

SUPPORTING INFORMATION

Synthesis of Selenochromenes via Dehydration of Arylalkynols Promoted by

Iron(III) Chloride and Diorganyl Diselenides

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X-ray diffraction analysis

Single crystals of **2a** and **3b** were obtained using CH₂Cl₂/MeOH (9:1) through slow evaporation by controlled temperature (20–25 °C) over a period of seven days. All single crystals were colorless and of tabular habit. Data were collected on a Bruker Venture Photon 100 diffractometer equipped with an Incoatec IμS high brilliance Mo-Kα X-ray tube with two-dimensional Montel micro-focusing optics. The structure was solved by direct methods using SHELXS¹. Subsequent Fourier-difference map analyses yielded the positions of the non-hydrogen atoms. Refinements were carried out with the SHELXL package¹. All refinements were made by full-matrix least-squares on F² with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were included in the refinement in calculated positions but the atoms (of hydrogens) that are commentating performing special bond were located in the Fourier map. Drawings were done using ORTEP 3.1 for Windows² Crystal data and more details of the data collection and refinements of the structures are presented in Table TS1.

1. G. M. Sheldrick, *Acta Cryst.* A64, 2008, 6, 112–122.
2. ORTEP3 for Windows - L. J. Farrugia, *J. Appl. Crystallogr.* 1997, 30, 565.

Supplementary data

CCDC- 1990021 to 1990022 contain the supplementary crystallographic data for molecule **2a** and **3b** respectively.

These data can be obtained free of charge via
<http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223–336–033; or e-mail: deposit@ccdc.cam.ac.uk.

Table S1. Data collection and refinements of the structures **2a** and **3b**.

| Molecule | 2a | 3b |
|-------------------|---|--|
| Empirical formula | C ₂₂ H ₁₆ Se ₂ | C ₁₆ H ₉ BrCl ₂ OSe |
| Formula weight | 438.27 | 447.00 |
| Temperature (K) | 127(2) | 294(2) |
| Wavelength | 0.71073 | 0.71073 |

| Crystal system | Triclinic | Monoclinic |
|---|---|---|
| Space group | <i>P</i> -1 | <i>P</i> 21/n |
| <i>a</i> (Å) | 7.0078(4) | 16.0762(7) |
| <i>b</i> (Å) | 9.6334(6) | 4.1491(2) |
| <i>c</i> (Å) | 13.8589(8) | 23.3019(11) |
| α (°) | 110.327(2) | 90 |
| β (°) | 92.316(2) | 95.784(2) |
| γ (°) | 96.373(2) | 90(2) |
| Volume (Å ³) | 868.78(9) | 1546.36(12) |
| <i>Z</i> | 2 | 4 |
| Calculated density (mg.m ⁻³) | 1.675 | 1.920 |
| Absorption coefficient (nm ⁻¹) | 4.255 | 5.351 |
| <i>F</i> (000) | 432 | 864 |
| Crystal size (mm) | 0.31 x 0.30 x 0.09 | 0.13 x 0.11 x 0.10 |
| Theta range for data collection (°) | 2.26 - 27.57 | 2.55 - 27.24 |
| Limiting indices | -7 ≤ <i>h</i> ≤ 9, -12 ≤ <i>k</i> ≤ 12, -17 ≤ <i>l</i> ≤ 18 | -15 ≤ <i>h</i> ≤ 20, -5 ≤ <i>k</i> ≤ 5, -29 ≤ <i>l</i> ≤ 29 |
| Reflections collected | 10067 | 27712 |
| Reflections unique | 3941 | 3473 |
| Completeness to theta | 99.8% | 99.7% |
| Absorption correction | Numerical | Numerical |
| Max. Transmission | 0.7007 | 0.6267 |
| Min. Transmission | 0.3522 | 0.5530 |
| Data / restraints / parameters | 3941 / 0 / 217 | 3473 / 0 / 190 |
| Goodness-of-fit on <i>F</i> ² | 1.056 | 1.089 |
| Índice <i>R</i> _{int} | 0.0250 | 0.0455 |
| Final <i>R</i> indices <i>R</i> ₁ and <i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)] | 0.0225/0.0535 | 0.0561/0.1659 |
| <i>R</i> indices (all data) <i>R</i> ₁ and <i>wR</i> ₂ | 0.0268/0.0551 | 0.0752/0.1758 |
| Largest diff. peak (e ⁻ Å ⁻³) and hole | 0.424– 0.481 | 0.705 – 1.749 |

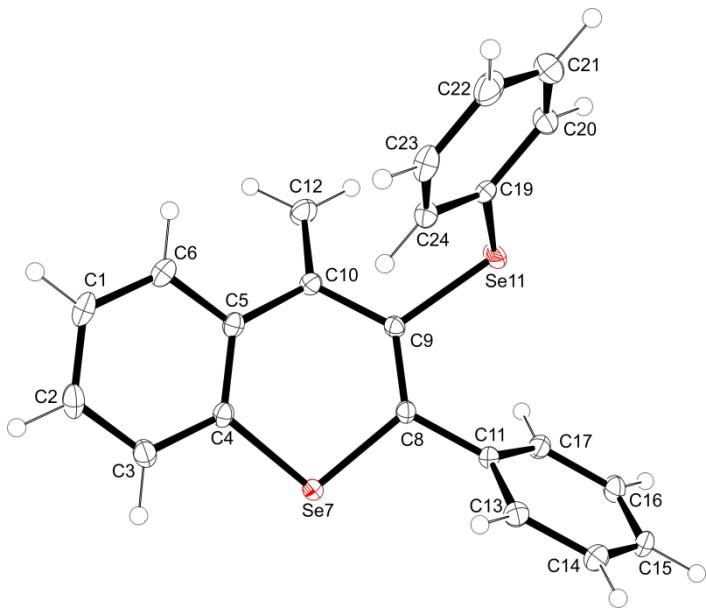


Figure S1. ORTEP drawings (ellipsoids set at 50 % probability) of the compound **2a** (CCDC 1990021).

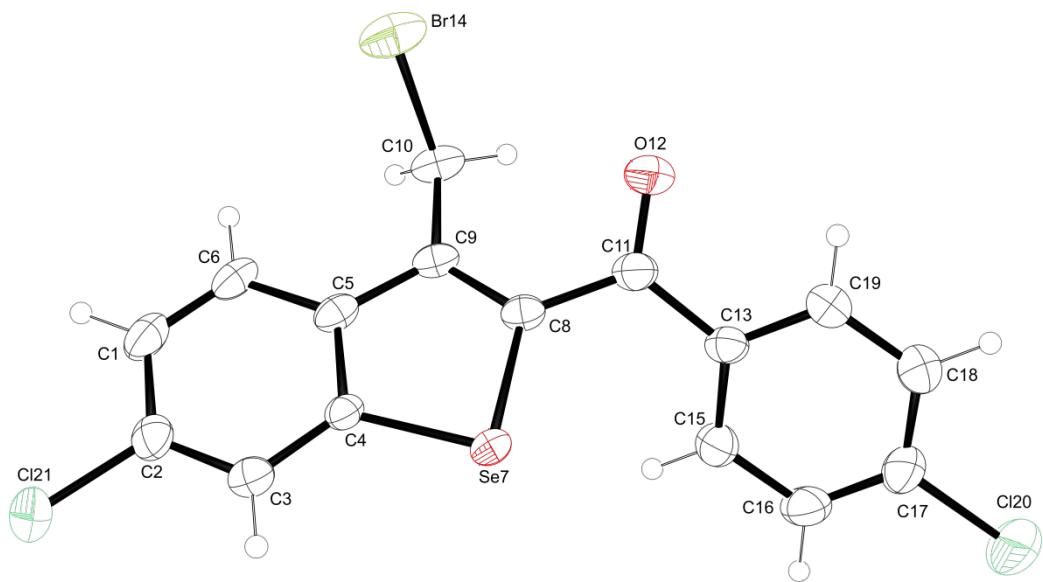
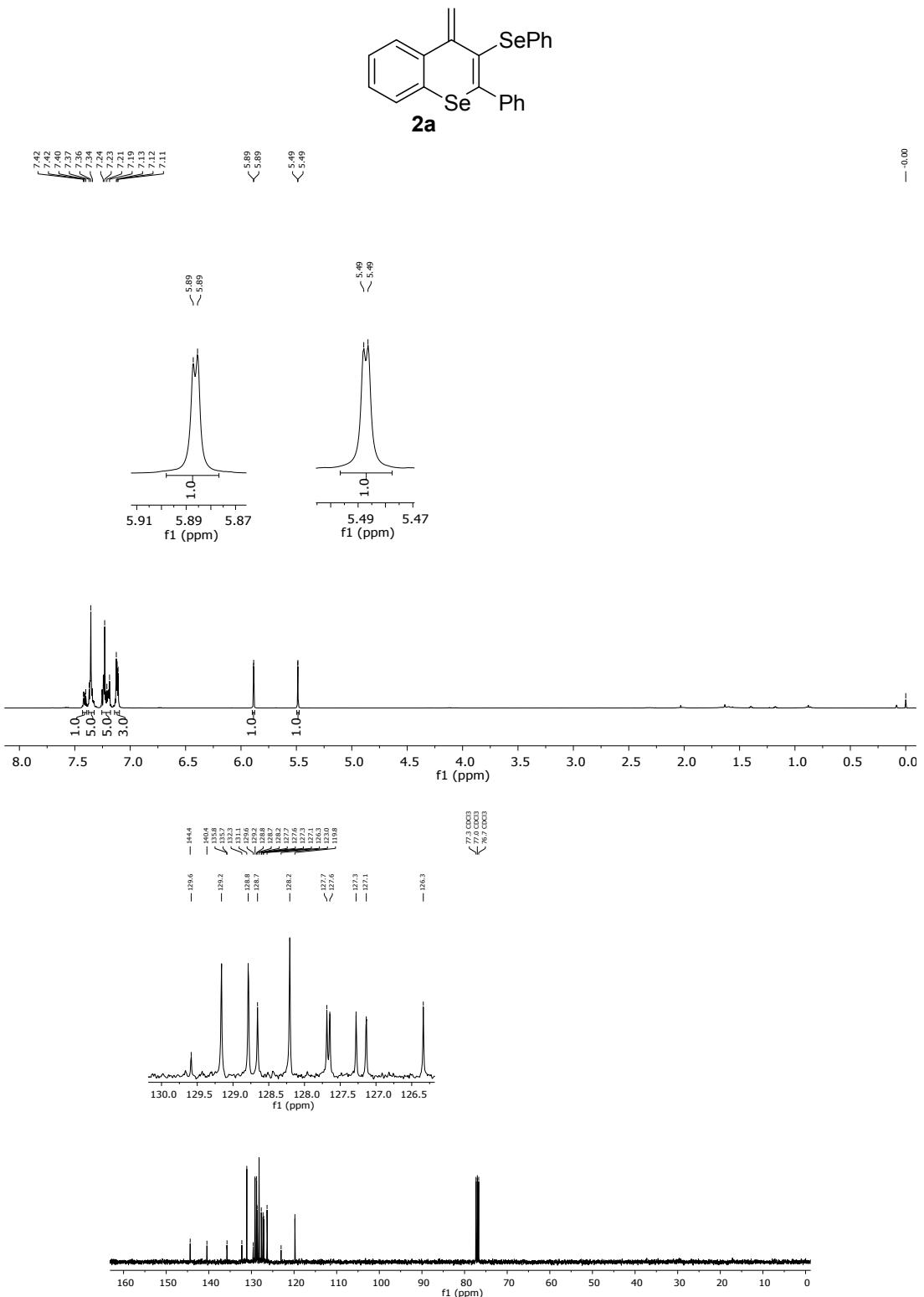
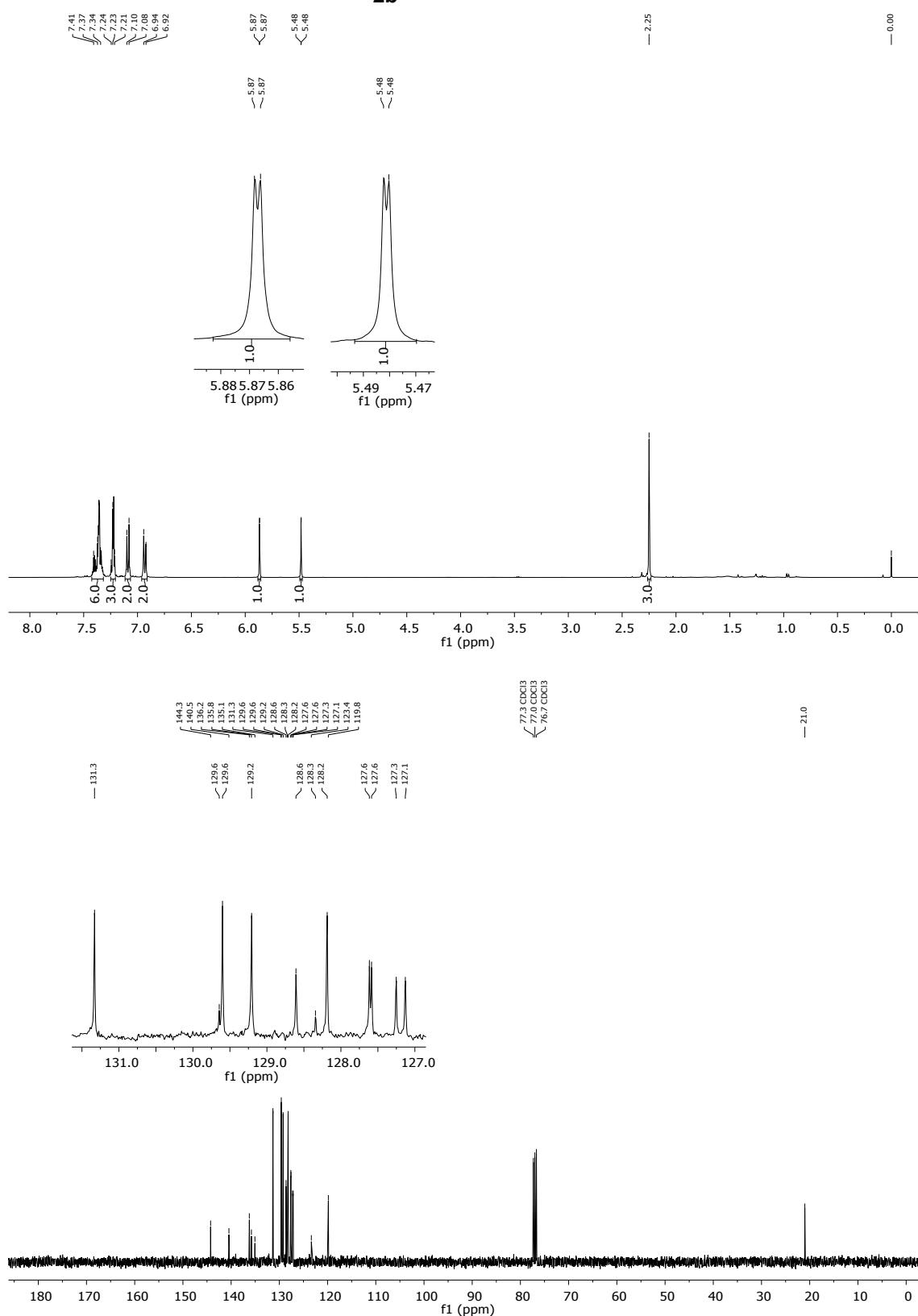
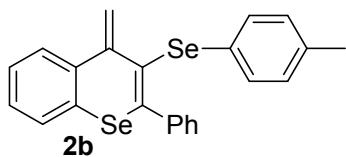


Figure S2. ORTEP drawings (ellipsoids set at 50 % probability) of the compound **3b** (CCDC 1990022).

