Supplementary Material

Ultrasound and Oxone® promoting regioselective selenofunctionalization of chromone

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1. General Remarks

The reactions were monitored by TLC carried out on Merck silica gel (60 F_{254}) by using UV light as visualizing agent and 5% vanillin in 10% H_2SO_4 and heat as developing agents. Baker silica gel (particle size 0.040-0.063 mm) was used for flash chromatography. The nuclear magnetic resonance (NMR) analyses were carried out in a Bruker Avance III HD spectrometer employing a direct broadband observe probe (F-BBO). Hydrogen nuclear magnetic resonance spectra (^{1}H NMR) were obtained at 400 MHz. Spectra were recorded in deuterated DMSO-d_6 solutions. ^{1}H NMR Chemical shifts are reported in ppm, referenced to tetramethylsilane (TMS) as the internal reference (0.0 ppm). Coupling constant (*J*) are reported in Hertz (Hz). Abbreviations to denote the multiplicity of a signal are s (singlet), d (doublet), dd (doublet of doublet) and m (multiplet). Carbon-13 nuclear magnetic resonance spectra (^{13}C-{^{1}H} NMR) were obtained at 100 MHz. ^{13}C NMR Chemical shifts are reported in ppm, referenced to tetramethylsilane (TMS) as the internal reference (0.0 ppm). Selenium-77 nuclear magnetic resonance spectra (^{77}Se-{^{1}H} NMR were obtained at 76.0 MHz. The ^{77}Se NMR chemical shifts are reported in ppm relative to external standard, the $C_6H_5SeSeC_6H_5$ in $CDCl_3$ (δ 463 ppm). Low-resolution mass spectra (MS) were obtained with a Shimadzu GC-MS-QP2010 mass spectrometer. The HRMS analyses were performed in a Bruker micrOTOF-QII spectrometer equipped with an APCI source operating in positive mode. The samples were solubilized in acetonitrile and analyzed by direct infusion. The ultrasound-promoted reactions were performed using a Cole Parmer-ultrasonic processor Model CPX 130, with a maxim power of 130 W, operating at amplitude of 60% and a frequency of 20 kHz. The temperature of the reaction under US was monitored using an Incoterm digital infrared thermometer Model Infraterm (Brazil). Melting point (mp) values were measured in a Marte PFD III instrument with a 0.1 ^{o}C precision. Oxone® was purchased from Sigma Aldrich.

2. General procedure for synthesis of 3-(phenylselanyl)-4*H*-chromen-4-ones 3

To a 10 mL round-bottomed glass vial, the chromone **1** (0.250 mmol), diselenide **2a**-**h** (0.125 mmol), Oxone® (0.077 g; 0.250 mmol) and DMF (2.0 mL) were added. The US probe was placed in the reaction vial, which was sonicated (20 KHz, 60% of sonic amplitude) for the time indicated in Table 2. The reaction progress was monitored by TLC in order to evaluate the starting materials consumption. After that, the reaction mixture was extracted with ethyl acetate (3x 15.0 mL), the organic phase was separated, dried over $MgSO_4$ and the solvent was evaporated under reduced pressure. The product was isolated by column chromatography using silica gel 60A (0.060-0.200 mm-Across) and using a mixture of hexane and ethyl acetate (90:10).

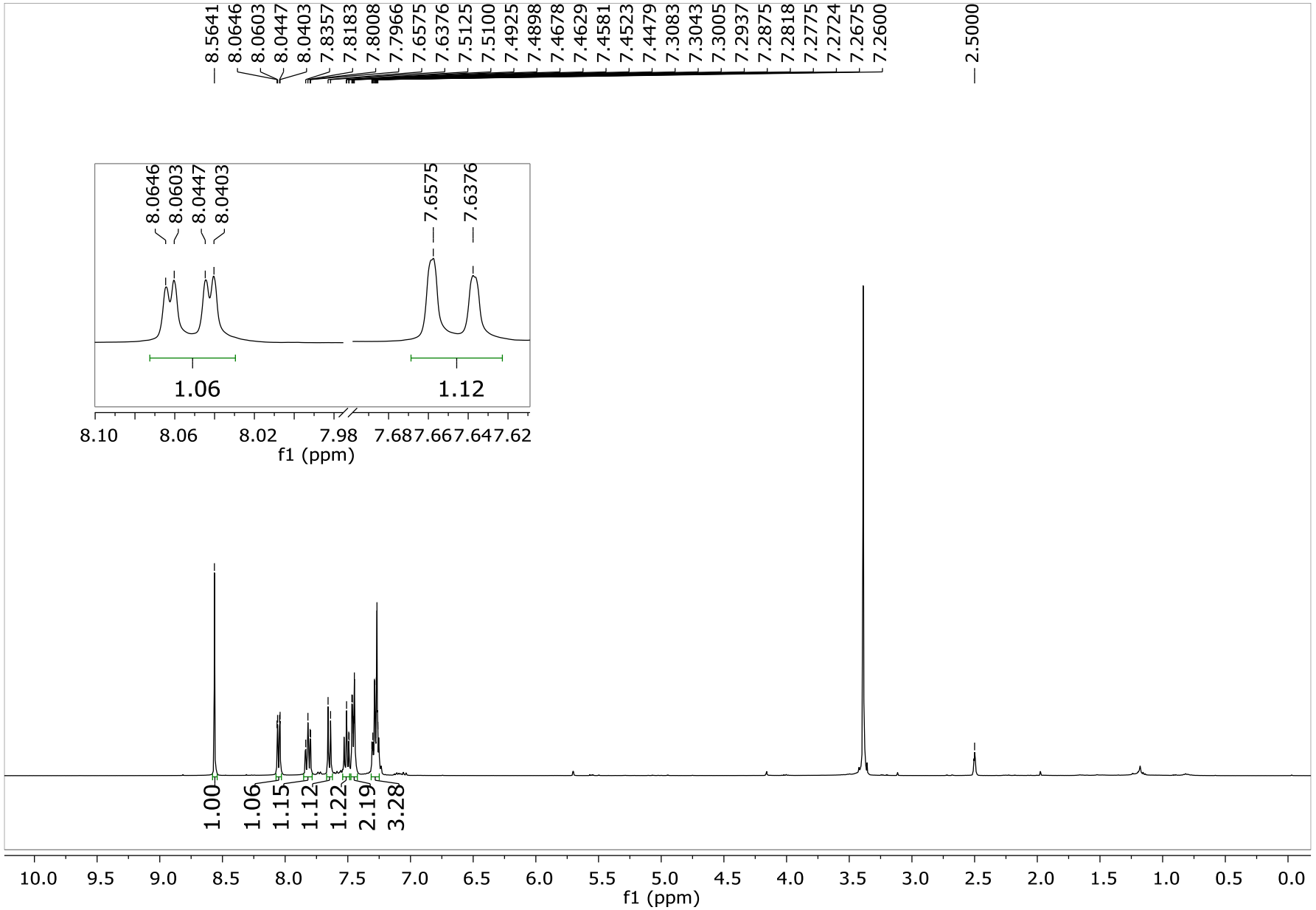


Figure 1S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3a**.

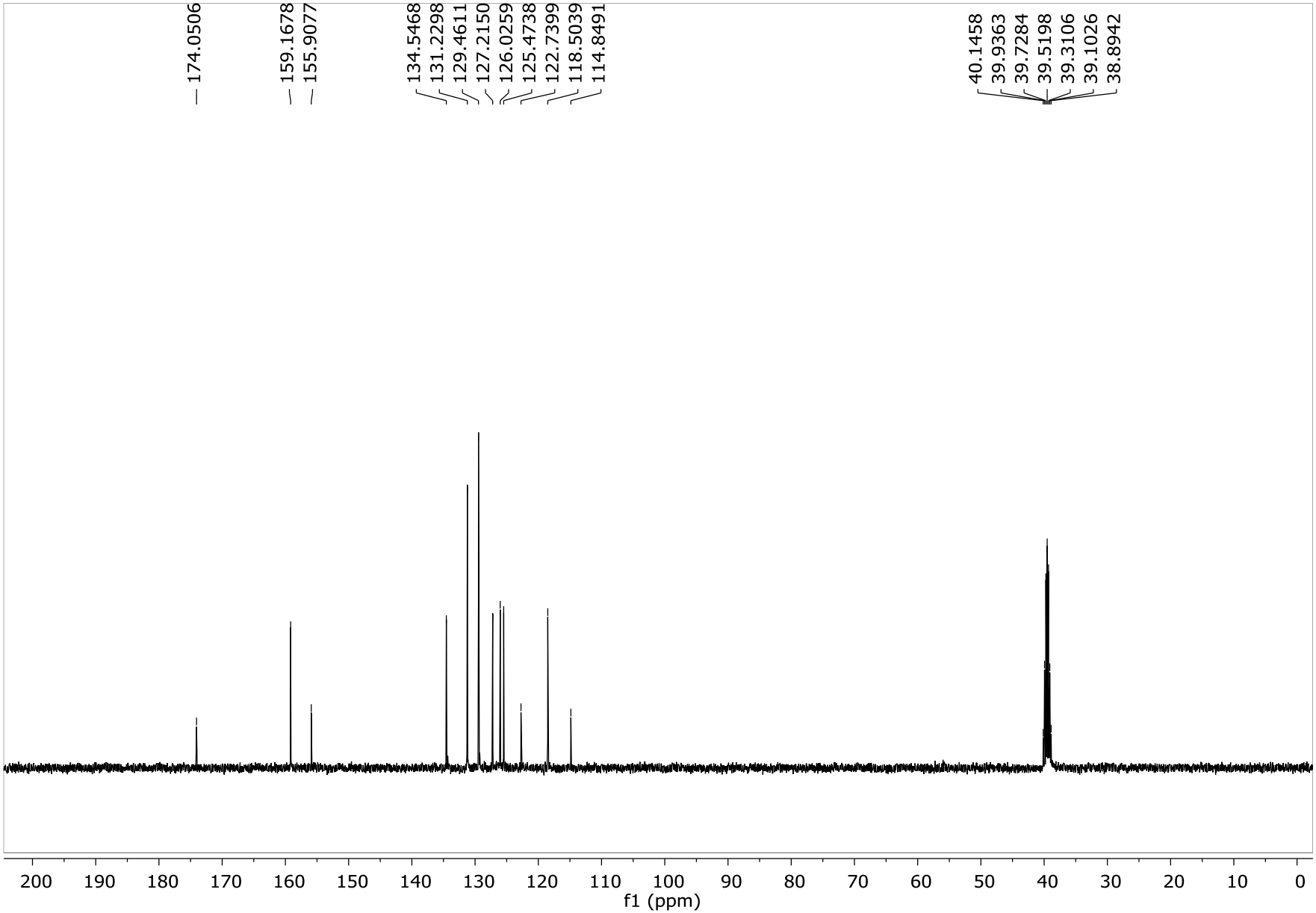


Figure 2S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3a**.

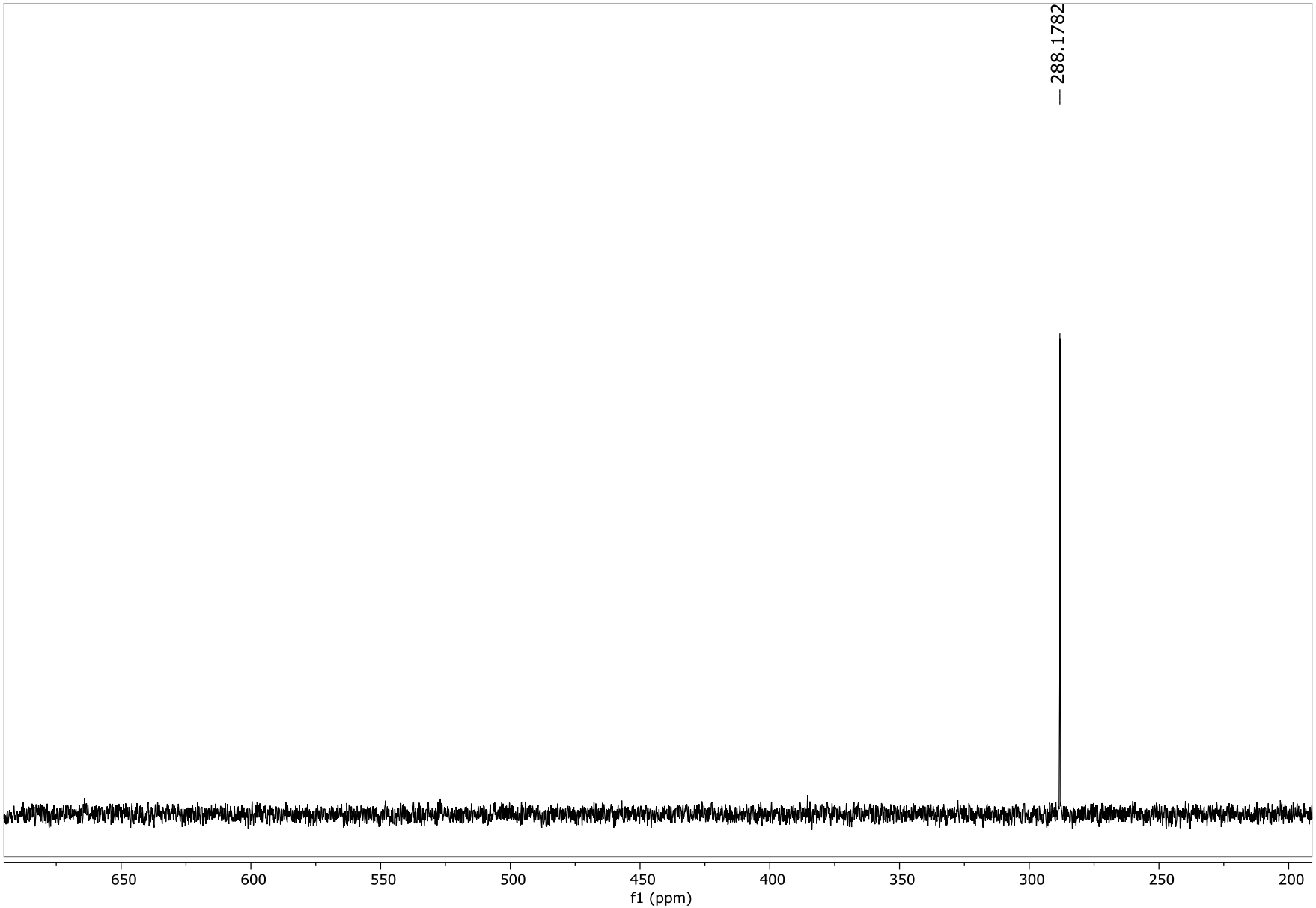


Figure 3S. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3a**.

