



Supplementary Materials

Leveraging SARS-CoV-2 Main Protease (M^{pro}) for COVID-19 Mitigation with Selenium-Based Inhibitors

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¹H, ¹³C ⁷⁷Se Spectra of compounds **1a**, **2a-c** and **3a-c**

S2–S8

Citation: De Luca, V.; Angeli, A.; Nocentini, A.; Gratterer, P.; Pratesi, S.; Tanini, D.; Carginale, V.; Capperucci, A.; Supuran, C.T.; Capasso, C. Leveraging SARS-CoV-2 Main Protease (M^{pro}) for COVID-19 Mitigation with Selenium-Based Inhibitors. *Int. J. Mol. Sci.* **2024**, *25*, 971. <https://doi.org/10.3390/ijms25020971>

Academic Editor: Barbara Ruaro

Received: 7 December 2023

Revised: 5 January 2024

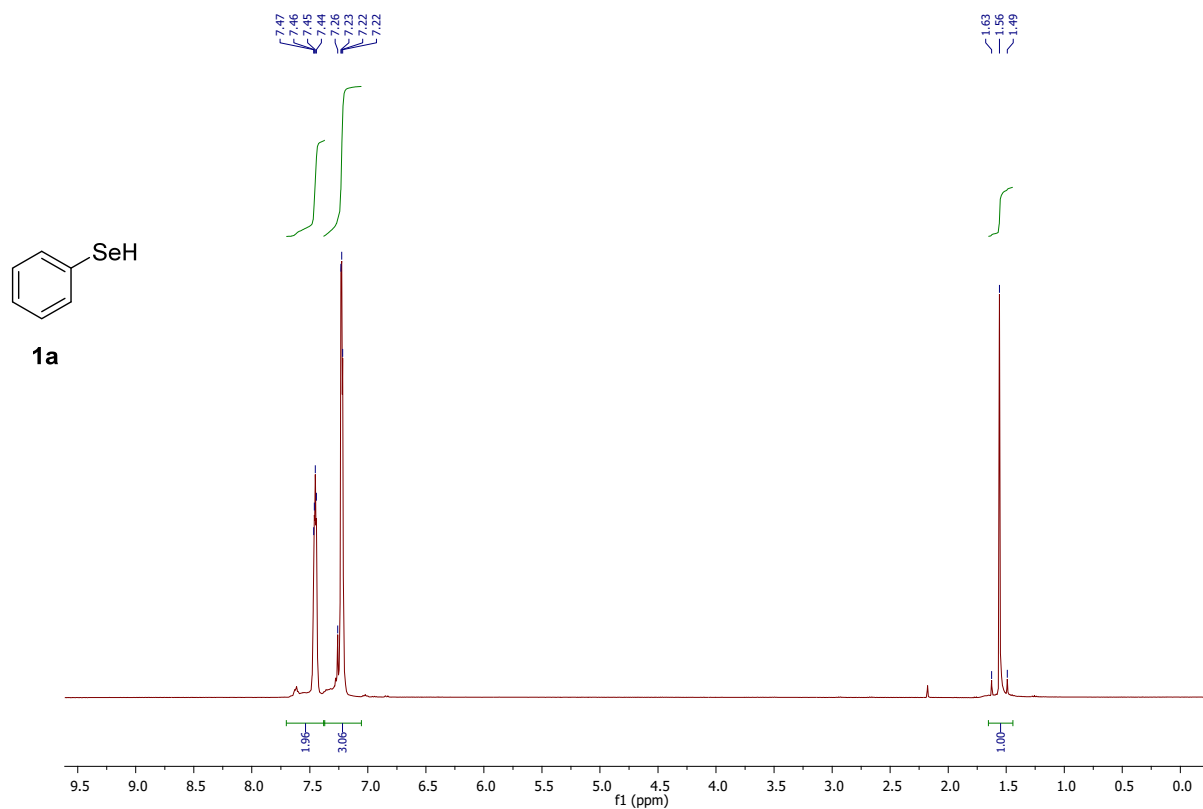
Accepted: 9 January 2024

Published: 12 January 2024



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Copy of NMR Spectra of synthesised compounds