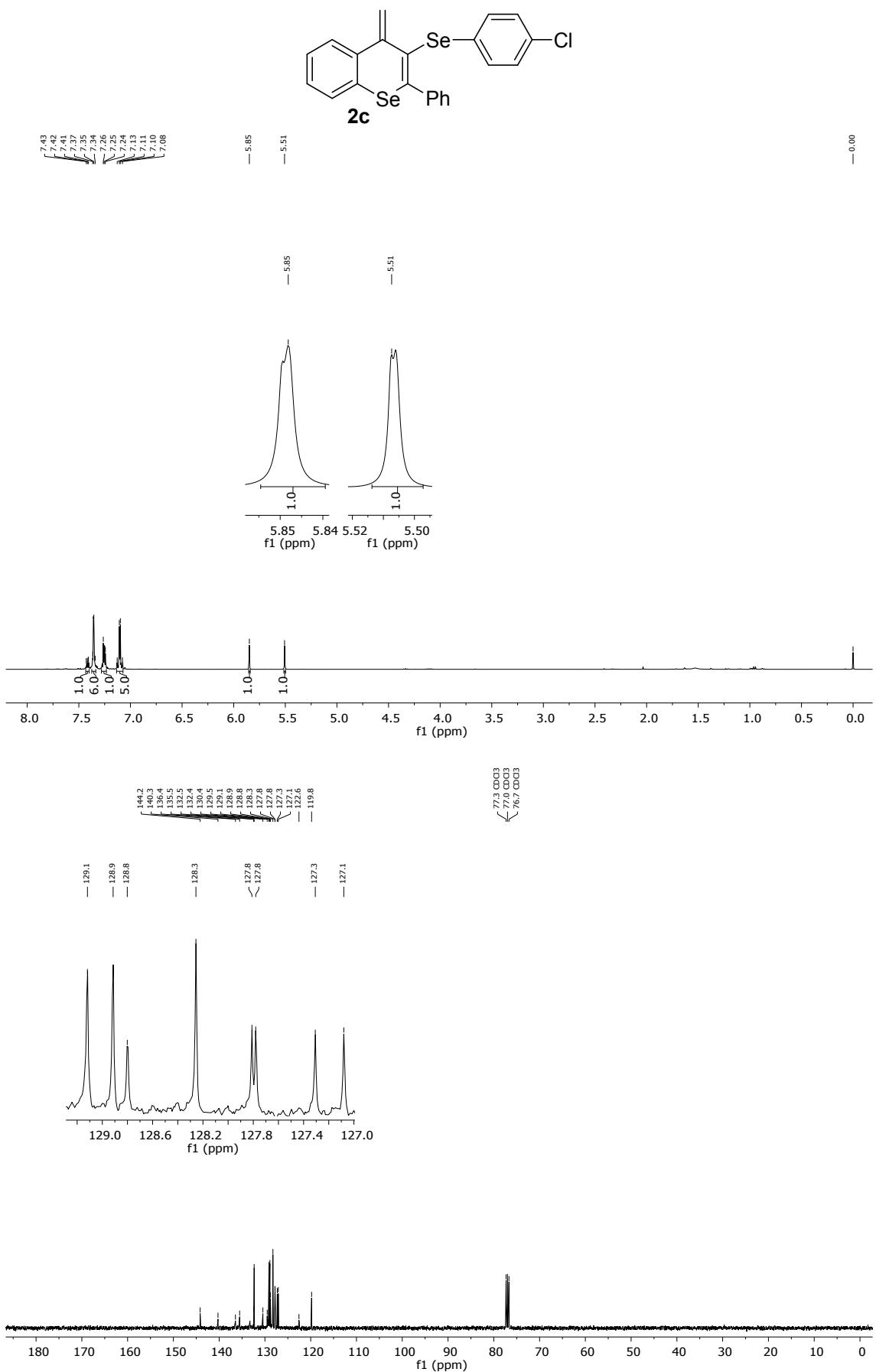
Spectra



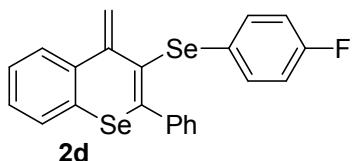
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2a** in CDCl₃.



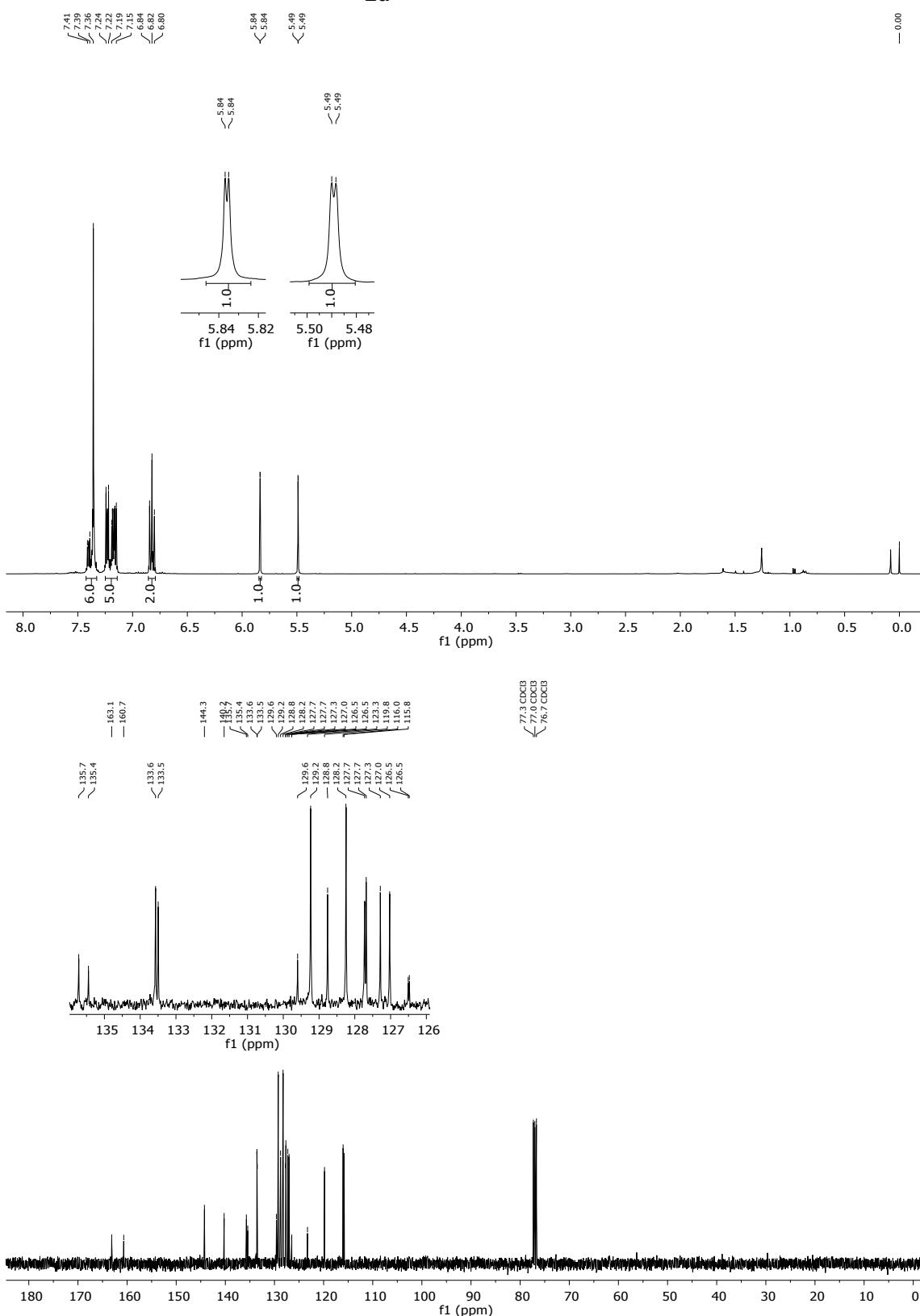
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2b** in CDCl₃.



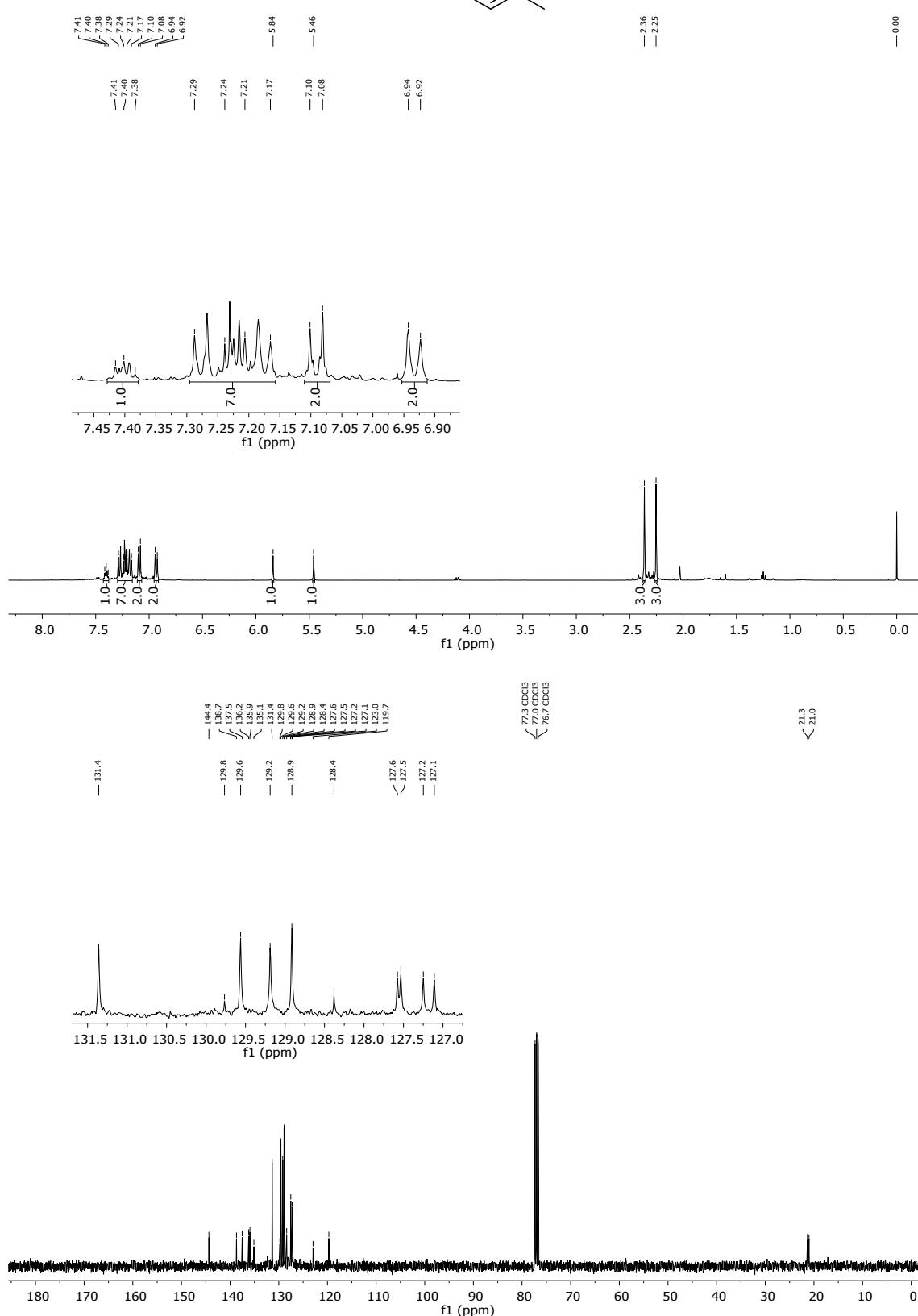
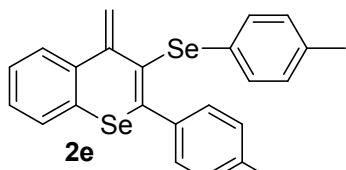
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2c** in CDCl₃.



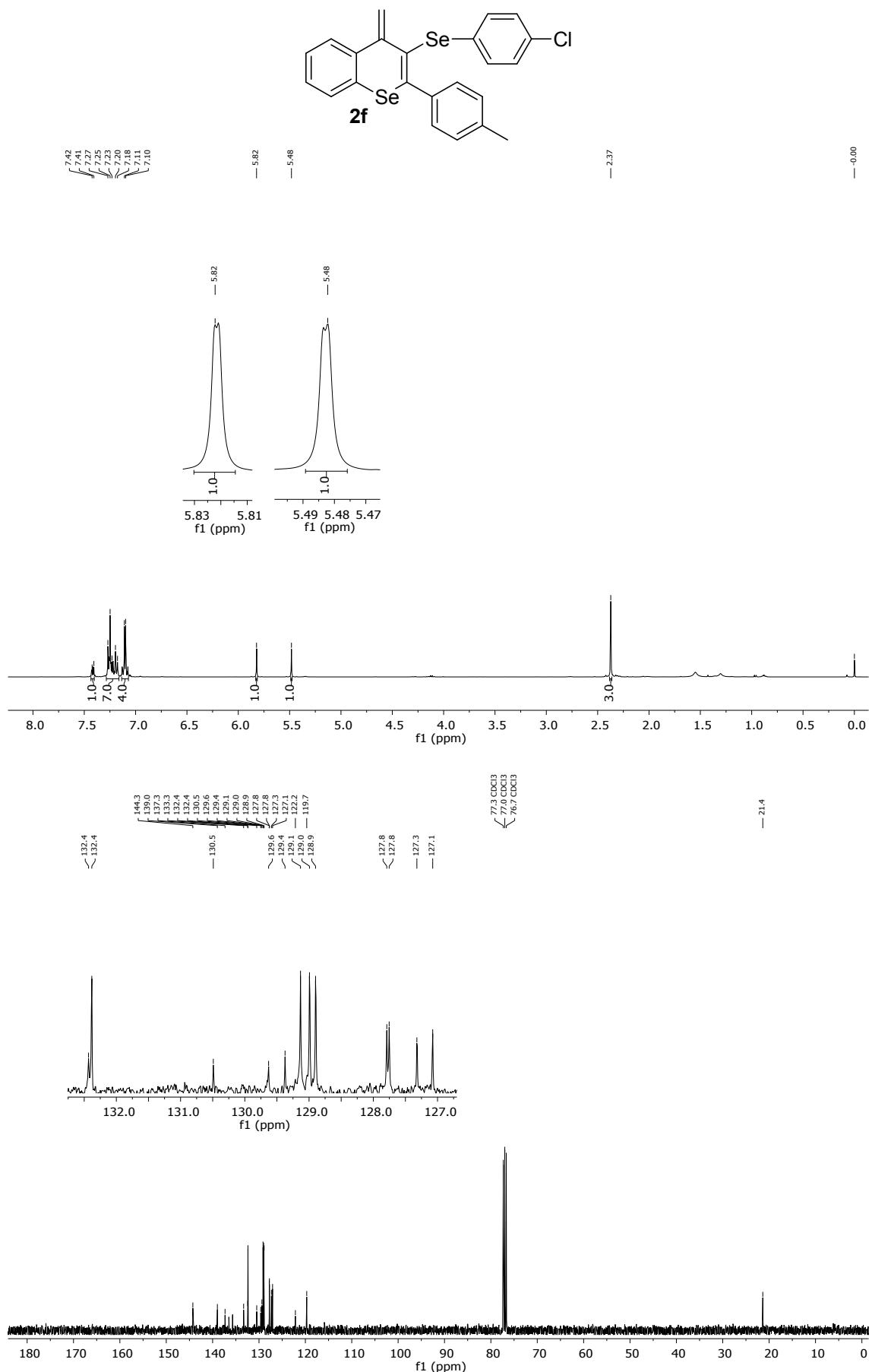
2d



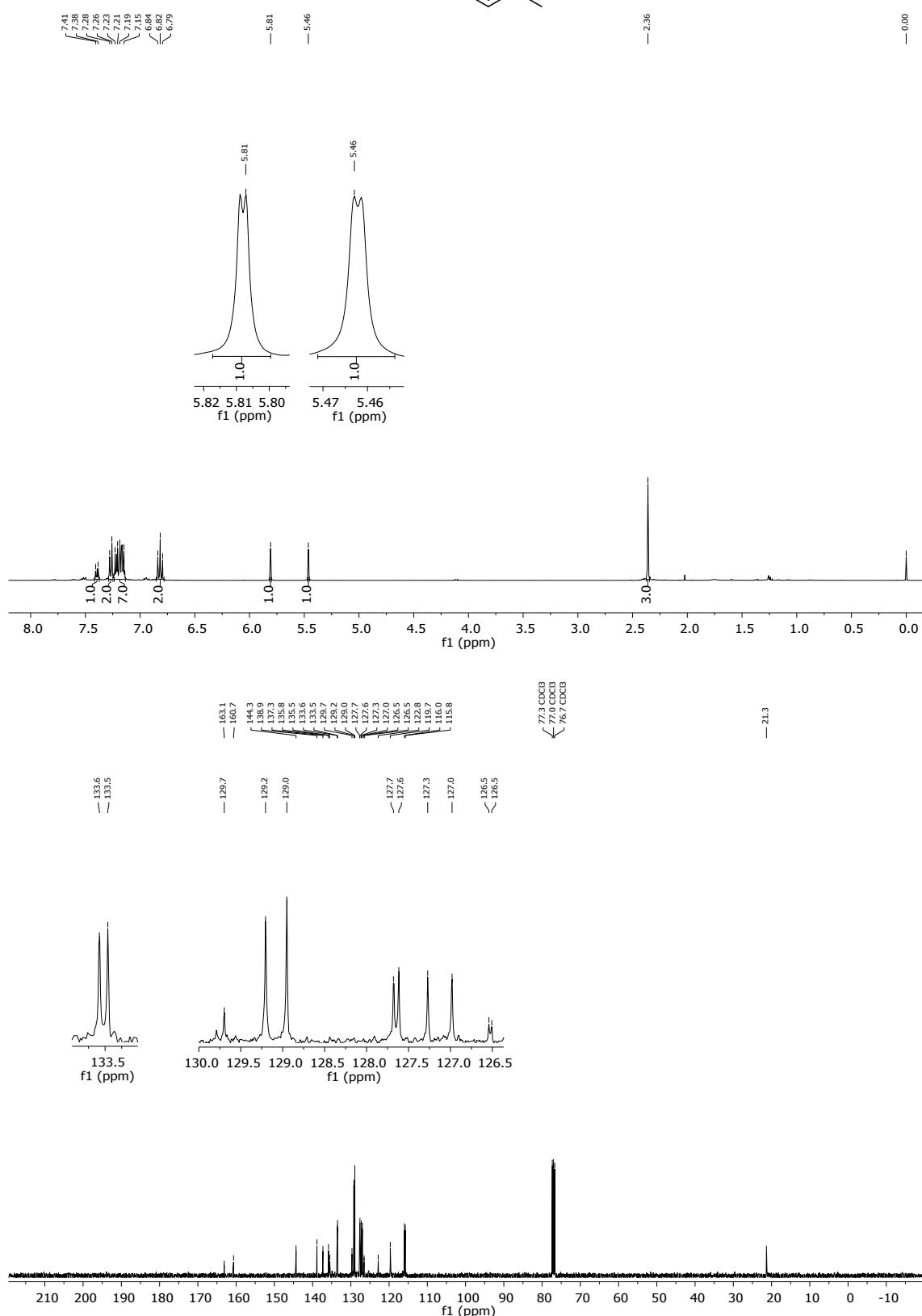
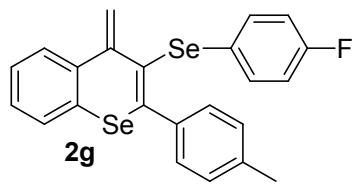
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2d** in CDCl_3 .