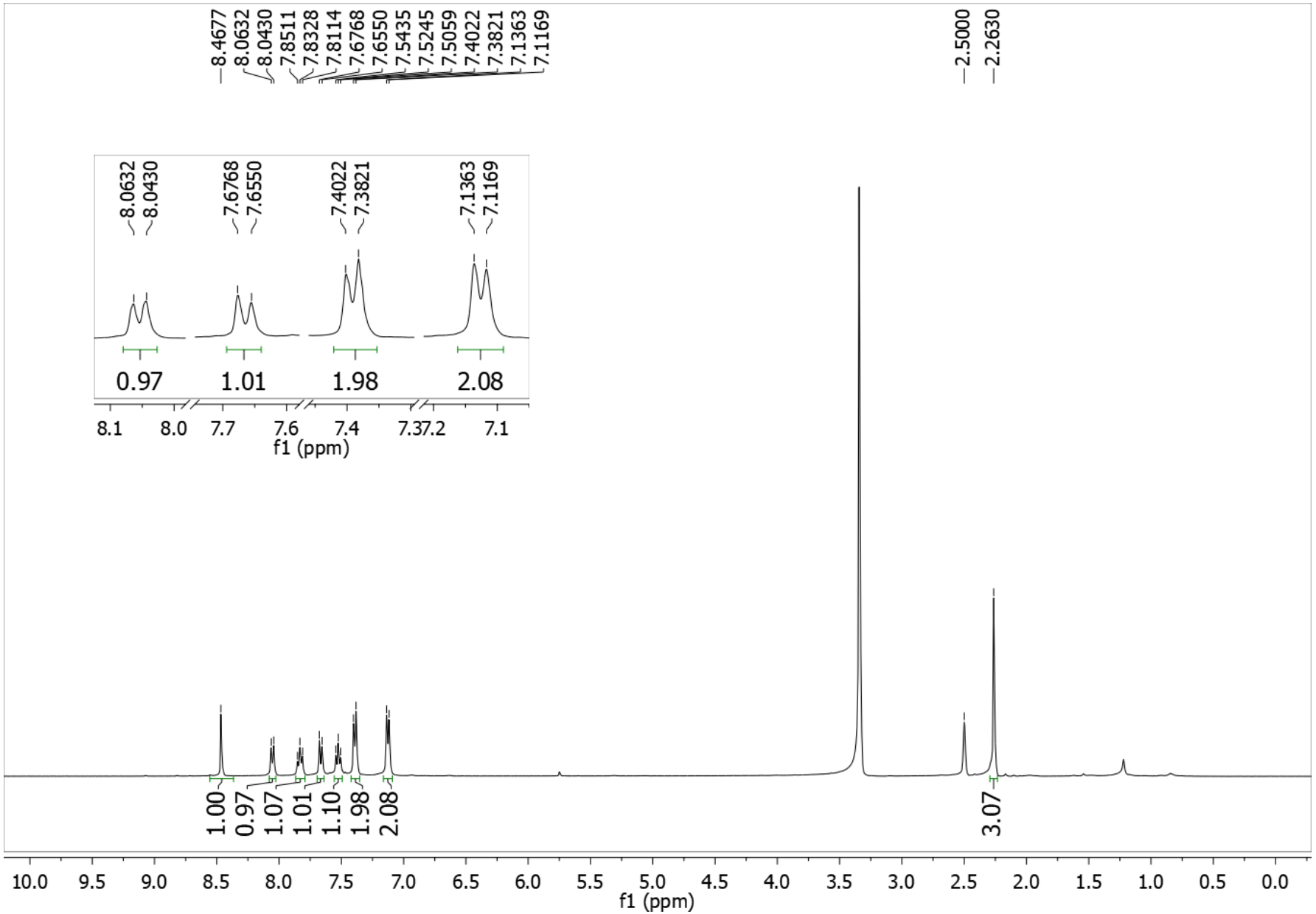


Figure 4S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3b**.

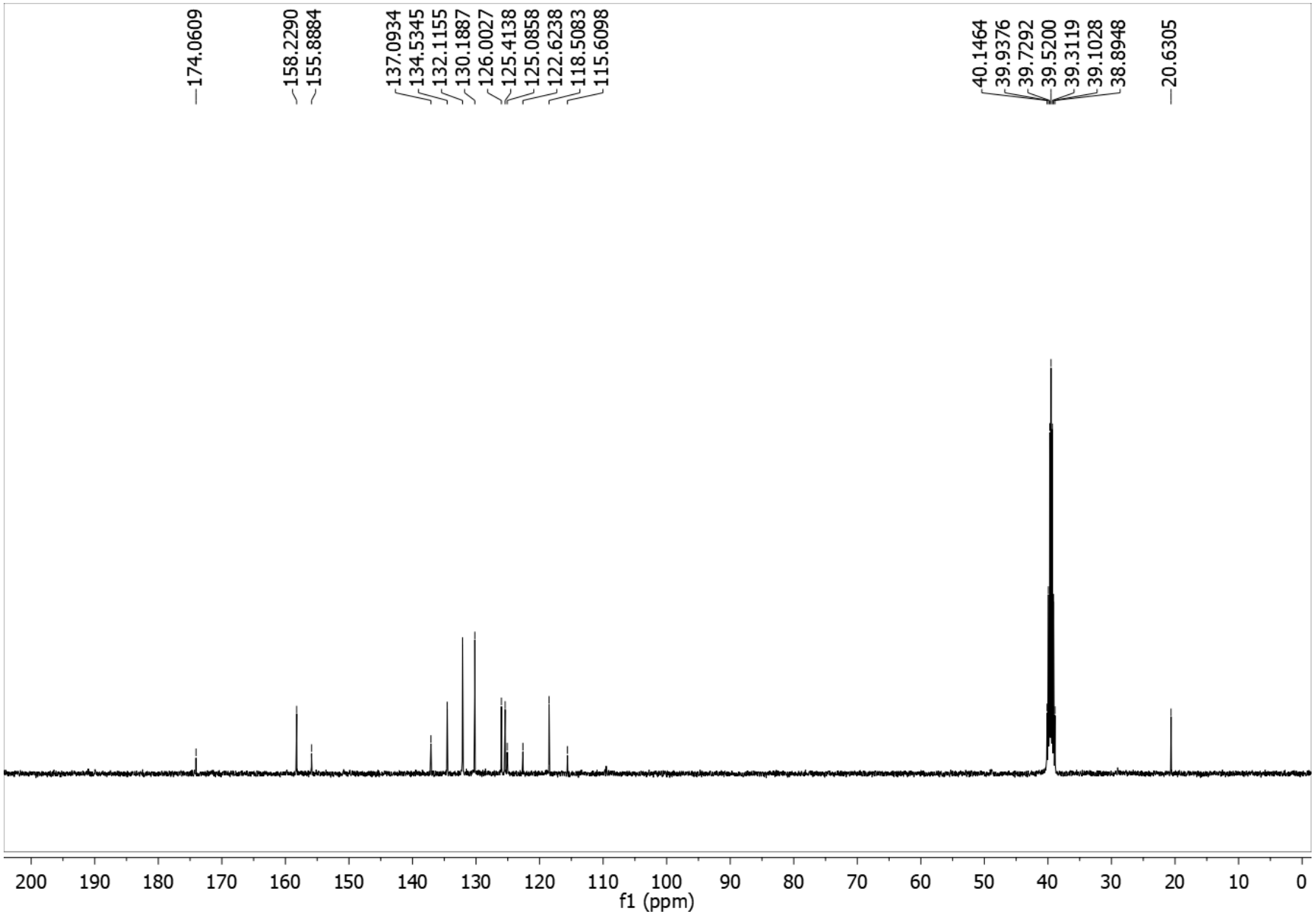


Figure 5S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3b**.

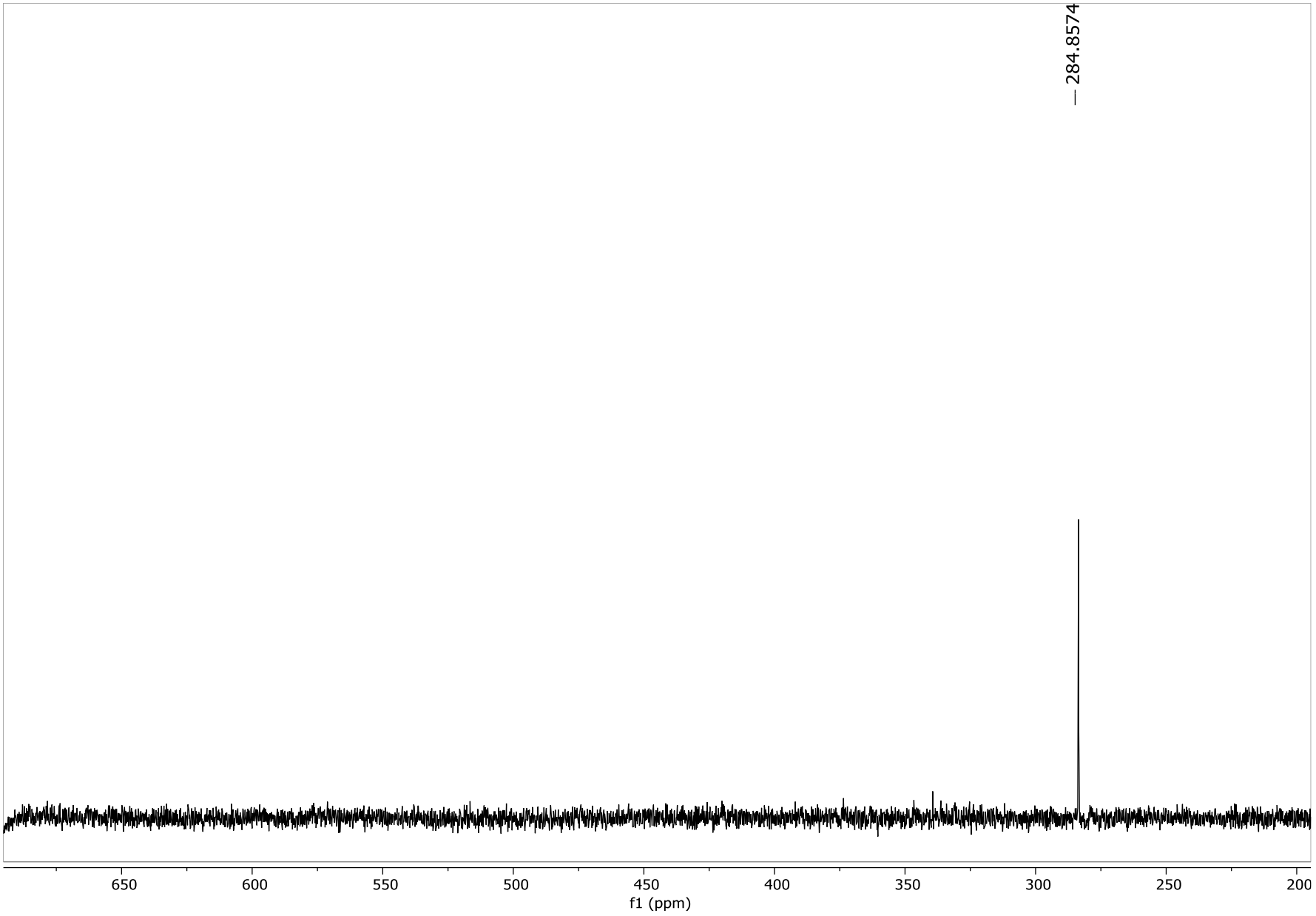


Figure 6S. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3b**.

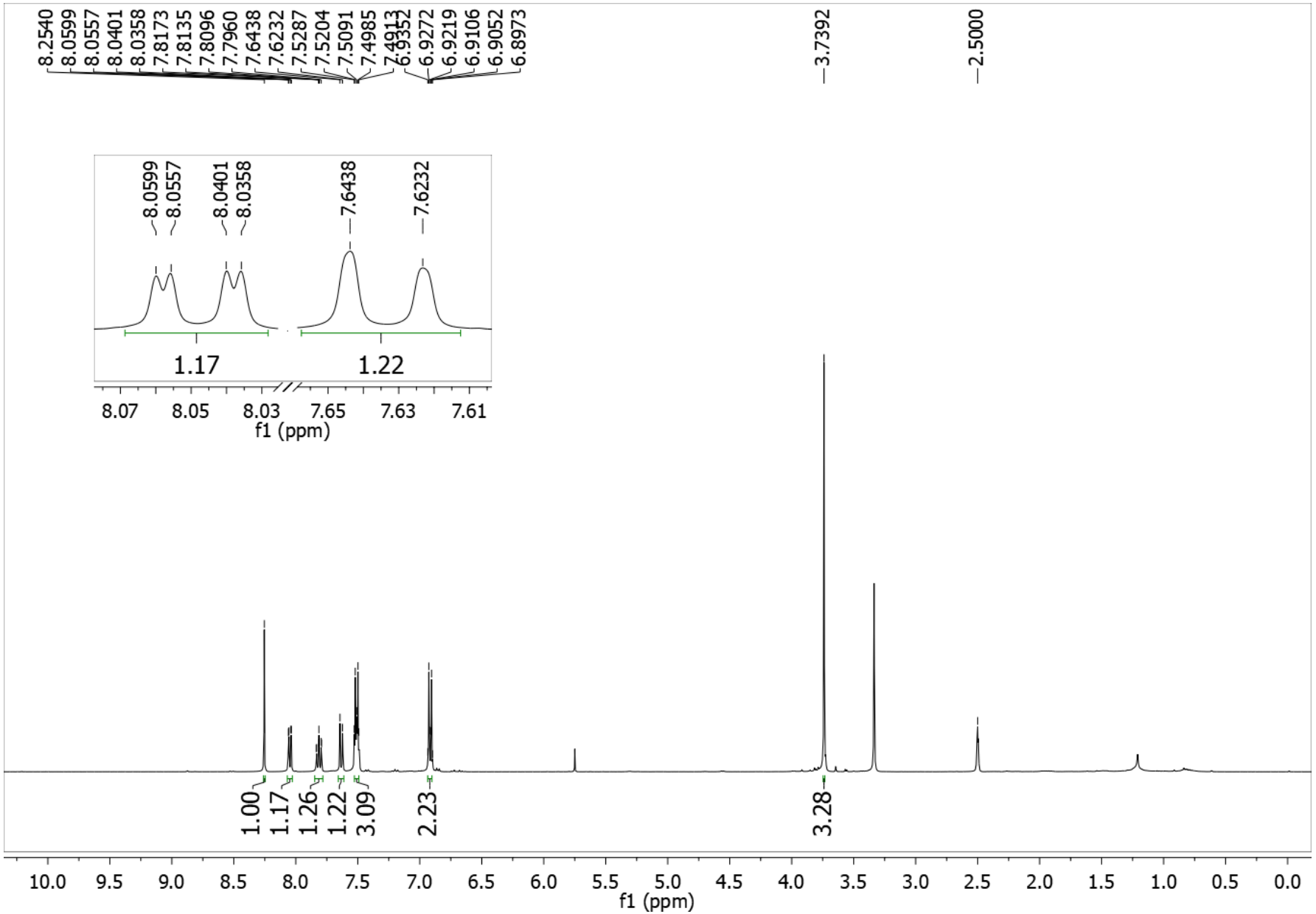


Figure 7S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3c**.