**Figure S1.** ¹H NMR Spectrum of compound **1a** (CDCl₃, 400 MHz).

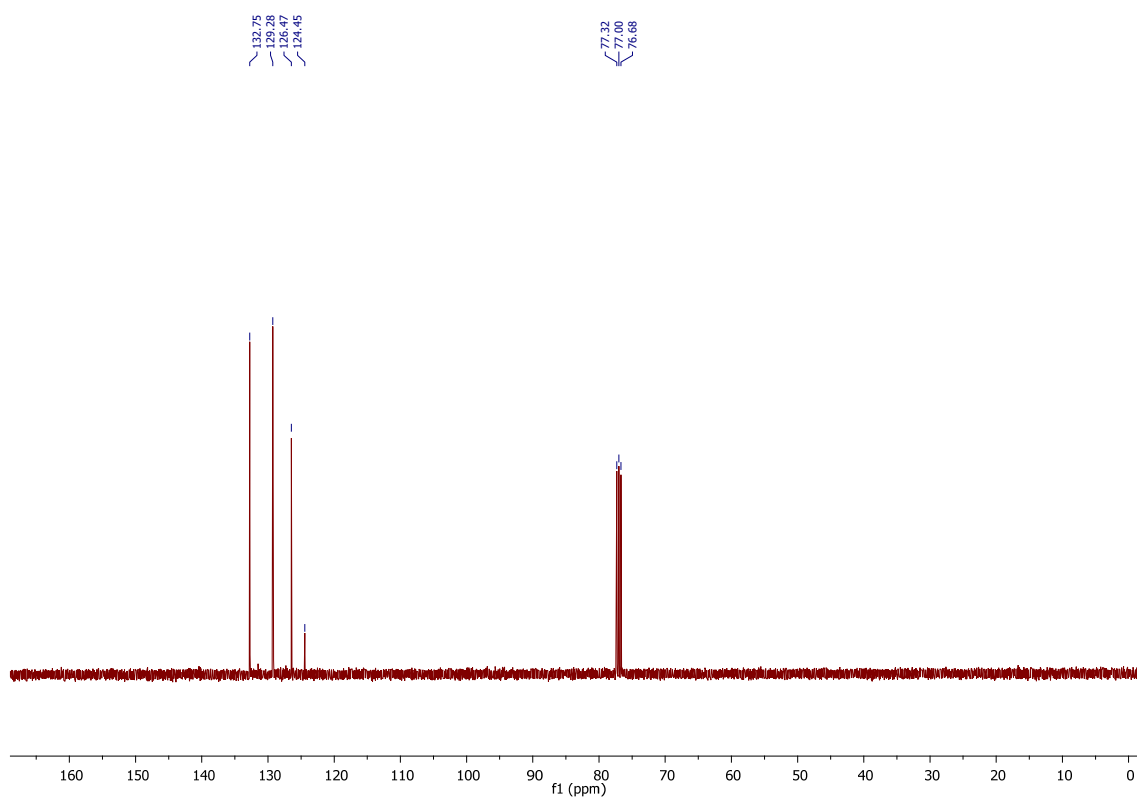
