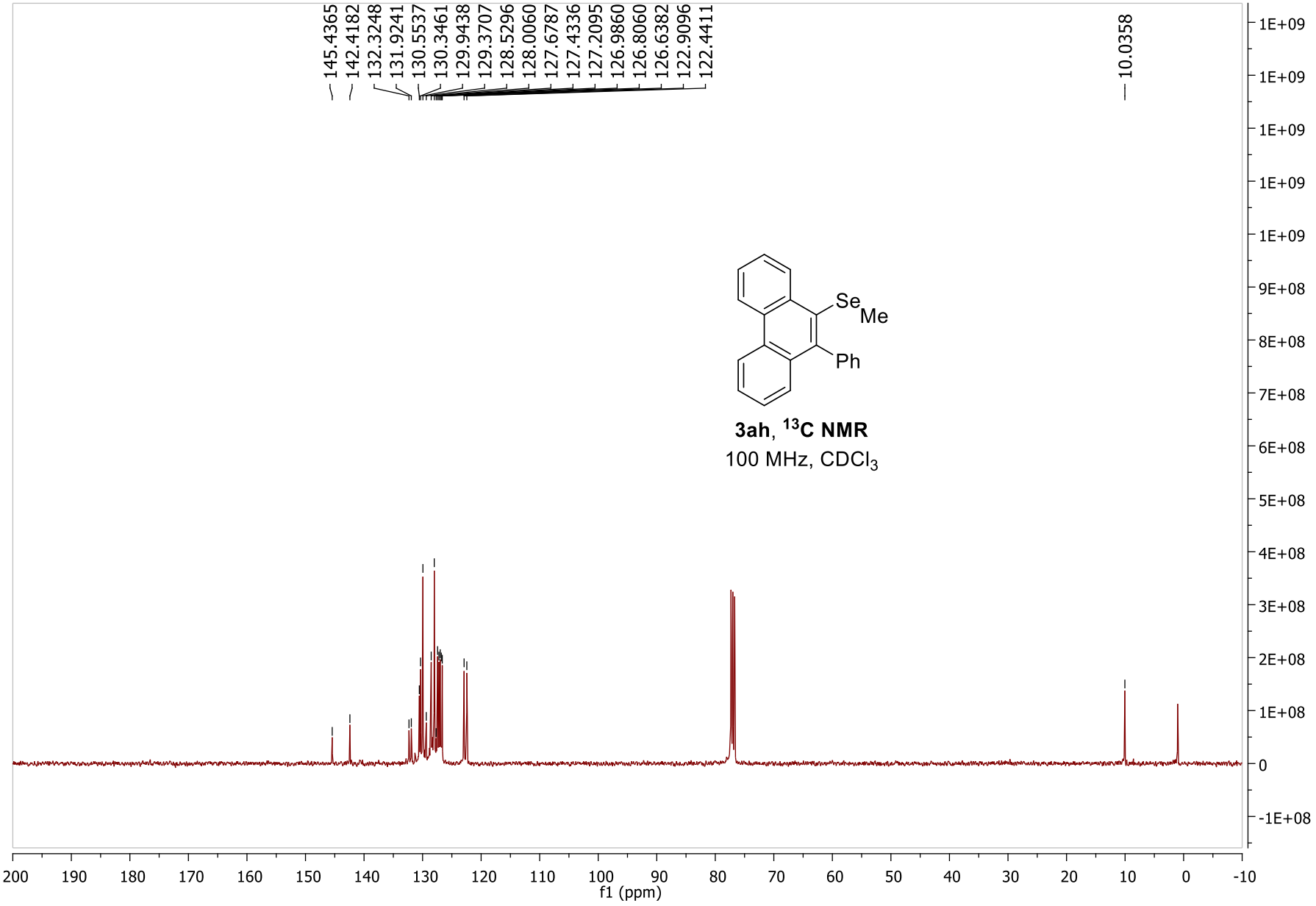

147.7432
145.6056
145.1319
141.4973
131.9856
131.7872
131.3477
130.9275
129.7877
129.2933
129.1160
128.3931
128.1305
128.0947
127.9944
127.7130
127.4932
127.0501
125.8215
123.7878
123.0434
122.6839
Se
Ph
NO2
3af, 13C NMR
100 MHz, CDCl3
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


350.1990
Se
Ph
NO2
3af, 77Se NMR
76 MHz, CDCl3
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


8.8220
8.7992
8.7770
8.7747
8.7563
8.7535
7.7168
7.7120
7.7027
7.6994
7.6961
7.6822
7.6787
7.6333
7.6302
7.6126
7.6096
7.5299
7.5251
7.5234
7.5204
7.5069
7.5045
7.4961
7.4891
7.4856
7.4828
7.4798
7.3174
7.3114
7.3059
7.3026
7.2936
7.0200
6.9995
6.9203
6.9003
2.2430
Se
Ph
Me
3ag, 1H NMR
400 MHz, CDCl3
3.00
2.00
1.07
5.01
1.96
1.95
1.95
3.06
f1 (ppm)

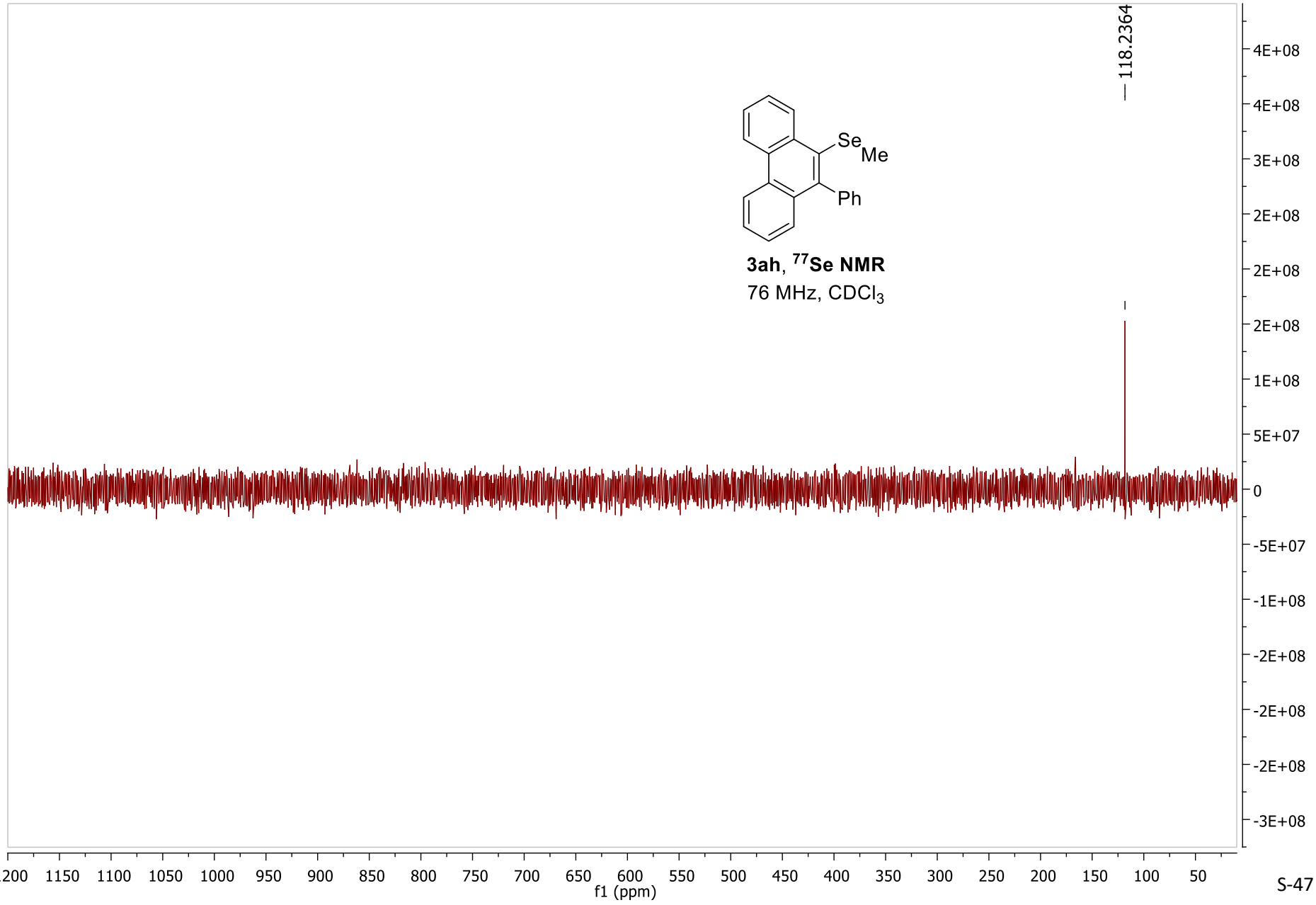

146.6188
142.0285
135.2605
132.4467
132.1326
131.0210
130.6907
130.3210
129.7262
129.2816
128.8493
127.9345
127.5120
127.3405
127.2523
126.9439
126.6796
122.6462
122.5249
20.8771
Se
Ph
Me
3ag, 13C NMR
100 MHz, CDCl3
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

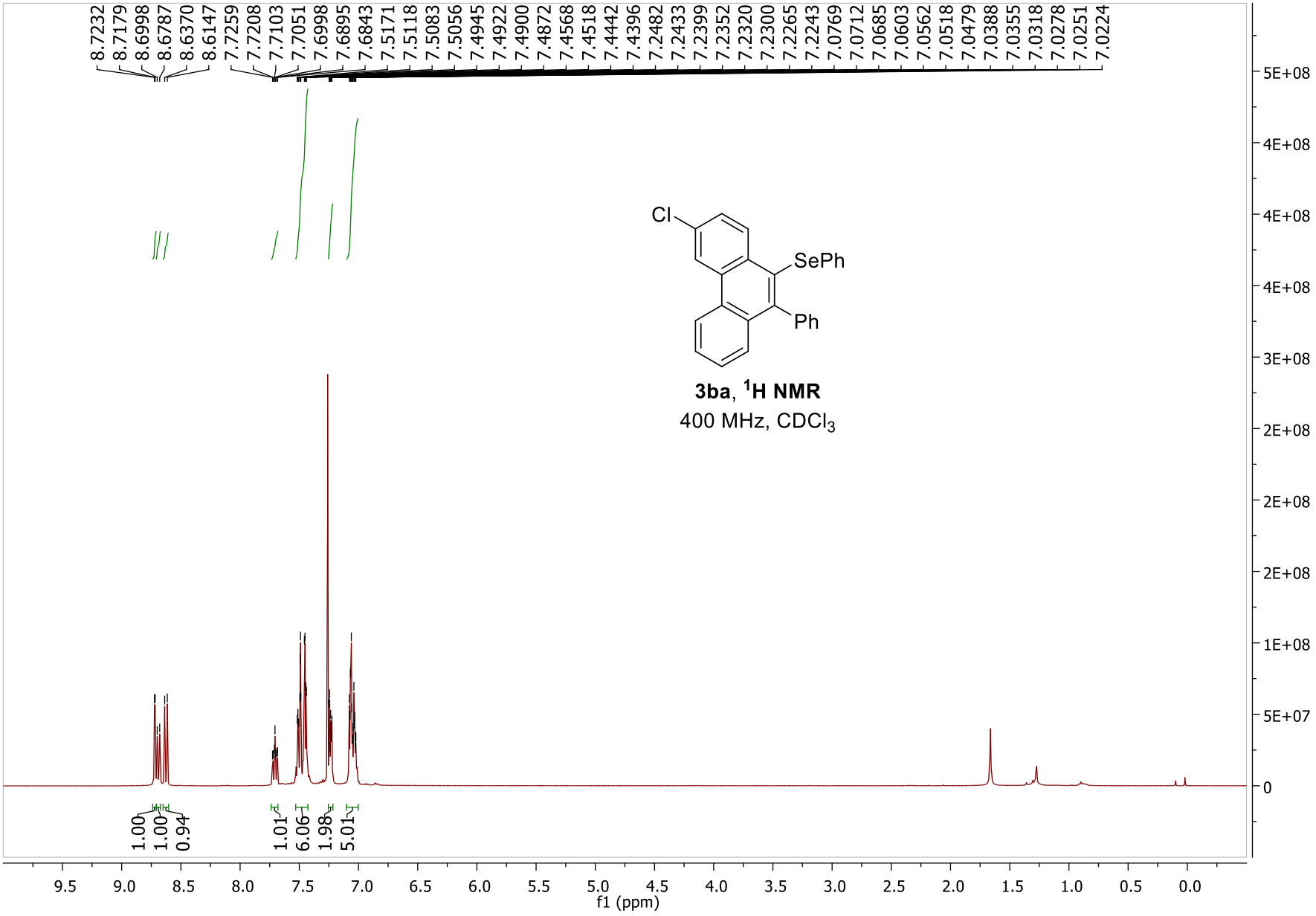

8.7821
8.7634
7.6320
7.6274
7.6179
7.6102
7.5635
7.5565
7.5492
7.5429
7.5355
7.5289
7.5226
7.4375
7.4241
7.4197
7.3475
7.3413
7.3360
7.2398
7.2352
7.2254
7.2227
7.1500
7.1441
1.9639
Se
Me
Ph
3ah, 1H NMR
400 MHz, CDCl3
1.00
2.05
2.00
1.03
2.05
2.06
1.99
1.00
3.04
f1 (ppm)

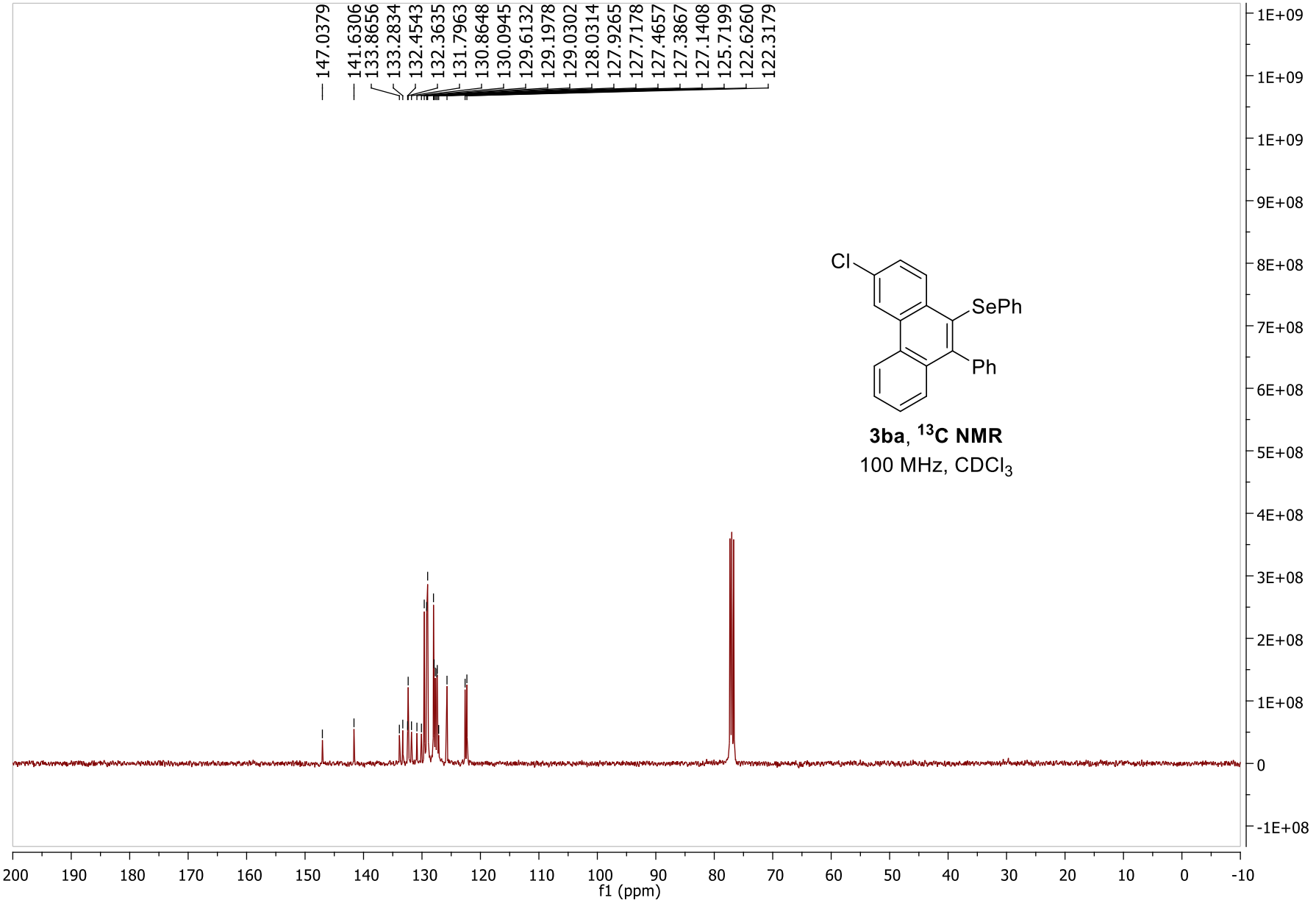


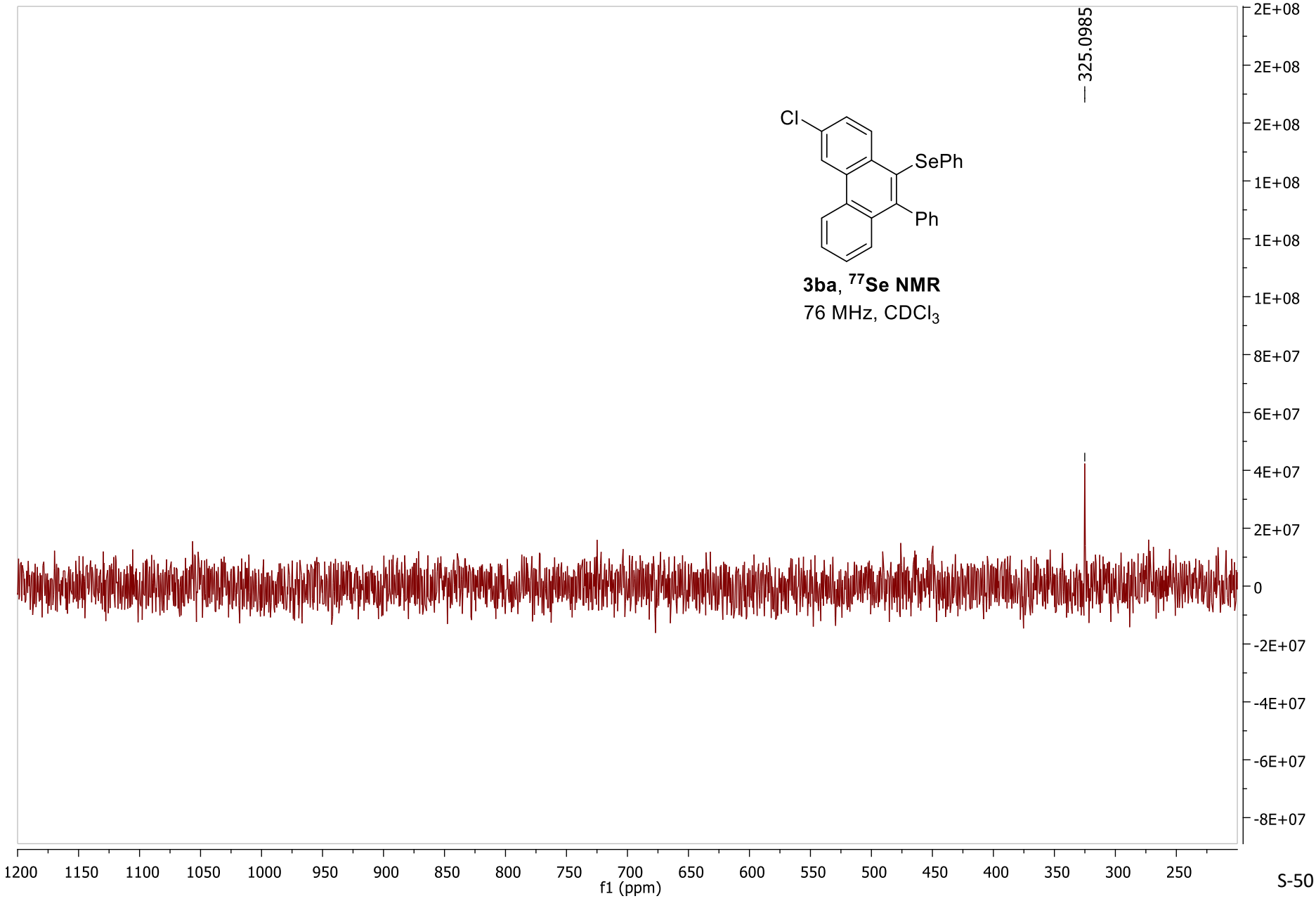

**3ah**, **$^{13}$C NMR**

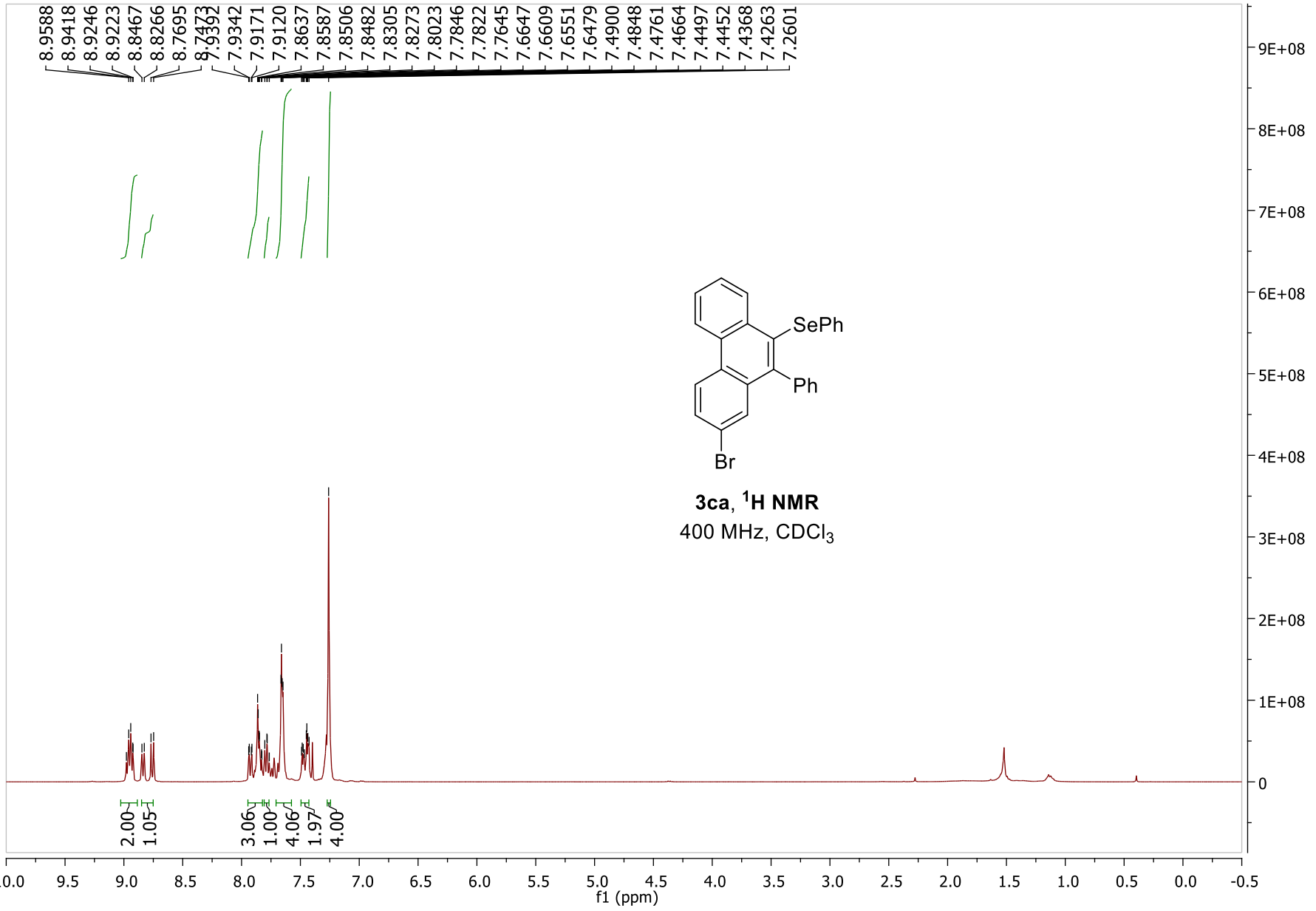
100 MHz, $CDCl_3$

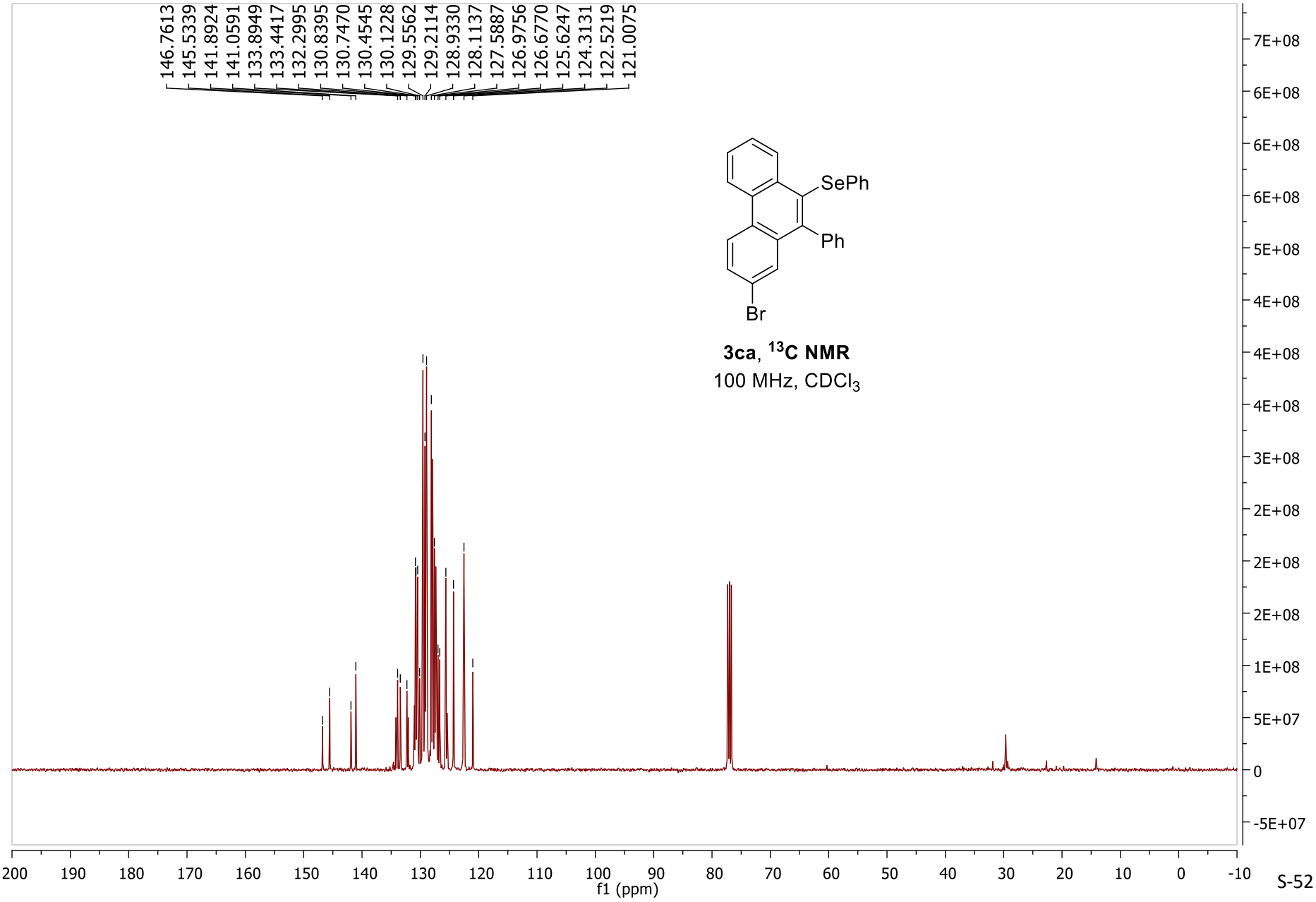

118.2364
Se
Me
Ph
3ah, 77Se NMR
76 MHz, CDCl3
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
-2E+08
-2E+08
-3E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50
f1 (ppm)

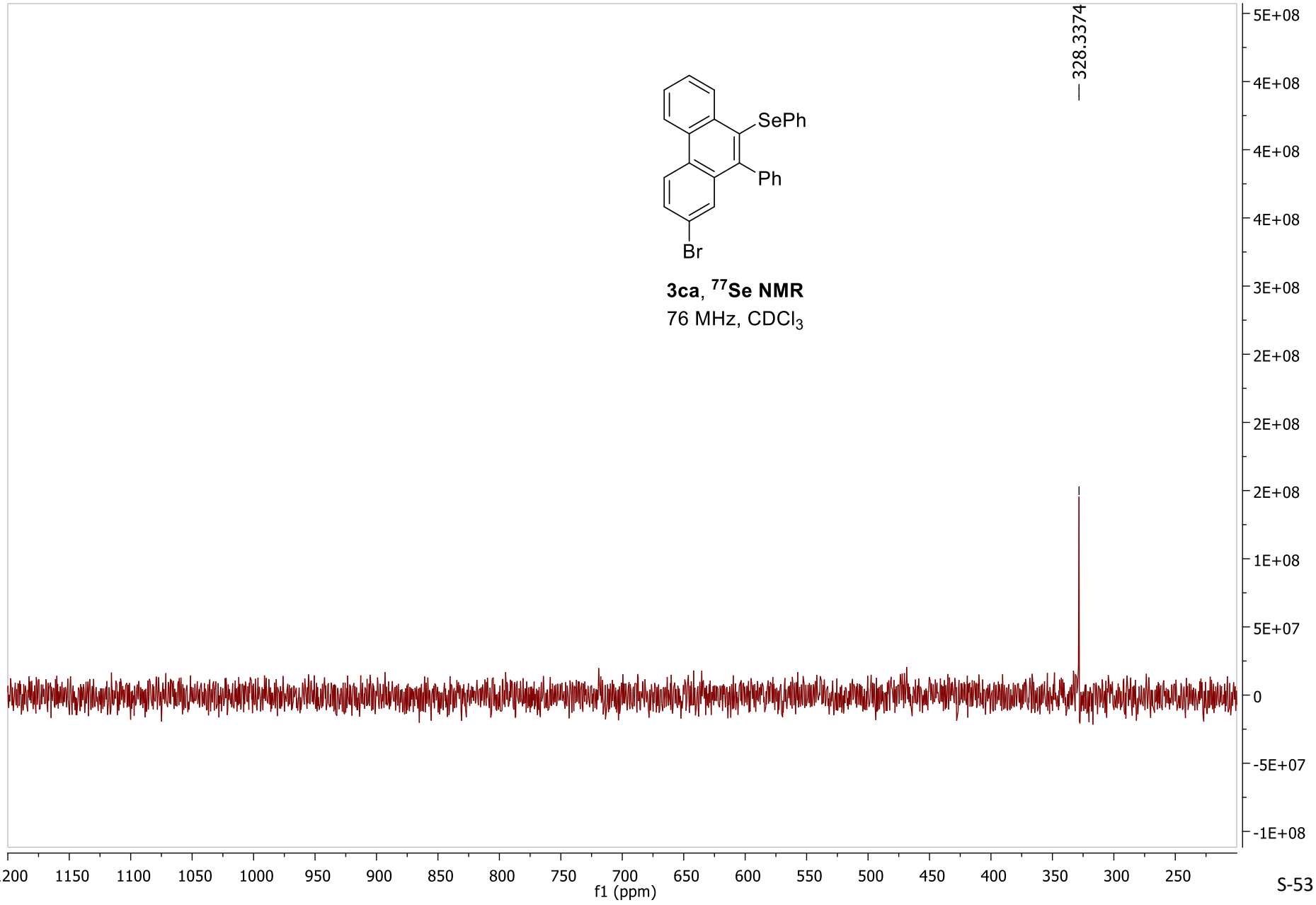

8.7232
8.7179
8.6998
8.6787
8.6370
8.6147
7.7259
7.7208
7.7103
7.7051
7.6998
7.6895
7.6843
7.5171
7.5118
7.5083
7.5056
7.4945
7.4922
7.4900
7.4872
7.4568
7.4518
7.4442
7.4396
7.2482
7.2433
7.2399
7.2352
7.2320
7.2300
7.2265
7.2243
7.0769
7.0712
7.0685
7.0603
7.0562
7.0518
7.0479
7.0388
7.0355
7.0318
7.0278
7.0251
7.0224
Cl
SePh
Ph
3ba, 1H NMR
400 MHz, CDCl3
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
1.00
0.94
1.01
6.06
1.98
5.01
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
f1 (ppm)