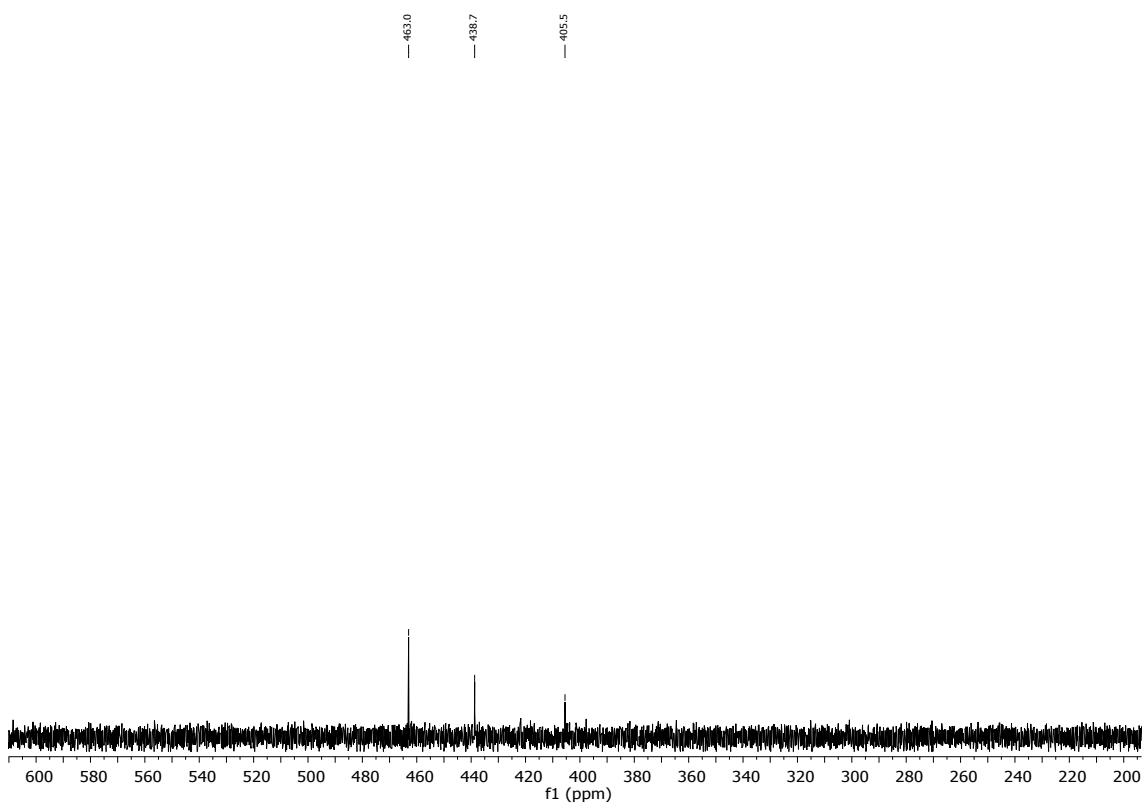
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2e** in CDCl_3 .



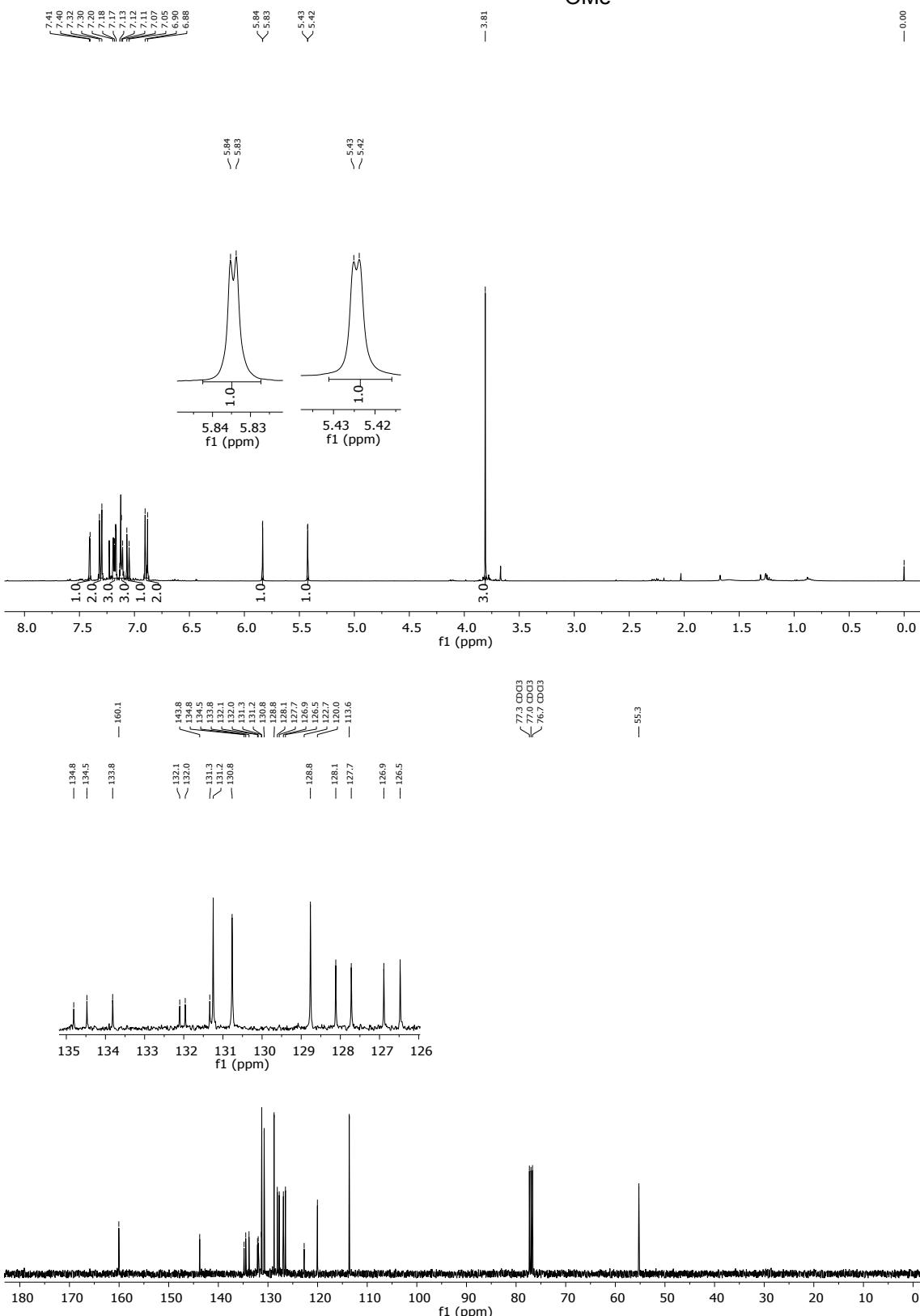
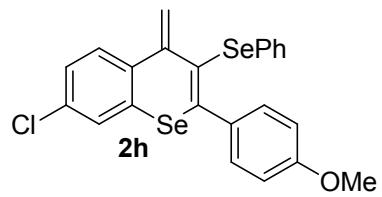
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2f** in CDCl₃.



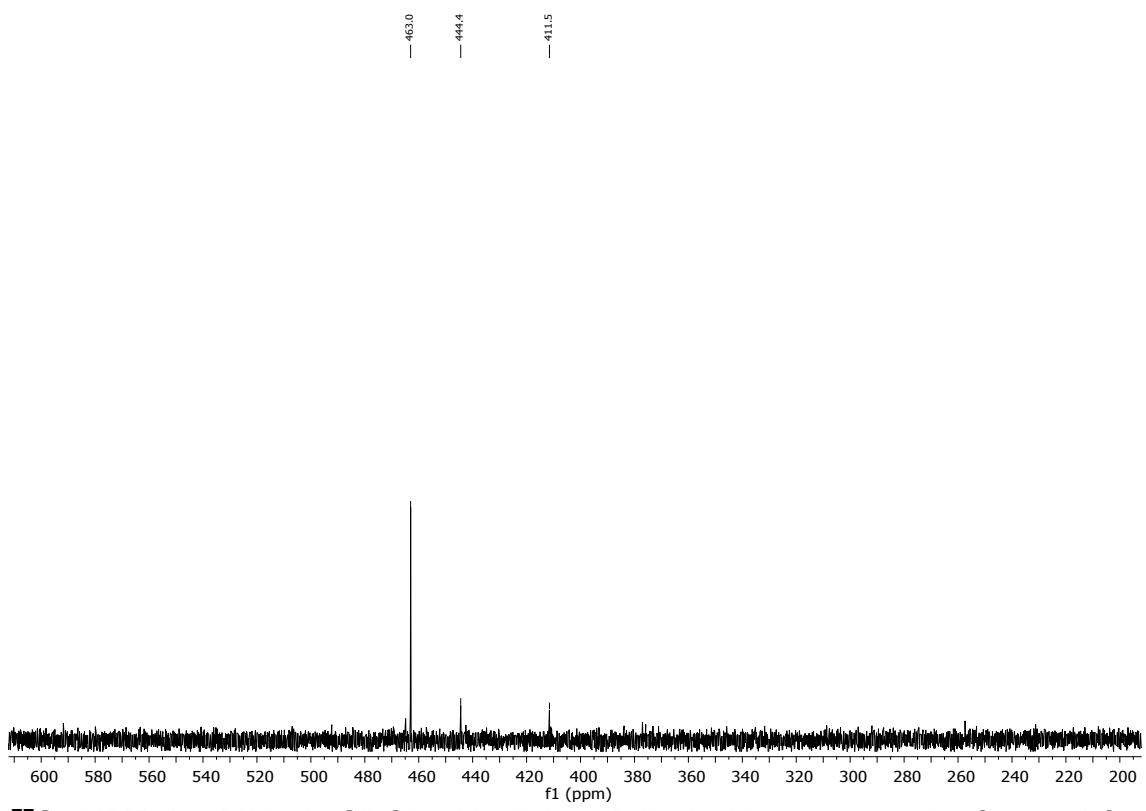
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2g** in CDCl_3 .



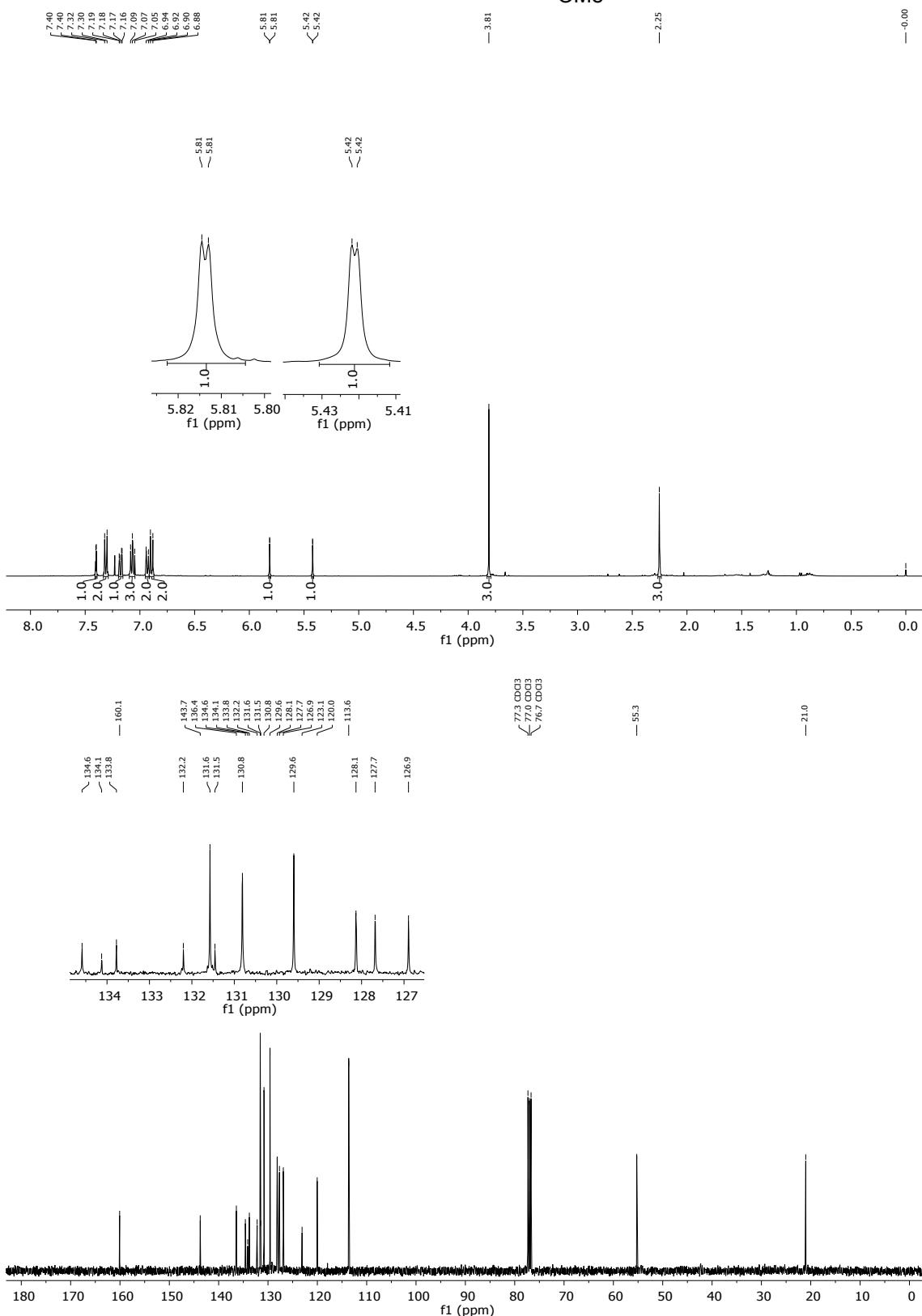
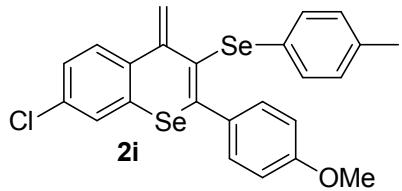
^{77}Se NMR (77 MHz, in CDCl_3 with diphenyl diselenide as external reference) for **2g**.



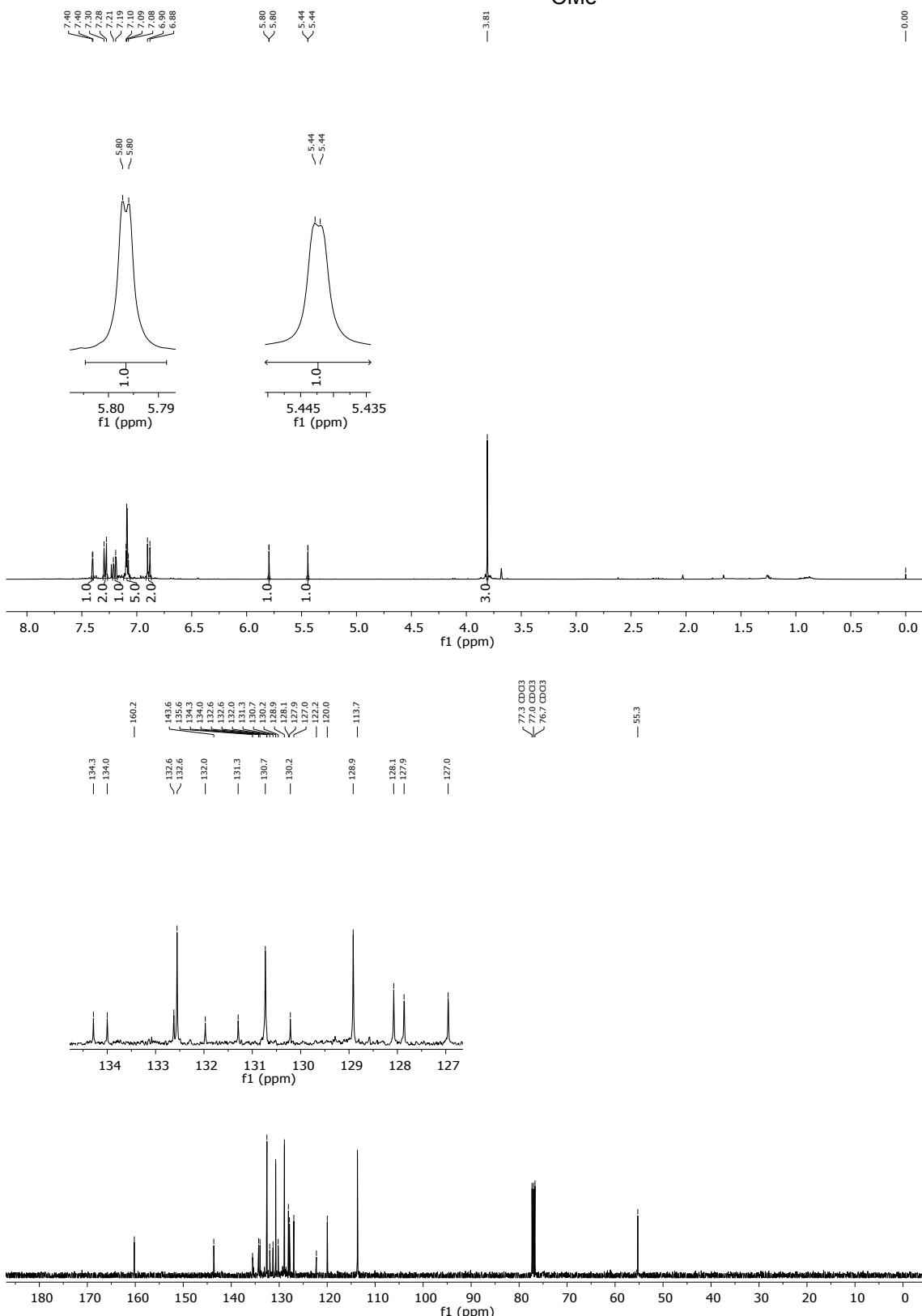
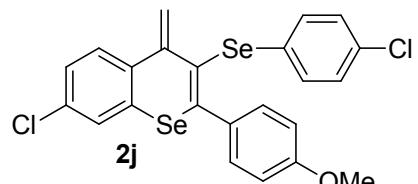
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2h** in CDCl_3 .