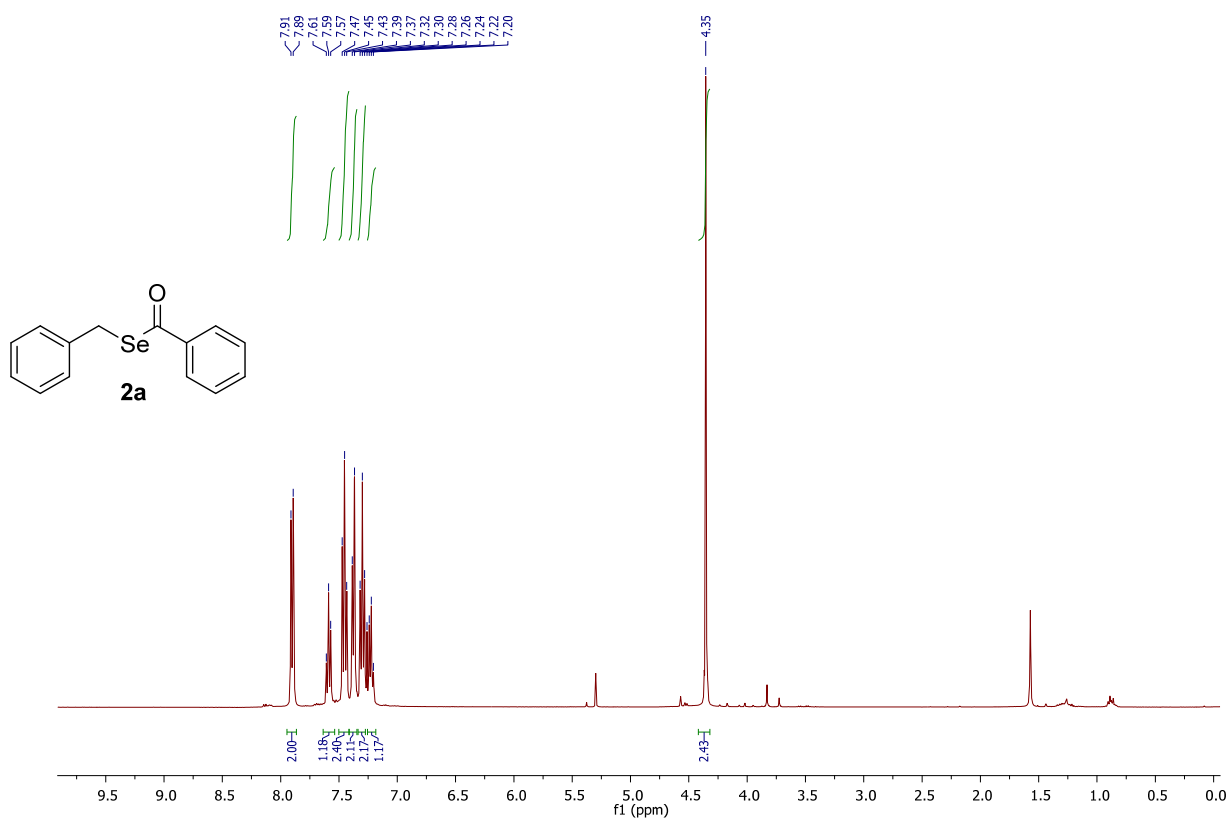
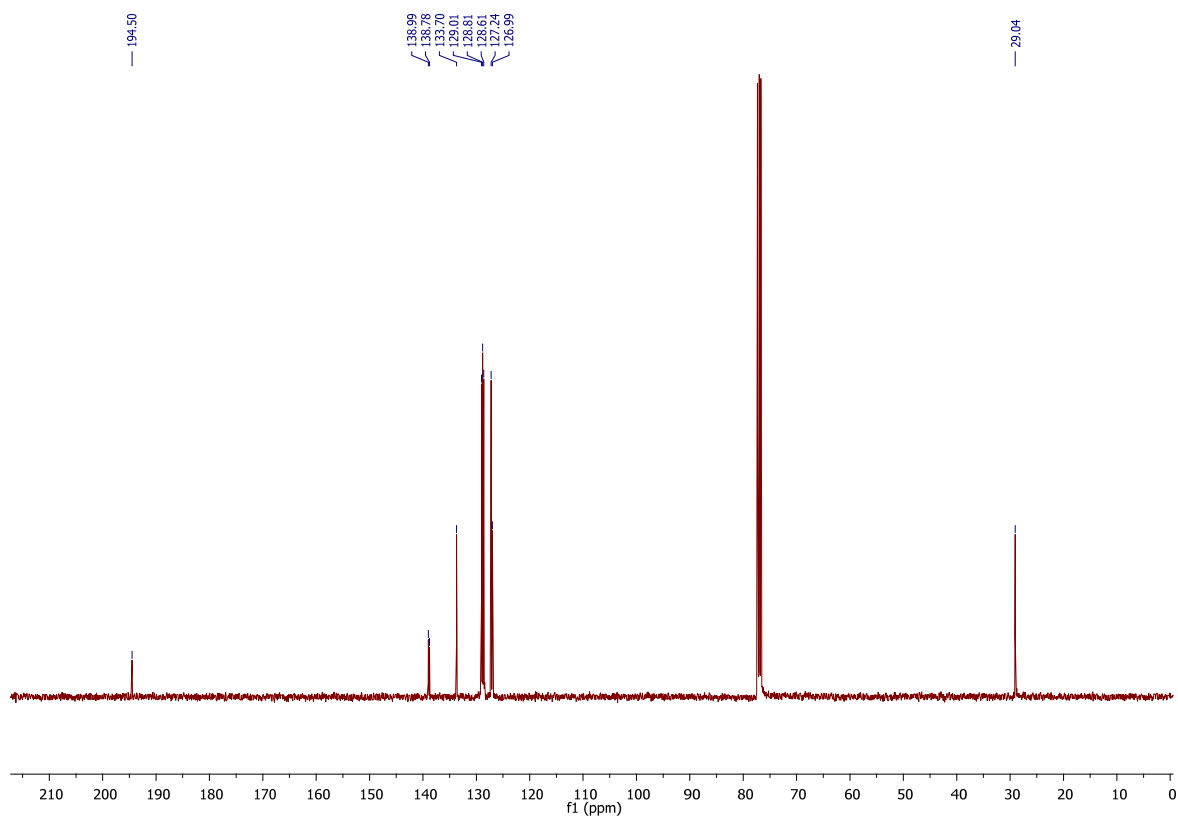
