Supporting information

The Short Route to Chalcogenurea-substituted 3a,6-Epoxyisoindoles *via* an Intramolecular Diels–Alder Furan (IMDAF) Reaction. Antibacterial and Antifungal activity

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The single-crystal X-ray diffraction data for **5a** and **7p** were collected on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (T = 100 K, λ(Cu$K\alpha$)-radiation, graphite monochromator, shutterless ω-scan mode). The data were integrated and corrected for absorption by the *CrysAlisPro* program [1]. The single-crystal X-ray diffraction data for **7g** were collected at the 'Belok/XSA' beamline (λ = 0.74500 Å, T = 100 K) of the National Research Center 'Kurchatov Institute' (Moscow, Russian Federation) using a single-axis MARdtb goniometer equipped with a Rayonix SX-165 position-sensitive CCD detector. In total, 480-720 frames for two different orientations of the crystal were collected in direct geometry (θ = 0°) with an oscillation range of 1.0° in the φ scanning mode. The data were indexed and integrated using the utility *iMOSFLM* from the CCP4 software suite [2] and then scaled and corrected for absorption using the Scala program [3]. The single-crystal X-ray diffraction data for **6e** were collected on a four-circle area-detector Bruker KAPPA APEX II diffractometer (T = 296 K, λ(Mo$K\alpha$)-radiation, graphite monochromator). The data were integrated by the SAINT-Plus program [4] and corrected for absorption by the *SADABS* program [5]. For details, see Table 1.

The structures were solved by intrinsic phasing modification of direct methods [6] and refined by a full-matrix least squares technique on F^2 with anisotropic displacement parameters for non-hydrogen atoms. The absolute configuration of **7p** was objectively determined by the refinement of Flack parameter, which became equal to -0.029(16). The hydrogen atoms of the NH-groups were objectively localized in the difference-Fourier maps and refined isotropically with fixed displacement parameters [U_{iso}(H) = 1.2U_{eq}(N)]. The other hydrogen atoms in all compounds were placed in calculated positions and refined within riding model with fixed isotropic displacement parameters [U_{iso}(H) = 1.5U_{eq}(C) for the CH_3-groups and 1.2U_{eq}(C) for the other groups]. All calculations were carried out using the SHELXTL program [7].

Crystallographic data for all investigated compounds have been deposited with the Cambridge Crystallographic Data Center, CCDC 2265781 (**5a**), CCDC 2283074 (**6e**), CCDC 2265782 (**7g**), and CCDC 2265783 (**7p**). Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

References

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[4] SAINT-Plus (Version 7.68). Bruker AXS Inc., Madison, Wisconsin, USA, **2007**.

[5] SADABS. Bruker AXS Inc., Madison, Wisconsin, USA, *2008*.

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Table 1. Crystal data and structure refinement for **5a**, **6e**, **7g** and **7p**.

Identification code	**5a**	**6e**	**7g**	**7p**
Empirical formula	$C_{15}H_{16}N_2O_2$	$C_{15}H_{15}N_2OFS$	$C_{16}H_{18}N_2O_2Se$	$C_{15}H_{15}ClN_2OSe$
Formula weight	256.30	290.35	349.28	353.70
Crystal size, mm	0.06×0.18×0.24	0.04×0.20×0.40	0.02×0.10×0.12	0.09×0.11×0.14
Wavelength, Å	1.54184	0.71073	0.74500	1.54184
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$P2_12_12_1$	$P2_12_12_1$
a, Å	8.8352(8)	13.8056(6)	6.5229(11)	6.31793(12)
b, Å	23.420(2)	8.4418(5)	9.1181(15)	9.33602(18)
c, Å	5.8137(5)	11.6065(6)	24.346(4)	23.9880(5)
α, deg.	90	90	90	90
β, deg.	94.8340(10)	94.293(3)	90	90
γ, deg.	90	90	90	90
V, Å^3	1198.69(18)	1348.87(12)	1448.0(4)	1414.92(5)
Z	4	4	4	4
Density (calc.), Mg/m^3	1.420	1.430	1.602	1.660
μ, mm^{-1}	0.772	0.284	2.934	5.300
F(000)	544	608	712	712
Theta range, deg.	3.78 – 77.82	4.11 – 27.50	2.50 – 31.15	3.69 – 79.40
Index ranges	$-10 \le h \le 11$, $-29 \le k \le 29$, $-7 \le l \le 7$	$-17 \le h \le 17$, $-10 \le k \le 10$, $-14 \le l \le 15$	$-9 \le h \le 9$, $-12 \le k \le 12$, $-33 \le l \le 33$	$-6 \le h \le 8$, $-10 \le k \le 11$, $-30 \le l \le 30$
Reflections collected	24889	13238	28507	9337
Independent reflections, R_{int}	2531, 0.077	3079, 0.058	4019, 0.039	2870, 0.036
Reflections observed	2330	1876	3948	2771
R_1 / wR_2 ($I > 2\sigma(I)$)	0.058 / 0.145	0.044 / 0.084	0.039 / 0.093	0.029 / 0.075
R_1 / wR_2 (all data)	0.060 / 0.147	0.092 / 0.010	0.039 / 0.093	0.030 / 0.075

Goodness-of-fit on F^2	1.061	0.999	1.091	1.137
Extinction coefficient	—	—	0.037(4)	0.00081(8)
T_{min} / T_{max}	0.519 / 1.000	0.909 / 1.000	0.666 / 0.921	0.491 / 0.612
$\Delta\rho_{max}$ / $\Delta\rho_{min}$, e·Å^{-3}	0.497 / -0.303	0.18 / -0.19	0.649 / -0.897	0.529 / -0.441

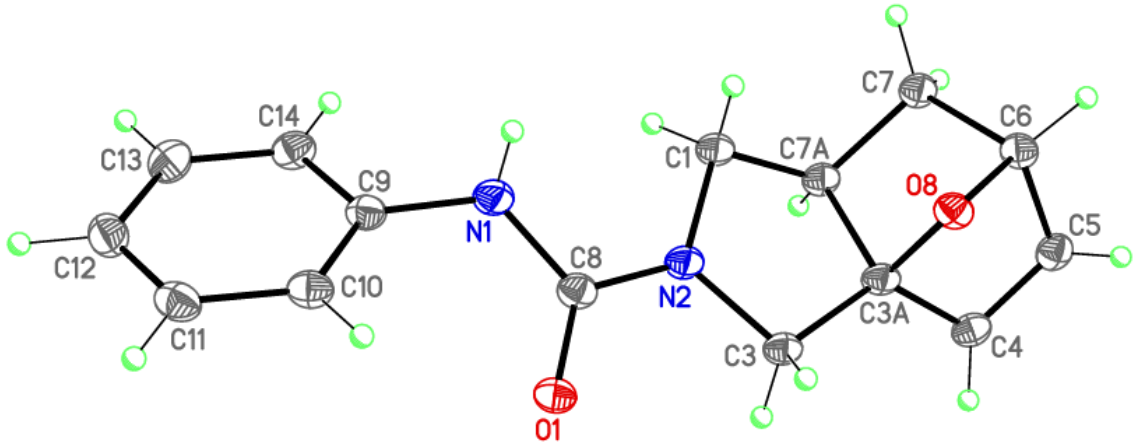


Fig. 1. Molecular structure of **5a** (50%-ellipsoids).

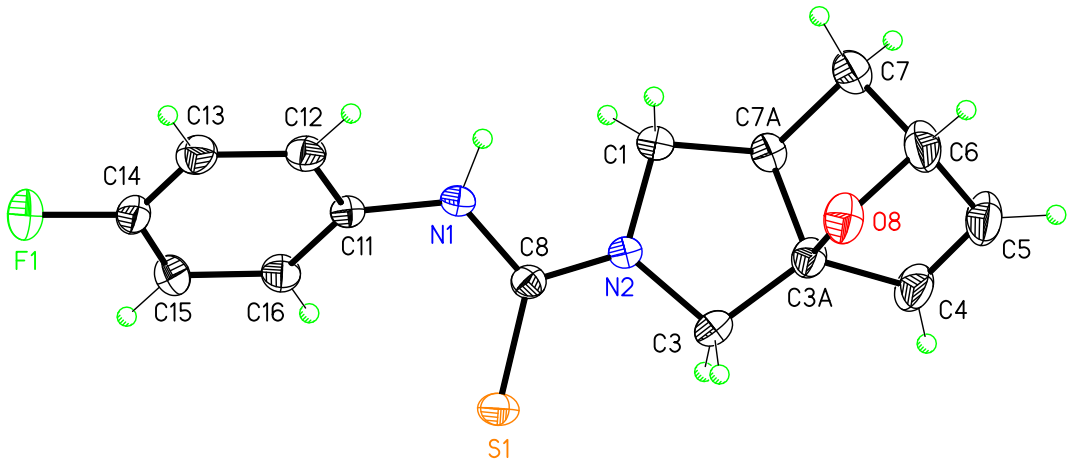


Fig. 2. Molecular structure of **6e** (30%-ellipsoids).

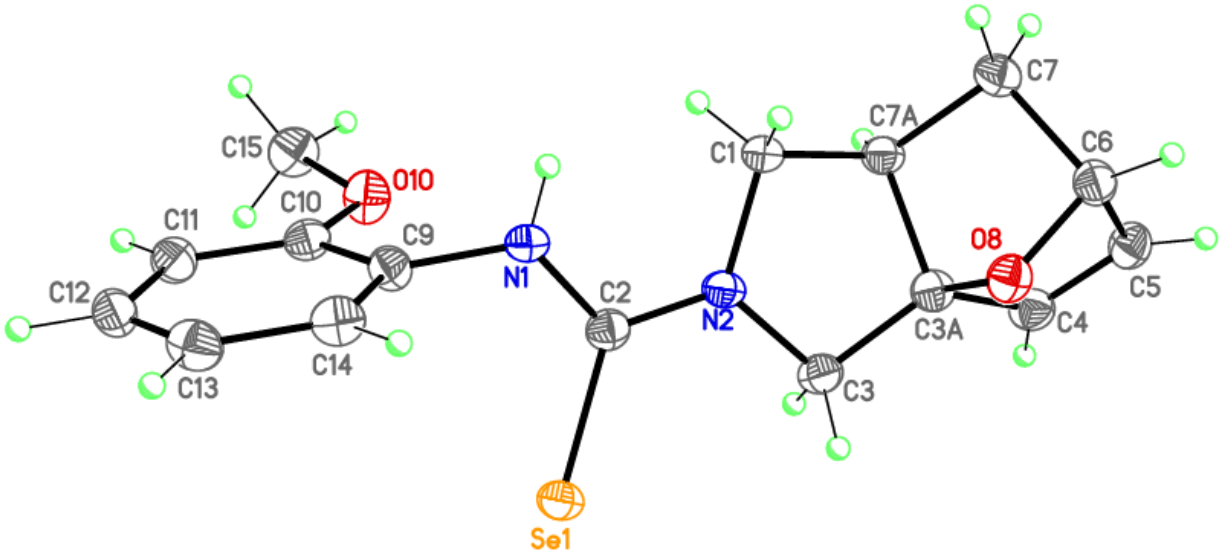


Fig. 3. Molecular structure of **7g** (50%-ellipsoids).

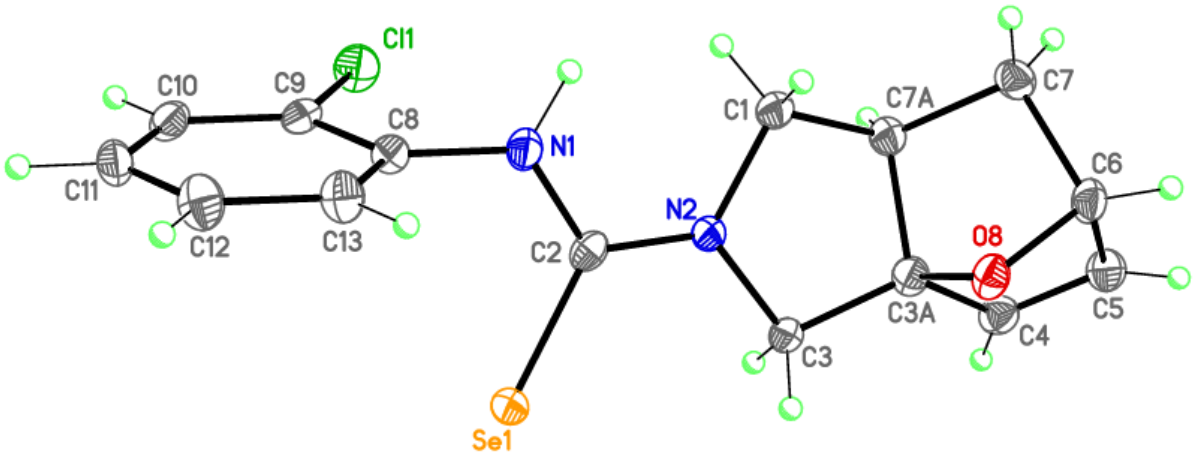


Fig. 4. Molecular structure of **7p** (50%-ellipsoids).

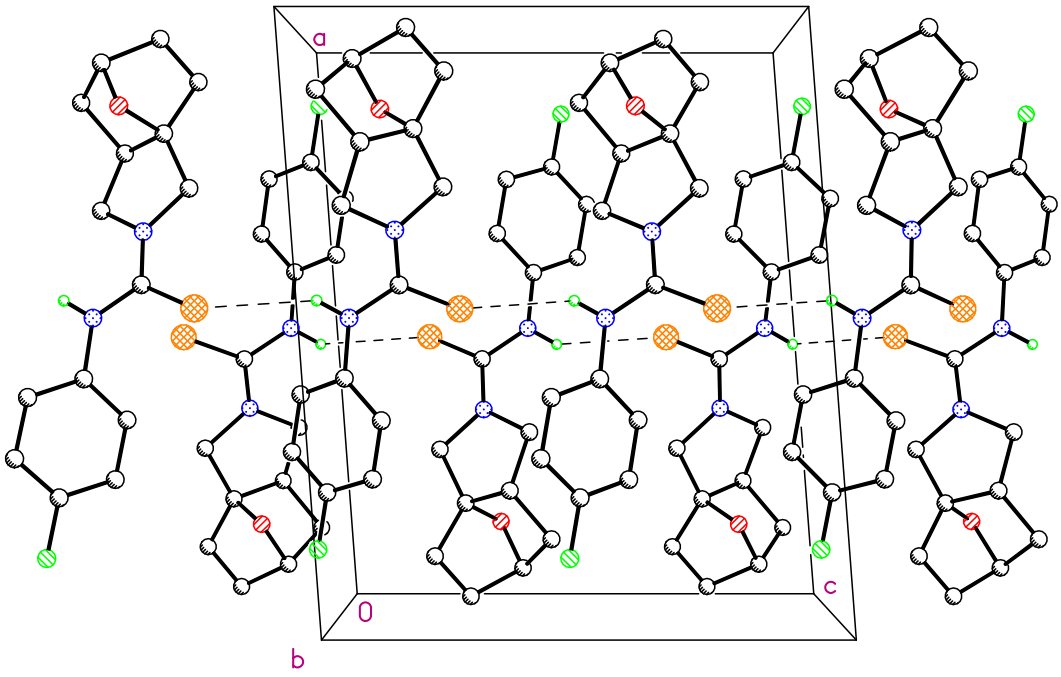


Fig. 5. Crystal structure of **6e**.

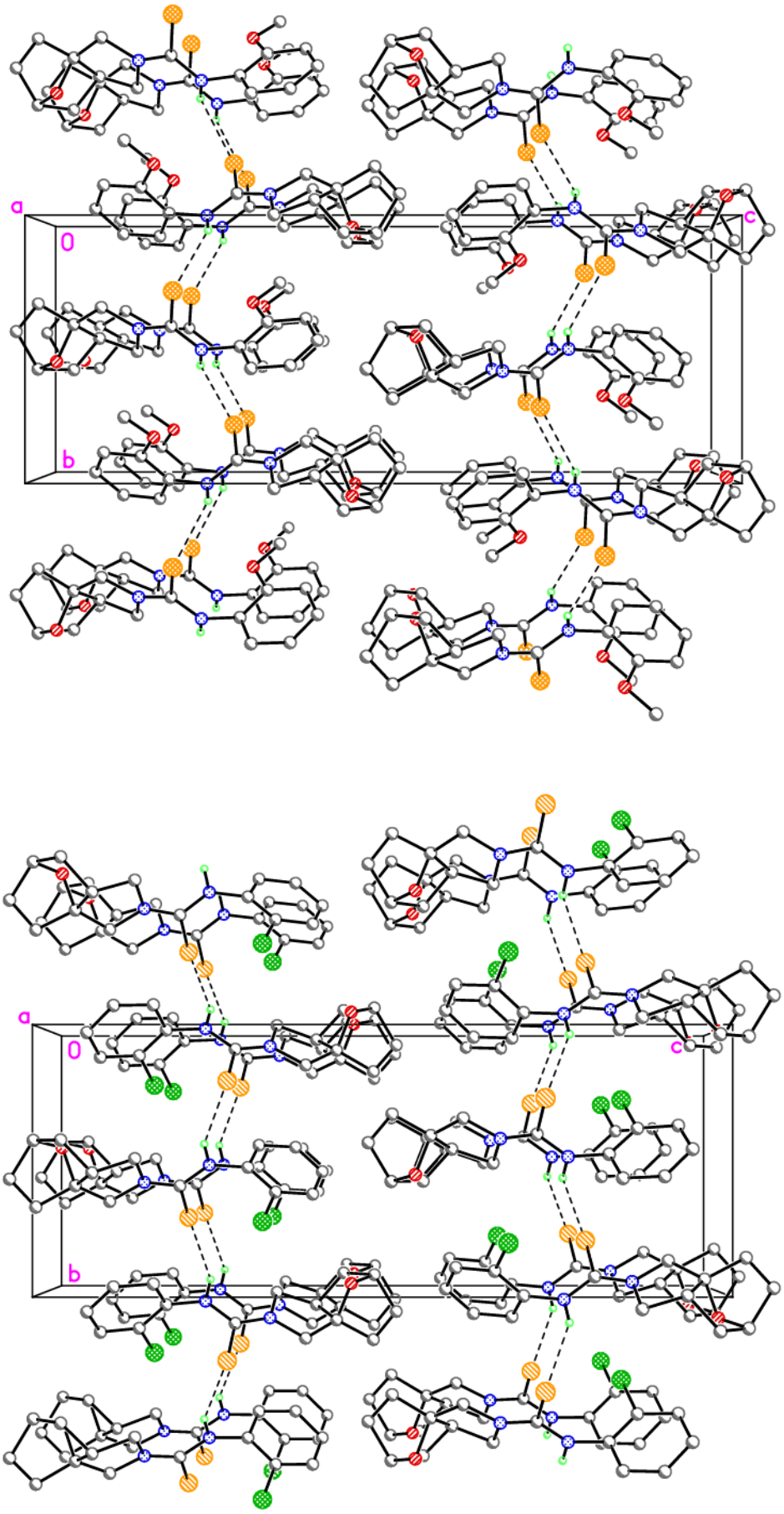


Fig. 6. Crystal structures of **7g** (top) and **7p** (bottom).

2. Experimental

2.1. General remarks

All reagents and solvents were purchased from commercial suppliers (Acros Organics, Aldrich, Alfa Aesar, AstaTech and Reachim) and used without further purification. No reactions require absolute solvents (CH_2Cl_2, EtOH, MeCN, MeOH, PhMe) and in an inert atmosphere. Thin layer chromatography, when necessary, was carried out on aluminum backed silica plates Sorbfil. The plates were visualized under UV light (254 nm) or in I_2 vapor. Organic layers were dried over anhydrous $MgSO_4$ or Na_2SO_4 and concentrated *in vacuo*. In rare cases, when the precipitate was not formed after 12 h standing at room temperature, the solvent was removed *in vacuo* and the residual was solidified by addition of hexane. Analytical samples for the new compounds were obtained by recrystallization from EtOAc, EtOH or EtOAc/hexane mixtures. Melting points for all crystalline compounds were measured on a capillary point apparatus Stuart SMP 10 equipped with a digital thermometer and were uncorrected. IR spectra were obtained in KBr pellets using an Infralum FT-801 IR-Fourier spectrometer. GC-MS mass spectra were taken on a Thermo Focus DSQ II GC-MS spectrometer (electron ionization, 70 eV, ion source temperature 200 °C, gas chromatographic inlet with a Varian Factor-Four VF-5ms column). LC-MS mass spectra were taken on Agilent 1100 series LC/MSD spectrometer with an API-ES/APCI ionization mode. NMR spectra were run in deuterated (>99%) solvents on Jeol JNM-ECA 600 (600.2 MHz for ^{1}H, 150.9 MHz for ^{13}C), Bruker Avance NEO 700 (700.2 MHz for ^{1}H and 176.1 MHz for ^{13}C and 658.8 MHz for ^{19}F) or Bruker Avance-III HD 300 (300.1 MHz for ^{1}H, 75.5 MHz for ^{13}C and 57.2 MHz for ^{77}Se) spectrometer for 2−8% solutions in $CDCl_3$ or DMSO-d_6 at 23−25 or 80-140 °C respectively. Residual signals of deuterated solvents were used as internal standards ($CDCl_3$: 7.25 ppm for ^{1}H nuclei, 77.2 ppm for ^{13}C nuclei; DMSO-d_6: 2.50 ppm for ^{1}H nuclei, 39.5 ppm for ^{13}C nuclei). Microanalyses were performed for C, H, N, and S with the elemental analysis system Eurovector EA 3000 (CHNS) and were within ±0.4 % of theoretical values.

2.2. *In vitro* antibacterial activity

All the synthesized compounds **5-7** were evaluated for their *in vitro* antimicrobial activity against *Staphylococcus aureus* (ATCC 25923), *Micrococcus luteus* (VKM-2665)*, Bacillus cereus (*VKM IP5832*), Enterococcus faecium spp.* as examples of Gram-positive bacteria, and *Escherichia coli* (ATCC 25922) and *Pseudomonas fluorescence* (VKM A1) as examples of Gram-negative bacteria with the requirements of the Institute of Clinical and Laboratory Standards (CLSI/NCCLS). Overnight cultures were grown at 37 °C in Lysogeny broth (LB) and diluted to obtain an opacity equivalent to 0.5 on the McFarland scale. Screening vials were filled with

solutions of the test compounds in 0.5% DMSO as prepared above with three replications for each treatment. API *pefloxacin* (0.5-256 μg/mL) and 0.5% DMSO served as positive and negative controls, respectively. The MICs of compounds were measured using the twofold serial broth dilution method. Twofold serial dilutions of solutions of the test compounds were prepared at 256, 128, 64, 32, 16, 8, 4, 2, 1 and 0.5 μg/mL. The tubes were then inoculated with the test microbe; each 5 mL received 0.1 mL of the above inoculums and were incubated at 37 °C. After incubation, the antibacterial activity of the test compounds was determined by measuring the absorption of the solution with a spectrophotometer on 500 nm.

2.3. *In vitro* antifungal activity

The antifungal activity of the tested compounds **5-7** and their minimum inhibitory concentrations (MICs) against yeasts and imperfect fungi were determined in vitro in a liquid culture medium RPMI 1640 with *L*-glutamine without sodium bicarbonate by the microdilution method of two-fold serial dilutions in accordance with the requirements of the Institute of Clinical and Laboratory Standards (CLSI/NCCLS) and according to previous studies [1-3]. The following collection test cultures were used: the yeast culture *Candida albicans* (ATCC 14053) and the culture of the imperfect fungus *Aspergillus niger* (ATCC 16404).

Definition of antifungal activity. Microbial cultures were grown on solid nutrient media, which were required for their maintenance, as well as to obtain the seed material necessary for setting up experiments. Yeast *Candida albicans* was grown on Sabouraud agar (peptone – 10 g, glucose – 40 g, agar – 20 g, distilled water – 1 L, pH 6.0), fungal culture *Aspergillus niger* – on potato-glucose agar (potato – 200 g, glucose – 20 g, agar – 15 g, distilled water – 1 L, pH 5.5-6.0). The media used were prepared from the appropriate ingredients and sterilized by autoclaving for 30 min at 110 °C, at 0.5 atm. The antifungal activity of the tested compounds was evaluated in a liquid nutrient medium RPMI 1640 with *L*-glutamine, without sodium bicarbonate (ICN Biomedicals Inc., Ohio, USA) by dilution in distilled water followed by buffering with 0.165 M morpholine propane sulfonic acid (MOPS; ACROS ORGANICS, New Jersey, USA) and bringing the pH to 7.0 with 1 N NaOH. Sterilization was carried out by pressure filtration through 0.22 μm Sterivex-GV filters (Millipore, USA). To set up the experiment, it was necessary to obtain seed material (inoculum), that was the cells or spores of cultures grown on appropriate solid nutrient media. For this purpose daily culture of the yeast *C. albicans*, grown at 35 °C, and a culture of the fungi *A. niger*, grown at 28 °C for 7 days, that showed abundant sporulation, were used. The preparation of yeast cell suspensions, as well as the preparation of a suspension of *A. niger* spores, was carried out in a sterile isotonic NaCl solution, bringing the

density of the suspensions to certain values. The optical density of the yeast suspension was controlled spectrophotometrically, reaching D = 0.11 at a wavelength of 530 nm. This yeast cell suspension was diluted 1:1000 with standard medium (RPMI 1640) to obtain an inoculum suspension containing twice the concentration of cells compared to the experiment. The final concentration of yeast cells in the experiment was $1 – 5 \times 10^3$ cells/ml. The suspension of fungal spores was adjusted to an optical density of 0.09 – 0.11 and diluted with a standard medium (RPMI 1640) by 100 times. The final concentration of fungal spores/cells in the experiment was $0.4 – 5 \times 10^4$ cells/ml. The number of cells in the inoculum for both cultures was checked by seeding on Sabouraud agar and counting the grown colonies [1,2]. To assess the biological activity of the test compounds, they were dissolved in DMSO at an initial concentration of 6.4 mM, after which a series of two-fold dilutions of these preparations in the same solvent was prepared up to a concentration of compounds of 12.5 μM. After the transfer of these solutions into a liquid nutrient medium and the introduction of inoculum, they were diluted 100 times, and the solvent concentration (DMSO) decreased to 1%. At the same time, the final concentration of drugs was in the range from 64 to 0.125 μM. Experiments to assess the antibiotic activity of the tested preparations were carried out using the micromethod in sterile 96-well flat-bottomed plates (Pan-Eco, Russia). The sample volume in the experiment was 200 μl [1,2].

Setting up an experiment. At a preliminary stage, a series of dilutions of each compound in 100% DMSO was diluted 10 times with a standard liquid nutrient medium and dilutions containing 10% DMSO were obtained for setting up the experiment. When setting up the experiment, first, 80 μl of liquid nutrient medium were added into the wells of the experimental 96-well plates, then, 20 μl of solutions of the tested compounds from preliminarily prepared series of dilutions with 10% DMSO were added. There was a 5-fold dilution and the solvent content was reduced to 2%. The subsequent introduction of 100 μl of the inoculum led to a further 2-fold dilution and the final concentration of drugs in the experiment reached from 64 to 0.125 μM at a concentration of DMSO of 1%. Each tested compound was present in the experiment at least in three repetitions. Wells containing no test drugs or solvent were included in the experimental panel as controls. *Amphotericin B* (Sigma, USA) was used as a reference drug. The plates were incubated in the dark in a humid atmosphere at 35 °C. Growth assessment was performed visually. The minimum inhibitory concentration (MIC) was defined as the minimum drug concentration that completely prevents growth of the test organism. The MICs of preparations for the yeast culture *C. albicans* were read after 24 hours, for *A. niger* - after 48 hours of cultivation. Statistical processing of the research results was carried out using the computer programs Statgraf and Microsoft Excel, calculating the arithmetic mean values,

confidence intervals and standard deviation. The significance of differences between the means was assessed using Student's t-test ($P<0.05$).

2.4. *N*-Prop-2-en-1-amines (1d-f); general procedures. Allylamine (27 mmol, 2.0 mL) was added to 27 mmol of the corresponding furfural in DCM (50 mL) in the presence of anhydrous $MgSO_4$ (54 mmol). The reaction mixtures were stirred (TLC control) at r.t, and after approx. 2 h, the $MgSO_4$ was filtered off, rinsed with DCM (3 × 15 mL), and the solutions were concentrated. The residues were dissolved in methanol (15 mL) and sodium borohydride (20 mmol, 0.76 g) was added portionwise over a 10 min period. The resulting mixtures were vigorously stirred at r.t for 12 h, then poured into H_2O (50 mL) and extracted with DCM (3 × 50 mL). The organic layers were dried with anhydrous $MgSO_4$, concentrated and purified by column chromatography (SiO_2, 23 × 1.6 cm, eluent: heptane).

***N*-[(5-Propyl-2-furyl)methyl]prop-2-en-1-amine (1d).** Yield: 2.95 g (61 %); light yellow oil; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) 6.02 (d, *J* = 2.5 Hz, 1H), 5.91-5.84 (m, 2H), 5.15 (dq, *J* = 17.2, 1.5 Hz, 1H), 5.08 (dq, *J* = 10.1, 1.5 Hz, 1H), 3.70 (s, 2H), 3.23 (d, *J* = 6.1 Hz, 2H), 2.54 (t, *J* = 7.6 Hz, 2H), 1.65-1.59 (m, 2H), 1.38 (s, 1H), 0.92 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150.9 MHz, $CDCl_3$): δ (ppm) 155.8, 151.9, 136.7, 116.2, 107.5, 105.2, 51.5, 45.6, 30.2, 21.5, 13.8. IR (KBr, cm^{-1}): ν_{max} = 3341 (NH). GC-MS (EI, 70 eV): *m/z* (%) = 179 (24) $[M]^+$, 150 (32), 136 (19), 123 (100), 108 (26), 96 (11), 94 (18), 81 (43), 68 (19), 57 (19), 41 (18). Anal. Calcd for $C_{11}H_{17}NO$: C, 73.70; H, 9.56; N, 7.81. Found: C, 73.81; H, 9.63; N, 7.65.

***N*-[(5-Phenyl-2-furyl)methyl]prop-2-en-1-amine (1e).** Yield: 3.51 g (61 %); light yellow oil; ^{1}H NMR (700.2 MHz, $CDCl_3$): δ (ppm) 7.66 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 6.59 (d, *J* = 3.1 Hz, 1H), 6.27 (d, *J* = 3.1 Hz, 1H), 5.96-5.91 (m, 1H), 5.24 (br.d, *J* = 17.2 Hz, 1H), 5.15 (d, *J* = 10.0 Hz, 1H), 3.86 (br.s, 2H), 3.33 (d, *J* = 5.7 Hz, 2H), 1.64 (s, 1H); ^{13}C NMR (176.1 MHz, $CDCl_3$): δ (ppm) 153.6, 153.2, 136.5, 130.9, 128.6 (2C), 127.1, 123.6 (2C), 116.4, 109.2, 105.6, 51.4, 45.5. IR (KBr, cm^{-1}): ν_{max} = 3081 (NH). GC-MS (EI, 70 eV): *m/z* (%) = 213 (26) $[M]^+$, 184 (40), 171 (21), 157 (100), 128 (38), 115 (22), 105 (22), 77 (18), 68 (20), 51 (15), 41 (18). Anal. Calcd for $C_{14}H_{15}NO$: C, 78.84; H, 7.09; N, 6.57. Found: C, 78.92; H, 6.89; N, 6.33.

***N*-[(5-Chloro-2-furyl)methyl]prop-2-en-1-amine (1f).** Yield: 3.32 g (72 %); light yellow oil; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) 6.17 (d, *J* = 3.0 Hz, 1H), 6.07 (d, *J* = 3.0 Hz, 1H), 5.91-5.84 (m, 1H), 5.18 (dq, *J* = 17.2, 1.5 Hz, 1H), 5.15 (dq, *J* = 10.0, 1.5 Hz, 1H), 3.73 (s, 2H), 3.26 (d, *J* = 6.1 Hz, 2H), 3.15 (s, 1H); ^{13}C NMR (150.9 MHz, $CDCl_3$): δ (ppm) 153.2, 135.9, 135.5, 116.9, 109.7, 106.7, 51.1, 45.1. IR (KBr, cm^{-1}): ν_{max} = 2963 (NH). MS (ESI): *m/z* = 172 $[M+H]^+$

for ^{35}Cl. Anal. Calcd for $C_8H_{10}ClNO$: C, 55.99; H, 5.87; N, 8.16. Found: C, 55.73; H, 6.09; N, 8.41.

2.5. Optimisation of IMDAF reaction conditions. A solution of the allylamine **1a** (0.1 g, 0.73 mmol) and phenylisocyanate (0.079 mL, 0.73 mmol) in various solvents (5 mL) was stirring or refluxed for 1−10 h (TLC monitoring). The resulting mixture was filtered off or evaporated, dried under vacuum and then at the air, studied by the NMR method (Table 1).

***N*-Allyl-*N*-(2-furylmethyl)-*N*'-phenylurea (2a).** ^{1}H NMR (700.2 MHz, $CDCl_3$): δ (ppm) 7.40 (dd, *J* = 1.7, 0.7 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 8.0 Hz, 2H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.78 (br.s, 1H), 6.36 (dd, *J* = 3.1, 1.7 Hz, 1H), 6.31 (br.d, *J* = 3.1 Hz, 1H), 5.86-5.81 (m, 1H), 5.31-5.26 (m, 2H), 4.52 (s, 2H), 4.00 (d, *J* = 5.5 Hz, 2H); ^{13}C NMR (176.1 MHz, $CDCl_3$): δ (ppm) 155.5, 151.3, 142.5, 139.2, 133.9, 128.8 (2C), 123.0, 119.8 (2C), 117.4, 110.6, 108.4, 49.8, 43.4.

2.6. General Procedure for the Synthesis of Products 5a-t and Characterization Data. A solution of the corresponding allylamine **1a-c,h-j** (4 mmol) and arylisocyanate (4 mmol) in toluene (10.0 mL) was refluxed for 4−6 h (TLC monitoring). The resulting mixture was cooled, and formation of solid was observed. The crystals were filtered off, washed with diethyl ether (3 × 5 mL), dried under vacuum and then at the air.

(3a*RS*,6*RS*,7a*RS*)-*N*-Phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5a). Yield: 0.71 g (69%); colourless plates. M.p. 158–160 °C; ^{1}H NMR (700.2 MHz, $CDCl_3$): δ (ppm) 7.41 (d, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.42 (dd, *J* = 5.7, 1.7 Hz, 1H), 6.38 (d, *J* = 5.7 Hz, 1H), 6.32 (br.s, 1H), 5.09 (dd, *J* = 4.5, 1.7 Hz, 1H), 3.97-3.91 (m, 3H), 3.12 (t, *J* = 9.5 Hz, 1H), 2.20-2.17 (m, 1H), 1.81 (ddd, *J* = 11.7, 4.5, 2.6 Hz, 1H), 1.48 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, $CDCl_3$): δ (ppm) 153.7, 139.1, 137.5, 134.0, 128.8 (2C), 122.9, 119.8 (2C), 94.8, 80.3, 51.4, 47.7, 42.1, 31.5. IR (KBr, cm^{-1}): ν_{max} = 3406 (NH), 1661 (NC=O). MS (ESI): *m/z* = 257 $[M+H]^+$. Anal. Calcd for $C_{15}H_{16}N_2O_2$: C, 70.29; H, 6.29; N, 10.93. Found: C, 70.26; H, 6.31; N, 10.90.

(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5b). Yield: 0.82 g (76%); colourless powder. M.p. 150–152 °C; ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) 8.15 (br.s, 1H), 7.49 (dd, *J* = 8.6, 1.0 Hz, 2H), 7.22 (dd, *J* = 8.6, 7.6 Hz, 2H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.49 (d, *J* = 5.6 Hz, 1H), 6.31 (d, *J* = 5.6 Hz, 1H), 3.94 (t, *J* = 9.3 Hz, 1H), 3.88 (d, *J* = 12.1 Hz, 1H), 3.71 (d, *J* = 12.1 Hz, 1H), 2.99 (t, *J* = 9.8 Hz, 1H), 2.23-2.19 (m, 1H), 1.55 (s, 3H), 1.53 (dd, *J* = 11.6, 7.6 Hz, 1H), 1.43 (dd, *J* = 11.6, 3.0 Hz, 1H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) 154.3, 141.0, 140.8, 135.4, 128.8 (2C), 122.2, 120.1 (2C), 94.6, 88.3, 52.0, 48.2, 45.1, 38.3, 19.5. IR (KBr, cm^{-1}): ν_{max} = 3336 (NH), 1649 (NC=O).

MS (ESI): *m/z* = 271 $[M+H]^+$. Anal. Calcd for $C_{16}H_{18}N_2O_2$: C, 71.09; H, 6.71; N, 10.36. Found: C, 71.26; H, 6.45; N, 10.47.

(3a*RS*,6*RS*,7a*RS*)-6-Ethyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5c). Yield: 0.67 g (59%); colourless powder. M.p. 138–139 °C; ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 8.15 (br.s, 0.2H), 7.49 (d, *J* = 8.6 Hz, 2H), 7.22 (t, *J* = 8.6 Hz, 2H), 6.92 (t, *J* = 8.6 Hz, 1H), 6.49 (d, *J* = 5.8 Hz, 1H), 6.38 (d, *J* = 5.8 Hz, 1H), 3.93 (t, *J* = 9.3 Hz, 1H), 3.88 (d, *J* = 12.3 Hz, 1H), 3.72 (d, *J* = 12.3 Hz, 1H), 2.97 (t, *J* = 9.8 Hz, 1H), 2.22-2.19 (m, 1H), 1.94-1.83 (m, 2H), 1.49-1.43 (m, 2H), 0.98 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) 154.3, 140.9, 139.4, 135.4, 128.8 (2C), 122.2, 120.0 (2C), 94.4, 92.4, 51.9, 48.2, 44.6, 36.1, 26.1, 9.8. IR (KBr, cm^{-1}): ν_{max} = 3339 (NH), 1649 (NC=O). MS (ESI): *m/z* = 285 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2O_2$: C, 71.81; H, 7.09; N, 9.85. Found: C, 71.99; H, 7.23; N, 9.98.

(3a*RS*,6*RS*,7a*RS*)-5,6-Dimethyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5d). Yield: 0.67 g (87%); colourless powder. M.p. 162–164 °C; ^{1}H NMR (700.2 MHz, $CDCl_3$, 50 °C): δ (ppm) 7.41 (d, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 7.6 Hz, 2H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.16 (br.s, 1H), 5.97 (s, 1H), 3.96 (t, *J* = 9.3 Hz, 1H), 3.88 (d, *J* = 12.3 Hz, 1H), 3.87 (d, *J* = 12.3 Hz, 1H), 3.18 (t, *J* = 9.4 Hz, 1H), 2.36-2.32 (m, 1H), 1.81 (s, 3H), 1.59 (s, 3H), 1.57 (dd, *J* = 11.7, 7.6 Hz, 1H), 1.50 (dd, *J* = 11.7, 2.5 Hz, 1H); ^{13}C NMR (176.1 MHz, $CDCl_3$, 50 °C): δ (ppm) 153.7, 149.5, 139.1, 128.8 (2C), 127.8, 122.9, 119.8 (2C), 93.7, 89.7, 51.6, 47.9, 47.2, 37.4, 17.5, 11.9. IR (KBr, cm^{-1}): ν_{max} = 3136 (NH), 1608 (NC=O). GC-MS (EI, 70 eV): *breaks down into an amine and an isocyanate*. MS (ESI): *m/z* = 285 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2O_2$: C, 71.81; H, 7.09; N, 9.85. Found: C, 71.68; H, 7.21; N, 9.63.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5e). Yield: 0.64 g (55%); colourless powder. M.p. 158–159 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) 8.08 (br.s, 1H), 7.56 (d, *J* = 8.8 Hz, 2H), 7.26 (d, *J* = 8.8 Hz, 2H), 6.49 (d, *J* = 5.7 Hz, 1H), 6.30 (dd, *J* = 5.7, 1.5 Hz, 1H), 5.06 (dd, *J* = 4.5, 1.5 Hz, 1H), 3.98 (t, *J* = 9.6 Hz, 1H), 3.96 (d, *J* = 12.3 Hz, 1H), 3.79 (d, *J* = 12.3 Hz, 1H), 2.98 (t, *J* = 9.6 Hz, 1H), 2.16-2.12 (m, 1H), 1.73 (ddd, *J* = 11.4, 4.2, 2.7 Hz, 1H), 1.44 (dd, *J* = 11.4, 7.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 154.1, 140.0, 137.6, 134.7, 128.5 (2C), 125.9, 121.5 (2C), 94.9, 80.1, 51.8, 47.9, 41.8, 31.7. IR (KBr, cm^{-1}): ν_{max} = 3396 (NH), 1660 (NC=O). GC-MS (EI, 70 eV): *breaks down into an amine and an isocyanate*. MS (ESI): *m/z* = 291 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2O_2$: C, 61.97; H, 5.20; N, 9.64. Found: C, 62.13; H, 5.48; N, 9.41.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5f). Yield: 0.94 g (77%); colourless powder. M.p. 98–99 °C; ^{1}H NMR

(700.2 MHz, DMSO-d_6): δ (ppm) 8.07 (br.s, 1H), 7.56 (d, J = 8.8 Hz, 2H), 7.26 (d, J = 8.8 Hz, 2H), 6.48 (d, J = 5.5 Hz, 1H), 6.30 (d, J = 5.5 Hz, 1H), 3.97 (t, J = 9.3 Hz, 1H), 3.90 (d, J = 12.3 Hz, 1H), 3.75 (d, J = 12.3 Hz, 1H), 3.04-3.00 (m, 1H), 2.25-2.21 (m, 1H), 1.59-1.57 (m, 1H), 1.58 (s, 3H), 1.46 (dd, J = 11.4, 2.5 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 154.2, 140.8, 140.1, 135.2, 128.5 (2C), 125.9, 121.6 (2C), 94.6, 88.3, 51.9, 48.2, 45.2, 38.4, 19.3. IR (KBr, cm^{-1}): ν_{max} = 3304 (NH), 1657 (NC=O). MS (ESI): *m/z* = 305 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{16}H_{17}ClN_2O_2$: C, 63.05; H, 5.62; N, 9.19. Found: C, 62.87; H, 5.39; N, 9.41.

(3a*RS*,6*RS*,7a*RS*)-*N*-(3-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5g). Yield: 0.81 g (70%); colourless powder. M.p. 138–139 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) 8.14 (br.s, 1H), 7.70 (s, 1H), 7.46 (d, J = 8.1 Hz, 1H), 7.24 (t, J = 8.1 Hz, 1H), 6.97 (d, J = 8.1 Hz, 1H), 6.49 (d, J = 5.7 Hz, 1H), 6.45 (br.d, J = 5.7 Hz, 1H), 5.06 (br.d, J = 4.5 Hz, 1H), 4.00-3.96 (m, 2H), 3.79 (d, J = 12.5 Hz, 1H), 2.99 (t, J = 9.8 Hz, 1H), 2.16-2.12 (m, 1H), 1.74-1.72 (m, 1H), 1.44 (dd, J = 11.4, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 154.0, 142.6, 137.6, 134.7, 133.3, 130.2, 121.7, 119.4, 118.2, 94.9, 80.1, 51.8, 47.9, 41.8, 31.7. IR (KBr, cm^{-1}): ν_{max} = 3196 (NH), 1588 (NC=O). GC-MS (EI, 70 eV): *breaks down into an amine and an isocyanate*. MS (ESI): *m/z* = 291 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2O_2$: C, 61.97; H, 5.20; N, 9.64. Found: C, 61.89; H, 5.31; N, 9.58.