147.0379
141.6306
133.8656
133.2834
132.4543
132.3635
131.7963
130.8648
130.0945
129.6132
129.1978
129.0302
128.0314
127.9265
127.7178
127.4657
127.3867
127.1408
125.7199
122.6260
122.3179
Cl
SePh
Ph
3ba, 13C NMR
100 MHz, CDCl3
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


325.0985
Cl
SePh
Ph
3ba, 77Se NMR
76 MHz, CDCl3
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
-4E+07
-6E+07
-8E+07
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


8.9588
8.9418
8.9246
8.9223
8.8467
8.8266
8.7695
7.9392
7.9342
7.9171
7.9120
7.8637
7.8587
7.8506
7.8482
7.8305
7.8273
7.8023
7.7846
7.7822
7.7645
7.6647
7.6609
7.6551
7.6479
7.4900
7.4848
7.4761
7.4664
7.4497
7.4452
7.4368
7.4263
7.2601
SePh
Ph
Br
3ca, 1H NMR
400 MHz, CDCl3
2.00
1.05
3.06
1.00
4.06
1.97
4.00
f1 (ppm)


146.7613
145.5339
141.8924
141.0591
133.8949
133.4417
132.2995
130.8395
130.7470
130.4545
130.1228
129.5562
129.2114
128.9330
128.1137
127.5887
126.9756
126.6770
125.6247
124.3131
122.5219
121.0075
SePh
Ph
Br
3ca, 13C NMR
100 MHz, CDCl3
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


328.3374
SePh
Ph
Br
3ca, 77Se NMR
76 MHz, CDCl3
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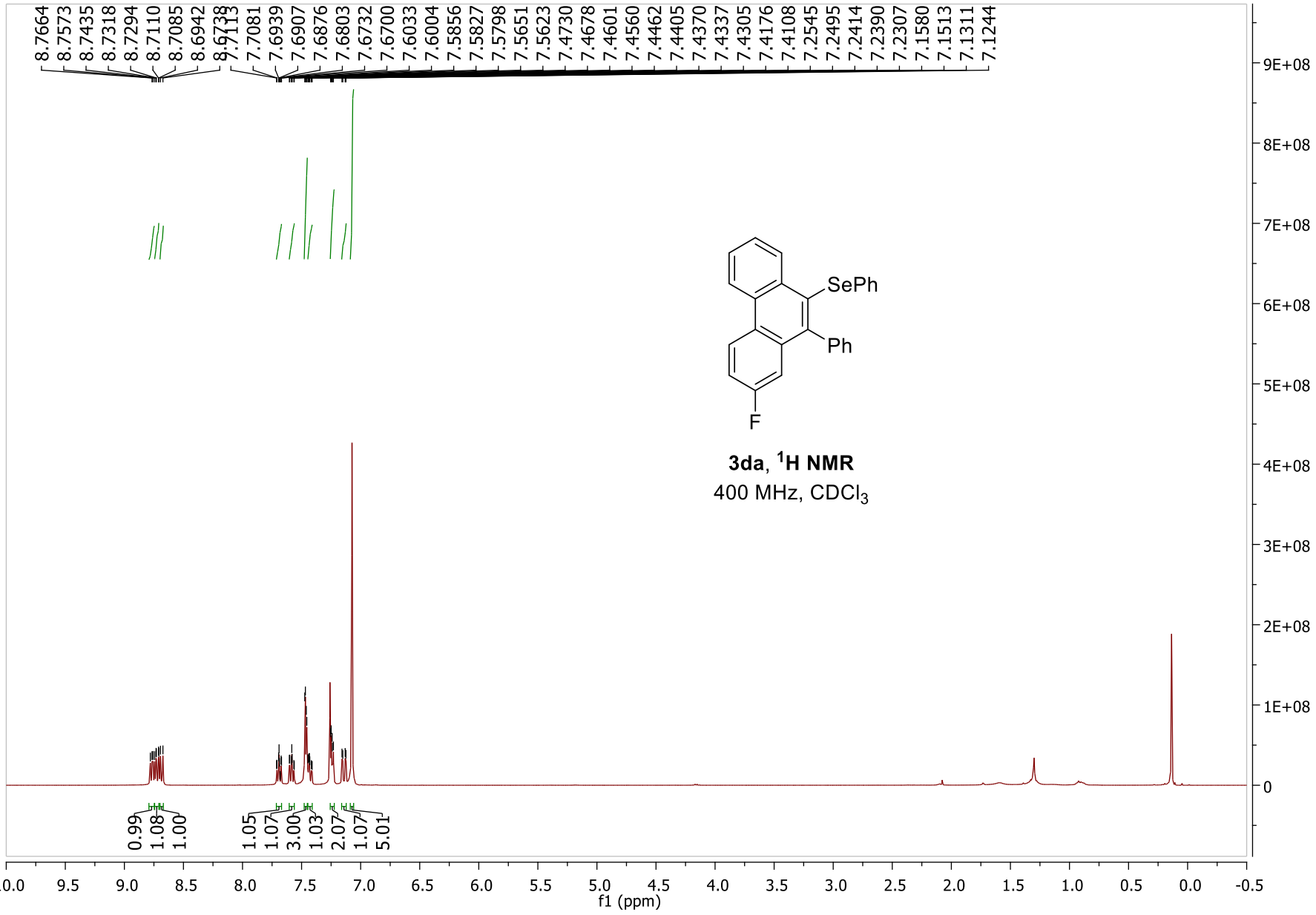
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)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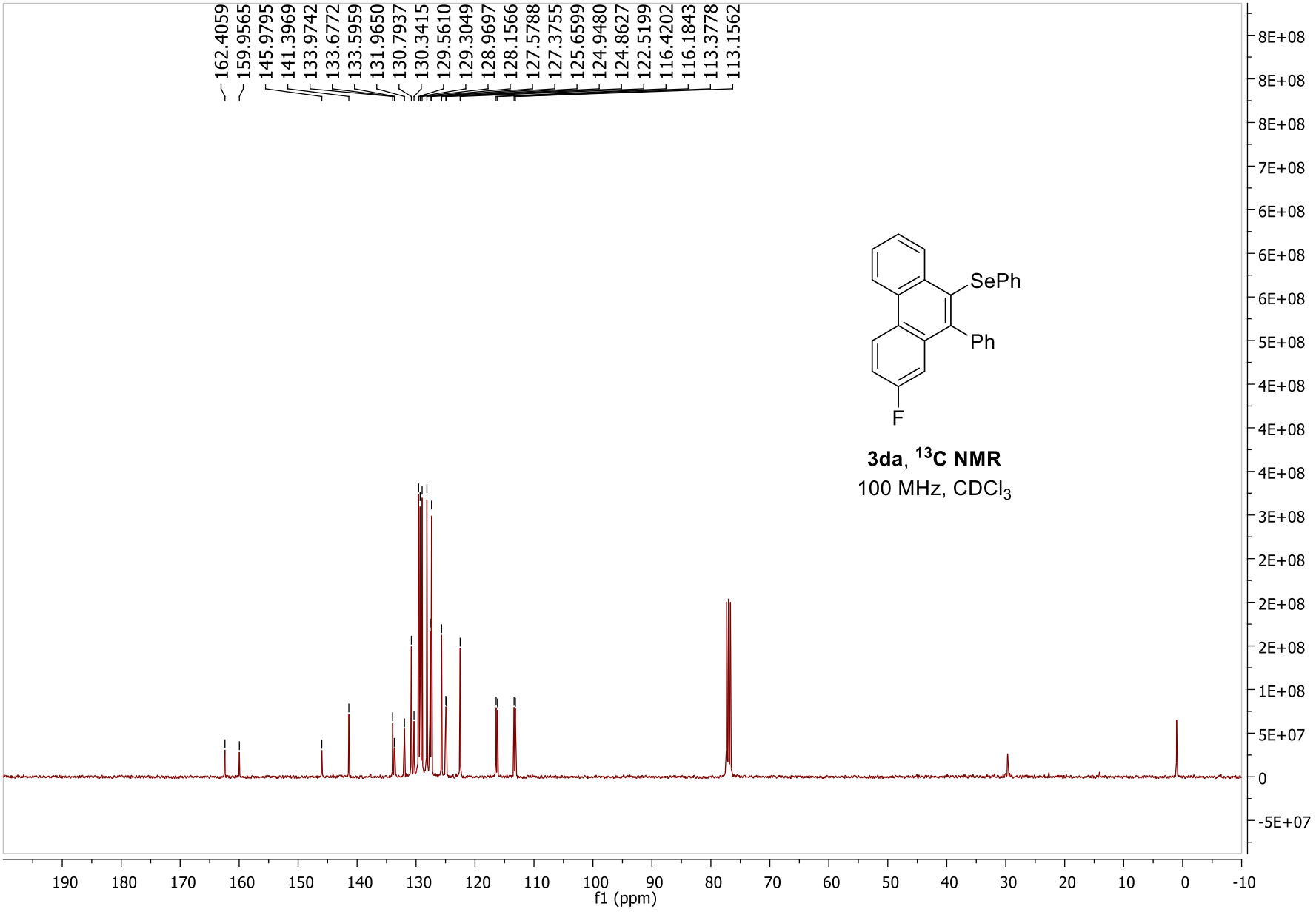
8.7573
8.7435
8.7318
8.7294
8.7110
8.7085
8.6942
8.6738
7.7113
7.7081
7.6939
7.6907
7.6876
7.6803
7.6732
7.6700
7.6033
7.6004
7.5856
7.5827
7.5798
7.5651
7.5623
7.4730
7.4678
7.4601
7.4560
7.4462
7.4405
7.4370
7.4337
7.4305
7.4176
7.4108
7.2545
7.2495
7.2414
7.2390
7.2307
7.1580
7.1513
7.1311
7.1244
SePh
Ph
F
3da, 1H NMR
400 MHz, CDCl3
0.99
1.08
1.00
1.05
1.07
3.00
1.03
2.07
1.07
5.01
f1 (ppm)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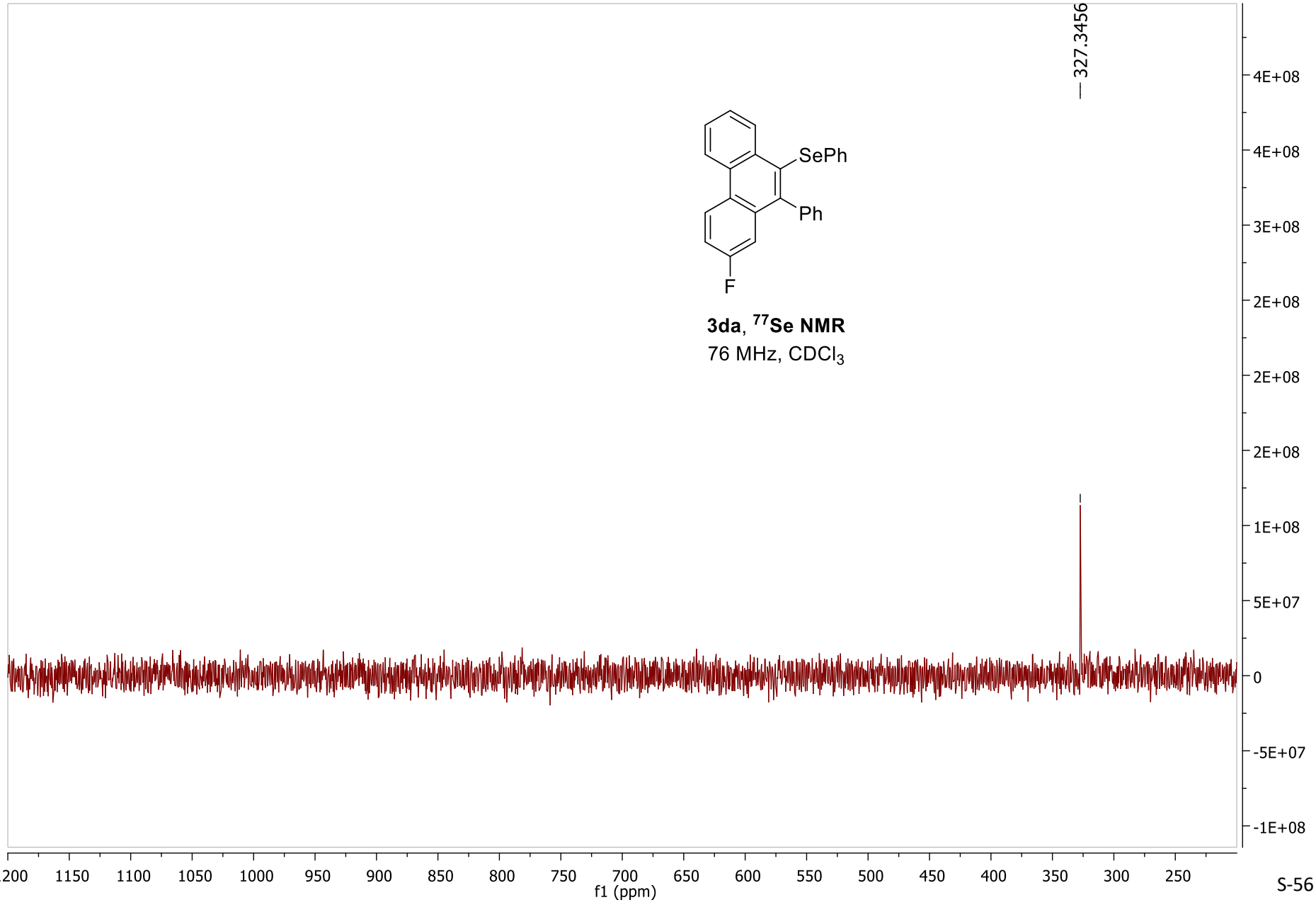
159.9565
145.9795
141.3969
133.9742
133.6772
133.5959
131.9650
130.7937
130.3415
129.5610
129.3049
128.9697
128.1566
127.5788
127.3755
125.6599
124.9480
124.8627
122.5199
116.4202
116.1843
113.3778
113.1562
SePh
Ph
F
3da, 13C NMR
100 MHz, CDCl3
8E+08
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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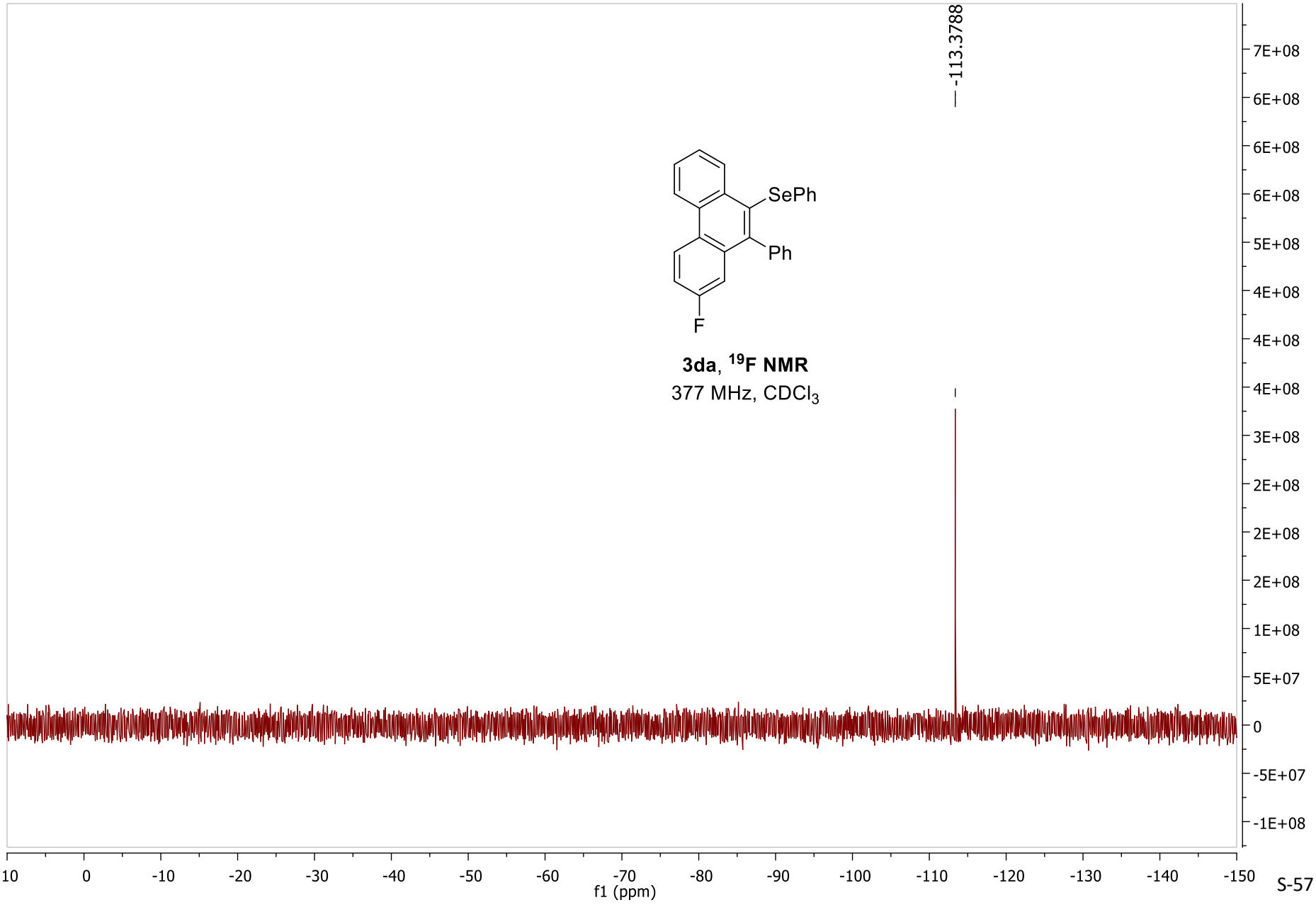
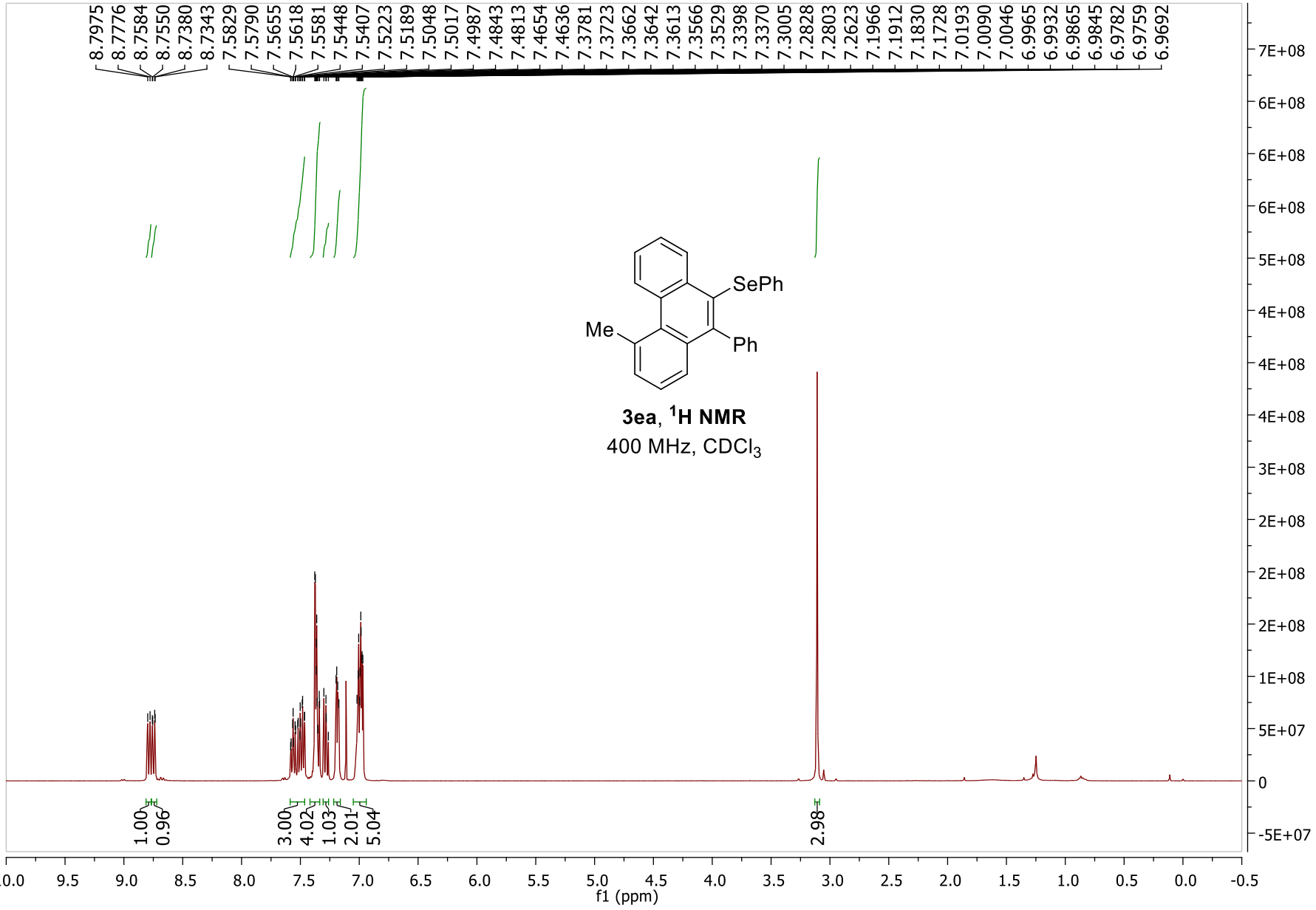
Ph
F
3da, 77Se NMR
76 MHz, CDCl3
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