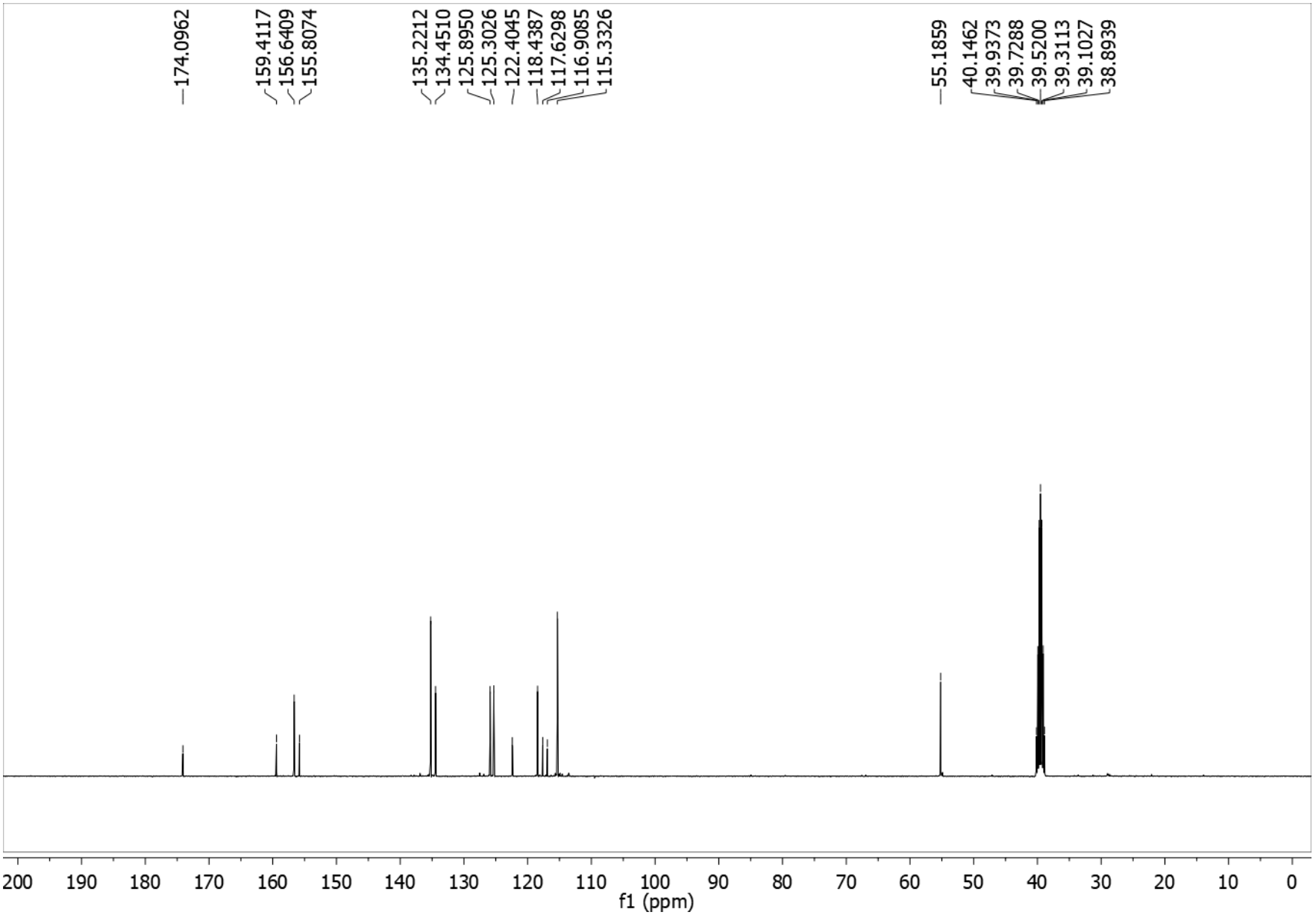


Figure 8S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3c**.

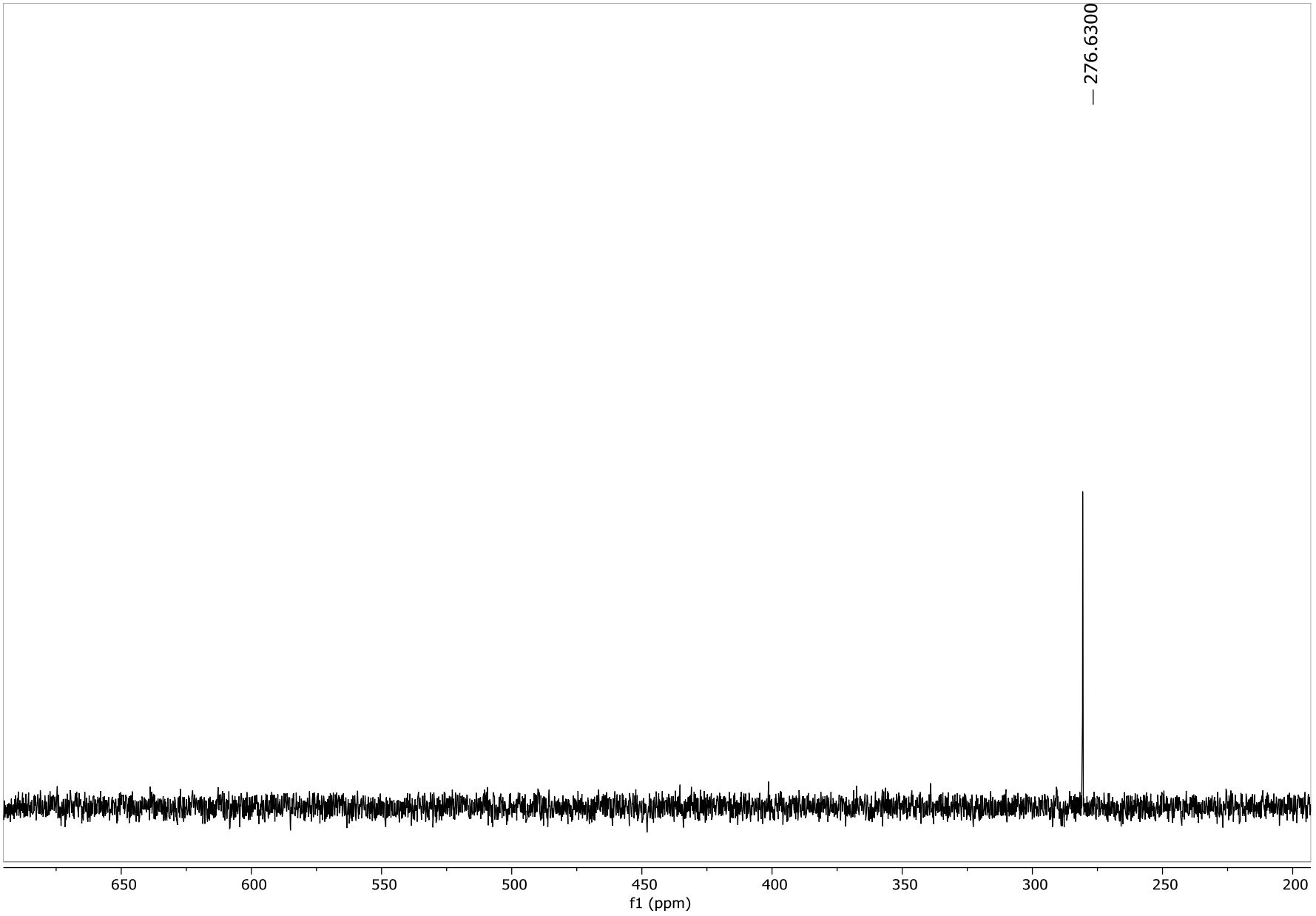


Figure 9S. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3c**.

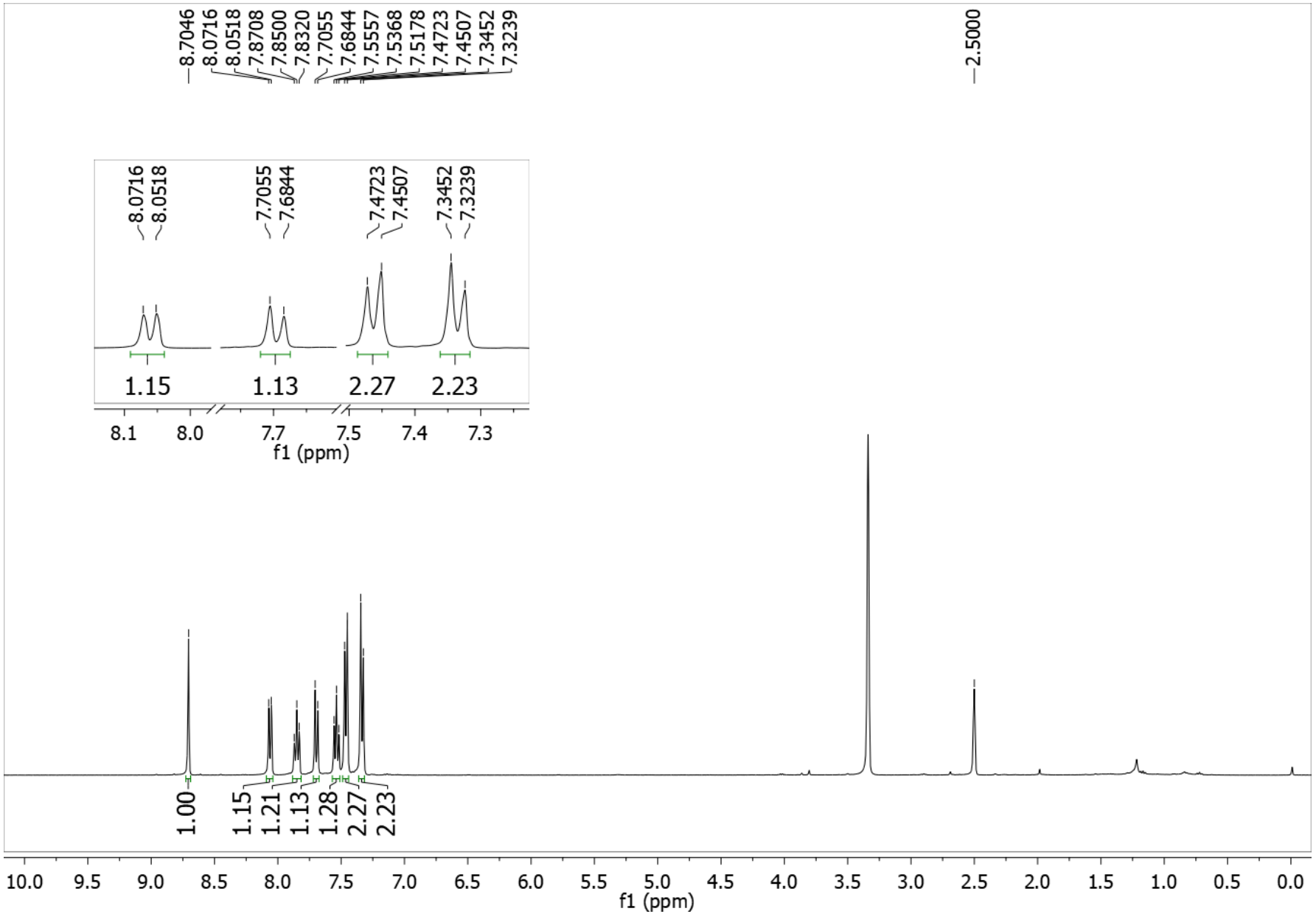


Figure 10S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3d**.