(3a*RS*,6*RS*,7a*RS*)-*N*-(3-Chlorophenyl)-6-ethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5h). Yield: 0.74 g (58%); colourless powder. M.p. 91–94 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.18 (br.s, 0.2H), 7.69 (s, 1H), 7.45 (d, J = 8.1 Hz, 1H), 7.24 (t, J = 8.1 Hz, 1H), 6.97 (d, J = 8.1 Hz, 1H), 6.49 (d, J = 5.6 Hz, 1H), 6.38 (d, J = 5.6 Hz, 1H), 3.96 (t, J = 9.3 Hz, 1H), 3.90 (d, J = 12.4 Hz, 1H), 3.76 (d, J = 12.4 Hz, 1H), 3.00 (t, J = 9.8 Hz, 1H), 2.25-2.21 (m, 1H), 1.95-1.86 (m, 2H), 1.53-1.47 (m, 2H), 1.01 (t, J = 7.6 Hz, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) 154.0, 142.5, 139.4, 135.3, 133.3, 130.2, 121.7, 119.3, 118.1, 94.4, 92.4, 51.9, 48.2, 44.6, 36.0, 25.9, 9.4. IR (KBr, cm^{-1}): ν_{max} = 3314 (NH), 1650 (NC=O). MS (ESI): *m/z* = 319 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{17}H_{19}ClN_2O_2$: C, 64.05; H, 6.01; N, 8.79. Found: C, 63.90; H, 5.84; N, 9.07.

(3a*RS*,6*RS*,7a*RS*)-*N*-Propyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5i). Yield: 0.37 g (42%); colourless powder. M.p. 138–140 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) 6.45 (d, J = 5.7 Hz, 1H), 6.40 (dd, J = 5.7, 1.4 Hz, 1H), 5.81 (br.s, 1H), 5.02 (dd, J = 4.5, 1.5 Hz, 1H), 3.80-3.77 (m, 2H), 3.60 (d, J = 12.4 Hz, 1H), 3.04-3.00 (m, 2H), 2.80 (t, J = 9.6 Hz, 1H), 2.07-2.03 (m, 1H), 1.67 (ddd, J = 11.7, 4.3, 3.1 Hz, 1H), 1.48-1.43 (m, 2H), 1.38 (dd, J = 11.4, 7.6 Hz, 1H), 0.86 (t, J = 7.4 Hz, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 157.0,

137.4, 134.9, 95.1, 80.0, 51.4, 47.6, 42.3, 41.9, 31.6, 23.6, 11.7. IR (KBr, cm^{-1}): ν_{max} = 3341 (NH), 1627, 1546 (NC=O). MS (ESI): *m/z* = 223 $[M+H]^+$. Anal. Calcd for $C_{12}H_{18}N_2O_2$: C, 64.84; H, 8.16; N, 12.60. Found: C, 64.89; H, 8.37; N, 12.79.

(3a*RS*,6*RS*,7a*RS*)-*N*-Hexyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5j). Yield: 0.32 g (30%); colourless powder. M.p. 102–104 °C; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) 6.36 (dd, *J* = 5.6, 1.5 Hz, 1H), 6.33 (d, *J* = 5.6 Hz, 1H), 5.03 (dd, *J* = 4.5, 1.5 Hz, 1H), 4.25 (br.t, *J* = 5.1 Hz, 1H), 3.83-3.74 (m, 3H), 3.18 (q, *J* = 7.1 Hz, 2H), 2.94 (t, *J* = 9.6 Hz, 1H), 2.12-2.07 (m, 1H), 1.74 (ddd, *J* = 11.6, 4.5, 3.0 Hz, 1H), 1.47-1.40 (m, 3H), 1.29-1.21 (m, 6H), 0.83 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (150.9 MHz, $CDCl_3$): δ (ppm) 156.7, 137.4, 134.3, 95.0, 80.3, 51.1, 47.5, 42.1, 40.7, 31.6, 31.3, 30.5, 26.7, 22.6, 14.1. IR (KBr, cm^{-1}): ν_{max} = 3339 (NH), 1618 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 264 (16) $[M]^+$, 223 (29), 96 (100), 81 (43), 56 (12), 53 (23), 41 (25). Anal. Calcd for $C_{15}H_{24}N_2O_2$: C, 68.15; H, 9.15; N, 10.60. Found: C, 68.07; H, 9.03; N, 10.69.

(3a*RS*,6*RS*,7a*RS*)-*N*-Hexyl-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5k). Yield: 0.31 g (28%); colourless powder. M.p. 137–138 °C; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) 6.36 (d, *J* = 5.8 Hz, 1H), 6.22 (d, *J* = 5.8 Hz, 1H), 4.15 (br.t, *J* = 5.6 Hz, 1H), 3.82-3.72 (m, 3H), 3.19 (q, *J* = 7.1 Hz, 2H), 3.01 (t, *J* = 9.4 Hz, 1H), 2.25-2.20 (m, 1H), 1.62 (s, 3H), 1.56 (ddd, *J* = 11.6, 7.6 Hz, 1H), 1.49-1.44 (m, 3H), 1.31-1.23 (m, 6H), 0.86 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150.9 MHz, $CDCl_3$): δ (ppm) 156.6, 140.6, 134.9, 94.8, 88.5, 51.3, 47.8, 45.5, 40.7, 37.9, 31.7, 30.5, 26.7, 22.7, 19.3, 14.1. IR (KBr, cm^{-1}): ν_{max} = 3340 (NH), 1617 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 278 (17) $[M]^+$, 237 (22), 110 (100), 95 (32), 43 (19). Anal. Calcd for $C_{16}H_{26}N_2O_2$: C, 69.03; H, 9.41; N, 10.06. Found: C, 68.89; H, 9.73; N, 9.84.

(3a*RS*,6*RS*,7a*RS*)-*N*-Benzyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5l). Yield: 0.44 g (41%); colourless powder. M.p. 155–156 °C; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) 7.31-7.22 (m, 5H), 6.39 (dd, *J* = 5.8, 1.5 Hz, 1H), 6.35 (d, *J* = 5.8 Hz, 1H), 5.06 (dd, *J* = 4.5, 1.5 Hz, 1H), 4.58 (t, *J* = 5.6 Hz, 1H), 4.44-4.38 (m, 2H), 3.87-3.80 (m, 3H), 2.98 (t, *J* = 9.6 Hz, 1H), 2.15-2.10 (m, 1H), 1.76 (ddd, *J* = 11.6, 4.5, 3.0 Hz, 1H), 1.43 (dd, *J* = 11.6, 7.6 Hz, 1H); ^{13}C NMR (150.9 MHz, $CDCl_3$): δ (ppm) 156.5, 139.8, 137.5, 134.2, 128.7 (2C), 127.8 (2C), 127.3, 95.0, 80.4, 51.2, 47.6, 44.8, 42.2, 31.4. IR (KBr, cm^{-1}): ν_{max} = 3325 (NH), 1624 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 270 (33) $[M]^+$, 229 (38), 122 (12), 106 (17), 96 (100), 91 (91), 81 (51), 65 (16), 56 (15), 53 (17), 41 (23). Anal. Calcd for $C_{16}H_{18}N_2O_2$: C, 71.09; H, 6.71; N, 10.36. Found: C, 71.38; H, 6.53; N, 10.48.

(3a*RS*,6*RS*,7a*RS*)-*N*-Benzyl-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5m). Yield: 0.33 g (29%); colourless powder. M.p. 126–128 °C; ^{1}H NMR (600.2

MHz, $CDCl_3$): δ (ppm) 7.33-7.24 (m, 5H), 6.36 (d, *J* = 5.8 Hz, 1H), 6.23 (d, *J* = 5.8 Hz, 1H), 4.50-4.42 (m, 3H), 3.85-3.77 (m, 3H), 3.04 (t, *J* = 9.4 Hz, 1H), 2.26-2.21 (m, 1H), 1.63 (s, 3H), 1.57 (dd, *J* = 11.6, 7.6 Hz, 1H), 1.48 (ddd, *J* = 11.6, 2.5 Hz, 1H); ^{13}C NMR (176.1 MHz, $CDCl_3$): δ (ppm) 156.3, 140.6, 139.6, 134.7, 128.6 (2C), 127.8 (2C), 127.3, 94.7, 88.4, 51.3, 47.9, 45.5, 44.7, 37.9, 19.2. IR (KBr, cm^{-1}): ν_{max} = 3306 (NH), 1621 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 284 (17) $[M]^+$, 243 (23), 110 (100), 95 (33), 91 (44), 65 (11), 41 (12). Anal. Calcd for $C_{17}H_{20}N_2O_2$: C, 71.81; H, 7.09; N, 9.85. Found: C, 71.63; H, 7.25; N, 9.51.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenethyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5n). Yield: 0.56 g (45%); colourless powder. M.p. 131–132 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) 7.11 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 6.47 (d, *J* = 5.7 Hz, 1H), 6.41 (dd, *J* = 5.7, 1.7 Hz, 1H), 6.22 (br.t, *J* = 5.5 Hz, 1H), 5.02 (dd, *J* = 4.5, 1.7 Hz, 1H), 3.77-3.72 (m, 2H), 3.72 (s, 3H), 3.57 (d, *J* = 12.2 Hz, 1H), 3.21-3.17 (m, 2H), 2.76 (t, *J* = 9.6 Hz, 1H), 2.65 (t, *J* = 7.6 Hz, 2H), 2.06-2.02 (m, 1H), 1.66 (ddd, *J* = 11.7, 4.5, 2.9 Hz, 1H), 1.36 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 158.0, 156.7, 137.5, 134.9, 132.2, 130.0 (2C), 114.2 (2C), 94.5, 79.9, 55.4, 51.3, 47.5, 42.4, 41.7, 35.8, 31.5. IR (KBr, cm^{-1}): ν_{max} = 3324 (NH), 1620 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 314 (46) $[M]^+$, 273 (25), 134 (100), 121 (49), 96 (23), 81 (45), 77 (10), 53 (13). Anal. Calcd for $C_{18}H_{22}N_2O_3$: C, 68.77; H, 7.05; N, 8.91. Found: C, 68.54; H, 7.06; N, 9.03.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenethyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5o). Yield: 0.54 g (41%); colourless powder. M.p. 122–123 °C; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) 7.12 (d, *J* = 8.6 Hz, 2H), 6.85 (d, *J* = 8.6 Hz, 2H), 6.36 (d, *J* = 5.6 Hz, 1H), 6.24 (d, *J* = 5.6 Hz, 1H), 4.20 (br.t, *J* = 5.5 Hz, 1H), 3.79 (s, 3H), 3.77-3.70 (m, 3H), 3.50-3.40 (m, 2H), 2.98 (t, *J* = 9.4 Hz, 1H), 2.76 (t, *J* = 6.8 Hz, 2H), 2.25-2.20 (m, 1H), 1.64 (s, 3H), 1.57 (dd, *J* = 11.6, 7.6 Hz, 1H), 1.48 (ddd, *J* = 11.6, 2.5 Hz, 1H); ^{13}C NMR (176.1 MHz, $CDCl_3$): δ (ppm) 158.2, 156.4, 140.5, 134.8, 131.4, 129.8 (2C), 114.0 (2C), 94.7, 88.4, 55.3, 51.1, 47.7, 45.4, 42.0, 37.9, 35.6, 19.2. IR (KBr, cm^{-1}): ν_{max} = 3340 (NH), 1624 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 328 (60) $[M]^+$, 287 (50), 134 (69), 121 (48), 110 (90), 95 (100), 41 (12). Anal. Calcd for $C_{19}H_{24}N_2O_3$: C, 69.49; H, 7.37; N, 8.53. Found: C, 69.66; H, 7.16; N, 8.41.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,2,2-Trichloroacetyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5p). Yield: 0.62 g (48%); colourless powder. M.p. 163–165 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) *E/Z isomers* 10.91 (br.s, 1.95H), 6.50-6.48 (m, 1.95H), 6.45 (dd, *J* = 5.7, 1.7 Hz, 1.95H), 5.05 (dd, *J* = 4.5, 1.7 Hz, 1.95H), 4.05 (d, *J* = 12.4 Hz, 0.95H), 4.02 (d, *J* = 13.7 Hz, 1H), 3.92 (dd, *J* = 11.4, 9.1 Hz, 0.95H), 3.82 (t, *J* = 9.4 Hz, 1H), 3.77 (d, *J* = 12.4 Hz,

0.95H), 3.68 (d, *J* = 13.7 Hz, 1H), 3.12 (t, *J* = 10.1 Hz, 1H), 2.98 (t, *J* = 10.5 Hz, 0.95H), 2.17-2.10 (m, 1.95H), 1.75 (ddd, *J* = 11.7, 4.1, 2.9 Hz, 0.95H), 1.68 (ddd, *J* = 11.7, 4.1, 2.9 Hz, 1H), 1.41 (dd, *J* = 11.7, 7.6 Hz, 0.95H), 1.36 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) *E/Z isomers* 159.7 (2C), 149.9 (2C), 137.8, 137.7, 134.5, 134.2, 94.9 (2C), 94.1, 92.7, 80.2, 80.1, 52.6, 52.4, 48.4, 48.3, 42.0, 40.8, 32.0, 31.5. IR (KBr, cm^{-1}): ν_{max} = 3275 (NH), 1746, 1672 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 285 (5) [M-40 (C_3H_4)]$^+$ for ^{35}Cl, 152 (8), 136 (13), 117 (16), 108 (42), 94 (11), 81 (93), 70 (100), 53 (23), 41 (16). Anal. Calcd for $C_{11}H_{11}Cl_3N_2O_3$: C, 40.58; H, 3.41; N, 8.60. Found: C, 40.13; H, 3.58; N, 8.70.

(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-(trichloroacetyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5q). Yield: 0.74 g (55%); colourless powder. M.p. 161–162 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) *E/Z isomers* 10.91 (br.s, 1.9H), 6.50-6.48 (m, 1.9H), 6.30 (d, *J* = 5.5 Hz, 1.9H), 4.00 (d, *J* = 12.4 Hz, 0.9H), 3.96 (d, *J* = 13.6 Hz, 1H), 3.91 (dd, *J* = 11.0, 9.3 Hz, 0.9H), 3.82 (t, *J* = 9.5 Hz, 1H), 3.73 (d, *J* = 12.4 Hz, 0.9H), 3.65 (d, *J* = 13.6 Hz, 1H), 3.18 (t, *J* = 10.1 Hz, 1H), 3.04 (t, *J* = 10.5 Hz, 0.9H), 2.27-2.20 (m, 1.9H), 1.57-1.49 (m, 8.5H), 1.43 (dd, *J* = 11.7, 2.1 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) *E/Z isomers* 159.7 (2C), 150.0 (2C), 140.8 (2C), 135.1, 134.7, 94.5 (2C), 93.7, 92.8, 88.5, 88.4, 52.7, 52.6, 48.7, 48.6, 45.3, 44.1, 38.6, 38.0, 19.3 (2C). IR (KBr, cm^{-1}): ν_{max} = 3200 (NH), 1732, 1676 (NC=O). GC-MS (EI, 70 eV): *m/z* (%) = 299 (5) [M-40 (C_3H_4)]$^+$ for ^{35}Cl, 151 (23), 122 (26), 108 (16), 95 (100), 70 (65), 41 (17). Anal. Calcd for $C_{12}H_{13}Cl_3N_2O_3$: C, 42.44; H, 3.86; N, 8.25. Found: C, 42.17; H, 3.57; N, 7.96.

(3a*RS*,6*RS*,7a*RS*)-6-Ethyl-*N*-(trichloroacetyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5r). Yield: 0.65 g (46%); colourless powder. M.p. 158–160 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) *E/Z isomers* 10.91 (br.s, 1.9H), 6.50-6.49 (m, 1.9H), 6.39 (d, *J* = 5.7 Hz, 1.9H), 4.00 (d, *J* = 12.4 Hz, 0.9H), 3.96 (d, *J* = 13.6 Hz, 1H), 3.91 (dd, *J* = 11.0, 9.3 Hz, 0.9H), 3.82 (t, *J* = 9.4 Hz, 1H), 3.75 (d, *J* = 12.4 Hz, 0.9H), 3.66 (d, *J* = 13.6 Hz, 1H), 3.16 (t, *J* = 10.1 Hz, 1H), 3.02 (t, *J* = 10.5 Hz, 0.9H), 2.26-2.20 (m, 1.9H), 1.94-1.83 (m, 3.8H), 1.51-1.43 (m, 3.8H), 0.99-0.97 (m, 5.7H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) *E/Z isomers* 159.7 (2C), 149.9 (2C), 139.4 (2C), 135.2, 134.8, 94.5 (2C), 93.5, 92.8, 92.6, 92.5, 52.7, 52.5, 48.7, 48.6, 44.8, 43.6, 36.5, 35.8, 25.9 (2C), 9.7 (2C). IR (KBr, cm^{-1}): ν_{max} = 3193 (NH), 1732, 1673 (NC=O). MS (ESI): *m/z* = 353 [M+H]$^+$ for ^{35}Cl. Anal. Calcd for $C_{13}H_{15}Cl_3N_2O_3$: C, 44.15; H, 4.28; N, 7.92. Found: C, 43.97; H, 3.94; N, 7.99.

(3a*SR*,6*RS*,7a*SR*)-7a-Chloro-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5s). Yield: 0.38 g (33%); colourless powder. M.p. 146–148 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) 8.34 (br.s, 1H), 7.50 (d, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.6 Hz, 2H), 6.96

(t, *J* = 7.6 Hz, 1H), 6.71 (dd, *J* = 5.7, 1.4 Hz, 1H), 6.62 (d, *J* = 5.7 Hz, 1H), 5.20 (dd, *J* = 4.3, 1.4 Hz, 1H), 4.20 (d, *J* = 11.9 Hz, 1H), 4.15 (d, *J* = 12.5 Hz, 1H), 3.86 (d, *J* = 12.5 Hz, 1H), 3.60 (d, *J* = 11.9 Hz, 1H), 2.67 (dd, *J* = 12.4, 4.8 Hz, 1H), 1.62 (d, *J* = 12.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 154.3, 140.6, 138.8, 133.5, 128.8 (2C), 122.4, 120.0 (2C), 96.4, 81.1, 73.5, 61.0, 46.1, 41.0. IR (KBr, cm^{-1}): ν_{max} = 3402 (NH), 1661 (NC=O), 753 (C-Cl). GC-MS (EI, 70 eV): 290 (26) $[M]^+$ for ^{35}Cl, 255 (26), 215 (24), 207 (12), 172 (14), 119 (13), 96 (75), 81 (100), 53 (19), 40 (45). Anal. Calcd for $C_{15}H_{15}ClN_2O_2$: C, 61.97; H, 5.20; N, 9.64. Found: C, 62.19; H, 5.00; N, 9.37.

(3a*SR*,6*RS*,7a*SR*)-7a-Bromo-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5t). Yield: 0.58 g (43%); colourless powder. M.p. 139–140 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6): δ (ppm) 8.34 (br.s, 1H), 7.50 (d, *J* = 7.4 Hz, 2H), 7.25 (t, *J* = 7.4 Hz, 2H), 6.96 (t, *J* = 7.4 Hz, 1H), 6.66 (dd, *J* = 5.7, 1.9 Hz, 1H), 6.62 (d, *J* = 5.7 Hz, 1H), 5.20 (dd, *J* = 4.8, 1.9 Hz, 1H), 4.30 (d, *J* = 12.4 Hz, 1H), 4.21 (d, *J* = 12.6 Hz, 1H), 3.86 (d, *J* = 12.4 Hz, 1H), 3.66 (d, *J* = 12.4 Hz, 1H), 2.65 (dd, *J* = 12.9, 4.8 Hz, 1H), 1.68 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6): δ (ppm) 154.3, 140.6, 138.1, 134.6, 128.8 (2C), 122.4, 120.0 (2C), 96.7, 81.0, 65.8, 62.2, 46.0, 40.8. IR (KBr, cm^{-1}): ν_{max} = 3402 (NH), 1661 (NC=O), 752 (C-Br). GC-MS (EI, 70 eV): 336 (18) $[M]^+$ for ^{81}Br, 255 (69), 215 (54), 122 (11), 119 (15), 96 (81), 81 (100), 77 (13), 53 (21), 40 (28). Anal. Calcd for $C_{15}H_{15}BrN_2O_2$: C, 53.75; H, 4.51; N, 8.36. Found: C, 53.46; H, 4.87; N, 8.37.

6.7. General Procedure for the Synthesis of Products 6a-p and Characterization Data. A solution of the corresponding allylamine **1a,b,e,h** (4 mmol) and arylisothiocyanate (4 mmol) in benzene (10 mL) was refluxed for 6 h (TLC monitoring). The resulting mixture was cooled, and formation of solid was observed. The crystals were filtered off, washed with diethyl ether (3 × 5 mL), dried under vacuum and then at the air.

(3a*RS*,6*RS*,7a*RS*)-*N*-Phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6a). Yield: 1.04 g (96%); colourless powder. M.p. 148–150 °C; ^{1}H NMR (600.2 MHz, DMSO-d_6, 100 °C): δ (ppm)) *the NH signal is less intense due to proton exchange* 8.71 (br.s, 0.8H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.51 (d, *J* = 6.1 Hz, 1H), 6.46 (br.d, *J* = 6.1 Hz, 1H), 5.08 (br.d, *J* = 5.1 Hz, 1H), 4.29 (br.t, *J* = 10.0 Hz, 1H), 4.23 (d, *J* = 13.5 Hz, 1H), 4.11 (d, *J* = 13.5 Hz, 1H), 3.23 (t, *J* = 10.5 Hz, 1H), 2.26-2.22 (m, 1H), 1.77 (ddd, *J* = 12.1, 4.0, 3.0 Hz, 1H), 1.47 (dd, *J* = 12.1, 8.1 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) 178.9, 141.2, 137.7, 134.5, 128.3 (2C), 126.0 (2C), 124.9, 94.3, 80.2, 55.8, 52.2, 41.5, 32.1. IR (KBr, cm^{-1}): ν_{max} = 3347 (NH), 1536 (NC=S). MS (ESI): *m/z* = 273 $[M+H]^+$.

Anal. Calcd for $C_{15}H_{16}N_2OS$: C, 66.15; H, 5.92; N, 10.29; S, 11.77. Found: C, 66.23; H, 5.87; N, 10.27; S, 11.69.

(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6b). Yield: 1.09 g (95%); colourless powder. M.p. 178–179 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 90 °C): δ (ppm)) 8.71 (br.s, 1H), 7.45 (d, J = 7.6 Hz, 2H), 7.31 (t, J = 7.6 Hz, 2H), 7.13 (t, J = 7.6 Hz, 1H), 6.50 (d, J = 5.6 Hz, 1H), 6.32 (d, J = 5.6 Hz, 1H), 4.29 (dd, J = 11.0, 9.0 Hz, 1H), 4.18 (d, J = 13.5 Hz, 1H), 4.09 (d, J = 13.5 Hz, 1H), 3.30 (dd, J = 11.0, 9.7 Hz, 1H), 2.39-2.30 (m, 1H), 1.63 (dd, J = 11.7, 7.3 Hz, 1H), 1.60 (s, 3H), 1.50 (dd, J = 11.7, 2.9 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 90 °C): δ (ppm) 179.1, 141.2, 140.9, 135.0, 128.2 (2C), 126.0 (2C), 124.8, 94.0, 88.4, 56.0, 52.5, 44.9, 38.7, 19.3. ^{1}H NMR (600.2 MHz, DMSO-d_6, 100 °C): δ (ppm)) *the NH signal is less intense due to proton exchange* 8.71 (br.s, 0.8H), 7.44 (d, J = 7.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.12 (t, J = 7.6 Hz, 1H), 6.50 (d, J = 5.1 Hz, 1H), 6.32 (d, J = 5.1 Hz, 1H), 4.28 (br.t, J = 10.1 Hz, 1H), 4.16 (d, J = 13.5 Hz, 1H), 4.08 (d, J = 13.5 Hz, 1H), 3.28 (t, J = 10.5 Hz, 1H), 2.36-2.32 (m, 1H), 1.64-1.60 (m, 1H), 1.60 (s, 3H), 1.50 (br.d, J = 11.1 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C): δ (ppm) 178.9, 141.2, 140.8, 135.0, 128.3 (2C), 126.1 (2C), 124.9, 94.0, 88.4, 56.0, 52.5, 44.9, 38.7, 19.3. IR (KBr, cm^{-1}): ν_{max} = 3305 (NH), 1535 (NC=S). MS (ESI): m/z = 287 $[M+H]^+$. Anal. Calcd for $C_{16}H_{18}N_2OS$: C, 67.10; H, 6.33; N, 9.78; S, 11.20. Found: C, 67.08; H, 6.12; N, 9.87; S, 11.34.

(3a*RS*,6*RS*,7a*RS*)-5,6-Dimethyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6c). Yield: 1.09 g (91%); colourless powder. M.p. 178–180 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 87 °C): δ (ppm) 8.72 (br.s, 1H), 7.42 (d, J = 7.9 Hz, 2H), 7.30 (t, J = 7.9 Hz, 2H), 7.13 (t, J = 7.9 Hz, 1H), 6.05 (d, J = 1.5 Hz, 1H), 4.25 (br.t, J = 8.9 Hz, 1H), 4.09 (d, J = 13.5 Hz, 1H), 4.02 (d, J = 13.5 Hz, 1H), 3.26 (t, J = 10.4 Hz, 1H), 2.38-2.34 (m, 1H), 1.78 (d, J = 1.5 Hz, 3H), 1.58 (dd, J = 11.7, 7.6 Hz, 1H), 1.51 (s, 3H), 1.44 (dd, J = 11.7, 2.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 87 °C): δ (ppm) 179.0, 149.2, 141.2, 128.7, 128.2 (2C), 126.0 (2C), 124.8, 93.2, 89.6, 56.2, 52.4, 46.5, 38.0, 17.6, 11.9. IR (KBr, cm^{-1}): ν_{max} = 3285 (NH), 1531 (NC=S). GC-MS (EI, 70 eV): *breaks down into an amine and an isothiocyanate*. MS (ESI): m/z = 301 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2OS$: C, 67.97; H, 6.71; N, 9.32; S, 10.67. Found: C, 68.03; H, 6.87; N, 9.16; S, 10.49.

(3a*RS*,6*RS*,7a*RS*)-*N*,6-Diphenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6d). Yield: 0.22 g (16%); colourless powder. M.p. 148–149 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.83 (br.s, 0.2H), 7.52 (d, J = 7.4 Hz, 2H), 7.45-7.41 (m, 4H), 7.37-7.30 (m, 3H), 7.13 (t, J = 7.4 Hz, 1H), 6.69 (d, J = 5.5 Hz, 1H), 6.65 (d, J = 5.5 Hz, 1H), 4.35 (br.s, 1H), 4.29 (d, J = 13.6 Hz,

1H), 4.21 (d, *J* = 13.6 Hz, 1H), 3.36 (t, *J* = 10.5 Hz, 1H), *the single proton signal is covered by the* DMSO *signal* 2.51 (br.s, 1H), 2.00 (dd, *J* = 11.7, 7.6 Hz, 1H), 1.43 (dd, *J* = 11.7, 2.1 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) 178.9, 141.0, 140.1, 139.8, 135.1, 128.8 (2C), 128.3 (2C), 128.1, 126.0 (4C), 124.9, 94.5, 92.1, 55.8, 52.4, 44.6, 39.2. IR (KBr, cm^{-1}): ν_{max} = 3339 (NH), 1530 (NC=S). GC-MS (EI, 70 eV): *breaks down into an amine and an isothiocyanate*. MS (ESI): *m/z* = 349 $[M+H]^+$. Anal. Calcd for $C_{21}H_{20}N_2OS$: C, 72.38; H, 5.79; N, 8.04; S, 9.20. Found: C, 72.23; H, 5.96; N, 7.89; S, 9.02.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Fluorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6e). Yield: 0.84 g (93%); colourless plates. M.p. 189–190 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C): δ (ppm)) *the NH signal is less intense due to proton exchange* 8.74 (br.s, 0.9H), 7.42 (dd, *J* = 8.9, 5.1 Hz, 2H), 7.10 (t, *J* = 8.9 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.08 (dd, *J* = 4.5, 1.5 Hz, 1H), 4.29 (br.t, *J* = 9.8 Hz, 1H), 4.22 (d, *J* = 13.5 Hz, 1H), 4.11 (d, *J* = 13.5 Hz, 1H), 3.23 (t, *J* = 10.4 Hz, 1H), 2.27-2.23 (m, 1H), 1.77 (ddd, *J* = 11.7, 4.5, 2.7 Hz, 1H), 1.48 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C): δ (ppm) 179.2, 159.8 (*J* = 241.6 Hz, 1H), 137.7, 137.5 (*J* = 2.5 Hz, 1C), 134.4, 128.2 (*J* = 7.6 Hz, 2C), 114.8 (*J* = 21.6 Hz, 2C), 94.3, 80.2, 55.8, 52.2, 41.6, 32.1; ^{19}F NMR (658.8 MHz, DMSO-d_6, 97 °C): δ (ppm) -118.2. IR (KBr, cm^{-1}): ν_{max} = 3226 (NH), 1532 (NC=S). GC-MS (EI, 70 eV): *breaks down into an amine and an isothiocyanate*. MS (ESI): *m/z* = 291 $[M+H]^+$. Anal. Calcd for $C_{15}H_{15}FN_2OS$: C, 62.05; H, 5.21; N, 9.65; S, 11.04. Found: C, 62.14; H, 5.19; N, 9.63; S, 10.92.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Fluorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6f). Yield: 0.84 g (69%); colourless powder. M.p. 196–198 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.74 (br.s, 0.9H), 7.42 (dd, *J* = 8.9, 5.1 Hz, 2H), 7.10 (t, *J* = 8.9 Hz, 2H), 6.50 (d, *J* = 5.5 Hz, 1H), 6.32 (d, *J* = 5.5 Hz, 1H), 4.27 (br.t, *J* = 9.8 Hz, 1H), 4.16 (d, *J* = 13.5 Hz, 1H), 4.07 (d, *J* = 13.5 Hz, 1H), 3.27 (t, *J* = 10.4 Hz, 1H), 2.38-2.32 (m, 1H), 1.62 (dd, *J* = 11.7, 7.4 Hz, 1H), 1.60 (s, 3H), 1.50 (dd, *J* = 11.7, 2.7 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C): δ (ppm) 179.2, 159.8 (*J* = 241.6 Hz, 1H), 140.9, 137.5 (*J* = 2.5 Hz, 1C), 135.0, 128.3 (*J* = 8.9 Hz, 2C), 114.8 (*J* = 21.6 Hz, 2C), 94.0, 88.4, 55.9, 52.5, 44.9, 38.7, 19.3; ^{19}F NMR (658.8 MHz, DMSO-d_6, 97 °C): δ (ppm) -118.4. IR (KBr, cm^{-1}): ν_{max} = 3206 (NH), 1530 (NC=S). GC-MS (EI, 70 eV): *breaks down into an amine and an isothiocyanate*. MS (ESI): *m/z* = 305 $[M+H]^+$. Anal. Calcd for $C_{16}H_{17}FN_2OS$: C, 63.13; H, 5.63; N, 9.20; S, 10.53. Found: C, 63.06; H, 5.47; N, 9.08; S, 10.60.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6g). Yield: 0.82 g (67%); colourless powder. M.p. 203–204 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.80 (br.s, 0.9H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (br.d, *J* = 5.7 Hz, 1H), 5.08 (br.d, *J* = 3.4 Hz, 1H), 4.29 (br.t, *J* = 9.5 Hz, 1H), 4.23 (d, *J* = 13.4 Hz, 1H), 4.11 (d, *J* = 13.4 Hz, 1H), 3.24 (t, *J* = 10.2 Hz, 1H), 2.27-2.23 (m, 1H), 1.77 (br.d, *J* = 11.4 Hz, 1H), 1.48 (dd, *J* = 11.4, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C): δ (ppm) 178.9, 140.2, 137.7, 134.4, 128.9, 128.2 (2C), 127.5 (2C), 94.3, 80.2, 55.9, 52.2, 41.5, 32.1. IR (KBr, cm^{-1}): ν_{max} = 3193 (NH), 1529 (NC=S). MS (ESI): *m/z* = 307 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2OS$: C, 58.72; H, 4.93; N, 9.13; S, 10.45. Found: C, 58.69; H, 8.05; N, 9.12; S, 10.43.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6h). Yield: 0.73 g (57%); colourless powder. M.p. 201–202 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 87 °C): δ (ppm) 8.82 (br.s, 1H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 2H), 6.50 (d, *J* = 5.5 Hz, 1H), 6.32 (d, *J* = 5.5 Hz, 1H), 4.27 (br.t, *J* = 9.0 Hz, 1H), 4.16 (d, *J* = 13.4 Hz, 1H), 4.07 (d, *J* = 13.4 Hz, 1H), 3.28 (t, *J* = 10.5 Hz, 1H), 2.36-2.32 (m, 1H), 1.62 (dd, *J* = 11.7, 7.6 Hz, 1H), 1.59 (s, 3H), 1.50 (dd, *J* = 11.7, 2.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 87 °C): δ (ppm) 178.2, 140.8, 140.0, 135.0, 128.9, 128.3 (2C), 127.8 (2C), *4 signals of the epoxyisoindole moiety are duplicated* 95.0 and 92.9 (1C), 88.4, 55.8 and 54.6 (1C), 54.0 and 50.6 (1C), 45.6 and 43.5 (1C), 38.7, 19.3. IR (KBr, cm^{-1}): ν_{max} = 3208 (NH), 1527 (NC=S). GC-MS (EI, 70 eV) *breaks down into an amine and an isothiocyanate*. MS (ESI): *m/z* = 321 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{16}H_{17}ClN_2OS$: C, 59.90; H, 5.34; N, 8.73; S, 9.99. Found: C, 59.82; H, 5.15; N, 8.98; S, 9.78.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Bromophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6i). Yield: 0.70 g (50%); colourless plates. M.p. 210–212 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.80 (br.s, 0.9H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.42 (d, *J* = 8.7 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.08 (dd, *J* = 4.5, 1.8 Hz, 1H), 4.29 (br.t, *J* = 10.0 Hz, 1H), 4.24 (d, *J* = 13.4 Hz, 1H), 4.11 (d, *J* = 13.4 Hz, 1H), 3.24 (t, *J* = 10.0 Hz, 1H), 2.27-2.23 (m, 1H), 1.77 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.48 (dd, *J* = 11.7, 7.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C): δ (ppm) 178.8, 140.6, 137.7, 134.4, 131.1 (2C), 127.8 (2C), 117.0, 94.3, 80.2, 56.0, 52.2, 41.5, 32.1. IR (KBr, cm^{-1}): ν_{max} = 3208 (NH), 1526 (NC=S). MS (ESI): *m/z* = 352 $[M+H]^+$ for ^{79}Br. Anal. Calcd for $C_{15}H_{15}BrN_2OS$: C, 51.29; H, 4.30; N, 7.98; S, 9.13. Found: C, 51.13; H, 4.76; N, 8.12; S, 9.18.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6j). Yield: 0.92 g (70%); colourless powder. M.p. 190–191 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.61 (br.s, 0.2H), 6.94 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.84-6.81 (m, 1H), 6.76 (d, *J* = 8.6 Hz, 1H), 6.49 (d, *J* = 5.7 Hz, 1H), 6.45 (dd, *J* = 5.7, 1.4 Hz, 1H), 5.07 (dd, *J* = 4.3, 1.4 Hz, 1H), 4.24-4.22 (m, 5H), 4.19 (d, *J* = 13.5 Hz, 1H), 4.07 (d, *J* = 13.5 Hz, 1H), 3.18 (t, *J* = 10.4 Hz, 1H), 2.24-2.21 (m, 1H), 1.76 (ddd, *J* = 11.7, 4.3, 2.9 Hz, 1H), 1.45 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *4 signals are duplicated* 179.0 and 178.9 (1C), 143.0, 141.2, 137.7, 134.5, 134.5 and 134.4 (1C), 119.6 and 119.5 (1C), 116.4, 115.5 and 115.4 (1C), 94.3, 80.1, 64.6 (2C), 55.6, 52.1, 41.5, 32.1. IR (KBr, cm^{-1}): ν_{max} = 3221 (NH), 1526 (NC=S). GC-MS (EI, 70 eV): *breaks down into an amine and an isothiocyanate*. MS (ESI): *m/z* = 331 $[M+H]^+$. Anal. Calcd for $C_{17}H_{18}N_2O_3S$: C, 61.80; H, 5.49; N, 8.48; S, 9.70. Found: C, 61.75; H, 5.60; N, 8.49; S, 9.86.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6k). Yield: 1.13 g (82%); colourless powder. M.p. 163–165 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.49 (br.s, 1H), 6.96 (d, *J* = 2.4 Hz, 1H), 6.85 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.76 (d, *J* = 8.6 Hz, 1H), 6.49 (d, *J* = 5.6 Hz, 1H), 6.31 (d, *J* = 5.6 Hz, 1H), 4.29-4.24 (m, 5H), 4.14 (d, *J* = 13.5 Hz, 1H), 4.05 (d, *J* = 13.5 Hz, 1H), 3.26 (dd, *J* = 10.7, 9.9 Hz, 1H), 2.37-2.27 (m, 1H), 1.62 (dd, *J* = 11.5, 7.3 Hz, 1H), 1.60 (s, 3H), 1.49 (dd, *J* = 11.5, 2.8 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 179.3, 143.1, 141.3, 140.9, 135.0, 134.6, 119.5, 116.3, 115.4, 94.1, 88.4, 65.7, 64.6, 55.9, 52.4, 44.9, 38.7, 19.2. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.60 (br.s, 0.2H), 6.94 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.83-6.81 (m, 1H), 6.76 (d, *J* = 8.5 Hz, 1H), 6.49 (d, *J* = 5.5 Hz, 1H), 6.31 (d, *J* = 5.5 Hz, 1H), 4.23 (br.s, 5H), 4.12 (d, *J* = 13.3 Hz, 1H), 4.03 (d, *J* = 13.3 Hz, 1H), 3.23 (t, *J* = 10.4 Hz, 1H), 2.34-2.30 (m, 1H), 1.61 (dd, *J* = 11.4, 7.4 Hz, 1H), 1.58 (s, 3H), 1.45 (dd, *J* = 11.4, 2.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *4 signals are duplicated* 179.0 and 178.9 (1C), 143.0, 141.2, 140.8, 135.0, 134.5 and 134.4 (1C), 119.6 and 119.5 (1C), 116.3, 115.5 and 115.4 (1C), 94.0, 88.4, 64.6 (2C), 56.0, 52.3, 44.8, 38.7, 19.3. IR (KBr, cm^{-1}): ν_{max} = 3280 (NH), 1534 (NC=S). GC-MS (EI, 70 eV): *breaks down into an amine and an isothiocyanate*. MS (ESI): *m/z* = 345 $[M+H]^+$. Anal. Calcd for $C_{18}H_{20}N_2O_3S$: C, 62.77; H, 5.85; N, 8.13; S, 9.31. Found: C, 62.76; H, 5.73; N, 8.00; S, 9.37.

(3a*RS*,6*RS*,7a*RS*)-*N*-Ethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6l). Yield: 0.74 g (83%); colourless powder. M.p. 179–181 °C; ^{1}H NMR (700.2 MHz, DMSO-

d_6, 77 °C): δ (ppm) 7.08 (br.s, 1H), 6.48 (d, *J* = 5.7 Hz, 1H), 6.43 (dd, *J* = 5.7, 1.5 Hz, 1H), 5.04 (dd, *J* = 4.5, 1.5 Hz, 1H), 4.10 (br.s, 1H), 4.04 (d, *J* = 13.1 Hz, 1H), 3.93 (d, *J* = 13.1 Hz, 1H), 3.55-3.51 (m, 2H), 3.02 (t, *J* = 10.2 Hz, 1H), 2.18-2.14 (m, 1H), 1.72 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.42 (dd, *J* = 11.7, 7.4 Hz, 1H), 1.13 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 77 °C): δ (ppm) 179.5, 137.6, 134.5, 94.3, 80.1, 54.9, 51.5, 41.5, 39.9, 31.9, 15.0. IR (KBr, cm^{-1}): ν_{max} = 3372 (NH), 1547 (NC=S). GC-MS (EI, 70 eV): *m/z* (%) = 224 (51) $[M]^+$, 183 (37), 143 (100), 108 (11), 96 (96), 88 (22), 81 (85), 69 (11), 60 (32), 56 (92), 41 (27). Anal. Calcd for $C_{11}H_{16}N_2OS$: C, 58.90; H, 7.19; N, 12.49; S, 14.29. Found: C, 58.68; H, 7.13; N, 12.56; S, 14.37.

(3a*RS*,6*RS*,7a*RS*)-*N*-Butyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6m). Yield: 0.64 g (63%); colourless powder. M.p. 149–150 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 6.88 (br.s, 1H), 6.47 (d, *J* = 5.7 Hz, 1H), 6.43 (dd, *J* = 5.7, 1.2 Hz, 1H), 5.04 (br.d, *J* = 2.9 Hz, 1H), 4.16-3.94 (m, 3H), 3.56-3.49 (m, 2H), 3.05 (t, *J* = 10.1 Hz, 1H), 2.21-2.12 (m, 1H), 1.76-1.29 (m, 6H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 179.9, 137.6, 134.5, 94.3, 80.1, 55.0, 51.6, 45.0, 41.5, 32.0, 31.5, 20.0, 14.0; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 7.03 (br.s, 0.3H), 6.48 (d, *J* = 5.7 Hz, 1H), 6.43 (dd, *J* = 5.7, 1.3 Hz, 1H), 5.04 (dd, *J* = 4.3, 1.3 Hz, 1H), 4.09-3.92 (m, 3H), 3.51-3.48 (m, 2H), 3.02 (t, *J* = 10.2 Hz, 1H), 2.17-2.14 (m, 1H), 1.72 (ddd, *J* = 11.7, 4.3, 2.9 Hz, 1H), 1.57-1.53 (m, 2H), 1.42 (dd, *J* = 11.7, 7.6 Hz, 1H), 1.35-1.29 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *2 signals are duplicated* 179.4 and 179.4 (1C), 137.6, 134.5, 94.2, 80.1, 55.0, 51.5, 45.0 and 44.8 (1C), 41.4, 31.9, 31.5, 19.9, 14.1. IR (KBr, cm^{-1}): ν_{max} = 3352 (NH), 1553 (NC=S). GC-MS (EI, 70 eV): *m/z* (%) = 252 (34) $[M]^+$, 211 (51), 171 (100), 115 (19), 108 (12), 96 (71), 81 (77), 72 (12), 56 (86), 41 (39). Anal. Calcd for $C_{13}H_{20}N_2OS$: C, 61.87; H, 7.99; N, 11.10; S, 12.71. Found: C, 61.99; H, 8.27; N, 11.39; S, 12.56.