-113.3788
SePh
Ph
F
3da, 19F NMR
377 MHz, CDCl3
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)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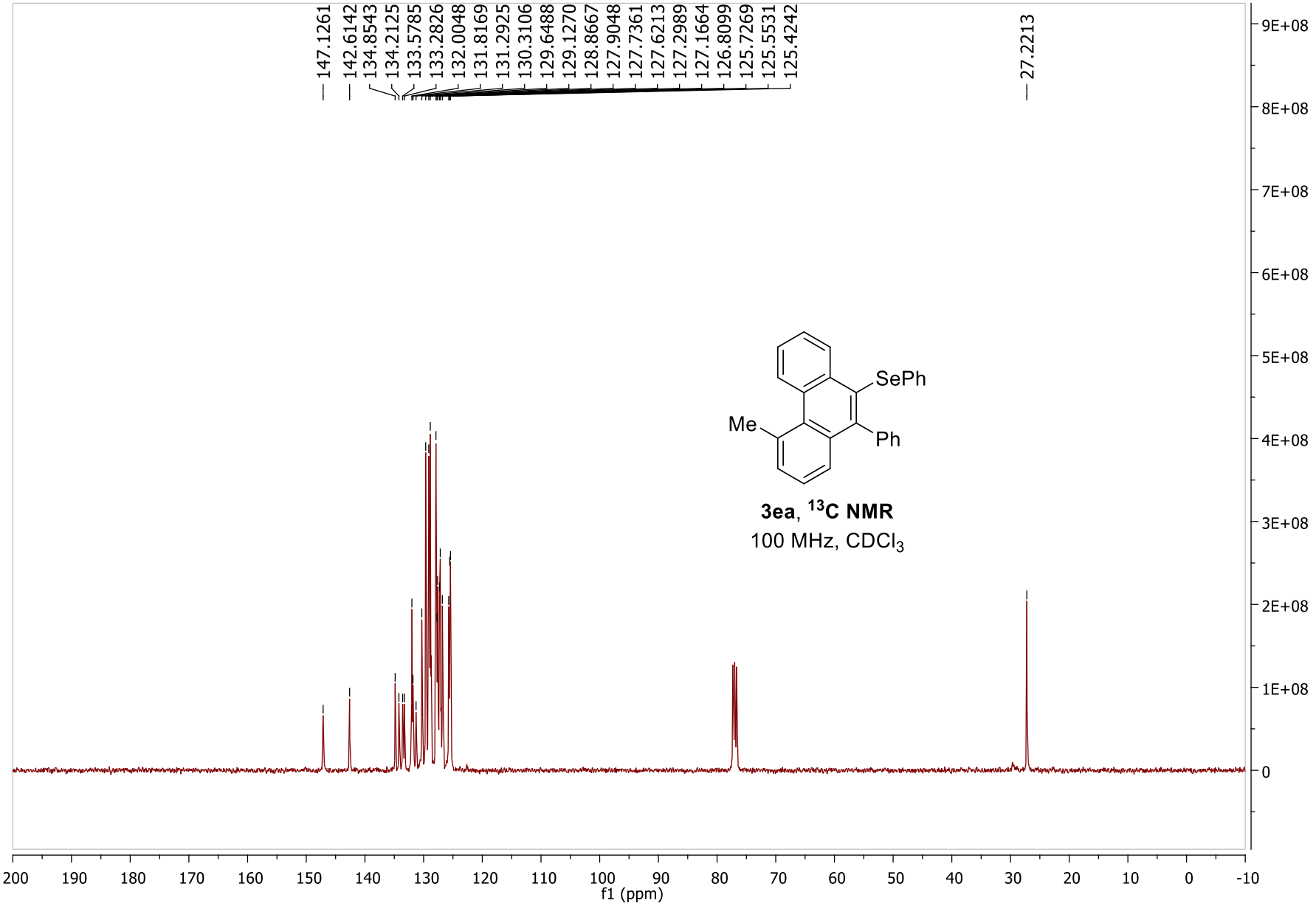
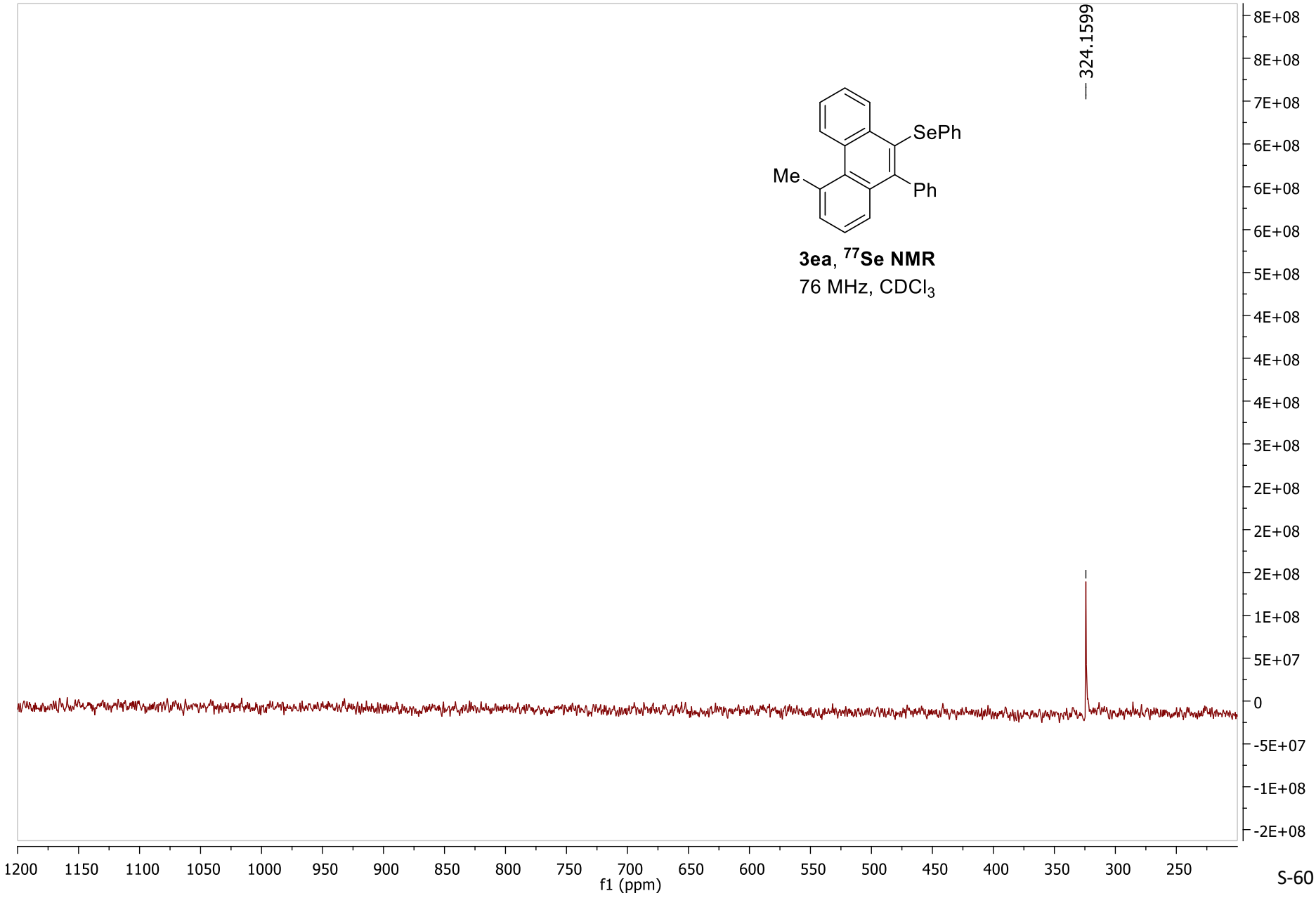
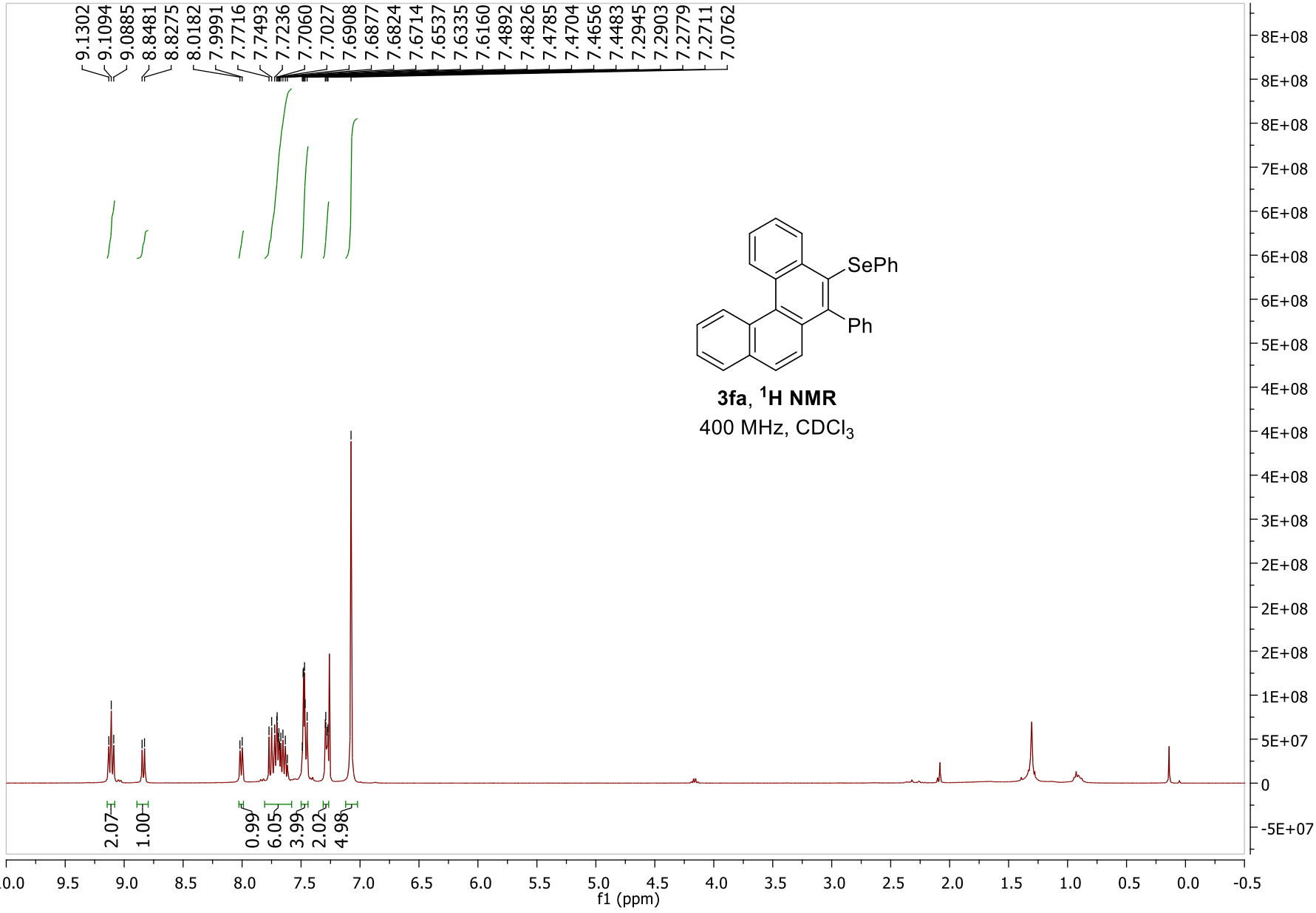
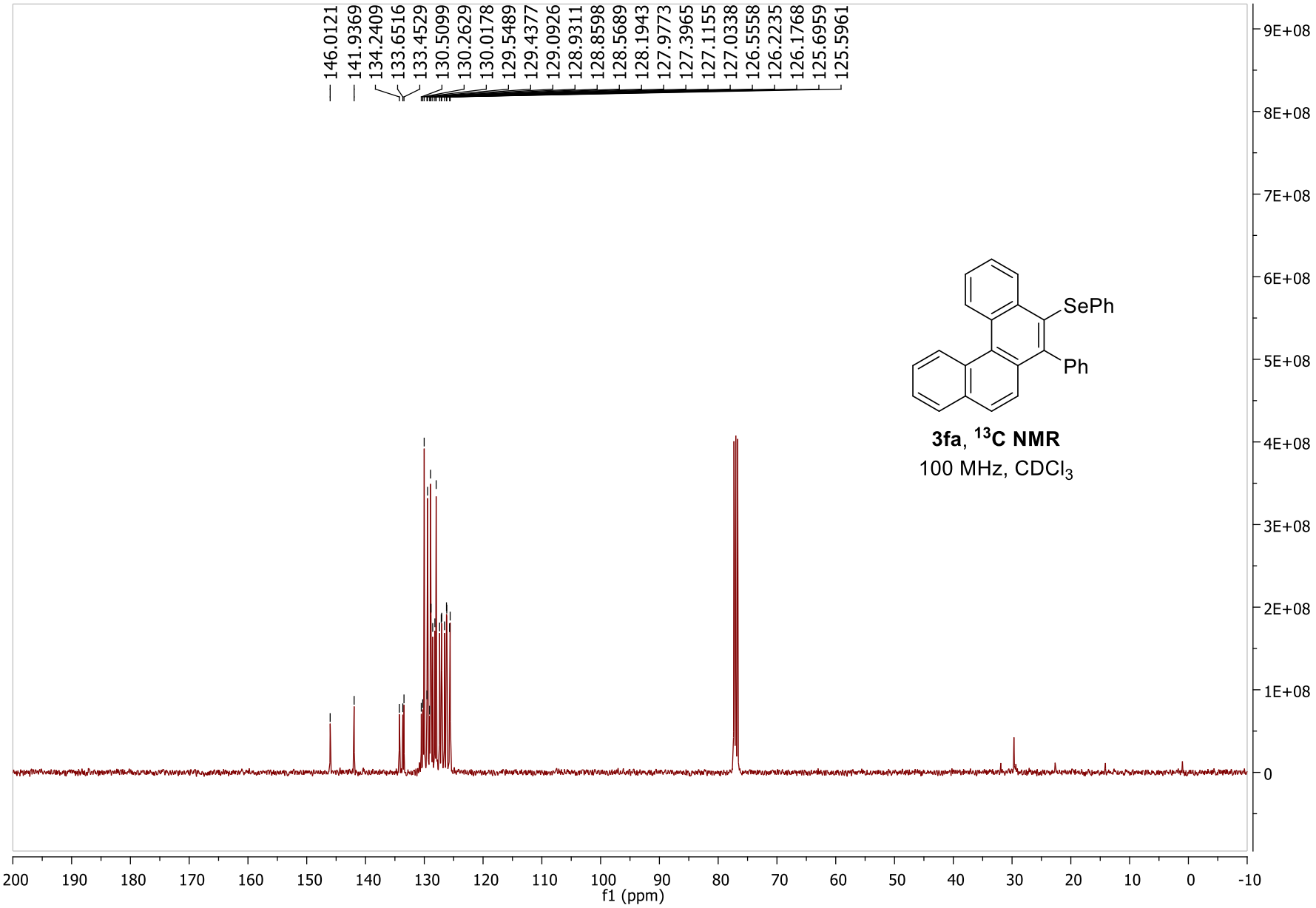
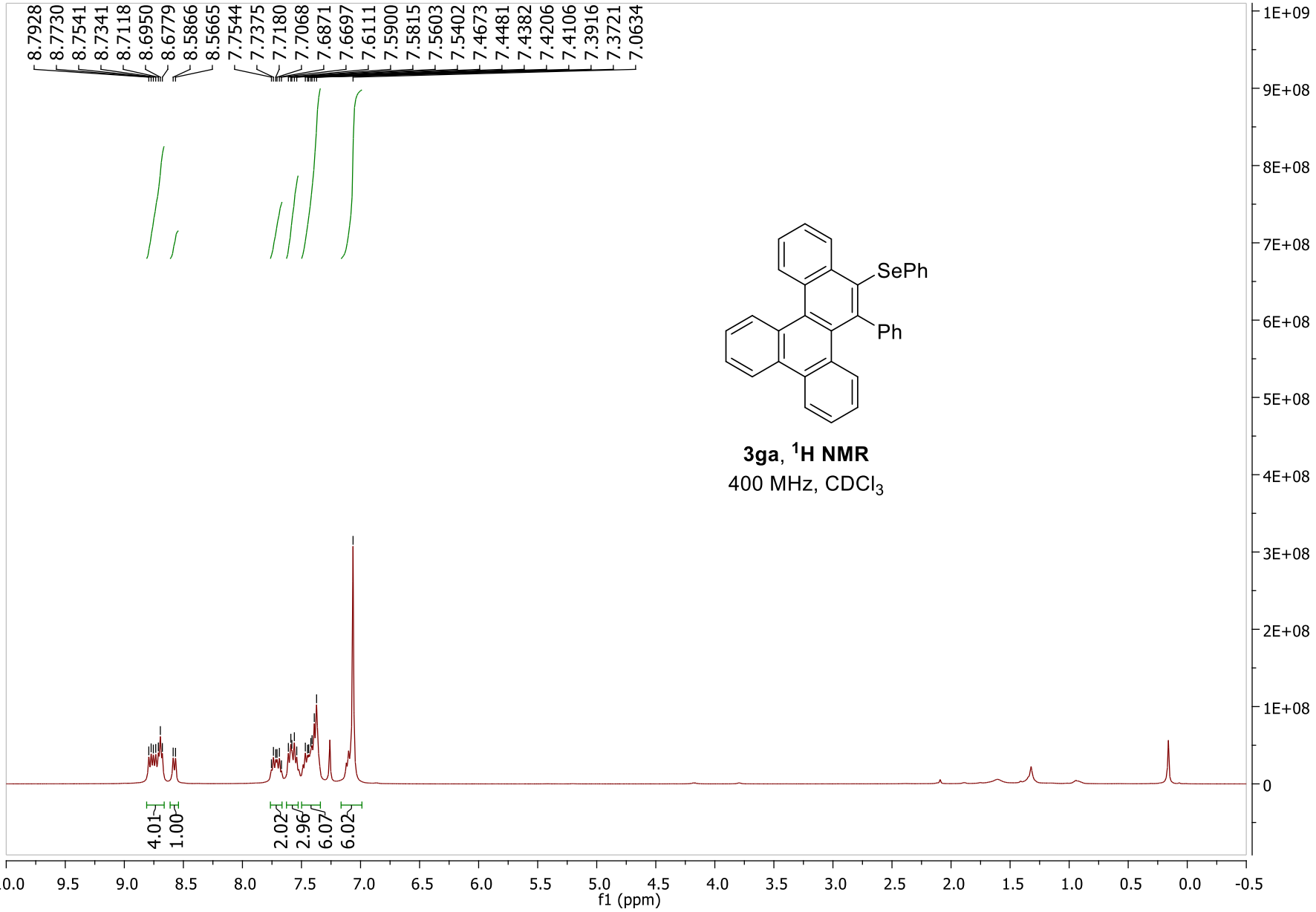
8.7776
8.7584
8.7550
8.7380
8.7343
7.5829
7.5790
7.5655
7.5618
7.5581
7.5448
7.5407
7.5223
7.5189
7.5048
7.5017
7.4987
7.4843
7.4813
7.4654
7.4636
7.3781
7.3723
7.3662
7.3642
7.3613
7.3566
7.3529
7.3398
7.3370
7.3005
7.2828
7.2803
7.2623
7.1966
7.1912
7.1830
7.1728
7.0193
7.0090
7.0046
6.9965
6.9932
6.9865
6.9845
6.9782
6.9759
6.9692
SePh
Me
Ph
3ea, 1H NMR
400 MHz, CDCl3
1.00
0.96
3.00
4.02
1.03
2.01
5.04
2.98
f1 (ppm)


147.1261
142.6142
134.8543
134.2125
133.5785
133.2826
132.0048
131.8169
131.2925
130.3106
129.6488
129.1270
128.8667
127.9048
127.7361
127.6213
127.2989
127.1664
126.8099
125.7269
125.5531
125.4242
27.2213
SePh
Me
Ph
3ea, 13C NMR
100 MHz, CDCl3
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


324.1599
SePh
Me
Ph
3ea, 77Se NMR
76 MHz, CDCl3
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


9.1302
9.1094
9.0885
8.8481
8.8275
8.0182
7.9991
7.7716
7.7493
7.7236
7.7060
7.7027
7.6908
7.6877
7.6824
7.6714
7.6537
7.6335
7.6160
7.4892
7.4826
7.4785
7.4704
7.4656
7.4483
7.2945
7.2903
7.2779
7.2711
7.0762
SePh
Ph
3fa, 1H NMR
400 MHz, CDCl3
2.07
1.00
0.99
6.05
3.99
2.02
4.98
f1 (ppm)


146.0121
141.9369
134.2409
133.6516
133.4529
130.5099
130.2629
130.0178
129.5489
129.4377
129.0926
128.9311
128.8598
128.5689
128.1943
127.9773
127.3965
127.1155
127.0338
126.5558
126.2235
126.1768
125.6959
125.5961
SePh
Ph
3fa, 13C NMR
100 MHz, CDCl3
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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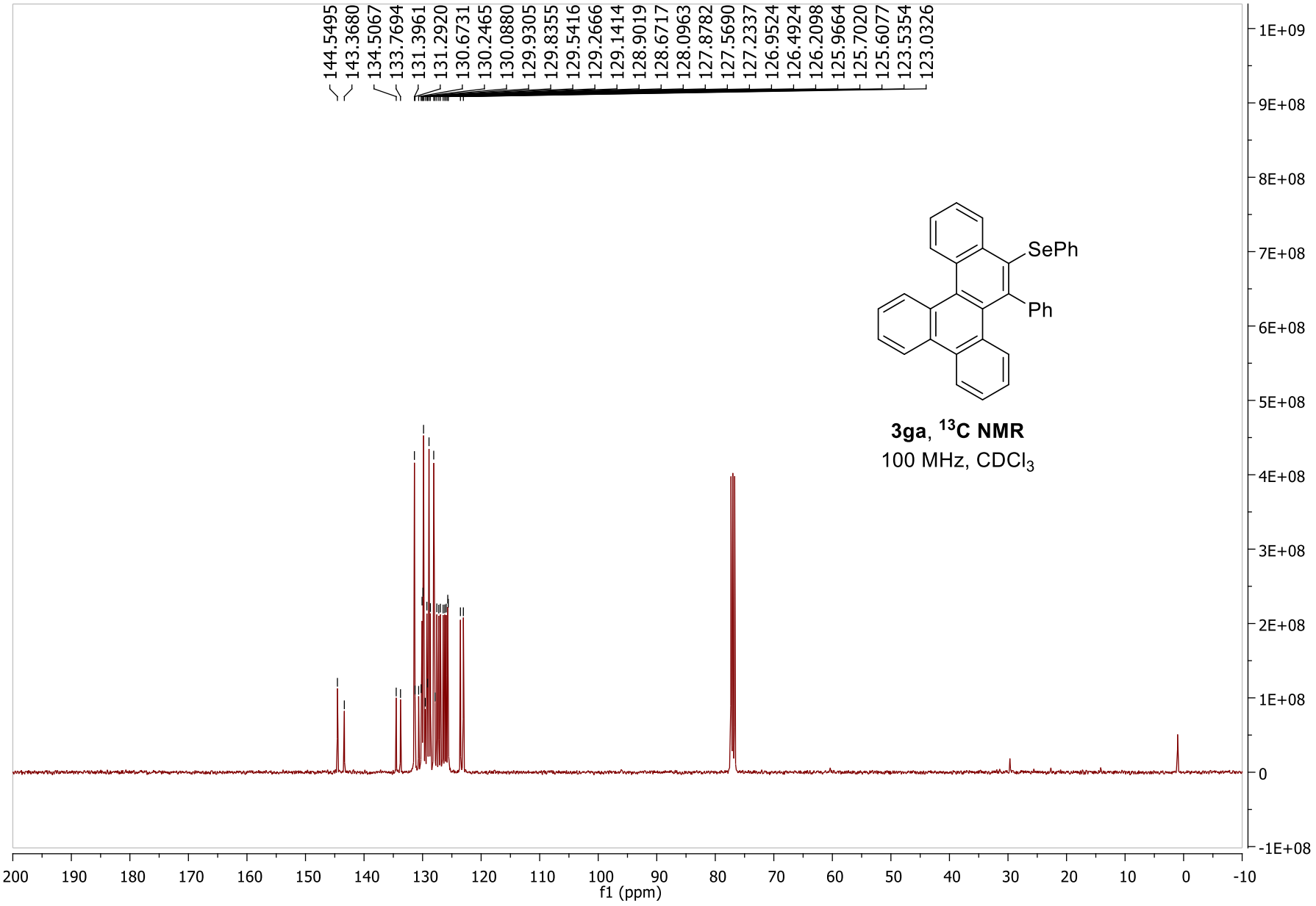
8.7730
8.7541
8.7341
8.7118
8.6950
8.6779
8.5866
8.5665
7.7544
7.7375
7.7180
7.7068
7.6871
7.6697
7.6111
7.5900
7.5815
7.5603
7.5402
7.4673
7.4481
7.4382
7.4206
7.4106
7.3916
7.3721
7.0634
SePh
Ph
3ga, 1H NMR
400 MHz, CDCl3
4.01
1.00
2.02
2.96
6.07
6.02
f1 (ppm)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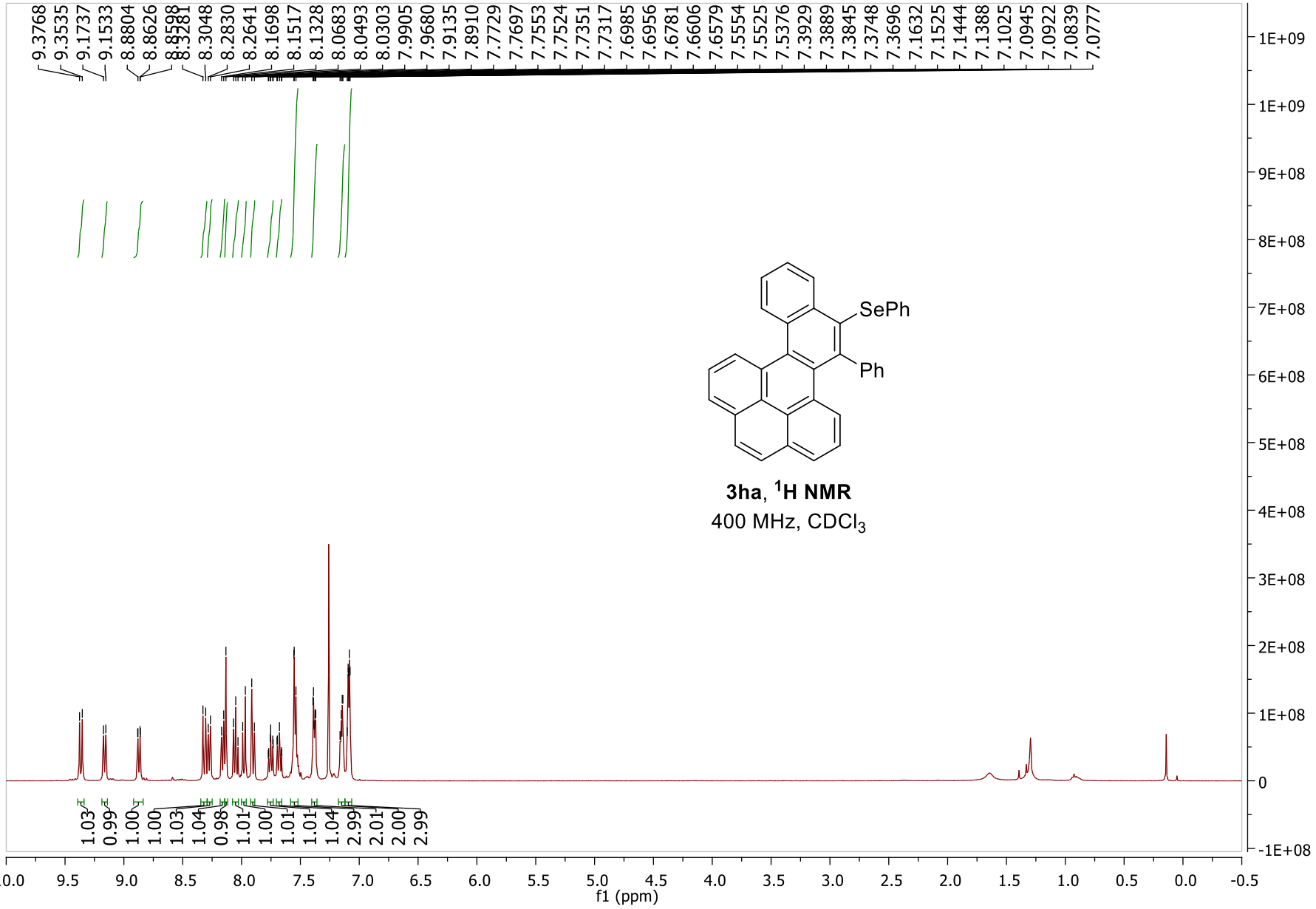
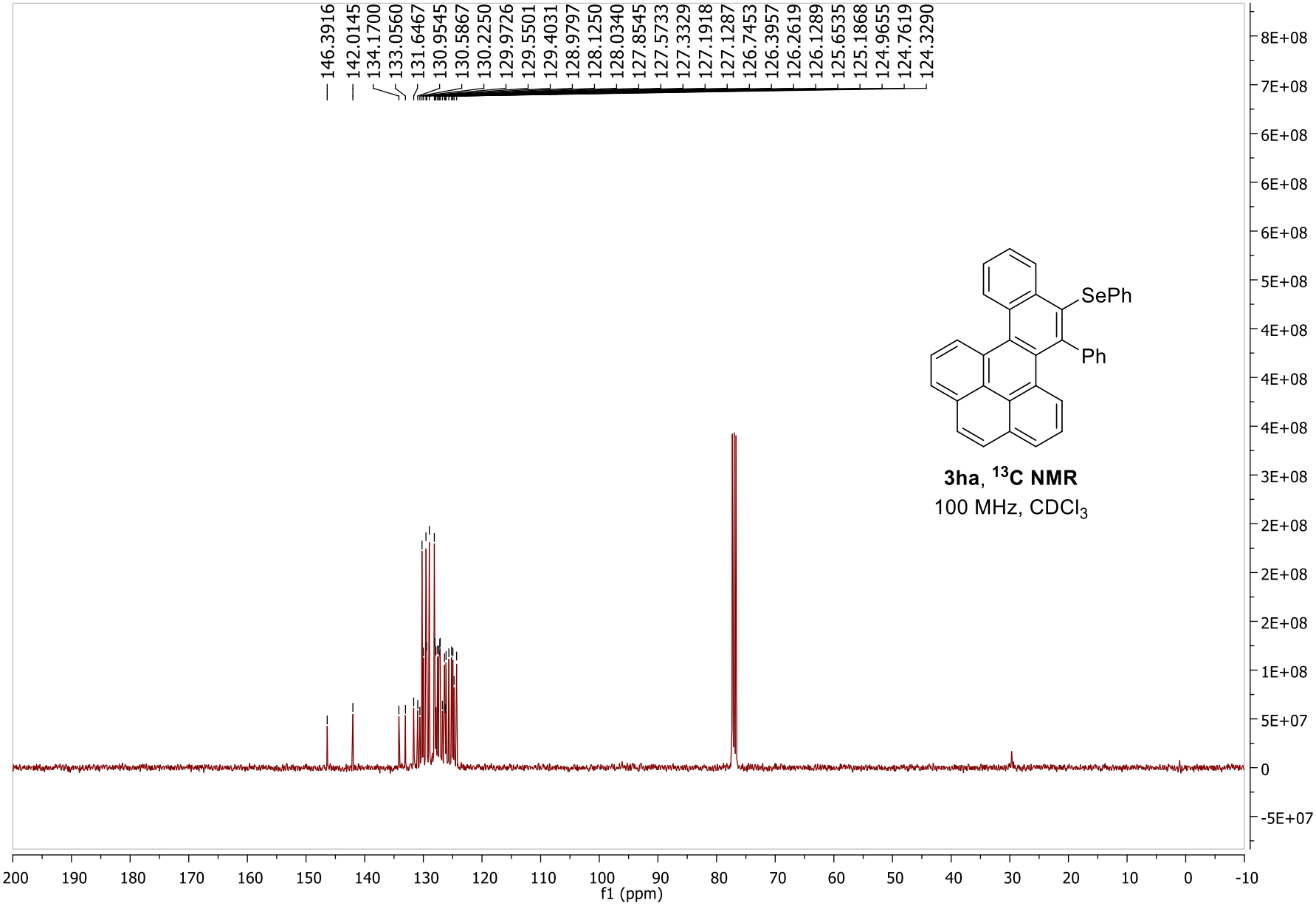
143.3680
134.5067
133.7694
131.3961
131.2920
130.6731
130.2465
130.0880
129.9305
129.8355
129.5416
129.2666
129.1414
128.9019
128.6717
128.0963
127.8782
127.5690
127.2337
126.9524
126.4924
126.2098
125.9664
125.7020
125.6077
123.5354
123.0326
SePh
Ph
3ga, 13C NMR
100 MHz, CDCl3
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