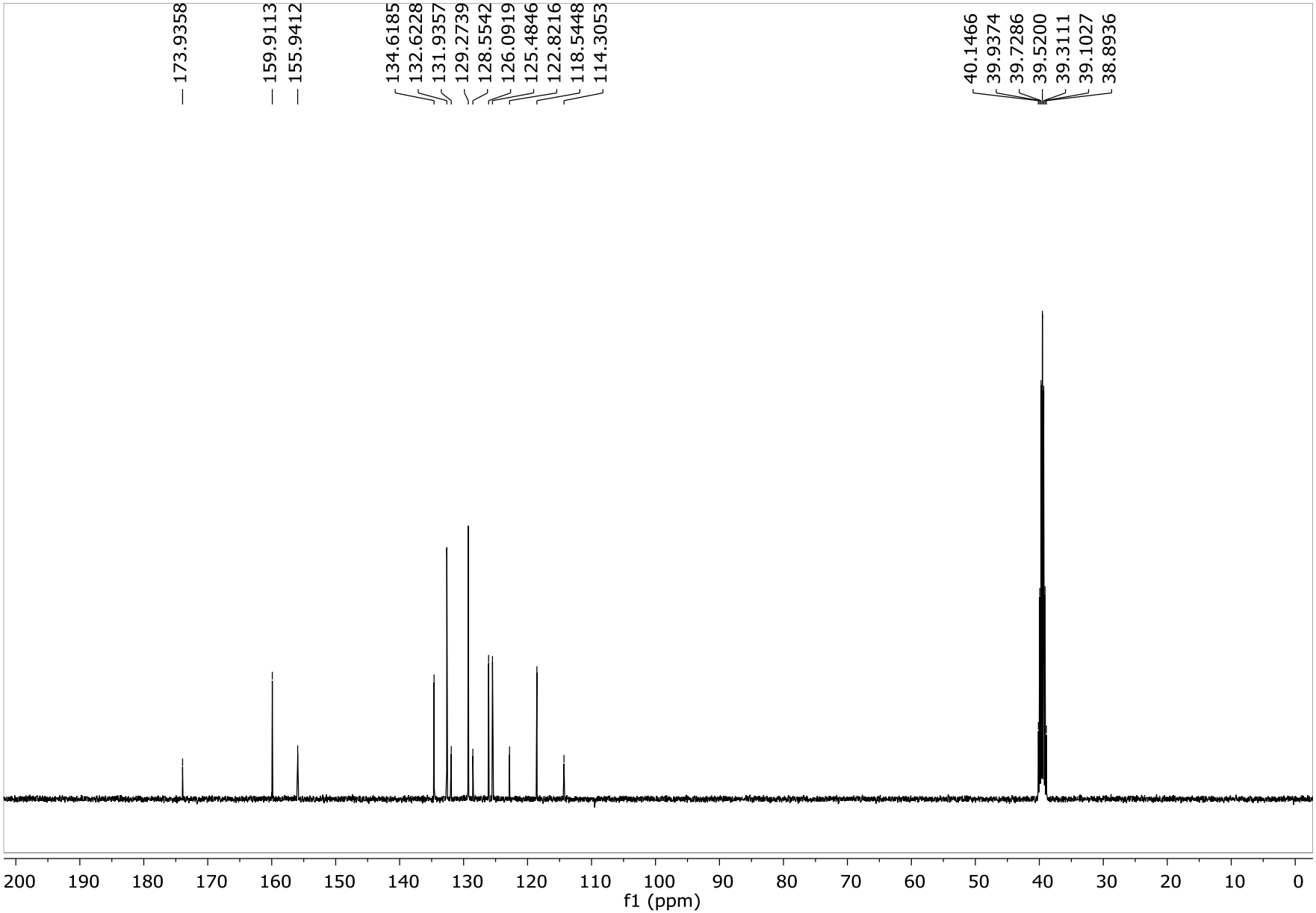


Figure 11S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3d**.

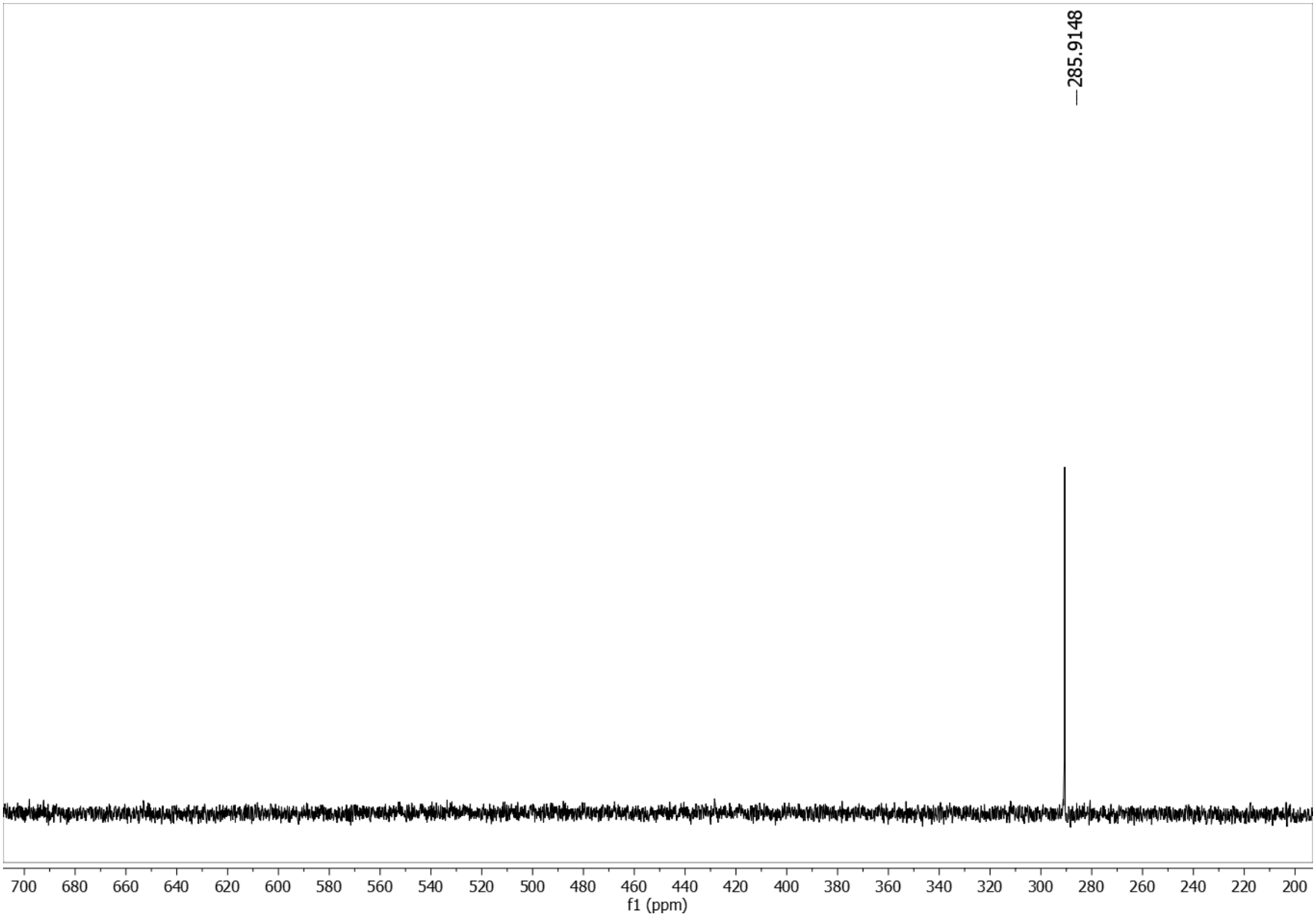


Figure 12S. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3d**.

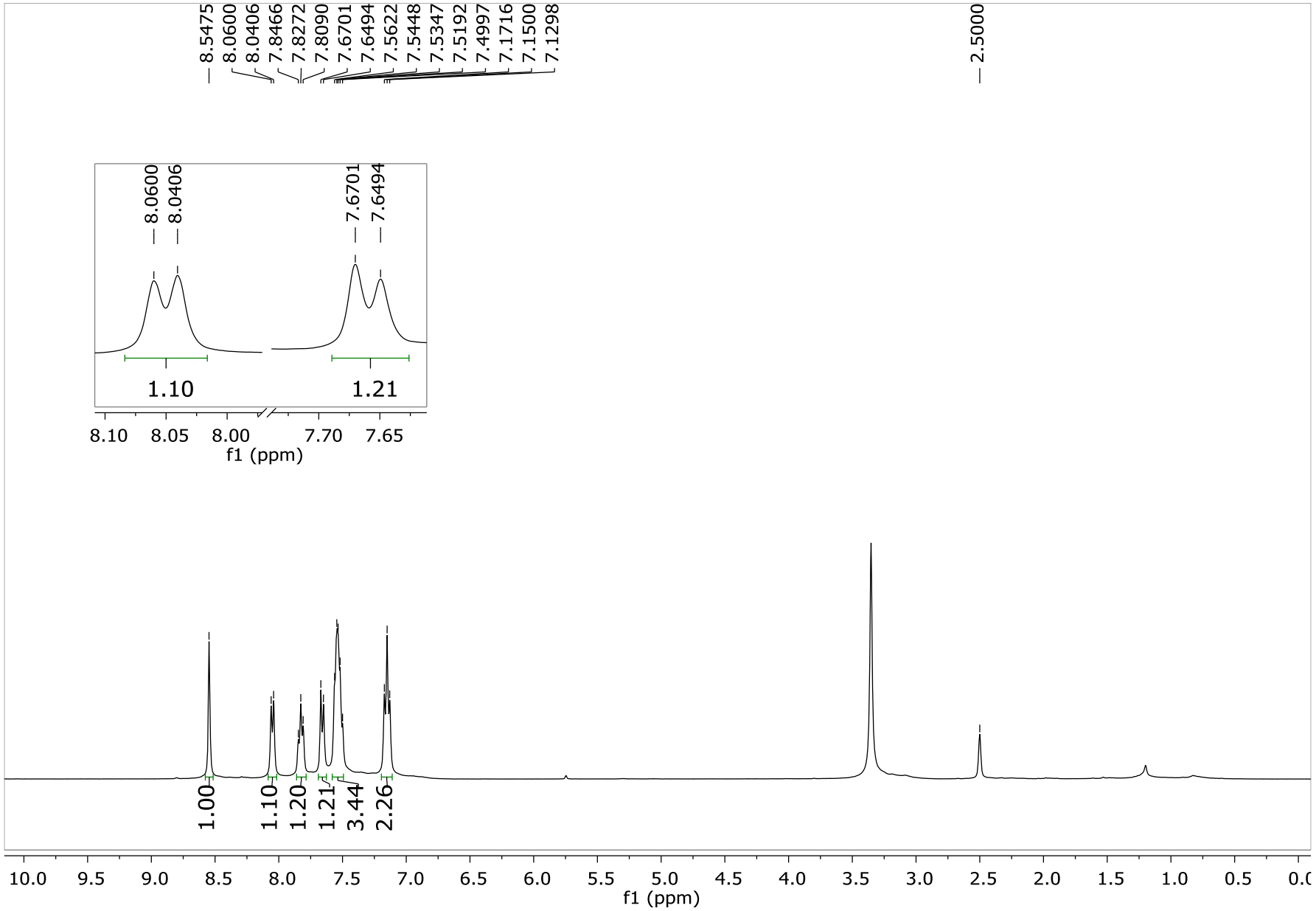


Figure 13S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3e**.

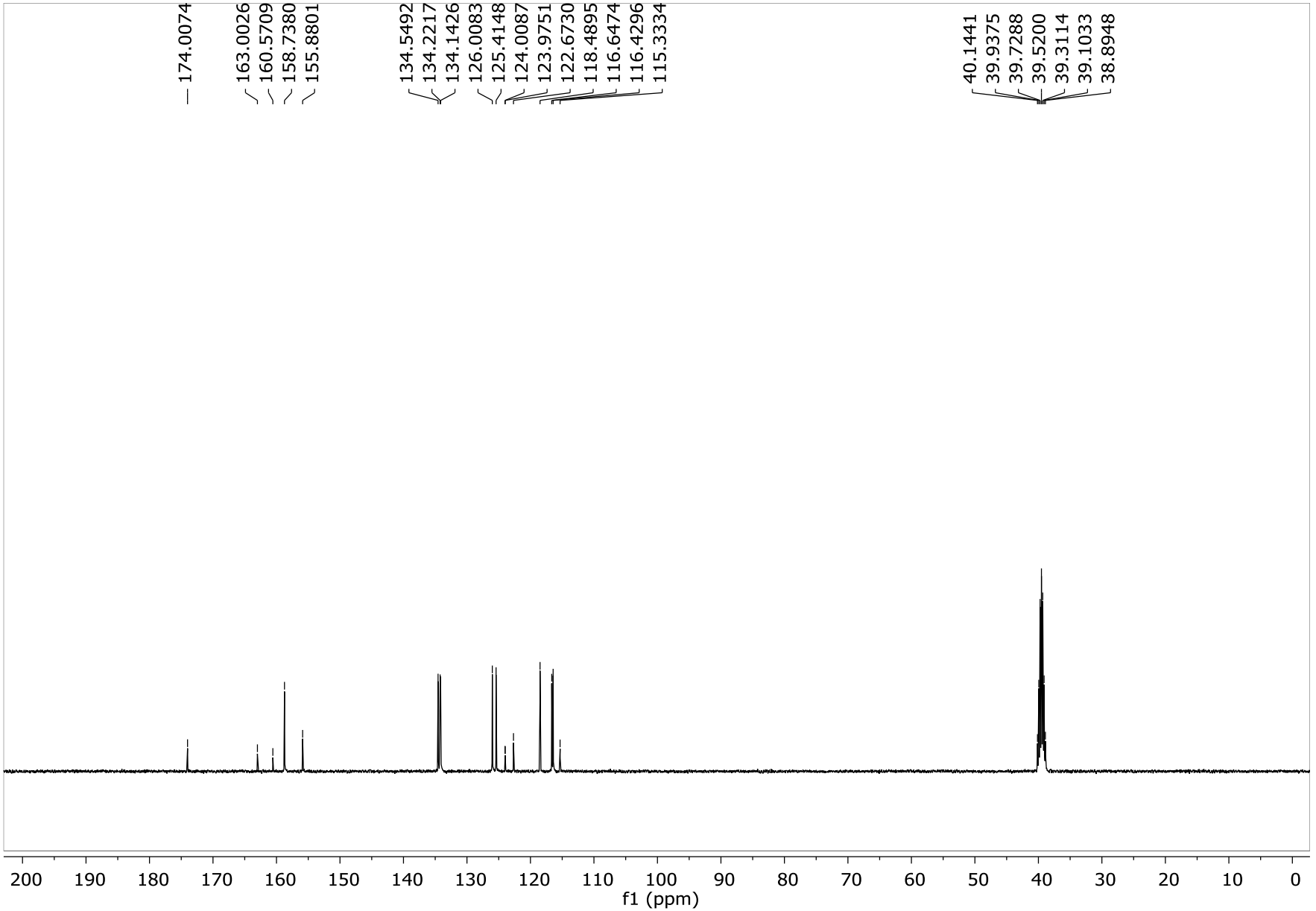


Figure 14S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3e**.