(3a*RS*,6*RS*,7a*RS*)-*N*-Butyl-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6n). Yield: 0.33 g (31%); colourless powder. M.p. 66–68 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 7.01 (br.s, 0.2H), 6.46 (d, *J* = 4.8 Hz, 1H), 6.29 (d, *J* = 4.8 Hz, 1H), 4.08-3.89 (m, 3H), 3.51-3.48 (m, 2H), 3.07 (t, *J* = 9.8 Hz, 1H), 2.27-2.23 (m, 1H), 1.58-1.52 (m, 3H), 1.56 (s, 3H), 1.45 (br.d, *J* = 11.4 Hz, 1H), 1.33-1.31 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *2 signals are duplicated* 179.4 and 179.3 (1C), 140.7, 135.1, 94.0, 88.3, 55.2, 51.8, 44.9 and 44.8 (1C), 44.7, 38.6, 31.5, 19.9, 19.3, 14.1. IR (KBr, cm^{-1}): ν_{max} = 3289 (NH), 1535 (NC=S). GC-MS (EI, 70 eV): *m/z* (%) = 266 (76) $[M]^+$, 225 (33), 171 (60), 115 (11), 110 (73),

95 (100), 56 (96), 41 (43). Anal. Calcd for $C_{14}H_{22}N_2OS$: C, 63.12; H, 8.32; N, 10.52; S, 12.04. Found: C, 62.86; H, 8.10; N, 10.81; S, 12.38.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2-Methylallyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6o). Yield: 0.85 g (85%); colourless powder. M.p. 148–149 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 7.09 (br.s, 1H), 6.48 (d, J = 5.7 Hz, 1H), 6.44 (dd, J = 5.7, 1.5 Hz, 1H), 5.04 (dd, J = 4.4, 1.5 Hz, 1H), 4.81 (d, J = 10.7 Hz, 2H), 4.20-4.13 (m, 3H), 4.11 (d, J = 13.2 Hz, 1H), 3.99 (d, J = 13.2 Hz, 1H), 3.10 (t, J = 10.1 Hz, 1H), 2.23-2.14 (m, 1H), 1.77-1.71 (m, 1H), 1.74 (s, 3H), 1.45 (dd, J = 11.5, 7.5 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 180.3, 143.1, 137.6, 134.5, 110.4, 94.3, 80.1, 55.1, 51.7, 50.6, 41.5, 32.0, 20.6. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 7.24 (br.s, 0.6H), 6.47 (d, J = 5.7 Hz, 1H), 6.44 (br.d, J = 5.7 Hz, 1H), 5.04 (d, J = 4.3 Hz, 1H), 4.79(d, J = 15.7 Hz, 2H), 4.17-4.11 (m, 3H), 4.09 (d, J = 13.1 Hz, 1H), 3.97 (d, J = 13.1 Hz, 1H), 3.07 (t, J = 10.1 Hz, 1H), 2.19-2.16 (m, 1H), 1.74-1.71 (m, 1H), 1.71 (s, 3H), 1.44 (dd, J = 11.4, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *2 signals are duplicated* 179.9 and 179.8 (1C), 143.1, 137.6, 134.5, 110.3, 94.2, 80.1, 55.1, 51.7, 50.4 and 50.3 (1C), 41.4, 32.0, 20.6. IR (KBr, cm^{-1}): ν_{max} = 3357 (NH), 1551 (NC=S). GC-MS (EI, 70 eV): *m/z* (%) = 250 (47) [M]$^+$, 235 (12), 209 (44), 169 (100), 108 (11), 96 (64), 81 (96), 70 (19), 56 (65), 41 (30). Anal. Calcd for $C_{13}H_{18}N_2OS$: C, 62.37; H, 7.25; N, 11.19; S, 12.81. Found: C, 62.36; H, 7.11; N, 11.24; S, 12.93.

(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-(2-methylallyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6p). Yield: 0.84 g (80%); colourless powder. M.p. 107–109 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 7.22 (br.s, 0.4H), 6.47 (d, J = 5.5 Hz, 1H), 6.29 (d, J = 5.5 Hz, 1H), 4.79 (d, J = 16.2 Hz, 2H), 4.17-4.10 (m, 3H), 4.02 (d, J = 12.8 Hz, 1H), 3.93 (d, J = 12.8 Hz, 1H), 3.12 (br. s, 1H), 2.29-2.25 (m, 1H), 1.71 (s, 3H), 1.59-1.57 (m, 1H), 1.57 (s, 3H), 1.46 (br.d, J = 11.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *2 signals are duplicated* 179.9 and 179.8 (1C), 143.1, 140.8, 135.1, 110.3, 94.0, 88.3, 55.4, 51.9, 50.4 and 50.3 (1C), 44.8, 38.6, 20.6, 19.3. IR (KBr, cm^{-1}): ν_{max} = 3421 (NH), 1536 (NC=S). GC-MS (EI, 70 eV): *m/z* (%) = 264 (71) [M]$^+$, 223 (45), 169 (67), 110 (66), 95 (100), 70 (25), 56 (58), 41 (29). Anal. Calcd for $C_{14}H_{20}N_2OS$: C, 63.60; H, 7.62; N, 10.60; S, 12.13. Found: C, 63.57; H, 7.65; N, 10.71; S, 12.14.

Methyl 2-{[(3a*RS*,6*RS*,7a*RS*)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindol-2-ylcarbonothioyl]amino}benzoate (6q). Yield: 1.08 g (82%); colourless powder. M.p. 138–140 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 70 °C): δ (ppm) 10.04 (br.s, 1H), 8.38 (d, J = 8.4 Hz, 1H), 7.92 (dd, J = 7.9, 1.7 Hz, 1H), 7.57 (dt, J = 7.6, 1.7 Hz, 1H), 7.22 (dt, J = 8.1, 1.2 Hz, 1H), 6.55

(d, *J* = 5.7 Hz, 1H), 6.49 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.08 (dd, *J* = 4.5, 1.7 Hz, 1H), 4.33-4.26 (m, 2H), 4.15-4.11 (m, 1H), 3.87 (s, 3H), 3.26 (t, *J* = 10.2 Hz, 1H), 2.31 (br.s, 1H), 1.81 (ddd, *J* = 11.7, 4.5, 2.9 Hz, 1H), 1.49 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 70 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 177.7, 167.9, 142.1, 137.8, 134.4, 133.0, 130.6, 125.3, 124.0, 121.0, 80.2, 52.8, 40.8, 32.2. IR (KBr, cm^{-1}): ν_{max} = 3116 (NH), 1694 (CO_2), 1545 (NC=S). MS (ESI): *m/z* = 331 $[M+H]^+$. Anal. Calcd for $C_{17}H_{18}N_2O_3S$: C, 61.80; H, 5.49; N, 8.48; S, 9.71. Found: C, 62.03; H, 5.27; N, 8.31; S, 9.90.

***N*-[(3a*RS*,6*RS*,7a*RS*)-1,6,7,7a-Tetrahydro-3a,6-epoxyisoindol-2-ylcarbonothioyl]benzamide (6r).** Yield: 1.04 g (87%); colourless powder. M.p. 144–145 °C; ^{1}H NMR (600.2 MHz, $CDCl_3$): δ (ppm) *E/Z isomers* 8.48 (br.s, 1H), 8.45 (br.s, 0.7H), 7.84-7.82 (m, 3.4H), 7.59-7.56 (m, 1.7H), 7.49-7.46 (m, 3.4H), 6.44-6.40 (m, 2.4H), 6.32 (d, *J* = 6.1 Hz, 1H), 5.11-5.09 (m, 1.7H), 4.58 (d, *J* = 15.6 Hz, 0.7H), 4.43 (d, *J* = 14.1 Hz, 1H), 4.30 (dd, *J* = 13.1, 9.1 Hz, 1H), 4.23 (d, *J* = 15.1 Hz, 0.7H), 4.07-4.02 (m, 1.7H), 3.64 (dd, *J* = 13.1, 9.6 Hz, 1H), 3.54 (dd, *J* = 13.1, 11.1 Hz, 0.7H), 2.32-2.21 (m, 1.7H), 1.92 (ddd, *J* = 11.6, 4.5, 2.5 Hz, 1H), 1.78 (ddd, *J* = 11.6, 4.5, 3.0 Hz, 0.7H), 1.57 (dd, *J* = 12.1, 7.6 Hz, 1H), 1.43 (dd, *J* = 12.1, 7.6 Hz, 0.7H); ^{13}C NMR (150.9 MHz, $CDCl_3$): δ (ppm) *E/Z isomers* 177.1 (2C), 163.6, 163.5, 137.8 (2C), 134.0, 133.3, 133.2, 133.1, 132.6 (2C), 129.1 (2C), 129.0 (2C), 128.0 (4C), 94.8, 93.4, 80.7, 80.5, 60.1, 58.3, 55.7, 53.8, 42.9, 40.9, 32.4, 31.1. IR (KBr, cm^{-1}): ν_{max} = 3253 (NH), 1659 (NC=O), 1531 (NC=S). MS (ESI): *m/z* = 301 $[M+H]^+$. Anal. Calcd for $C_{16}H_{16}N_2O_2S$: C, 63.98; H, 5.37; N, 9.33; S, 10.68. Found: C, 64.09; H, 5.21; N, 9.31; S, 10.87.

(3a*SR*,6*RS*,7a*SR*)-7a-Chloro-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carbothioamide (6s). Yield: 0.56 g (46%); colourless powder. M.p. 159–161 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) 8.99 (br.s, 1H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 6.72 (dd, *J* = 5.7, 1.7 Hz, 1H), 6.62 (d, *J* = 5.7 Hz, 1H), 5.21 (dd, *J* = 4.5, 1.4 Hz, 1H), 4.58 (d, *J* = 13.1 Hz, 1H), 4.42 (d, *J* = 13.6 Hz, 1H), 4.17 (d, *J* = 13.6 Hz, 1H), 3.88 (d, *J* = 13.1 Hz, 1H), 2.73 (dd, *J* = 12.6, 4.8 Hz, 1H), 1.67 (d, *J* = 12.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) 179.7, 140.9, 138.8, 133.2, 128.4 (2C), 126.0 (2C), 125.1, 95.9, 81.2, 72.9, 65.2, 50.0, 41.7. IR (KBr, cm^{-1}): ν_{max} = 3358 (NH), 1537 (NC=S). MS (ESI): *m/z* = 307 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2OS$: C, 58.72; H, 4.93; N, 9.13; S, 10.45. Found: C, 58.68; H, 5.09; N, 8.89; S, 10.31.

(3a*SR*,6*RS*,7a*SR*)-7a-Bromo-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carbothioamide (6t). Yield: 0.88 g (63%); colourless powder. M.p. 179–181 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) 8.99 (br.s, 1H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 6.67 (dd, *J* = 5.7, 1.7 Hz, 1H), 6.63 (d, *J* = 5.7 Hz, 1H), 5.22

(dd, *J* = 4.5, 1.7 Hz, 1H), 4.70 (d, *J* = 13.4 Hz, 1H), 4.48 (d, *J* = 13.6 Hz, 1H), 4.18 (d, *J* = 13.6 Hz, 1H), 3.95 (d, *J* = 13.4 Hz, 1H), 2.70 (dd, *J* = 12.6, 4.5 Hz, 1H), 1.74 (d, *J* = 12.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) 179.7, 140.9, 138.2, 134.2, 128.4 (2C), 126.0 (2C), 125.1, 96.2, 81.1, 66.4, 64.9, 49.9, 41.5. IR (KBr, cm^{-1}): ν_{max} = 3330 (NH), 1534 (NC=S). MS (ESI): *m/z* = 352 $[M+H]^+$ for ^{79}Br. Anal. Calcd for $C_{15}H_{15}BrN_2OS$: C, 51.29; H, 4.30; N, 7.98; S, 9.13. Found: C, 51.11; H, 4.47; N, 7.76; S, 9.00.

6.8. General Procedure for the Synthesis of Products 7a-w and Characterization Data. A solution of the corresponding allylamine **1a-d,f-h** (0.4 mmol) and arylisoselenocyanate (0.4 mmol) in benzene or toluene (5.0 mL) was refluxed for 4−6 h (TLC monitoring). The resulting mixture was cooled, and formation of solid was observed. The crystals were filtered off, washed with diethyl ether (3 × 5 mL), dried under vacuum and then at the air.

(3a*RS*,6*RS*,7a*RS*)-*N*-Phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7a). Yield: 0.11 g (88%); colourless powder. M.p. 128–130 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.98 (br.s, 1H), 7.44-7.15 (m, 5H), 6.52 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.5 Hz, 1H), 5.09 (dd, *J* = 4.4, 1.5 Hz, 1H), 4.35 (dd, *J* = 10.4, 9.8 Hz, 1H), 4.26 (d, *J* = 13.7 Hz, 1H), 4.19 (d, *J* = 13.7 Hz, 1H), 3.26 (dd, *J* = 11.0, 10.0 Hz, 1H), 2.32-2.23 (m, 1H), 1.78 (ddd, *J* = 11.7, 4.4, 2.8 Hz, 1H), 1.50 (dd, *J* = 11.7, 7.5 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.3, 141.9, 137.7, 134.4, 128.3 (2C), 127.0 (2C), 125.5, 94.2, 80.2, 57.4, 54.0, 41.6, 32.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 299.0. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 9.09 (br.s, 0.2H), 7.40 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 6.52 (d, *J* = 5.7 Hz, 1H), 6.47 (br.d, *J* = 5.7 Hz, 1H), 5.09 (dd, *J* = 4.1, 1.0 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.45 – 4.00 (m, 3H), 3.23 (t, *J* = 10.1 Hz, 1H), 2.27 (s, 1H), 1.77 (br.d, *J* = 11.7 Hz, 1H), 1.48 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 177.8, 141.7, 137.7, 134.4, 128.7 (2C), 128.3 (2C), 127.0, 125.6, 80.2, 32.2, 15.5. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 282.4, 279.6. IR (KBr, cm^{-1}): ν_{max} = 3193 (NH), 1527 (NC=Se). MS (ESI): *m/z* = 320 $[M+H]^+$. Anal. Calcd for $C_{15}H_{16}N_2OSe$: C, 67.55; H, 4.54; N, 6.30. Found: C, 56.43; H, 5.05; N, 8.77.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Ethylphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7b). Yield: 0.10 g (73%); colourless powder. M.p. 146–148 °C; ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *there are no NH signal* 7.24 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.51 (br.s, 1H), 6.47 (dd, *J* = 5.5, 1.5 Hz, 1H), 5.08 (dd, *J* = 4.0, 1.0 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.50 – 3.93 (br.m, 3H), ~ 3.21 – 3.12 (br.m, 1H), 2.59 (q,

J = 7.6 Hz, 2H), *broadening of proton signals H-7,7a* ~ 2.33 – 2.15 (br.m, 1H), 1.74 (br.s, 1H), 1.45 (br.s, 1H), 1.18 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 177.1, 141.3, 139.3, 137.8, 134.5 (2C), 127.8 (2C), 127.4 (2C), 40.5, 28.3, 16.2. IR (KBr, cm^{-1}): ν_{max} = 3159 (NH), 1531 (NC=Se). MS (ESI): *m/z* = 348 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2OSe$: C, 58.79; H, 5.80; N, 8.07. Found: C, 59.00; H, 5.86; N, 7.91.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,6-Dimethylphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7c). Yield: 0.12 g (86%); colourless powder. M.p. 214–216 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.74 (br.s, 1H), 7.10-7.05 (m, 3H), 6.53 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.7 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.7 Hz, 1H), 4.34 (t, *J* = 10.0 Hz, 1H), 4.23 (d, *J* = 13.5 Hz, 1H), 4.16 (d, *J* = 13.5 Hz, 1H), 3.23 (dd, *J* = 11.0, 10.0 Hz, 1H), 2.36-2.26 (m, 1H), 2.22 (s, 3H), 2.21 (s, 3H), 1.79 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.50 (dd, *J* = 11.7, 7.5 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.0, 139.4, 137.7, 137.0, 136.9, 134.5, 128.0 (2C), 127.1, 94.4, 80.2, 57.1, 53.7, 41.7, 32.2, 18.7 (2C). ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 263.8. ^{1}H NMR (600.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.82 (br.s, 0.2H), 7.10-7.07 (m, 3H), 6.53 (br.d, *J* = 5.5 Hz, 1H), 6.47 (br.d, *J* = 5.5 Hz, 1H), 5.09 (br.d, *J* = 3.3 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.55 – 3.95 (m, 3H), 3.20 (br.s, 1H), 2.30 (br.s, 1H), 2.19 (s, 3H), 2.18 (s, 3H), 1.78 (br.d, *J* = 11.4 Hz, 1H), 1.49 (dd, *J* = 11.4, 7.9 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 177.5, 139.3, 139.2, 137.7, 137.0, 136.9, 134.5, 128.0 (2C), 127.1, 80.2, 32.2, 18.7 (2C). ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 249.4, 246.1. IR (KBr, cm^{-1}): ν_{max} = 3160 (NH), 1521 (NC=Se). MS (ESI): *m/z* = 348 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2OSe$: C, 58.79; H, 5.80; N, 8.07. Found: C, 59.13; H, 5.67; N, 8.22.

(3a*RS*,6*RS*,7a*RS*)-*N*-(3,5-Dimethylphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7d). Yield: 0.09 g (68%); colourless powder. M.p. 101–103 °C; ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *there are no NH signal* 6.95 (s, 2H), 6.81 (s, 1H), 6.51 (br.s, 1H), 6.45 (dd, *J* = 5.5, 1.5 Hz, 1H), 5.08 (br.d, *J* = 3.0 Hz, 1H), *broadening of proton signals H-1,3,7,7a* ~ 4.49 – 3.92 (br.m, 3H), ~ 3.21 – 3.11 (br.m, 1H), ~ 2.32 – 2.14 (br.m, 1H), 2.25 (s, 6H), 1.73 (br.s, 1H), 1.43 (br.s, 1H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *no 2 C signals were reasonably attributed to an epoxyisoindole moiety* 176.5, 140.9, 137.4, 137.3, 136.9 (2C), 134.0 (2C), 129.8 (2C), 124.6 (2C), 40.1, 21.1, 20.9. IR (KBr, cm^{-1}): ν_{max} = 3176 (NH), 1533 (NC=Se). MS (ESI): *m/z* = 348 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2OSe$: C, 58.79; H, 5.80; N, 8.07. Found: C, 58.63; H, 5.64; N, 8.04.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7e). Yield: 0.09 g (67%); colourless powder. M.p. 168–170 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.87 (br.s, 1H), 7.29 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.51 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.7 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.6 Hz, 1H), 4.34 (br.t, *J* = 10.0 Hz, 1H), 4.24 (d, *J* = 13.6 Hz, 1H), 4.17 (d, *J* = 13.6 Hz, 1H), 3.79 (s, 3H), 3.23 (dd, *J* = 11.2, 9.8 Hz, 1H), 2.31-2.22 (m, 1H), 1.78 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.49 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.6, 157.7, 137.7, 135.0, 134.4, 128.7 (2C), 113.9 (2C), 94.2, 80.2, 57.3, 55.9, 54.0, 41.6, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 290.9. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.97 (br.s, 0.3H), 7.25 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.6 Hz, 2H), 6.50 (d, *J* = 5.7 Hz, 1H), 6.47 (br.d, *J* = 5.7 Hz, 1H), 5.08 (br.d, *J* = 3.6 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.40 – 4.05 (m, 3H), 3.77 (s, 3H), 3.20 (br.t, *J* = 10.1 Hz, 1H), 2.26 (br.s, 1H), 1.78-1.75 (m, 1H), 1.48 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 178.1, 157.6, 137.7, 134.7, 134.4, 128.8 (2C), 113.8 (2C), 80.2, 55.8, 40.8, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 277.0, 274.2. IR (KBr, cm^{-1}): ν_{max} = 3171 (NH), 1535 (NC=Se). MS (ESI): *m/z* = 350 $[M+H]^+$. Anal. Calcd for $C_{16}H_{18}N_2O_2Se$: C, 55.02; H, 5.19; N, 8.02. Found: C, 54.91; H, 5.01; N, 7.85.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7f). Yield: 0.05 g (36%); colourless powder. M.p. 179–180 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.96 (br.s, 0.2H), 7.25 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.6 Hz, 2H), 6.50 (d, *J* = 5.7 Hz, 1H), 6.32 (d, *J* = 5.7 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.45 – 3.95 (m, 3H), 3.77 (s, 3H), 3.24 (br.t, *J* = 9.5 Hz, 1H), 2.35 (br.s, 1H), 1.62 (dd, *J* = 11.4, 7.4 Hz, 1H), 1.50 (dd, *J* = 11.4, 1.9 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 178.1, 157.6, 140.8, 134.9, 134.7, 128.8 (2C), 113.8 (2C), 88.4, 55.8, 40.8, 38.8, 19.2. IR (KBr, cm^{-1}): ν_{max} = 3181 (NH), 1535 (NC=Se). MS (ESI): *m/z* = 364 $[M+H]^+$. Anal. Calcd for $C_{17}H_{20}N_2O_2Se$: C, 56.20; H, 5.55; N, 7.71. Found: C, 56.42; H, 5.34; N, 7.89.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2-Methoxyphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7g). Yield: 0.10 g (74%); colourless plates. M.p. 179–181 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.49 (br.s, 1H), 7.22 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.22 (ddd, *J* = 9.1, 7. 4, 1.7 Hz, 1H), 7.05 (dd, *J* = 8.3, 1.3 Hz, 1H), 6.92 (dt, *J* = 7.6, 1.4 Hz, 1H), 6.52 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.7 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.7 Hz, 1H), 4.33 (br.t, *J* =

10.0 Hz, 1H), 4.23 (d, *J* = 13.6 Hz, 1H), 4.16 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.23 (dd, *J* = 11.0, 9.8 Hz, 1H), 2.34-2.24 (m, 1H), 1.79 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.50 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.6, 154.5, 137.7, 134.4, 130.8, 129.5, 127.4, 120.3, 112.8, 94.2, 80.2, 57.1, 56.5, 53.9, 41.6, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 293.8; ^{1}H NMR (700.2 MHz, DMSO-d_6, 77 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 8.61 (br.s, 0.9H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (br.d, *J* = 5.7 Hz, 1H), 5.08 (br.d, *J* = 4.1 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.50 – 3.95 (m, 3H), 3.80 (s, 3H), 3.19 (br.s, 1H), 2.28 (br.s, 1H), 1.76 (dt, *J* = 11.4, 2.8 Hz, 1H), 1.47 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 77 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 178.4, 154.7, 137.7, 134.4, 130.6, 130.0, 128.7, 127.6, 120.2, 112.6, 80.2, 56.3, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 277.0, 273.9. IR (KBr, cm^{-1}): ν_{max} = 3225 (NH), 1530 (NC=Se). MS (ESI): *m/z* = 350 $[M+H]^+$. Anal. Calcd for $C_{16}H_{18}N_2O_2Se$: C, 55.02; H, 5.19; N, 8.02. Found: C, 55.13; H, 5.03; N, 8.13.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Fluorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7h). Yield: 0.06 g (45%); colourless powder. M.p. 197–199 °C; ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 9.09 (br.s, 0.2H), 7.38 (dd, *J* = 8.8, 5.3 Hz, 2H), 7.12 (t, *J* = 8.8 Hz, 2H), 6.52 (d, *J* = 5.7 Hz, 1H), 6.47 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.08 (dd, *J* = 4.5, 1.7 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.55 – 3.85 (m, 3H), 3.21 (br.t, *J* = 10.0 Hz, 1H), 2.27 (br.s, 1H), 1.78 (ddd, *J* = 11.7, 4.3, 2.9 Hz, 1H), 1.48 (dd, *J* = 11.7, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 178.1, 160.2 (d, *J* = 241.7 Hz), 138.1, 137.8, 134.4, 129.3 (d, *J* = 9.5 Hz, 2C), 114.9 (d, *J* = 23.0 Hz, 2C), 80.2, 40.8, 32.2. ^{19}F NMR (658.8 MHz, DMSO-d_6, 25 °C): δ (ppm) -117.3. IR (KBr, cm^{-1}): ν_{max} = 3169 (NH), 1536 (NC=Se). MS (ESI): *m/z* = 338 $[M+H]^+$. Anal. Calcd for $C_{15}H_{15}FN_2OSe$: C, 53.42; H, 4.48; N, 8.31. Found: C, 53.57; H, 4.64; N, 8.15.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7i). Yield: 0.10 g (73%); colourless powder. M.p. 208–209 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.03 (br.s, 1H), 7.45 (d, *J* = 8.8 Hz, 2H), 7.35 (d, *J* = 8.8 Hz, 2H), 6.52 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.7 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.7 Hz, 1H), 4.35 (br.t, *J* = 10.0 Hz, 1H), 4.25 (d, *J* = 13.7 Hz, 1H), 4.18 (d, *J* = 13.7 Hz, 1H), 3.26 (dd, *J* = 11.3, 9.8 Hz, 1H), 2.33-2.23 (m, 1H), 1.79 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.49 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.3, 140.9, 137.8, 134.3,

129.8, 128.5 (2C), 128.2 (2C), 94.2, 80.2, 57.5, 54.2, 41.6, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 302.5. ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.32 (br.s, 0.2H), 7.40-7.36 (m, 4H), 6.51 (br.m, 1H), 6.46 (dd, *J* = 5.5, 1.5 Hz, 1H), 5.08 (dd, *J* = 4.0, 1.5 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.51 – 3.96 (m, 3H), 3.24-3.13 (br.m, 1H), 2.33-2.15 (br.m, 1H), 1.78-1.72 (br.m, 1H), 1.47-1.40 (br.m, 1H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *6 signals of the epoxyisoindole moiety are duplicated* 177.2, 140.6, 137.9, 134.4 (2C), 129.8, 128.9, 128.4 (2C), 95.5 and 93.0 (1C), 80.3 and 80.1 (1C), 60.8 and 56.7 (1C), 54.9 and 50.9 (1C), 42.4 and 40.6 (1C), 32.4 and 32.0 (1C). ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 285.8, 283.2. IR (KBr, cm^{-1}): ν_{max} = 3143 (NH), 1535 (NC=Se). MS (ESI): *m/z* = 355 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2OSe$: C, 50.94; H, 4.27; N, 7.92. Found: C, 50.77; H, 4.14; N, 7.62.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7j). Yield: 0.10 g (69%); colourless powder. M.p. 201–203 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.02 (br.s, 1H), 7.45 (dd, *J* = 8.7, 1.0 Hz, 2H), 7.35 (dd, *J* = 8.7, 1.0 Hz, 2H), 6.50 (d, *J* = 5.6 Hz, 1H), 6.32 (dd, *J* = 5.6, 1.0 Hz, 1H), 4.34 (br.t, *J* = 9.8 Hz, 1H), 4.21-4.12 (m, 2H), 3.30 (br.t, *J* = 10.4 Hz, 1H), 2.33-2.11 (m, 1H), 1.64 (dd, *J* = 11.7, 7.4 Hz, 1H), 1.61 (s, 3H), 1.52 (dd, *J* = 11.7, 2.5 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.2, 140.9 (2C), 134.9, 129.8, 128.6 (2C), 128.2 (2C), 93.9, 88.5, 57.7, 54.4, 44.8, 38.8, 19.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 302.2. ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.27 (br.s, 0.2H), 7.39-7.36 (m, 4H), 6.51 (br.s, 1H), 6.33 (d, *J* = 6.1 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.47 – 3.93 (m, 3H), 3.30-3.18 (br.m, 1H), 2.43-2.25 (br.m, 1H), 1.62-1.46 (br.m, 2H), 1.57 (s, 3H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *6 signals of the epoxyisoindole moiety are duplicated* 177.1, 140.9, 140.7, 135.0 (2C), 129.8, 128.9, 128.4 (2C), 95.0 and 92.7 (1C), 88.6 and 88.5 (1C), 61.0 and 57.0 (1C), 55.1 and 51.1 (1C), 45.7 and 43.5 (1C), 39.0 and 38.5 (1C), 19.4. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 285.7, 283.1. IR (KBr, cm^{-1}): ν_{max} = 3157 (NH), 1535 (NC=Se). MS (ESI): *m/z* = 369 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{16}H_{17}ClN_2OSe$: C, 52.26; H, 4.66; N, 7.62. Found: C, 51.94; H, 4.78; N, 7.99.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-ethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7k). Yield: 0.07 g (45%); colourless powder. M.p. 201–203 °C; ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.30 (br.s, 0.2H), 7.39-7.36 (m, 4H), 6.52-6.50 (br.m, 1H), 6.40 (d, *J* = 5.6 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.47 – 3.94 (m, 3H), 3.27-3.15 (br.m, 1H), 2.43-2.24 (br.m, 1H), 1.96-1.84 (m, 2H), 1.57-1.47 (m, 2H), 0.98 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ

(ppm) *6 signals of the epoxyisoindole moiety are duplicated* 177.1, 140.7, 139.5, 135.1 (2C), 129.8, 129.1 and 128.9 (1C), 128.4 (2C), 94.9 and 92.7 (1C), 92.5, 61.0 and 57.0 (1C), 55.1 and 51.1 (1C), 45.2 and 42.9 (1C), 36.8 and 36.3 (1C), 25.9, 9.8. IR (KBr, cm^{-1}): ν_{max} = 3154 (NH), 1532 (NC=Se). MS (ESI): *m/z* = 383 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{17}H_{19}ClN_2OSe$: C, 53.48; H, 5.02; N, 7.34. Found: C, 53.65; H, 4.98; N, 7.12.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-propyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7l). Yield: 0.09 g (57%); colourless powder. M.p. 200–202 °C; ^1H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.29 (br.s, 0.2H), 7.39-7.36 (m, 4H), 6.51-6.49 (br.m, 1H), 6.40 (d, *J* = 5.6 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.47 – 3.93 (m, 3H), 3.27-3.15 (br.m, 1H), 2.42-2.23 (br.m, 1H), 1.91-1.80 (m, 2H), 1.57-1.40 (m, 4H), 0.94 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *6 signals of the epoxyisoindole moiety are duplicated* 177.1, 140.6, 139.8, 134.9 (2C), 129.8, 129.1 and 128.9 (1C) , 128.4 (2C), 92.5, 92.1 and 91.9 (1C), 61.0 and 57.0 (1C), 55.1 and 51.1 (1C), 45.0 and 42.8 (1C), 37.3 and 36.8 (1C), 35.4, 18.6, 15.1. IR (KBr, cm^{-1}): ν_{max} = 3148 (NH), 1533 (NC=Se). MS (ESI): *m/z* = 397 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{18}H_{21}ClN_2OSe$: C, 54.62; H, 5.35; N, 7.08. Found: C, 54.60; H, 4.99; N, 7.17.

(3a*RS*,6*SR*,7a*RS*)-6-Chloro-*N*-(4-chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7m). Yield: 0.06 g (39%); colourless powder. M.p. 203–205 °C; ^1H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.12 (br.s, 1H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.35 (d, *J* = 8.8 Hz, 2H), 6.75 (d, *J* = 5.6 Hz, 1H), 6.52 (d, *J* = 5.6 Hz, 1H), 4.41 (br.t, *J* = 10.0 Hz, 1H), 4.30-4.20 (m, 2H), 3.42 (dd, *J* = 11.5, 10.0 Hz, 1H), 2.61-2.50 (m, 1H), 2.19 (dd, *J* = 11.7, 7.3 Hz, 1H), 2.04 (dd, *J* = 11.7, 2.8 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.6, 140.8, 139.7, 136.2, 129.9, 128.6 (2C), 128.2 (2C), 100.7, 92.9, 57.2, 54.1, 45.3, 42.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 308.4. ^1H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.39 (br.s, 0.2H), 7.38 (br.s, 4H), 6.76 (br.s, 1H), 6.55 (d, *J* = 5.6 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.54 – 4.00 (m, 3H), 3.34-3.33 (br.m, 1H), 2.62-2.44 (br.m, 1H), 2.17-1.98 (br.m, 2H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *6 signals of the epoxyisoindole moiety are duplicated* 177.4, 140.6, 139.6, 136.3 (2C), 130.0, 129.0 and 128.9 (1C), 128.4 (2C), 100.8 and 100.7 (1C), 94.2 and 91.8 (1C), 60.6 and 56.6 (1C), 54.7 and 50.8 (1C), 46.0 and 43.8 (1C), 42.3 and 41.9 (1C). ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 291.6, 288.6. IR (KBr, cm^{-1}): ν_{max} = 3142 (NH), 1533 (NC=Se). MS (ESI): *m/z* = 388 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{14}Cl_2N_2OSe$: C, 46.42; H, 3.64; N, 7.22. Found: C, 46.12; H, 3.79; N, 6.86.

Ethyl (3a*RS*,6*RS*,7a*RS*)-2-((4-chlorophenyl)carbamoselenoyl)-2,3,7,7a-tetrahydro-3a,6-epoxyisoindole-6(1*H*)-carboxylate (7n). Yield: 0.11 g (66%); colourless powder. M.p. 155 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.11 (br.s, 1H), 7.46 (d, *J* = 8.7 Hz, 2H), 7.35 (d, *J* = 8.7 Hz, 2H), 6.67 (d, *J* = 5.6 Hz, 1H), 6.57 (d, *J* = 5.6 Hz, 1H), 4.41-4.26 (m, 5H), 3.34 (dd, *J* = 11.3, 9.7 Hz, 1H), 2.51-2.41 (m, 1H), 1.95 (dd, *J* = 11.7, 2.8 Hz, 1H), 1.85 (dd, *J* = 11.7, 7.3 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.5, 169.1, 140.9, 136.9, 135.4, 129.1, 128.6 (2C), 128.2 (2C), 95.1, 89.0, 61.5, 57.2, 53.7, 43.0, 36.6, 14.4. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 305.6. ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.37 (br.s, 0.2H), 7.40-7.36 (m, 4H), 6.69-6.57 (br.m, 1H), 6.57 (d, *J* = 5.6 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.49 – 4.04 (m, 3H), 4.24 (q, *J* = 7.1 Hz, 2H), 3.32-3.21 (br.m, 1H), 2.52-2.33 (br.m, 1H), 1.96-1.76 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *7 signals of the epoxyisoindole moiety are duplicated* 177.4, 169.4, 140.6, 136.8, 135.6 (2C), 129.9, 129.1 and 128.9 (1C) , 128.4 (2C), 100.0 and 96.2 (1C), 93.9 and 88.7 (1C), 61.7, 60.5 and 56.4 (1C), 54.6 and 50.7 (1C), 43.8 and 41.5 (1C), 36.9 and 36.5 (1C), 14.6. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 288.9, 286.2. IR (KBr, cm^{-1}): ν_{max} = 3362 (NH), 1728 (CO_2), 1526 (NC=Se). MS (ESI): *m/z* = 397 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{18}H_{19}ClN_2O_3Se$: C, 50.78; H, 4.50; N, 6.58. Found: C, 50.96; H, 4.81; N, 6.78.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-5,6-dimethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7o). Yield: 0.10 g (68%); colourless powder. M.p. 211–213 °C (decomp.); ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.00 (br.s, 1H), 7.45 (dd, *J* = 8.7, 1.4 Hz, 2H), 7.34 (dd, *J* = 8.7, 1.4 Hz, 2H), 6.05 (d, *J* = 1.7 Hz, 1H), 4.31 (br.t, *J* = 10.2 Hz, 1H), 4.10 (br.s, 2H), 3.28 (dd, *J* = 11.0, 10.0 Hz, 1H), 2.44-2.34 (m, 1H), 1.78 (d, *J* = 1.7 Hz, 3H), 1.60 (dd, *J* = 11.6, 7.4 Hz, 1H), 1.52 (s, 3H), 1.46 (dd, *J* = 11.7, 2.8 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.2, 149.3, 140.9, 129.7, 128.5 (2C), 128.2 (2C), 121.6, 93.1, 89.7, 57.9, 54.4, 46.5, 38.1, 17.6, 11.9. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 301.1. ^{1}H NMR (600.2 MHz, DMSO-d_6): δ (ppm) *the NH signal is less intense due to proton exchange* 9.28 (br.s, 0.2H), 7.40-7.36 (m, 4H), 6.05 (s, 1H), *broadening of proton signals H-1,3* ~ 4.45 – 3.87 (m, 3H), 3.27-3.16 (br.m, 1H), 2.45-2.27 (br.m, 1H), 1.74 (s, 3H), 1.74 (s, 3H), 1.59-1.40 (m, 2H); ^{13}C NMR (150.9 MHz, DMSO-d_6): δ (ppm) *6 signals of the epoxyisoindole moiety are duplicated* 177.1, 149.3, 140.7, 129.8, 129.0 and 128.9 (1C), 128.4 (4C), 128.0, 94.2 and 91.9 (1C), 89.7 and 89.6 (1C), 61.1 and 56.9 (1C), 55.2 and 51.1 (1C), 47.3 and 45.1 (1C), 38.3 and 37.8 (1C), 17.7, 12.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 285.0, 281.3. IR (KBr, cm^{-1}): ν_{max} = 3147 (NH), 1536 (NC=Se).

MS (ESI): *m/z* = 383 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{17}H_{19}ClN_2OSe$: C, 53.48; H, 5.02; N, 7.34. Found: C, 53.50; H, 4.79; N, 7.45.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7p). Yield: 0.12 g (87%); colourless prisms. M.p. 179–181 °C; ^1H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.95 (br.s, 1H), 7.50-7.26 (m, 4H), 6.53 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.7 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.6 Hz, 1H), 4.35 (br.t, *J* = 9.7 Hz, 1H), 4.25 (d, *J* = 13.6 Hz, 1H), 4.17 (d, *J* = 13.6 Hz, 1H), 3.25 (dd, *J* = 11.1, 9.9 Hz, 1H), 2.36-2.26 (m, 1H), 1.80 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.50 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.6, 139.2, 137.7, 134.4, 132.4, 129.7, 128.7, 128.3, 127.3, 94.3, 80.2, 57.4, 54.1, 41.7, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 306.5; ^1H NMR (700.2 MHz, DMSO-d_6, 77 °C): δ (ppm) 9.09 (br.s, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 6.53 (d, *J* = 5.7 Hz, 1H), 6.47 (dd, *J* = 5.7, 1.4 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.4 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.60 – 3.90 (m, 3H), 3.21 (br.s, 1H), 2.31 (br.s, 1H), 1.79 (br.d, *J* = 11.4 Hz, 1H), 1.49 (dd, *J* = 11.4, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 77 °C): δ (ppm) *no 3 C signals were reasonably attributed to an epoxyisoindole moiety* 178.5, 139.2, 137.7, 134.4, 132.5, 132.3, 129.7, 128.7, 128.5, 127.4, 80.2, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 292.8, 290.2. IR (KBr, cm^{-1}): ν_{max} = 3168 (NH), 1530 (NC=Se). MS (ESI): *m/z* = 355 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2OSe$: C, 50.94; H, 4.27; N, 7.92. Found: C, 51.12; H, 4.06; N, 8.11.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Bromophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7q). Yield: 0.07 g (44%); colourless powder. M.p. 217–218 °C; ^1H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.99 (br.s, 1H), 7.50-7.38 (m, 4H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.08 (dd, *J* = 4.4, 1.7 Hz, 1H), 4.38-4.16 (m, 3H), 3.25 (br.dd, *J* = 11.4, 9.7 Hz, 1H), 2.33-2.23 (m, 1H), 1.79 (ddd, *J* = 11.7, 4.4, 2.8 Hz, 1H), 1.50 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.2, 141.3, 137.8, 134.3, 131.1 (2C), 128.9 (2C), 122.0, 94.1, 80.2, 57.3, 54.0, 41.5, 32.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 303.0; ^1H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) 9.12 (br.s, 1H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 6.52 (br.d, *J* = 5.2 Hz, 1H), 6.48 (br.d, *J* = 5.2 Hz, 1H), 5.06 (br.d, *J* = 2.9 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.50 – 4.00 (m, 3H), 3.23 (br.s, 1H), 2.28 (br.s, 1H), 1.78 (br.d, *J* = 10.5 Hz, 1H), 1.49 (br.dd, *J* = 11.0, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 177.8, 141.3, 137.8, 134.3, 131.2 (2C), 129.0 (2C), 117.9, 80.2, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 286.0, 283.5. IR

(KBr, cm^{-1}): ν_{max} = 3142 (NH), 1530 (NC=Se). MS (ESI): *m/z* = 399 $[M+H]^+$ for ^{79}Br. Anal. Calcd for $C_{15}H_{15}BrN_2OSe$: C, 45.25; H, 3.80; N, 7.04. Found: C, 45.21; H, 4.00; N, 6.97.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Bromophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7r). Yield: 0.06 g (34%); colourless powder. M.p. 211–213 °C; ^1H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) 9.12 (br.s, 1H), 7.49 (d, *J* = 7.2 Hz, 2H), 7.38 (d, *J* = 7.2 Hz, 2H), 6.51 (br.d, *J* = 4.1 Hz, 1H), 6.33 (br.d, *J* = 4.1 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.65 – 3.85 (m, 3H), 3.28 (br.s, 1H), 2.37 (br.s, 1H), 1.64-1.50 (m, 2H), 1.59 (s, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 177.8, 141.3, 140.9, 134.9, 131.2 (2C), 129.0 (2C), 117.9, 88.5, 38.8, 19.2. IR (KBr, cm^{-1}): ν_{max} = 3157 (NH), 1536 (NC=Se). MS (ESI): *m/z* = 413 $[M+H]^+$ for ^{79}Br. Anal. Calcd for $C_{16}H_{17}BrN_2OSe$: C, 46.62; H, 4.16; N, 6.80. Found: C, 46.28; H, 3.99; N, 6.91.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Iodophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7s). Yield: 0.11 g (59%); colourless powder. M.p. 200 °C (decomp.); ^1H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.01 (br.s, 1H), 7.65 (d, *J* = 8.7 Hz, 2H), 7.27 (d, *J* = 8.7 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.08 (dd, *J* = 4.5, 1.7 Hz, 1H), 4.34 (br.d, *J* = 9.9 Hz, 1H), 4.25 (d, *J* = 13.7 Hz, 1H), 4.17 (d, *J* = 13.7 Hz, 1H), 3.25 (dd, *J* = 11.4, 9.7 Hz, 1H), 2.32-2.23 (m, 1H), 1.79 (ddd, *J* = 11.7, 4.4, 2.7 Hz, 1H), 1.49 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.1, 141.9, 137.8, 137.1 (2C), 129.0 (2C), 133.1, 94.1, 89.6, 80.2, 57.5, 54.2, 41.5, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 304.4; ^1H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 9.10 (br.s, 0.2H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.3 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.46 (dd, *J* = 5.7, 1.4 Hz, 1H), 5.08 (dd, *J* = 4.5, 1.2 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.55 – 4.00 (m, 3H), 3.22 (br.t, *J* = 9.8 Hz, 1H), 2.27 (br.s, 1H), 1.77 (br.d, *J* = 11.4 Hz, 1H), 1.47 (dd, *J* = 11.4, 7.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 177.6, 141.7, 137.8, 137.1 (2C), 133.1, 129.1 (2C), 89.8, 80.2, 32.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 286.8, 284.2. IR (KBr, cm^{-1}): ν_{max} = 3156 (NH), 1529 (NC=Se). MS (ESI): *m/z* = 447 $[M+H]^+$. Anal. Calcd for $C_{15}H_{15}IN_2OSe$: C, 40.47; H, 3.40; N, 6.29. Found: C, 40.69; H, 3.07; N, 6.03.

(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Iodophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7t). Yield: 0.06 g (31%); colourless powder. M.p. 209–211 °C; ^1H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 9.09 (br.s, 0.2H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.3 Hz, 2H), 6.50 (d, *J* = 5.5 Hz,

1H), 6.33 (d, *J* = 5.5 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.60 – 3.90 (m, 3H), 3.27 (br.t, *J* = 9.1 Hz, 1H), 2.36 (br.s, 1H), 1.62 (dd, *J* = 11.4, 7.6 Hz, 1H), 1.59 (s, 3H), 1.51 (br.d, *J* = 11.4 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 177.8, 141.7, 140.9, 137.1 (2C), 134.9, 129.1 (2C), 89.9, 88.5, 38.8, 19.2. IR (KBr, cm^{-1}): ν_{max} = 3156 (NH), 1532 (NC=Se). MS (ESI): *m/z* = 461 $[M+H]^+$. Anal. Calcd for $C_{16}H_{17}IN_2OSe$: C, 41.85; H, 3.73; N, 6.10. Found: C, 41.75; H, 3.92; N, 6.01.