**3ha**, **$^{1}$H NMR**

400 MHz, $CDCl_3$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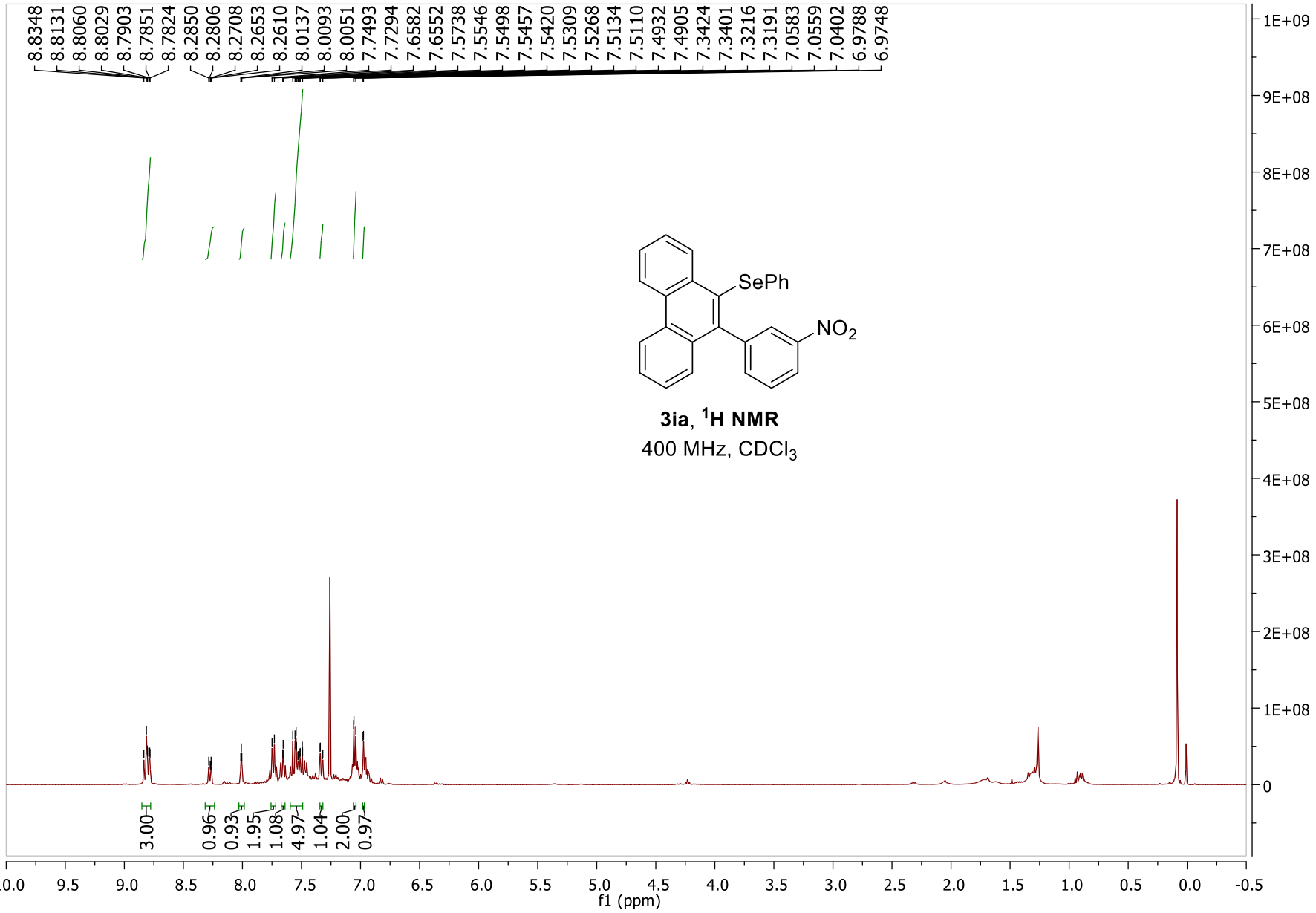
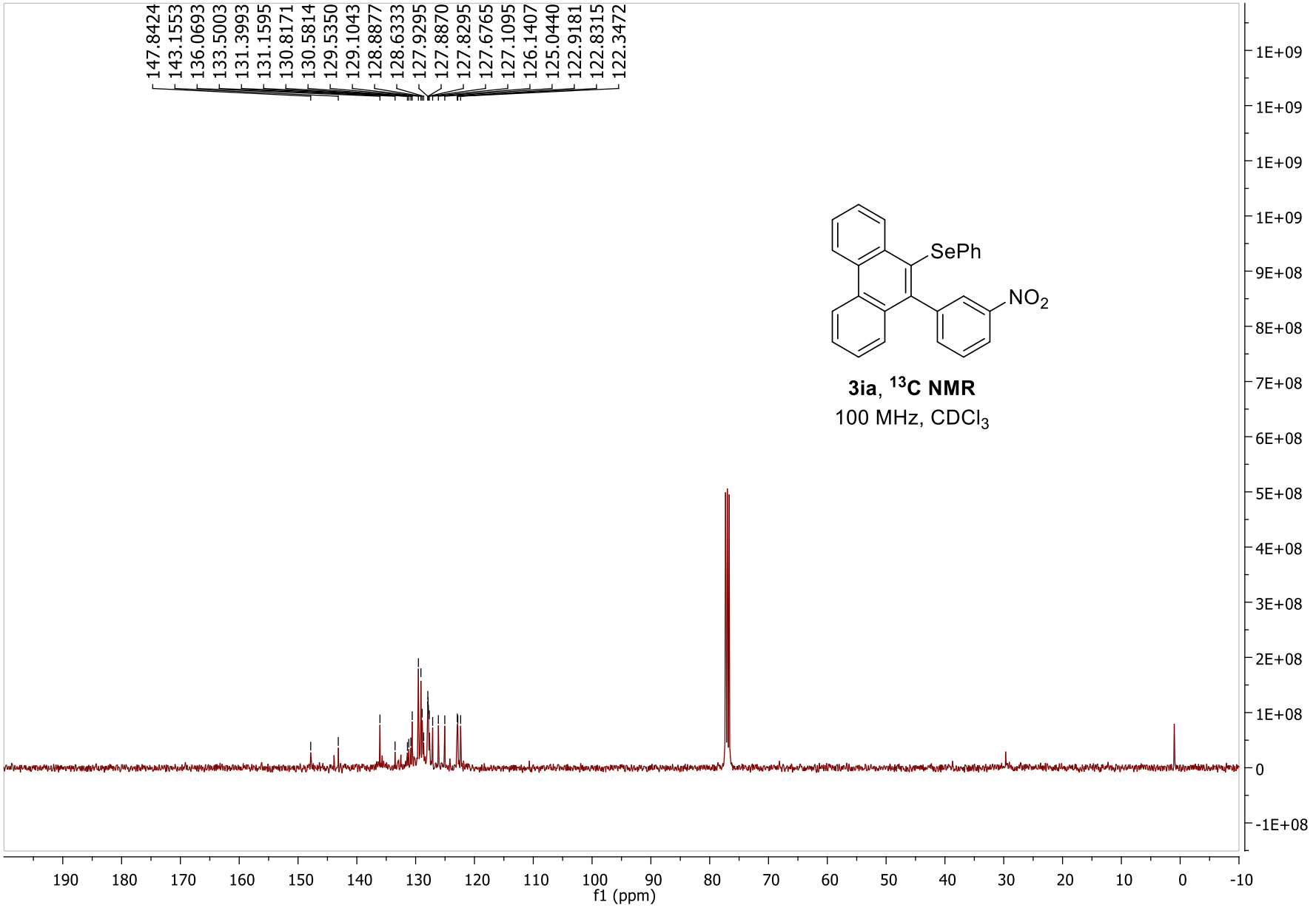
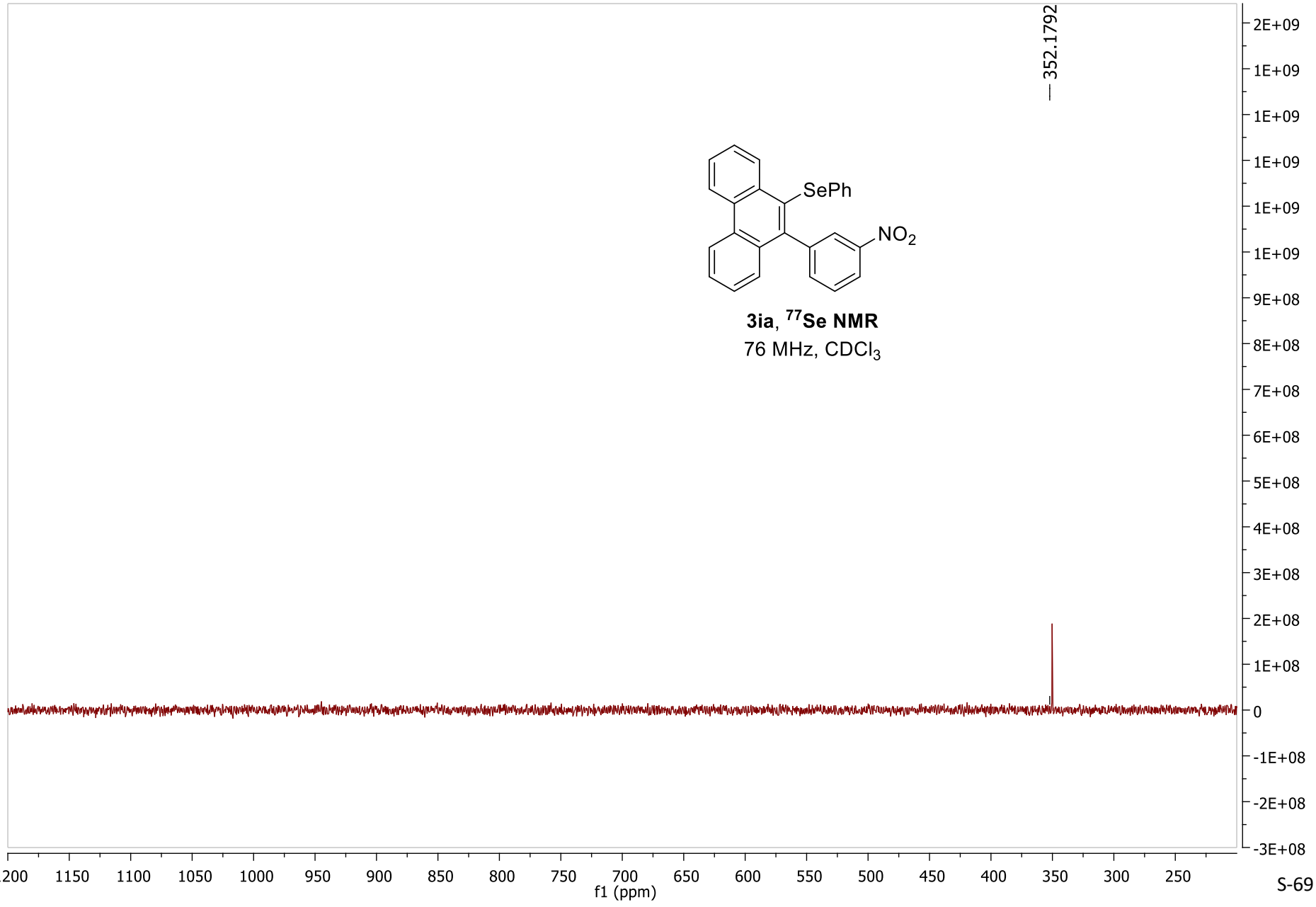
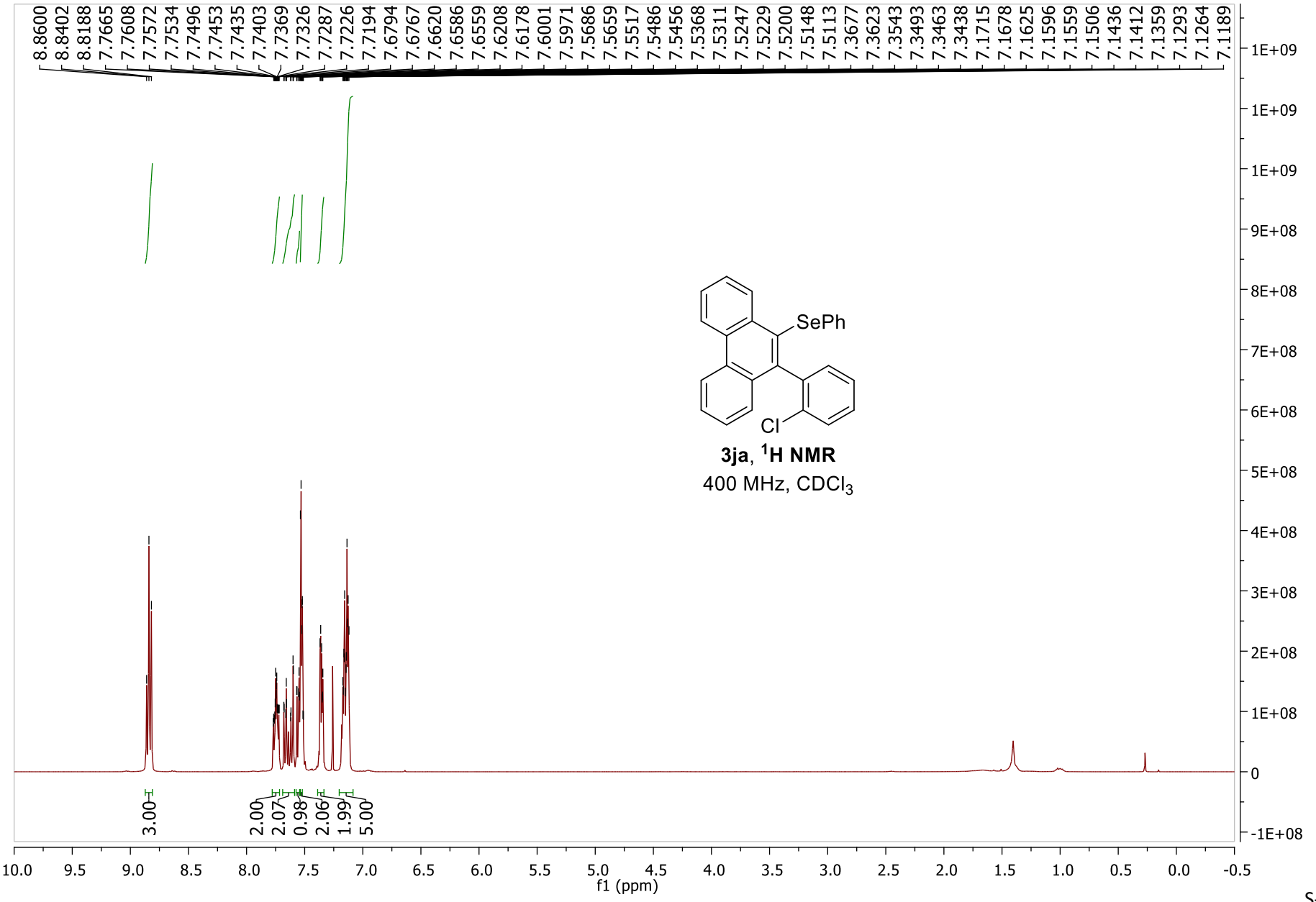
142.0145
134.1700
133.0560
131.6467
130.9545
130.5867
130.2250
129.9726
129.5501
129.4031
128.9797
128.1250
128.0340
127.8545
127.5733
127.3329
127.1918
127.1287
126.7453
126.3957
126.2619
126.1289
125.6535
125.1868
124.9655
124.7619
124.3290
SePh
Ph
3ha, 13C NMR
100 MHz, CDCl3
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.8348
8.8131
8.8060
8.8029
8.7903
8.7851
8.7824
8.2850
8.2806
8.2708
8.2653
8.2610
8.0137
8.0093
8.0051
7.7493
7.7294
7.6582
7.6552
7.5738
7.5546
7.5498
7.5457
7.5420
7.5309
7.5268
7.5134
7.5110
7.4932
7.4905
7.3424
7.3401
7.3216
7.3191
7.0583
7.0559
7.0402
6.9788
6.9748
SePh
NO2
3ia, 1H NMR
400 MHz, CDCl3
3.00
0.96
0.93
1.95
1.08
4.97
1.04
2.00
0.97
f1 (ppm)

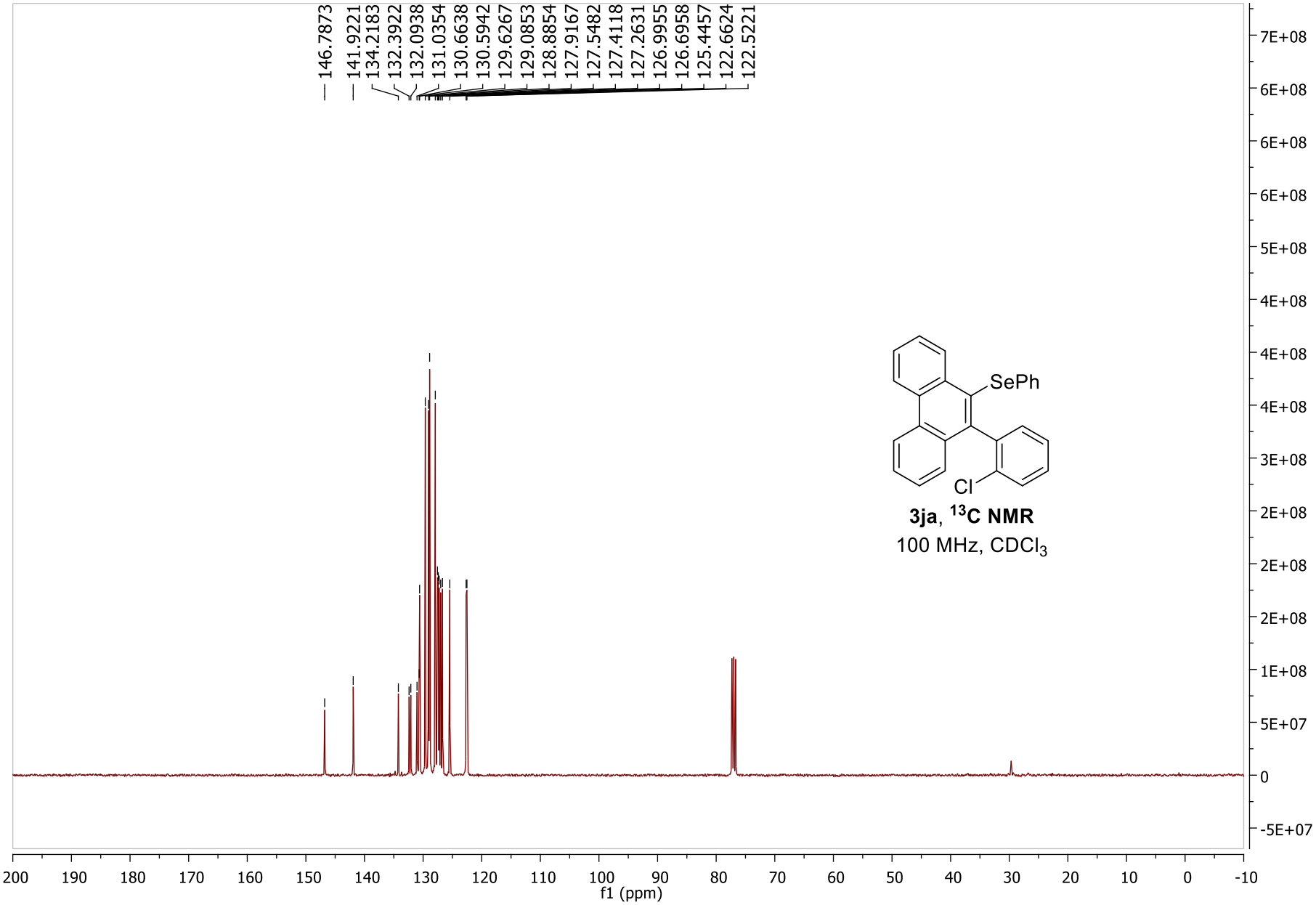

147.8424
143.1553
136.0693
133.5003
131.3993
131.1595
130.8171
130.5814
129.5350
129.1043
128.8877
128.6333
127.9295
127.8870
127.8295
127.6765
127.1095
126.1407
125.0440
122.9181
122.8315
122.3472
SePh
NO2
3ia, 13C NMR
100 MHz, CDCl3
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


352.1792
SePh
NO2
3ia, 77Se NMR
76 MHz, CDCl3
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
-2E+08
-3E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)




**3ja**, **$^{1}$H NMR**

400 MHz, $CDCl_3$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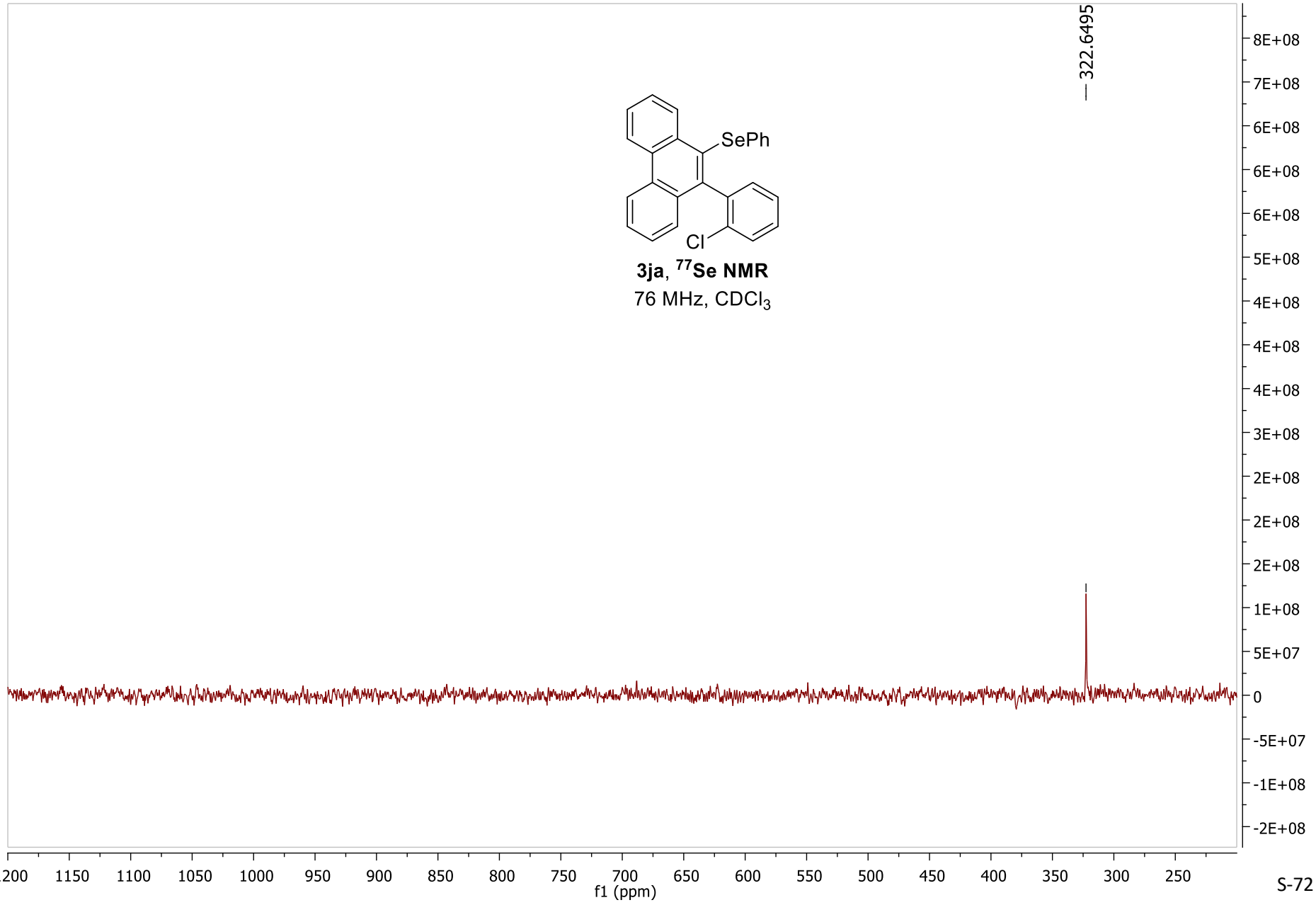
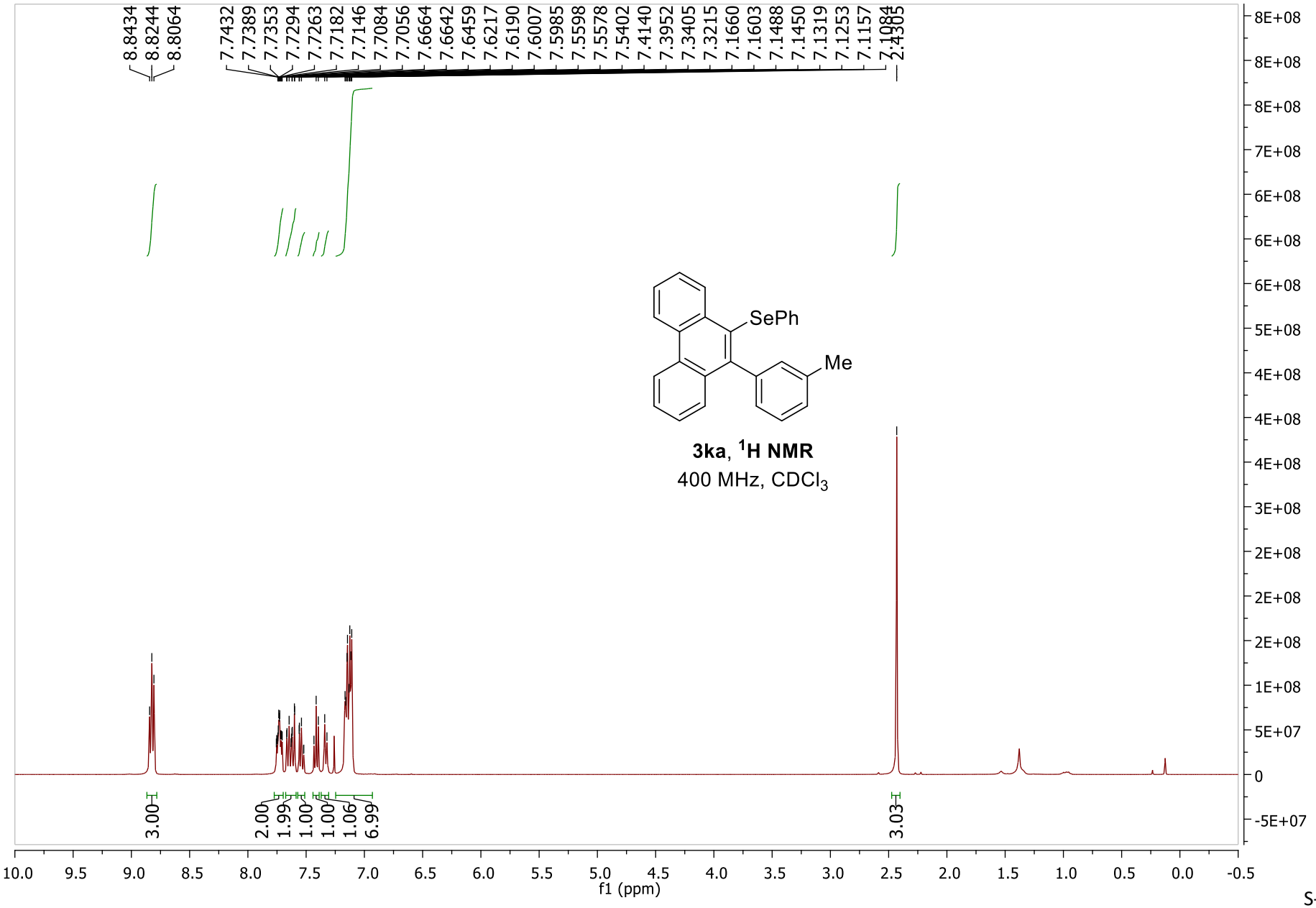
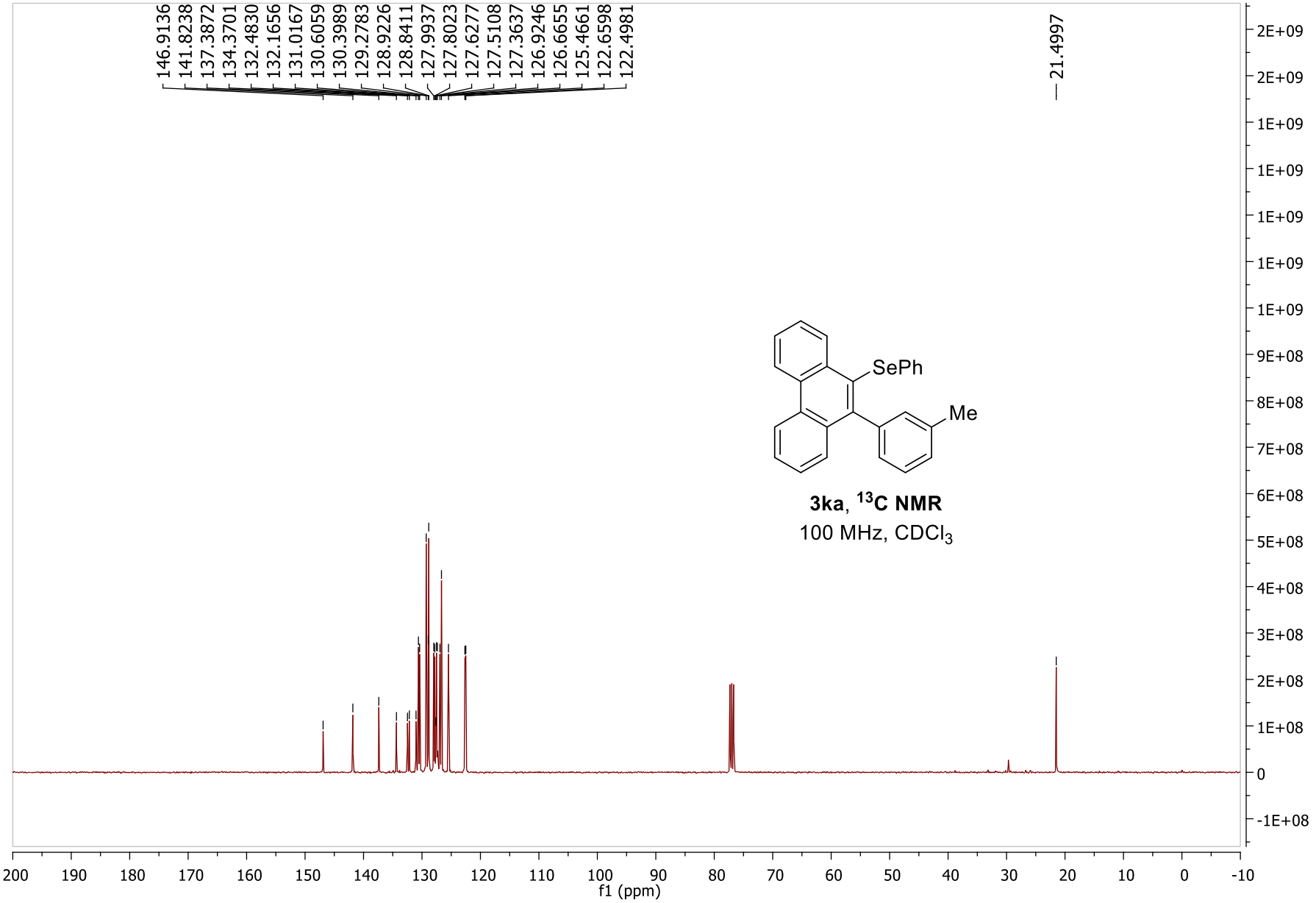
134.2183
132.3922
132.0938
131.0354
130.6638
130.5942
129.6267
129.0853
128.8854
127.9167
127.5482
127.4118
127.2631
126.9955
126.6958
125.4457
122.6624
122.5221
SePh
Cl
3ja, 13C NMR
100 MHz, CDCl3
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


322.6495
SePh
Cl
3ja, 77Se NMR
76 MHz, CDCl3
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)


8.8434
8.8244
8.8064
7.7432
7.7389
7.7353
7.7294
7.7263
7.7182
7.7146
7.7084
7.7056
7.6664
7.6642
7.6459
7.6217
7.6190
7.6007
7.5985
7.5598
7.5578
7.5402
7.4140
7.3952
7.3405
7.3215
7.1660
7.1603
7.1488
7.1450
7.1319
7.1253
7.1157
2.4305
SePh
Me
3ka, 1H NMR
400 MHz, CDCl3
3.00
2.00
1.99
1.00
1.00
1.06
6.99
3.03
f1 (ppm)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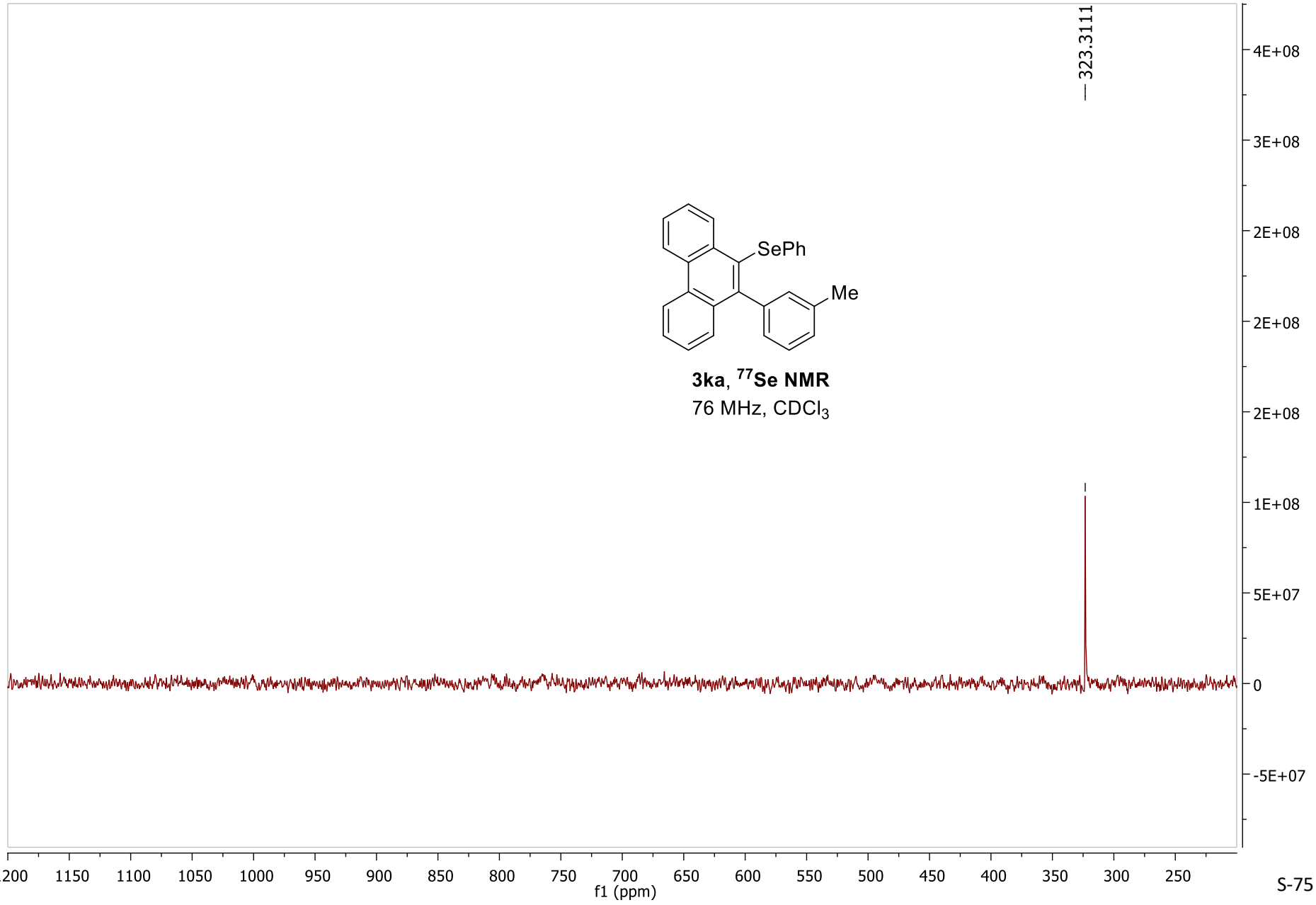
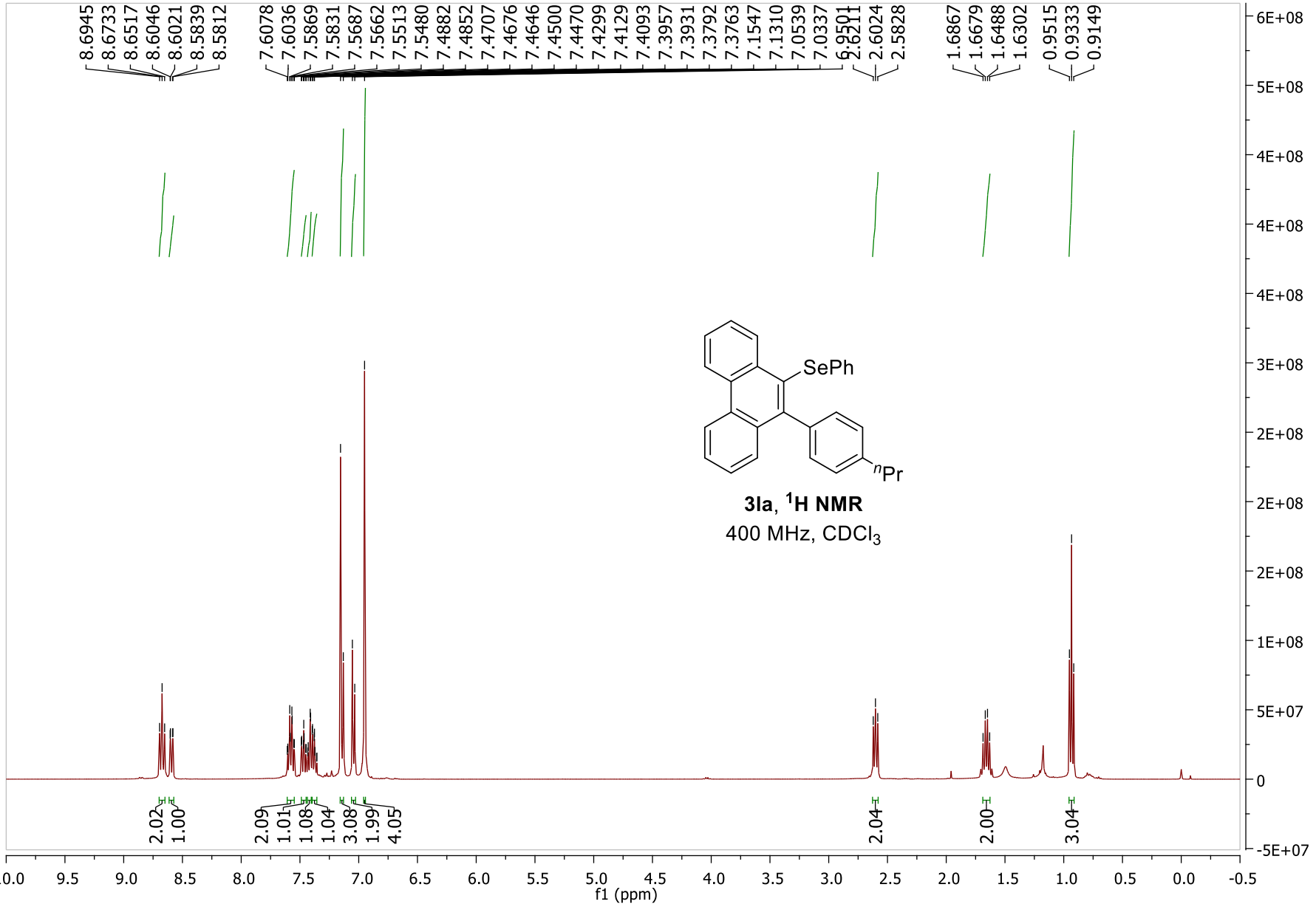
137.3872
134.3701
132.4830
132.1656
131.0167
130.6059
130.3989
129.2783
128.9226
128.8411
127.9937
127.8023
127.6277
127.5108
127.3637
126.9246
126.6655
125.4661
122.6598
122.4981
21.4997
SePh
Me
3ka, 13C NMR
100 MHz, CDCl3
f1 (ppm)