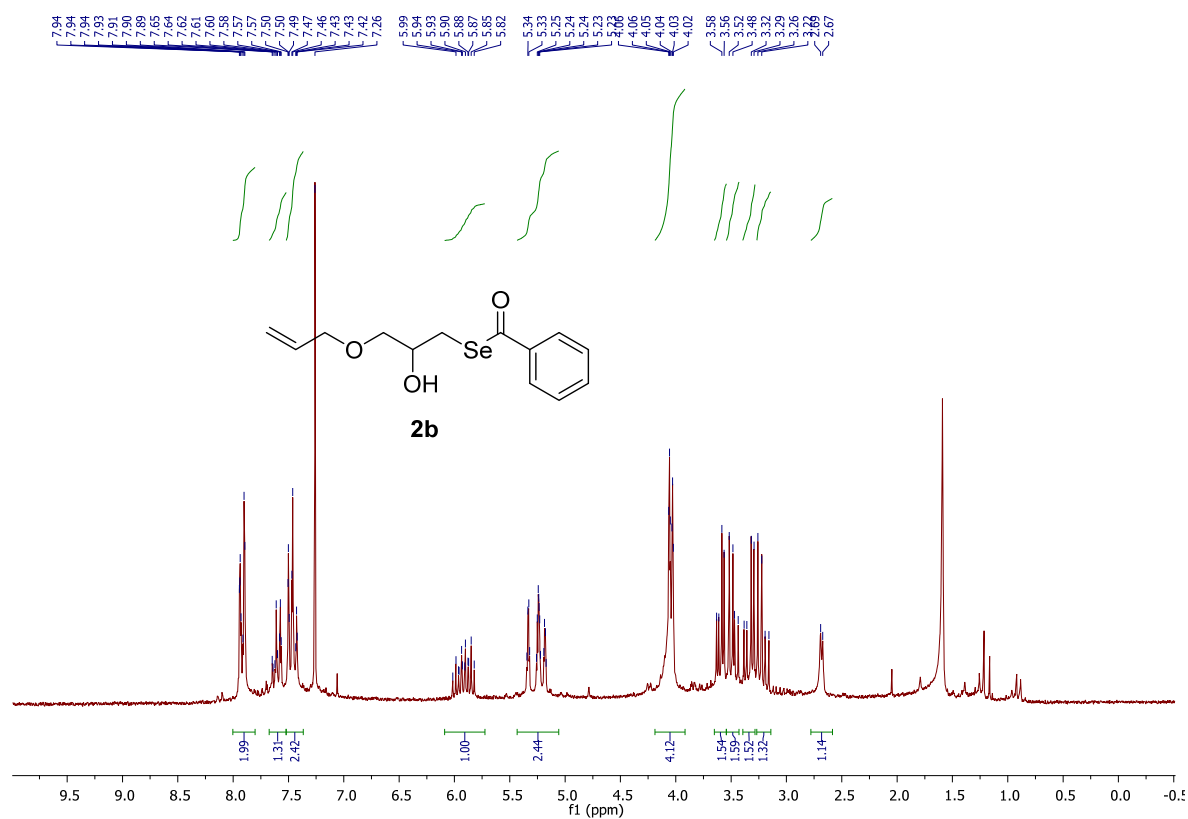
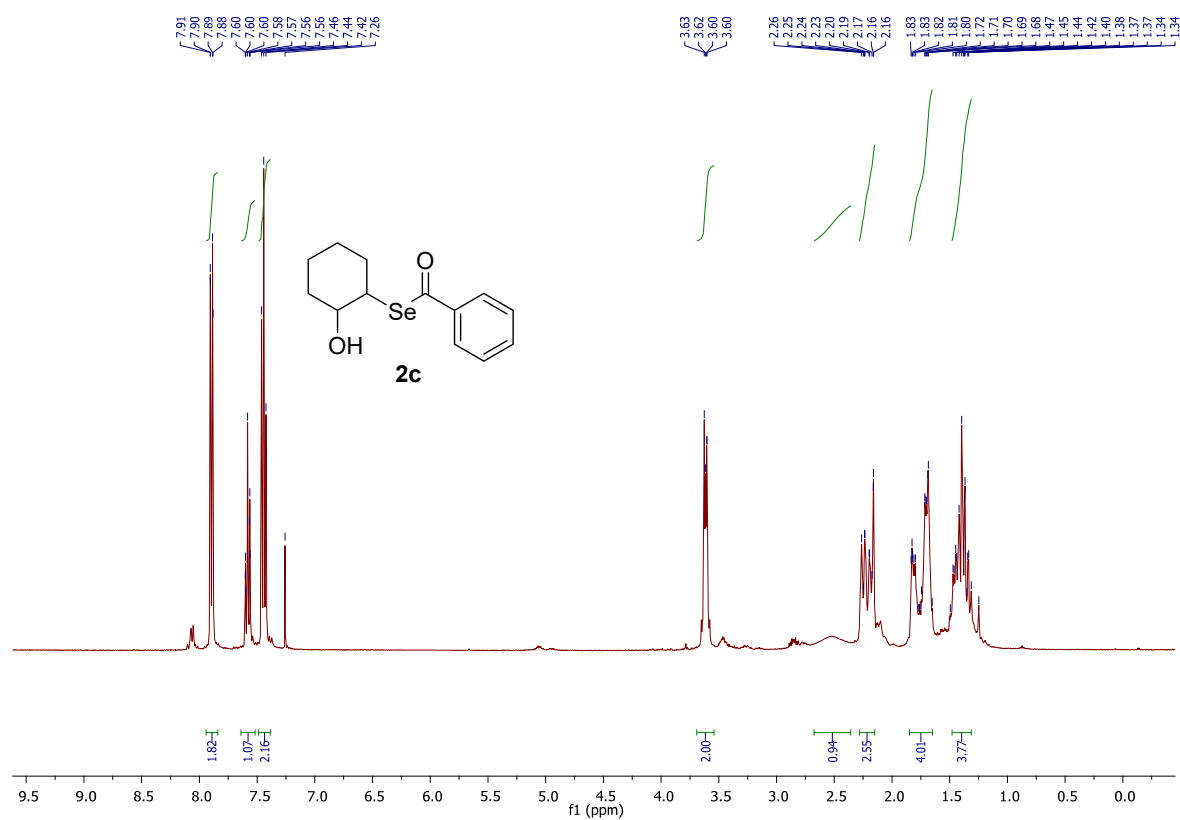