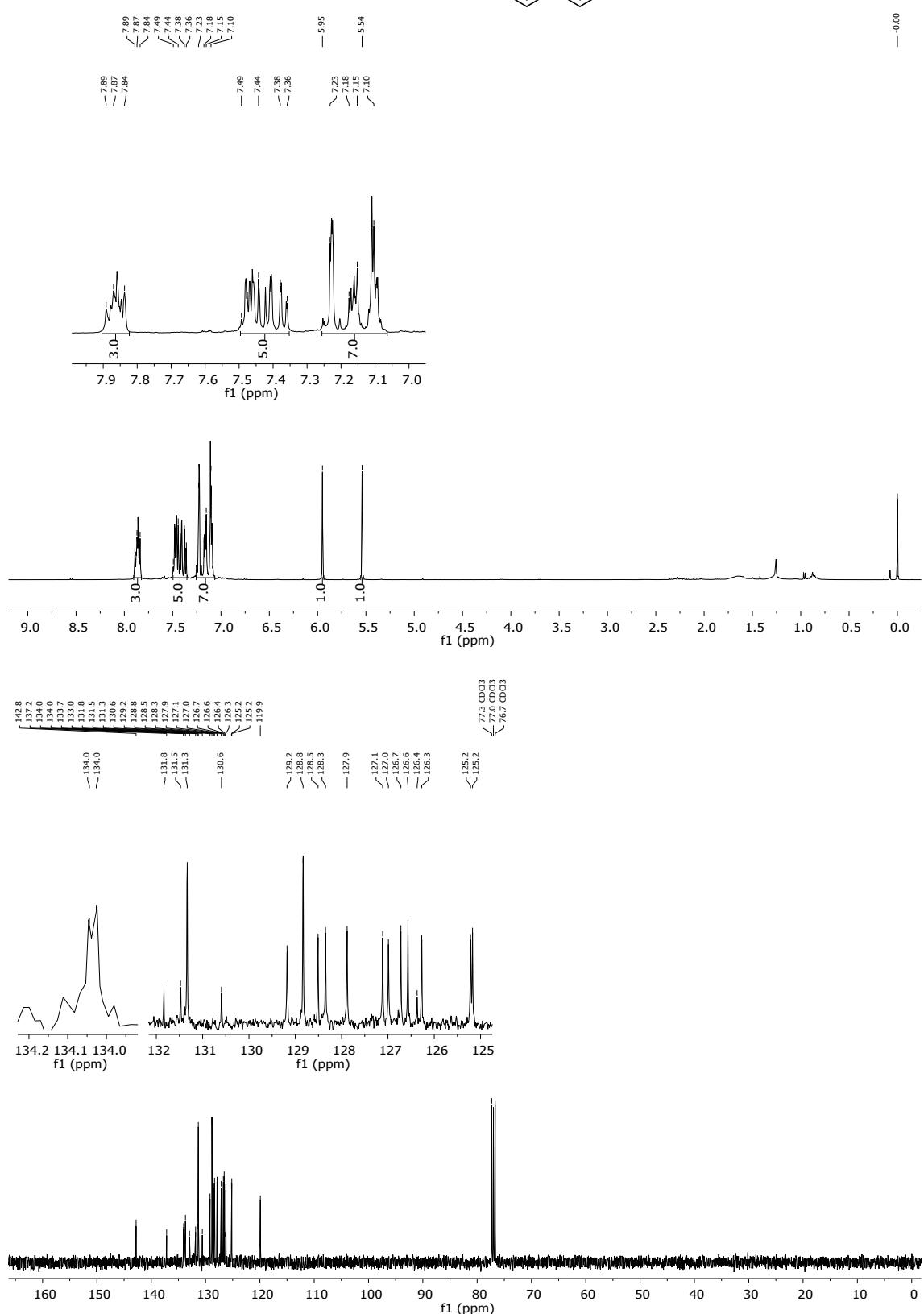
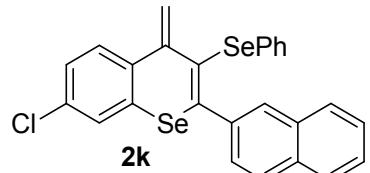
^{77}Se NMR (77 MHz, in CDCl_3 with diphenyl diselenide as external reference) for **2h**.



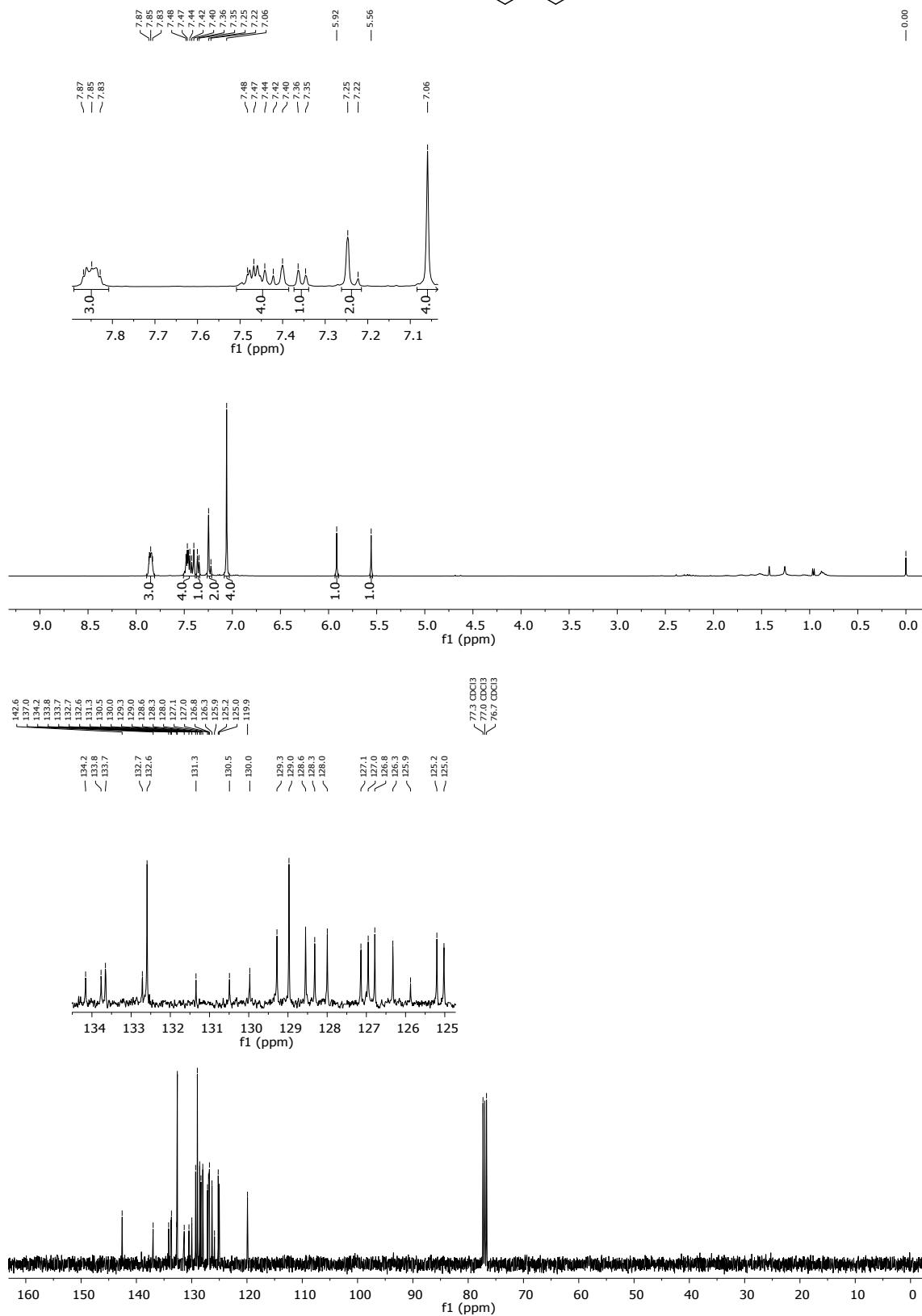
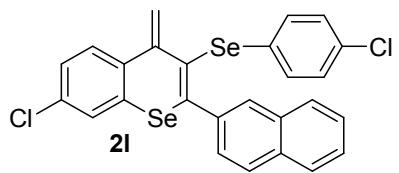
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2i** in CDCl_3 .



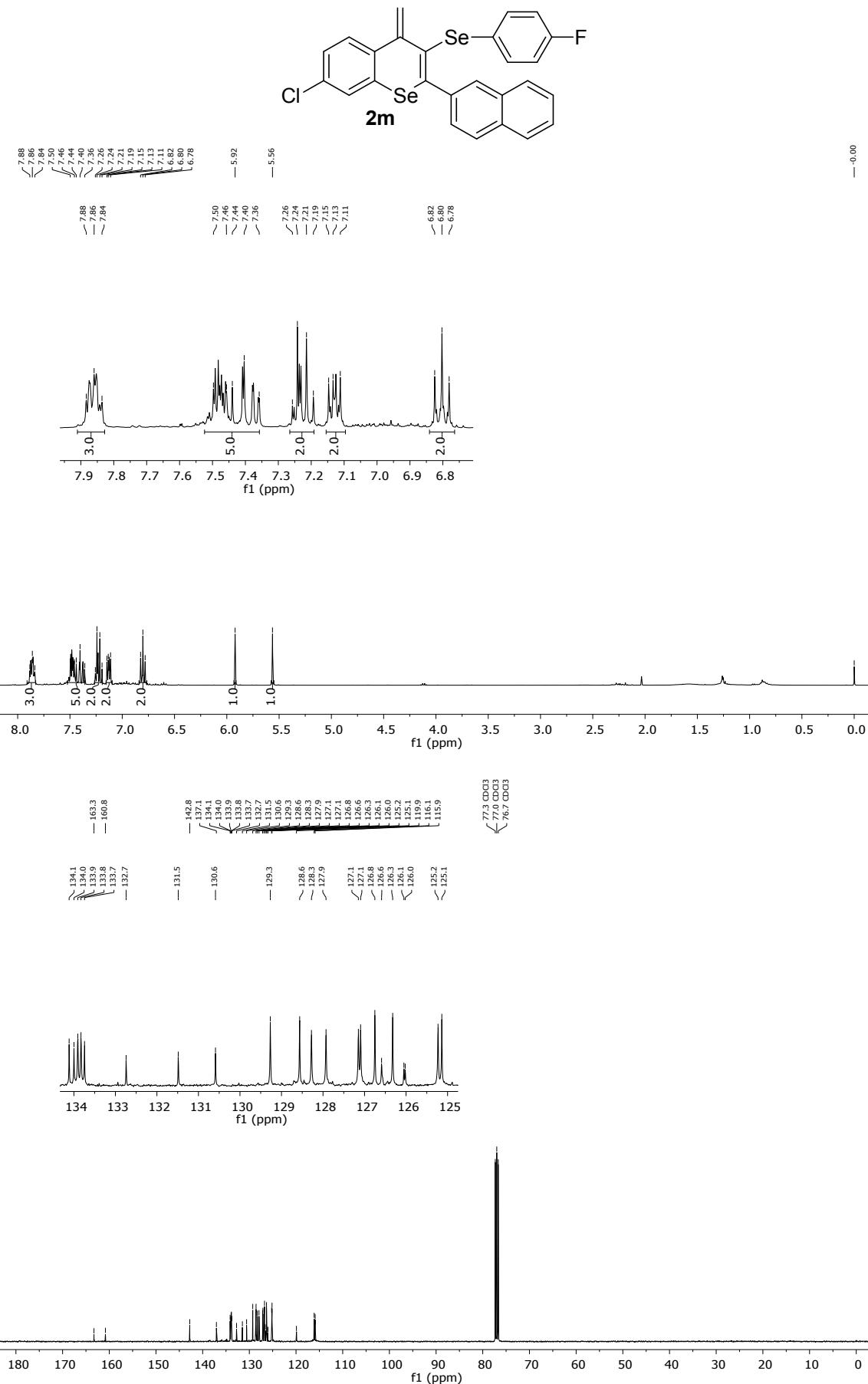
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2j** in CDCl_3 .



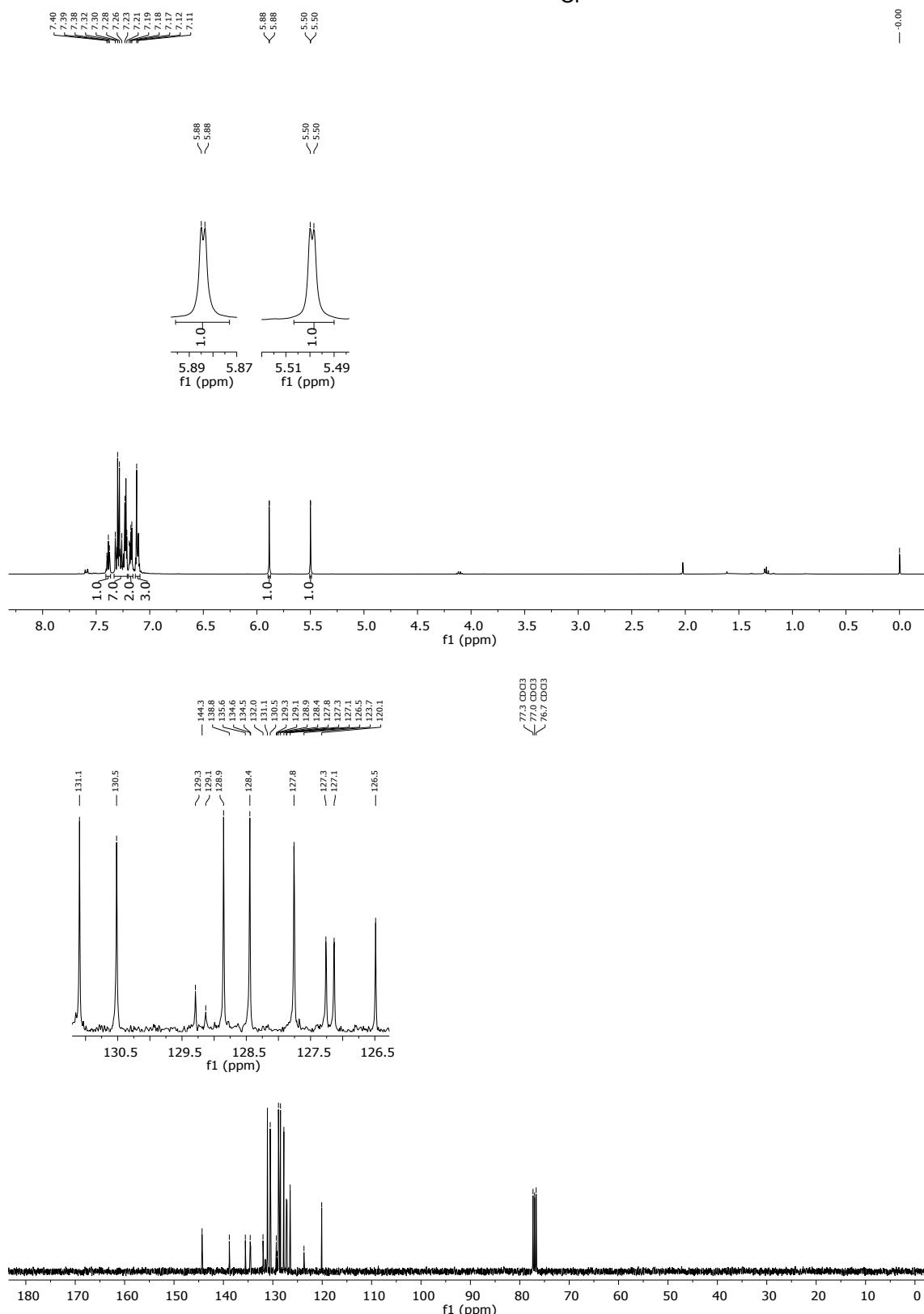
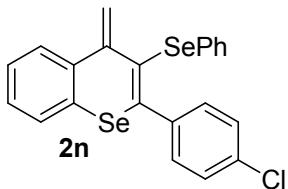
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2k** in CDCl_3 .