323.3111
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
SePh
Me
3ka, 77Se NMR
76 MHz, CDCl3
1200
1150
1100
1050
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
f1 (ppm)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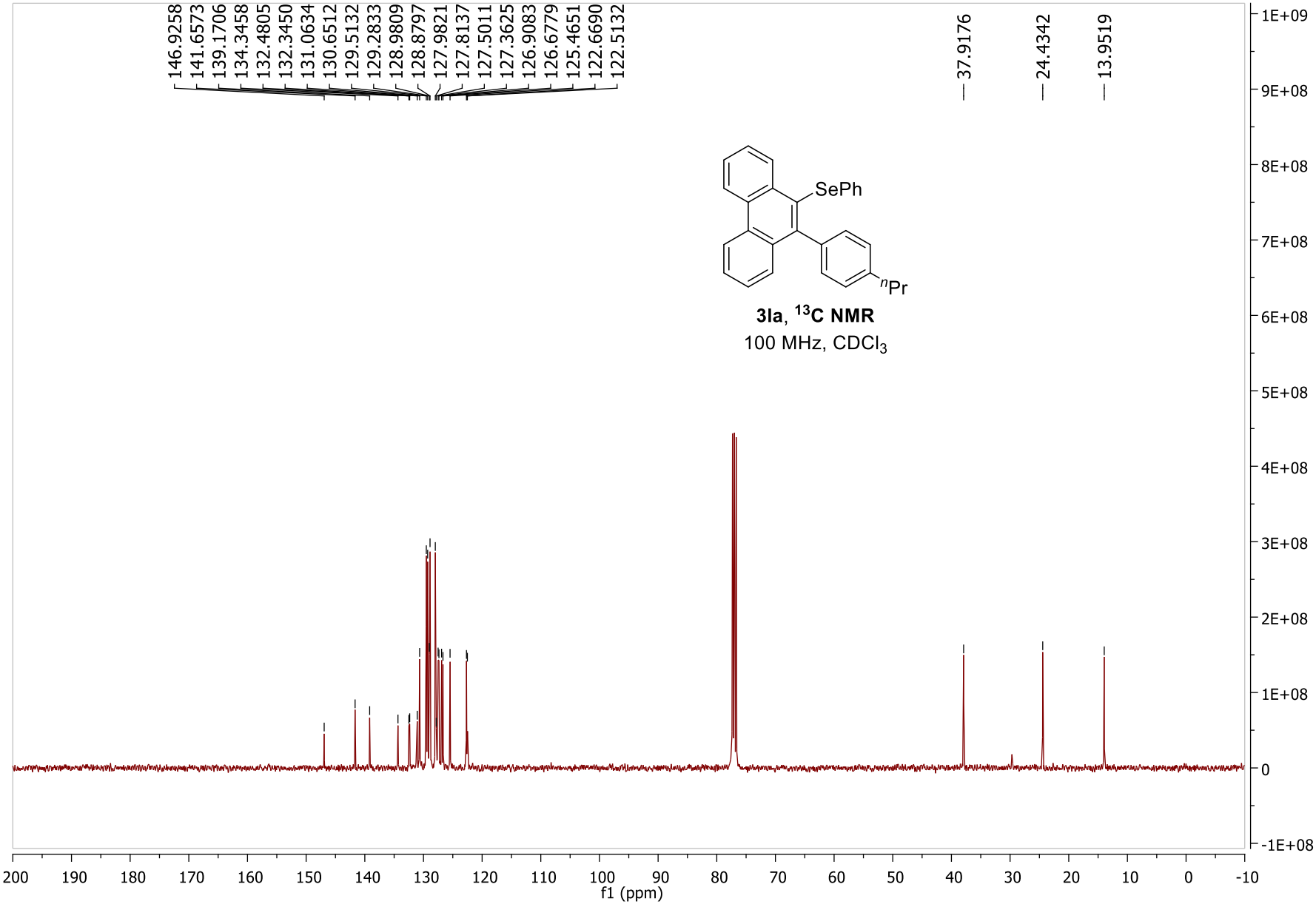
8.6733
8.6517
8.6046
8.6021
8.5839
8.5812
7.6078
7.6036
7.5869
7.5831
7.5687
7.5662
7.5513
7.5480
7.4882
7.4852
7.4707
7.4676
7.4646
7.4500
7.4470
7.4299
7.4129
7.4093
7.3957
7.3931
7.3792
7.3763
7.1547
7.1310
7.0539
7.0337
6.9501
2.6211
2.6024
2.5828
1.6867
1.6679
1.6488
1.6302
0.9515
0.9333
0.9149
SePh
nPr
3Ia, 1H NMR
400 MHz, CDCl3
2.02
1.00
2.09
1.01
1.08
1.04
3.08
1.99
4.05
2.04
2.00
3.04
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
10.0
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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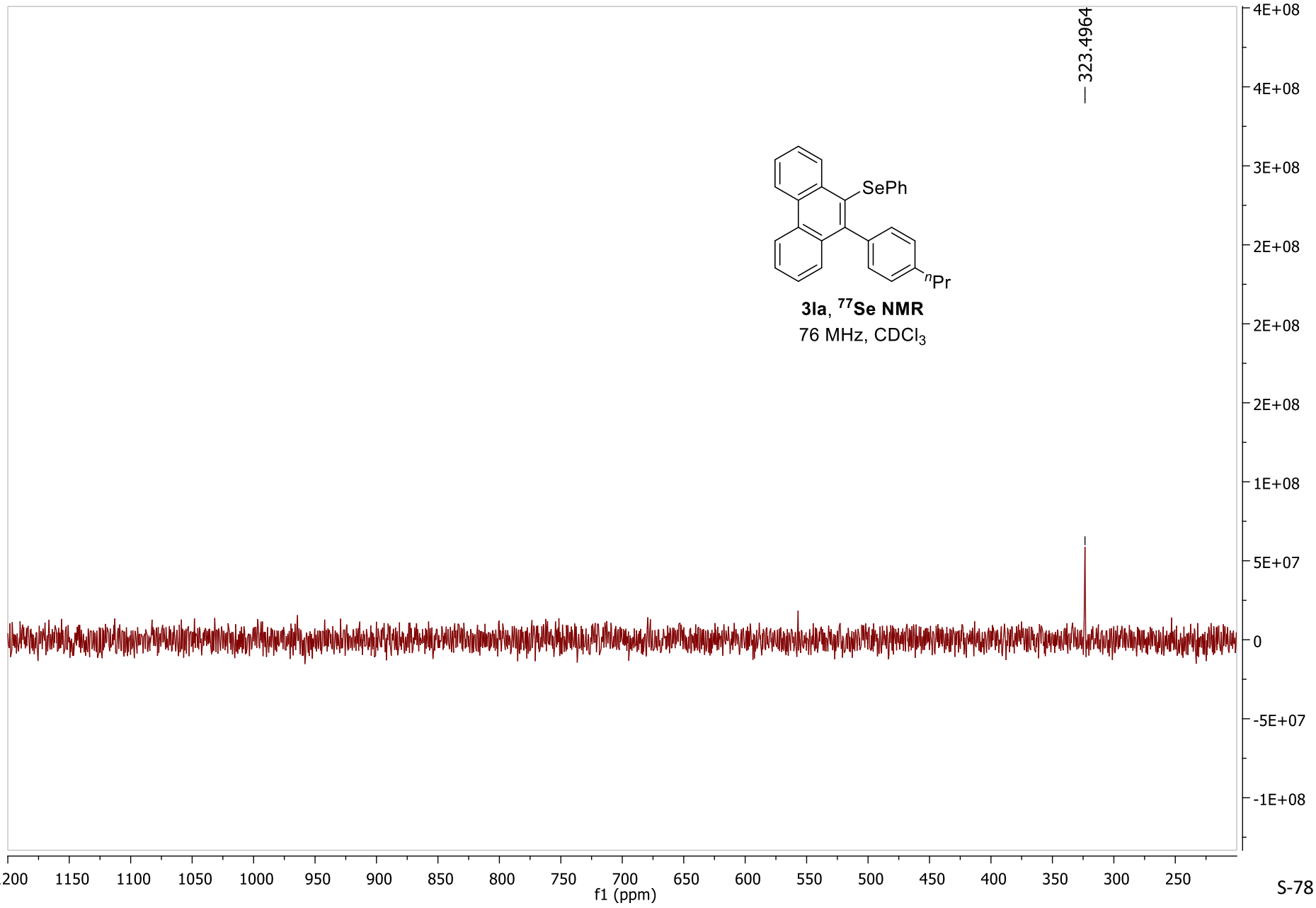
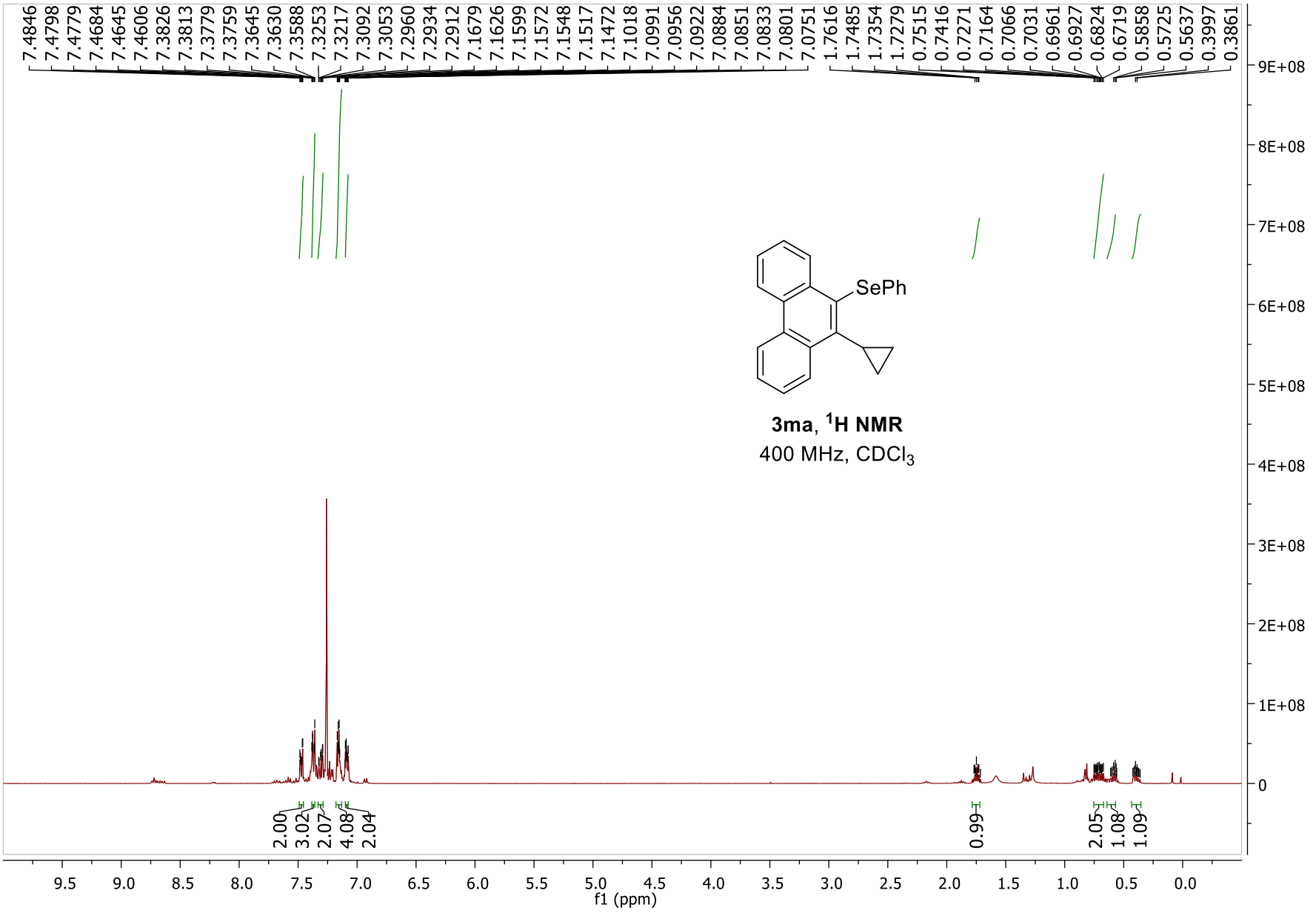
141.6573
139.1706
134.3458
132.4805
132.3450
131.0634
130.6512
129.5132
129.2833
128.9809
128.8797
127.9821
127.8137
127.5011
127.3625
126.9083
126.6779
125.4651
122.6690
122.5132
37.9176
24.4342
13.9519
SePh
nPr
3la, 13C NMR
100 MHz, CDCl3
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


323.4964
SePh
nPr
3Ia, 77Se NMR
76 MHz, CDCl3
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
1200
1150
1100
1050
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
f1 (ppm)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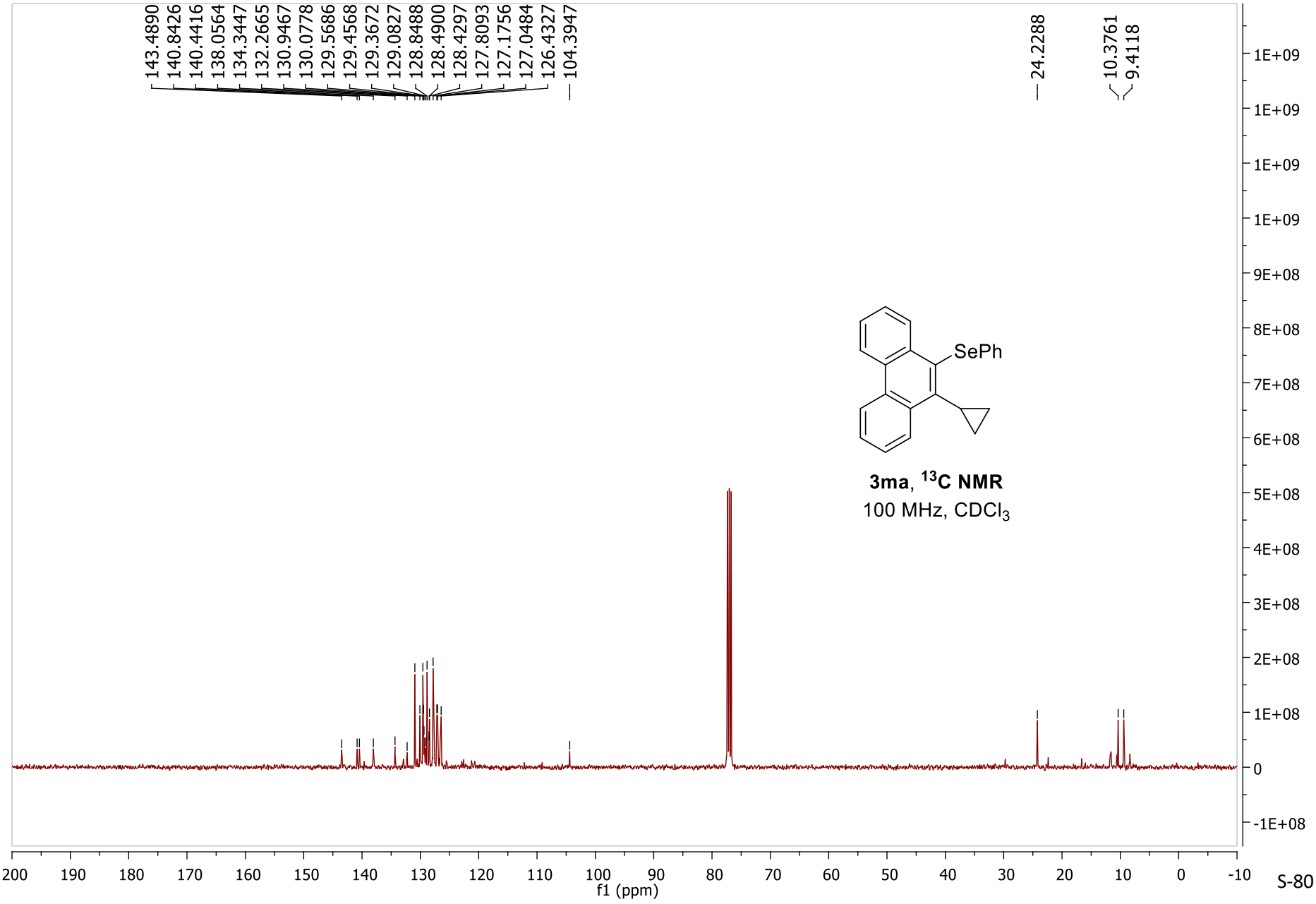
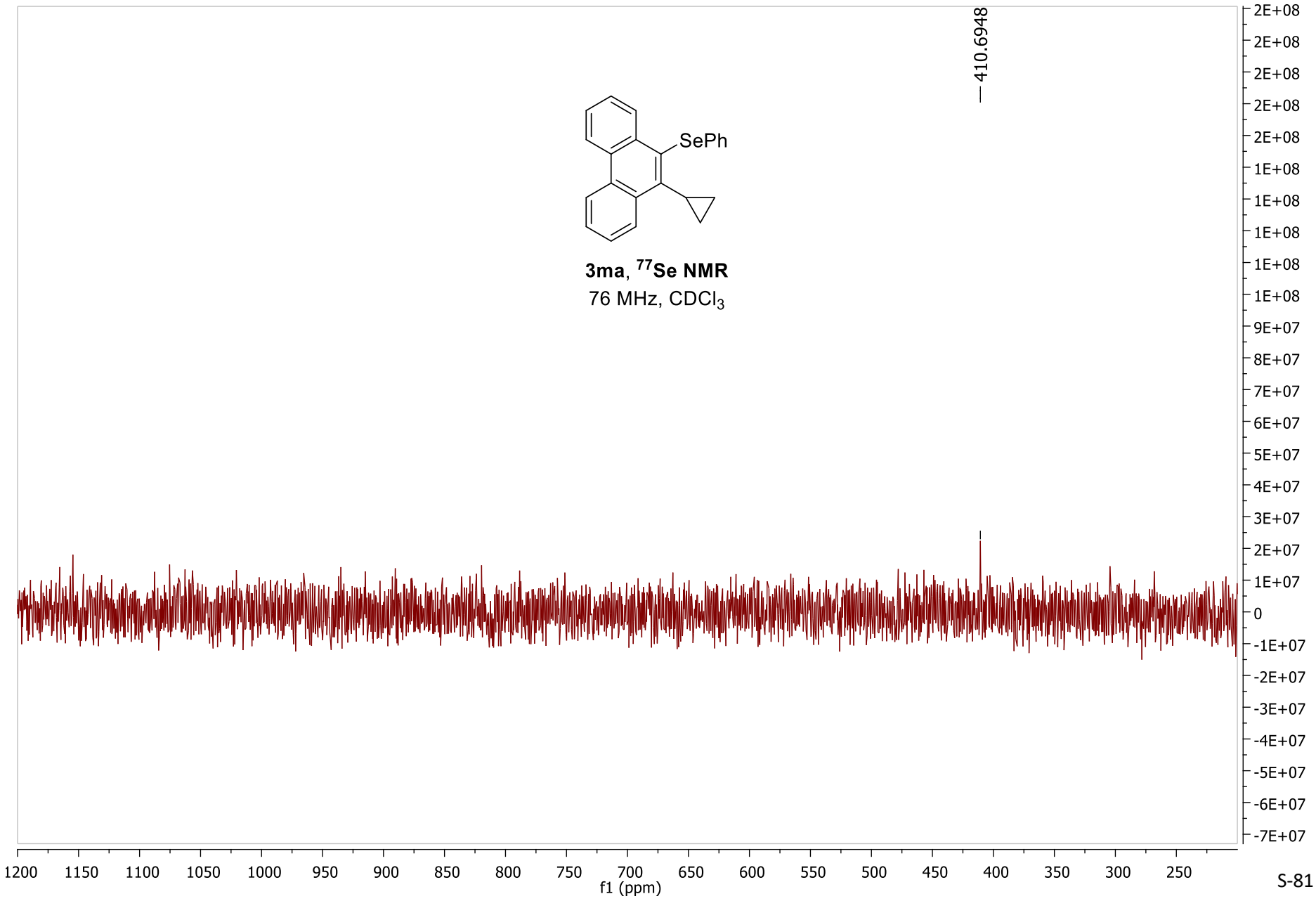
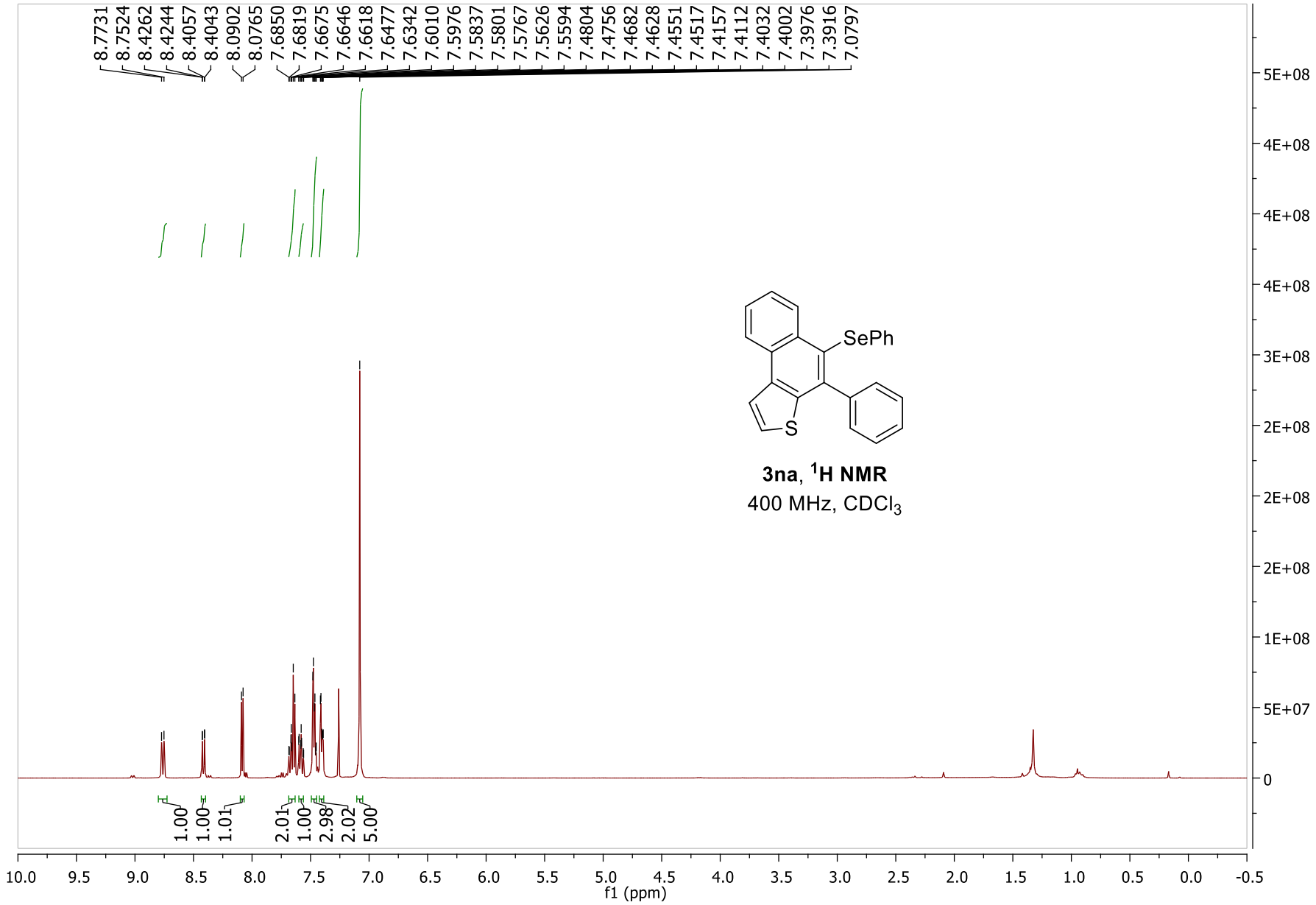
7.4798
7.4779
7.4684
7.4645
7.4606
7.3826
7.3813
7.3779
7.3759
7.3645
7.3630
7.3588
7.3253
7.3217
7.3092
7.3053
7.2960
7.2934
7.2912
7.1679
7.1626
7.1599
7.1572
7.1548
7.1517
7.1472
7.1018
7.0991
7.0956
7.0922
7.0884
7.0851
7.0833
7.0801
7.0751
1.7616
1.7485
1.7354
1.7279
0.7515
0.7416
0.7271
0.7164
0.7066
0.7031
0.6961
0.6927
0.6824
0.6719
0.5858
0.5725
0.5637
0.3997
0.3861
SePh
3ma, 1H NMR
400 MHz, CDCl3
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
2.00
3.02
2.07
4.08
2.04
0.99
2.05
1.08
1.09
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
f1 (ppm)


143.4890
140.8426
140.4416
138.0564
134.3447
132.2665
130.9467
130.0778
129.5686
129.4568
129.3672
129.0827
128.8488
128.4900
128.4297
127.8093
127.1756
127.0484
126.4327
104.3947
24.2288
10.3761
9.4118
SePh
3ma, 13C NMR
100 MHz, CDCl3
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