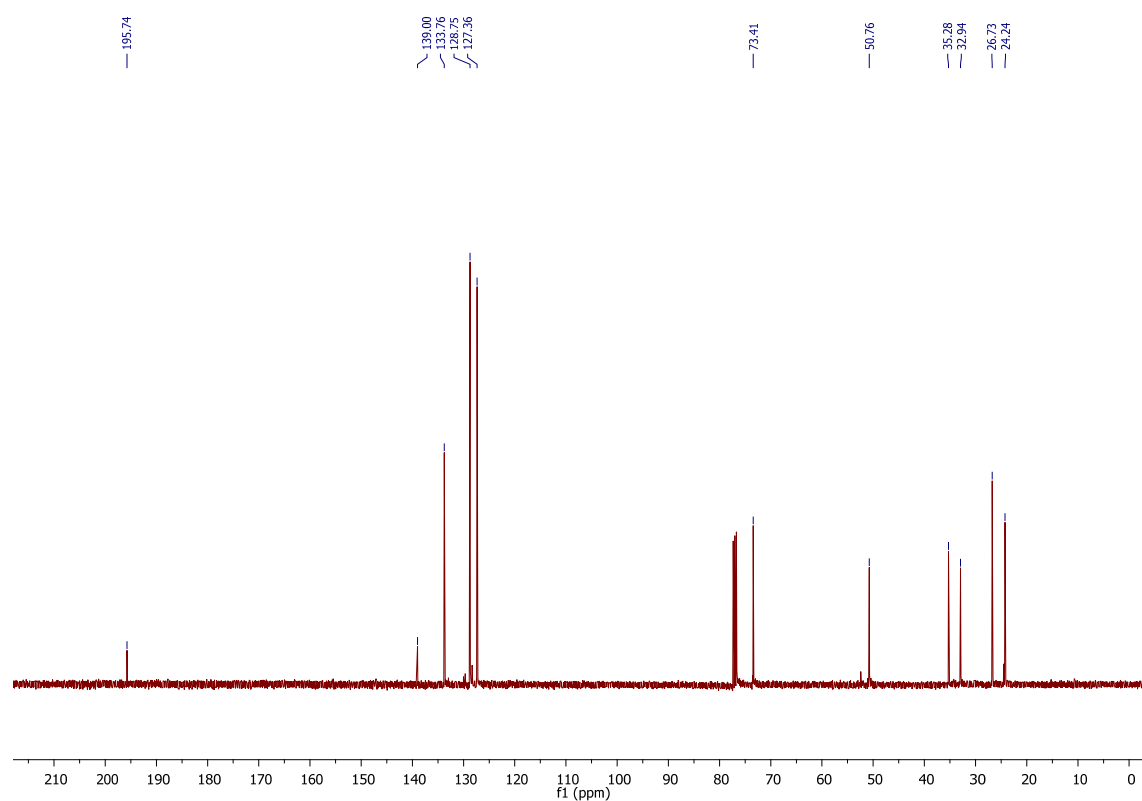
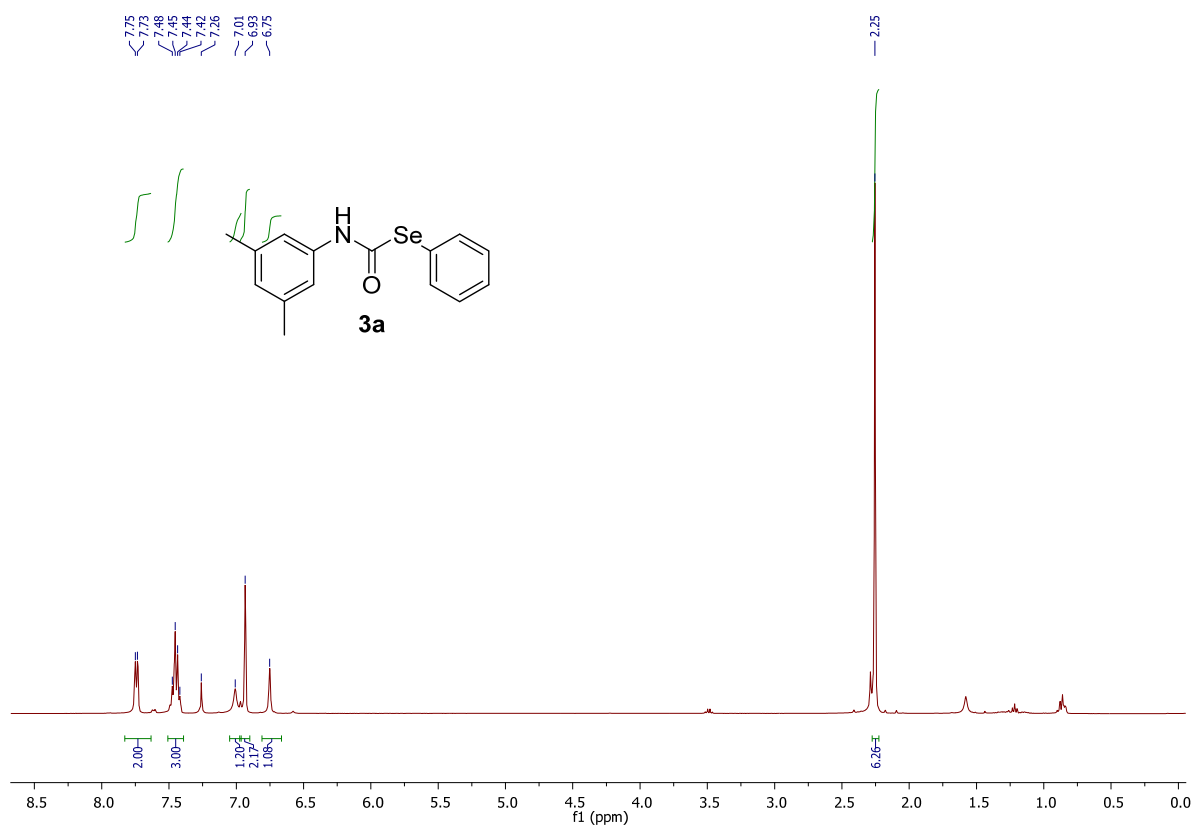