(3a*RS*,6*RS*,7a*RS*)-6-Ethyl-*N*-(4-iodophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7u). Yield: 0.12 g (65%); colourless powder. M.p. 181–183 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 8.99 (br.s, 1H), 7.65 (d, *J* = 8.7 Hz, 2H), 7.27 (d, *J* = 8.7 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.39 (dd, *J* = 5.7 Hz, 1H), 4.34 (br.t, *J* = 9.6 Hz, 1H), 4.21-4.12 (m, 2H), 3.27 (br.t, *J* = 10.5 Hz, 1H), 2.41-2.32 (m, 1H), 2.04-1.86 (m, 2H), 1.61-1.50 (m, 2H), 1.03 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.0, 141.9, 139.5, 137.1 (2C), 135.0, 129.0 (2C), 93.6, 92.6, 89.6, 57.7, 54.4, 44.4, 36.5, 25.9, 9.3. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 304.0. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) *the NH signal is less intense due to proton exchange* 9.09 (br.s, 0.2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 6.51 (d, *J* = 5.7 Hz, 1H), 6.39 (d, *J* = 5.7 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.60 – 3.90 (m, 3H), 3.25 (br.t, *J* = 9.5 Hz, 1H), 2.35 (br.s, 1H), 1.97-1.89 (m, 2H), 1.57-1.51 (m, 2H), 1.02 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 177.5, 141.8, 139.5, 137.1 (2C), 135.0, 129.1 (2C), 92.3, 89.8, 36.5, 25.9, 9.4. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 286.7, 284.0. IR (KBr, cm^{-1}): ν_{max} = 3187 (NH), 1523 (NC=Se). MS (ESI): *m/z* = 474 $[M+H]^+$. Anal. Calcd for $C_{17}H_{19}IN_2OSe$: C, 43.15; H, 4.05; N, 5.92. Found: C, 42.97; H, 3.95; N, 6.11.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,6-Dichlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3H)-carboselenoamide (7v). Yield: 0.09 g (57%); colourless powder. M.p. 223–224 °C (decomp.); ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.12 (br.s, 1H), 7.49 (d, *J* = 7.9 Hz, 2H), 7.33 (t, *J* = 7.9 Hz, 1H), 6.54 (d, *J* = 5.7 Hz, 1H), 6.48 (br.d, *J* = 5.8 Hz, 1H), 5.10 (br.d, *J* = 4.3 Hz, 1H), 4.33 (br.t, *J* = 9.7 Hz, 1H), 4.26-4.13 (m, 2H), 3.25 (br.t, *J* = 10.4 Hz, 1H), 2.39-2.29 (m, 1H), 1.84-1.77 (m, 1H), 1.51 (dd, *J* = 11.7, 7.6 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.8, 137.7, 137.1, 136.0, 134.4, 129.3 (2C), 128.6 (2C), 94.4, 80.2, 57.3, 54.1, 41.8, 32.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 296.2. ^{1}H NMR (300.1 MHz, DMSO-d_6, 140 °C): δ (ppm) 8.95 (br.s, 1H), 7.46 (dd, *J* = 8.3, 0.9 Hz, 2H), 7.31 (dd, *J* = 8.7, 7.3 Hz, 1H), 6.53 (d, *J* = 5.7 Hz, 1H), 6.47 (dd, *J* = 5.7, 1.6 Hz, 1H), 5.10 (dd, *J* = 4.4, 1.6 Hz, 1H),

4.36 (dd, *J* = 11.3, 9.0 Hz, 1H), 4.25 (d, *J* = 13.7 Hz, 1H), 4.18 (d, *J* = 13.7 Hz, 1H), 3.27 (dd, *J* = 11.2, 9.8 Hz, 1H), 2.37-2.28 (m, 1H), 1.81 (ddd, *J* = 11.7, 4.4, 2.8 Hz, 1H), 1.52 (dd, *J* = 11.7, 7.5 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 140 °C): δ (ppm) 179.3, 137.7, 137.3, 136.0, 134.4, 129.2 (2C), 128.6 (2C), 94.5, 80.3, 57.4, 54.1, 41.9, 32.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 140°C): δ (ppm) 305.1. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) 9.22 (br.s, 1H), 7.50 (dd, *J* = 8.1, 2.4 Hz, 2H), 7.34 (t, *J* = 8.1 Hz, 1H), 6.55 (d, *J* = 5.7 Hz, 1H), 6.47 (dd, *J* = 5.7, 1.7 Hz, 1H), 5.10 (dd, *J* = 4.5, 1.4 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.55 – 3.90 (m, 3H), 3.21 (br.s, 1H), 2.33 (br.s, 1H), 1.80 (br.d, *J* = 11.2 Hz, 1H), 1.49 (dd, *J* = 11.2, 7.6 Hz, 1H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 178.4, 137.7, 137.0, 135.9, 134.4 (2C), 129.5, 128.7 (2C), 80.2, 32.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 283.3, 280.9. IR (KBr, cm^{-1}): ν_{max} = 3147 (NH), 1524 (NC=Se). MS (ESI): *m/z* = 388 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{14}Cl_2N_2OSe$: C, 46.42; H, 3.64; N, 7.22. Found: C, 46.57; H, 3.82; N, 7.13.

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,6-Dichlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7w). Yield: 0.08 g (47%); colourless powder. M.p. 224–225 °C (decomp.); ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.12 (br.s, 1H), 7.49-7.47 (m, 2H), 7.33 (t, *J* = 8.3 Hz, 1H), 6.53 (d, *J* = 5.6 Hz, 1H), 6.33 (d, *J* = 5.6 Hz, 1H), 4.33 (br.t, *J* = 9.5 Hz, 1H), 4.20-4.08 (m, 2H), 3.29 (br.t, *J* = 10.4 Hz, 1H), 2.47-2.37 (m, 1H), 1.65 (dd, *J* = 11.5, 7.3 Hz, 1H), 1.62 (s, 3H), 1.53 (dd, *J* = 11.5, 2.8 Hz, 1H). ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.7, 140.9, 137.1, 136.0, 135.0, 129.3 (2C), 128.6 (2C), 94.1, 88.5, 57.4, 54.1, 45.1, 38.8, 19.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 302.2. ^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C): δ (ppm) 9.21 (br.s, 1H), 7.50-7.49 (m, 2H), 7.34 (t, *J* = 8.1 Hz, 1H), 6.54 (d, *J* = 5.5 Hz, 1H), 6.33 (d, *J* = 5.5 Hz, 1H), *broadening of proton signals H-1,3* ~ 4.55 – 3.85 (m, 3H), 3.25 (br.s, 1H), 2.42 (br.s, 1H), 1.65-1.53 (m, 2H), 1.61 (s, 3H); ^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C): δ (ppm) *no 4 C signals were reasonably attributed to an epoxyisoindole moiety* 178.3, 140.8, 137.0, 135.9, 135.0 (2C), 129.5, 128.7 (2C), 88.5, 38.8, 19.2. ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 283.1, 280.4. IR (KBr, cm^{-1}): ν_{max} = 3166 (NH), 1524 (NC=Se). MS (ESI): *m/z* = 402 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{16}H_{16}Cl_2N_2OSe$: C, 47.78; H, 4.01; N, 6.97. Found: C, 47.53; H, 3.81; N, 7.18.

(3a*RS*,6*RS*,7a*RS*)-*N*-(3-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7x). Yield: 0.12 g (53%); colourless powder. M.p. 121–123 °C; ^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C): δ (ppm) 9.07 (br.s, 1H), 7.58 (t, *J* = 1.8 Hz, 1H), 7.44-7.31 (m, 2H), 7.20 (ddd, *J* = 7.9, 1.8, 1.0 Hz, 1H), 6.52 (d, *J* = 5.8 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.6 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.6 Hz, 1H), 4.36 (br.t, *J* = 9.9 Hz, 1H), 4.27 (d, *J* = 13.8 Hz, 1H), 4.20 (d, *J* =

13.8 Hz, 1H), 3.27 (dd, *J* = 11.2, 9.9 Hz, 1H), 2.33-2.23 (m, 1H), 1.79 (ddd, *J* = 11.7, 4.5, 2.8 Hz, 1H), 1.50 (dd, *J* = 11.7, 7.5 Hz, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C): δ (ppm) 178.1, 143.4, 137.8, 134.3, 132.6, 129.7, 128.7, 126.5, 125.1, 94.1, 80.2, 57.5, 54.2, 41.6, 32.2; ^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C): δ (ppm) 307.3; ^{1}H NMR (300.1 MHz, DMSO-d_6): δ (ppm) 9.33 (br.s, 1H), 7.54 (br.s, 1H), 7.40-7.32 (m, 2H), 7.23 (dt, *J* = 7.0, 1.8 Hz, 1H), 6.53 (d, *J* = 5.7 Hz, 1H), 6.47 (dd, *J* = 5.8, 1.6 Hz, 1H), 5.09 (dd, *J* = 4.5, 1.6 Hz, 1H), *broadening of proton signals H-1,3,7,7a* ~ 4.52 – 4.00 (m, 3H), 3.30-3.15 (br.m, 1H), 2.38-2.14 (br.m, 1H), 1.77 (br.s, 1H), 1.46 (br.s, 1H); ^{13}C NMR (75.5 MHz, DMSO-d_6): δ (ppm) *5 signals of the epoxyisoindole moiety and aromatic ring are duplicated* 177.2, 143.2, 137.8, 134.3, 132.4, 129.9, 128.8. 126.8, 125.5 and 125.3 (1C), 95.4 and 93.0 (1C), 80.1, 60.7 and 56.6 (1C), 55.0 and 50.9 (1C), 42.4, 32.4 and 32.0 (1C); ^{77}Se NMR (57.2 MHz, DMSO-d_6): δ (ppm) *signals of the Se are duplicated* 290.0, 287.3. IR (KBr, cm^{-1}): ν_{max} = 3185 (NH), 1531 (NC=Se). MS (ESI): *m/z* = 355 $[M+H]^+$ for ^{35}Cl. Anal. Calcd for $C_{15}H_{15}ClN_2OSe$: C, 50.94; H, 4.27; N, 7.92. Found: C, 50.76; H, 4.09; N, 8.09.

References

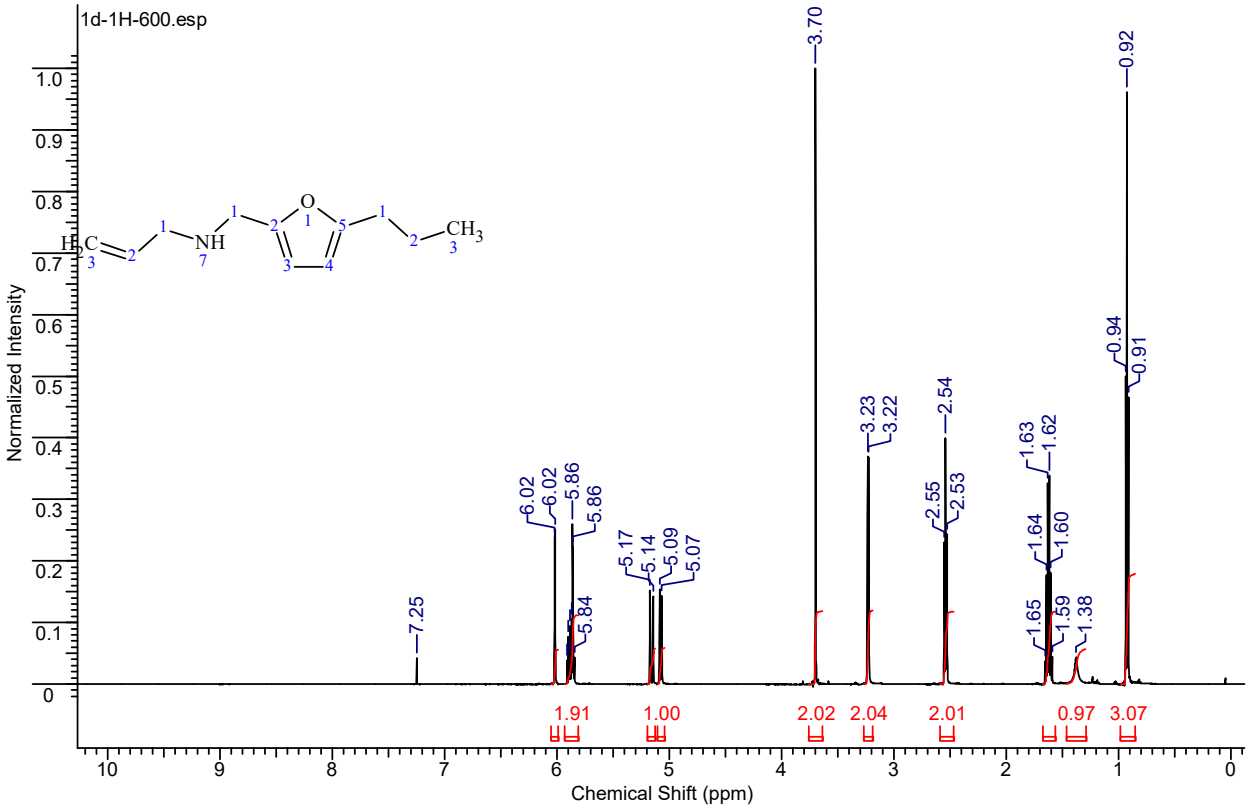
[1]. *CLSI M38-A2*. Ed. 2. Reference method for broth dilution antifungal susceptibility testing of filamentous fungi. Approved standart. Clinical and Laboratory Standards Institute. *Pensylvania*, **2008**.

[2]. *CLSI M27-S3*. Reference method for broth dilution antifungal susceptibility testing of yeasts. Clinical and Laboratory Standards Institute. *Pensylvania*, **2013**.

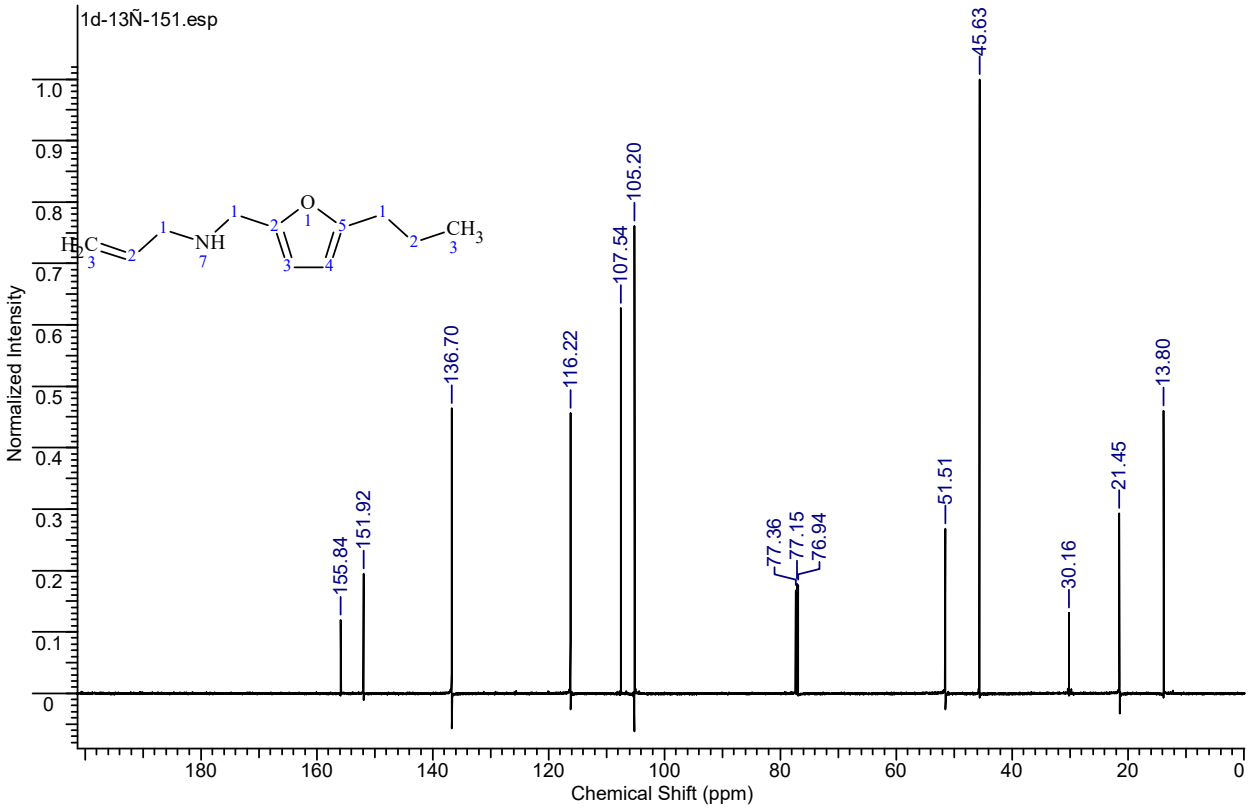
[3]. Trenin, A.S.; Isakova, E.B.; Treshchalin M.I.; Polozkova, V.A.; Mirchink, E.P.; Panov, A.A.; Simonov, A.Yu.; Bychkova, O.P.; Tatarskiy, V.V.; Lavrenov, S.N. *Pharmaceuticals*, **2022**, *15*, 118–130.

3. Copies of NMR spectra

N-[(5-Propyl-2-furyl)methyl]prop-2-en-1-amine (1d). ^{1}H NMR (600.2 MHz, $CDCl_3$)

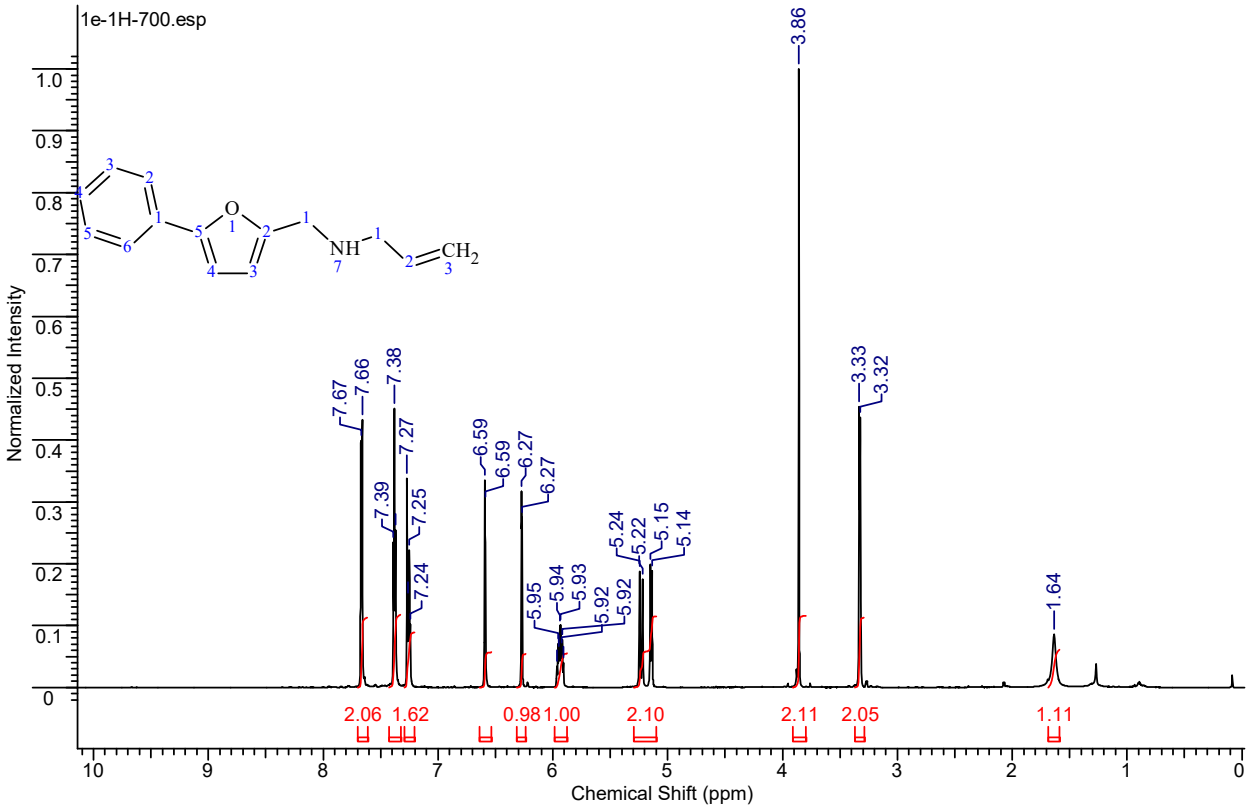


^{13}C NMR (150.9 MHz, $CDCl_3$)

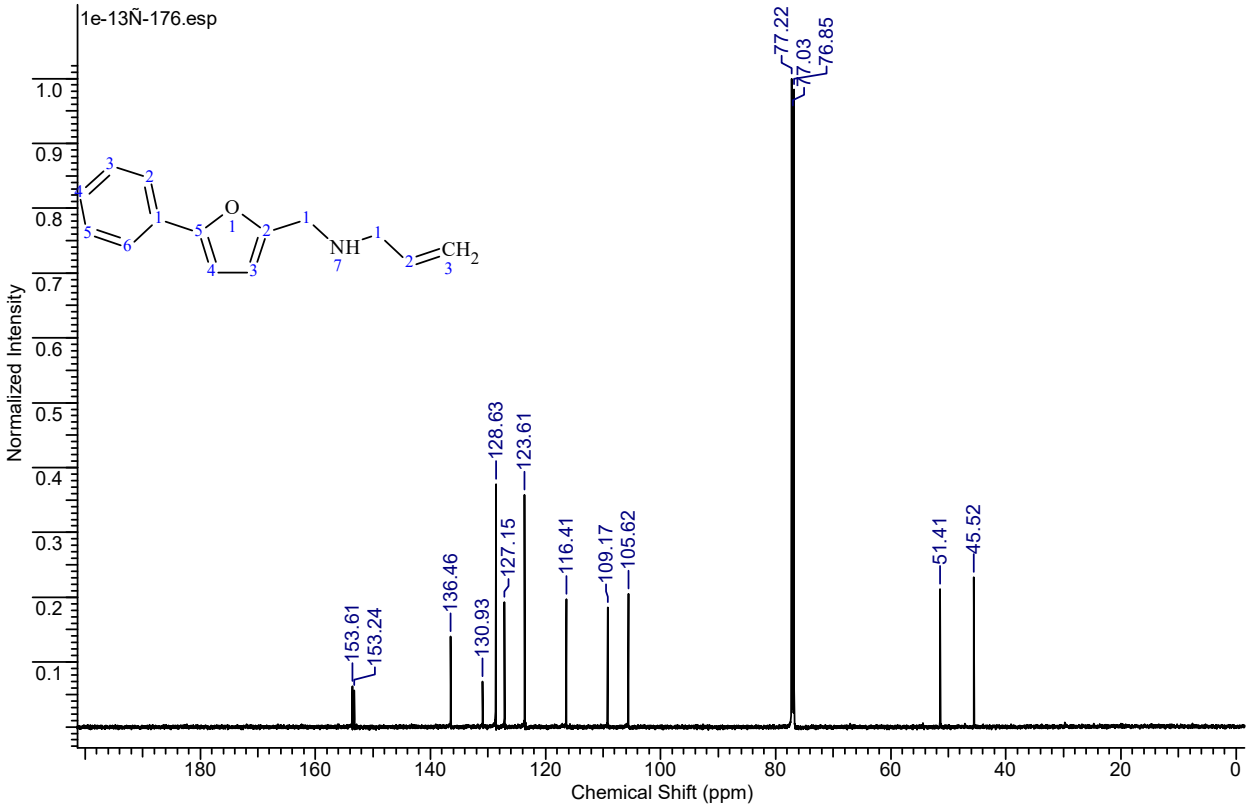


***N*-[(5-Phenyl-2-furyl)methyl]prop-2-en-1-amine (1e).**

^{1}H NMR (700.2 MHz, $CDCl_3$)

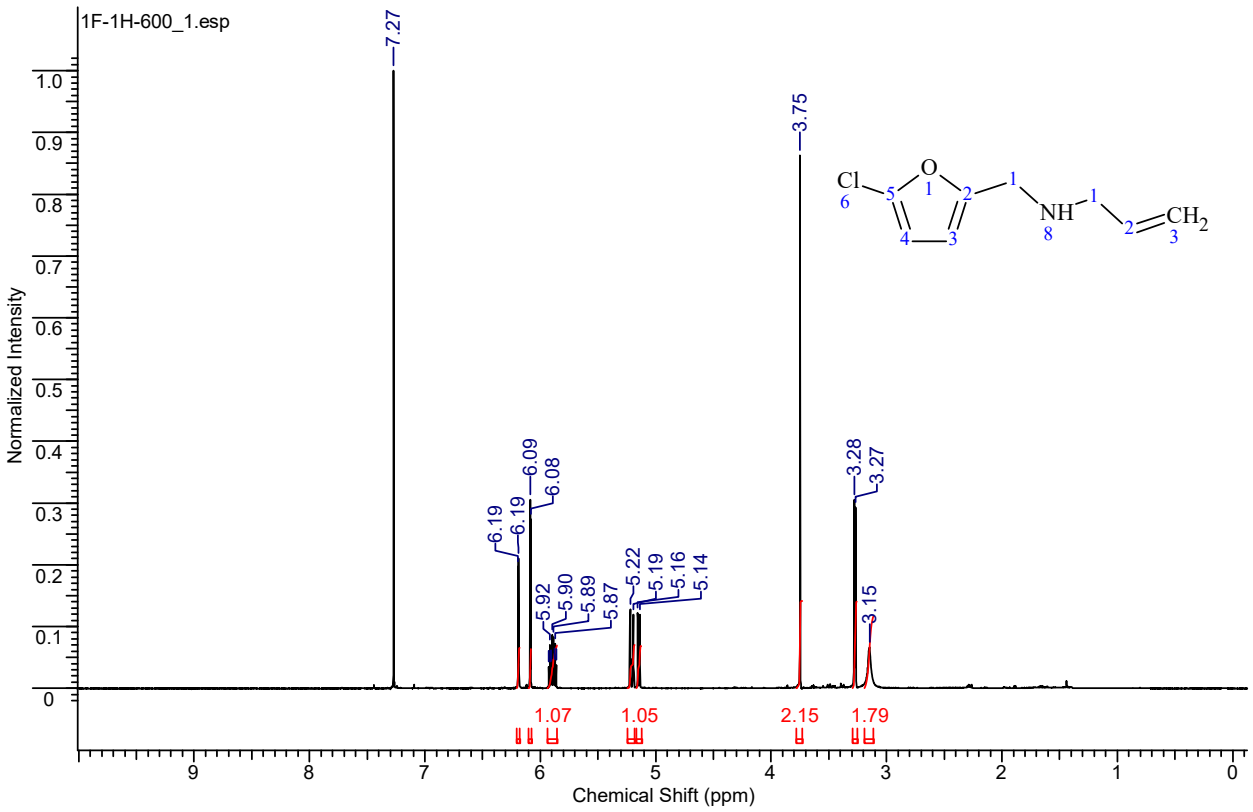


^{13}C NMR (176.1 MHz, $CDCl_3$)

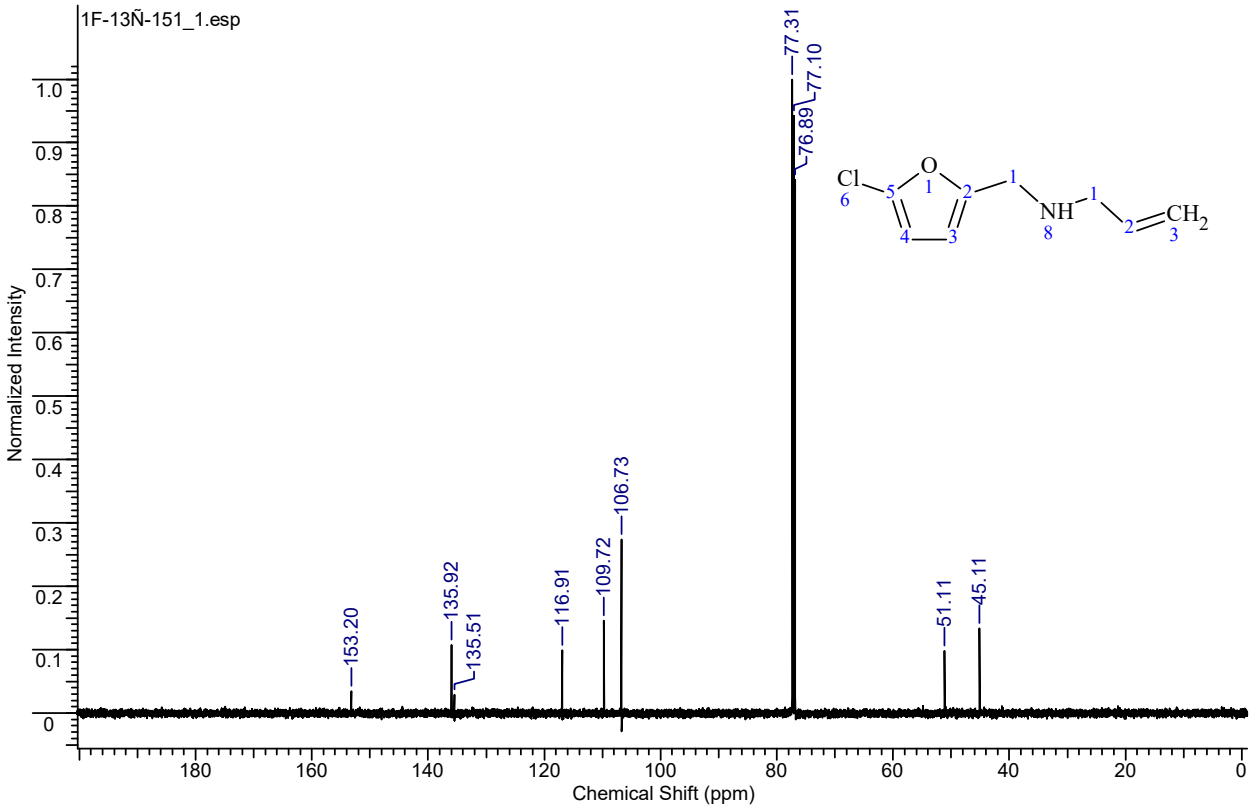


***N*-[(5-Chloro-2-furyl)methyl]prop-2-en-1-amine (1f).**

^{1}H NMR (600.2 MHz, $CDCl_3$)

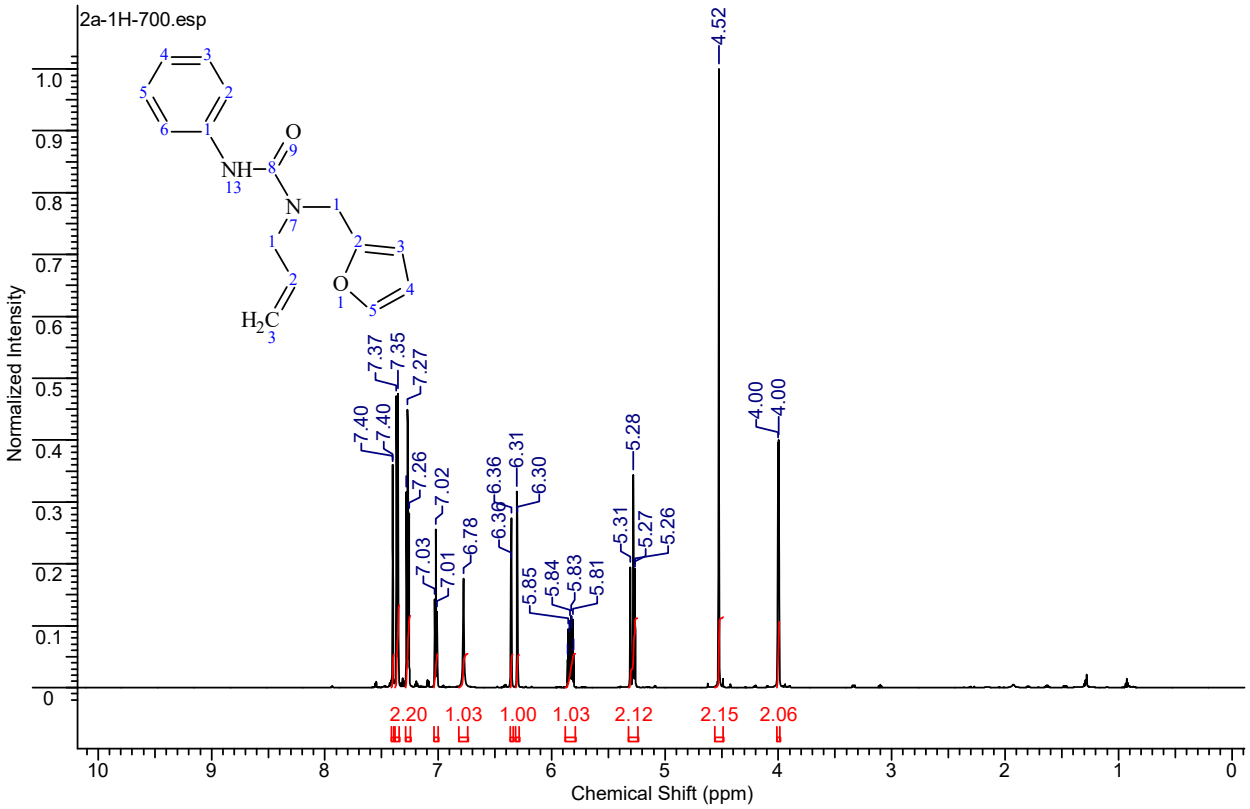


^{13}C NMR (150.9 MHz, $CDCl_3$)

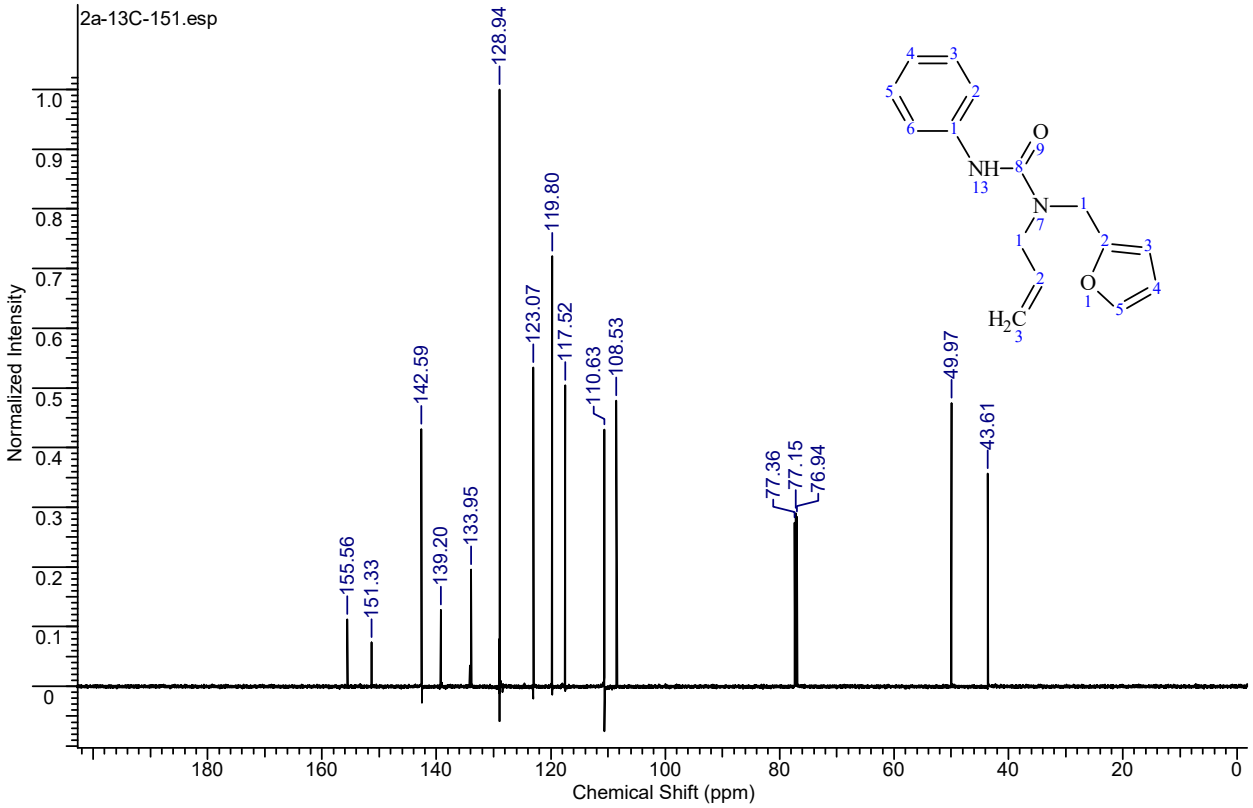


N-Allyl-*N*-(2-furylmethyl)-*N*'-phenylurea (2a).

^{1}H NMR (700.2 MHz, $CDCl_3$)

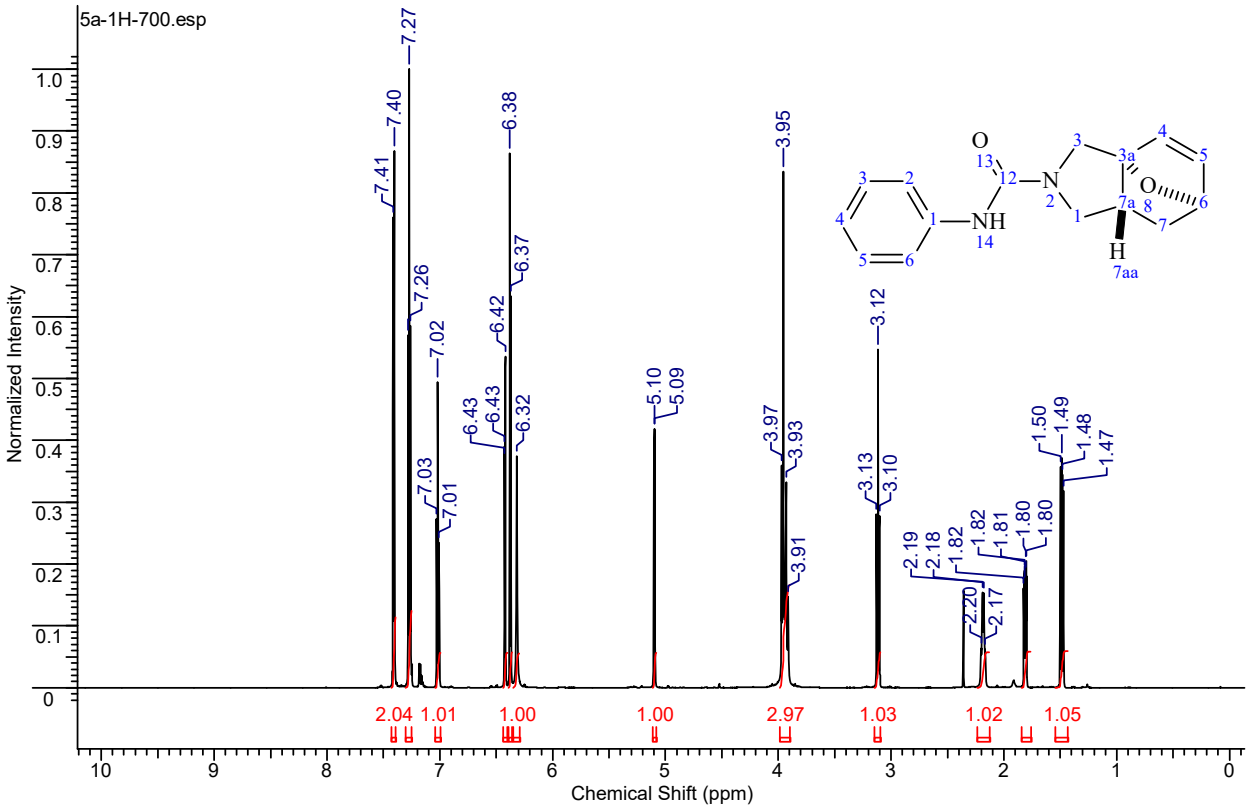


^{13}C NMR (150.9 MHz, $CDCl_3$)

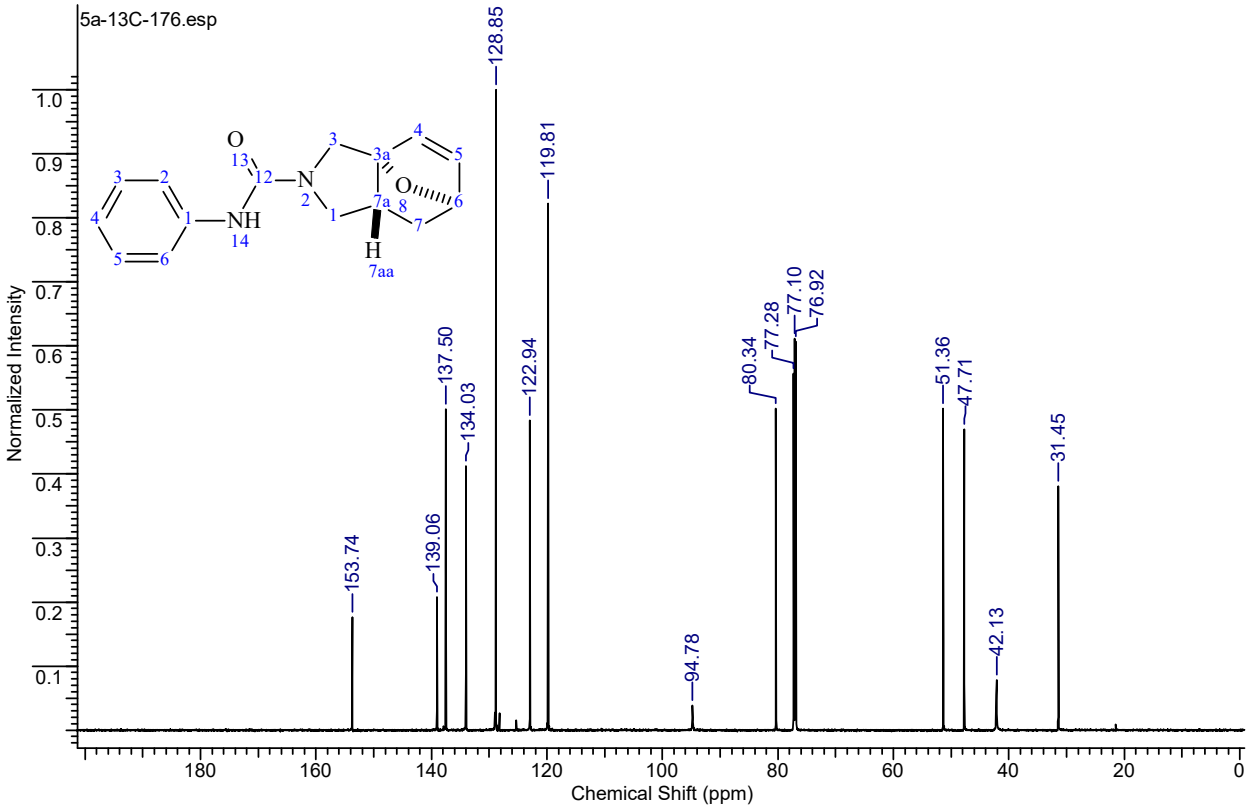


(3a*RS*,6*RS*,7a*RS*)-*N*-Phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5a).