410.6948
SePh
3ma, 77Se NMR
76 MHz, CDCl3
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
1E+08
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
-2E+07
-3E+07
-4E+07
-5E+07
-6E+07
-7E+07
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)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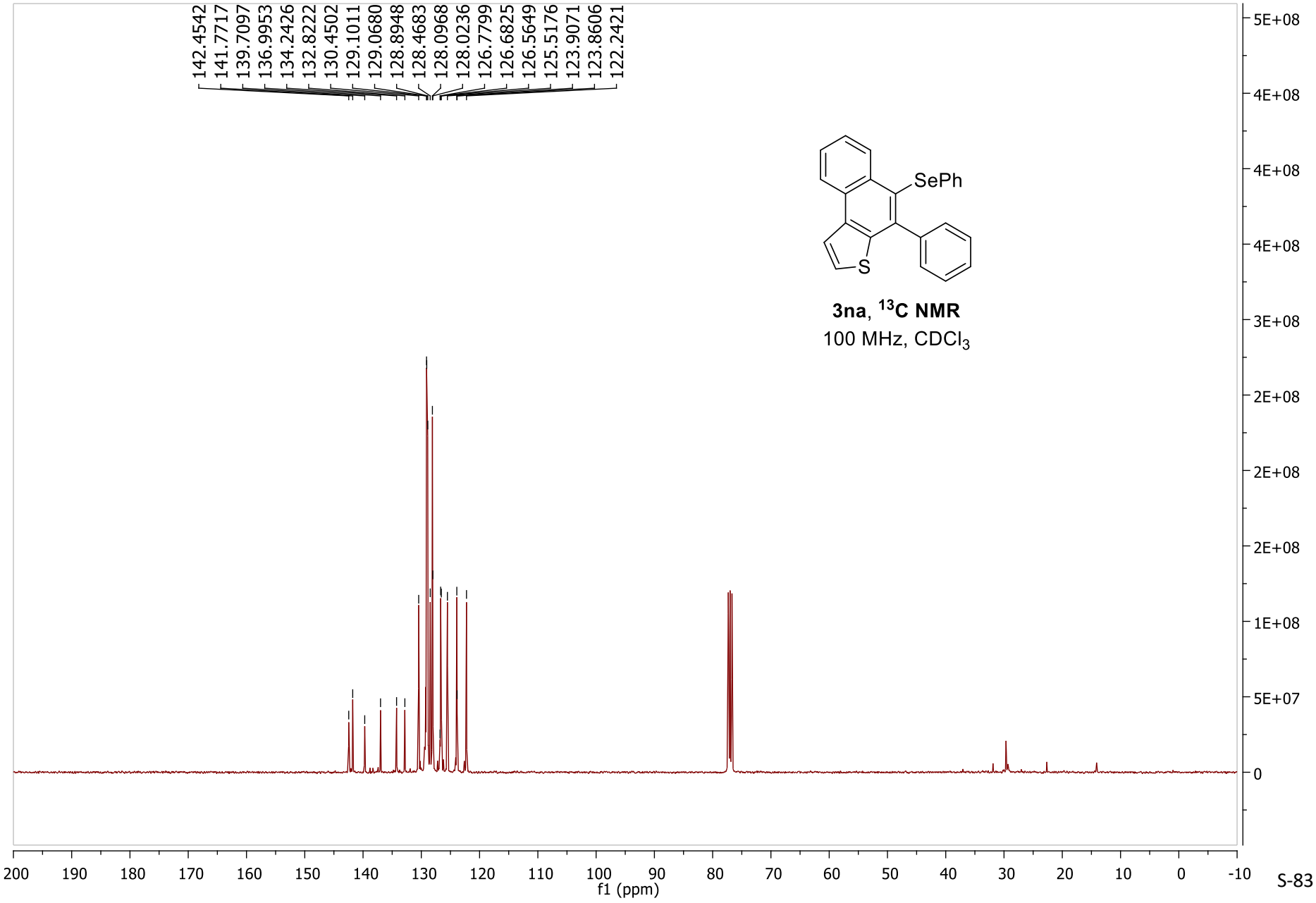
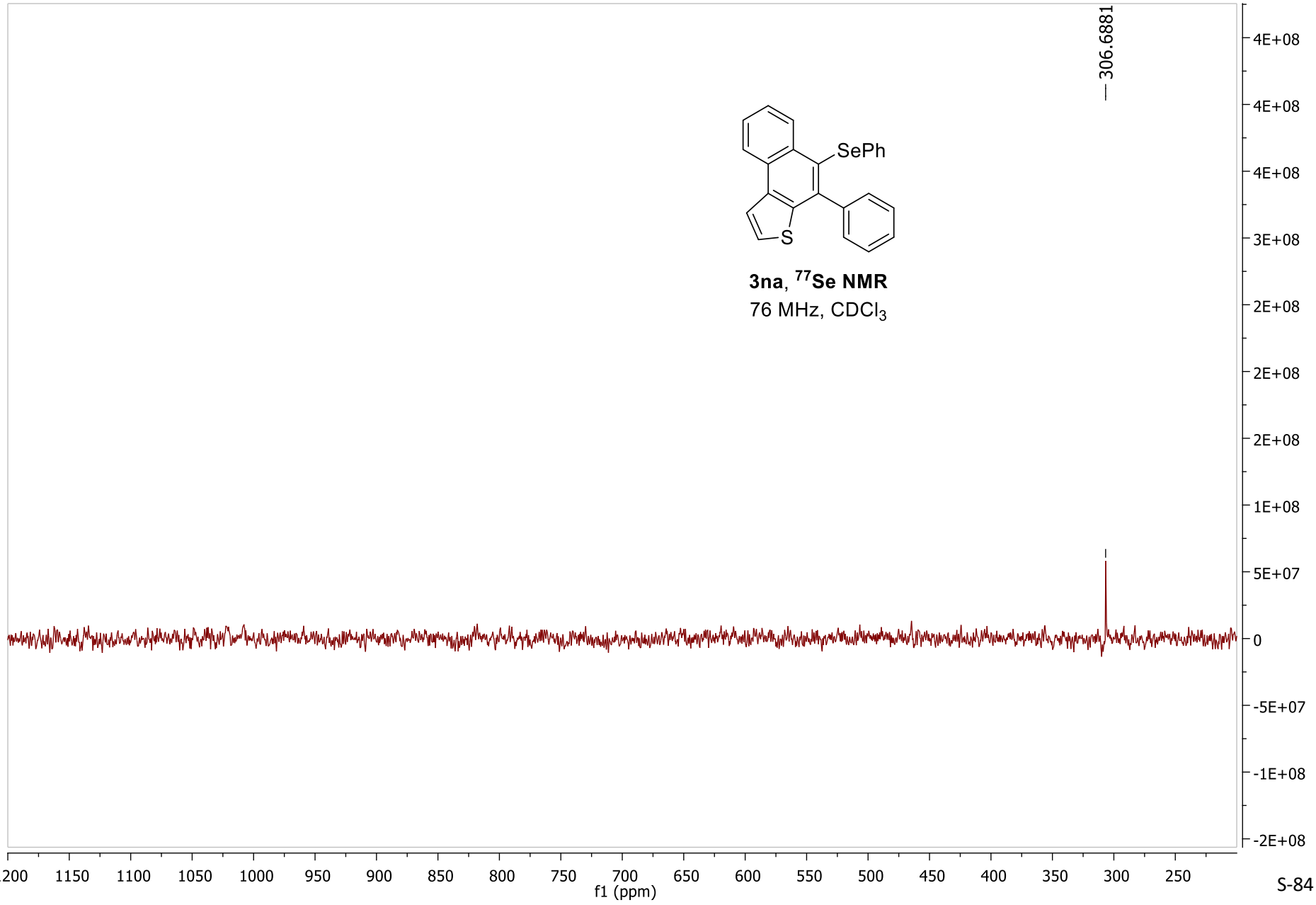
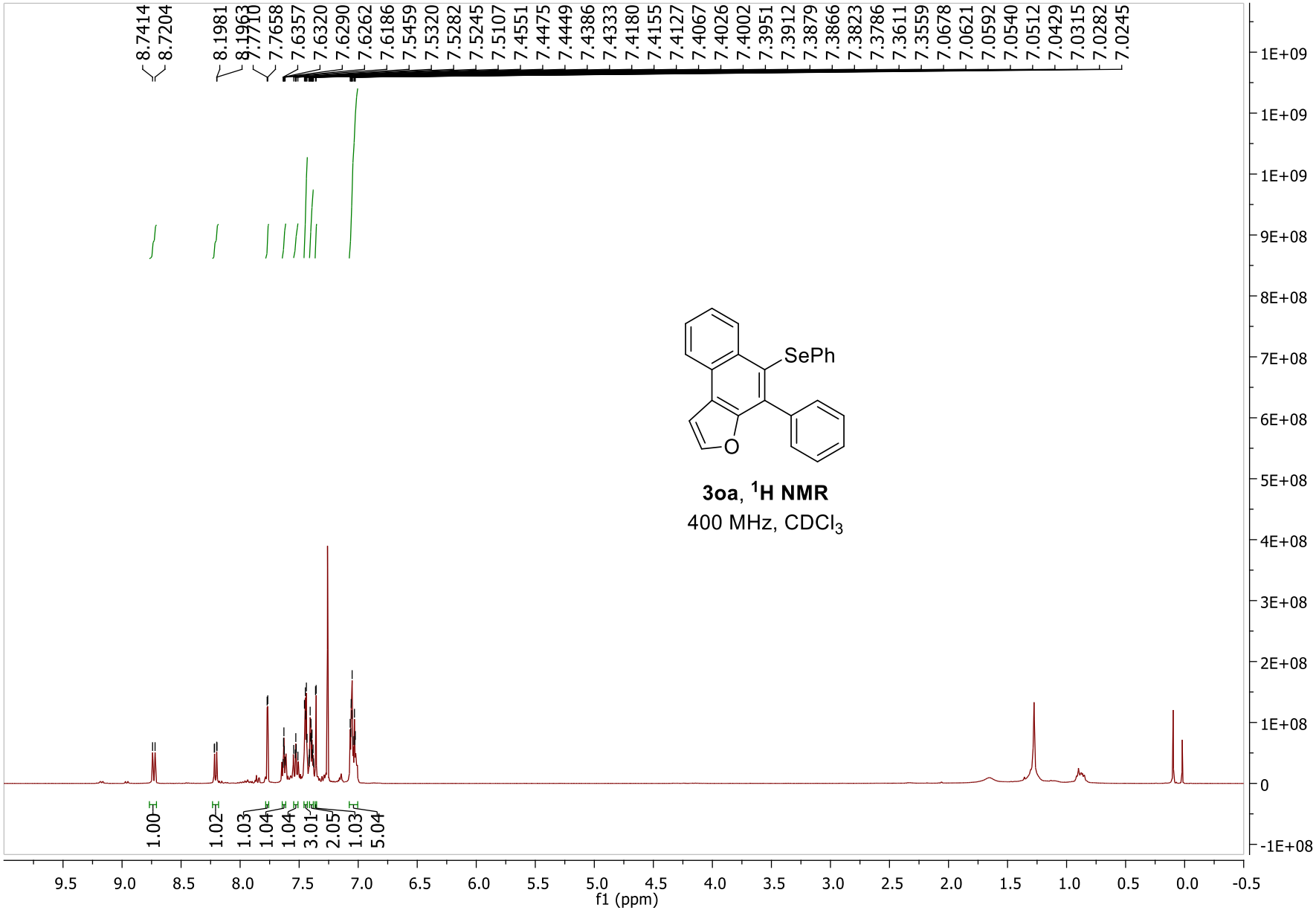
8.7524
8.4262
8.4244
8.4057
8.4043
8.0902
8.0765
7.6850
7.6819
7.6675
7.6646
7.6618
7.6477
7.6342
7.6010
7.5976
7.5837
7.5801
7.5767
7.5626
7.5594
7.4804
7.4756
7.4682
7.4628
7.4551
7.4517
7.4157
7.4112
7.4032
7.4002
7.3976
7.3916
7.0797
SePh
S
3na, 1H NMR
400 MHz, CDCl3
1.00
1.00
1.01
2.01
1.00
2.98
2.02
5.00
f1 (ppm)


142.4542
141.7717
139.7097
136.9953
134.2426
132.8222
130.4502
129.1011
129.0680
128.8948
128.4683
128.0968
128.0236
126.7799
126.6825
126.5649
125.5176
123.9071
123.8606
122.2421
SePh
S
3na, 13C NMR
100 MHz, CDCl3
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


306.6881
SePh
S
3na, 77Se NMR
76 MHz, CDCl3
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
1200
1150
1100
1050
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
f1 (ppm)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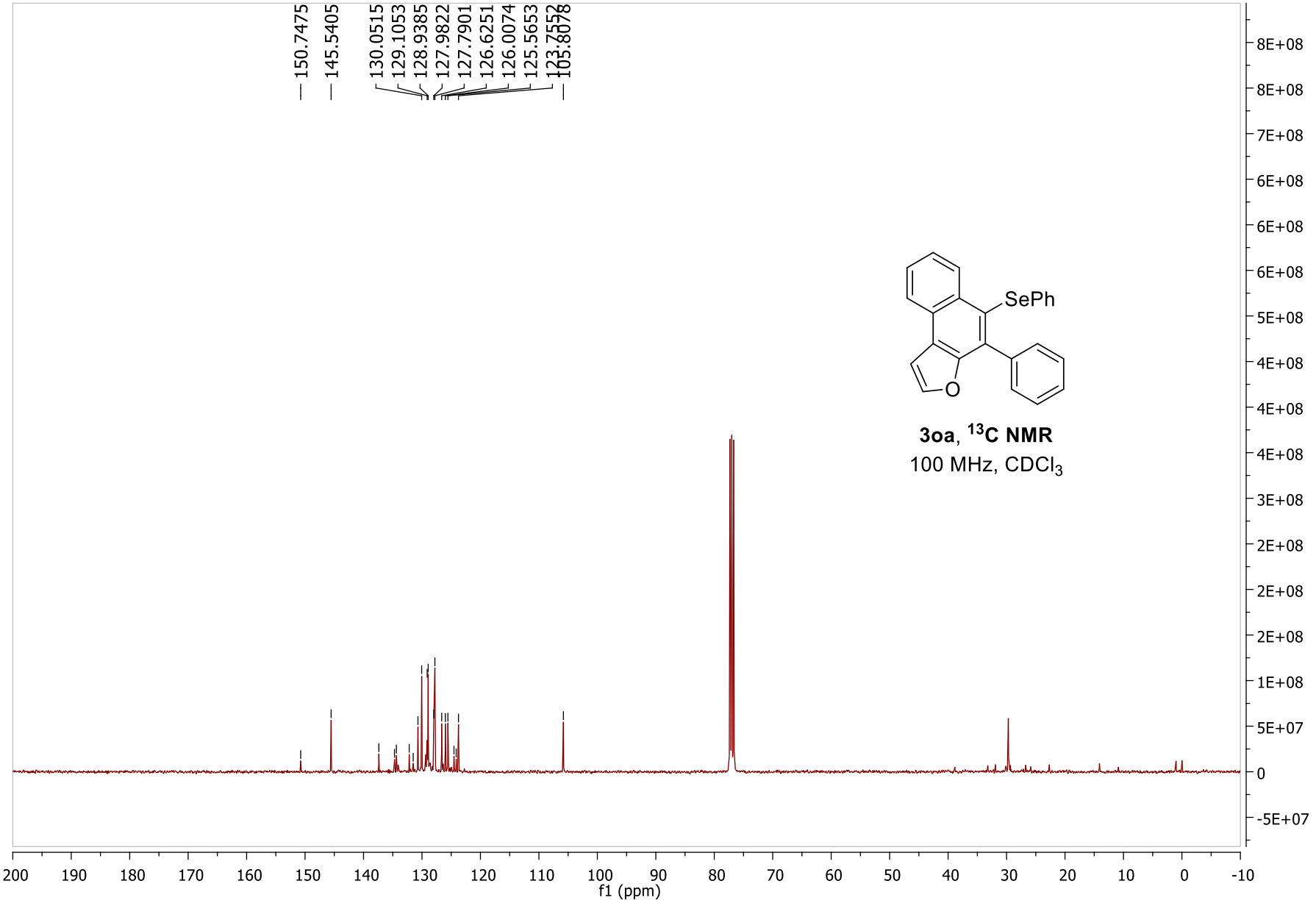
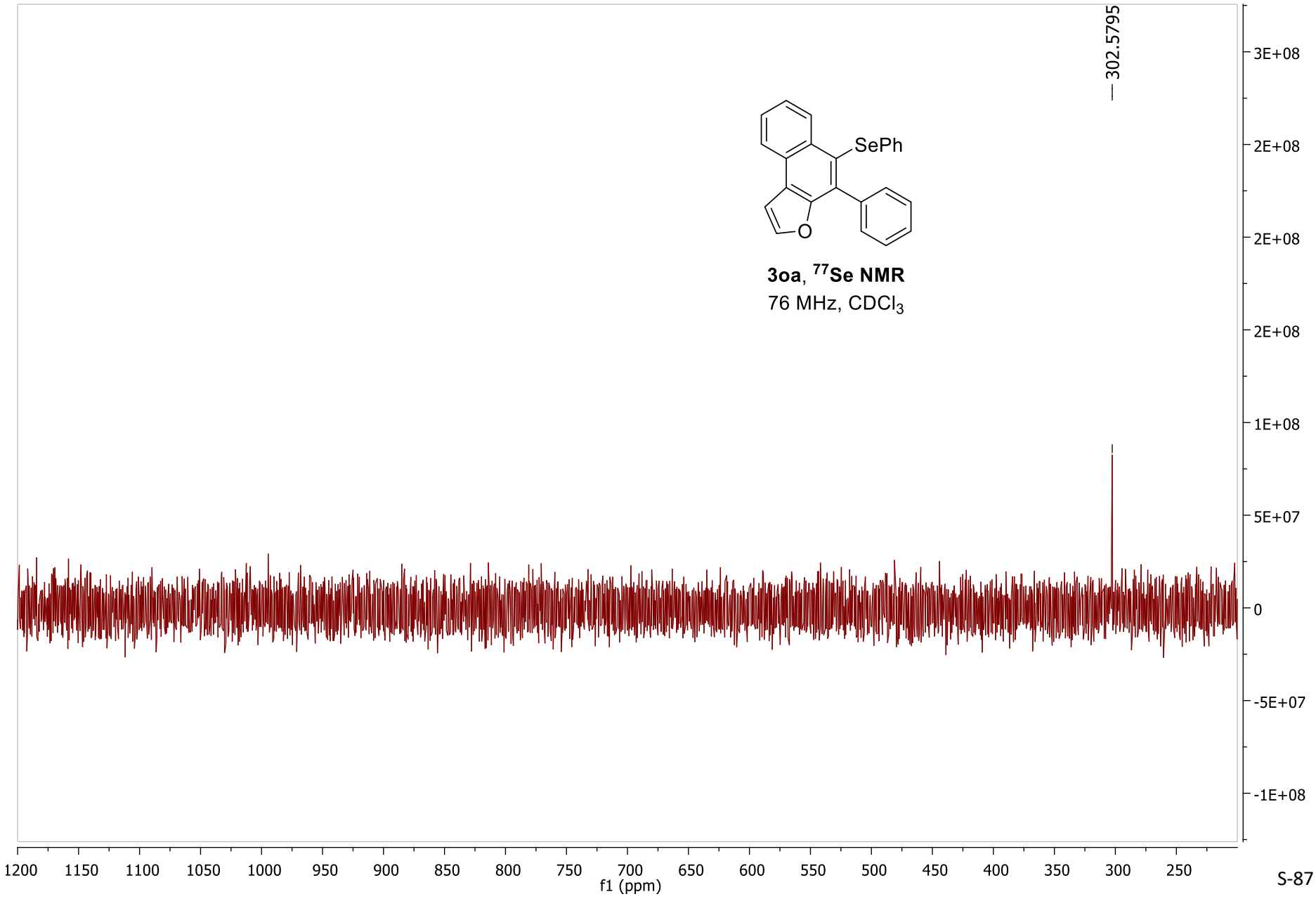
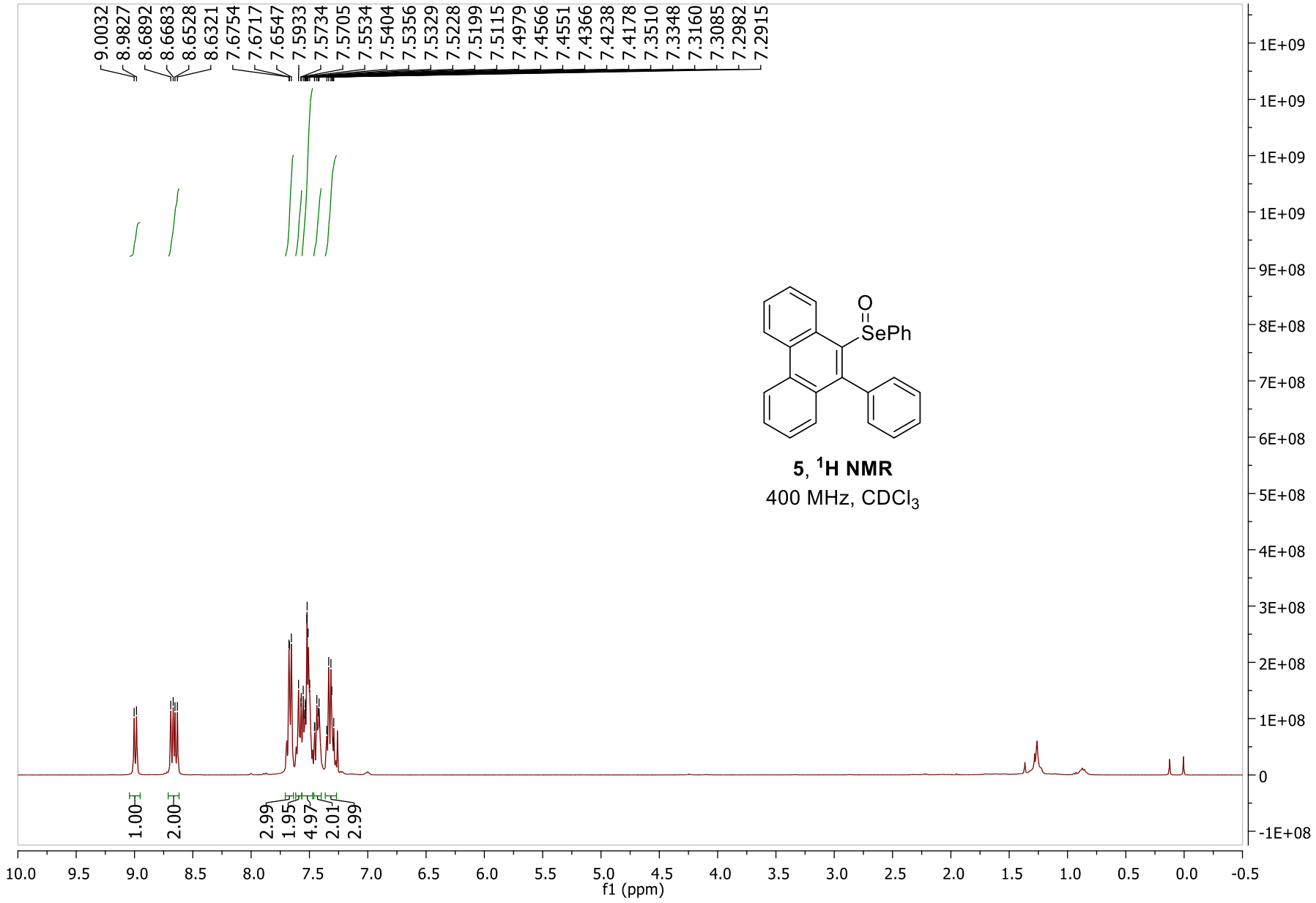
8.7204
8.1981
8.1963
7.7710
7.7658
7.6357
7.6320
7.6290
7.6262
7.6186
7.5459
7.5320
7.5282
7.5245
7.5107
7.4551
7.4475
7.4449
7.4386
7.4333
7.4180
7.4155
7.4127
7.4067
7.4026
7.4002
7.3951
7.3912
7.3879
7.3866
7.3823
7.3786
7.3611
7.3559
7.0678
7.0621
7.0592
7.0540
7.0512
7.0429
7.0315
7.0282
7.0245
SePh
O
3oa, 1H NMR
400 MHz, CDCl3
1.00
1.02
1.03
1.04
1.04
3.01
2.05
1.03
5.04
f1 (ppm)


150.7475
145.5405
130.0515
129.1053
128.9385
127.9822
127.7901
126.6251
126.0074
125.5653
123.7552
105.8078
SePh
O
3oa, 13C NMR
100 MHz, CDCl3
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


302.5795
SePh
O
3oa, 77Se NMR
76 MHz, CDCl3
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)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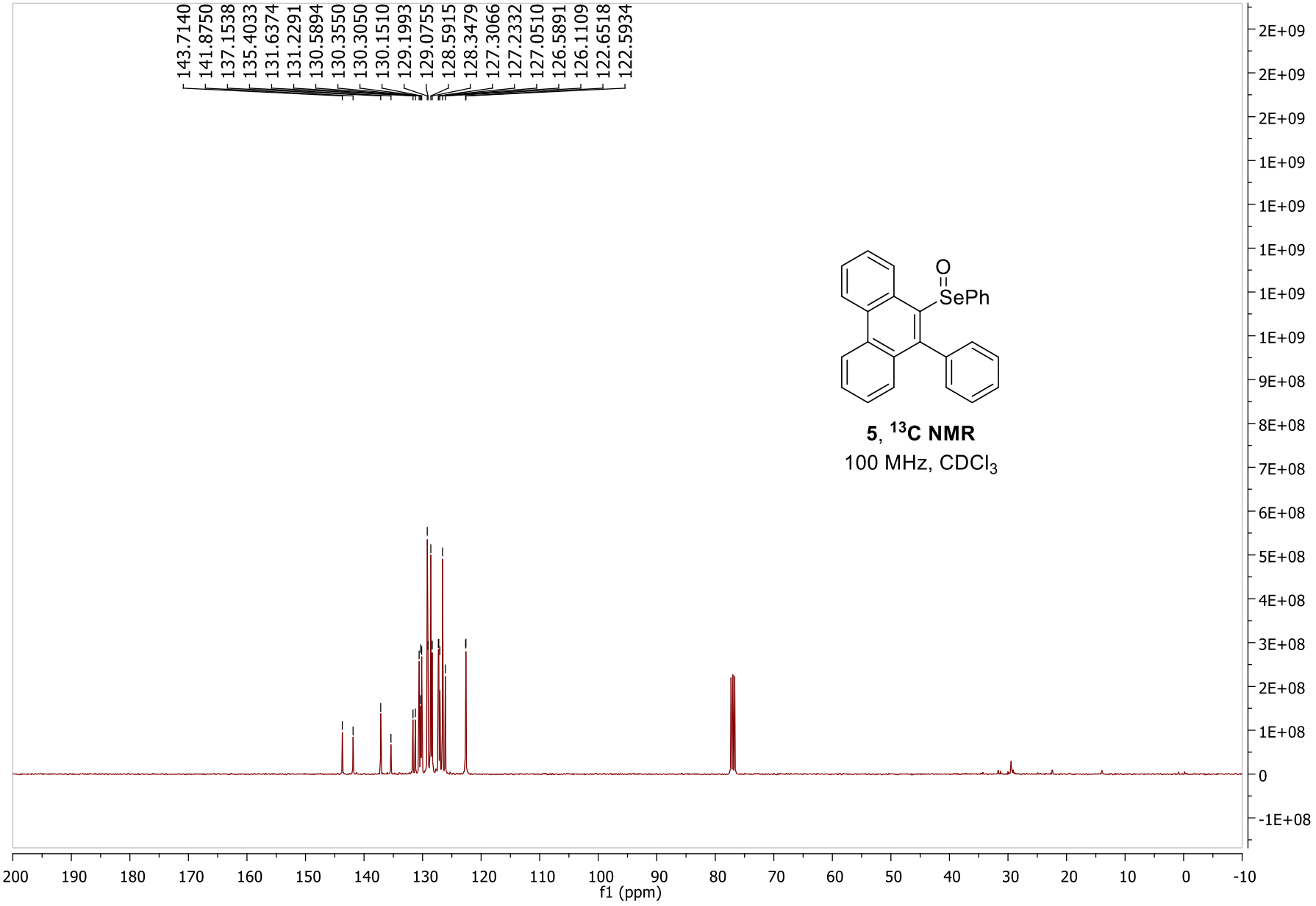
8.6892
8.6683
8.6528
8.6321
7.6754
7.6717
7.6547
7.5933
7.5734
7.5705
7.5534
7.5404
7.5356
7.5329
7.5228
7.5199
7.5115
7.4979
7.4566
7.4551
7.4366
7.4238
7.4178
7.3510
7.3348
7.3160
7.3085
7.2982
7.2915
O
SePh
5, 1H NMR
400 MHz, CDCl3
1.00
2.00
2.99
1.95
4.97
2.01
2.99
f1 (ppm)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141.8750
137.1538
135.4033
131.6374
131.2291
130.5894
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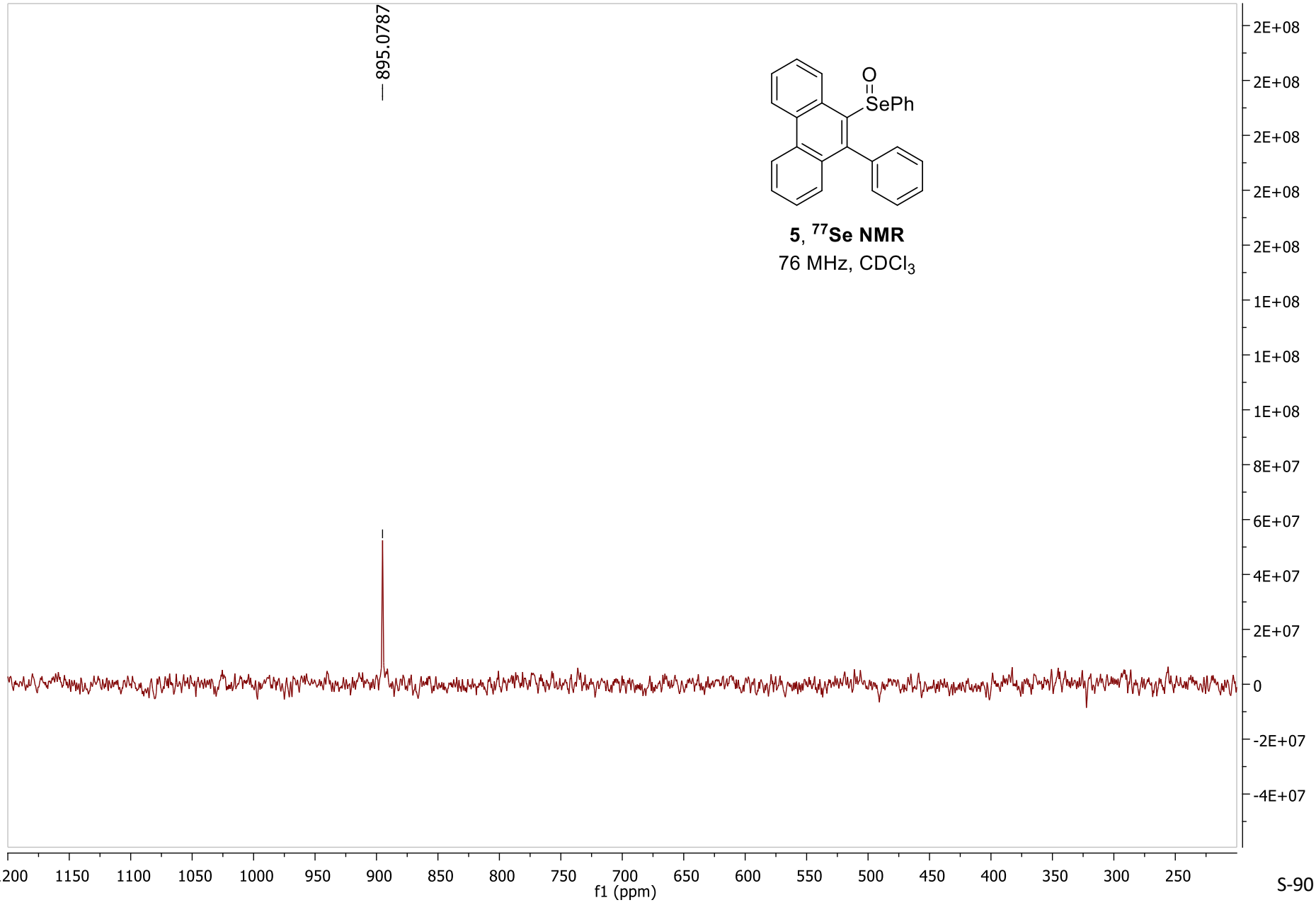
130.3050
130.1510
129.1993
129.0755
128.5915
128.3479
127.3066
127.2332
127.0510
126.5891
126.1109
122.6518
122.5934
O
SePh
5, 13C NMR
100 MHz, CDCl3
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