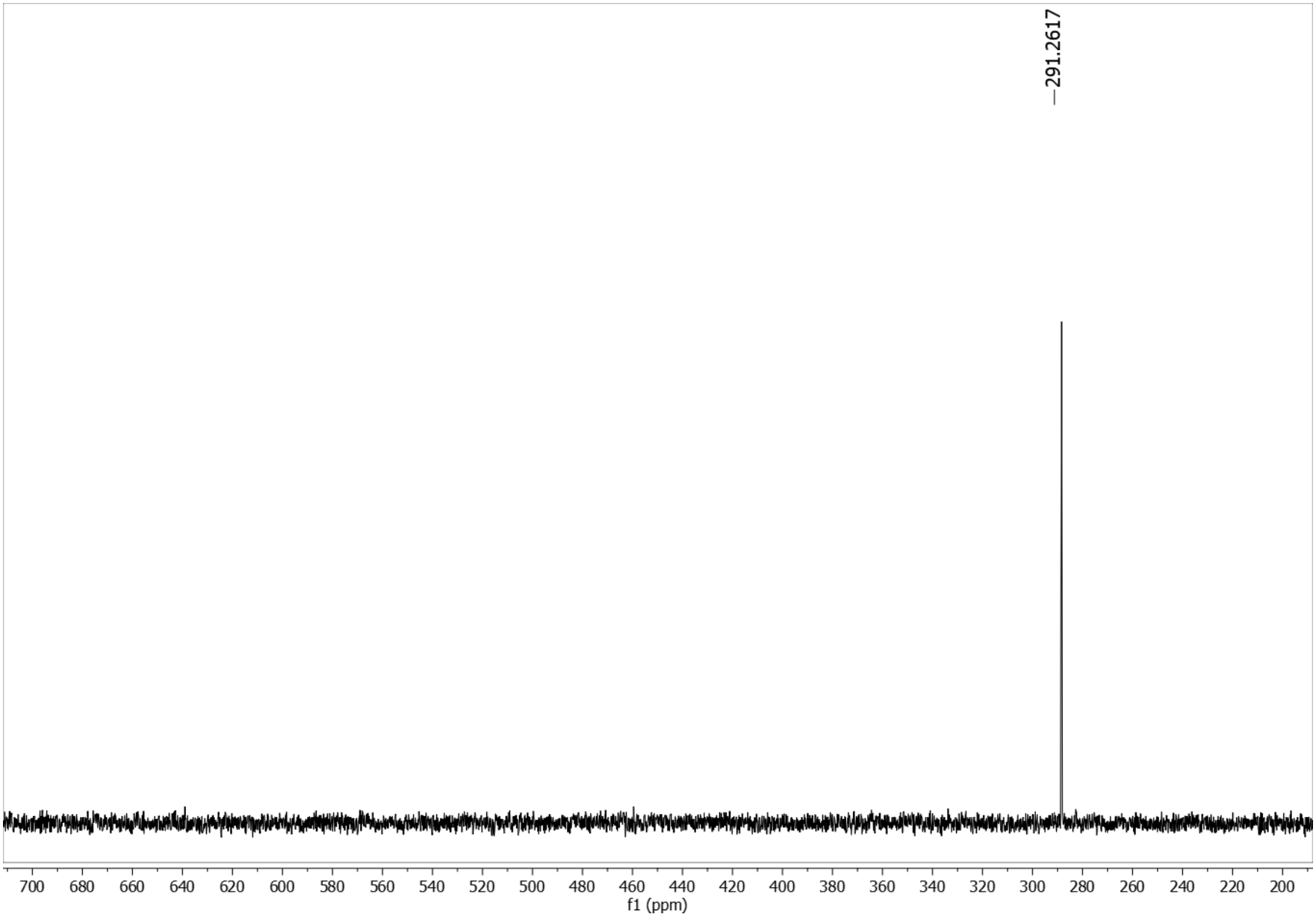


Figure 15S. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3e**.

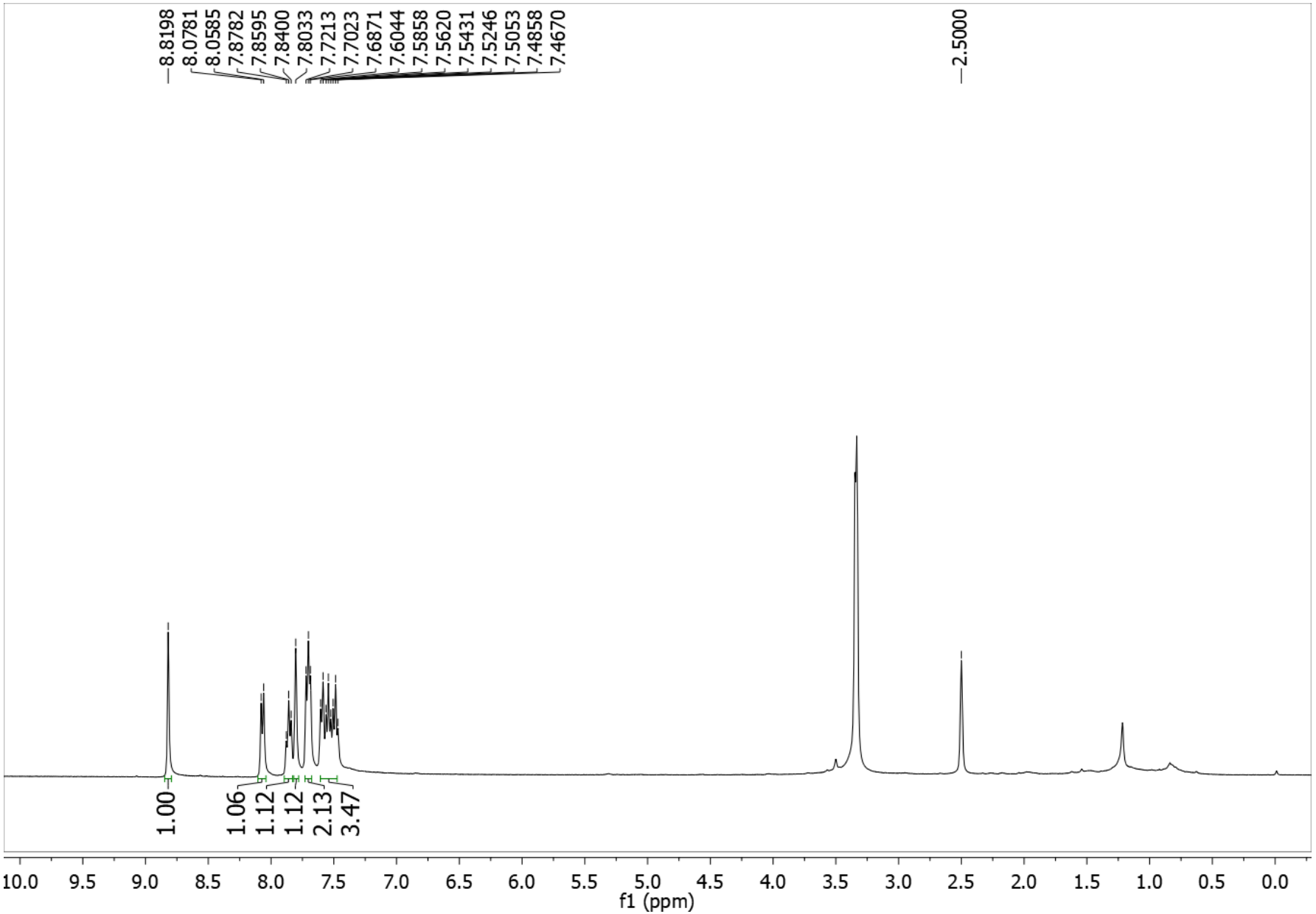


Figure 16S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3f**.

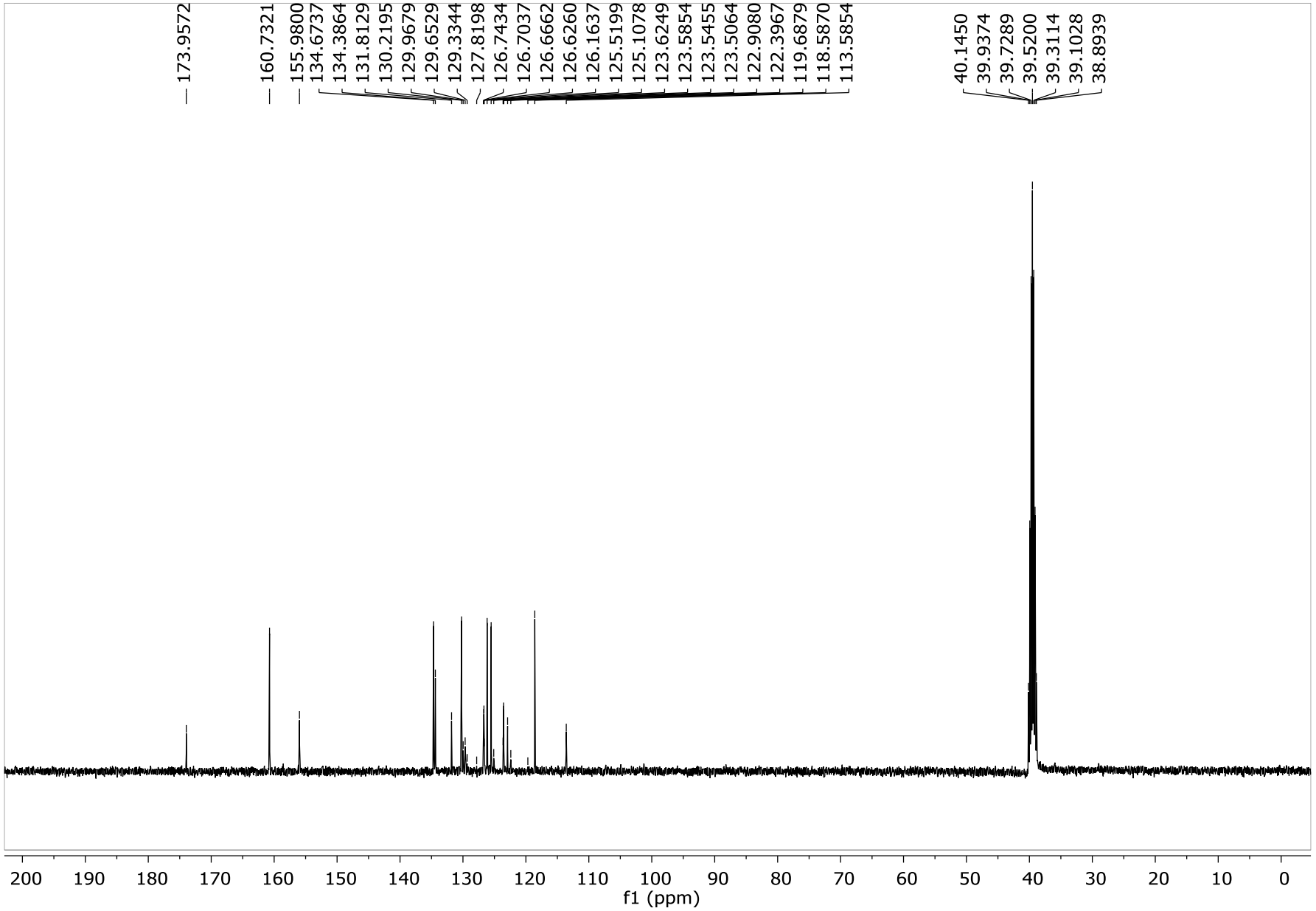


Figure 17S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3f**.

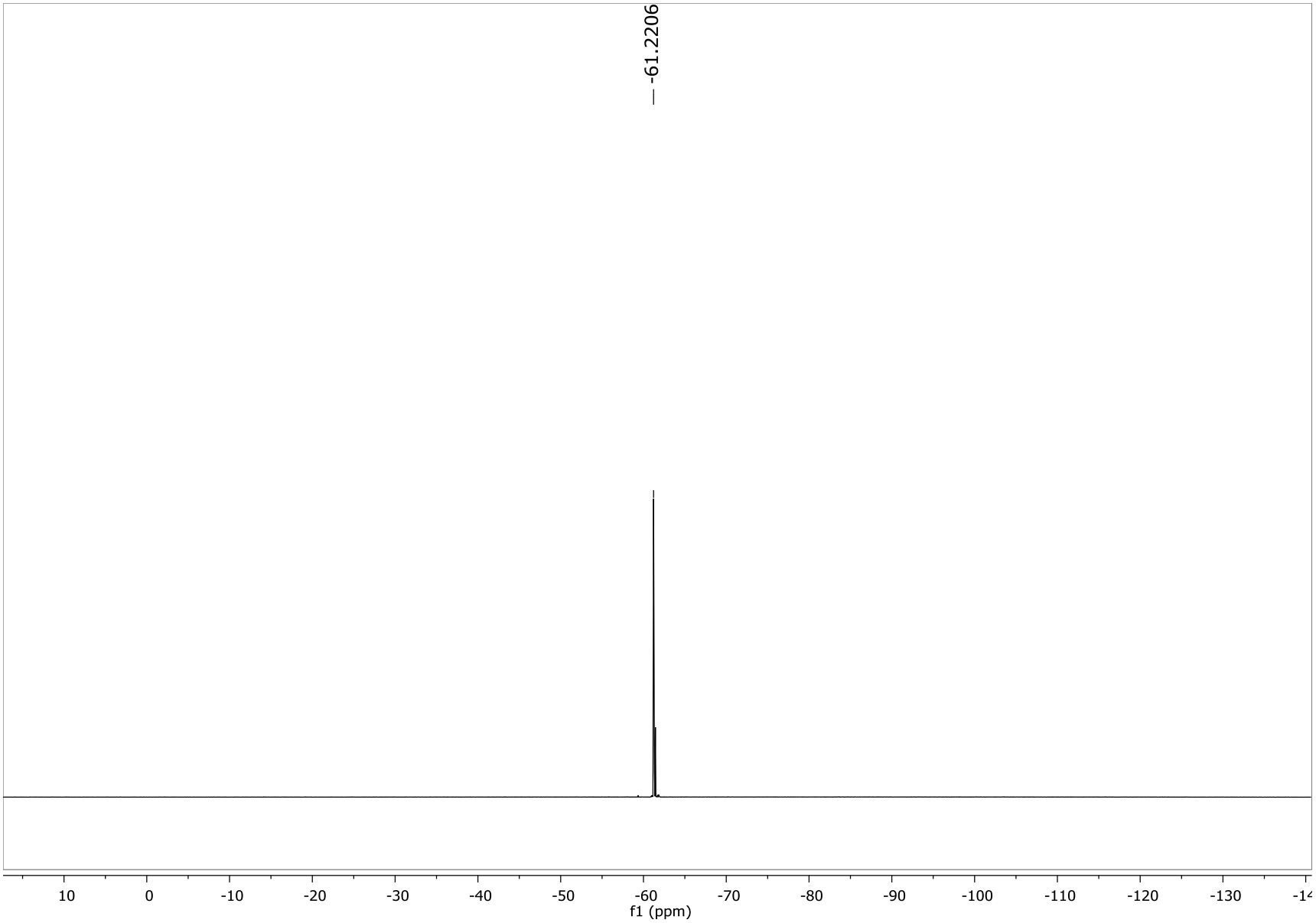


Figure 18S. ^{19}F NMR (376 MHz, DMSO-d_6) spectrum of the product **3f**.