Figure S2. ^{13}C NMR Spectrum of compound **1a** (CDCl_3 , 100 MHz).

Figure S3. ¹H NMR Spectrum of compound **2a** (CDCl₃, 400 MHz).Figure S4. ¹³C NMR Spectrum of compound **2a** (CDCl₃, 100 MHz).

Figure S5. ¹H NMR Spectrum of compound **2b** (CDCl₃, 200 MHz).Figure S6. ¹H NMR Spectrum of compound **2c** (CDCl₃, 400 MHz).

Figure S7. ¹³C NMR Spectrum of compound **2c** (CDCl₃, 100 MHz).Figure S8. ¹H NMR spectrum of compound **3a** (CDCl₃, 400 MHz).

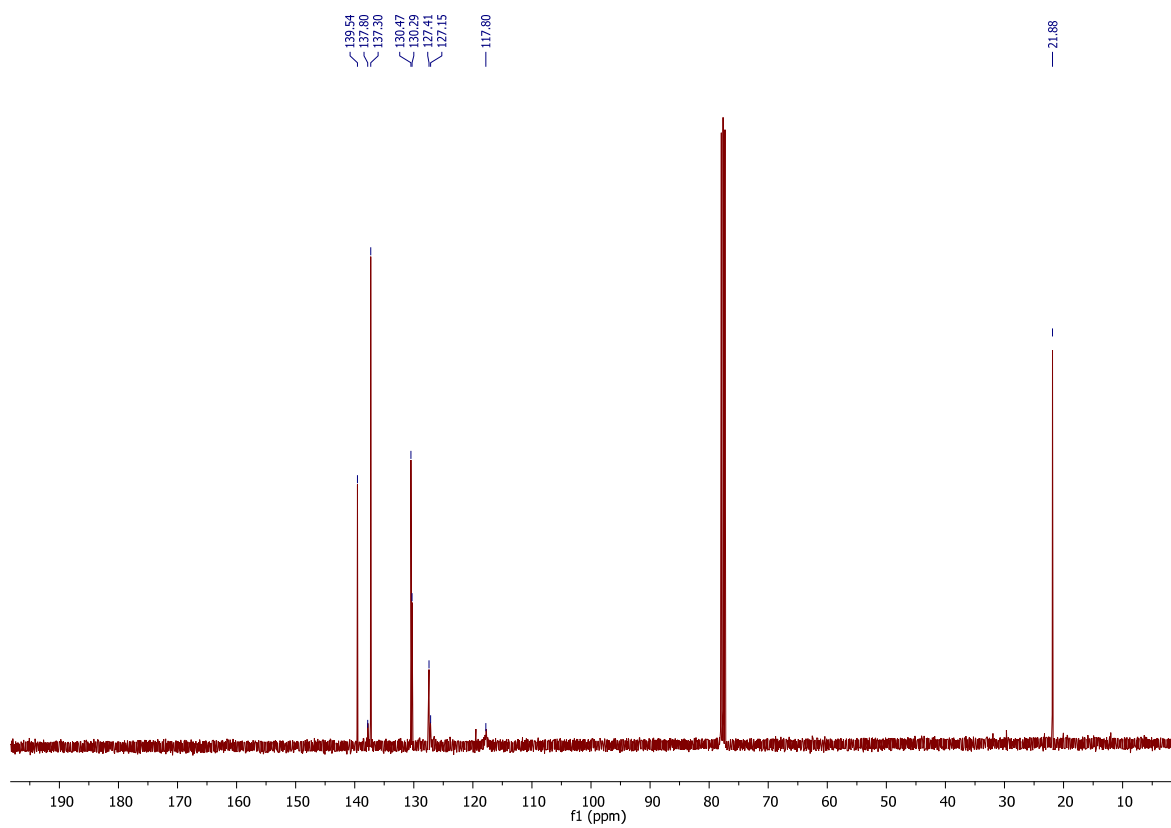
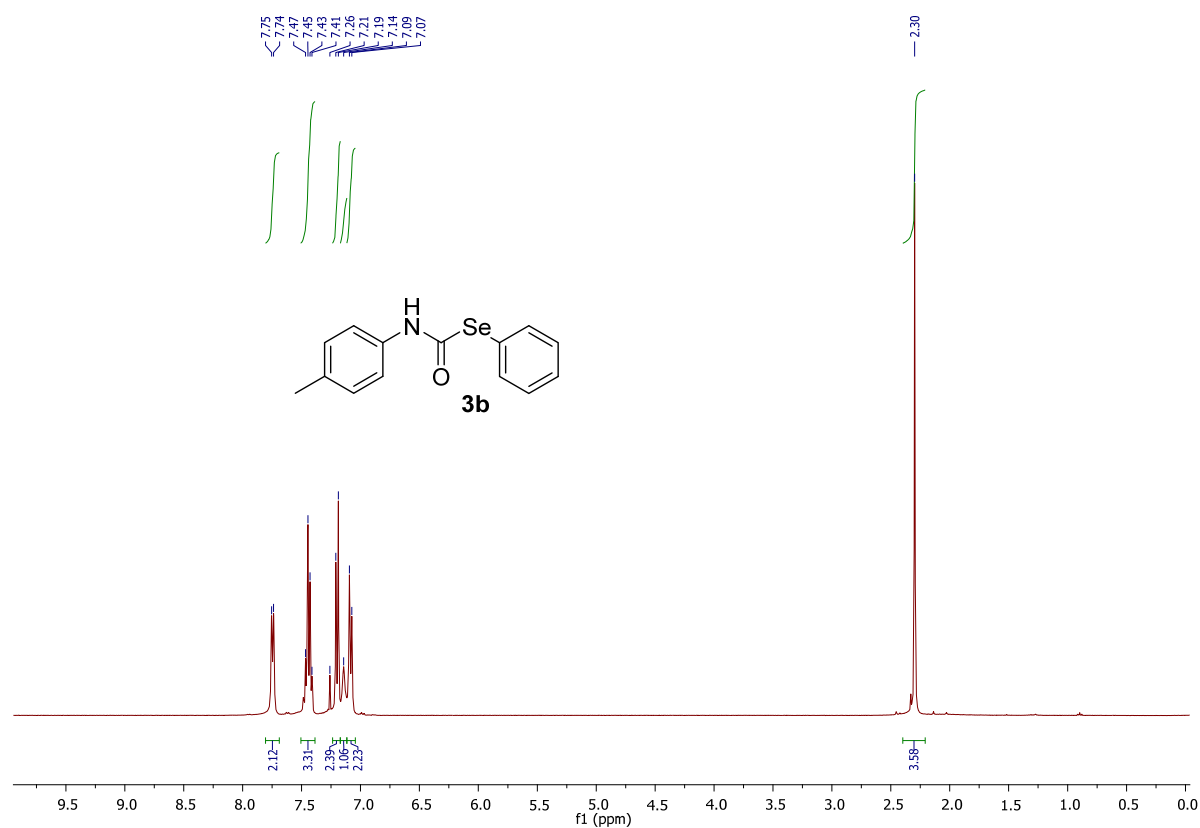
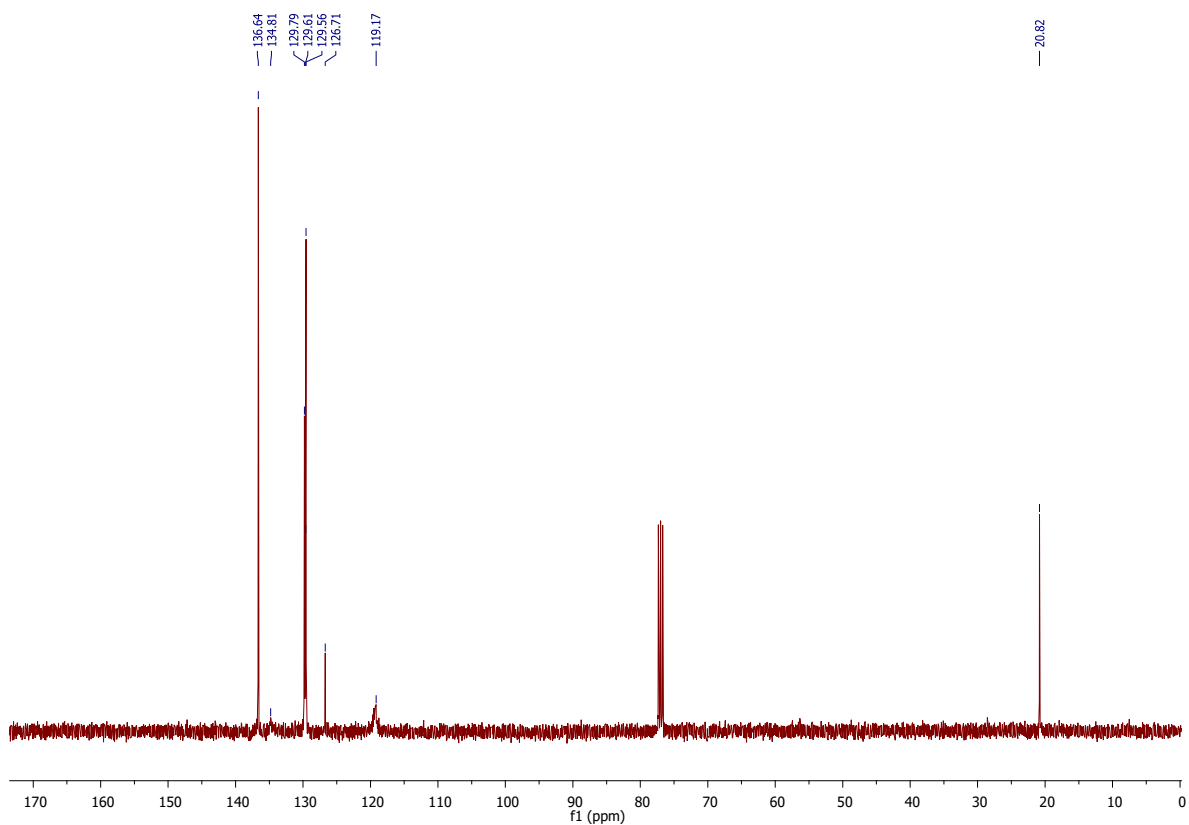