895.0787
O
SePh
5, 77Se NMR
76 MHz, CDCl3
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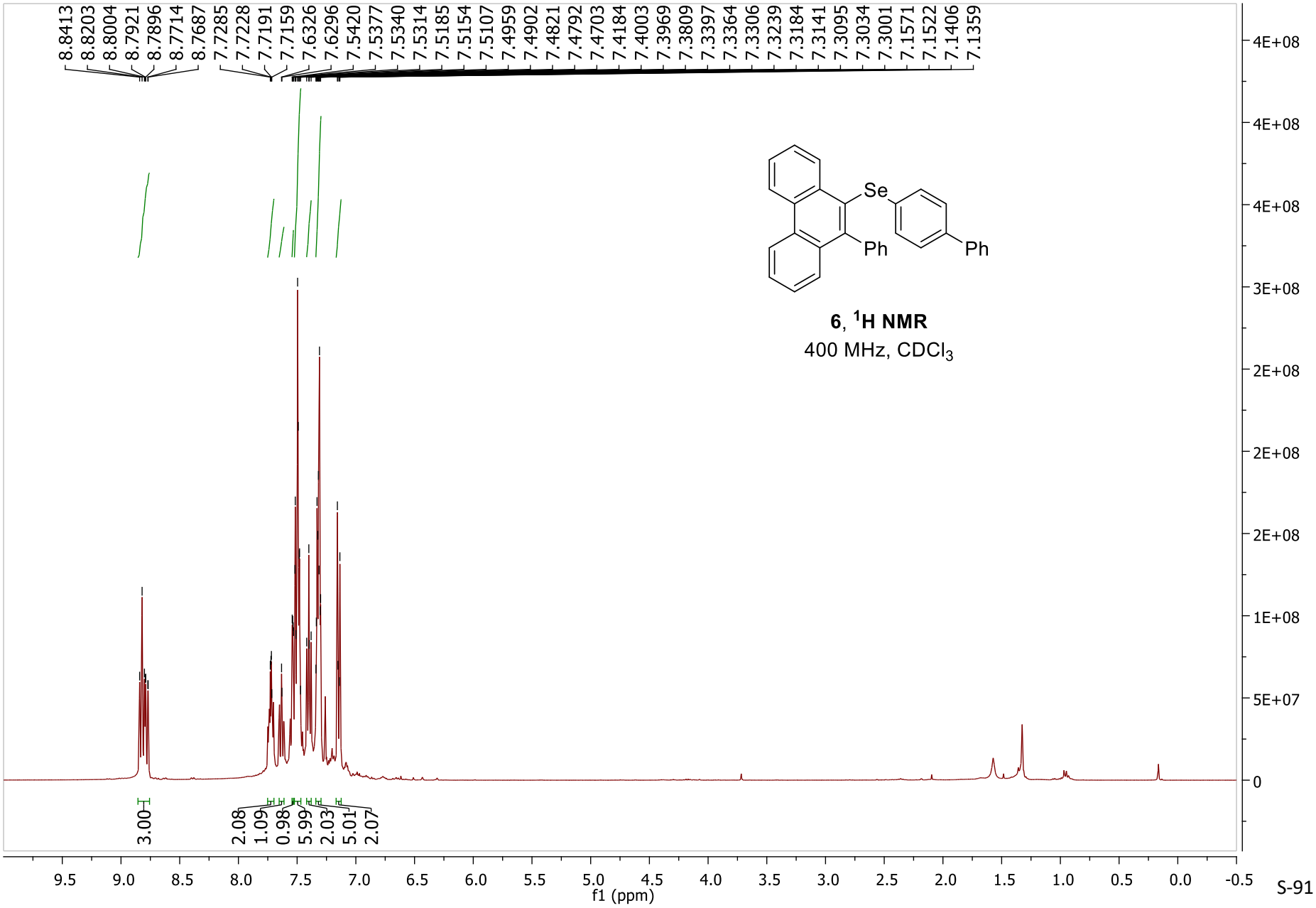
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
-4E+07
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)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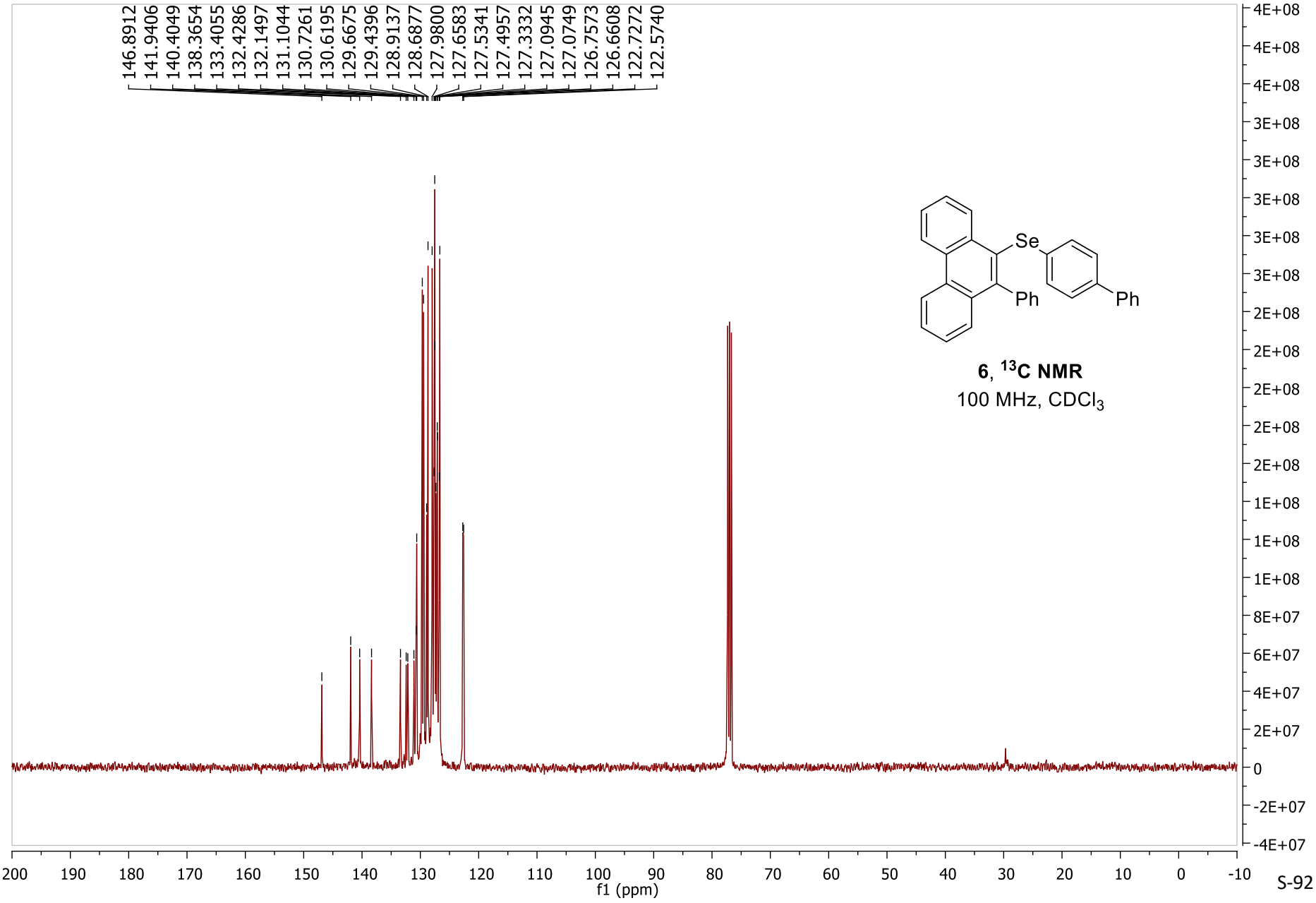
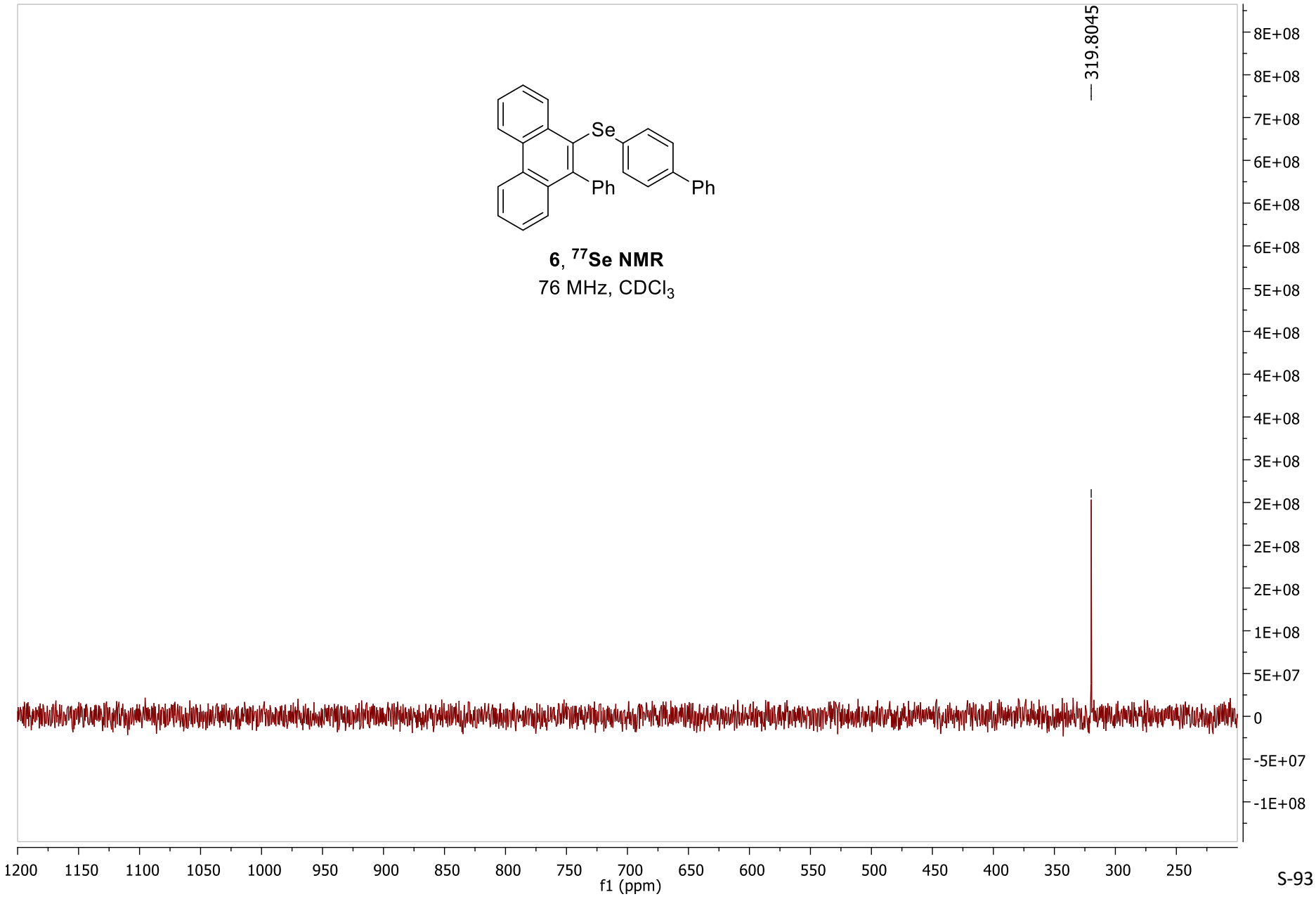
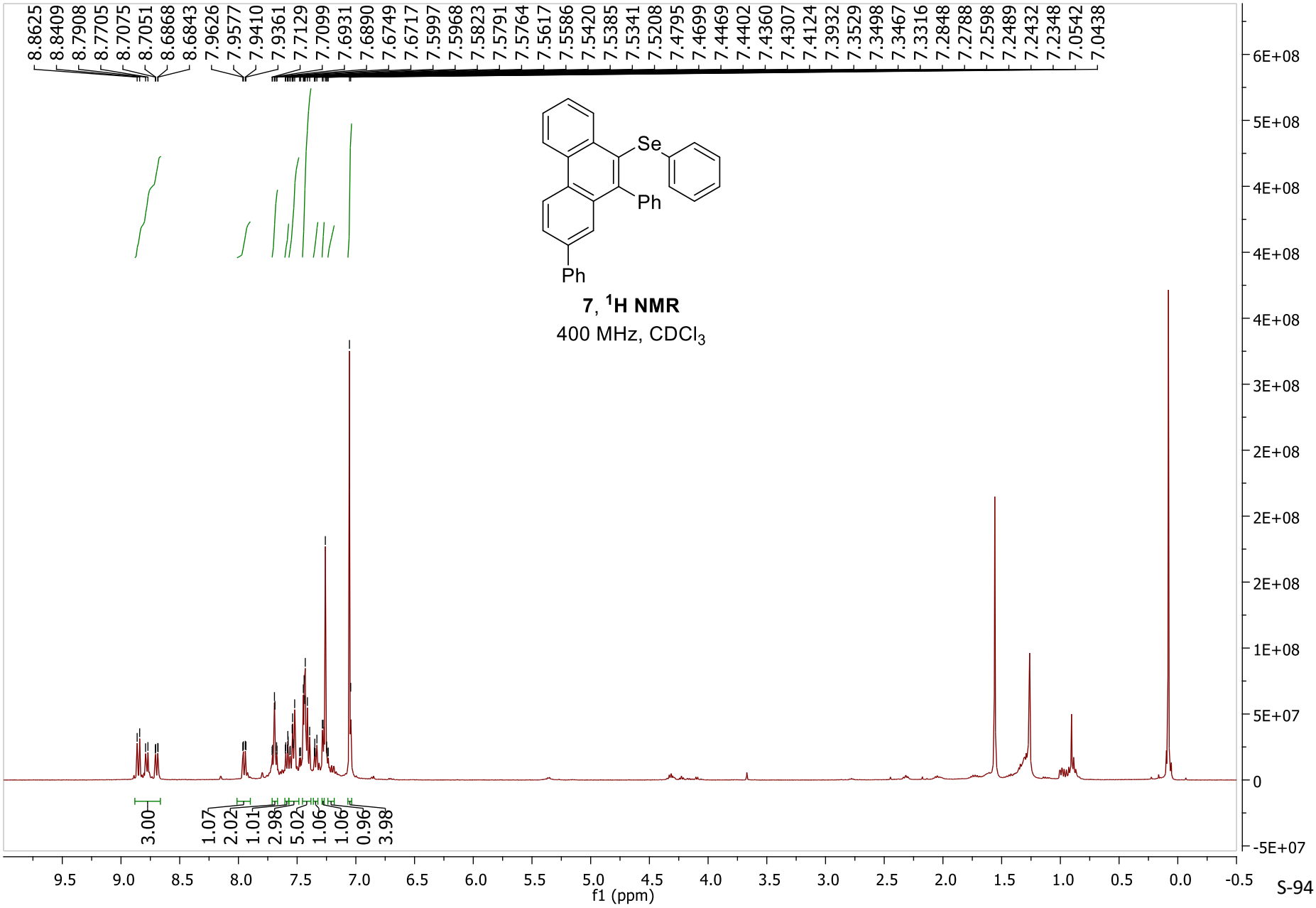
7.7159
7.6326
7.6296
7.5420
7.5377
7.5340
7.5314
7.5185
7.5154
7.5107
7.4959
7.4902
7.4821
7.4792
7.4703
7.4184
7.4003
7.3969
7.3809
7.3397
7.3364
7.3306
7.3239
7.3184
7.3141
7.3095
7.3034
7.3001
7.1571
7.1522
7.1406
7.1359
Se
Ph
Ph
6, 1H NMR
400 MHz, CDCl3
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
3.00
2.08
1.09
0.98
5.99
2.03
5.01
2.07
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)


146.8912
141.9406
140.4049
138.3654
133.4055
132.4286
132.1497
131.1044
130.7261
130.6195
129.6675
129.4396
128.9137
128.6877
127.9800
127.6583
127.5341
127.4957
127.3332
127.0945
127.0749
126.7573
126.6608
122.7272
122.5740
Se
Ph
Ph
6, 13C NMR
100 MHz, CDCl3
4E+08
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
-4E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




**6**, **$^{77}$Se NMR**

76 MHz, $CDCl_3$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8.7908
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8.7075
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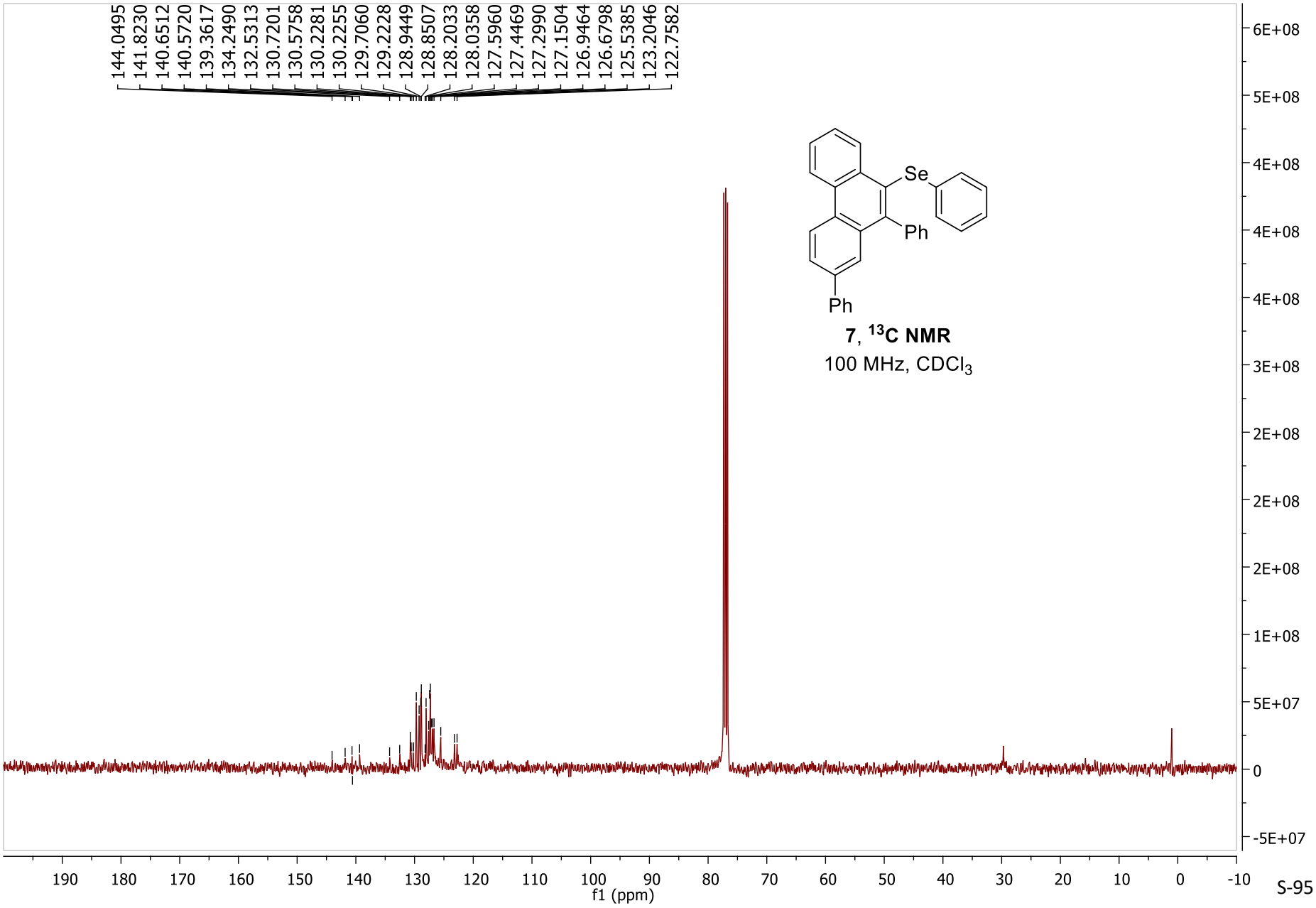
7.9410
7.9361
7.7129
7.7099
7.6931
7.6890
7.6749
7.6717
7.5997
7.5968
7.5823
7.5791
7.5764
7.5617
7.5586
7.5420
7.5385
7.5341
7.5208
7.4795
7.4699
7.4469
7.4402
7.4360
7.4307
7.4124
7.3932
7.3529
7.3498
7.3467
7.3316
7.2848
7.2788
7.2598
7.2489
7.2432
7.2348
7.0542
7.0438
Se
Ph
Ph
7, 1H NMR
400 MHz, CDCl3
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
3.00
1.07
2.02
1.01
2.98
5.02
1.06
1.06
0.96
3.98
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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132.5313
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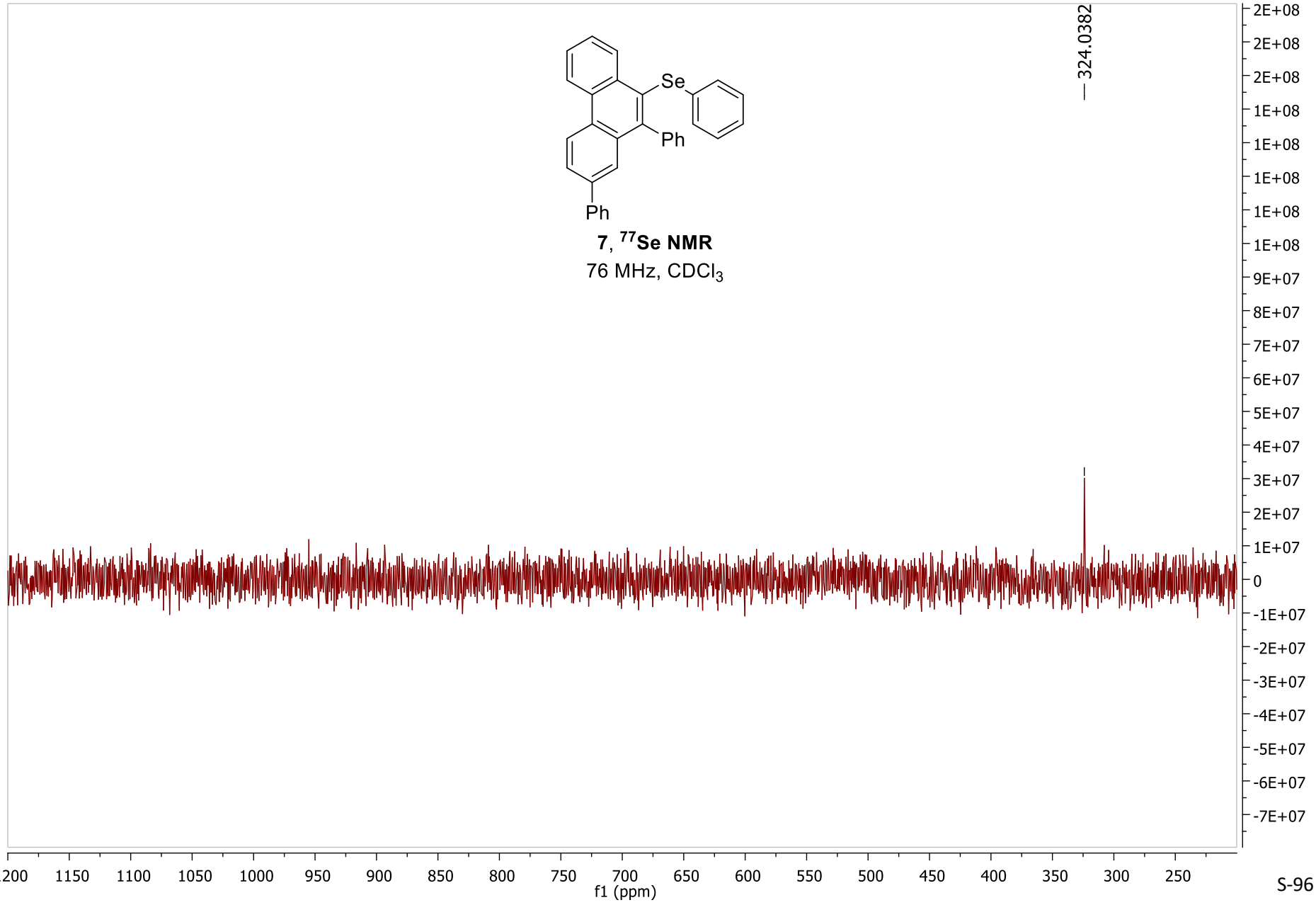
130.5758
130.2281
130.2255
129.7060
129.2228
128.9449
128.8507
128.2033
128.0358
127.5960
127.4469
127.2990
127.1504
126.9464
126.6798
125.5385
123.2046
122.7582
Se
Ph
Ph
7, 13C NMR
100 MHz, CDCl3
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Se
Ph
Ph
324.0382
7, 77Se NMR
76 MHz, CDCl3
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2E+08
2E+08
1E+08
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1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
-2E+07
-3E+07
-4E+07
-5E+07
-6E+07
-7E+07
1200 1150 1100 1050 1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250
f1 (ppm)

## 14. Table *S4*. Cartesian coordinates for various intermediates and transition states.

**Radical pathway:**

**A**:

| | | | |
|---|---|---|---|
| C | 4.48255900 | -2.73744300 | 0.87458600 |
| C | 4.38739100 | -1.41710000 | 0.41435600 |
| C | 3.24733100 | -0.63019800 | 0.66647100 |
| C | 2.17519900 | -1.21155100 | 1.39671200 |
| C | 2.27641100 | -2.54299600 | 1.85645600 |
| C | 3.42303100 | -3.30296000 | 1.60269200 |
| H | 5.37642100 | -3.31687800 | 0.67087800 |
| H | 5.21784200 | -0.97931500 | -0.13101500 |
| H | 1.44428700 | -2.97213900 | 2.40476400 |
| H | 3.48927600 | -4.32329800 | 1.96342400 |
| C | 3.20865200 | 0.76854300 | 0.15024100 |
| C | 3.65443900 | 1.04118700 | -1.16028100 |
| C | 2.79455800 | 1.84537900 | 0.96108900 |
| C | 3.69324100 | 2.35685900 | -1.64683200 |
| H | 3.95971100 | 0.22000300 | -1.80263200 |
| C | 2.83050500 | 3.16115100 | 0.47529200 |
| H | 2.47051500 | 1.65778600 | 1.97987900 |
| C | 3.28271700 | 3.42305900 | -0.82896900 |
| H | 4.03728400 | 2.54691100 | -2.65797000 |

| | | | |
|---|---|---|---|
| H | 2.51671000 | 3.97916000 | 1.11554900 |
| H | 3.31378500 | 4.44120900 | -1.20219400 |
| C | 0.95251100 | -0.49270900 | 1.63179700 |
| C | -0.09558100 | 0.11248600 | 1.81398000 |
| C | -1.28906000 | 0.89032400 | 1.98179200 |
| C | -1.21494900 | 2.29802800 | 1.89010100 |
| C | -2.53552800 | 0.27066200 | 2.21918000 |
| C | -2.37040600 | 3.07249300 | 2.04007300 |
| H | -0.25567000 | 2.76901800 | 1.69535100 |
| C | -3.68943800 | 1.05219400 | 2.36126200 |
| H | -2.59019200 | -0.81140600 | 2.28395800 |
| C | -3.61025400 | 2.45308700 | 2.27391500 |
| H | -2.30807400 | 4.15302300 | 1.96366000 |
| H | -4.64620100 | 0.57331200 | 2.54002000 |
| H | -4.50609000 | 3.05508900 | 2.38401900 |
| C | -0.62674800 | 3.43237500 | -1.45682100 |
| C | -2.02381700 | 3.53773300 | -1.34034700 |
| C | -2.81623600 | 2.37964400 | -1.23285300 |
| C | -2.22026700 | 1.11368700 | -1.24443700 |
| C | -0.81759000 | 1.00847100 | -1.37629100 |
| C | -0.01880200 | 2.17122700 | -1.47648200 |
| H | -0.01229700 | 4.32349700 | -1.52911900 |
| H | -2.49307300 | 4.51578800 | -1.32495200 |

| | | | |
|---|---|---|---|
| H | -3.89260900 | 2.46398500 | -1.13114400 |
| H | -2.82926800 | 0.21962700 | -1.15266800 |
| H | 1.06111600 | 2.08696700 | -1.56773300 |
| Se | 0.07542700 | -0.68182300 | -1.43632800 |
| I | -2.15843800 | -2.74985200 | -0.65560400 |

**TSa:**

| | | | |
|---|---|---|---|
| C | -3.93178900 | 3.27782800 | 1.24237500 |
| C | -4.12253200 | 1.96982900 | 0.77194000 |
| C | -3.05002100 | 1.06400300 | 0.68862600 |
| C | -1.76092900 | 1.50615700 | 1.07478100 |
| C | -1.56982300 | 2.81720100 | 1.54819400 |
| C | -2.65423500 | 3.70090600 | 1.64181200 |
| H | -4.77427200 | 3.95832400 | 1.30158700 |
| H | -5.11504200 | 1.63799400 | 0.48249500 |
| H | -0.57177800 | 3.13758300 | 1.82951300 |
| H | -2.50232600 | 4.70835700 | 2.01283500 |
| C | -3.29337700 | -0.32963700 | 0.21711200 |
| C | -3.97274300 | -0.56175100 | -0.99485200 |
| C | -2.89438600 | -1.43376800 | 0.99846200 |
| C | -4.24228300 | -1.87173100 | -1.42293700 |
| H | -4.27879600 | 0.28325000 | -1.60542600 |
| C | -3.16894500 | -2.74217500 | 0.57528900 |

| | | | |
|---|---|---|---|
| H | -2.39500300 | -1.26551700 | 1.94800900 |
| C | -3.84134500 | -2.96611500 | -0.63844700 |
| H | -4.75980400 | -2.03594300 | -2.36204600 |
| H | -2.86554800 | -3.58289200 | 1.19083300 |
| H | -4.05205900 | -3.97855900 | -0.96645600 |
| C | -0.58524900 | 0.63886700 | 0.88186200 |
| C | 0.22484000 | -0.10278300 | 1.52657500 |
| C | 1.22526600 | -1.02576200 | 1.88909800 |
| C | 0.96425900 | -2.42066600 | 1.77745800 |
| C | 2.49532500 | -0.58531200 | 2.35392700 |
| C | 1.95528300 | -3.34369500 | 2.11305600 |
| H | -0.00274100 | -2.75198800 | 1.40960700 |
| C | 3.47774100 | -1.52163500 | 2.68368100 |
| H | 2.69106000 | 0.47868400 | 2.43662000 |
| C | 3.21404200 | -2.90048400 | 2.56457200 |
| H | 1.75664600 | -4.40543400 | 2.01610000 |
| H | 4.44784100 | -1.18463100 | 3.03175500 |
| H | 3.98212800 | -3.62206700 | 2.82132100 |
| C | -0.00869500 | -3.44798100 | -1.61800300 |
| C | 1.35893000 | -3.77044100 | -1.59064100 |
| C | 2.32035700 | -2.75075400 | -1.49837900 |
| C | 1.92221100 | -1.40610400 | -1.41951200 |
| C | 0.55331600 | -1.09399500 | -1.44352400 |

| | | | |
|---|---|---|---|
| C | -0.41665100 | -2.10768100 | -1.54845100 |
| H | -0.75697900 | -4.23047000 | -1.69167900 |
| H | 1.67296900 | -4.80775200 | -1.64129900 |
| H | 3.37653300 | -2.99735200 | -1.47716500 |
| H | 2.66478500 | -0.61905200 | -1.33217200 |
| H | -1.47445700 | -1.85804700 | -1.57151100 |
| Se | -0.09542900 | 0.73638500 | -1.29312000 |
| I | 2.54735900 | 2.38763200 | -0.71908100 |