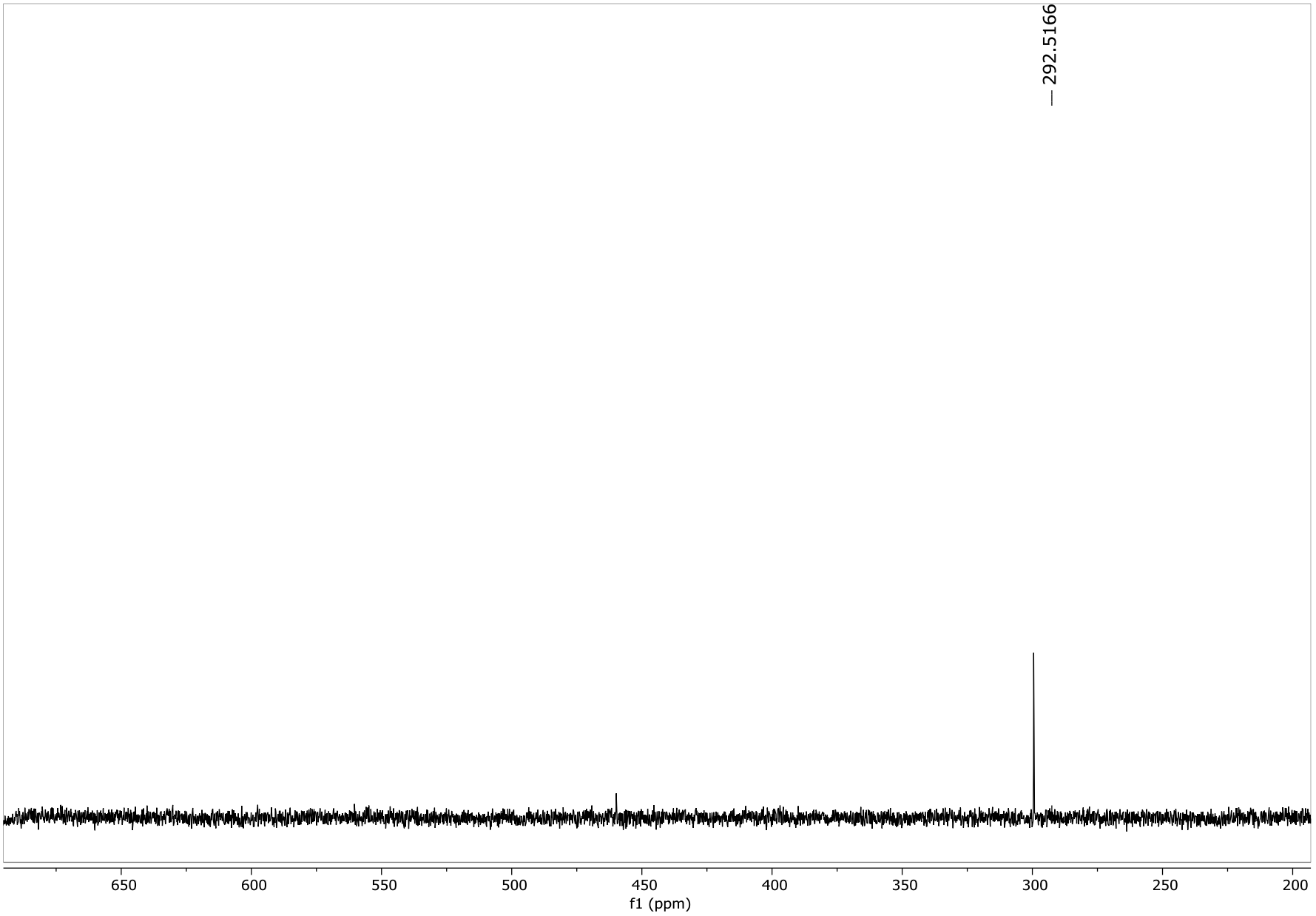


Figure 19S. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3f**.

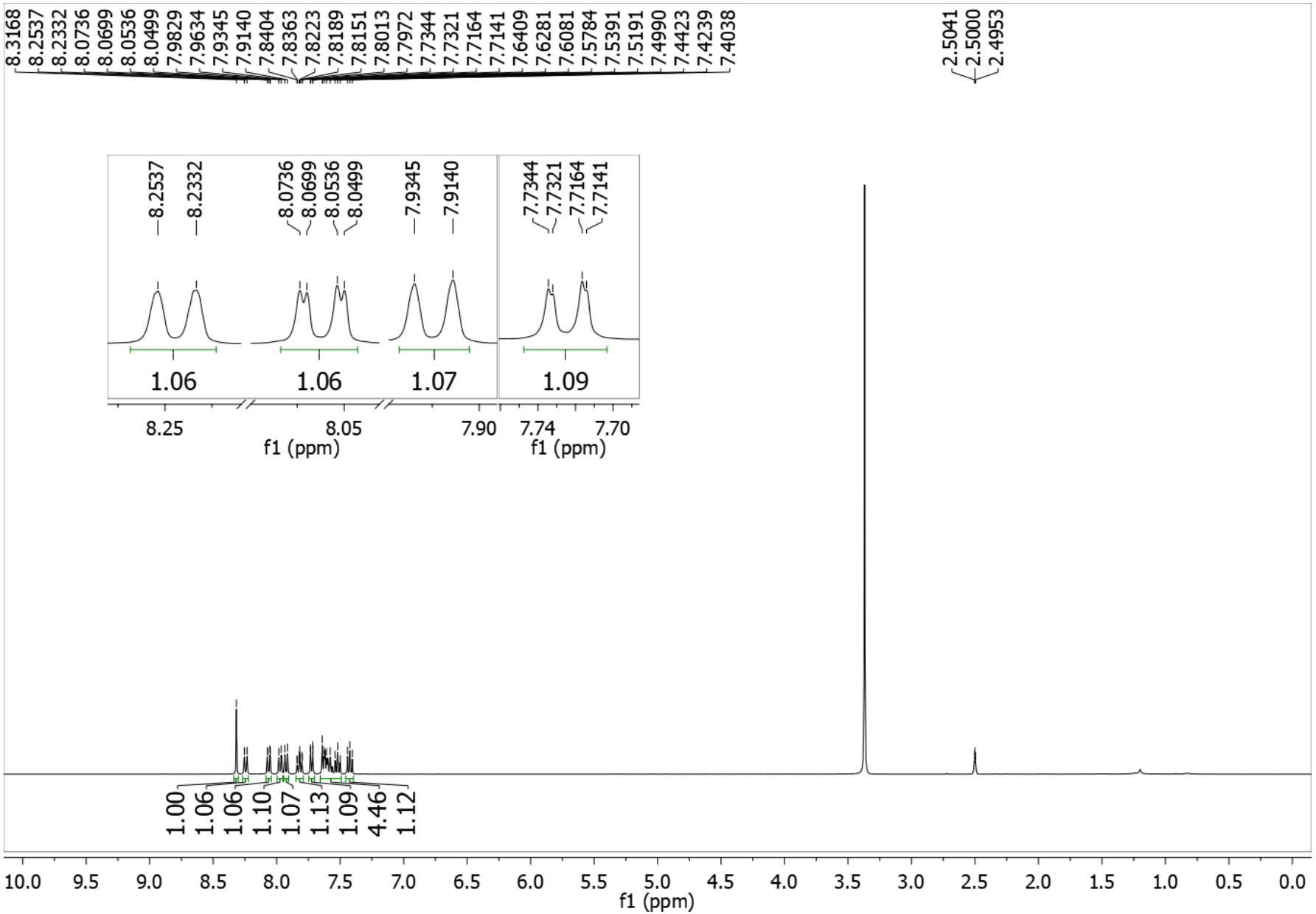


Figure 20S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3g**.

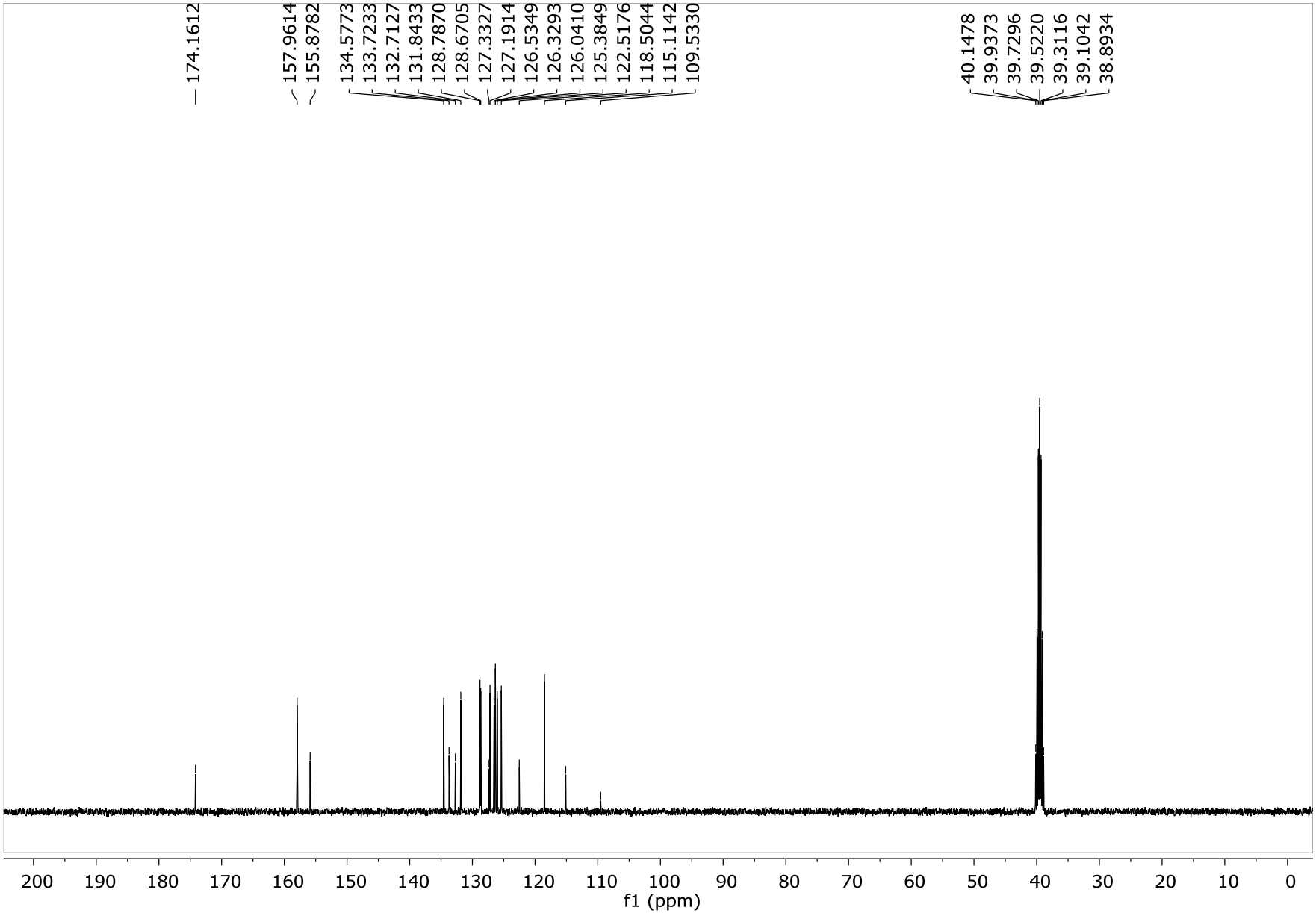


Figure 21S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3g**.

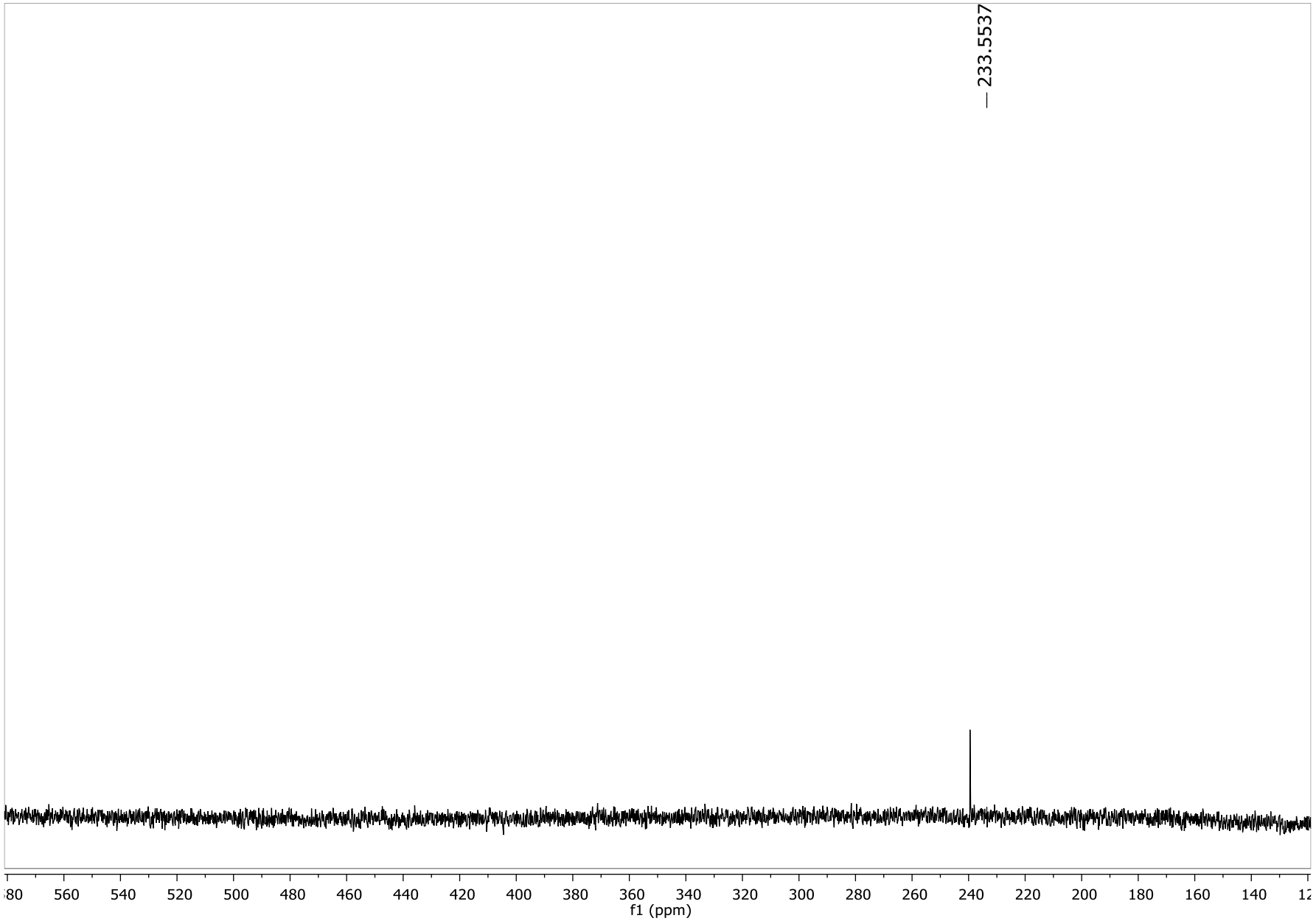


Figure S22. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3g**.