Figure S9. ^{13}C NMR spectrum of compound **3a** (CDCl_3 , 100 MHz).

Figure S10. ¹H NMR spectrum of compound **3b** (CDCl₃, 400 MHz).Figure S11. ¹³C NMR spectrum of compound **3b** (CDCl₃, 100 MHz).

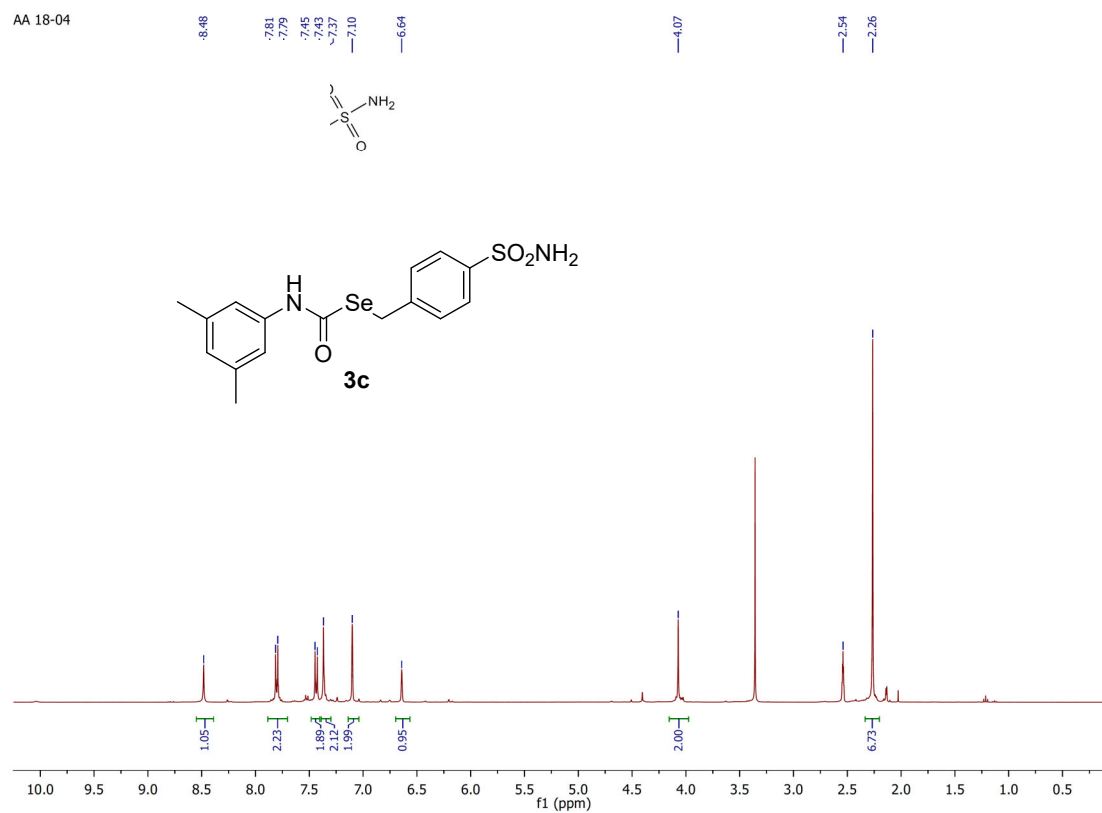


Figure S12. ^1H NMR spectrum of compound **3c** ($\text{DMSO-}d_6$, 400 MHz).