**B:**

| | | | |
|---|---|---|---|
| C | 3.88270800 | -3.30203800 | 1.30220200 |
| C | 4.09631900 | -2.00673200 | 0.80654700 |
| C | 3.03210200 | -1.09700800 | 0.67252700 |
| C | 1.72930000 | -1.52065900 | 1.03068900 |
| C | 1.51670100 | -2.81695200 | 1.53242200 |
| C | 2.59191700 | -3.70598000 | 1.67765600 |
| H | 4.71778900 | -3.98716300 | 1.40064800 |
| H | 5.09878800 | -1.68763000 | 0.53748100 |
| H | 0.50872200 | -3.12337400 | 1.79437900 |
| H | 2.42286600 | -4.70300500 | 2.06924200 |
| C | 3.29807700 | 0.28848800 | 0.18751600 |
| C | 3.97969200 | 0.50269500 | -1.02602800 |
| C | 2.91703900 | 1.40304500 | 0.96315700 |

| | | | |
|---|---|---|---|
| C | 4.26909500 | 1.80620200 | -1.46168500 |
| H | 4.27255300 | -0.35063000 | -1.63148900 |
| C | 3.21319300 | 2.70467300 | 0.53370200 |
| H | 2.41355900 | 1.24619700 | 1.91266200 |
| C | 3.88771800 | 2.91106600 | -0.68207100 |
| H | 4.78777800 | 1.95731300 | -2.40237200 |
| H | 2.92355700 | 3.55342600 | 1.14488200 |
| H | 4.11473500 | 3.91811000 | -1.01570200 |
| C | 0.55874000 | -0.64380000 | 0.77189000 |
| C | -0.19841200 | 0.08302900 | 1.52997900 |
| C | -1.19174600 | 1.00696300 | 1.90393200 |
| C | -0.92112800 | 2.40432900 | 1.82335400 |
| C | -2.46541800 | 0.56956000 | 2.36768900 |
| C | -1.90398600 | 3.32757700 | 2.18059600 |
| H | 0.04775700 | 2.73649500 | 1.46136100 |
| C | -3.43870400 | 1.50730200 | 2.71912700 |
| H | -2.67049800 | -0.49406300 | 2.43111600 |
| C | -3.16577700 | 2.88666800 | 2.62731500 |
| H | -1.69627100 | 4.38947100 | 2.10512900 |
| H | -4.41016900 | 1.17029700 | 3.06389300 |
| H | -3.92701100 | 3.60893100 | 2.90185100 |
| C | 0.00043600 | 3.48185100 | -1.61071000 |
| C | -1.36712000 | 3.80330100 | -1.57672100 |

| | | | |
|---|---|---|---|
| C | -2.32787600 | 2.78420700 | -1.47258300 |
| C | -1.92850800 | 1.44012300 | -1.38661300 |
| C | -0.56035900 | 1.13186600 | -1.41525500 |
| C | 0.40974300 | 2.14197600 | -1.53538900 |
| H | 0.74759000 | 4.26416400 | -1.69557300 |
| H | -1.68198900 | 4.84006300 | -1.63252700 |
| H | -3.38396400 | 3.03051900 | -1.44763300 |
| H | -2.66982000 | 0.65302400 | -1.28983000 |
| H | 1.46735800 | 1.89237500 | -1.56625600 |
| Se | 0.09375700 | -0.70078600 | -1.25604800 |
| I | -2.56138700 | -2.37053400 | -0.75877500 |

**B′:**

| | | | |
|---|---|---|---|
| C | -4.44609100 | -1.18843900 | 2.71254200 |
| C | -4.33288300 | -0.24380100 | 1.68250300 |
| C | -3.08910700 | 0.05420800 | 1.09468300 |
| C | -1.93069000 | -0.60210200 | 1.58489000 |
| C | -2.05323300 | -1.55958700 | 2.61052800 |
| C | -3.30158100 | -1.85753800 | 3.17177700 |
| H | -5.41715900 | -1.40462000 | 3.14463100 |
| H | -5.22104200 | 0.25692200 | 1.30888100 |
| H | -1.16271000 | -2.05055600 | 2.99182500 |

| | | | |
|---|---|---|---|
| H | -3.37777600 | -2.59296900 | 3.96501600 |
| C | -3.04640400 | 1.02267700 | -0.04004000 |
| C | -3.59144400 | 2.31273800 | 0.09747100 |
| C | -2.51310400 | 0.63479200 | -1.28535600 |
| C | -3.59043900 | 3.20557400 | -0.98724300 |
| H | -4.00245000 | 2.62208400 | 1.05453300 |
| C | -2.52088000 | 1.51995800 | -2.37157500 |
| H | -2.09692500 | -0.36238800 | -1.40420100 |
| C | -3.05707800 | 2.81205500 | -2.22507000 |
| H | -4.00495300 | 4.20092000 | -0.86556600 |
| H | -2.11194800 | 1.20302700 | -3.32605600 |
| H | -3.06050900 | 3.49973500 | -3.06421600 |
| C | -0.57631700 | -0.22390900 | 1.09503200 |
| C | -0.09363200 | 0.96624700 | 0.87547100 |
| C | 0.76827600 | 2.01540700 | 0.51719400 |
| C | 1.67199200 | 2.57335700 | 1.46846900 |
| C | 0.73917800 | 2.54352400 | -0.80737900 |
| C | 2.52906900 | 3.60856200 | 1.09274400 |
| H | 1.69572500 | 2.17288600 | 2.47691800 |
| C | 1.60326700 | 3.58009000 | -1.16505600 |
| H | 0.04184200 | 2.12614200 | -1.52762400 |
| C | 2.50245700 | 4.11649300 | -0.22148700 |
| H | 3.22358300 | 4.01991700 | 1.81746900 |

| | | | |
|---|---|---|---|
| H | 1.58099200 | 3.97325900 | -2.17567000 |
| H | 3.17126400 | 4.92148300 | -0.50601500 |
| C | 4.06379300 | -0.13817700 | 2.47535900 |
| C | 4.75373900 | 0.43737100 | 1.39539700 |
| C | 4.23676300 | 0.33377100 | 0.09420700 |
| C | 3.02552200 | -0.33991900 | -0.13403500 |
| C | 2.34359500 | -0.90916200 | 0.95118200 |
| C | 2.85478600 | -0.81722300 | 2.25704200 |
| H | 4.46103100 | -0.06130700 | 3.48144900 |
| H | 5.68709400 | 0.96267200 | 1.56757100 |
| H | 4.76555200 | 0.78017300 | -0.74096000 |
| H | 2.62008100 | -0.40953500 | -1.13841700 |
| H | 2.32124300 | -1.26100800 | 3.09179100 |
| Se | 0.63460800 | -1.82935400 | 0.71920000 |
| I | 0.40779400 | -1.95359700 | -2.45735200 |

**$TS_b$:**

| | | | |
|---|---|---|---|
| C | -4.13440200 | -3.49134700 | 0.64988900 |
| C | -4.38328300 | -2.17084700 | 0.25311300 |
| C | -3.32582400 | -1.27175100 | 0.02709200 |
| C | -1.98668500 | -1.69679600 | 0.24844700 |
| C | -1.75005700 | -3.03073000 | 0.63243700 |
| C | -2.81026600 | -3.92635900 | 0.82183500 |

| | | | |
|---|---|---|---|
| H | -4.95957100 | -4.17642800 | 0.81002900 |
| H | -5.40244200 | -1.83312900 | 0.09029400 |
| H | -0.73394200 | -3.38686200 | 0.78144300 |
| H | -2.60443900 | -4.95194300 | 1.10760600 |
| C | -3.57868100 | 0.10961700 | -0.43381500 |
| C | -4.48013300 | 0.96298500 | 0.21282100 |
| C | -2.77780600 | 0.60091300 | -1.51568100 |
| C | -4.62662100 | 2.29757900 | -0.20964800 |
| H | -5.05312900 | 0.59359100 | 1.05860600 |
| C | -2.97859600 | 1.94043100 | -1.96662800 |
| H | -2.34745000 | -0.11867700 | -2.21034500 |
| C | -3.87088200 | 2.78097500 | -1.30024500 |
| H | -5.32330400 | 2.95354900 | 0.30121800 |
| H | -2.42398900 | 2.29941500 | -2.82744800 |
| H | -4.00061100 | 3.80540100 | -1.63360400 |
| C | -0.87768100 | -0.70858300 | 0.15125000 |
| C | -0.87401900 | 0.40678000 | -0.57014700 |
| C | 0.01833000 | 1.47333800 | -0.95303800 |
| C | -0.20786500 | 2.79658600 | -0.50867900 |
| C | 1.09294300 | 1.21081400 | -1.83541600 |
| C | 0.64860000 | 3.82755300 | -0.90801000 |
| H | -1.03942400 | 2.99777200 | 0.16075600 |
| C | 1.94265500 | 2.25041900 | -2.23587800 |

| | | | |
|---|---|---|---|
| H | 1.25902600 | 0.19743600 | -2.18848700 |
| C | 1.72768400 | 3.55933900 | -1.77101200 |
| H | 0.48030600 | 4.83667000 | -0.54641400 |
| H | 2.77000100 | 2.04036100 | -2.90579000 |
| H | 2.38894300 | 4.36222300 | -2.07979500 |
| C | 0.82477300 | 2.75975500 | 2.98972400 |
| C | 2.05179000 | 3.26502500 | 2.52852700 |
| C | 2.87039200 | 2.47924000 | 1.70106400 |
| C | 2.46677100 | 1.18662200 | 1.32911300 |
| C | 1.24172100 | 0.69309300 | 1.79788700 |
| C | 0.41480200 | 1.46694200 | 2.62879900 |
| H | 0.18979300 | 3.36460500 | 3.62785900 |
| H | 2.36542700 | 4.26478800 | 2.80938000 |
| H | 3.81463400 | 2.86945100 | 1.33676700 |
| H | 3.09109900 | 0.58244800 | 0.67788200 |
| H | -0.53247900 | 1.07573700 | 2.98727200 |
| Se | 0.66595400 | -1.12415900 | 1.37346000 |
| I | 2.83220800 | -2.23420400 | -0.67471400 |

**C:**

| | | | |
|---|---|---|---|
| C | -4.07428100 | -3.48476300 | 0.76341100 |
| C | -4.37967000 | -2.18608700 | 0.34771500 |
| C | -3.35893500 | -1.24064100 | 0.10256400 |

| | | | |
|---|---|---|---|
| C | -2.00151400 | -1.61813600 | 0.30960000 |
| C | -1.70893900 | -2.93530100 | 0.71474700 |
| C | -2.73100700 | -3.86560600 | 0.93590700 |
| H | -4.86980600 | -4.20217500 | 0.93258200 |
| H | -5.41459900 | -1.90915800 | 0.17404100 |
| H | -0.68030300 | -3.25373000 | 0.85576000 |
| H | -2.48393400 | -4.87745900 | 1.23719000 |
| C | -3.64721700 | 0.10996300 | -0.37891600 |
| C | -4.85046500 | 0.76216800 | -0.13708300 |
| C | -2.56138000 | 0.75005200 | -1.21816200 |
| C | -5.09641800 | 2.06768000 | -0.60828400 |
| H | -5.61134500 | 0.26847400 | 0.46133400 |
| C | -2.87148800 | 2.17395500 | -1.61389500 |
| H | -2.49717500 | 0.16673200 | -2.16506000 |
| C | -4.07706900 | 2.76175600 | -1.34197300 |
| H | -6.03904100 | 2.55755000 | -0.39240900 |
| H | -2.11731800 | 2.70910000 | -2.18135500 |
| H | -4.26711700 | 3.77580000 | -1.67963200 |
| C | -0.94830300 | -0.58809100 | 0.12910400 |
| C | -1.15964100 | 0.54459400 | -0.59040000 |
| C | -0.09390400 | 1.52160000 | -0.94650400 |
| C | -0.09659500 | 2.83535900 | -0.43894600 |
| C | 0.91651600 | 1.12981500 | -1.84157100 |

| | | | |
|---|---|---|---|
| C | 0.91402400 | 3.73330100 | -0.80286100 |
| H | -0.87391300 | 3.14202900 | 0.25553000 |
| C | 1.92454300 | 2.03364100 | -2.21525400 |
| H | 0.91384700 | 0.11959300 | -2.24058200 |
| C | 1.92752800 | 3.33557100 | -1.69349200 |
| H | 0.91611100 | 4.73661900 | -0.38965400 |
| H | 2.70144700 | 1.71855900 | -2.90438300 |
| H | 2.70963200 | 4.03389000 | -1.97327100 |
| C | 0.96393600 | 2.71678300 | 3.06095000 |
| C | 2.18094800 | 3.25715300 | 2.61146700 |
| C | 2.96028900 | 2.55501500 | 1.67942300 |
| C | 2.52716100 | 1.31281000 | 1.18801400 |
| C | 1.31251000 | 0.78653600 | 1.64401500 |
| C | 0.52524500 | 1.47199900 | 2.58292000 |
| H | 0.36000900 | 3.25599500 | 3.78262900 |
| H | 2.51700200 | 4.21892000 | 2.98411800 |
| H | 3.89583000 | 2.97247600 | 1.32278900 |
| H | 3.11876700 | 0.77666000 | 0.45231700 |
| H | -0.41290800 | 1.05247700 | 2.93347100 |
| Se | 0.73610800 | -0.98748200 | 1.05975300 |
| I | 2.98362000 | -2.02518300 | -0.96135900 |

**$TS_C$:**

| | | | |
|---|---|---|---|
| C | -4.95731600 | 2.96904400 | 0.23383000 |
| C | -4.70576000 | 4.14827200 | -0.45669800 |
| C | -5.73896800 | 5.08255800 | -0.73149500 |
| C | -7.06238700 | 4.79057200 | -0.28790200 |
| C | -7.29734100 | 3.57822700 | 0.41228000 |
| C | -6.26724600 | 2.68186000 | 0.67496300 |
| H | -4.14891100 | 2.27573000 | 0.43747200 |
| H | -3.69069800 | 4.35703400 | -0.77122500 |
| H | -8.29347600 | 3.32831200 | 0.75880500 |
| H | -6.47249000 | 1.76595200 | 1.21754500 |
| C | -5.47076900 | 6.33013400 | -1.43756600 |
| C | -4.21353200 | 6.61487200 | -2.01754600 |
| C | -6.49591900 | 7.34841400 | -1.46585500 |
| C | -3.96769200 | 7.81966400 | -2.66945800 |
| H | -3.41938500 | 5.87889100 | -1.98001400 |
| C | -6.24264100 | 8.54688700 | -2.23621400 |
| H | -6.24877600 | 7.99937300 | 0.04646900 |
| C | -5.00111600 | 8.78600200 | -2.79123600 |
| H | -2.99481500 | 8.00747000 | -3.11020900 |
| H | -7.02924300 | 9.28542200 | -2.32994800 |
| H | -4.81842500 | 9.70674100 | -3.33446800 |
| C | -8.13832800 | 5.74756900 | -0.57424200 |

| | | | |
|---|---|---|---|
| C | -7.88944700 | 6.98330800 | -1.11125500 |
| C | -8.92881500 | 8.04690000 | -1.24119500 |
| C | -9.41538700 | 8.45529900 | -2.49723400 |
| C | -9.39286100 | 8.68325600 | -0.07809200 |
| C | -10.37772700 | 9.46818300 | -2.58500100 |
| H | -9.05617800 | 7.96509900 | -3.39793800 |
| C | -10.35662000 | 9.70207500 | -0.16559900 |
| H | -9.00997600 | 8.37544000 | 0.89087700 |
| C | -10.85201800 | 10.09408000 | -1.41797100 |
| H | -10.76080500 | 9.76450300 | -3.55586100 |
| H | -10.71467600 | 10.18315300 | 0.73897500 |
| H | -11.59986900 | 10.87735700 | -1.48795500 |
| C | -11.52059500 | 5.85666700 | -3.93583600 |
| C | -12.60388300 | 6.71888200 | -3.69309500 |
| C | -12.88615000 | 7.14198000 | -2.38512800 |
| C | -12.08526400 | 6.71348800 | -1.31371500 |
| C | -11.00952600 | 5.85455900 | -1.57118100 |
| C | -10.72070500 | 5.41313800 | -2.87221100 |
| H | -11.30084400 | 5.52588500 | -4.94511000 |
| H | -13.22105800 | 7.05787800 | -4.51830000 |
| H | -13.71639700 | 7.81356600 | -2.19499000 |
| H | -12.28927400 | 7.06046100 | -0.30494200 |
| H | -9.88730200 | 4.74263700 | -3.05874900 |

| | | | |
|---|---|---|---|
| Se | -9.94588900 | 5.14941700 | -0.09343900 |
| I | -11.05630400 | 6.48391900 | 2.58370700 |

**D (3aa):**

| | | | |
|---|---|---|---|
| C | -4.42392200 | -2.83665300 | 1.31273600 |
| C | -4.56981800 | -1.63938600 | 0.62618500 |
| C | -3.45175200 | -0.81986200 | 0.31487500 |
| C | -2.15409000 | -1.24442600 | 0.72769500 |
| C | -2.02957200 | -2.47365100 | 1.43501300 |
| C | -3.13814200 | -3.25834800 | 1.72097700 |
| H | -5.29361500 | -3.44358300 | 1.53861800 |
| H | -5.56456800 | -1.33560600 | 0.32638800 |
| H | -1.05773100 | -2.81152900 | 1.77374200 |
| H | -3.01677800 | -4.19031900 | 2.26158000 |
| C | -3.60431900 | 0.43868600 | -0.40974000 |
| C | -4.87354100 | 0.90171600 | -0.84954300 |
| C | -2.45456400 | 1.22635800 | -0.69765500 |
| C | -5.00278200 | 2.09065700 | -1.55556100 |
| H | -5.76768300 | 0.32830600 | -0.64071600 |
| C | -2.60656900 | 2.43455600 | -1.43685300 |
| H | -1.41588300 | -1.44866000 | -2.19155500 |
| C | -3.85657800 | 2.86326700 | -1.85887600 |
| H | -5.98243500 | 2.42315900 | -1.88073600 |

| | | | |
|---|---|---|---|
| H | -1.72942000 | 3.02294200 | -1.67788000 |
| H | -3.95534500 | 3.78536900 | -2.42078500 |
| C | -1.00152100 | -0.40330400 | 0.41291500 |
| C | -1.13080200 | 0.78305300 | -0.27396200 |
| C | 0.03917400 | 1.62510200 | -0.67040400 |
| C | 0.28494100 | 2.85835200 | -0.03818000 |
| C | 0.87428600 | 1.20571100 | -1.71742900 |
| C | 1.37404200 | 3.64720100 | -0.42892200 |
| H | -0.36477800 | 3.18588300 | 0.76889900 |
| C | 1.96648800 | 1.99675500 | -2.11172700 |
| H | 0.67643200 | 0.26201200 | -2.21754700 |
| C | 2.22049700 | 3.21599000 | -1.46605000 |
| H | 1.56642900 | 4.58831500 | 0.07556000 |
| H | 2.61185000 | 1.65893000 | -2.91622700 |
| H | 3.06733600 | 3.82516500 | -1.76519600 |
| C | 1.58300500 | 2.26211000 | 3.34661400 |
| C | 2.81754600 | 2.71885200 | 2.85294300 |
| C | 3.43365300 | 2.05733800 | 1.77946400 |
| C | 2.81931700 | 0.94106700 | 1.18763000 |
| C | 1.59020700 | 0.49764600 | 1.69112100 |
| C | 0.96568200 | 1.14210100 | 2.77095900 |
| H | 1.10416300 | 2.77000400 | 4.17676300 |
| H | 3.29271000 | 3.58495000 | 3.30097200 |

| | | | |
|---|---|---|---|
| H | 4.38131000 | 2.41361500 | 1.38999200 |
| H | 3.28253800 | 0.44617000 | 0.33879700 |
| H | 0.01380300 | 0.78576300 | 3.15325900 |
| Se | 0.74586400 | -1.10725200 | 0.96653100 |
| I | 2.54277600 | -2.18093700 | -1.43851600 |

**Polar Pathway:**

**Reactant Polar:**

| | | | |
|---|---|---|---|
| C | -2.87796200 | 1.27964200 | -1.02176200 |
| C | -1.65539700 | 1.77280100 | -1.50152400 |
| C | -0.92472900 | 2.73766400 | -0.78498800 |
| C | -1.45789500 | 3.22622400 | 0.43805500 |
| C | -2.68740100 | 2.72466300 | 0.91572100 |
| C | -3.39422100 | 1.75484200 | 0.19491900 |
| H | -3.41911200 | 0.52986500 | -1.58872100 |
| H | -1.25247100 | 1.39536000 | -2.43684400 |
| H | -3.08637100 | 3.11622100 | 1.84574900 |
| H | -4.33817200 | 1.37796000 | 0.57319800 |
| C | 0.35797400 | 3.25292500 | -1.33839500 |
| C | 0.42302700 | 3.68142100 | -2.67975800 |
| C | 1.52057100 | 3.32340300 | -0.54512900 |
| C | 1.61874800 | 4.18845300 | -3.21198000 |
| H | -0.46849800 | 3.63447600 | -3.29918400 |

| | | | |
|---|---|---|---|
| C | 2.71776200 | 3.82735700 | -1.07563000 |
| H | 1.48926100 | 2.97861400 | 0.48381400 |
| C | 2.76900500 | 4.26842600 | -2.40916300 |
| H | 1.65008000 | 4.52473900 | -4.24302700 |
| H | 3.60533700 | 3.87212700 | -0.45289100 |
| H | 3.69331800 | 4.66341000 | -2.81763600 |
| C | -0.80262400 | 4.27609800 | 1.17209800 |
| C | -0.25626100 | 5.19620700 | 1.76185400 |
| C | 0.41406200 | 6.29978000 | 2.39597100 |
| C | 1.80821900 | 6.25363700 | 2.61054800 |
| C | -0.30909600 | 7.45215500 | 2.77238100 |
| C | 2.46731500 | 7.34424900 | 3.19320400 |
| H | 2.36431800 | 5.36940600 | 2.31359700 |
| C | 0.35492000 | 8.54049900 | 3.35452200 |
| H | -1.37997200 | 7.48837000 | 2.59620300 |
| C | 1.74395800 | 8.49047800 | 3.56604100 |
| H | 3.53941700 | 7.30354100 | 3.35343400 |
| H | -0.20599200 | 9.42446500 | 3.63899700 |
| H | 2.25618700 | 9.33417400 | 4.01632600 |
| C | 1.66945300 | 7.85016600 | -0.57988400 |
| C | 1.43482900 | 9.23274200 | -0.63084700 |
| C | 0.16278300 | 9.72042800 | -0.98561900 |
| C | -0.86960500 | 8.82607400 | -1.30065500 |

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|---|---|---|---|
| C | -0.63244000 | 7.43933700 | -1.23277200 |
| C | 0.63285300 | 6.94717200 | -0.86873000 |
| H | 2.64586200 | 7.46878900 | -0.29907600 |
| H | 2.23362200 | 9.92763200 | -0.39361300 |
| H | -0.01979100 | 10.78869500 | -1.02634800 |
| H | -1.84607600 | 9.20112200 | -1.59186800 |
| H | 0.80555200 | 5.87717600 | -0.79920700 |
| Se | -2.01654300 | 6.16931700 | -1.74122600 |
| I | -3.74908000 | 6.55316900 | 0.28095200 |

**TS Polar:**

| | | | |
|---|---|---|---|
| C | -2.73612700 | 1.11165900 | -0.99243900 |
| C | -1.51897600 | 1.62658900 | -1.46475700 |
| C | -0.92980400 | 2.75829800 | -0.87687100 |
| C | -1.61286500 | 3.39116200 | 0.19882400 |
| C | -2.83253000 | 2.86157900 | 0.67989900 |
| C | -3.39008500 | 1.72331100 | 0.09008500 |
| H | -3.16410000 | 0.23104000 | -1.45884700 |
| H | -1.00660500 | 1.12950100 | -2.28241400 |
| H | -3.33291100 | 3.36462800 | 1.49980700 |
| H | -4.32379200 | 1.31960200 | 0.46455100 |
| C | 0.37900200 | 3.25305700 | -1.38215600 |
| C | 0.58884500 | 3.40343800 | -2.76759700 |

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|---|---|---|---|
| C | 1.43777800 | 3.53993600 | -0.49598500 |
| C | 1.82761300 | 3.84656700 | -3.25752700 |
| H | -0.22213900 | 3.19244200 | -3.45857900 |
| C | 2.67633100 | 3.97855300 | -0.98482300 |
| H | 1.30154100 | 3.39431700 | 0.57134800 |
| C | 2.87421900 | 4.13753600 | -2.36729400 |
| H | 1.97249000 | 3.96724700 | -4.32568100 |
| H | 3.48428700 | 4.18909400 | -0.29189400 |
| H | 3.83285200 | 4.47746300 | -2.74493400 |
| C | -1.12300000 | 4.59754000 | 0.79108300 |
| C | -0.70941200 | 5.57390100 | 1.42757100 |
| C | -0.07898900 | 6.61609200 | 2.16903200 |
| C | 1.29859100 | 6.86355900 | 1.96426000 |
| C | -0.81704600 | 7.40967000 | 3.07626300 |
| C | 1.93032200 | 7.89530900 | 2.66648400 |
| H | 1.85349300 | 6.25004400 | 1.26011900 |
| C | -0.17711200 | 8.44324700 | 3.76827800 |
| H | -1.87519000 | 7.20962800 | 3.21581500 |
| C | 1.19465000 | 8.68677400 | 3.56584000 |
| H | 2.98586400 | 8.08713400 | 2.50975200 |
| H | -0.73962300 | 9.05676300 | 4.46308600 |
| H | 1.68592800 | 9.48866400 | 4.10661100 |
| C | 2.04508200 | 7.58268000 | -1.57078500 |

| | | | |
|---|---|---|---|
| C | 2.17716500 | 8.89104700 | -1.06570300 |
| C | 1.09085800 | 9.52615000 | -0.43880000 |
| C | -0.13251200 | 8.85510700 | -0.31724300 |
| C | -0.27584700 | 7.54516400 | -0.83869000 |
| C | 0.82704200 | 6.90489500 | -1.45134100 |
| H | 2.88672700 | 7.09405100 | -2.04977200 |
| H | 3.12561500 | 9.41000300 | -1.15723700 |
| H | 1.19815800 | 10.52960300 | -0.04306700 |
| H | -0.97638300 | 9.33527300 | 0.16851000 |
| H | 0.72339400 | 5.89372700 | -1.83379200 |
| Se | -2.00820300 | 6.74077200 | -0.78825000 |
| I | -4.40097100 | 6.22235800 | 1.50766800 |

**Product Polar:**

| | | | |
|---|---|---|---|
| C | -2.42397700 | 1.37966700 | -0.91762400 |
| C | -1.16539700 | 1.89583500 | -1.25556500 |
| C | -0.74804100 | 3.16214400 | -0.80688300 |
| C | -1.65207500 | 3.90393300 | -0.00121600 |
| C | -2.92220400 | 3.38629100 | 0.34024500 |
| C | -3.30529000 | 2.12164600 | -0.11246100 |
| H | -2.71338900 | 0.39767800 | -1.27516400 |
| H | -0.48586400 | 1.30023500 | -1.85642000 |
| H | -3.59048700 | 3.99254900 | 0.94652700 |

| | | | |
|---|---|---|---|
| H | -4.27595100 | 1.71979100 | 0.15345800 |
| C | 0.60300100 | 3.66603900 | -1.17556600 |
| C | 1.07240200 | 3.50088400 | -2.49418000 |
| C | 1.44641300 | 4.27303900 | -0.22331700 |
| C | 2.34921900 | 3.94843700 | -2.85830500 |
| H | 0.42823100 | 3.04417800 | -3.24007400 |
| C | 2.72230800 | 4.72688600 | -0.58897600 |
| H | 1.13004000 | 4.34712000 | 0.81333800 |
| C | 3.17567600 | 4.57054400 | -1.90869500 |
| H | 2.69334800 | 3.82317100 | -3.87939000 |
| H | 3.36567000 | 5.18503800 | 0.15555000 |
| H | 4.16106100 | 4.92512100 | -2.19194200 |
| C | -1.34844900 | 5.22979900 | 0.47274000 |
| C | -1.00163000 | 6.17823800 | 1.25738400 |
| C | -0.36347800 | 6.74698700 | 2.42584300 |
| C | 1.01382400 | 7.04892900 | 2.37404500 |
| C | -1.11738200 | 6.99963400 | 3.58894800 |
| C | 1.63896000 | 7.59121800 | 3.50313200 |
| H | 1.57871800 | 6.85821200 | 1.46556400 |
| C | -0.47927000 | 7.54042300 | 4.71188800 |
| H | -2.17979800 | 6.77368900 | 3.59372300 |
| C | 0.89485300 | 7.83569000 | 4.67013800 |
| H | 2.69765400 | 7.82229700 | 3.47451100 |

| | | | |
|---|---|---|---|
| H | -1.04838000 | 7.73327400 | 5.61427700 |
| H | 1.38263400 | 8.25658200 | 5.54253100 |
| C | 1.25984400 | 7.14589800 | -3.23598700 |
| C | 2.11453200 | 8.15586900 | -2.76333800 |
| C | 1.80729500 | 8.84835600 | -1.58093300 |
| C | 0.63830600 | 8.53662600 | -0.86759800 |
| C | -0.20701500 | 7.52361400 | -1.35114000 |
| C | 0.09116400 | 6.82327500 | -2.53030600 |
| H | 1.50016200 | 6.60923700 | -4.14680600 |
| H | 3.01591200 | 8.40118500 | -3.31444100 |
| H | 2.46623500 | 9.62832500 | -1.21653800 |
| H | 0.39195100 | 9.08199000 | 0.03897200 |
| H | -0.56862200 | 6.04187700 | -2.89497400 |
| Se | -1.86988200 | 7.15896200 | -0.38602500 |
| I | -4.78920400 | 6.67576200 | 1.87946000 |