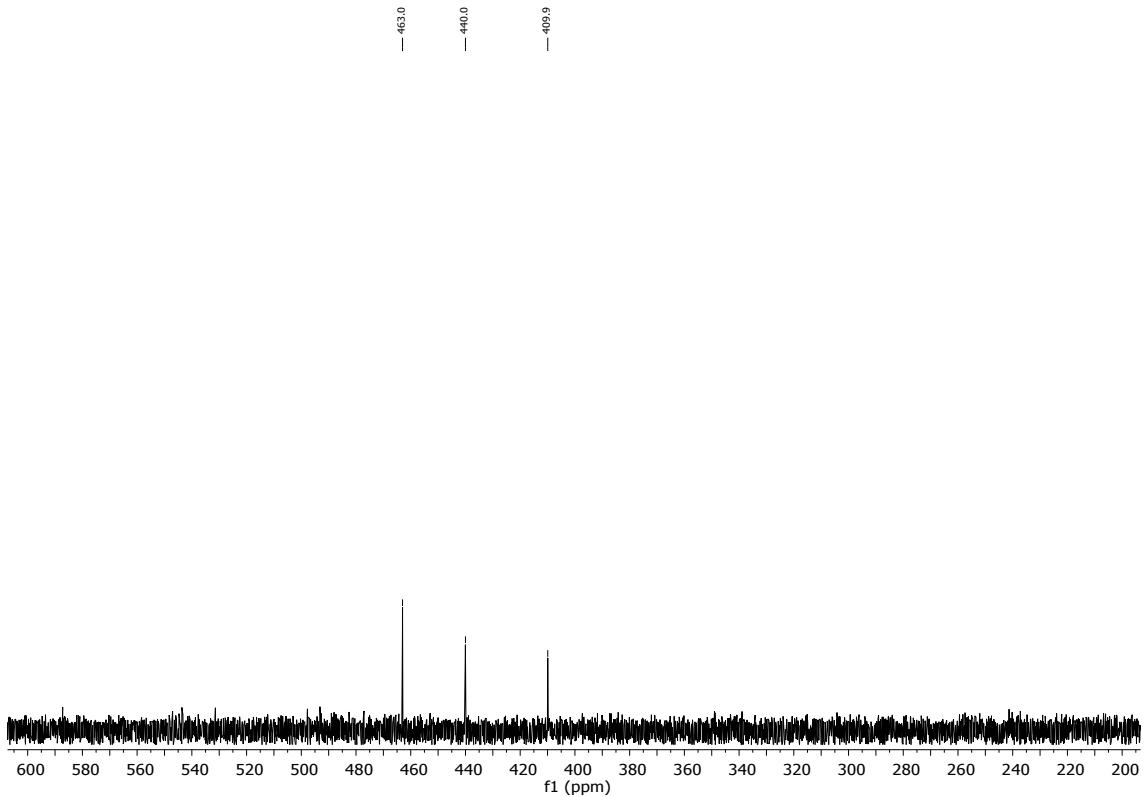
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2I** in CDCl_3 .



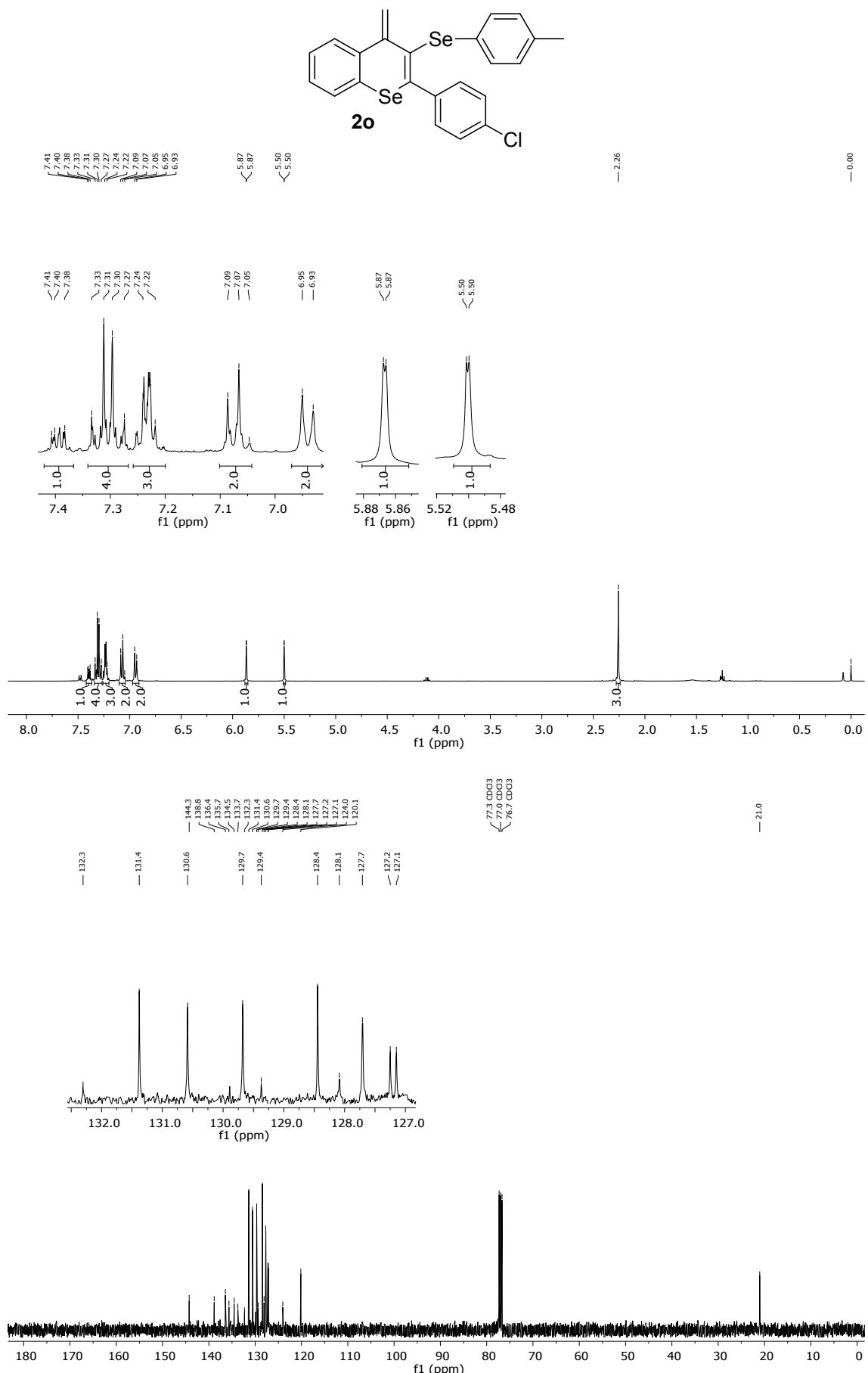
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2m** in CDCl₃.



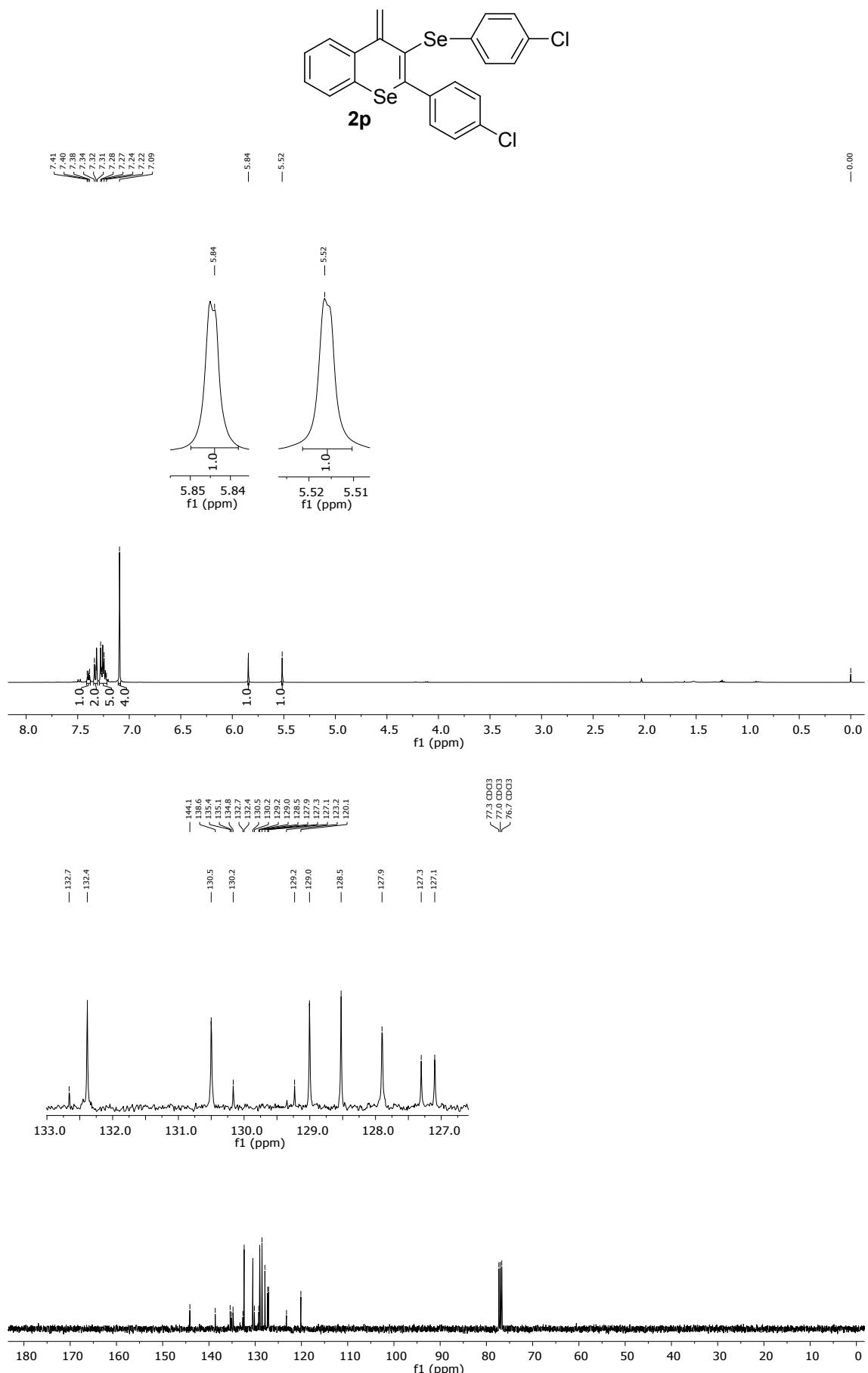
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2n** in CDCl_3 .



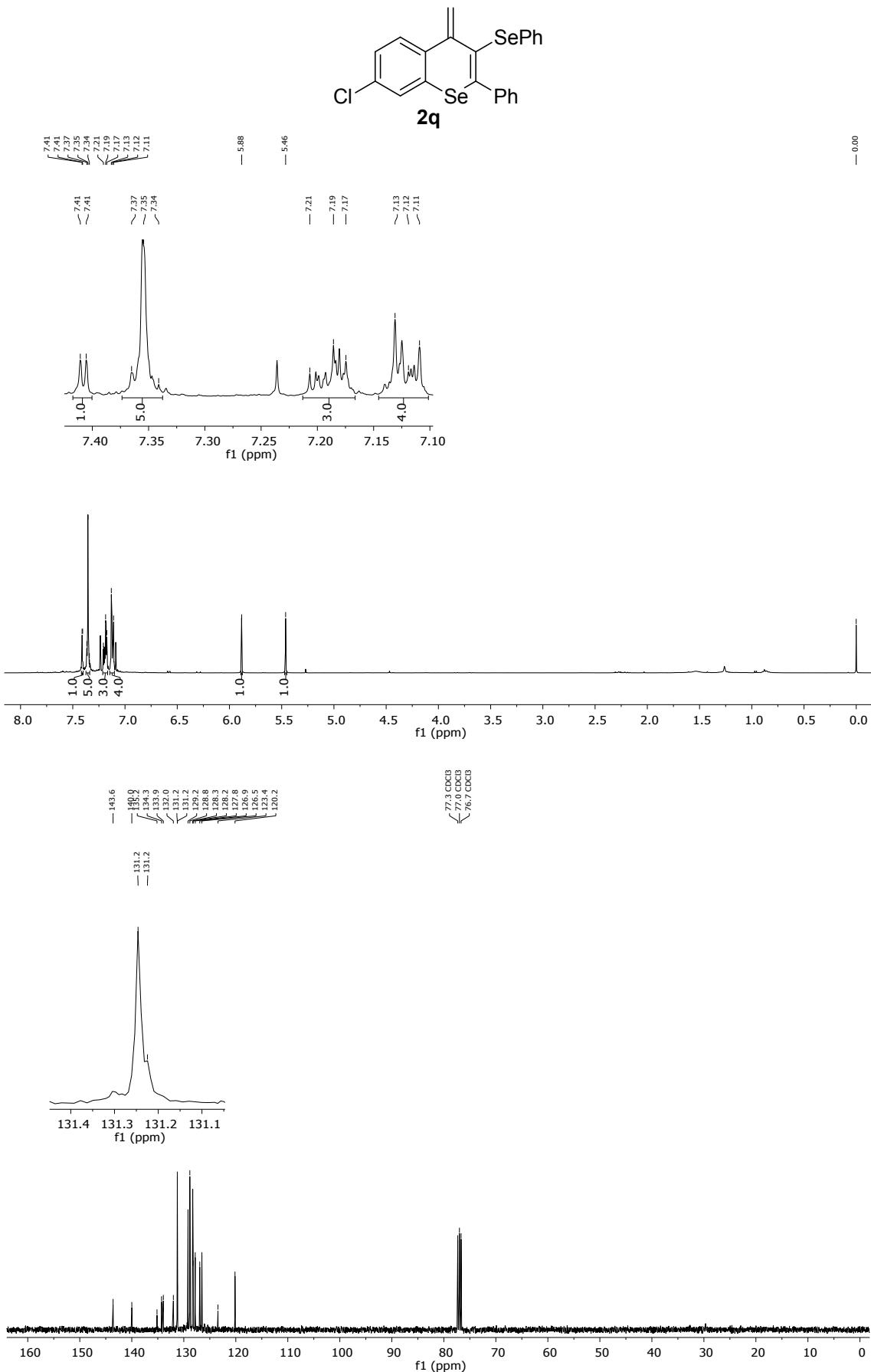
⁷⁷Se NMR (77 MHz, in CDCl₃ with diphenyl diselenide as external reference) for **2n**.



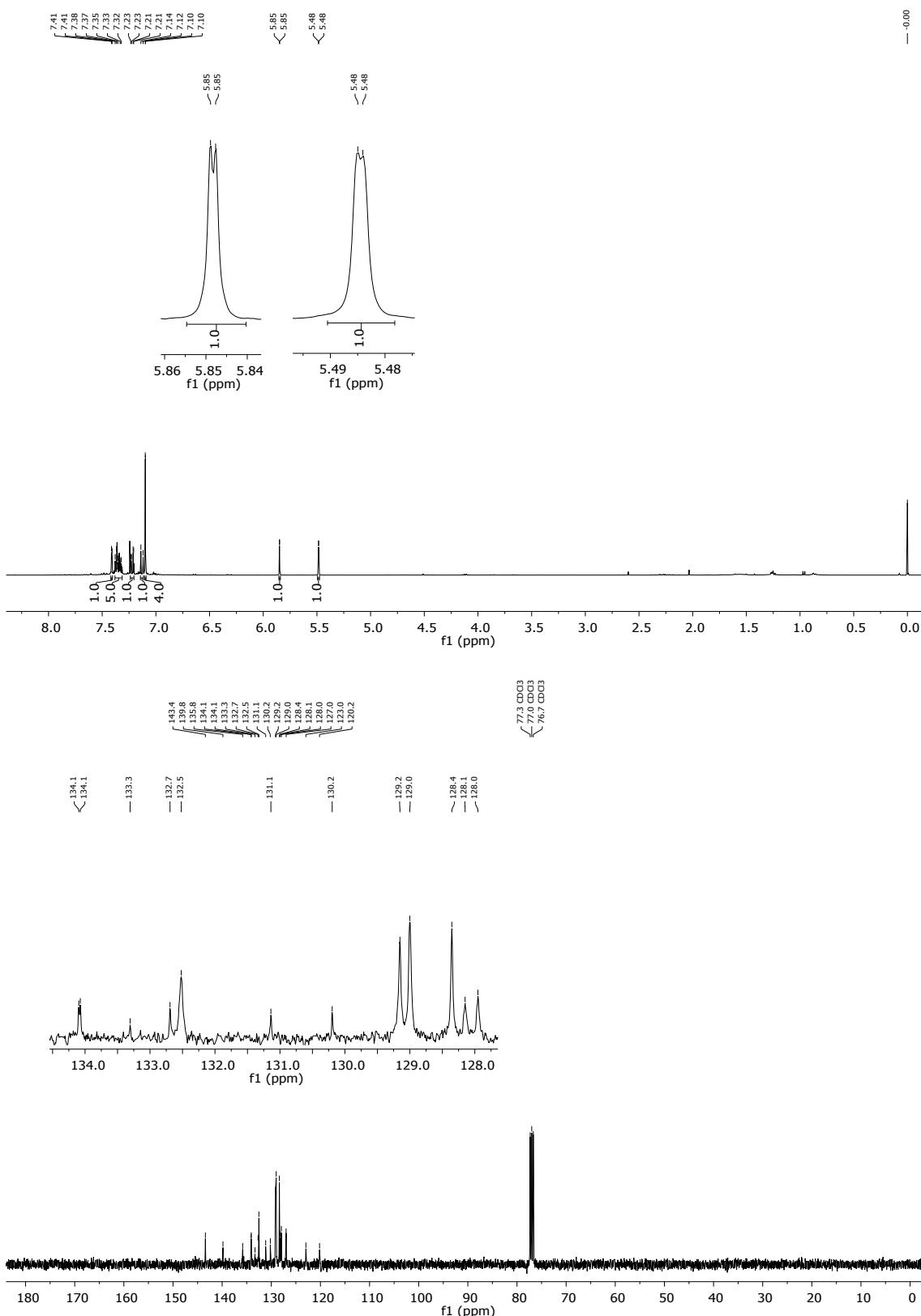
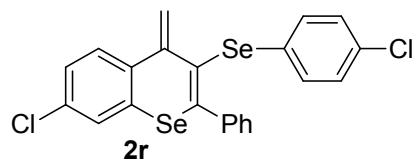
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2o** in CDCl₃.