^{1}H NMR (700.2 MHz, $CDCl_3$)

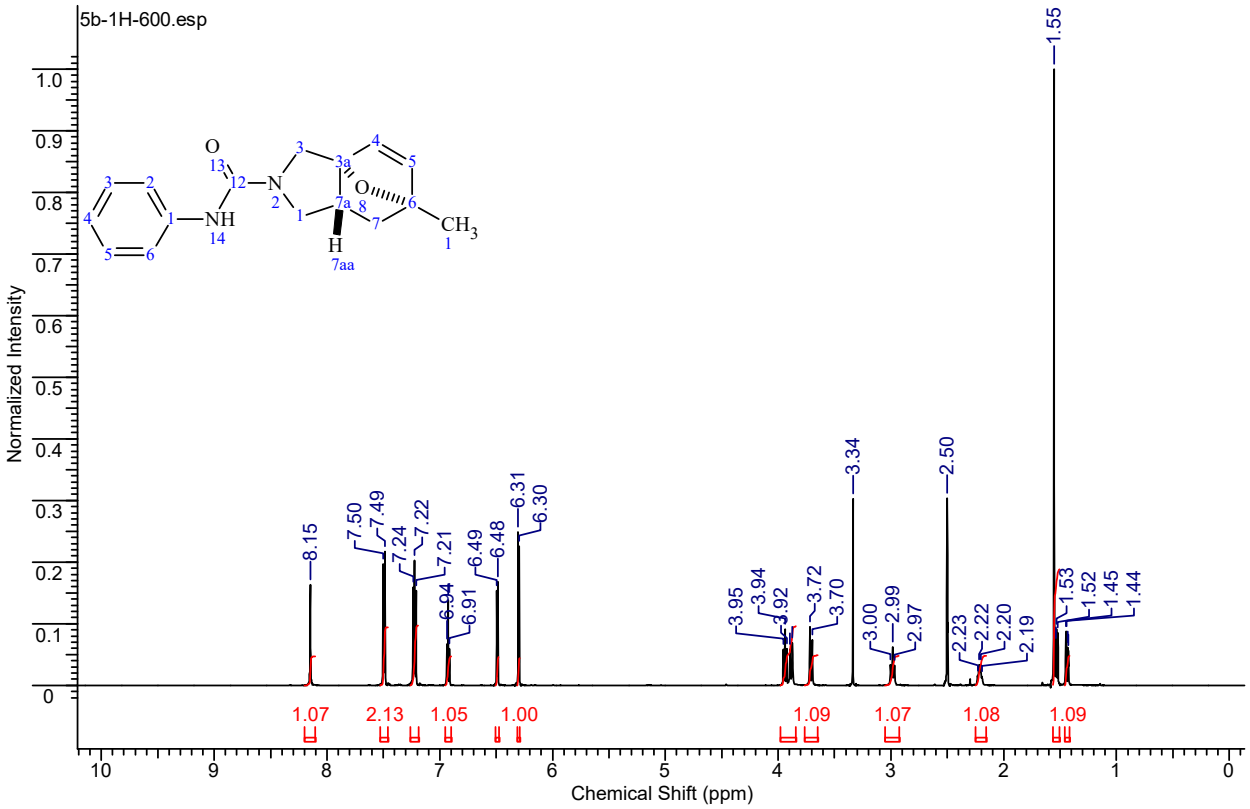


^{13}C NMR (176.1 MHz, $CDCl_3$)

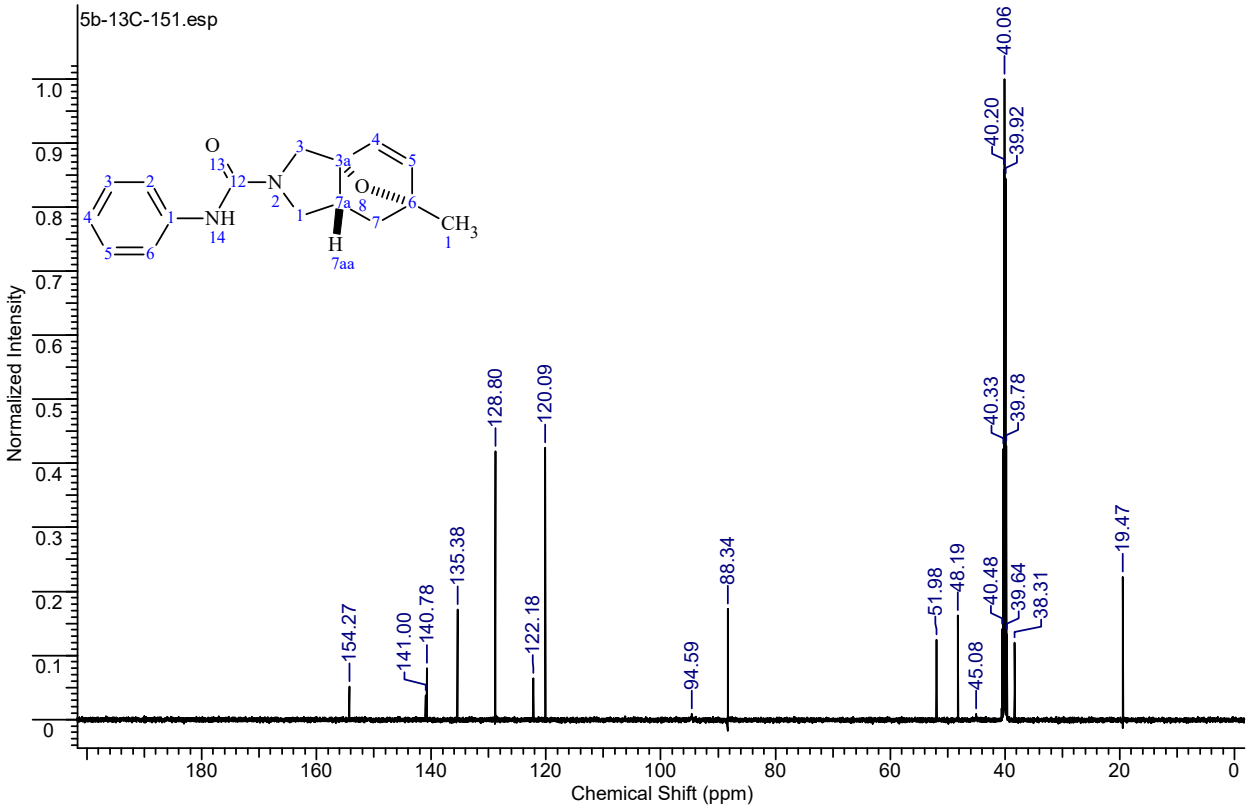


(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5b).

^{1}H NMR (600.2 MHz, DMSO-d_6)

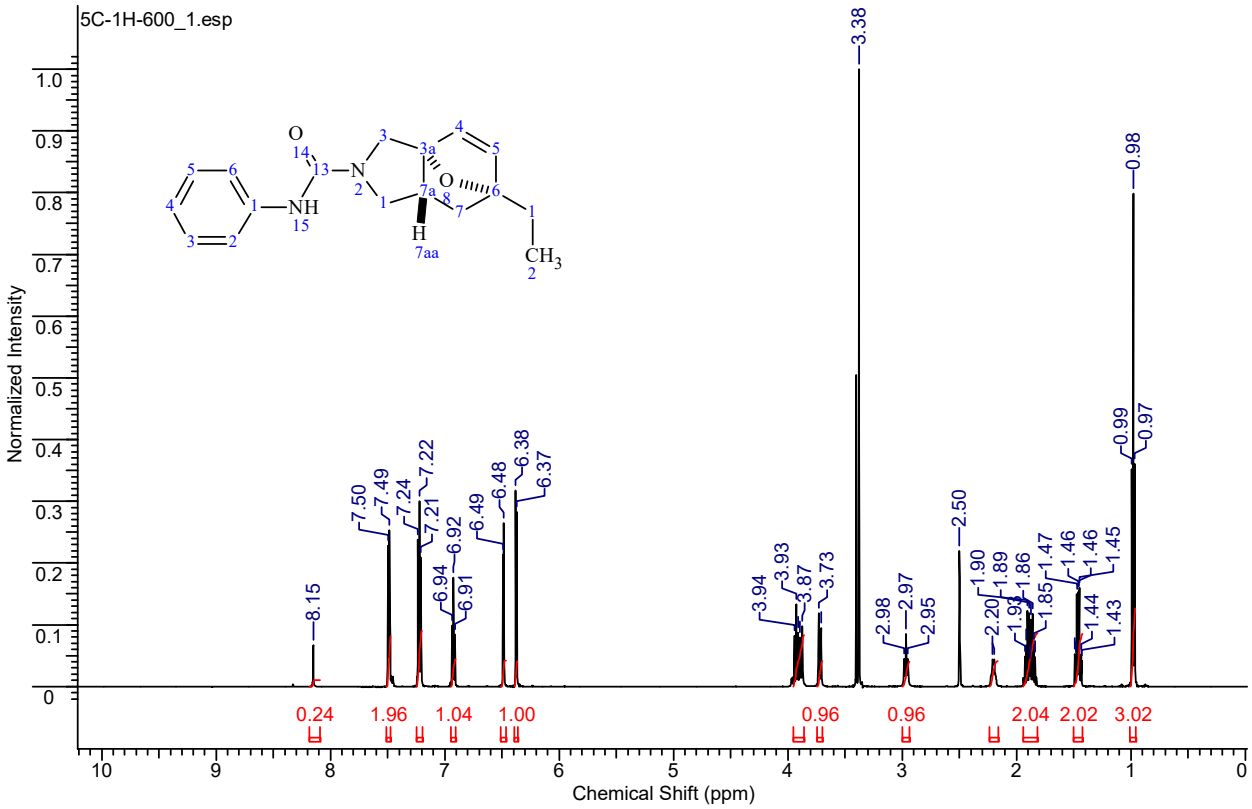


^{13}C NMR (150.9 MHz, DMSO-d_6)

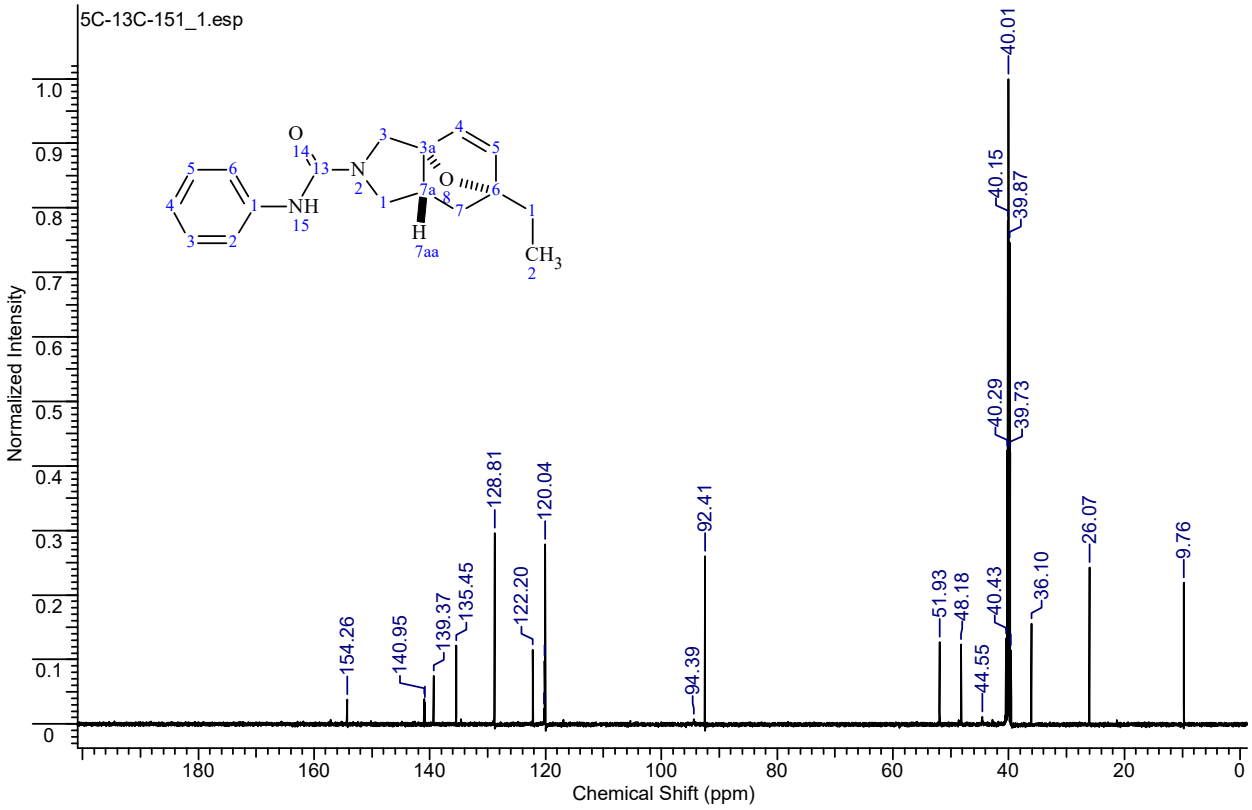


(3a*RS*,6*RS*,7a*RS*)-6-Ethyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5c).

^{1}H NMR (600.2 MHz, DMSO-d_6)

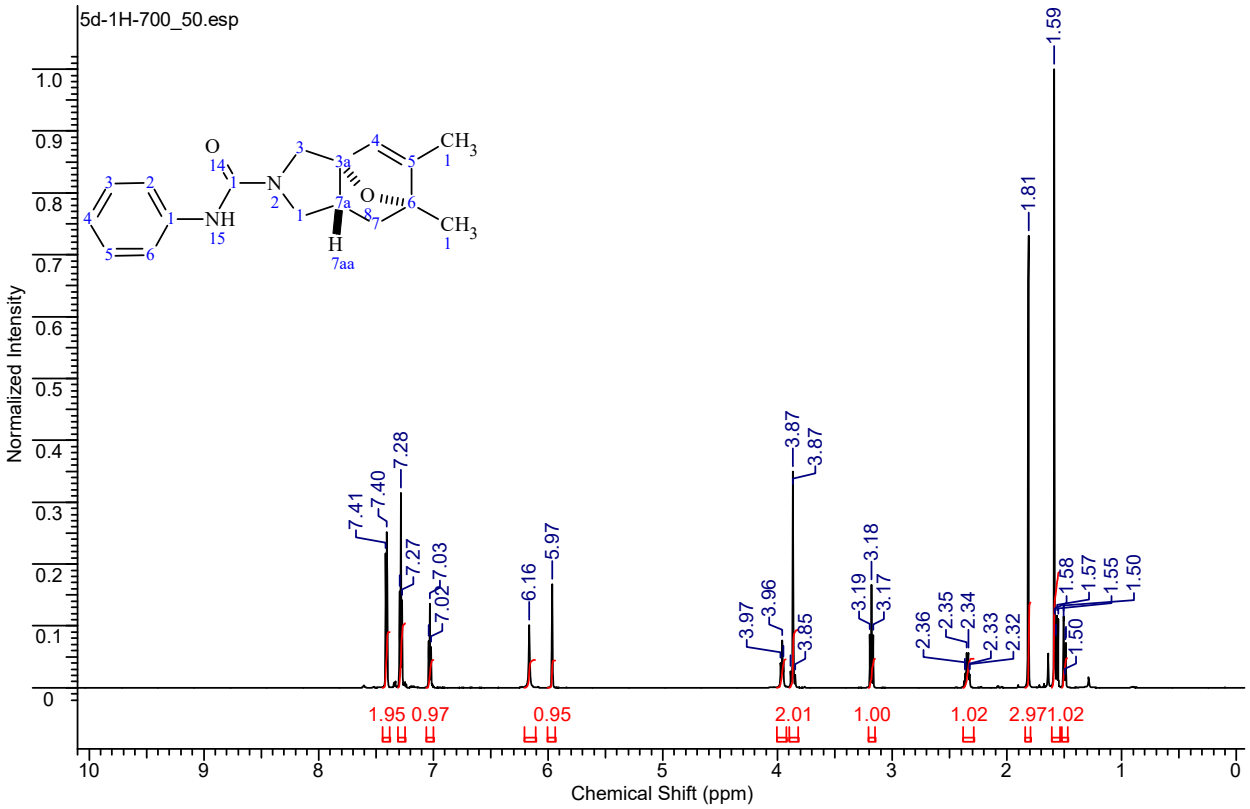


^{13}C NMR (150.9 MHz, DMSO-d_6)

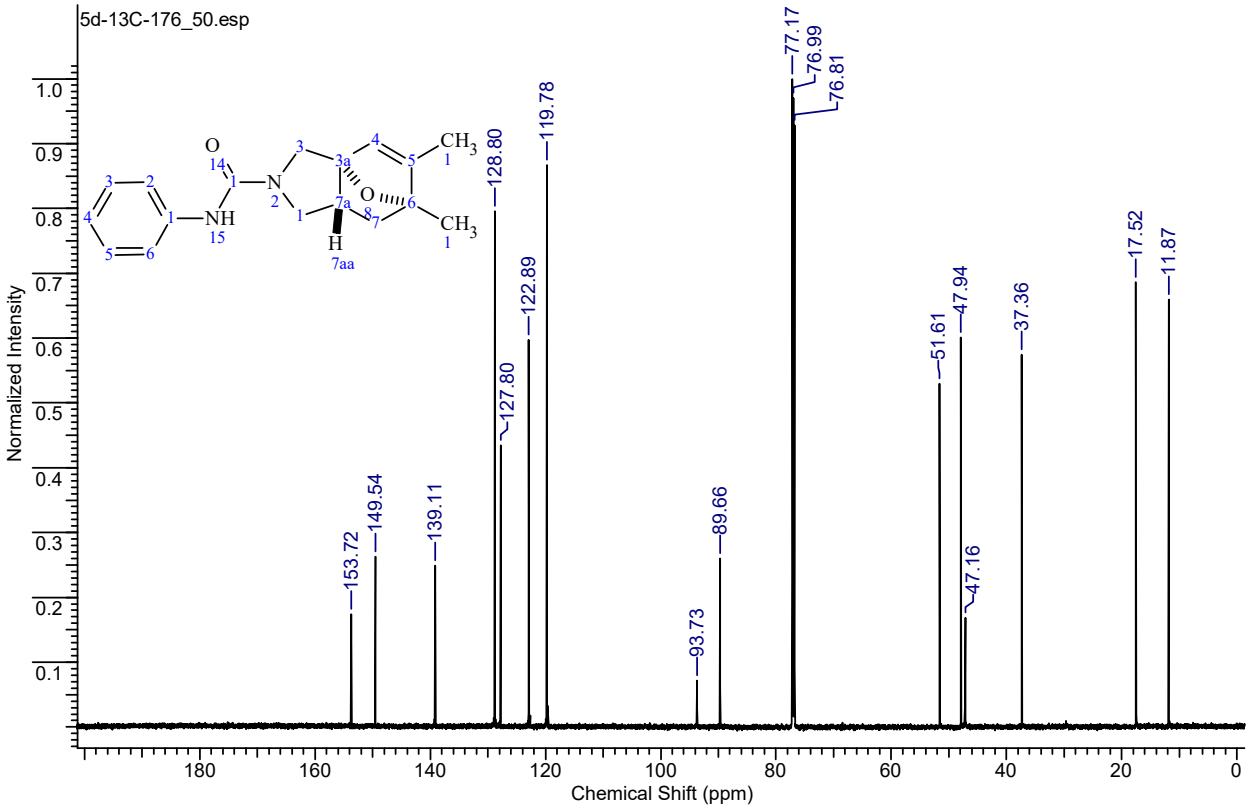


(3a*RS*,6*RS*,7a*RS*)-5,6-Dimethyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5d).

^{1}H NMR (700.2 MHz, $CDCl_3$, 50 °C)

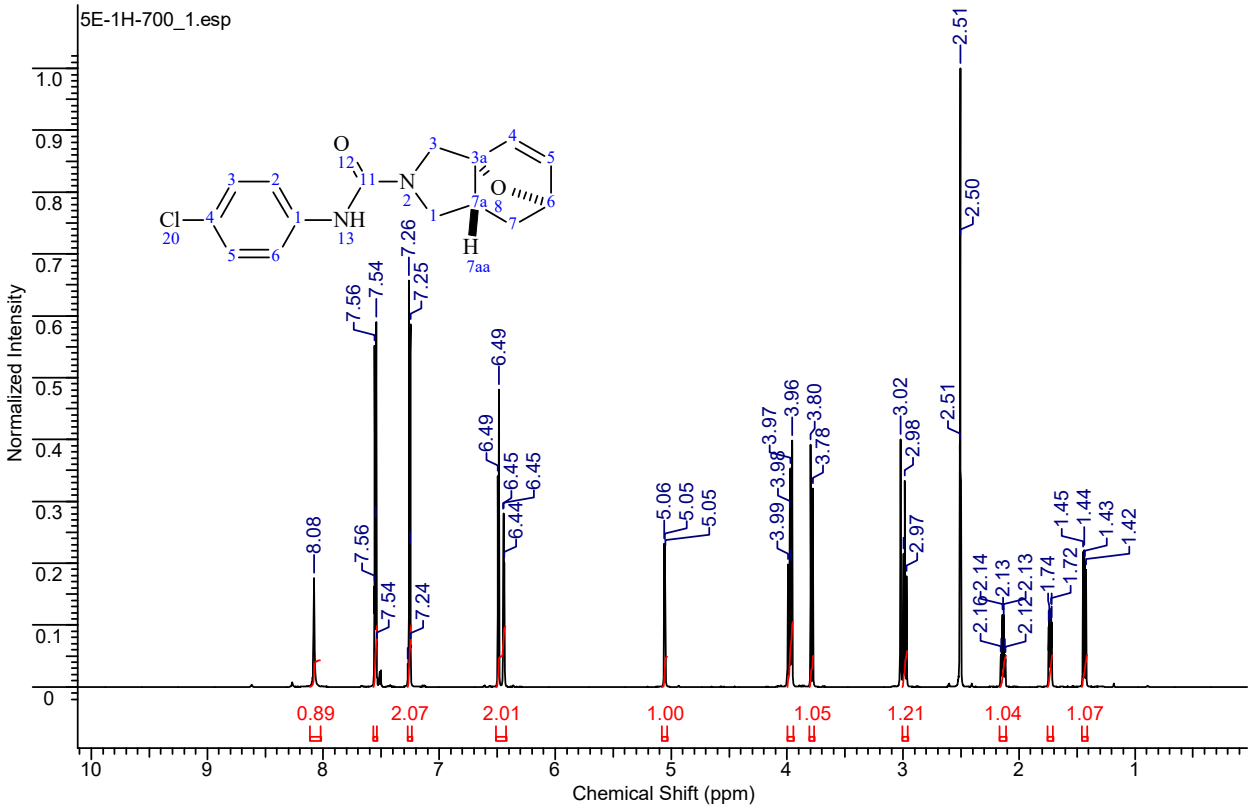


^{13}C NMR (176.1 MHz, $CDCl_3$, 50 °C)

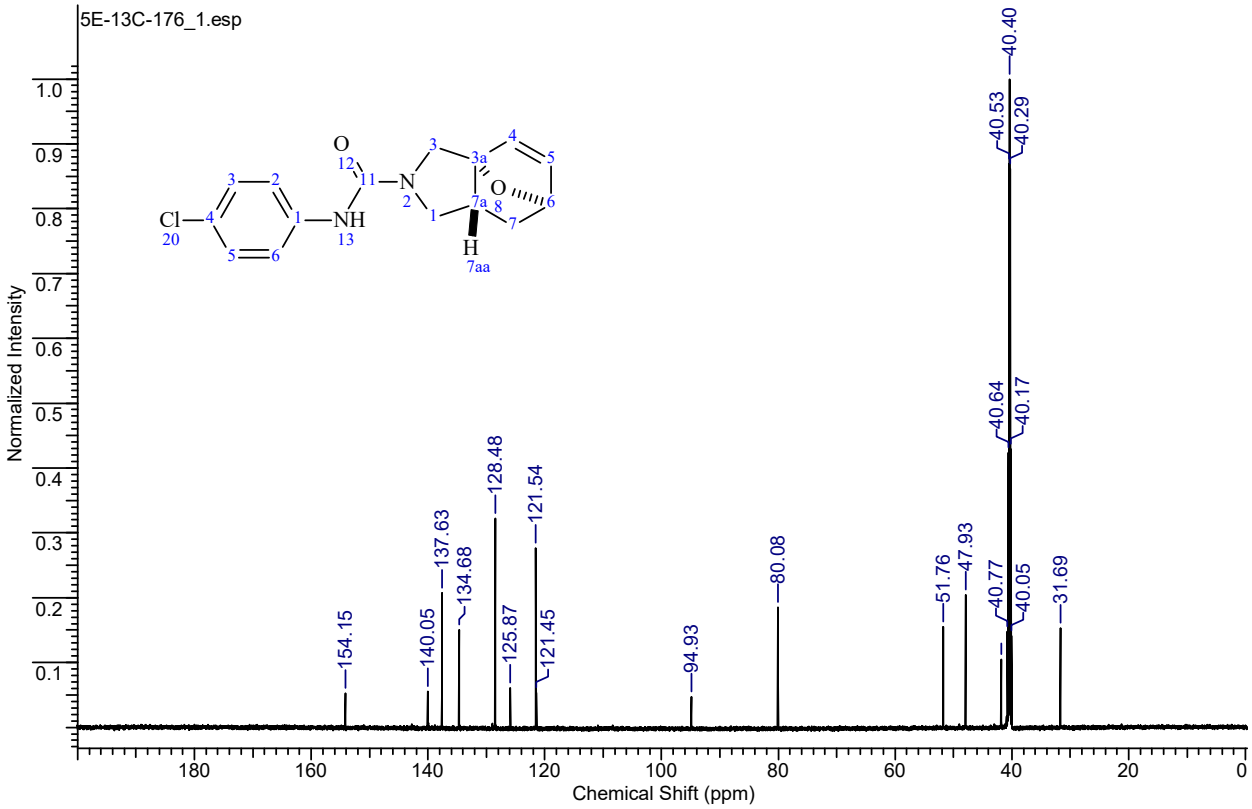


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5e).

^{1}H NMR (700.2 MHz, DMSO-d_6)

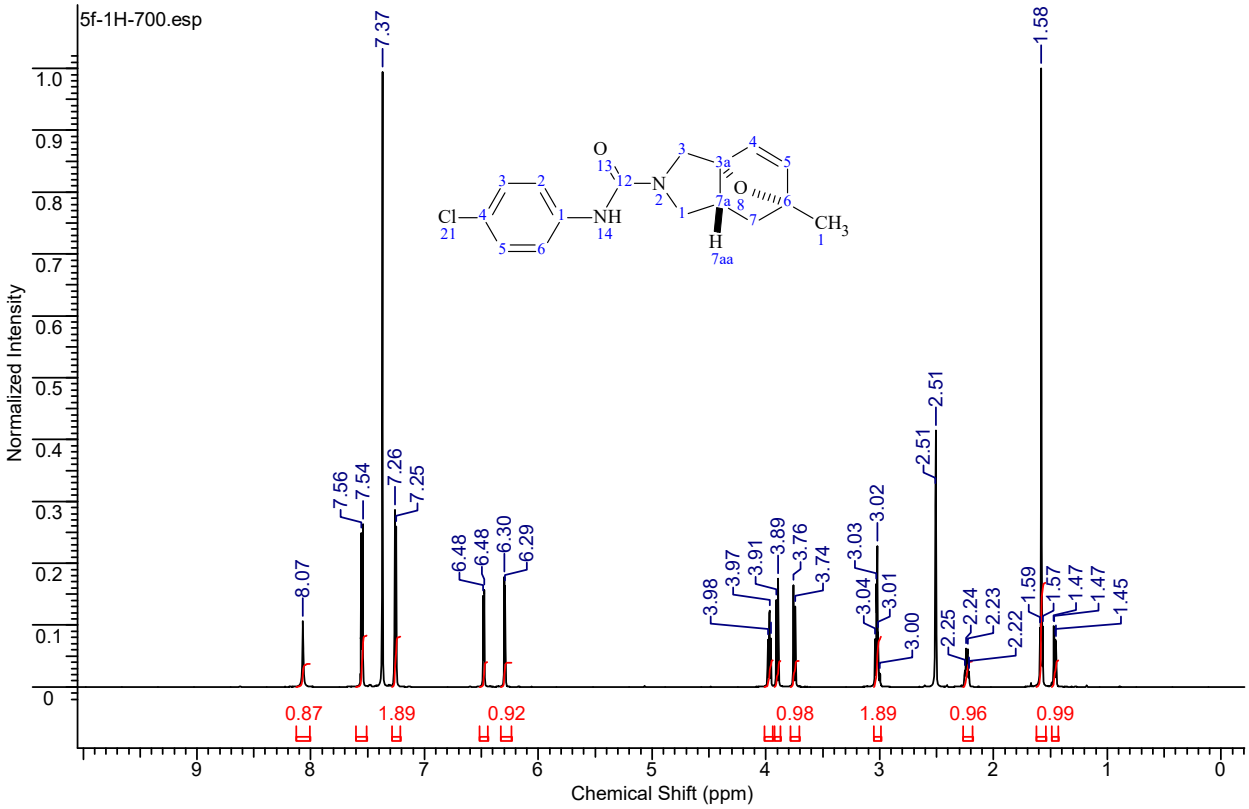


^{13}C NMR (176.1 MHz, DMSO-d_6)

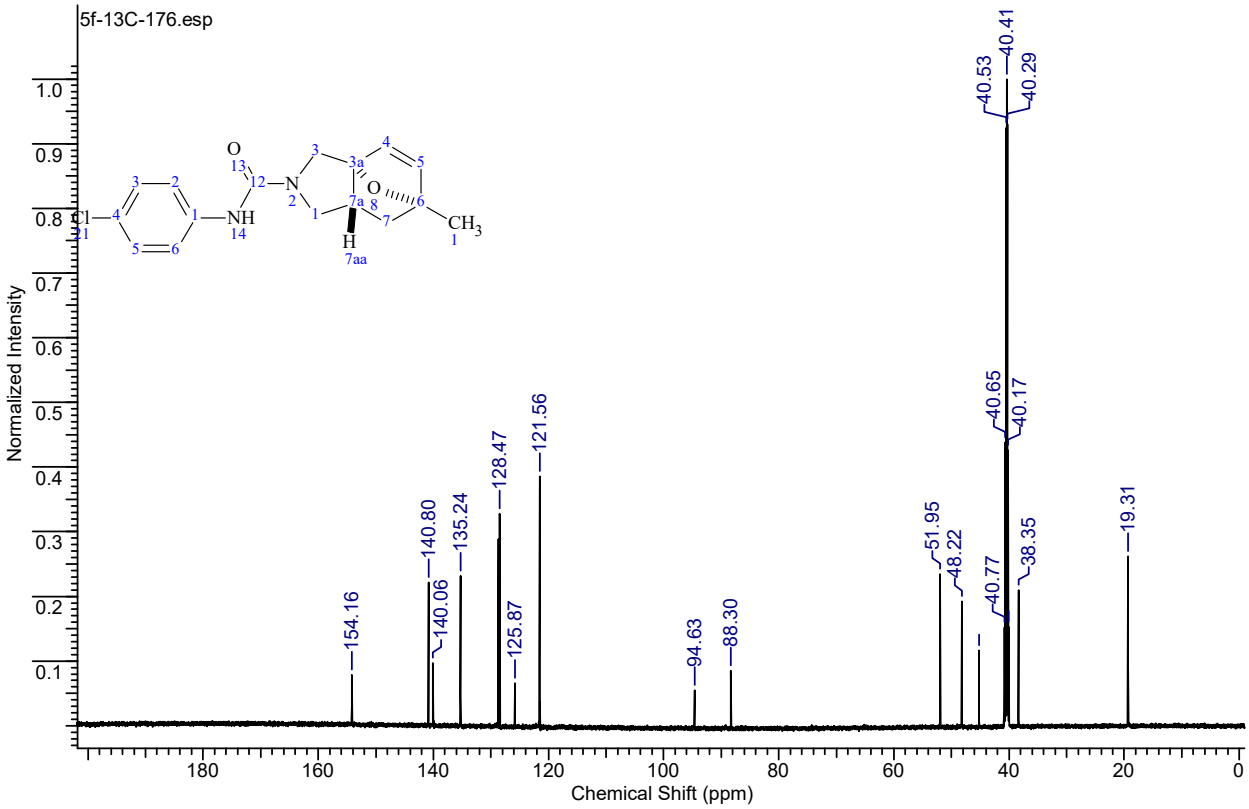


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-chlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5f). *Contains an impurity of benzene*

^{1}H NMR (700.2 MHz, DMSO-d_6)

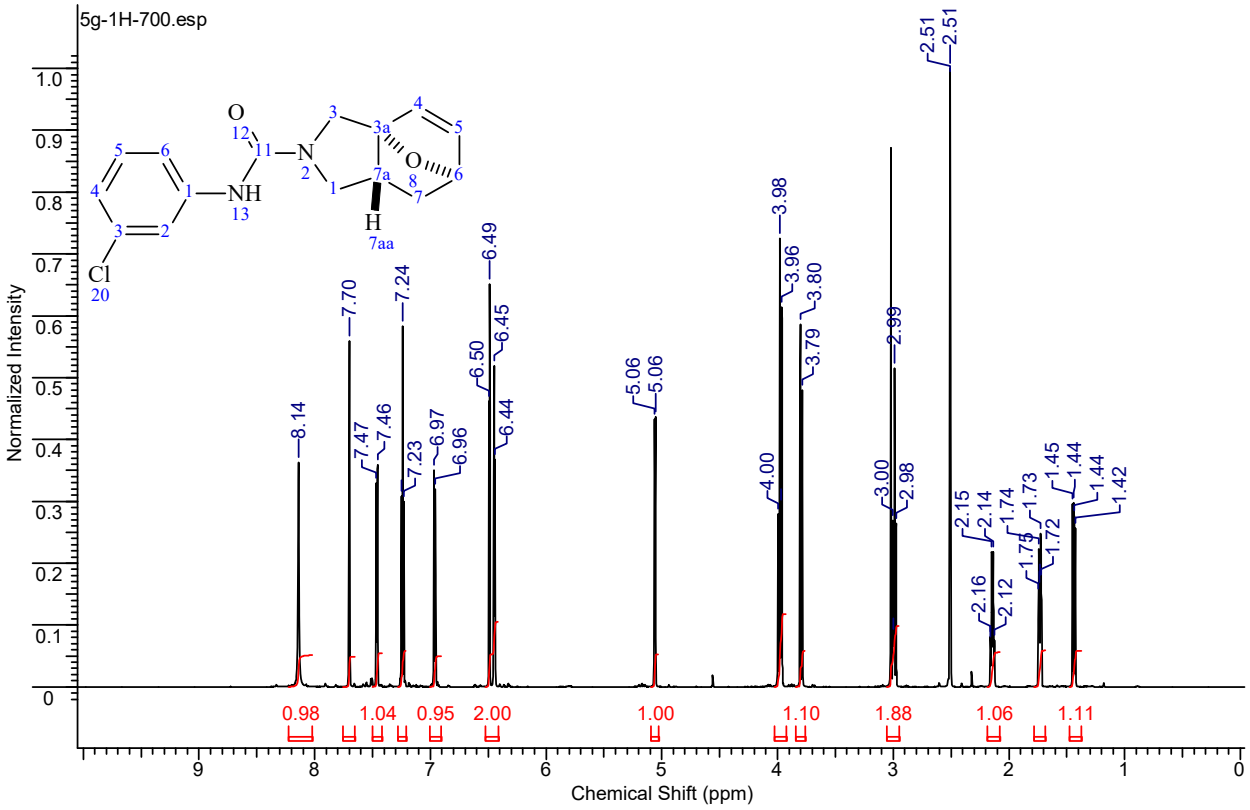


^{13}C NMR (176.1 MHz, DMSO-d_6)

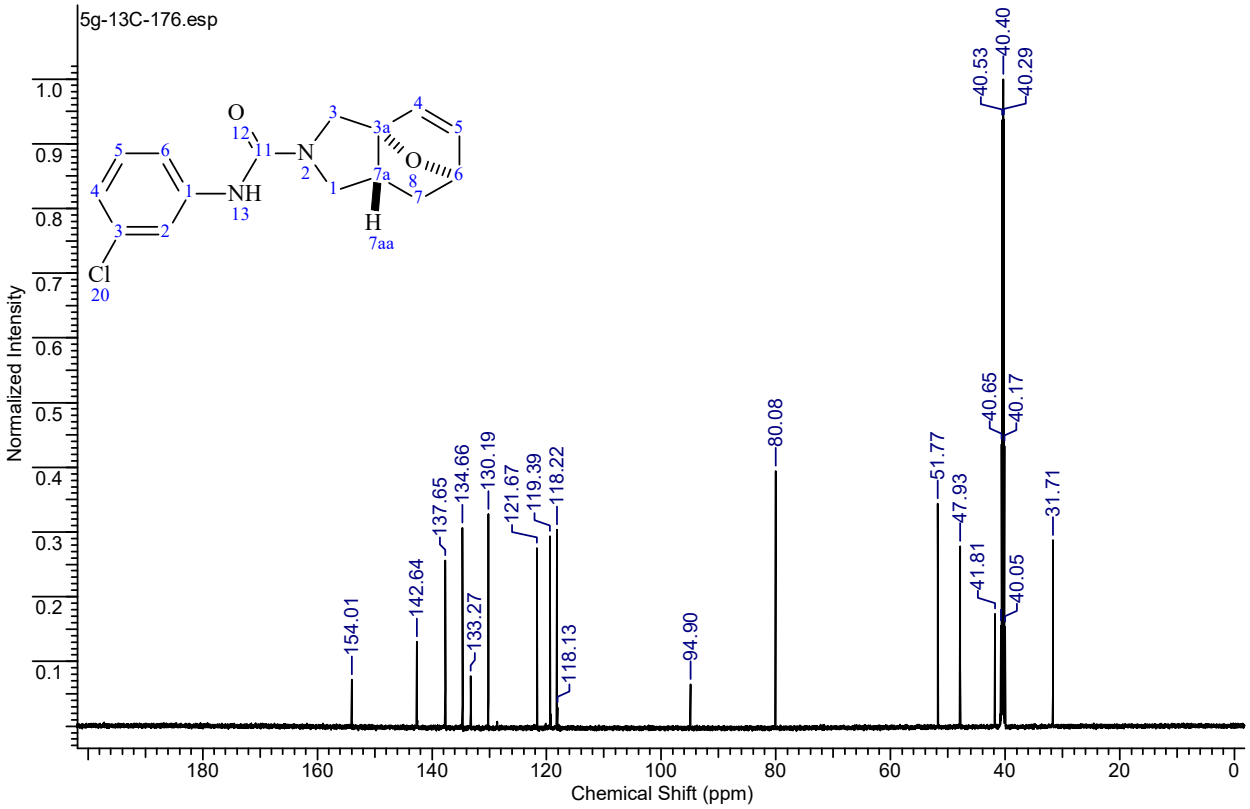


(3a*RS*,6*RS*,7a*RS*)-*N*-(3-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5g).