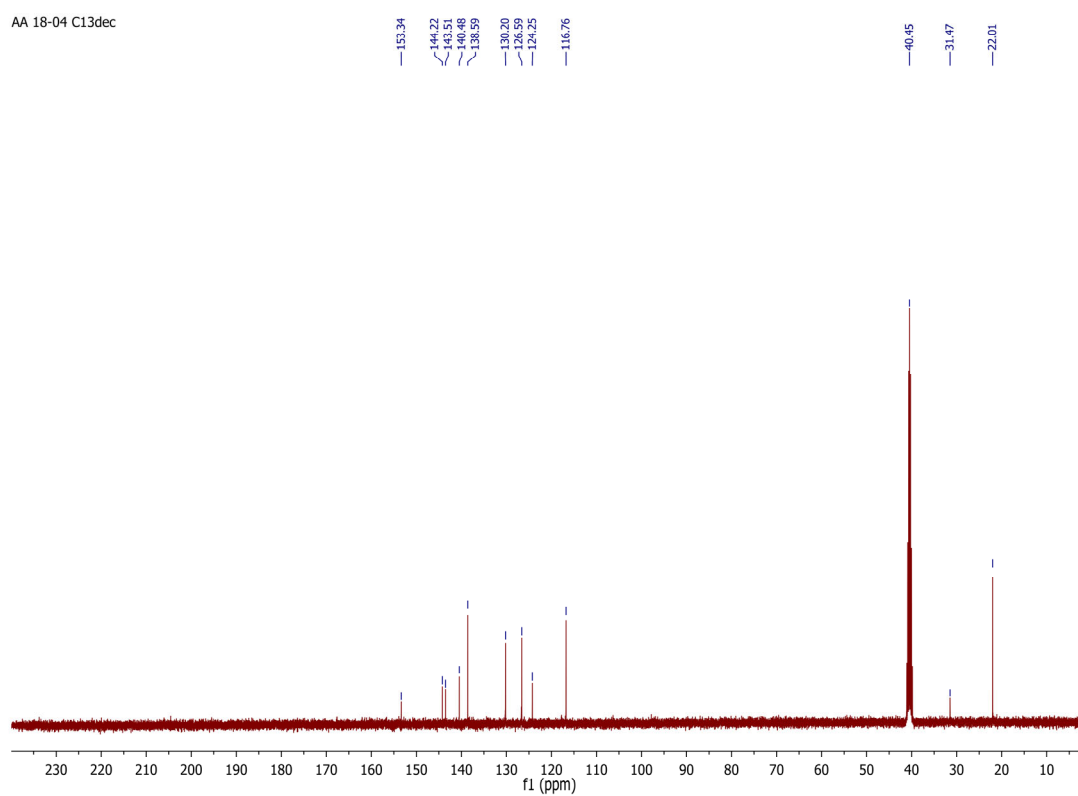


Figure S13. ^{13}C NMR spectrum of compound **3c** ($\text{DMSO-}d_6$, 100 MHz).

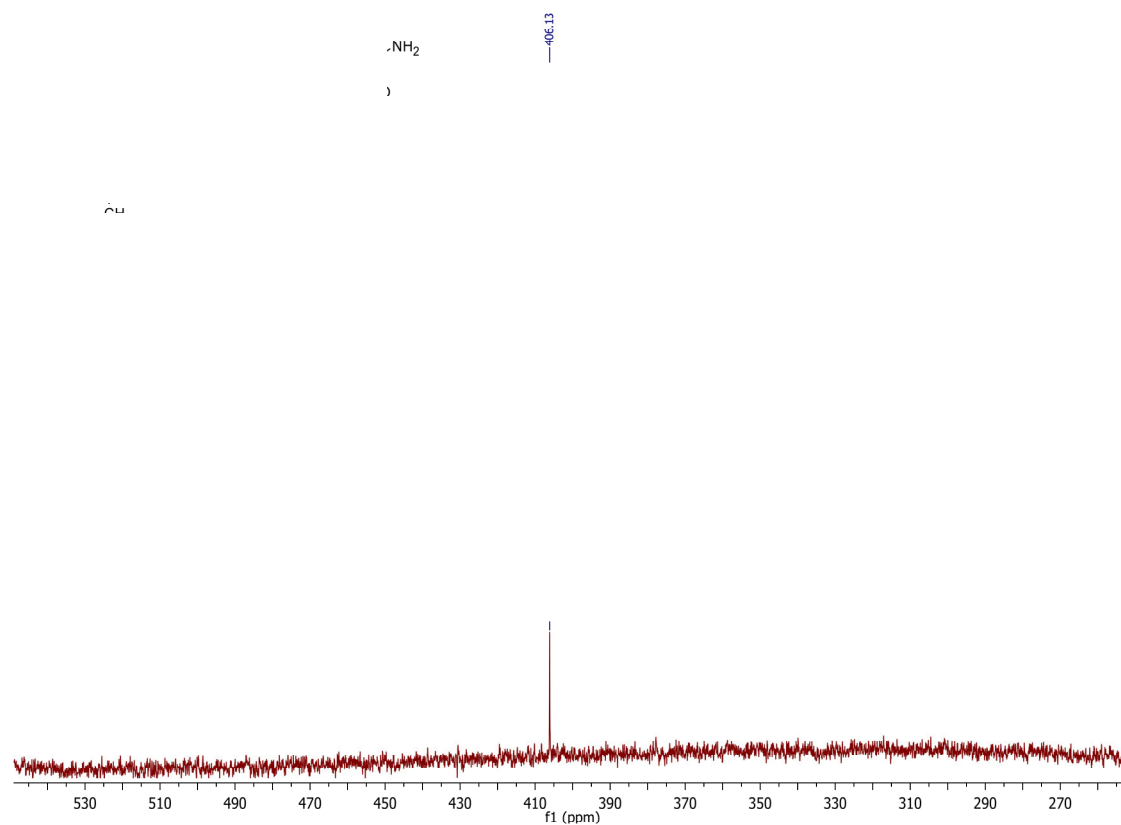


Figure S14. ^{77}Se NMR spectrum of compound **3c** ($\text{DMSO-}d_6$, 76 MHz).

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