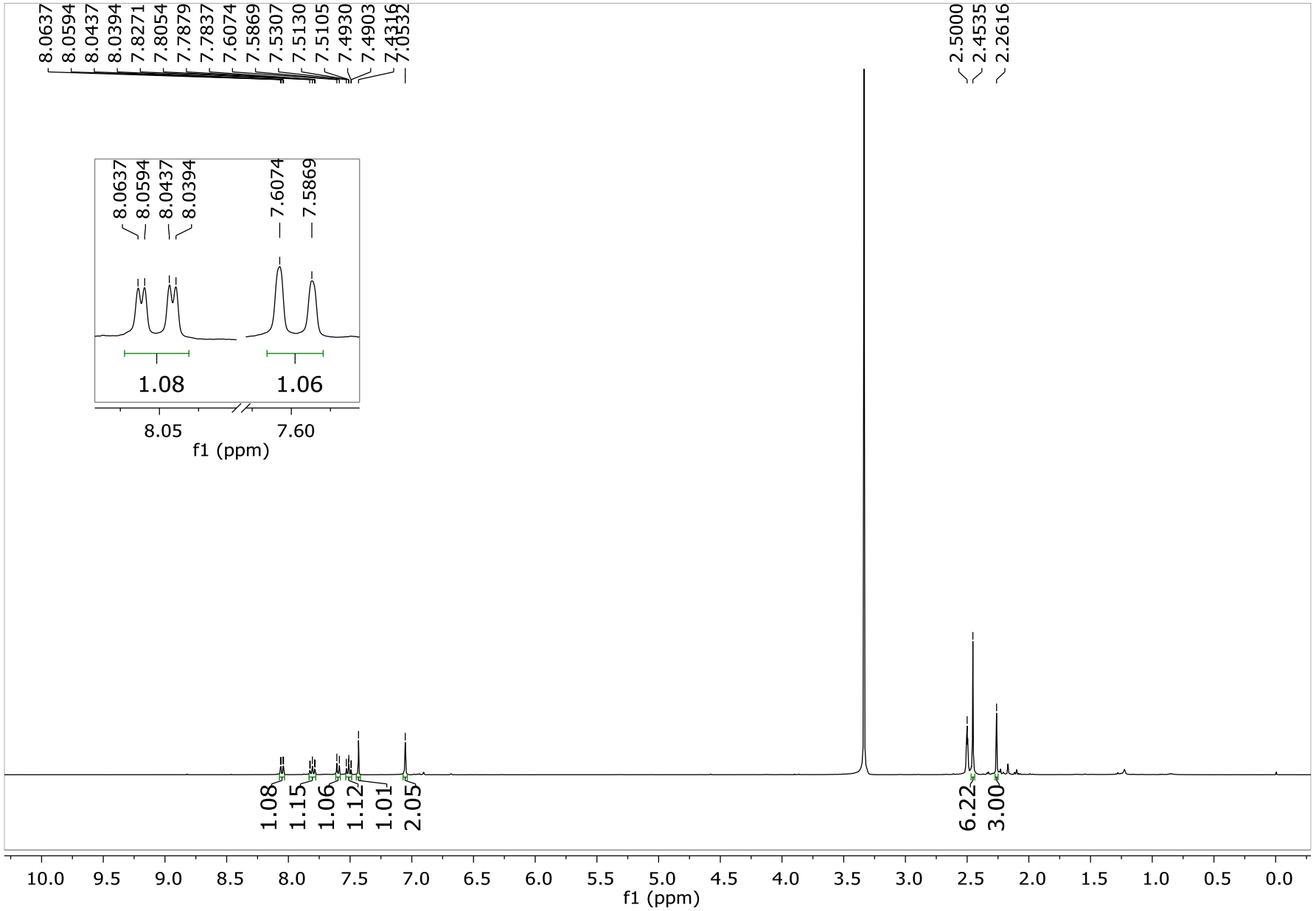


Figure 23S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the product **3h**.

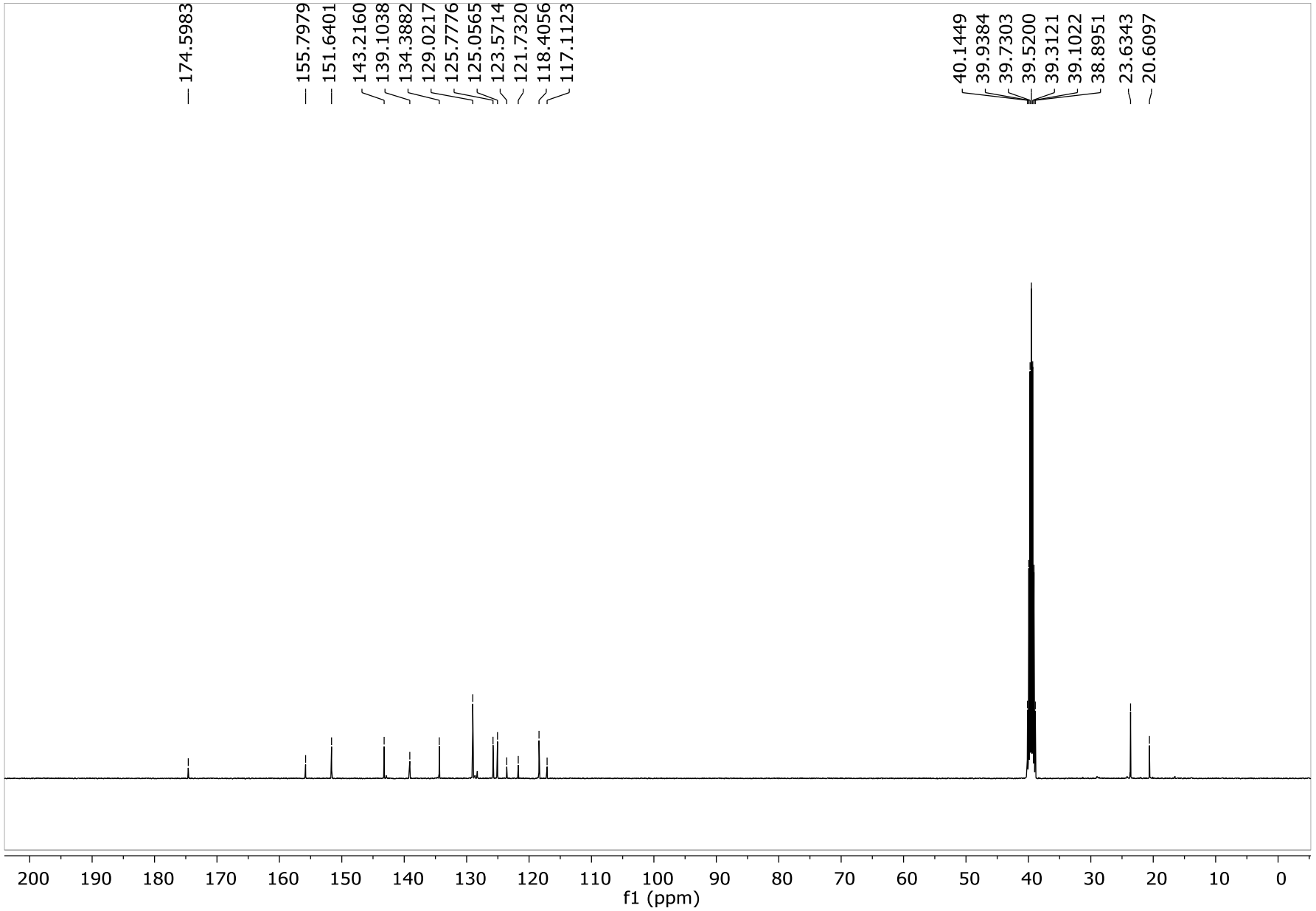


Figure 24S. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the product **3h**.

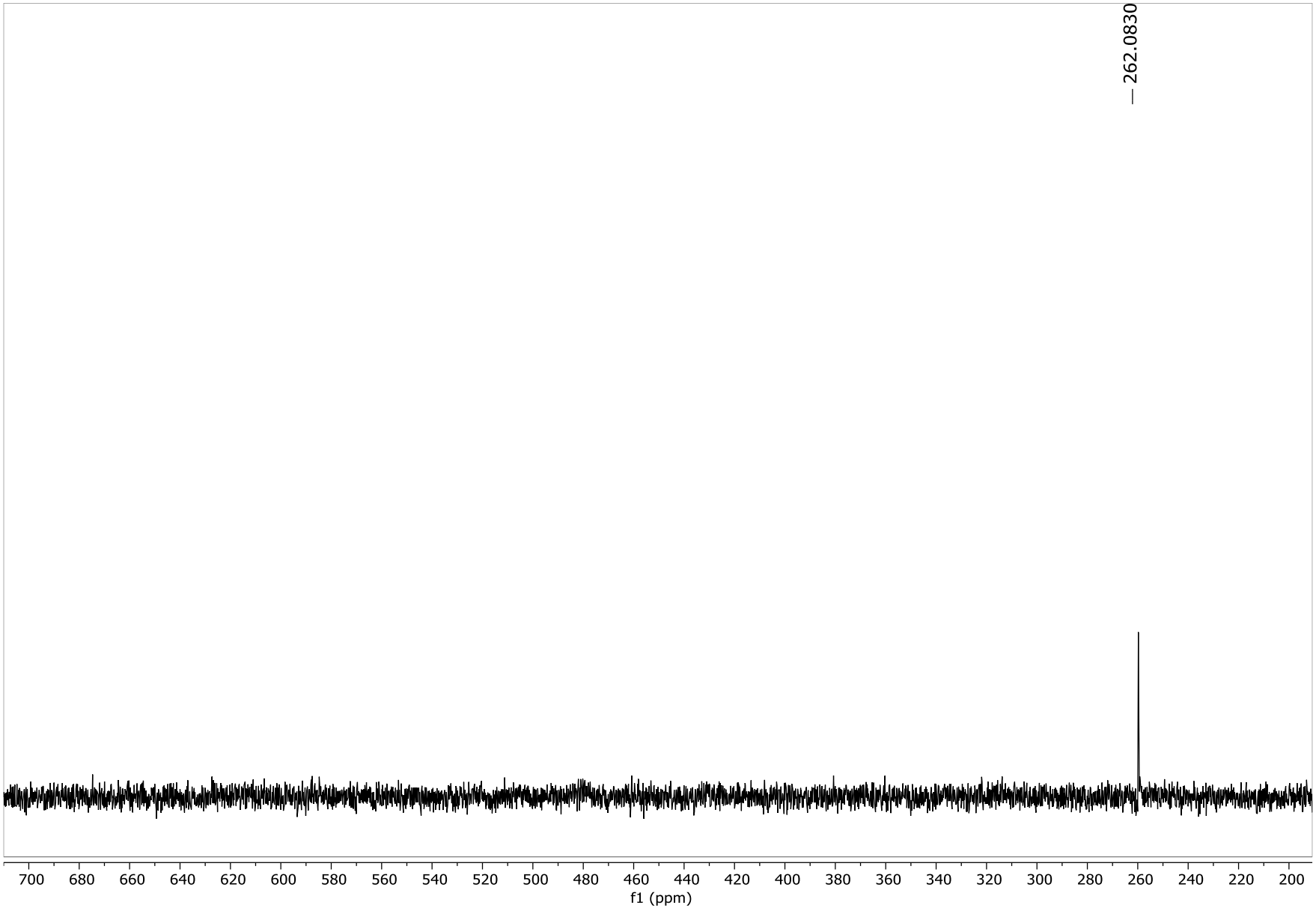
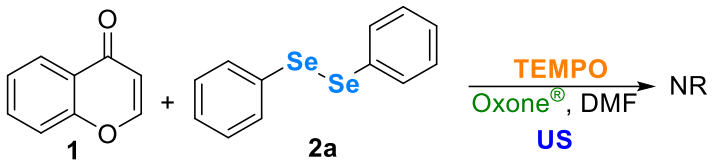
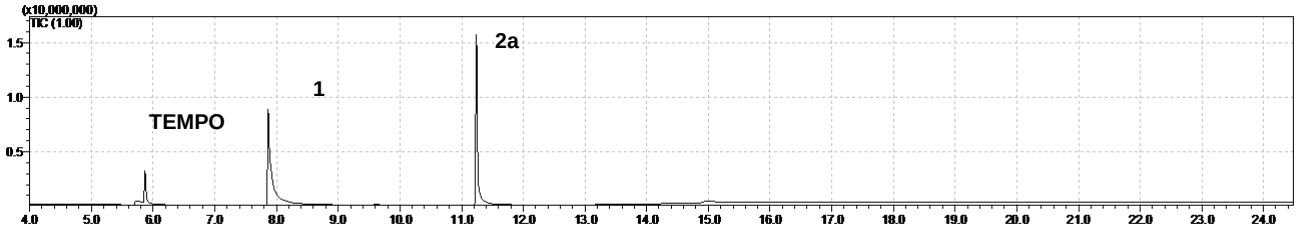


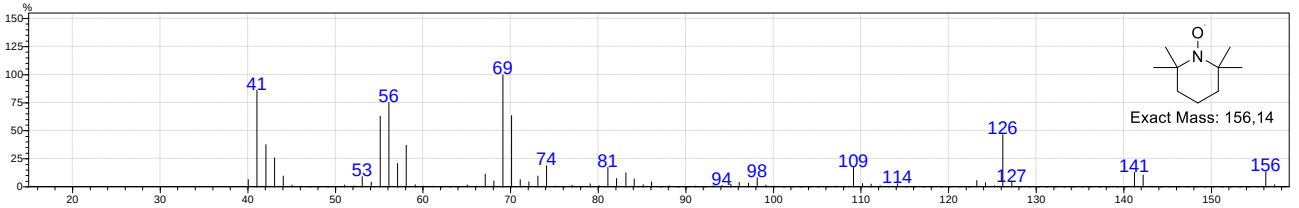
Figure S25. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the product **3h**.