^{1}H NMR (700.2 MHz, DMSO-d_6)

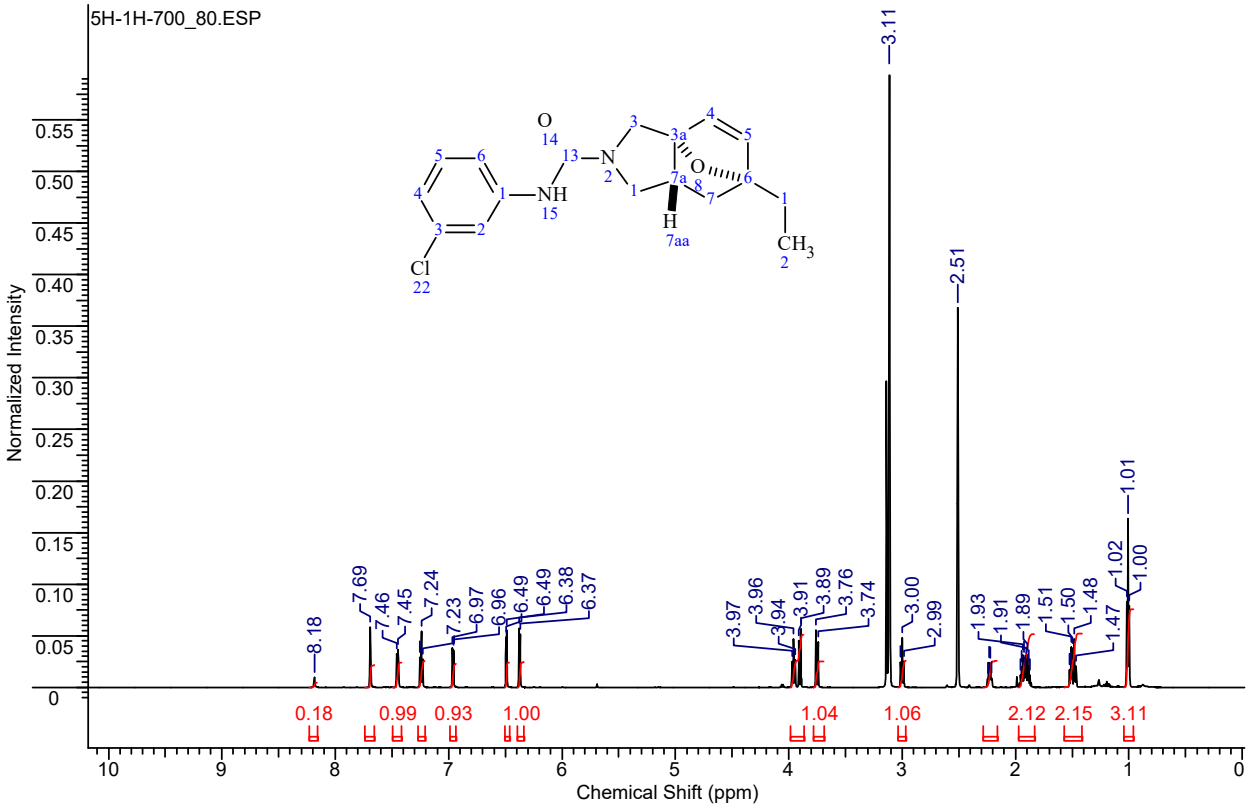


^{13}C NMR (176.1 MHz, DMSO-d_6)

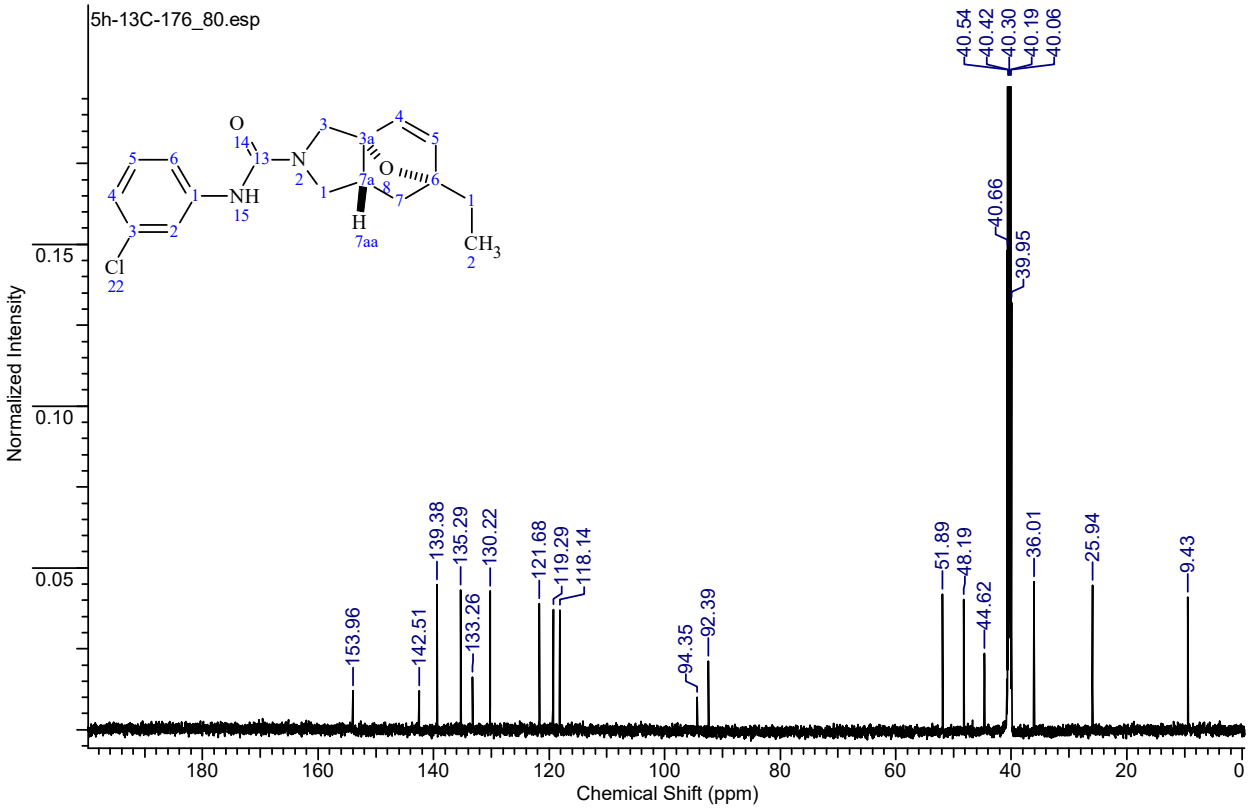


(3a*RS*,6*RS*,7a*RS*)-*N*-(3-Chlorophenyl)-6-ethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5h).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

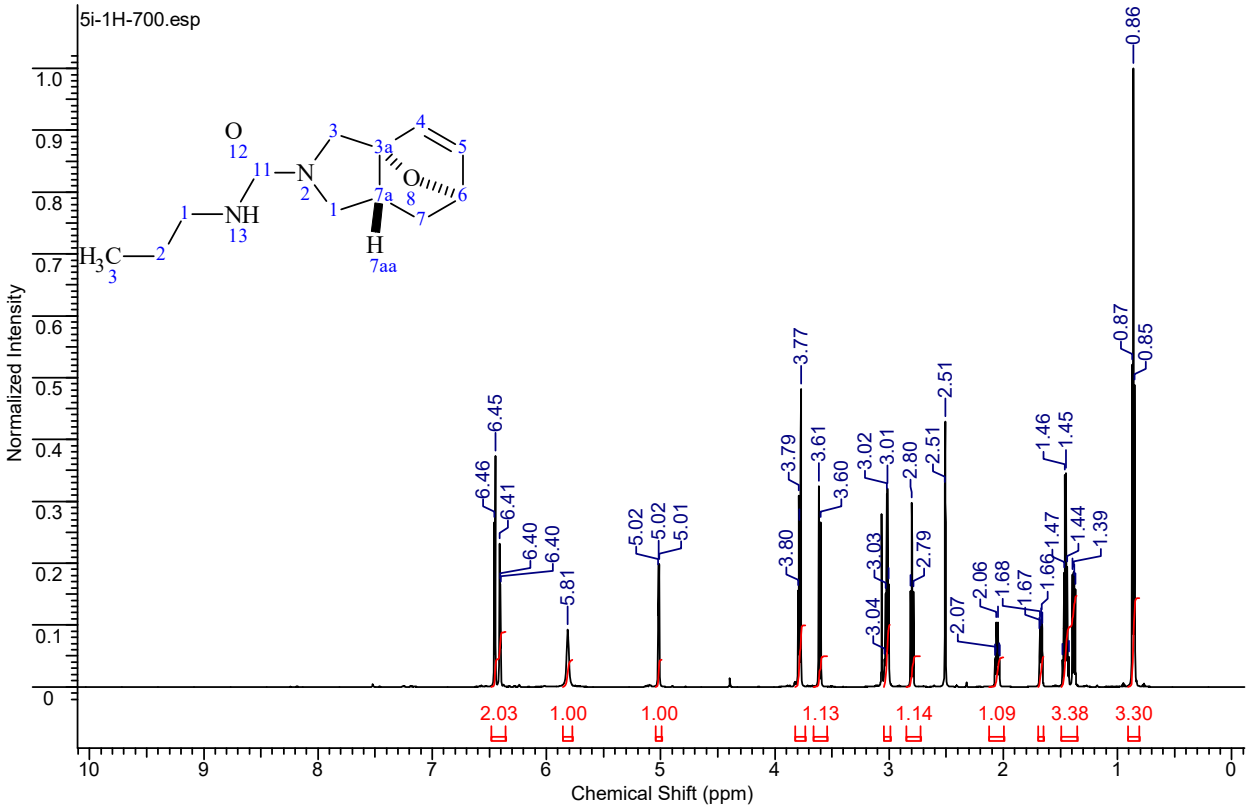


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

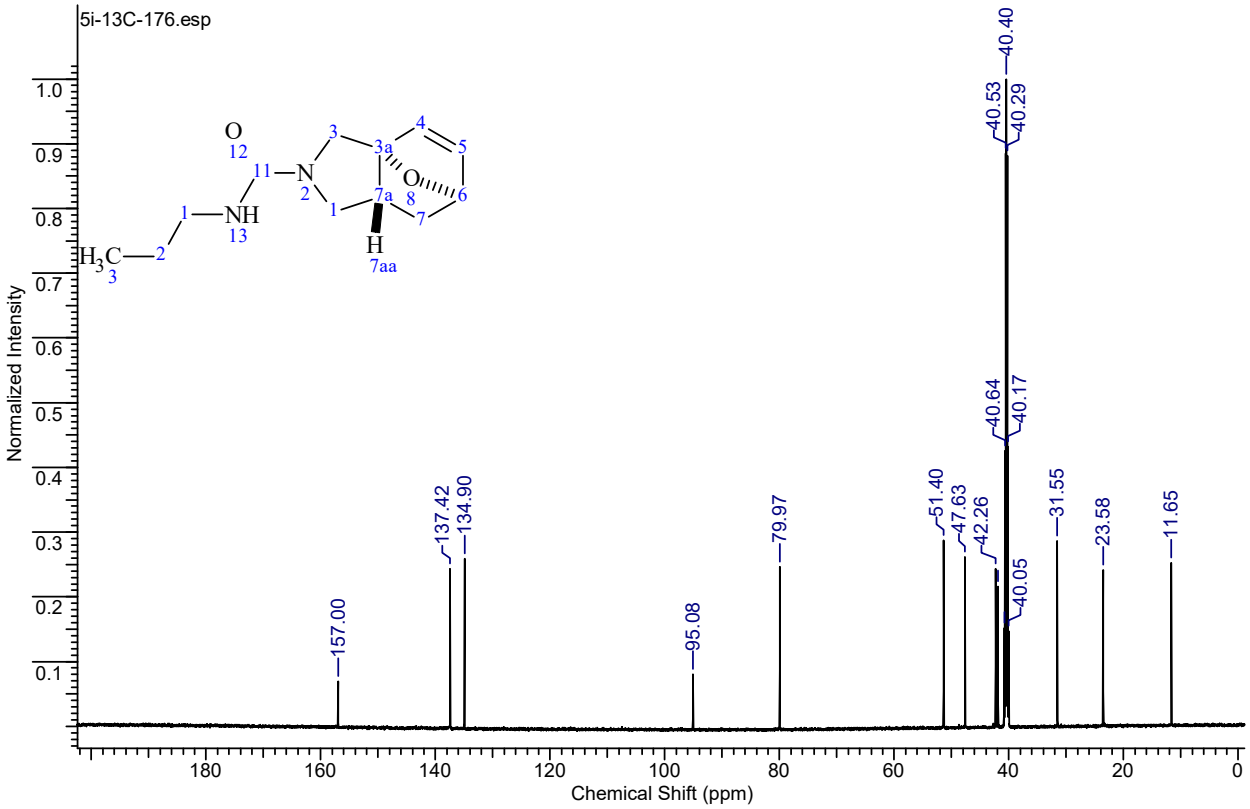


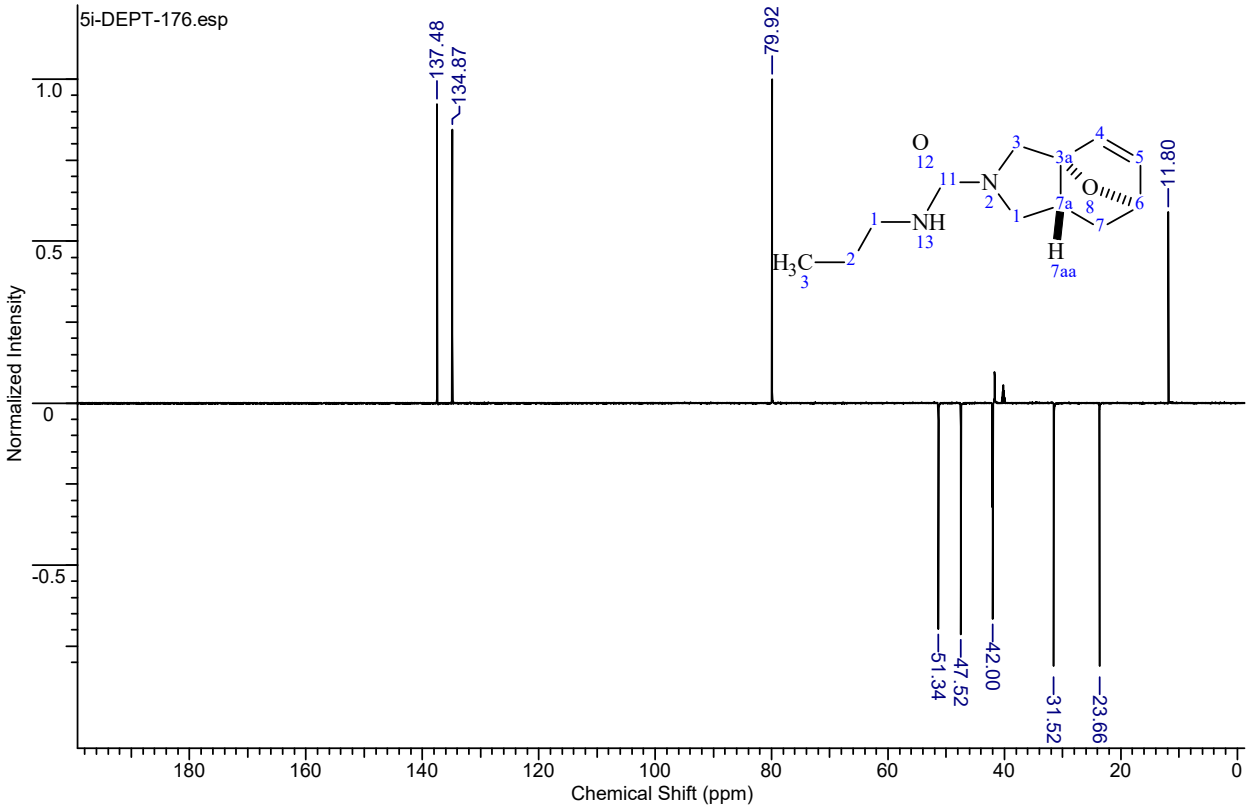
(3a*RS*,6*RS*,7a*RS*)-*N*-Propyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5i).

^{1}H NMR (700.2 MHz, DMSO-d_6)



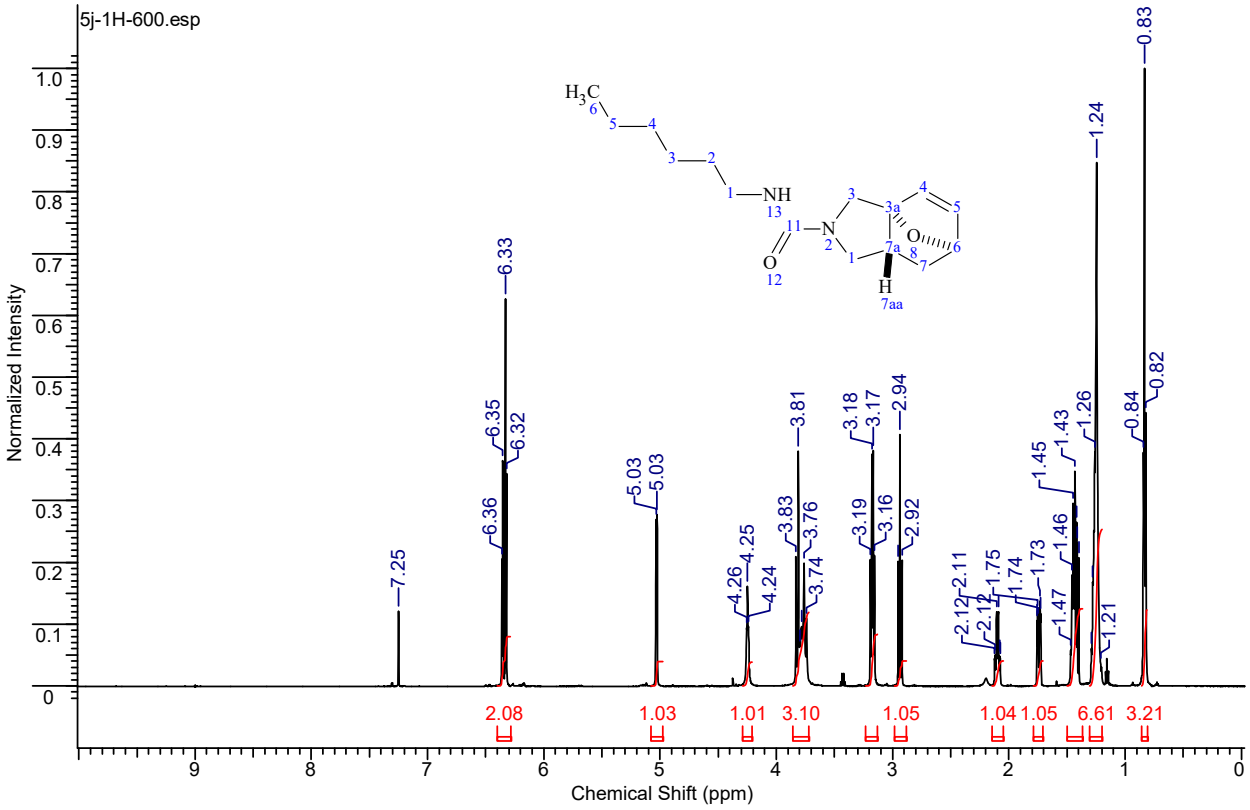
^{13}C NMR (176.1 MHz, DMSO-d_6)



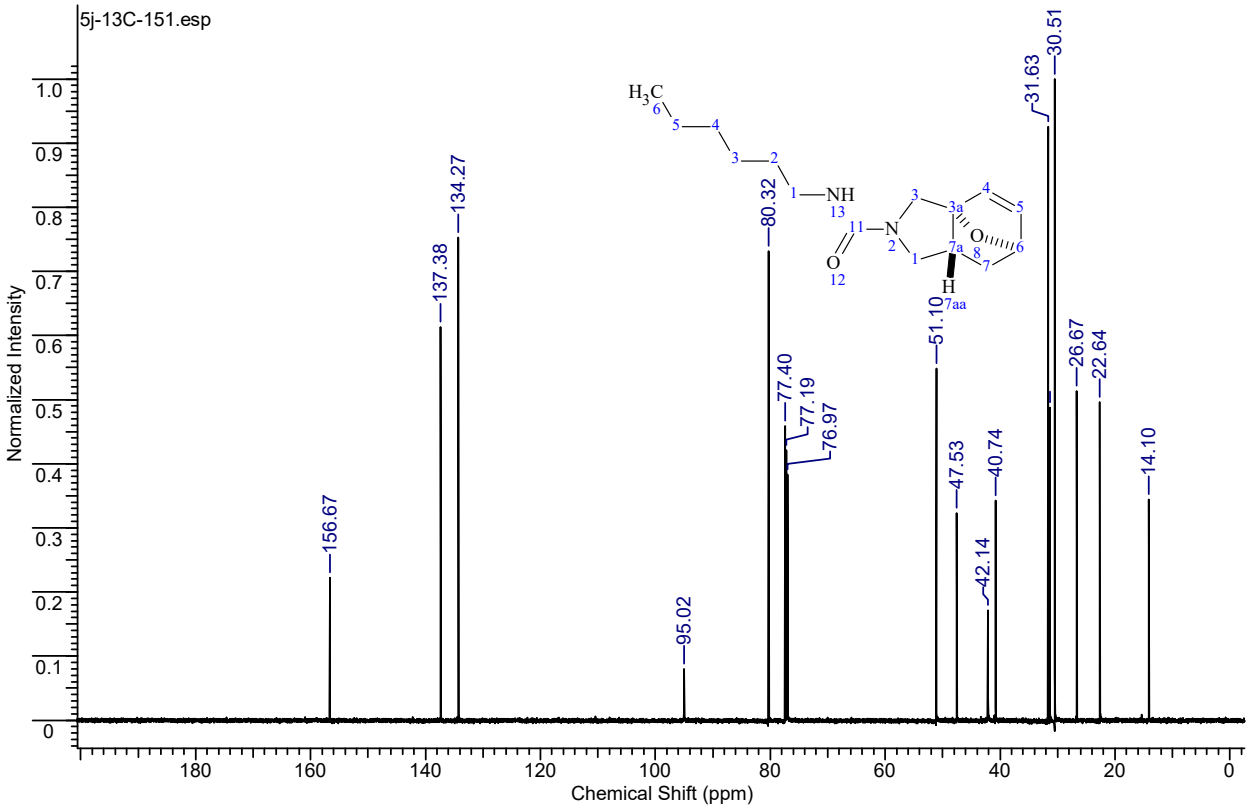

5i-DEPT-176.esp
137.48
134.87
79.92
11.80
51.34
47.52
42.00
31.52
23.66
Normalized Intensity
1.0
0.5
0
-0.5
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
12
11
N
2
3
3a
4
5
6
7a
8
7
1
NH
13
H3C
3
2
H
7aa

(3a*RS*,6*RS*,7a*RS*)-*N*-Hexyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5j).

^{1}H NMR (600.2 MHz, $CDCl_3$)

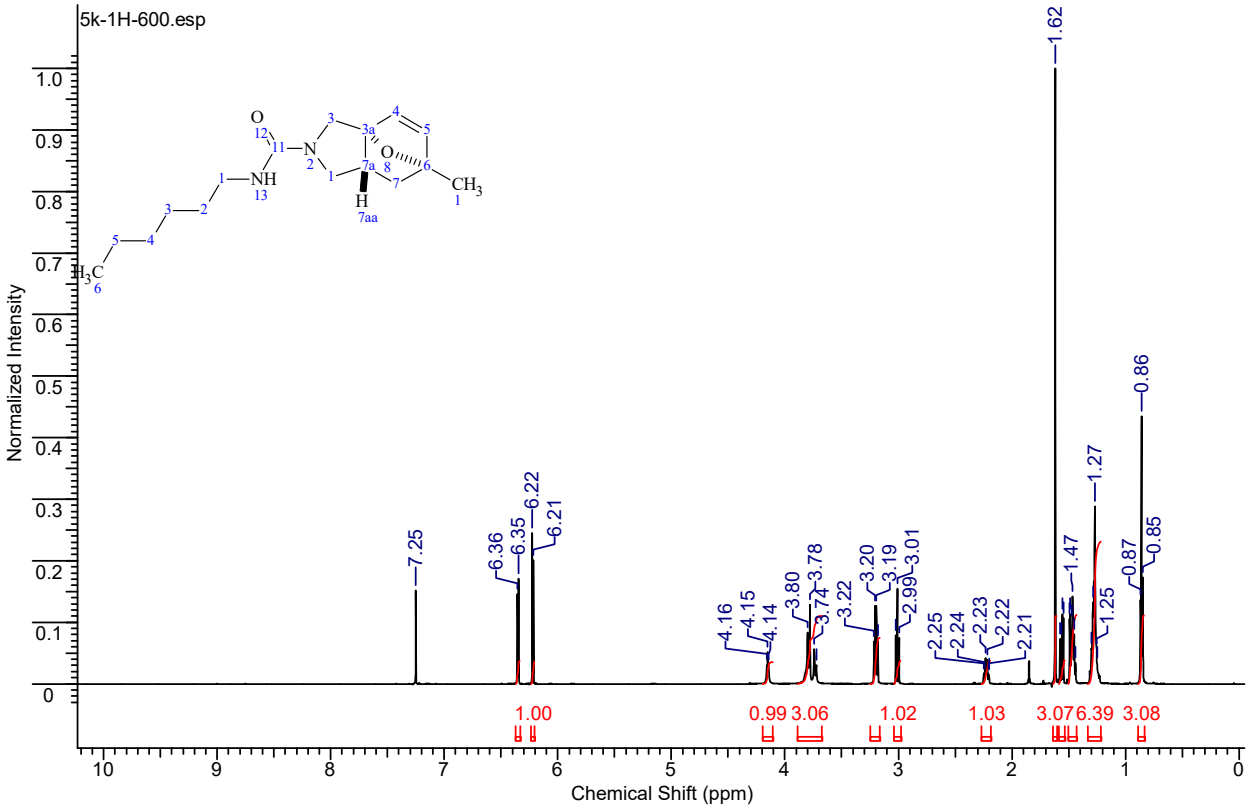


^{13}C NMR (150.9 MHz, $CDCl_3$)

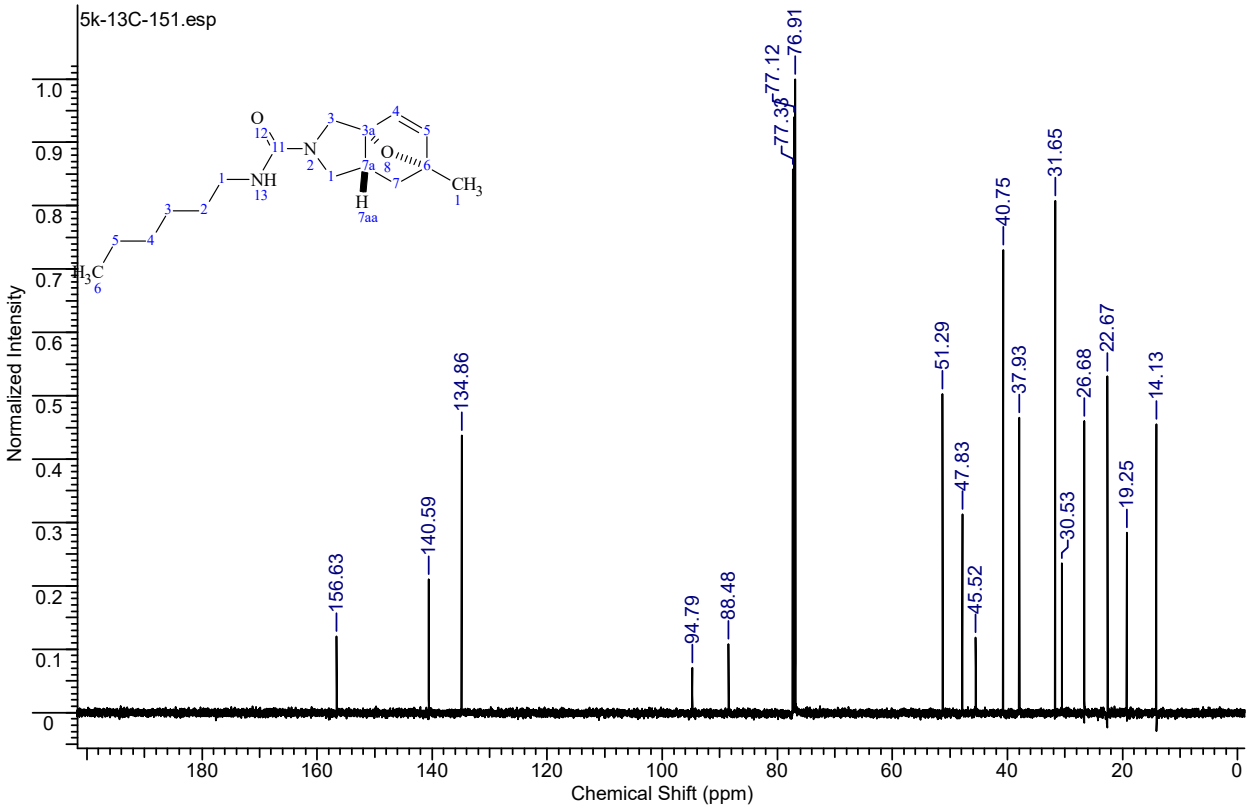


(3a*RS*,6*RS*,7a*RS*)-*N*-Hexyl-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5k).

^{1}H NMR (600.2 MHz, $CDCl_3$)

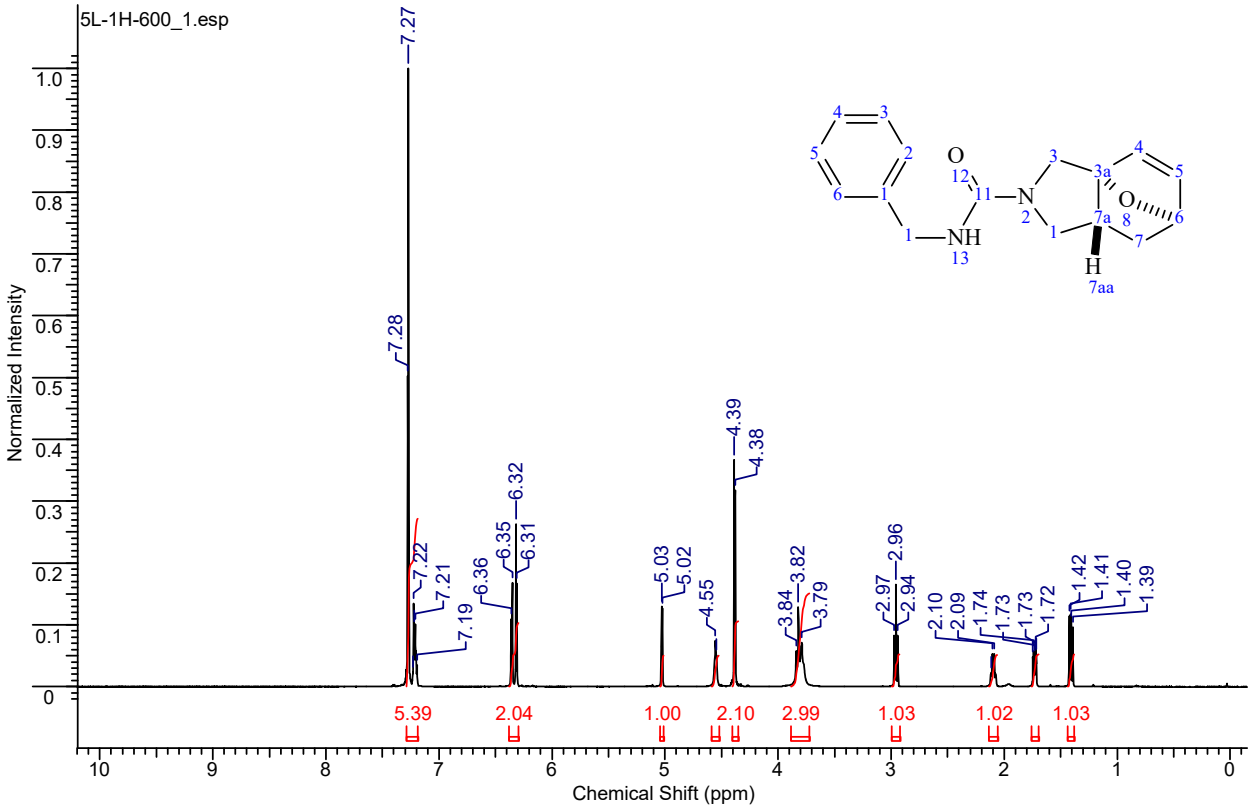


^{13}C NMR (150.9 MHz, $CDCl_3$)

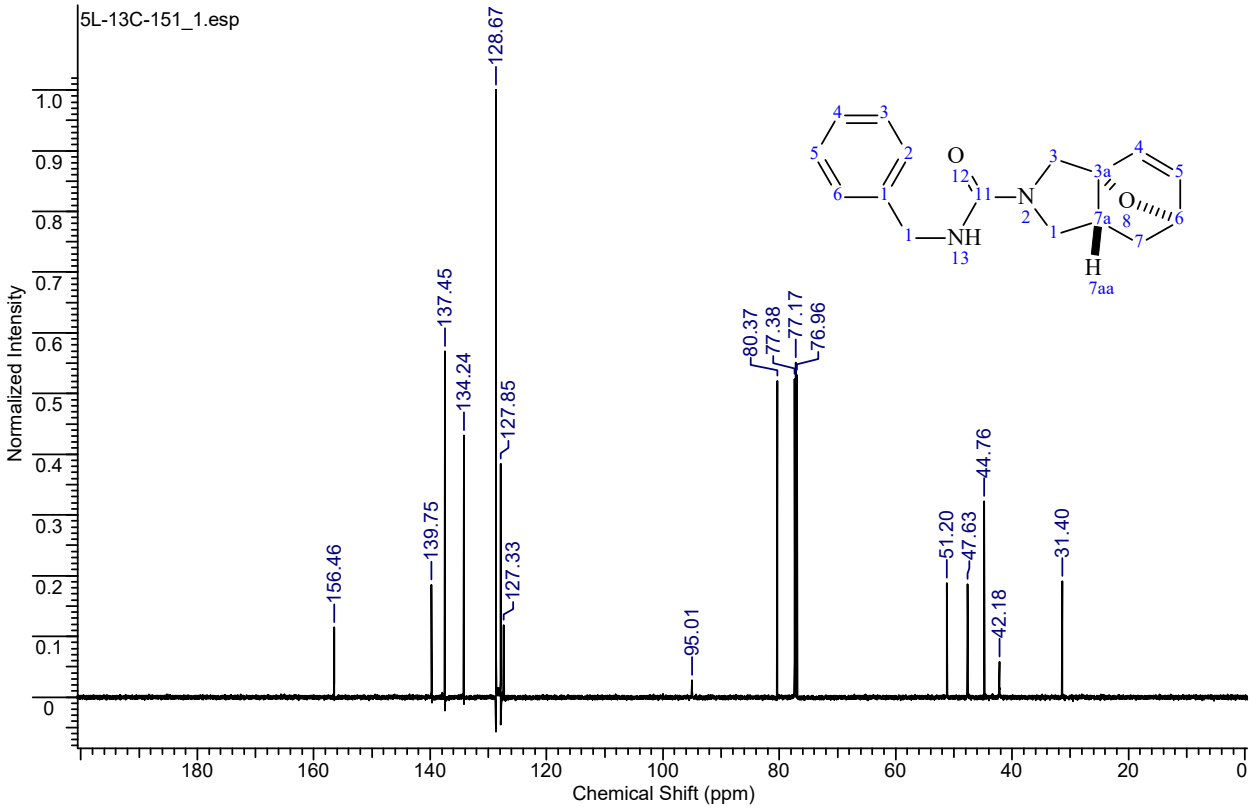


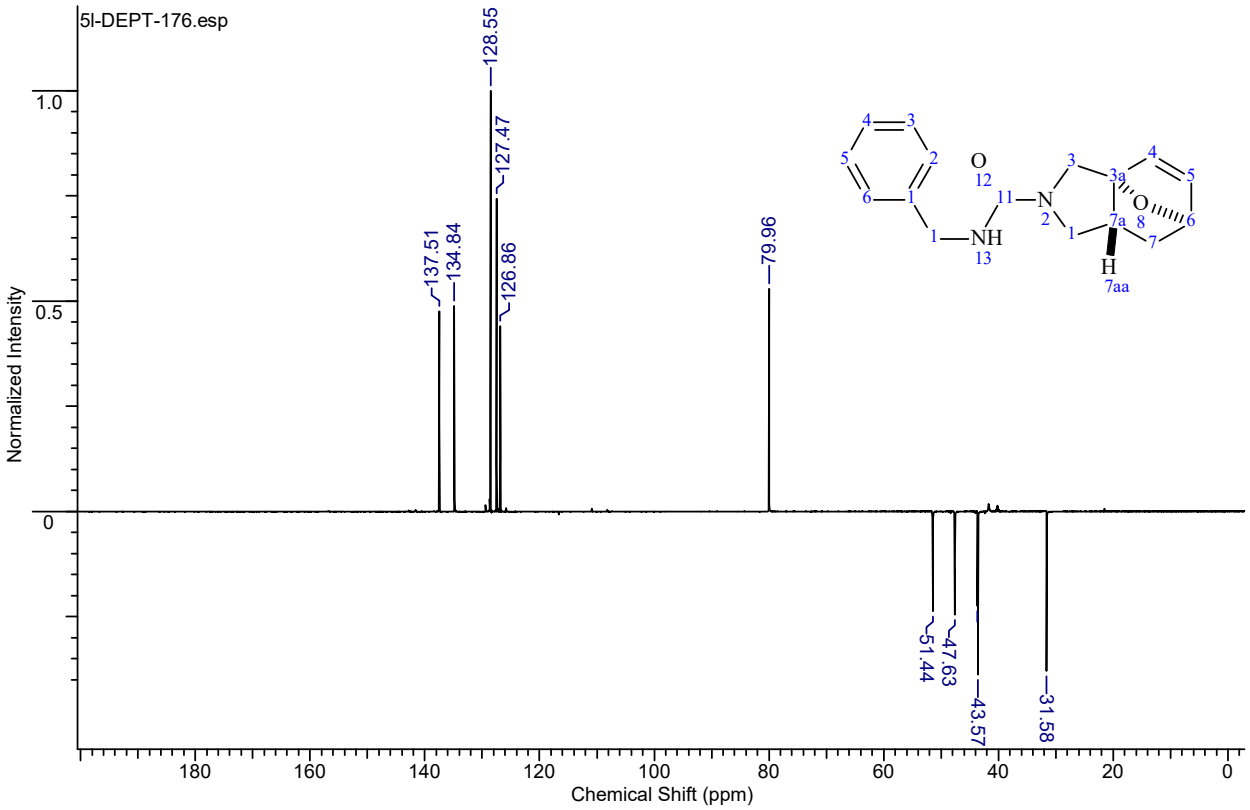
(3a*RS*,6*RS*,7a*RS*)-*N*-Benzyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5l).

^{1}H NMR (600.2 MHz, $CDCl_3$)



^{13}C NMR (150.9 MHz, $CDCl_3$)




5l-DEPT-176.esp
Normalized Intensity
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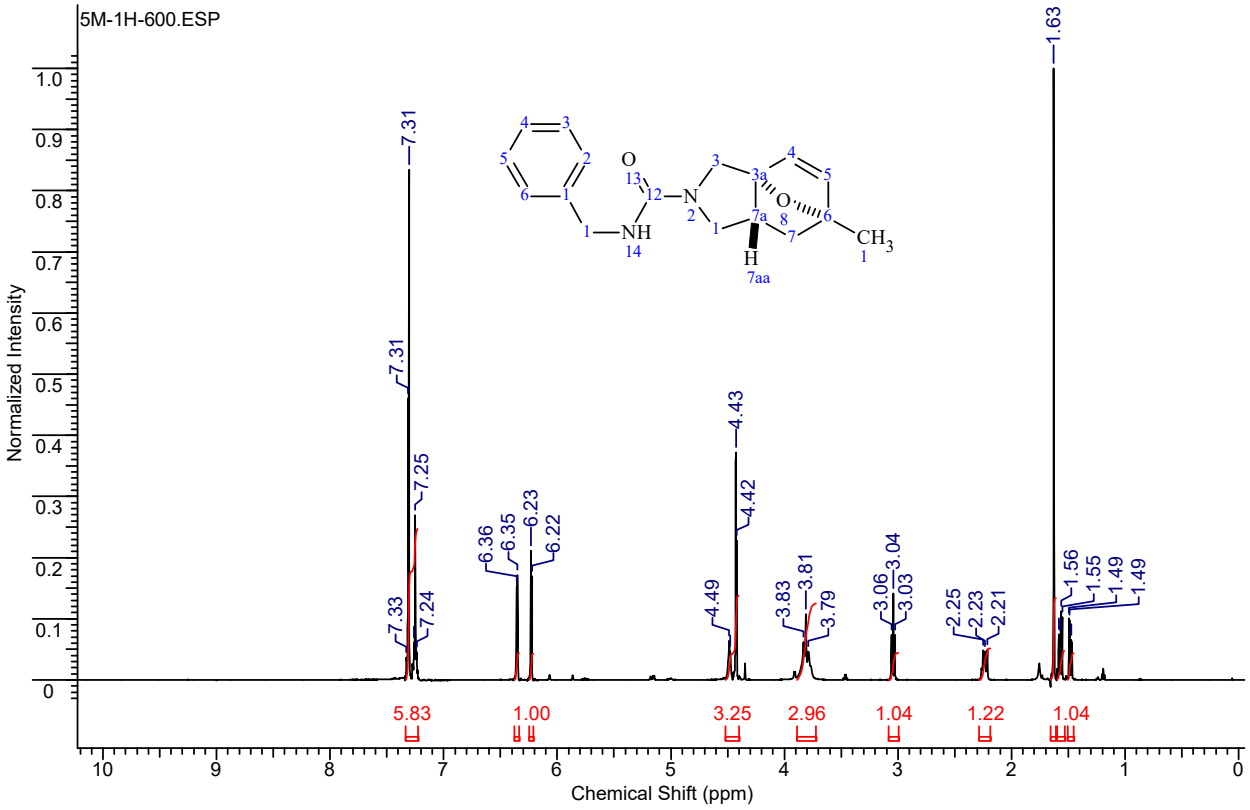
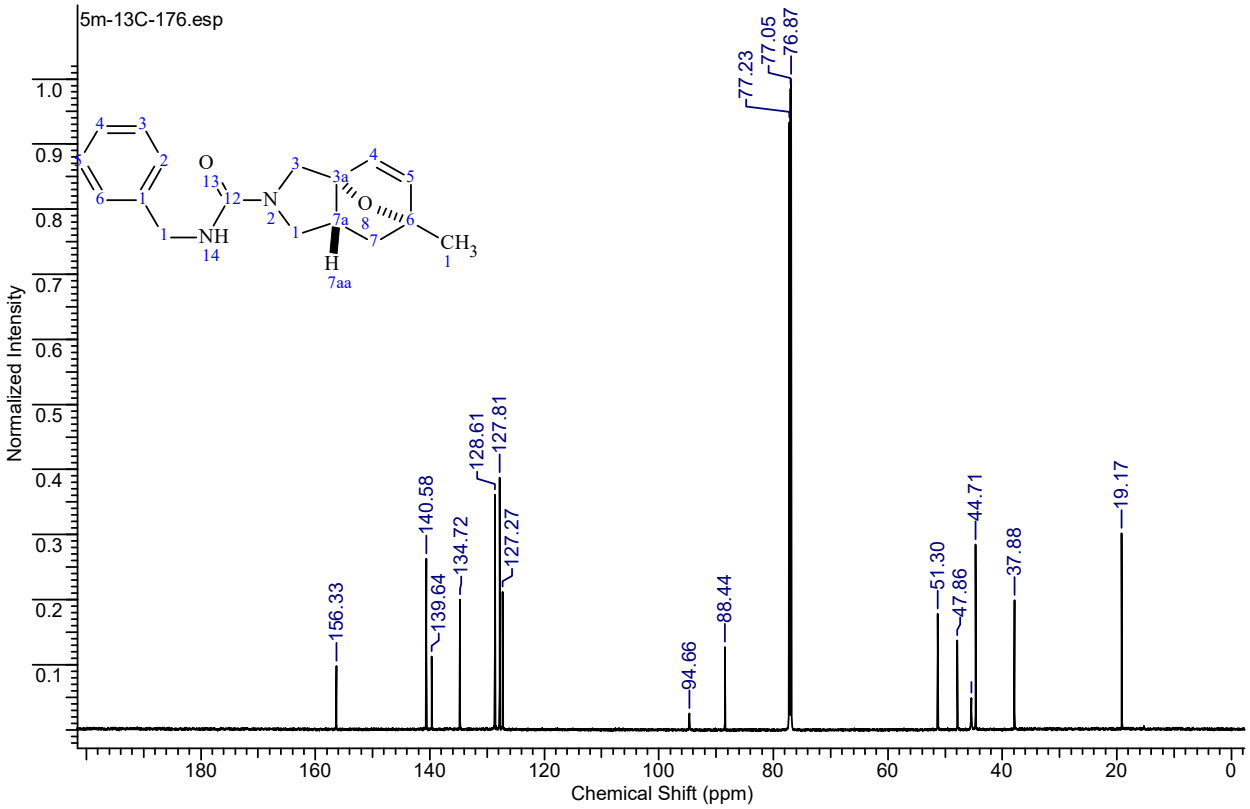
0.5
0
128.55
127.47
137.51
134.84
126.86
79.96
51.44
47.63
43.57
31.58
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
12
11
N
2
3
3a
4
5
6
7
7a
8
1
NH
13
H
7aa

(3a*RS*,6*RS*,7a*RS*)-*N*-Benzyl-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5m).

^{1}H NMR (600.2 MHz, $CDCl_3$)

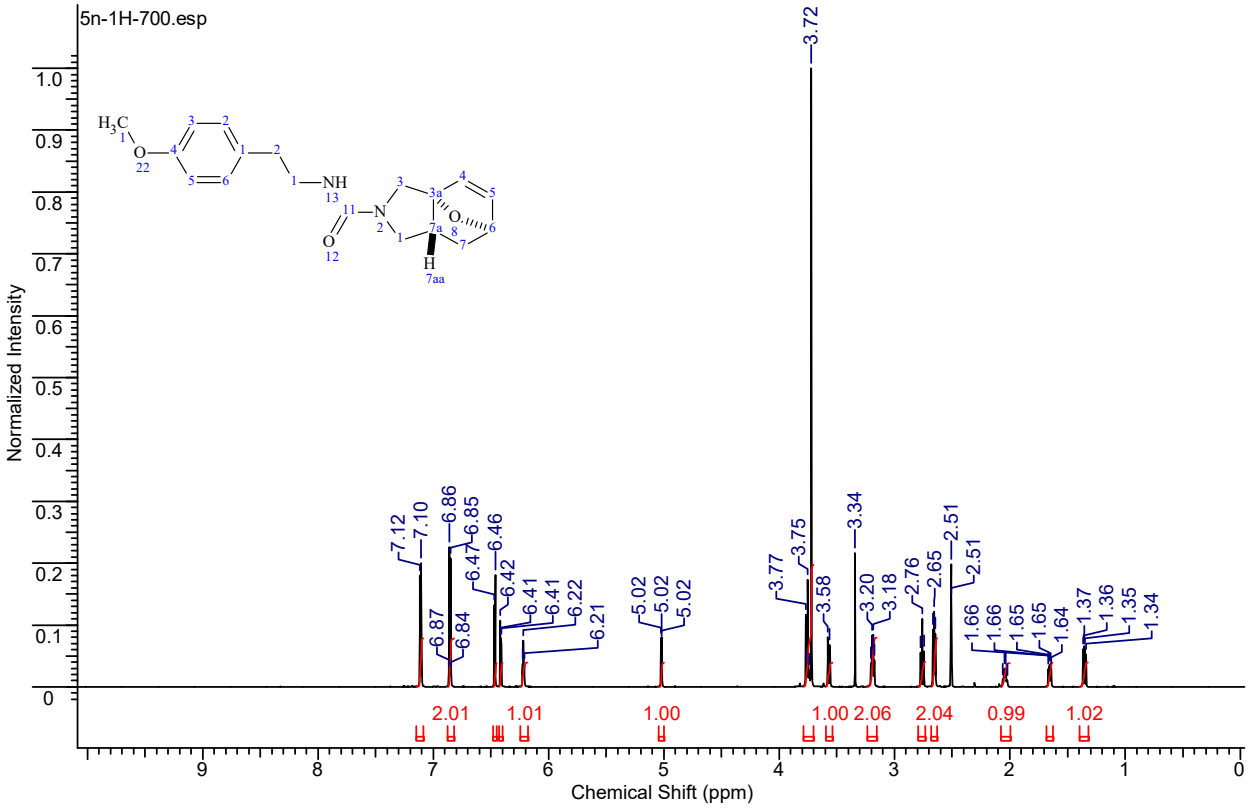


^{13}C NMR (176.1 MHz, $CDCl_3$)

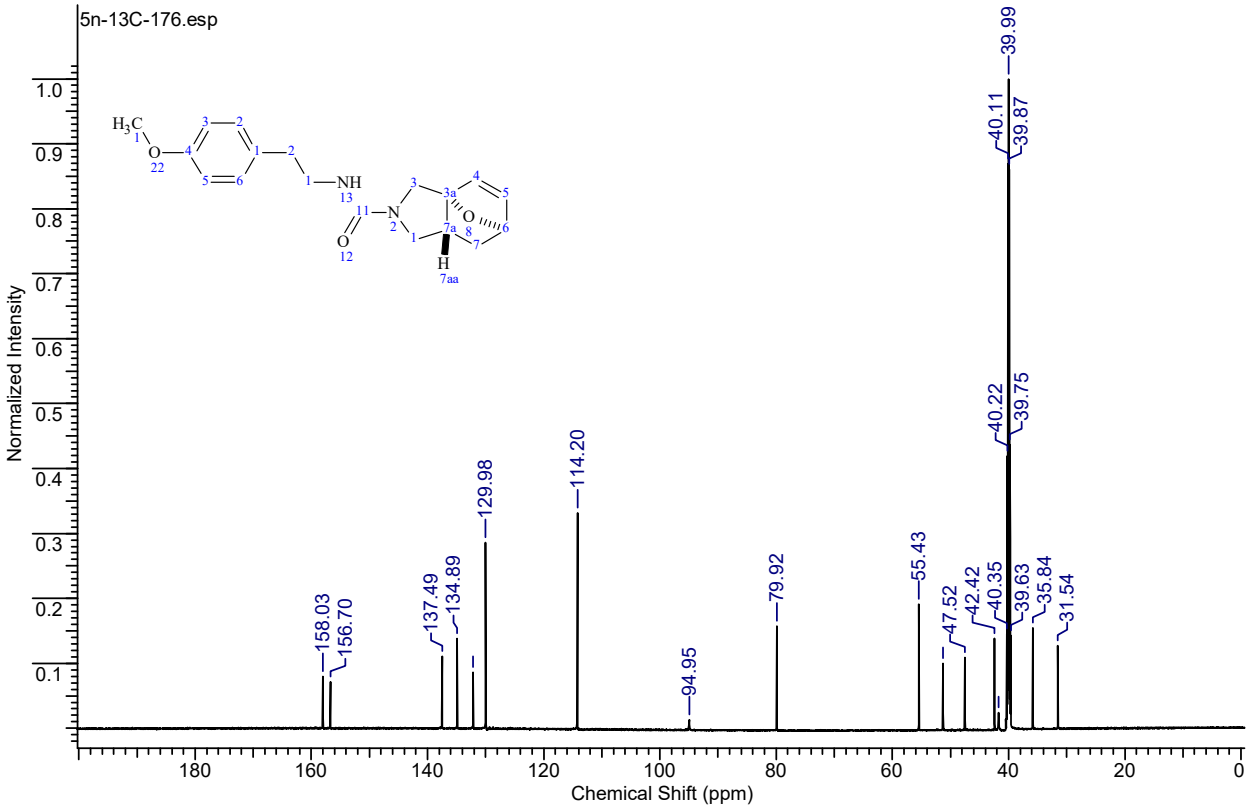


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenethyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5n).