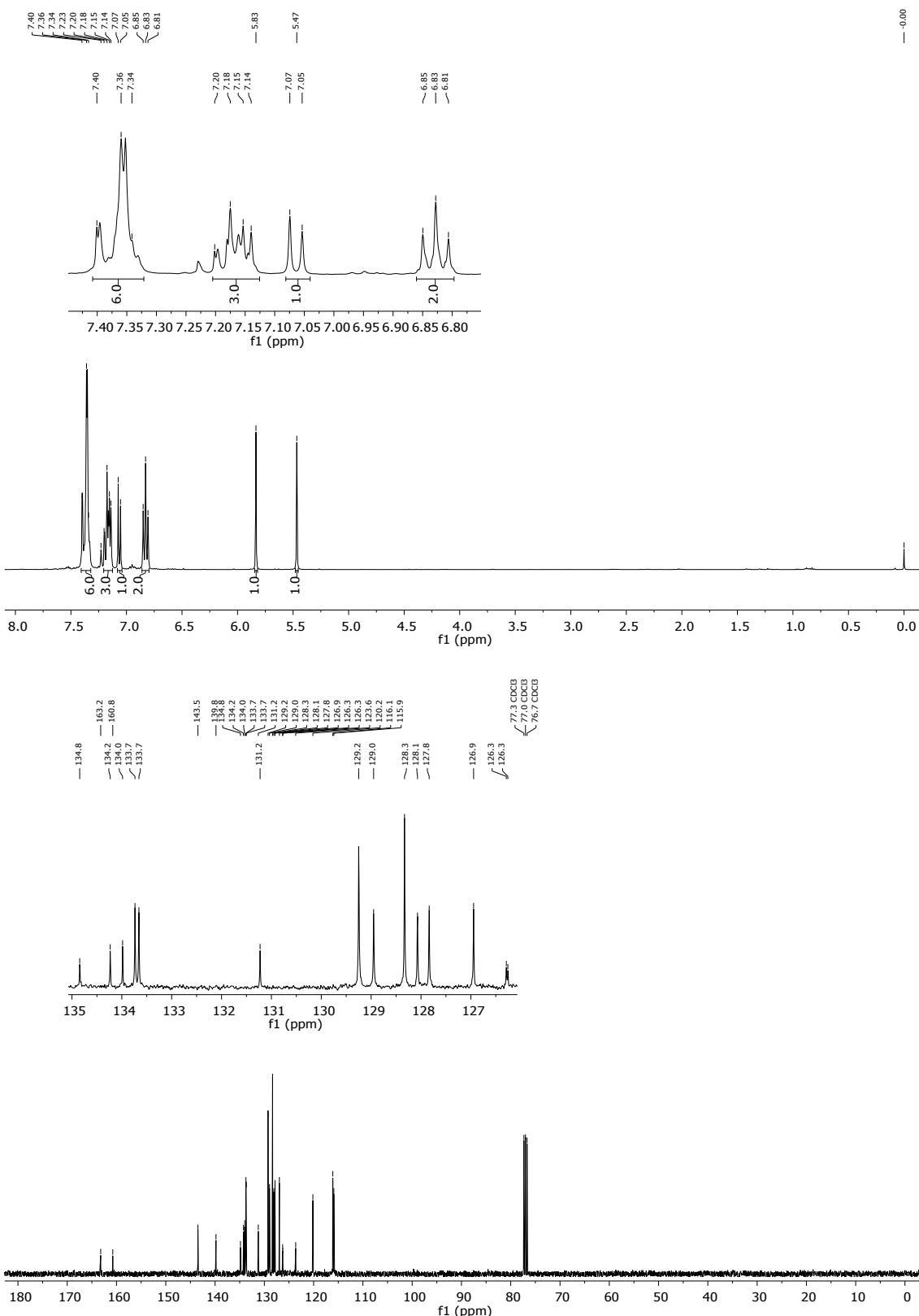
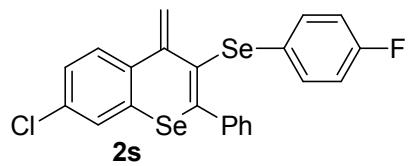
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2p** in CDCl_3 .



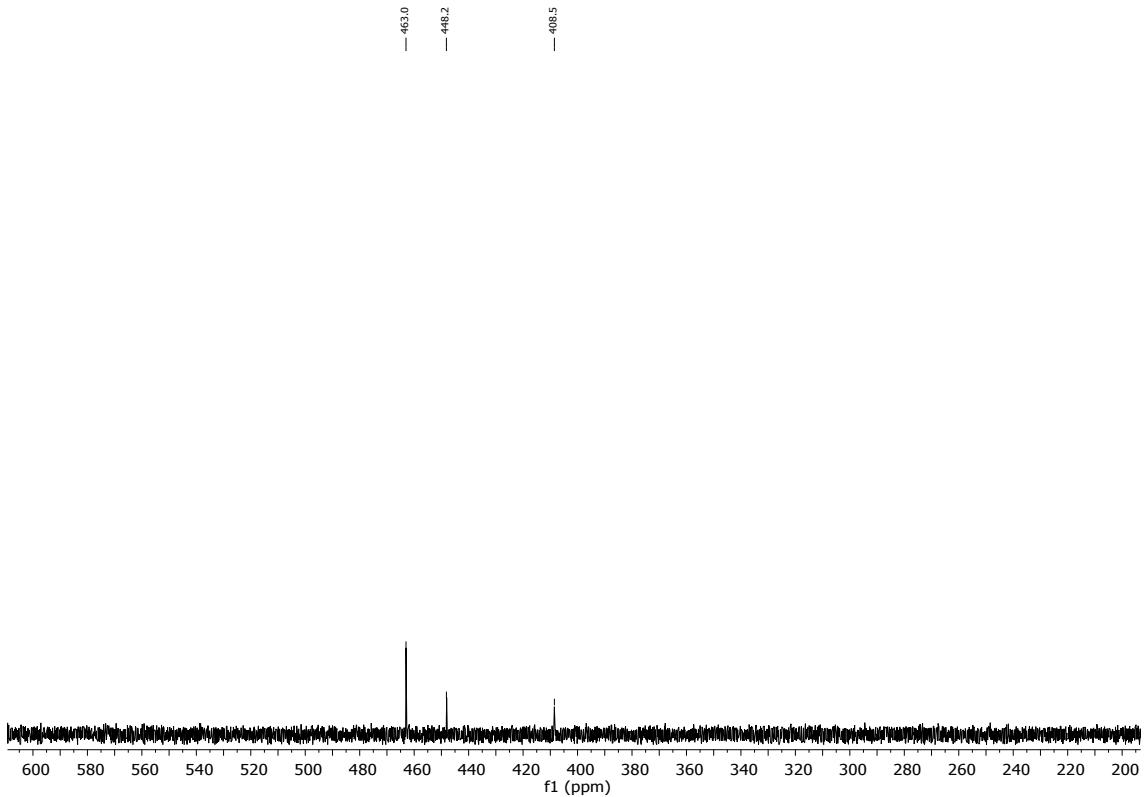
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2q** in CDCl₃.



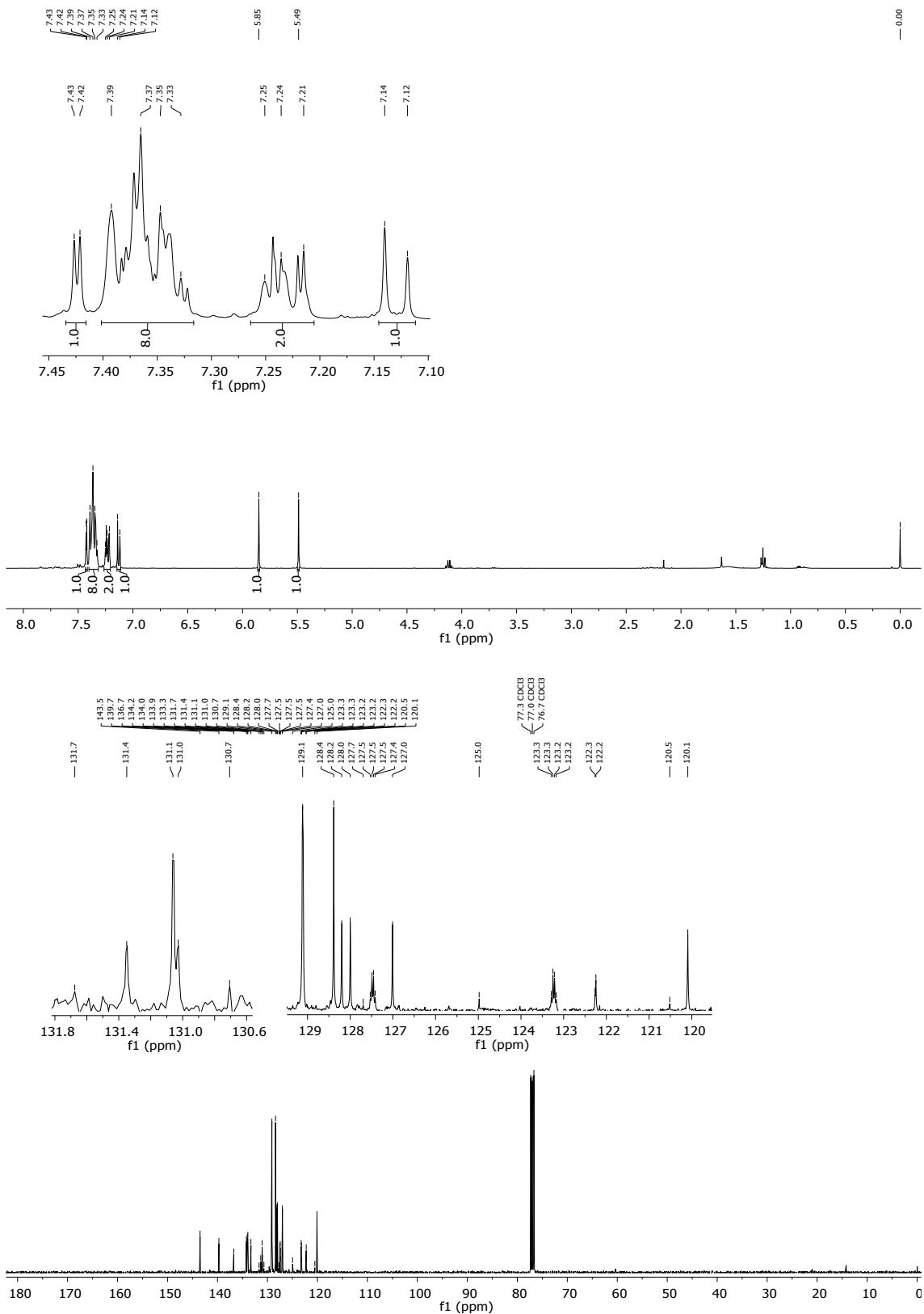
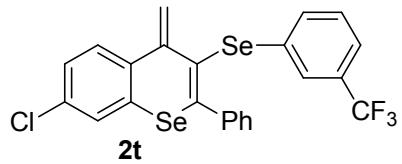
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2r** in CDCl_3 .



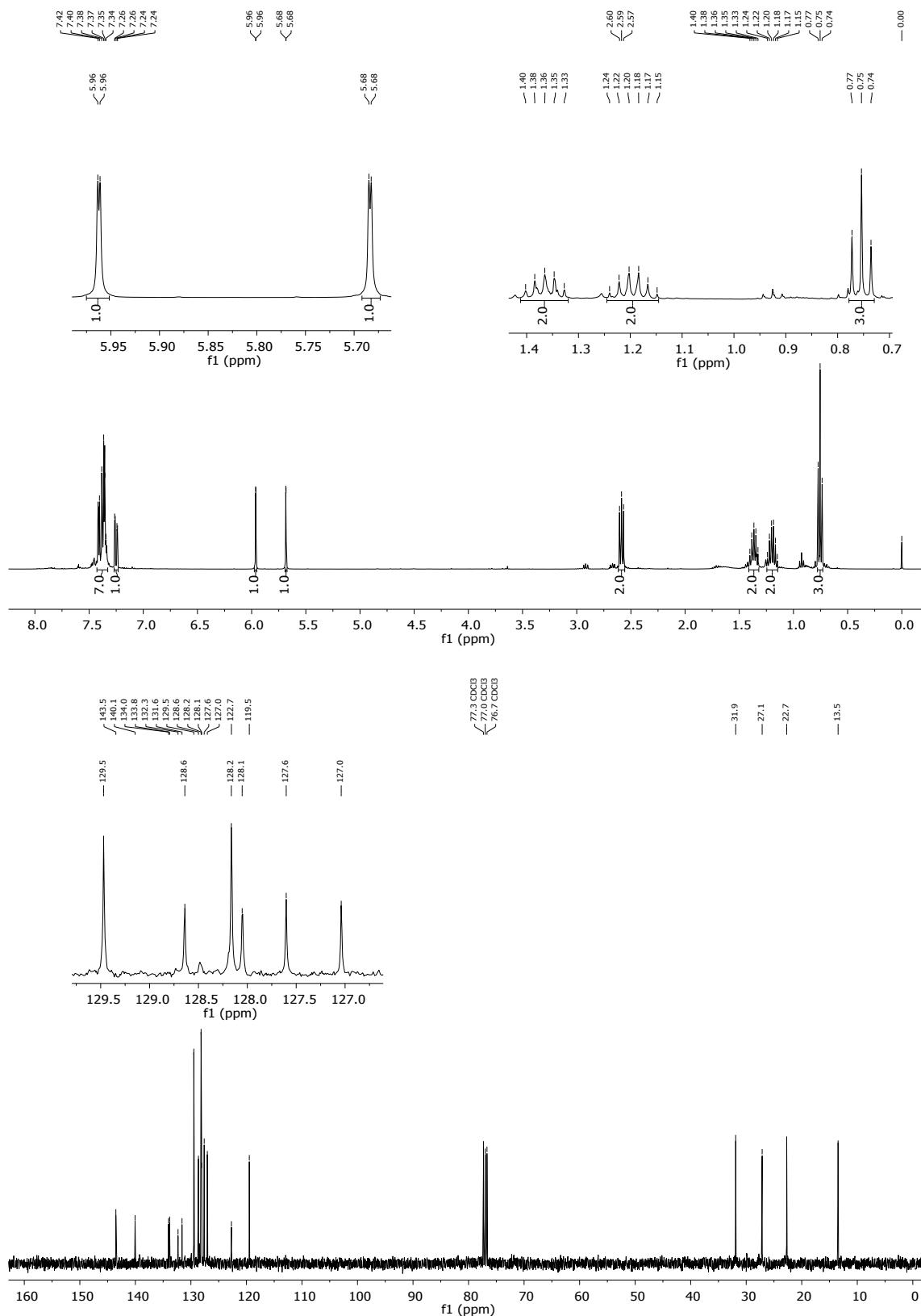
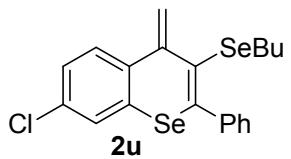
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2s** in CDCl_3 .