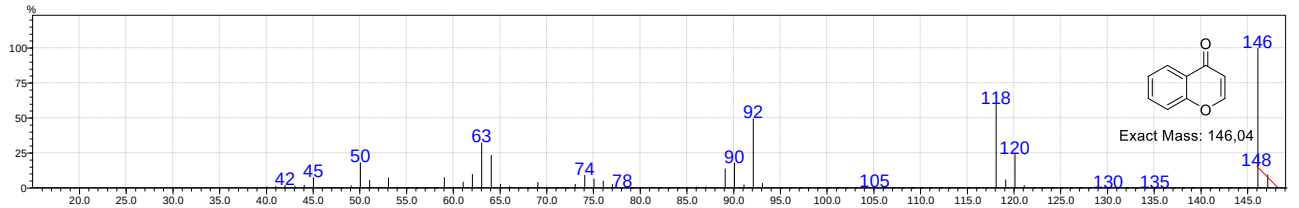
Control Experiments

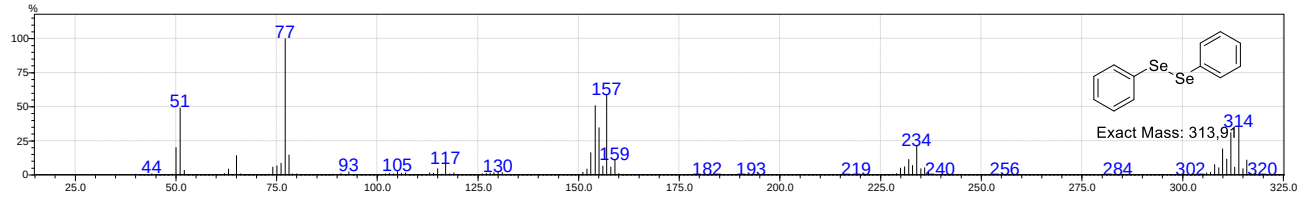


Scheme S1









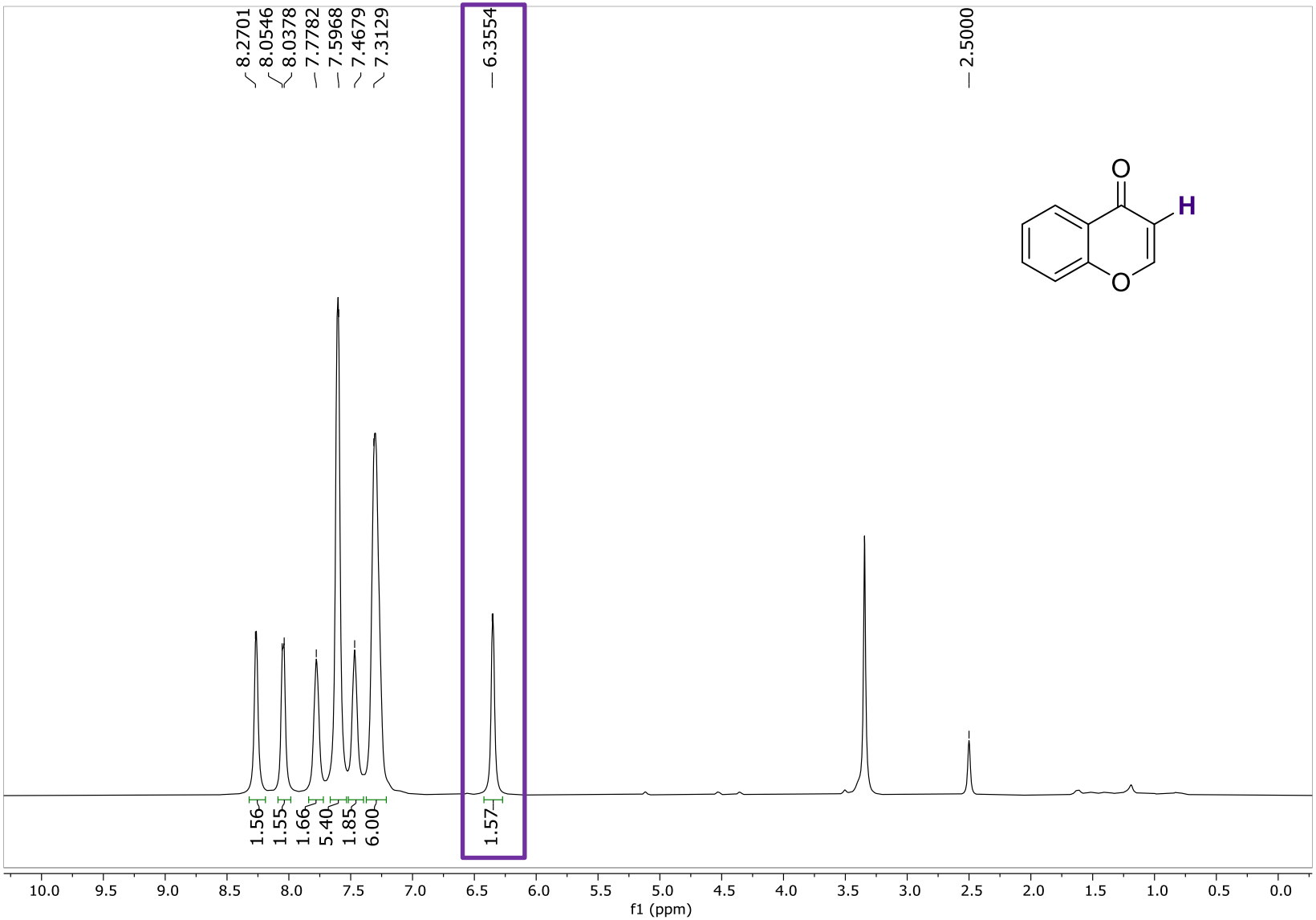


Figure S26. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the Scheme S1.

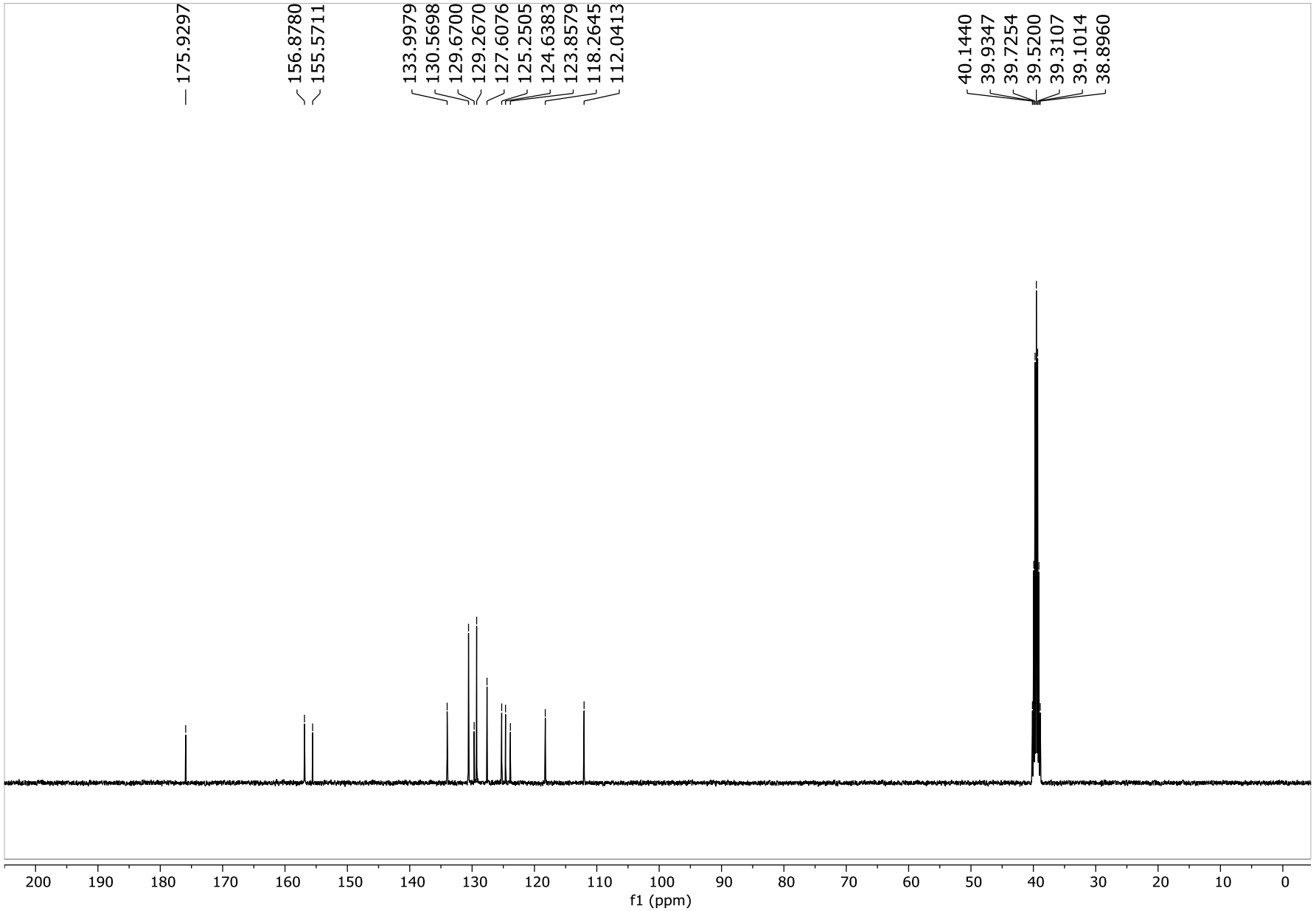


Figure S27. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the Scheme S1.

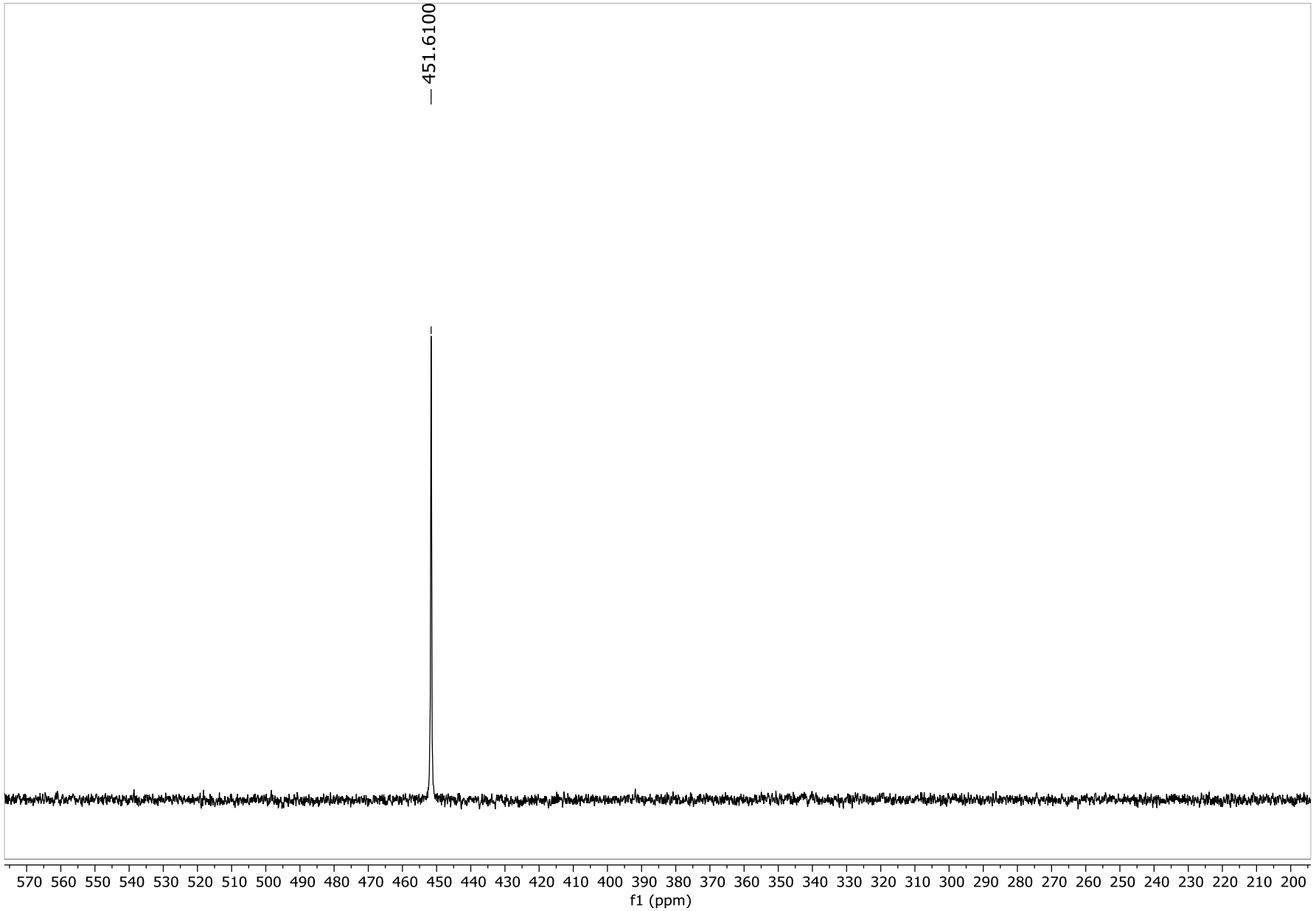


Figure S28. ^{77}Se NMR (76 MHz, DMSO-d_6) spectrum of the Scheme S1.