^{1}H NMR (700.2 MHz, DMSO-d_6)

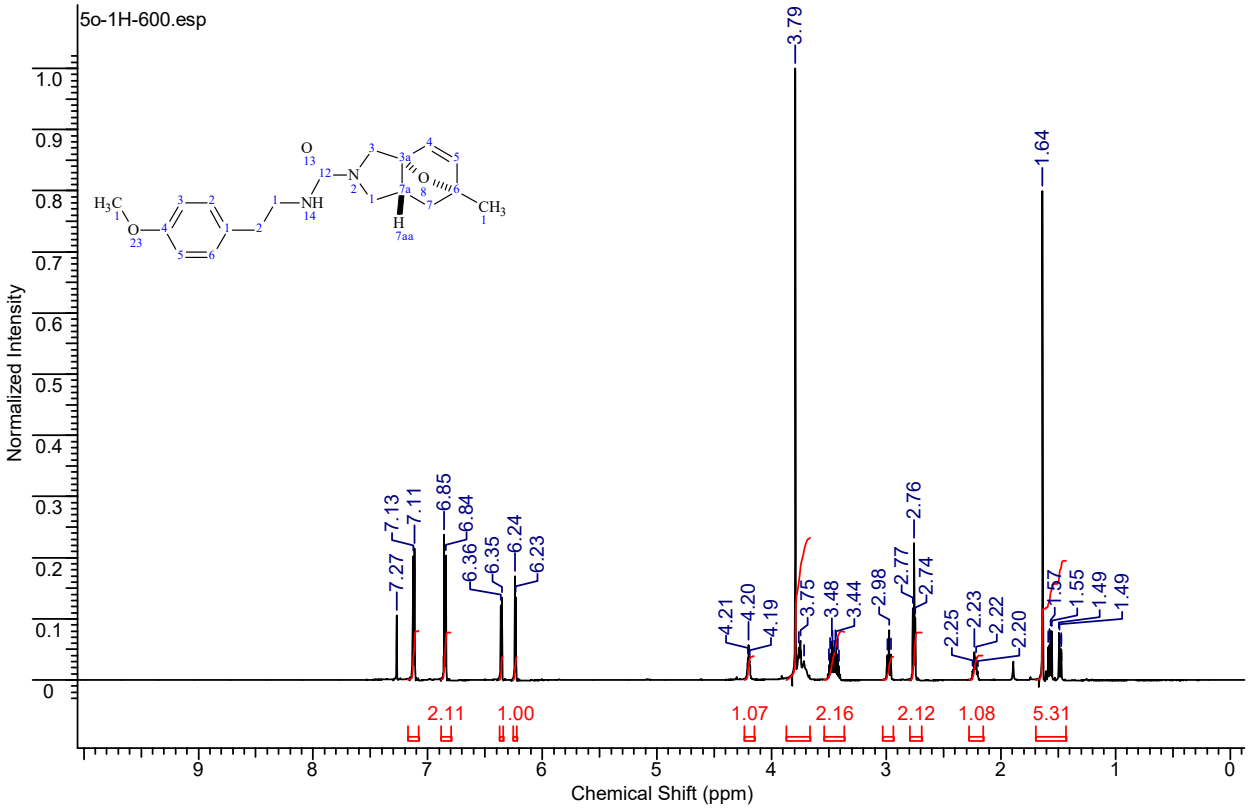


^{13}C NMR (176.1 MHz, DMSO-d_6)

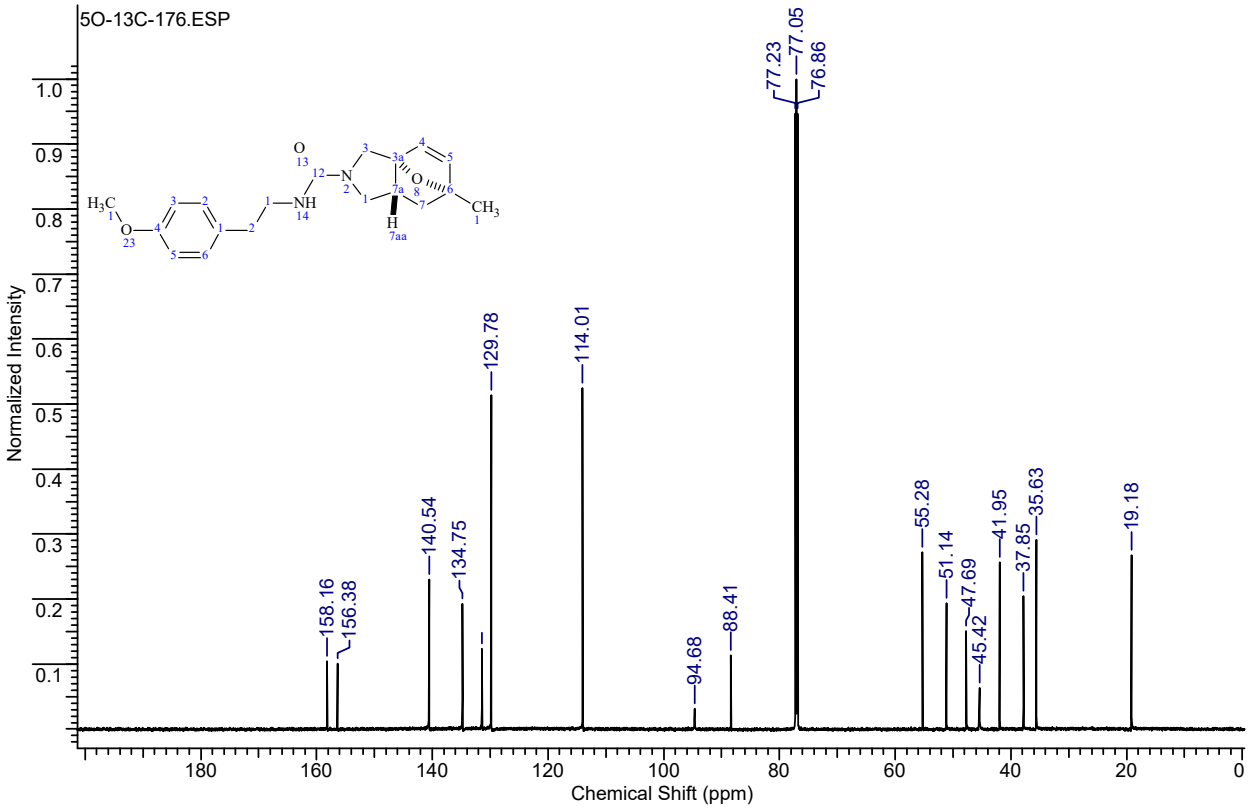


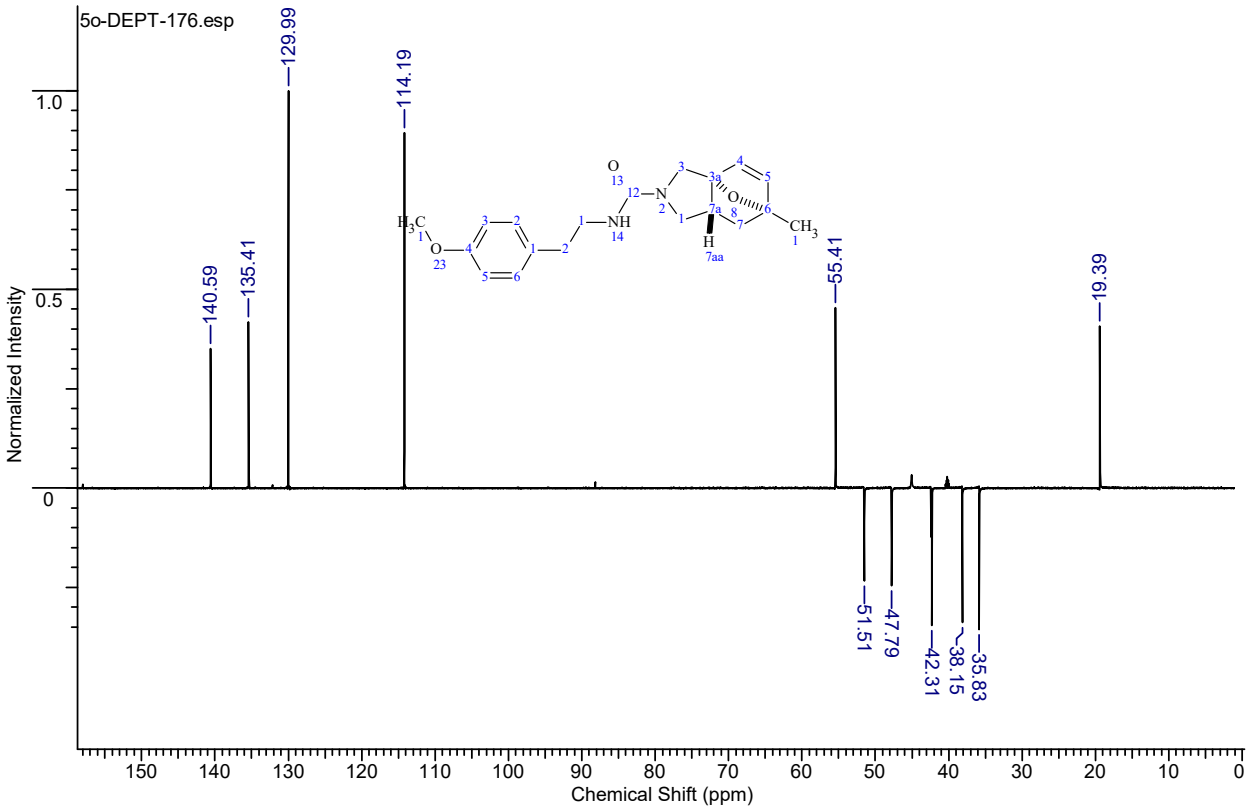
(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenethyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboxamide (5o).

^{1}H NMR (600.2 MHz, $CDCl_3$)

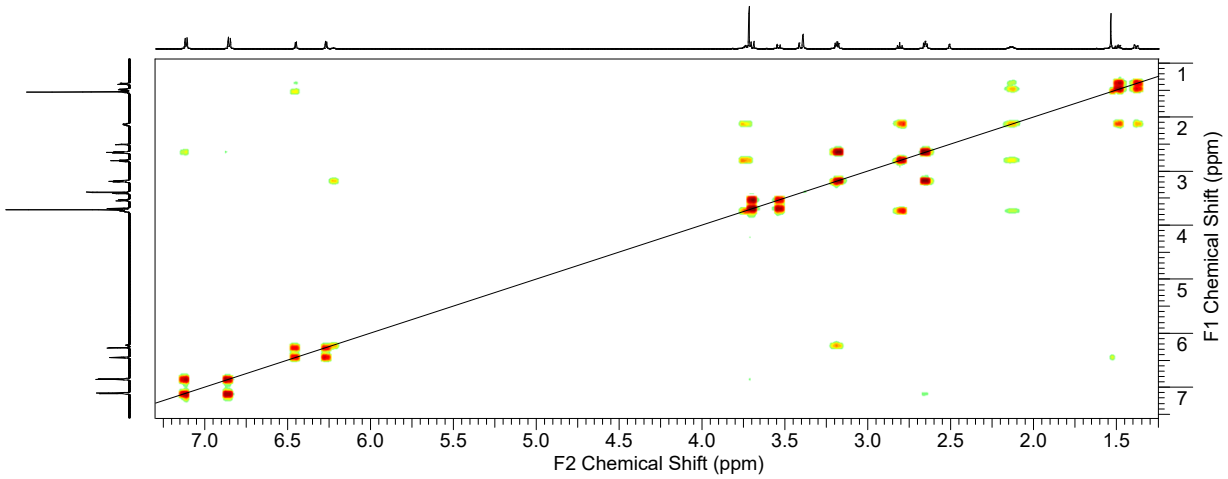


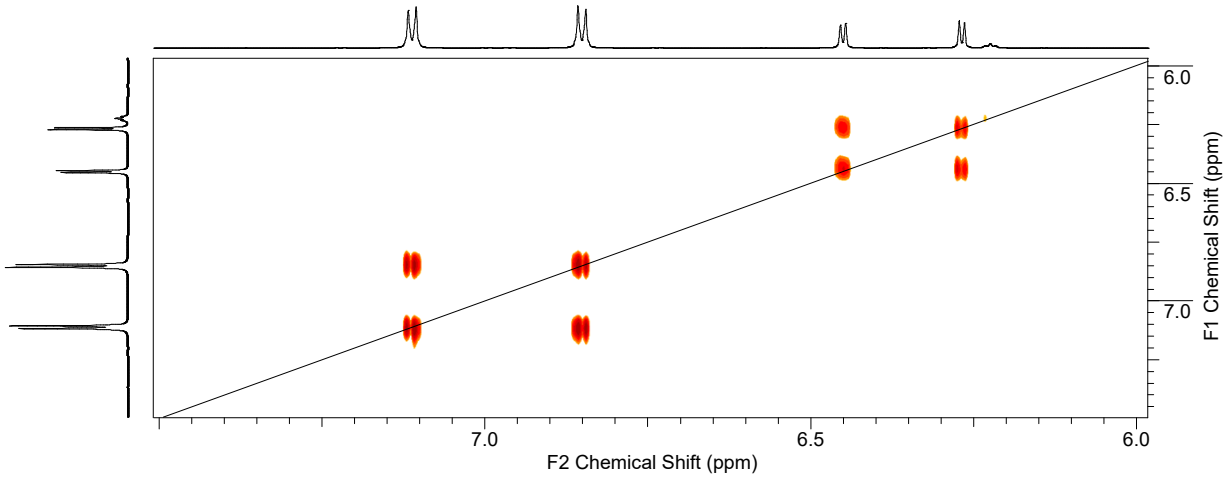
^{13}C NMR (176.1 MHz, $CDCl_3$)

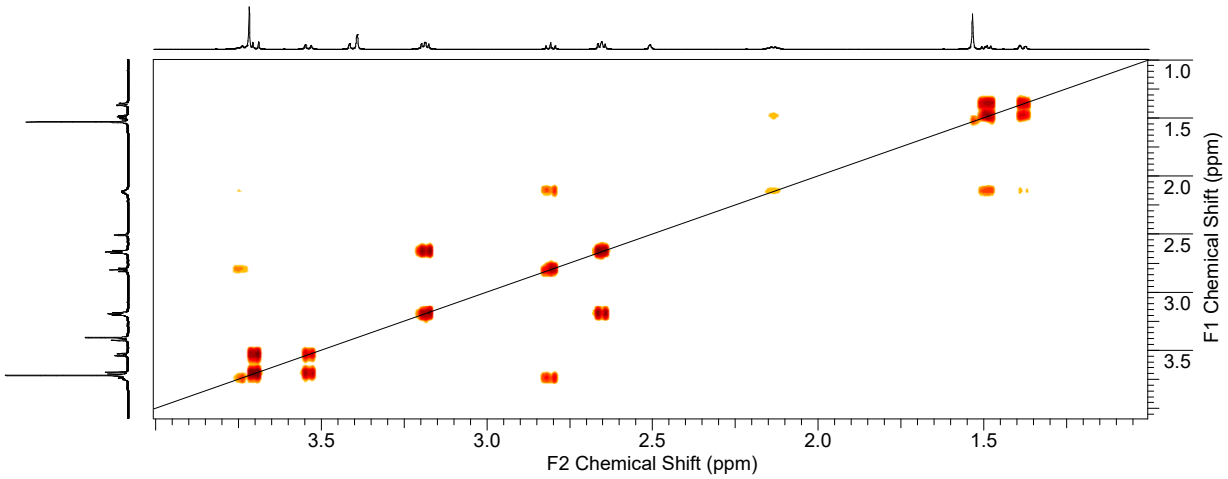



5o-DEPT-176.esp
129.99
114.19
140.59
135.41
55.41
19.39
51.51
47.79
42.31
38.15
35.83
1.0
0.5
0
Normalized Intensity
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

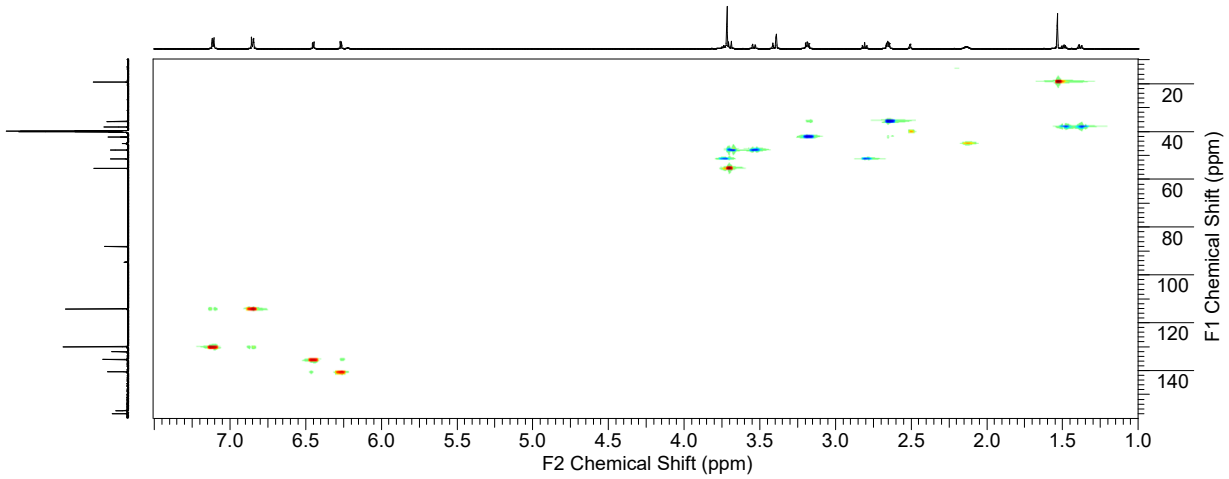
5o-COESY

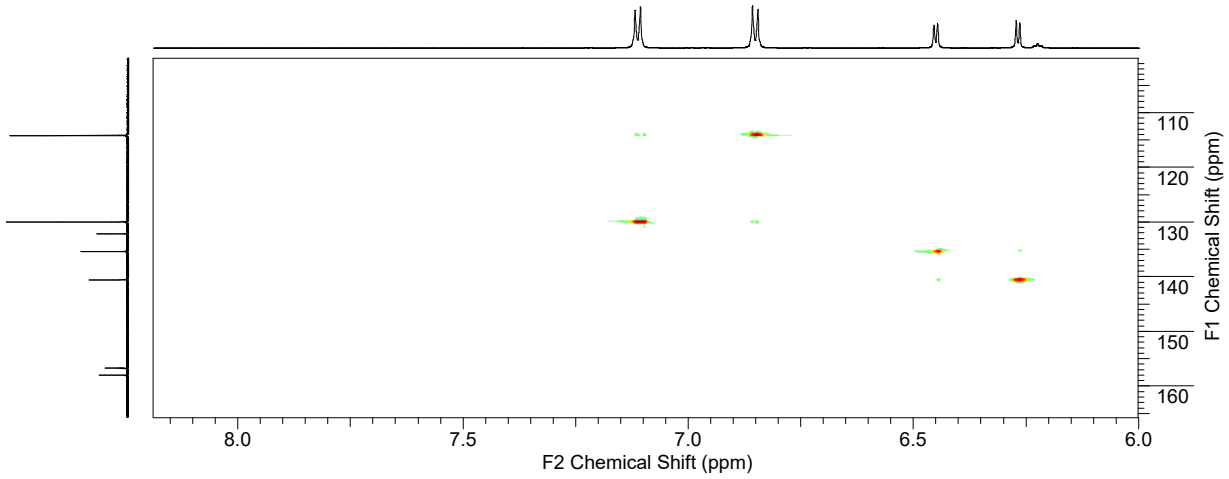

F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)

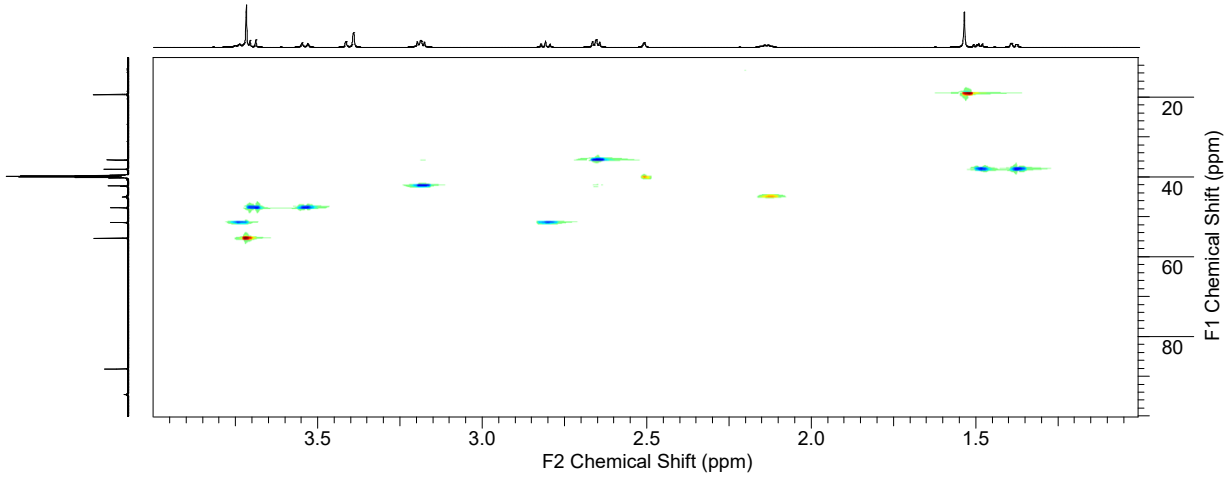

F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)


F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)

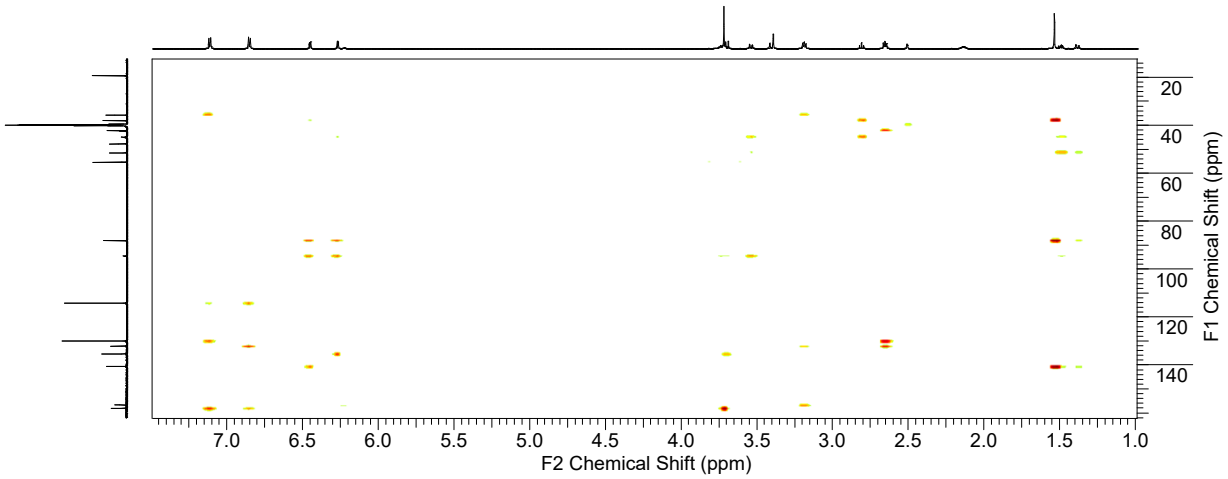
5o-HMQC

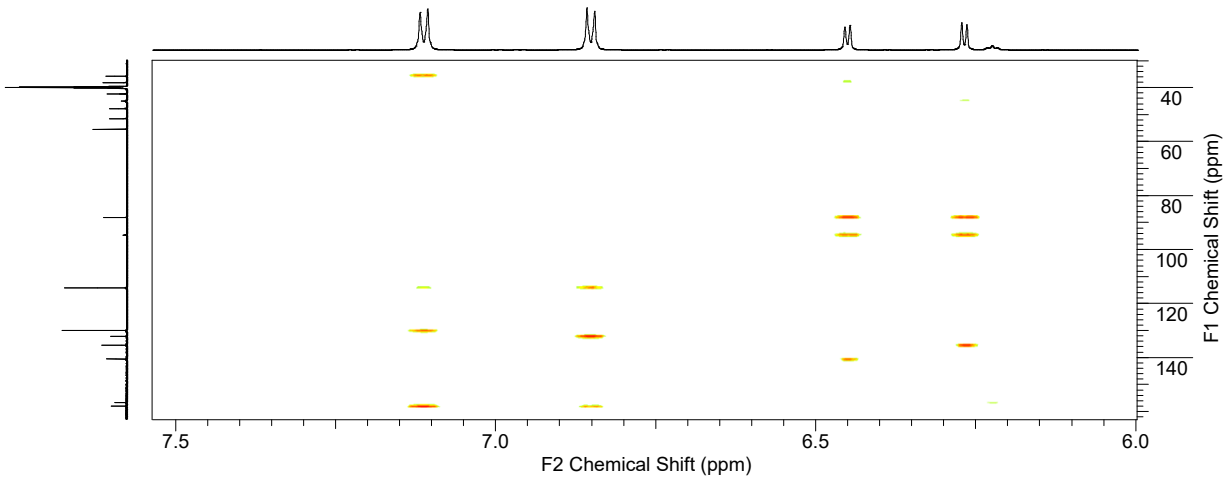

20
40
60
80
100
120
140
F1 Chemical Shift (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
F2 Chemical Shift (ppm)

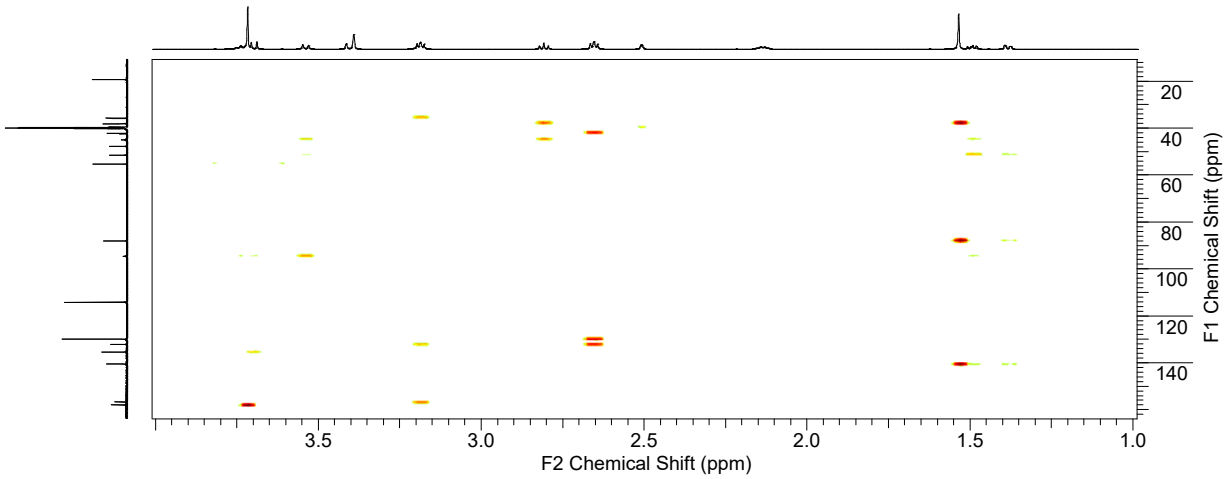

110
120
130
140
150
160
F1 Chemical Shift (ppm)
8.0
7.5
7.0
6.5
6.0
F2 Chemical Shift (ppm)


20
40
60
80
F1 Chemical Shift (ppm)
3.5
3.0
2.5
2.0
1.5
F2 Chemical Shift (ppm)

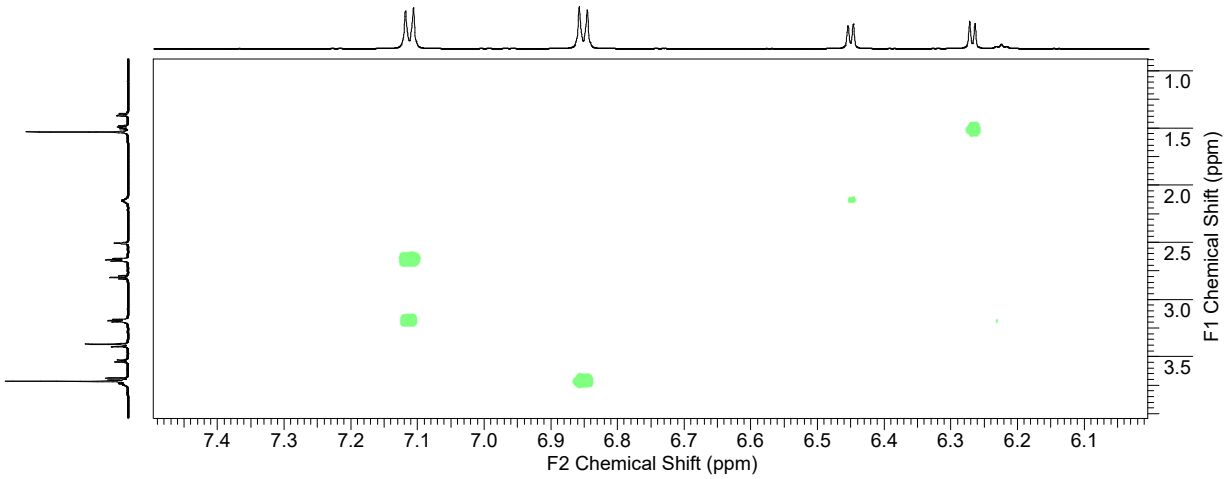
5o-HMBC

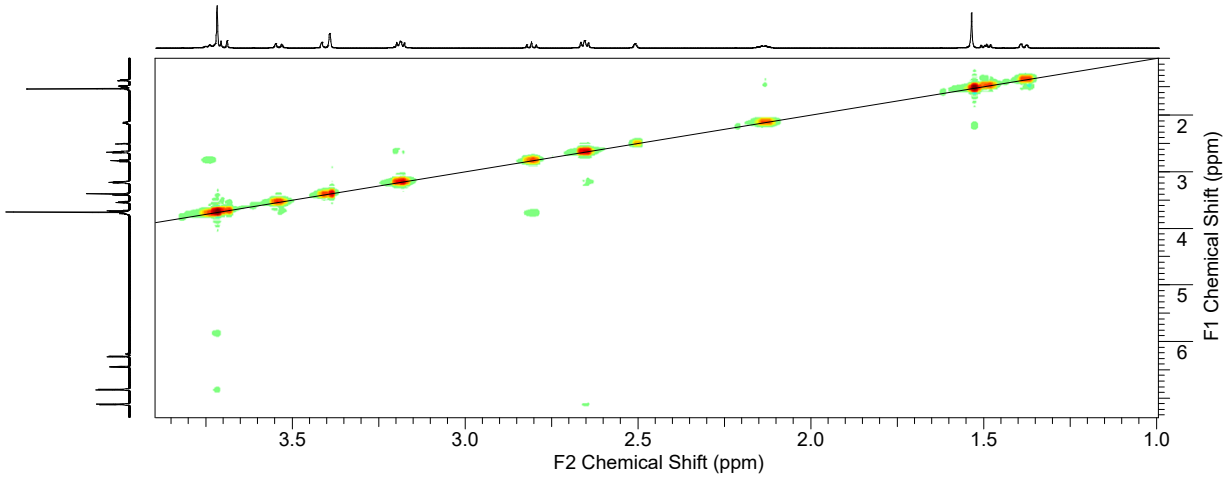

20
40
60
80
100
120
140
F1 Chemical Shift (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
F2 Chemical Shift (ppm)


40
60
80
100
120
140
F1 Chemical Shift (ppm)
7.5
7.0
6.5
6.0
F2 Chemical Shift (ppm)


20
40
60
80
100
120
140
F1 Chemical Shift (ppm)
3.5
3.0
2.5
2.0
1.5
1.0
F2 Chemical Shift (ppm)

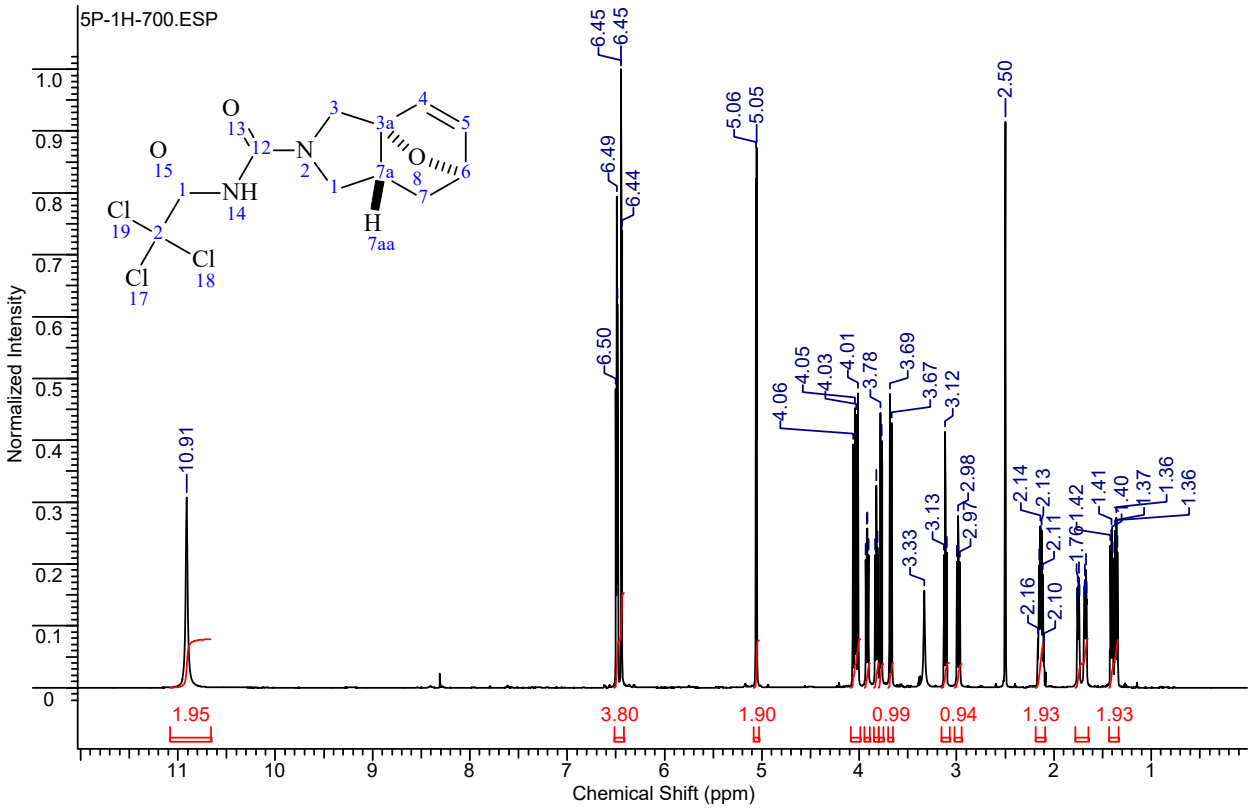
5o-NOESY


1.0
1.5
2.0
2.5
3.0
3.5
F1 Chemical Shift (ppm)
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
F2 Chemical Shift (ppm)

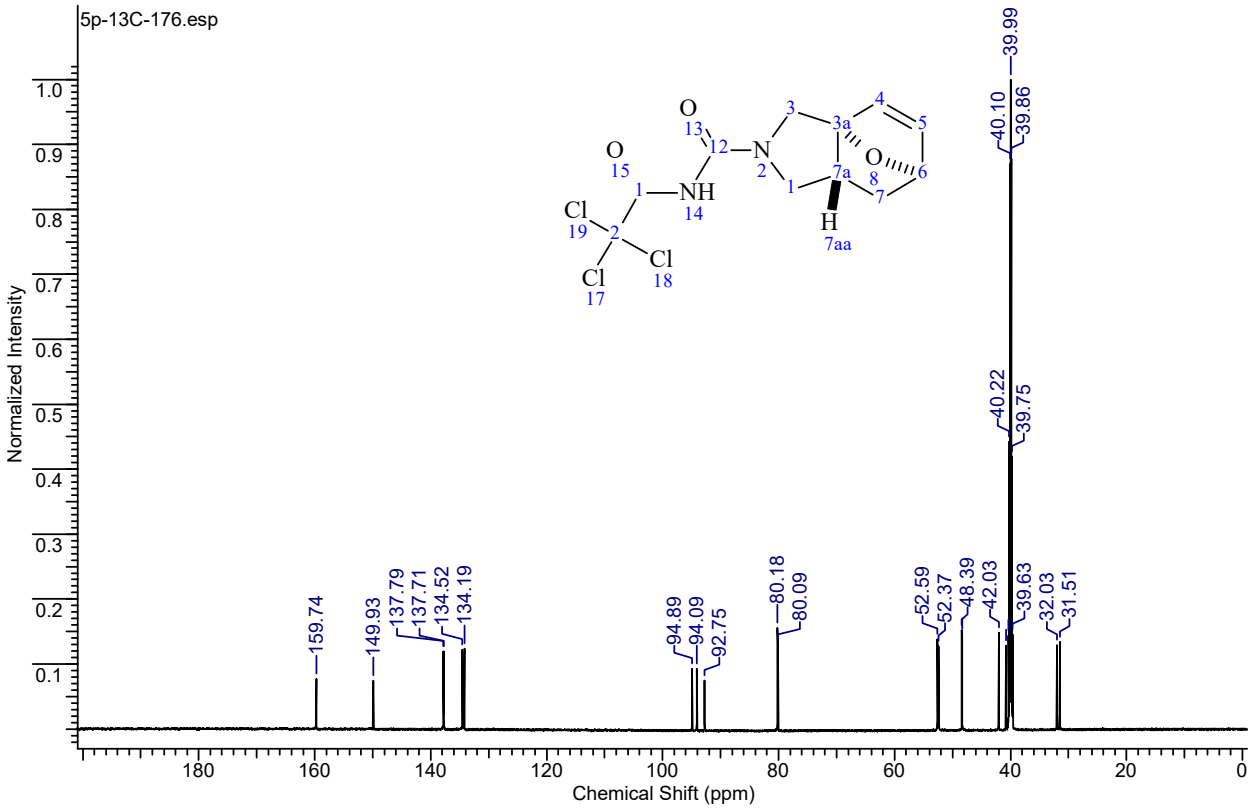

2
3
4
5
6
F1 Chemical Shift (ppm)
3.5
3.0
2.5
2.0
1.5
1.0
F2 Chemical Shift (ppm)

(3a*RS*,6*RS*,7a*RS*)-*N*-(2,2,2-Trichloroacetyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5p).