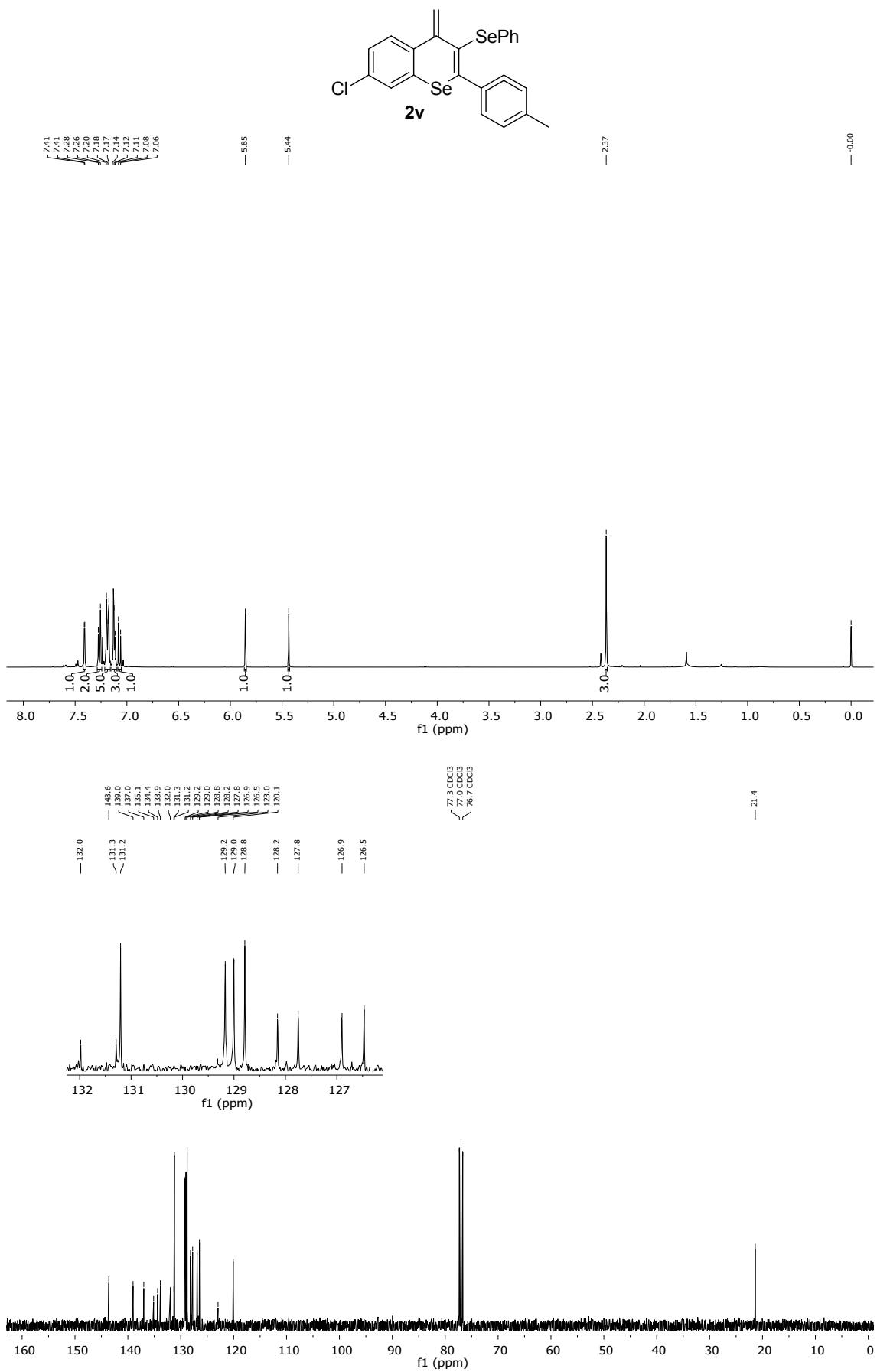
^{77}Se NMR (77 MHz, in CDCl_3 with diphenyl diselenide as external reference) for **2s**.



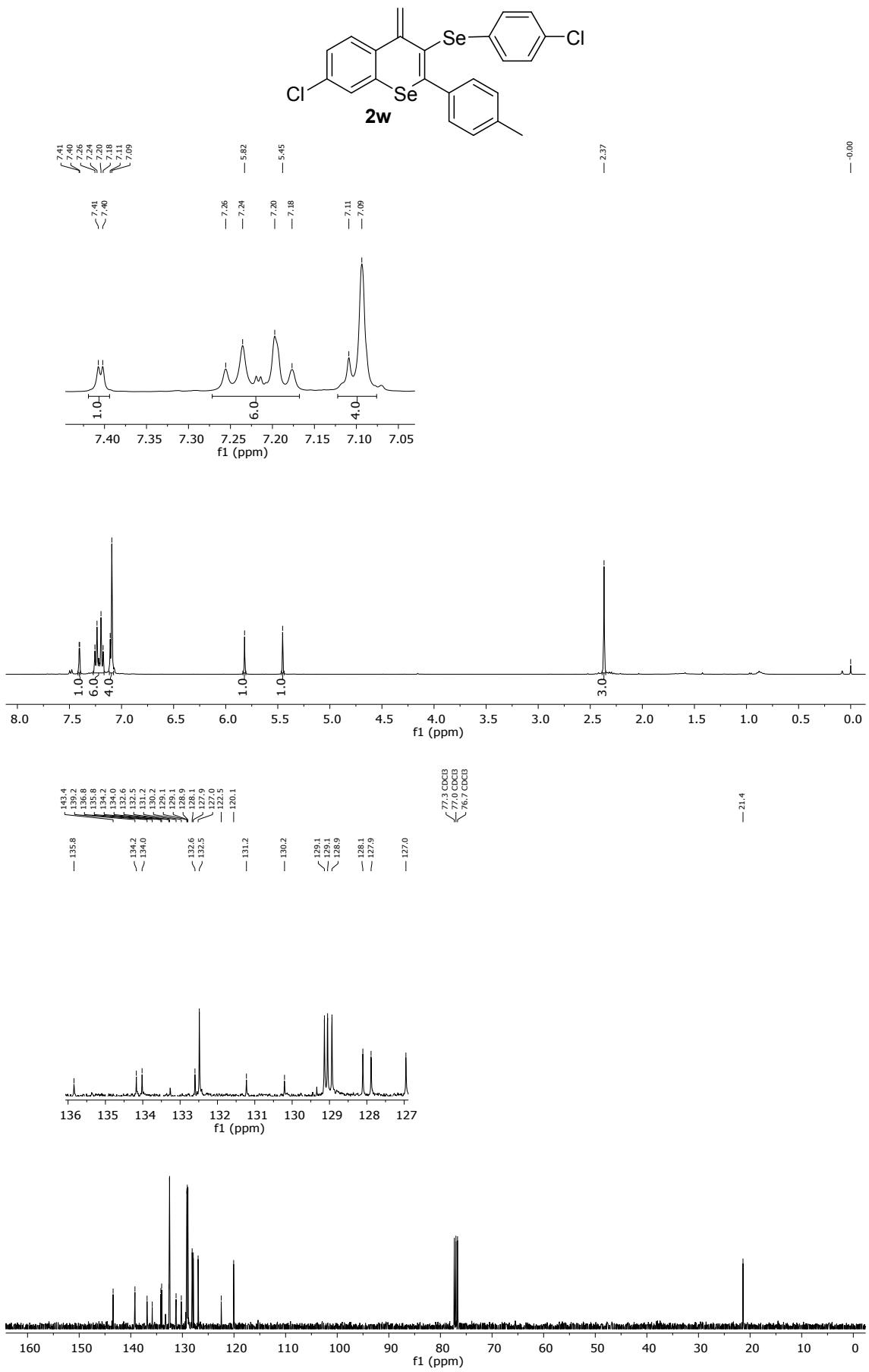
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2t** in CDCl_3 .



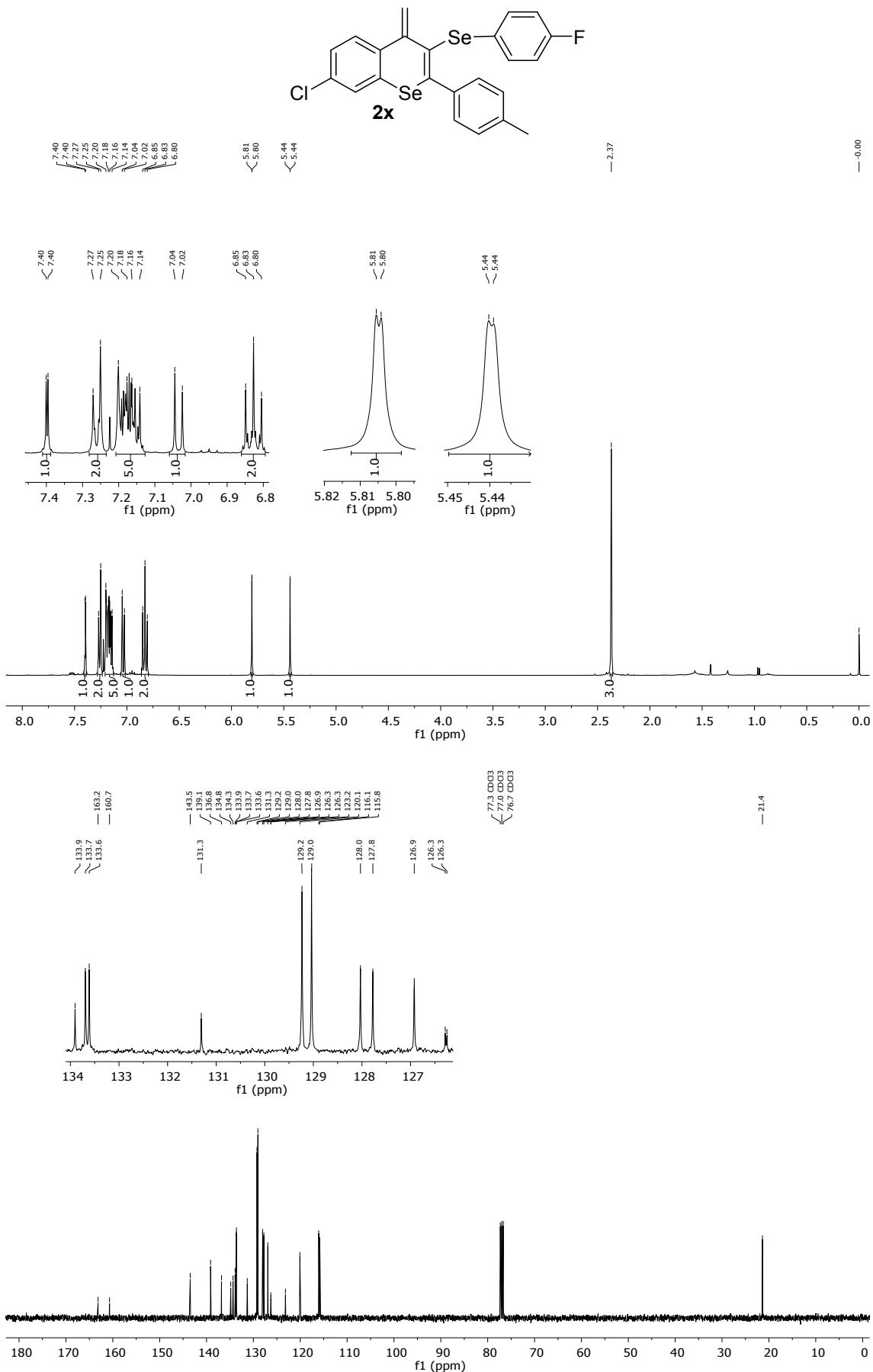
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2u** in CDCl_3 .



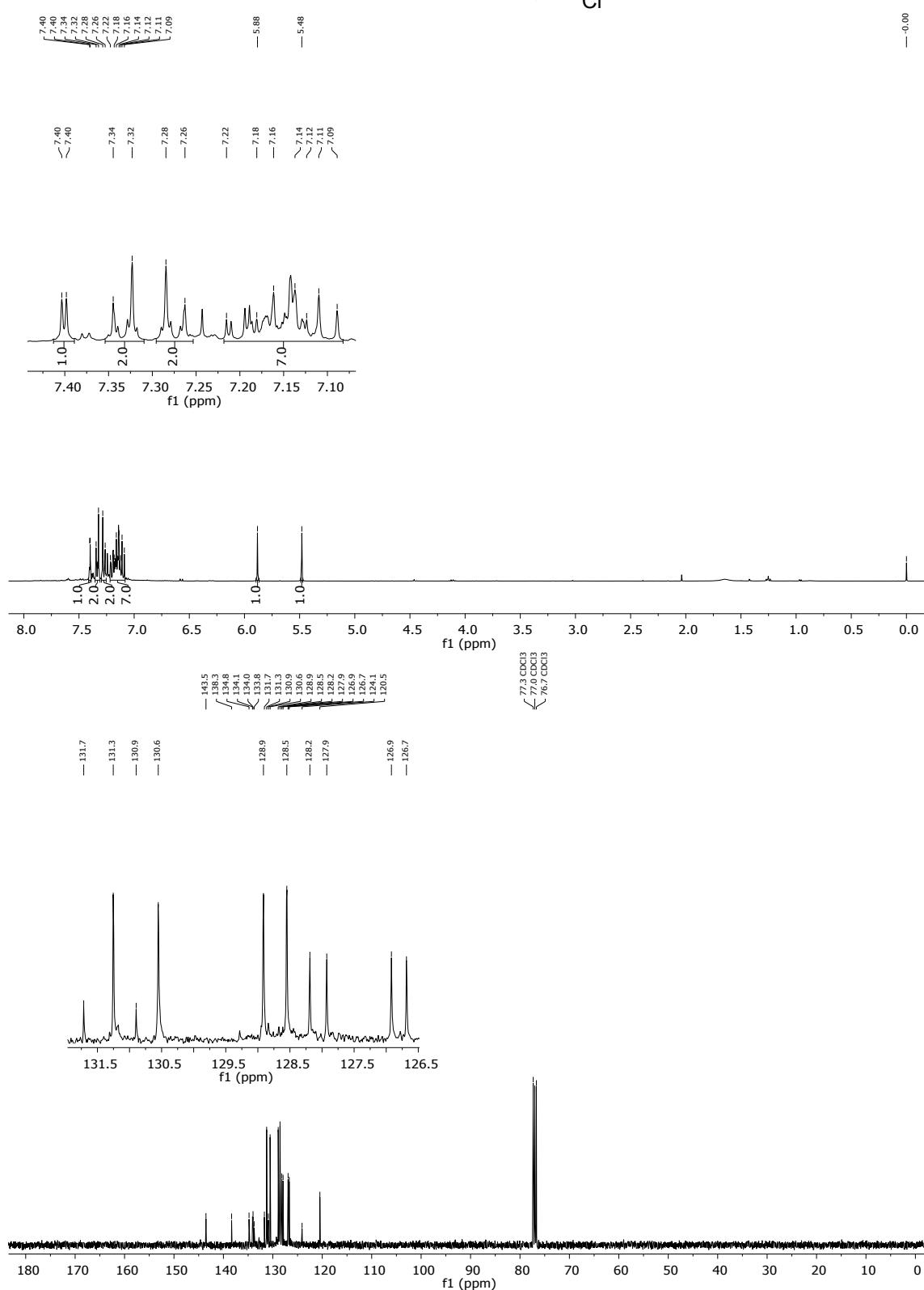
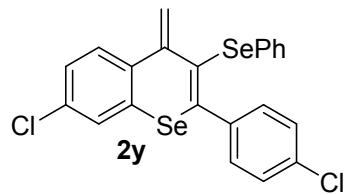
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2v** in CDCl₃.



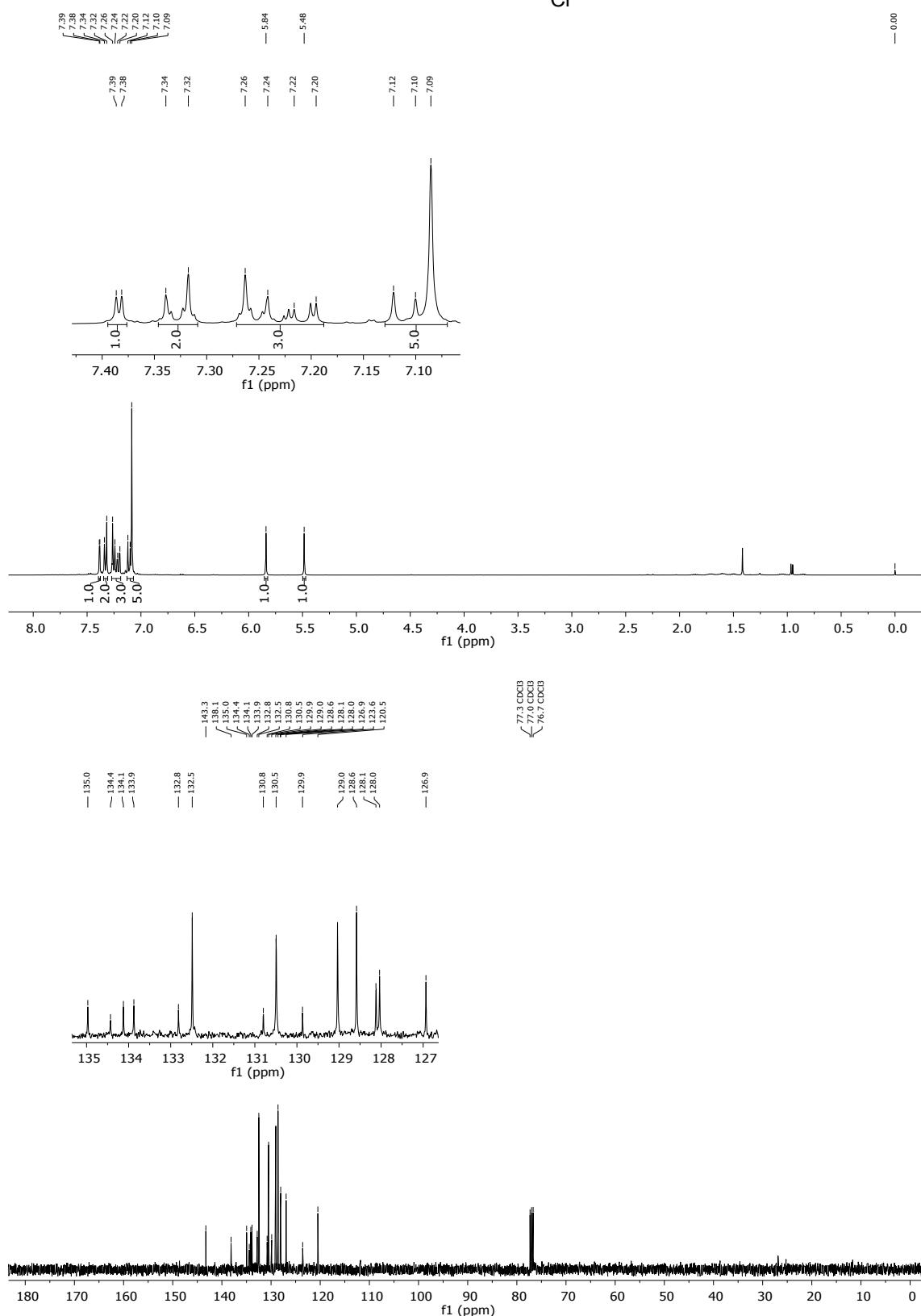
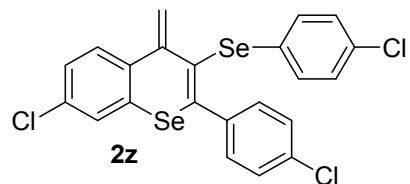
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2w** in CDCl₃.



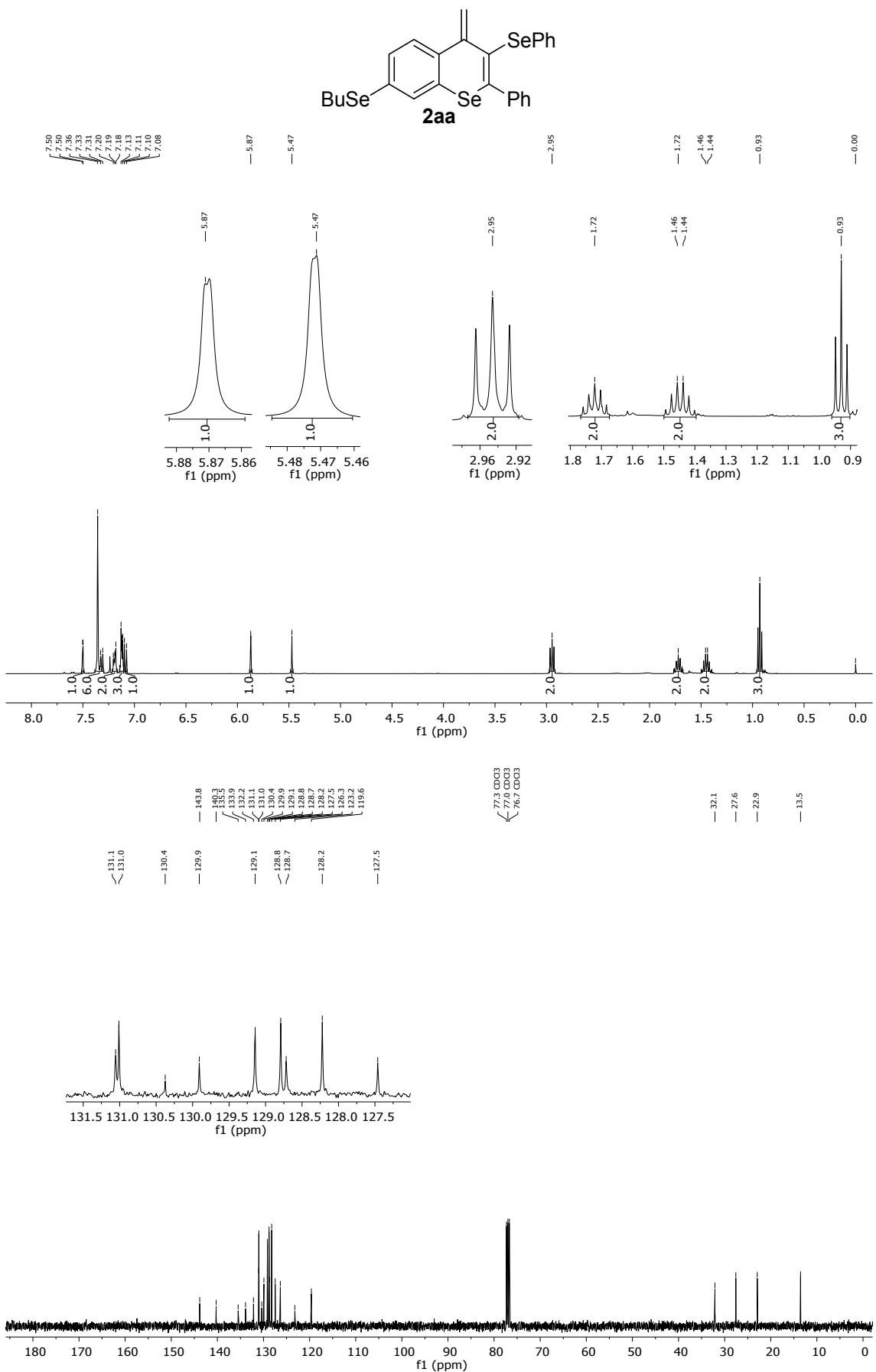
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2x** in CDCl₃.



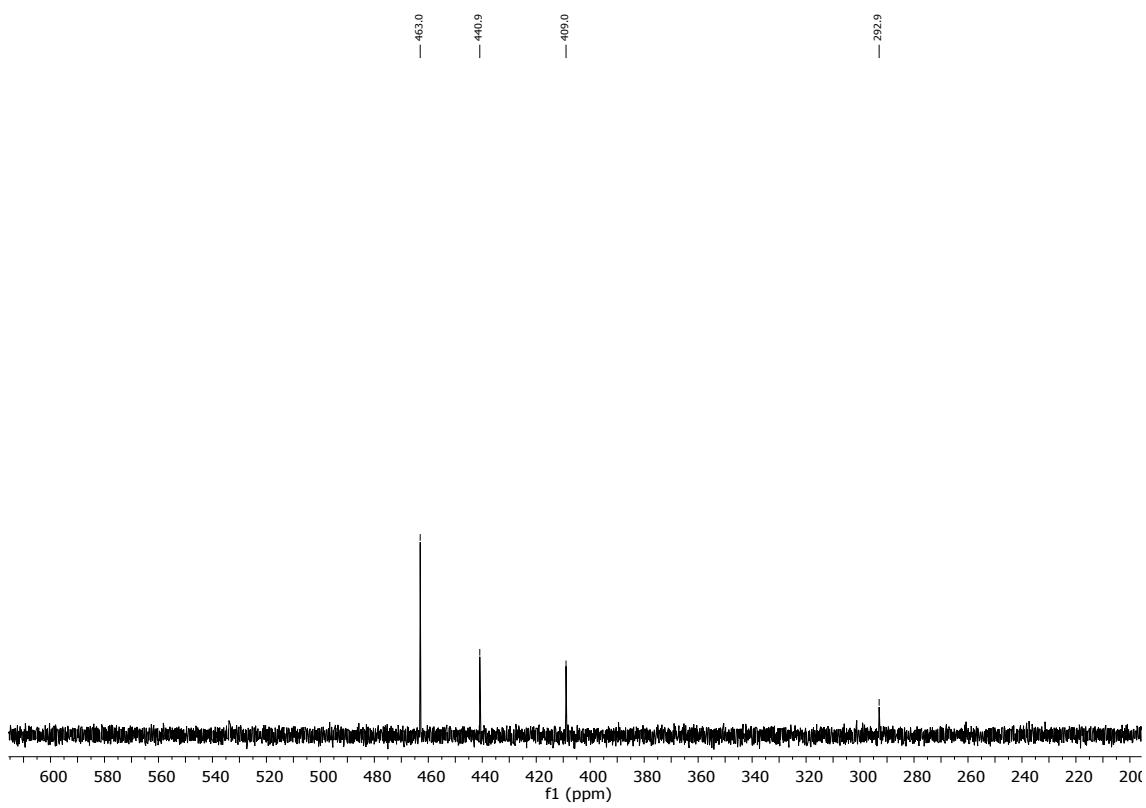
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2y** in CDCl_3 .



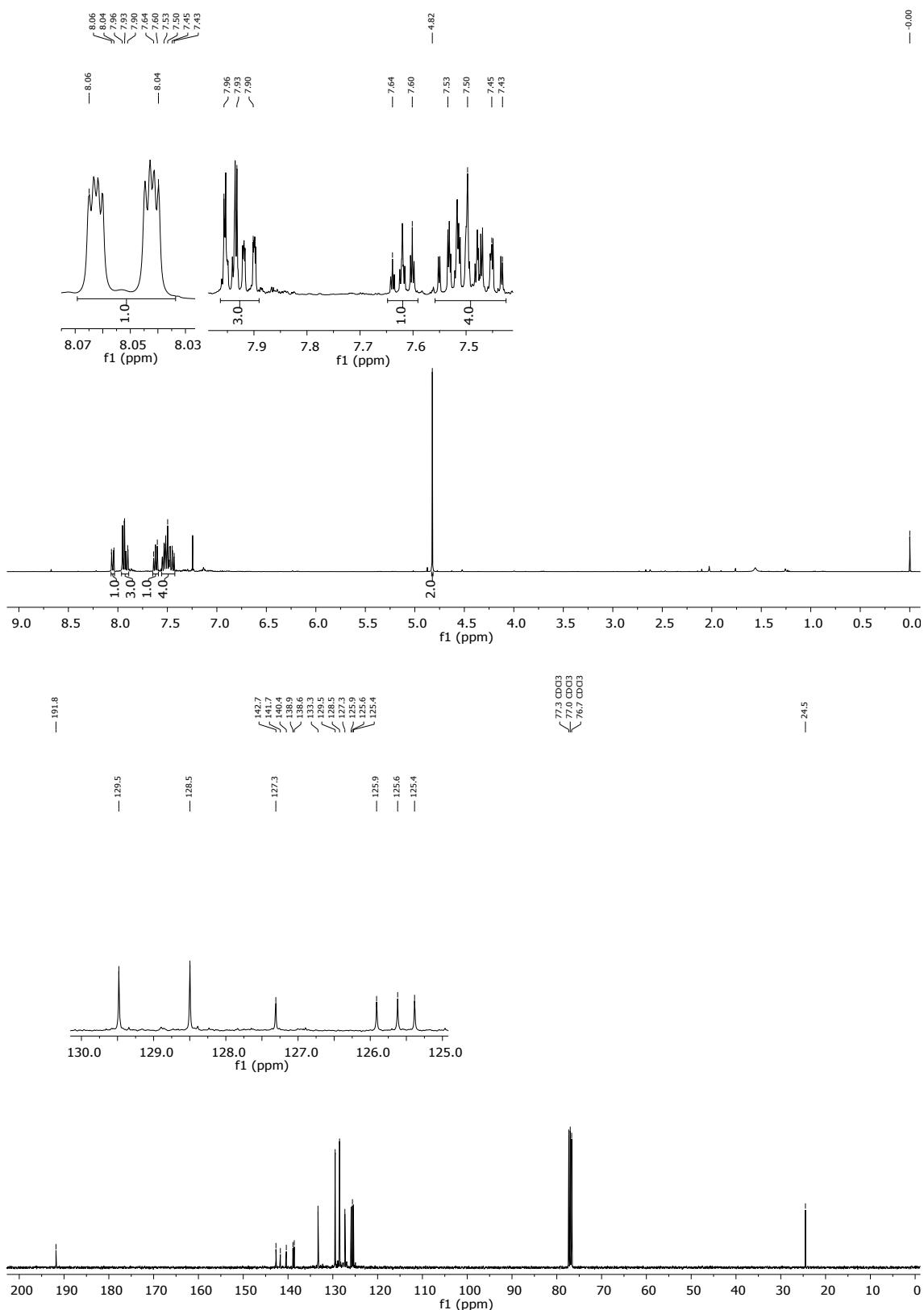
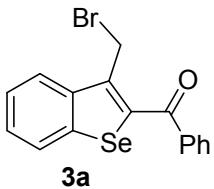
The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **2z** in CDCl_3 .



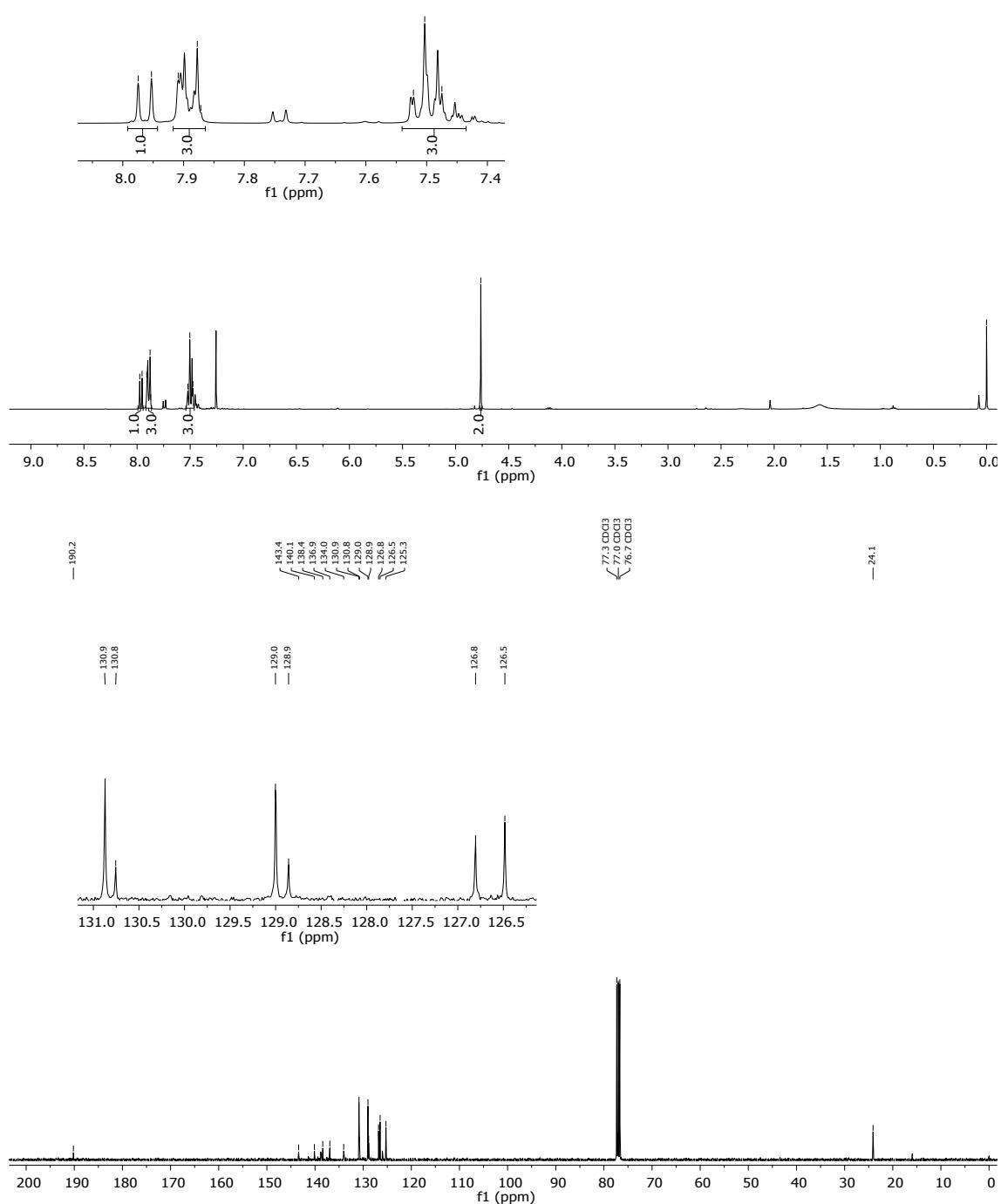
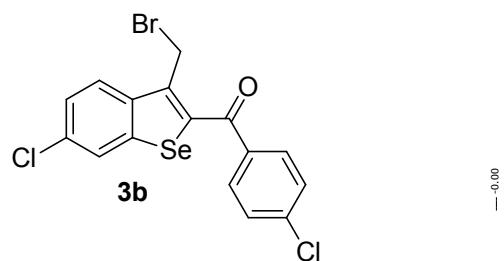
The ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra of **2aa** in CDCl_3 .



⁷⁷Se NMR (77 MHz, in CDCl₃ with diphenyl diselenide as external reference) for **2aa**.



The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **3a** in CDCl_3 .



The ^1H (400 MHz) and ^{13}C (100 MHz) NMR spectra of **3b** in CDCl_3 .