^{1}H NMR (700.2 MHz, DMSO-d_6)

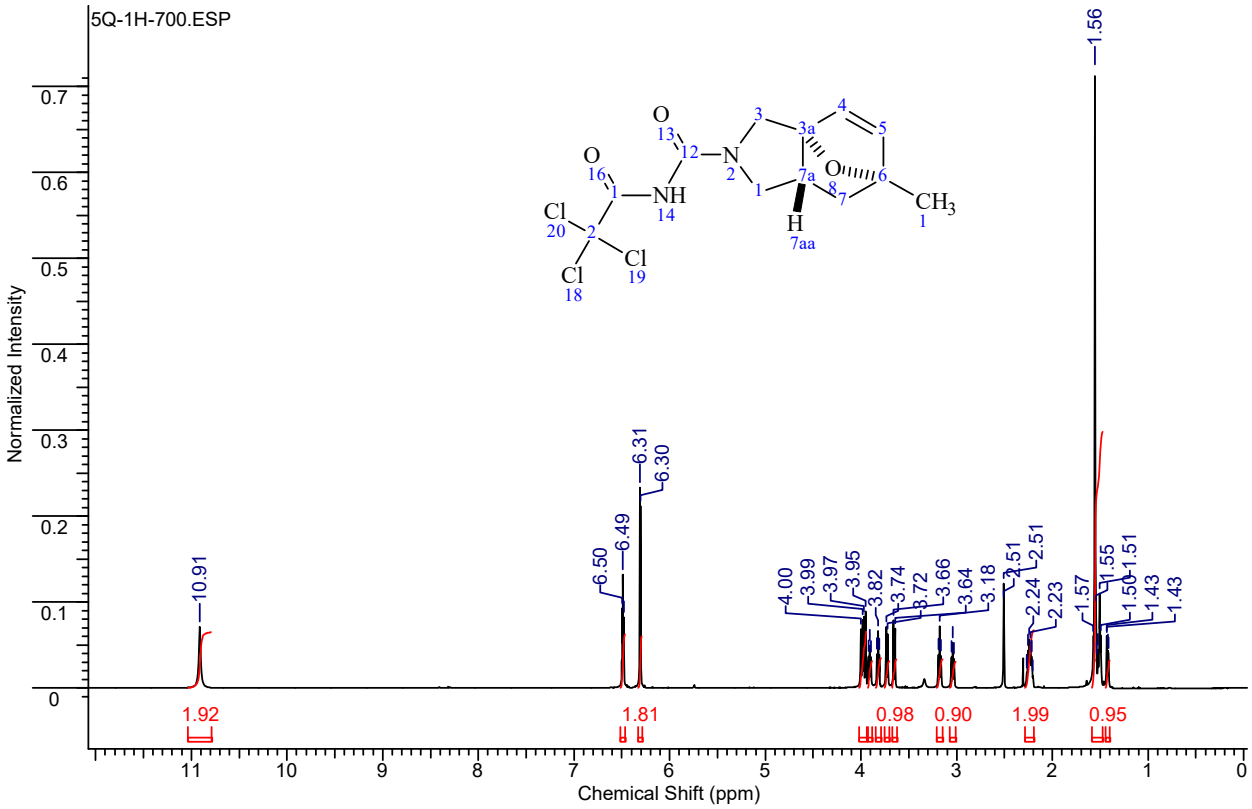


^{13}C NMR (176.1 MHz, DMSO-d_6)

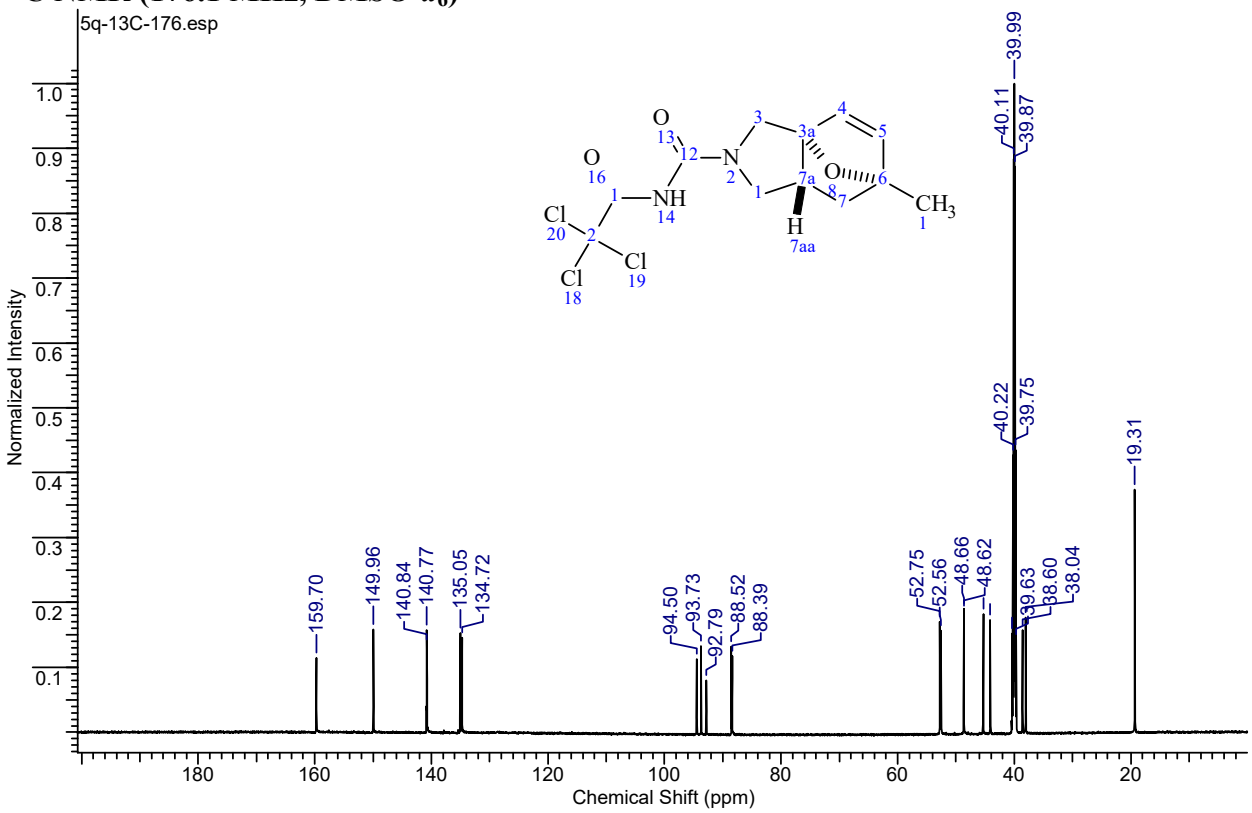


(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-(trichloroacetyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5q).

^{1}H NMR (700.2 MHz, DMSO-d_6)

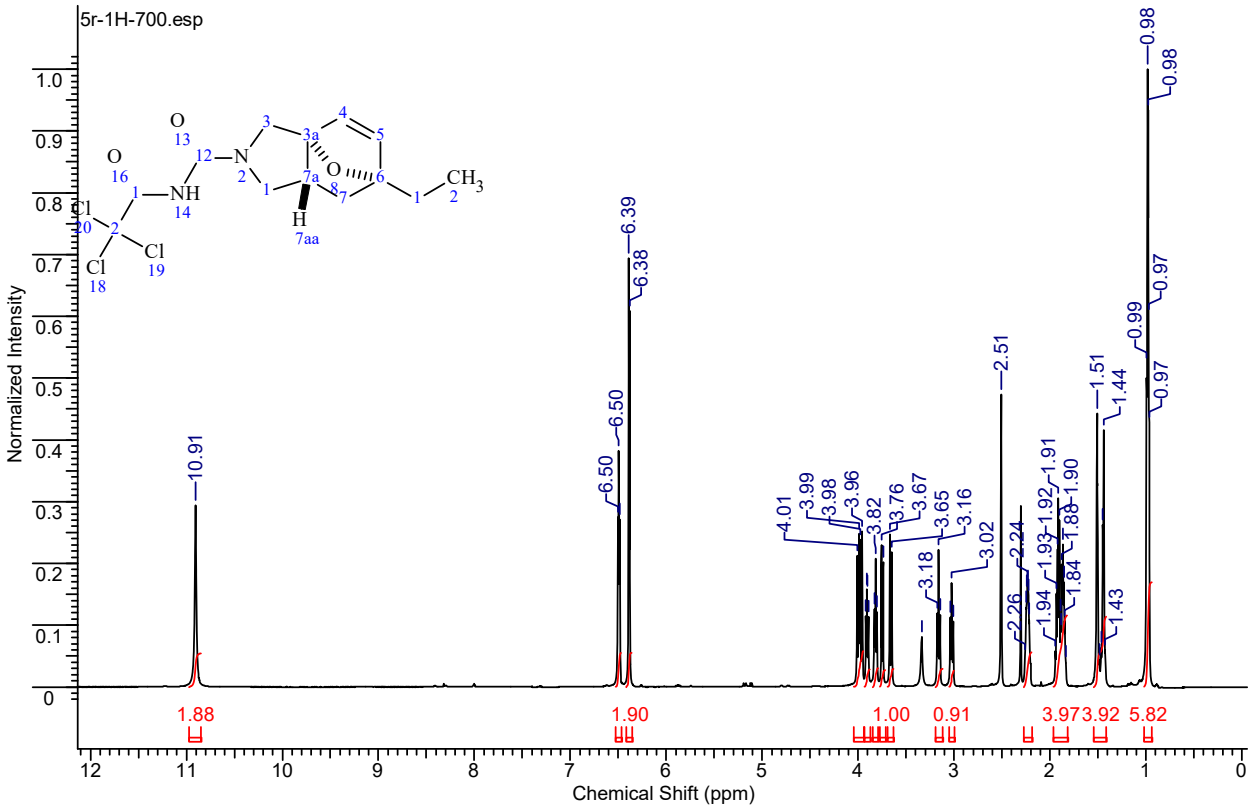


^{13}C NMR (176.1 MHz, DMSO-d_6)

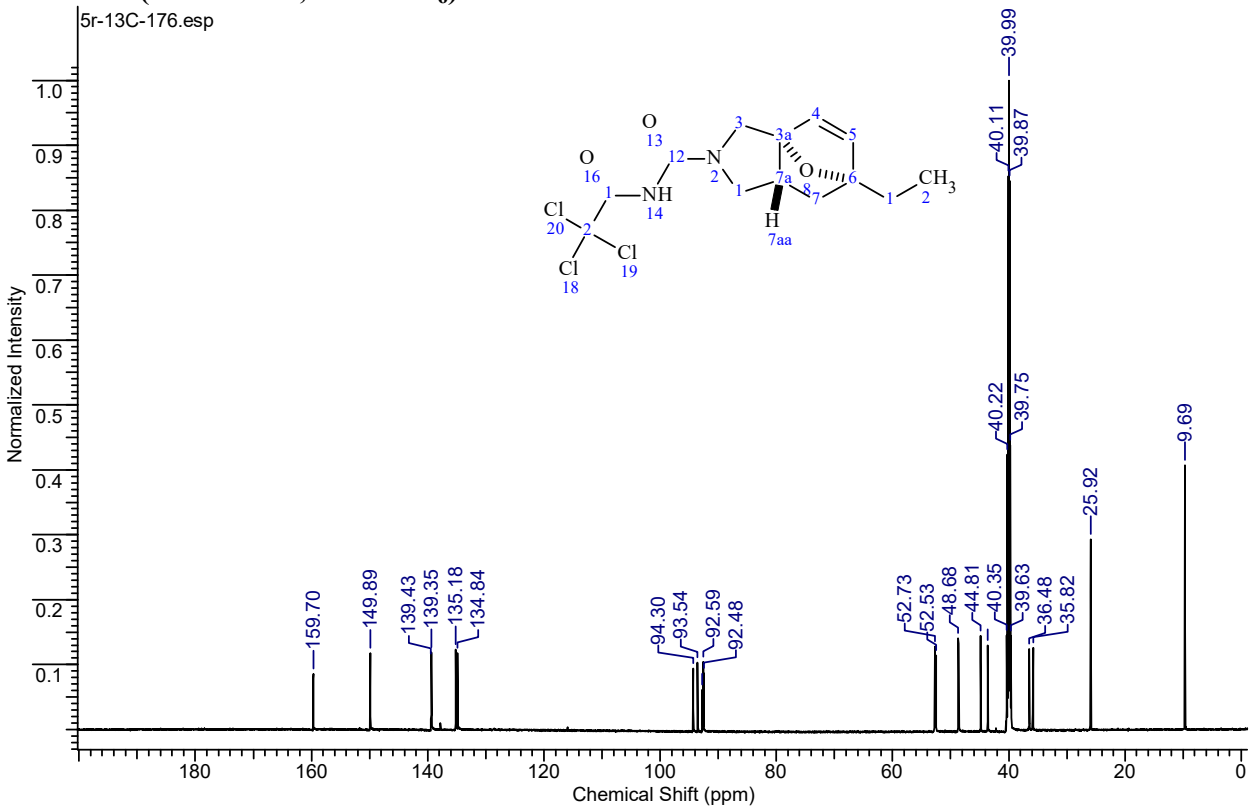


(3a*RS*,6*RS*,7a*RS*)-6-Ethyl-*N*-(trichloroacetyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5r).

^{1}H NMR (700.2 MHz, DMSO-d_6)

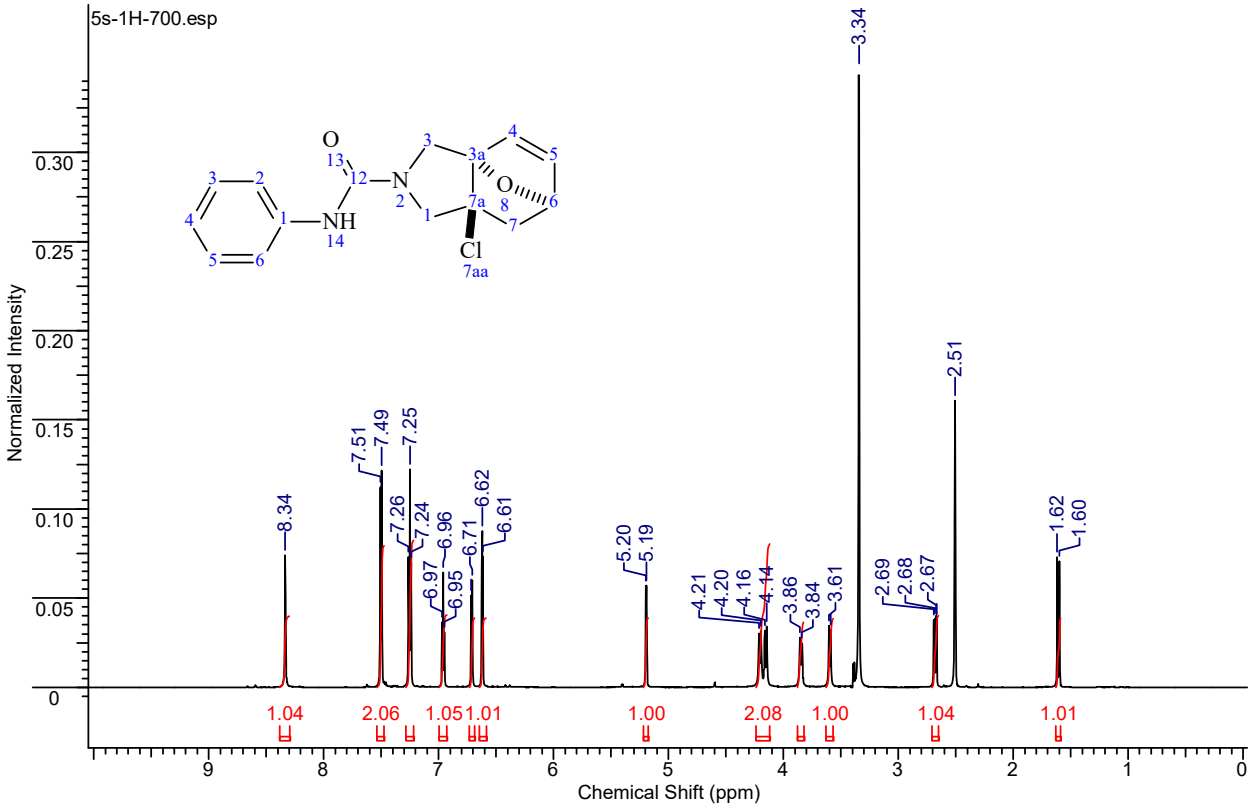


^{13}C NMR (176.1 MHz, DMSO-d_6)

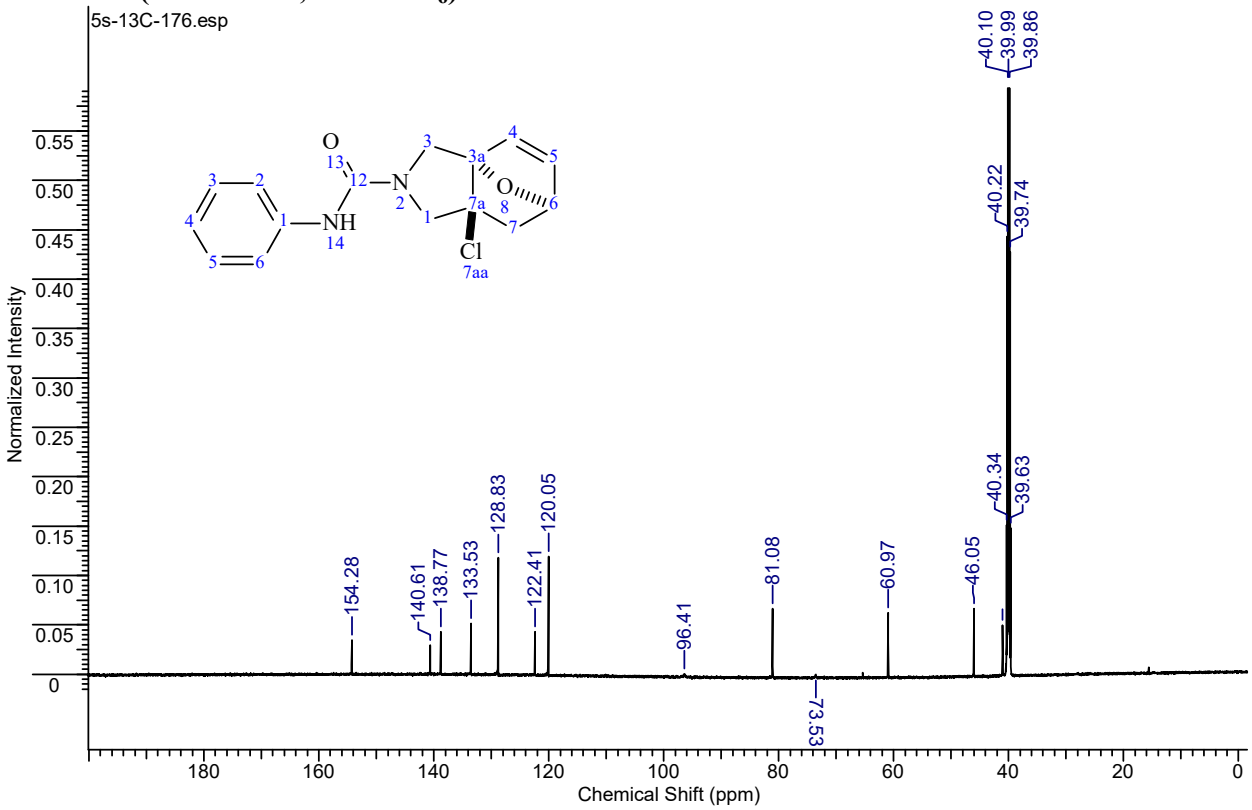


(3a*SR*,6*RS*,7a*SR*)-7a-Chloro-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5s).

^{1}H NMR (700.2 MHz, DMSO-d_6)

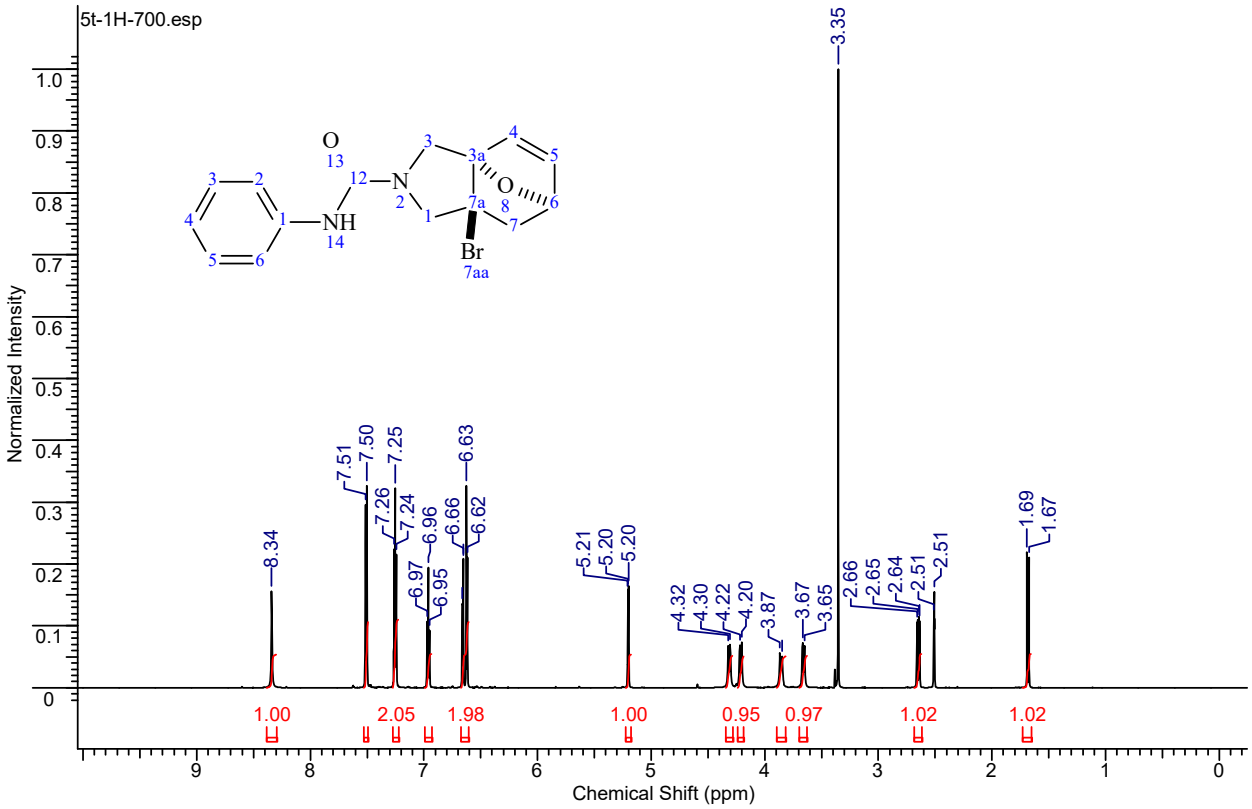


^{13}C NMR (176.1 MHz, DMSO-d_6)

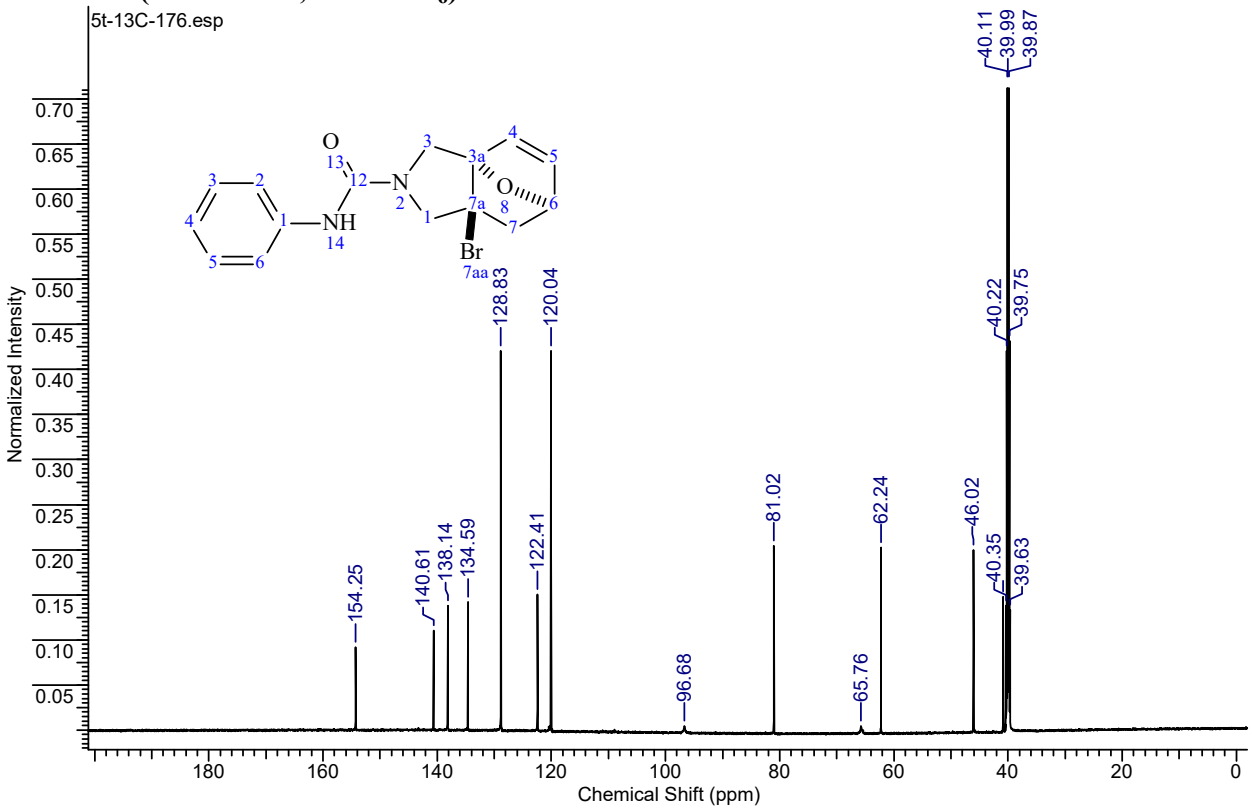


(3a*SR*,6*RS*,7a*SR*)-7a-Bromo-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carboxamide (5t).

^{1}H NMR (700.2 MHz, DMSO-d_6)

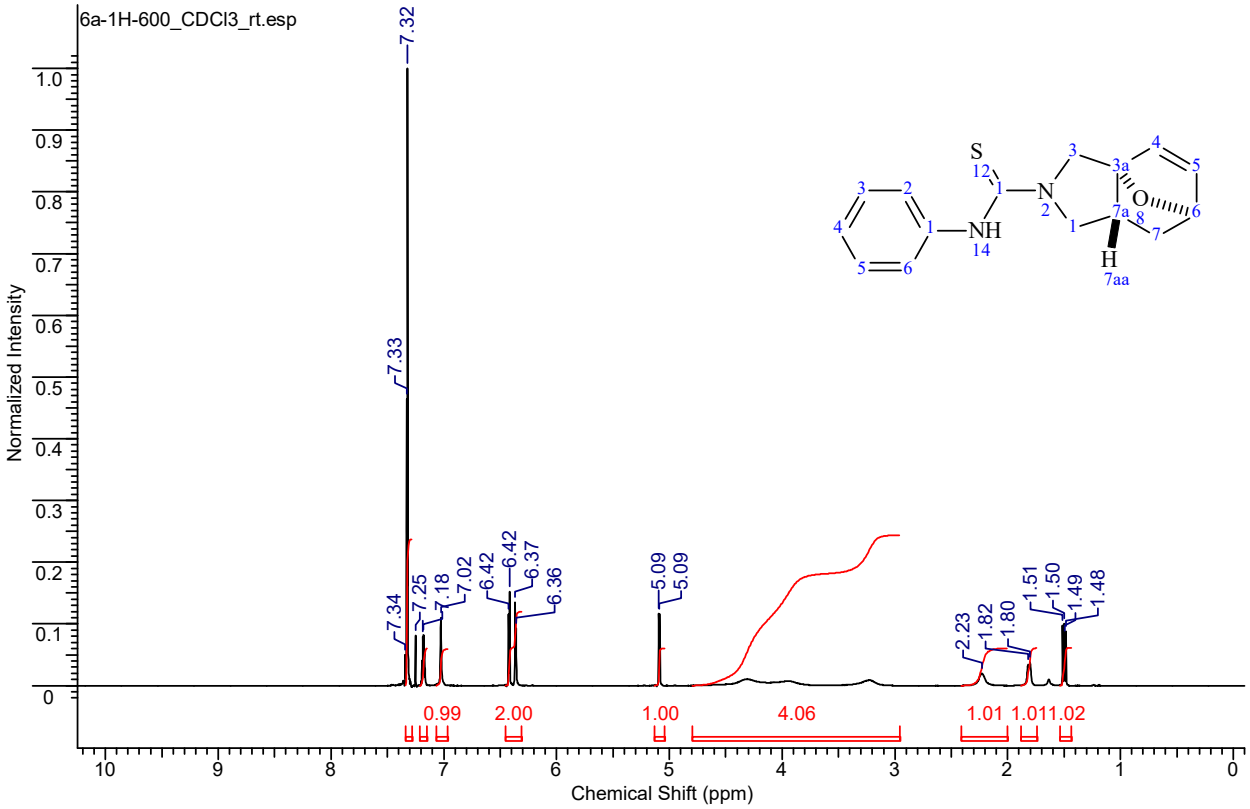


^{13}C NMR (176.1 MHz, DMSO-d_6)

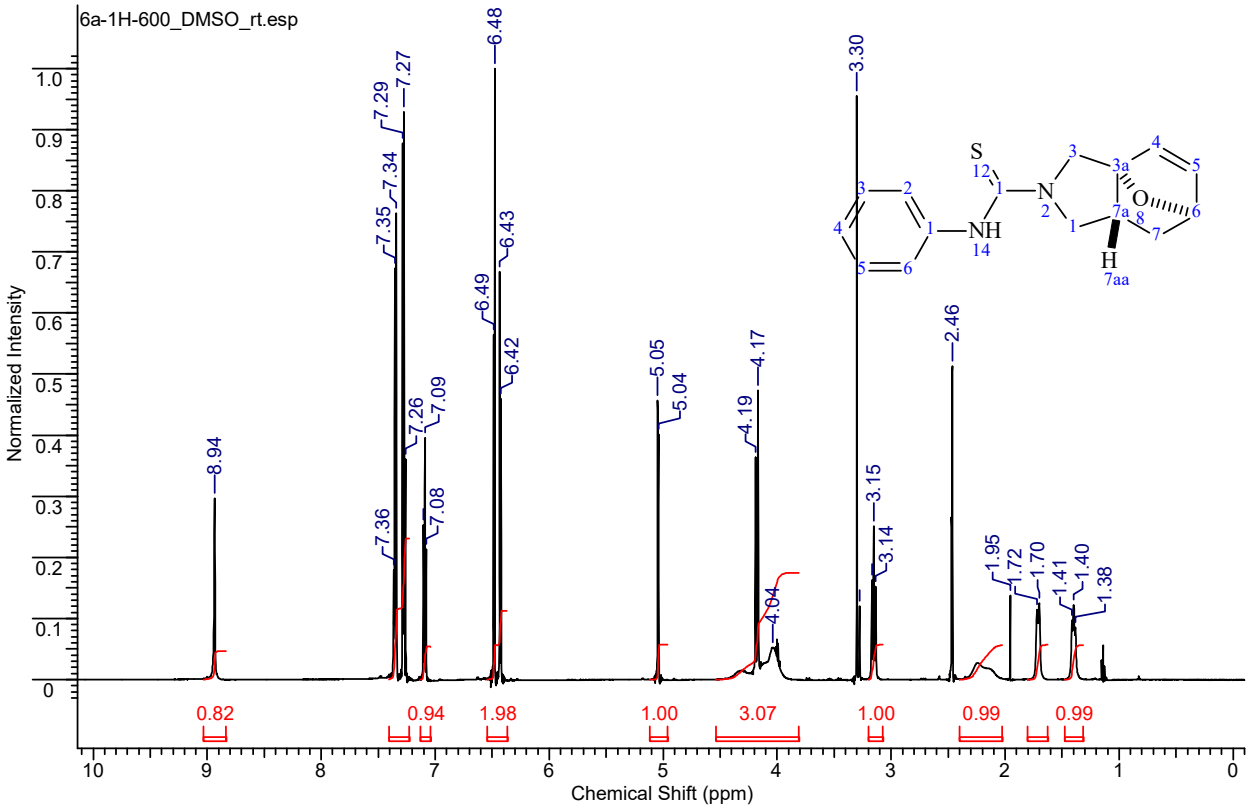


(3a*RS*,6*RS*,7a*RS*)-*N*-Phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6a).

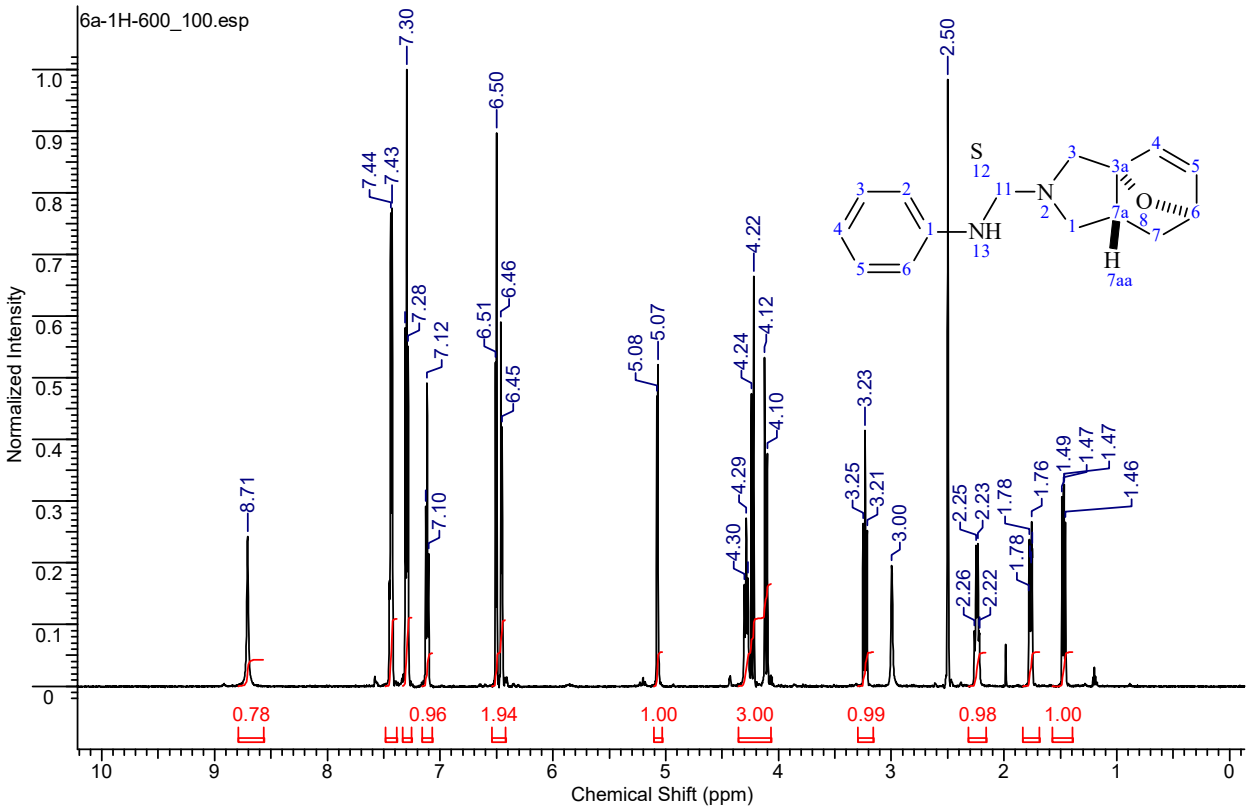
^{1}H NMR (600.2 MHz, $CDCl_3$)



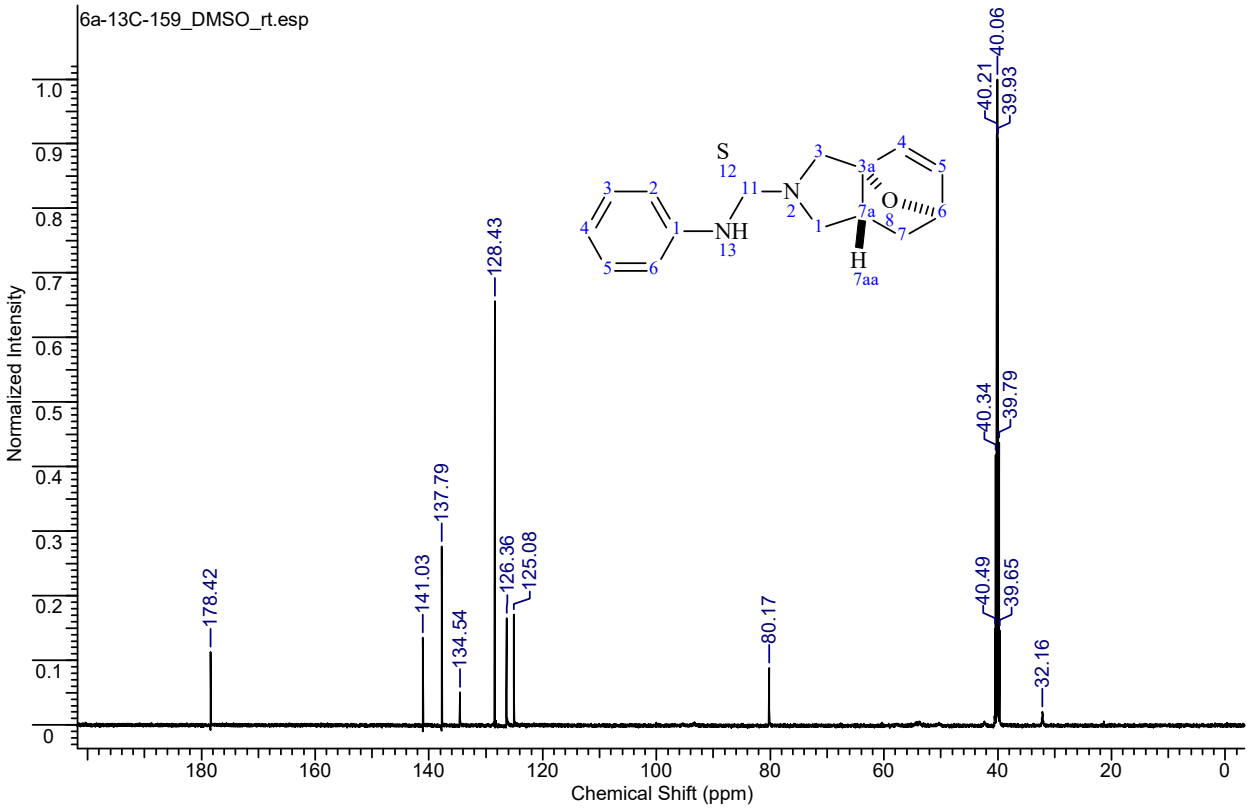
^{1}H NMR (600.2 MHz, DMSO-d_6, rt)



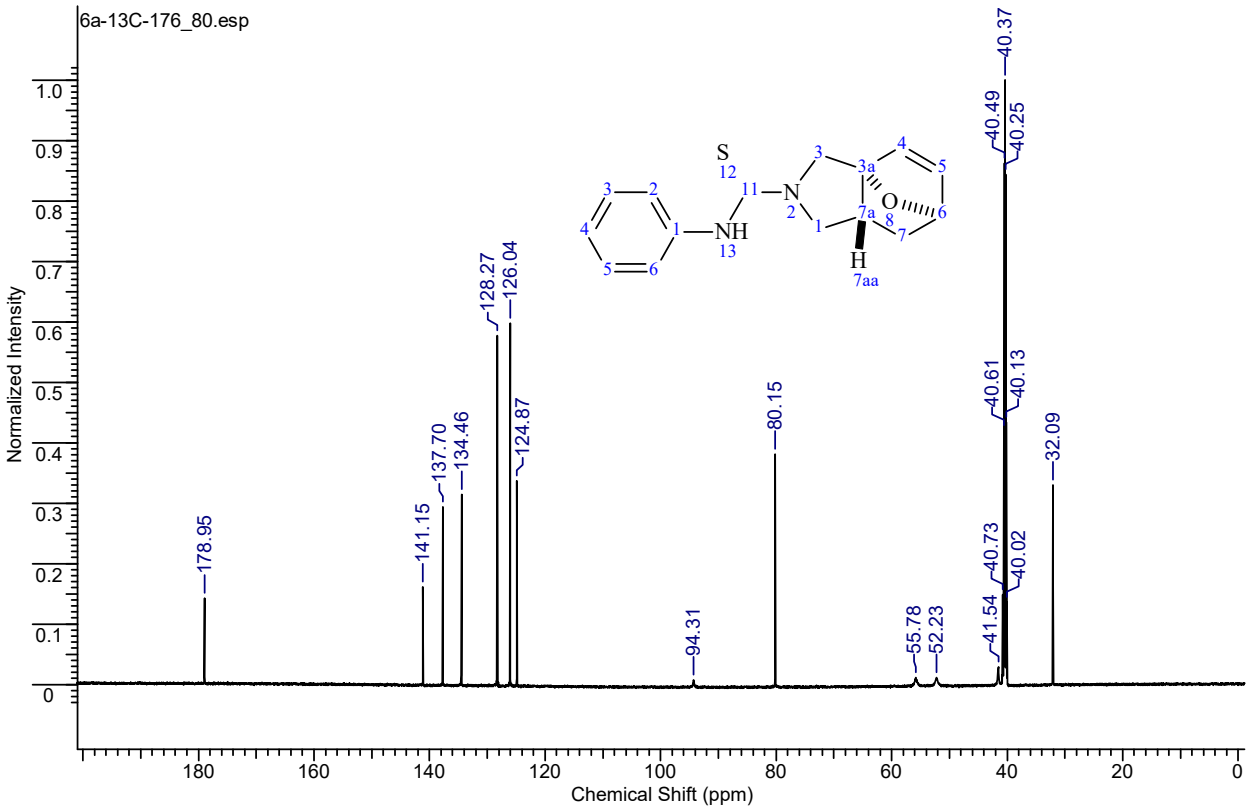
^{1}H NMR (600.2 MHz, DMSO-d_6, 100 °C)



^{13}C NMR (150.9 MHz, DMSO-d_6)

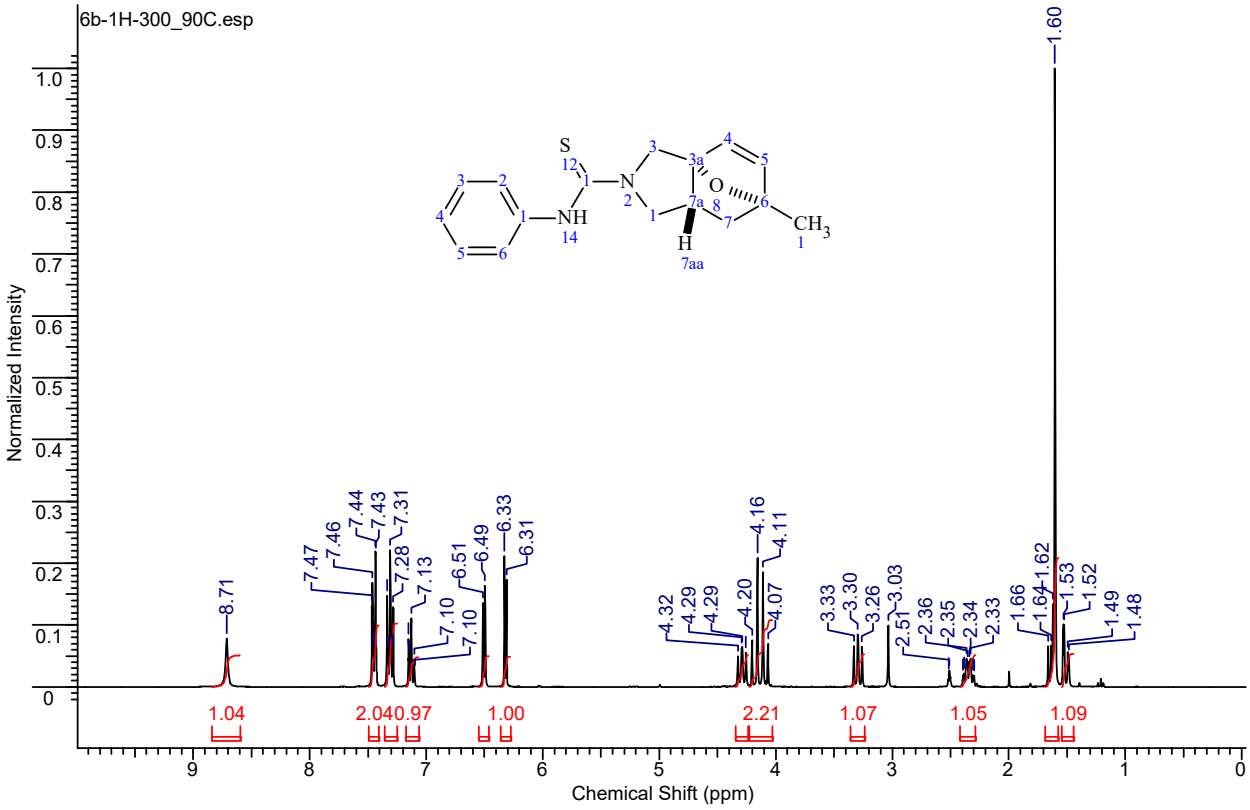


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

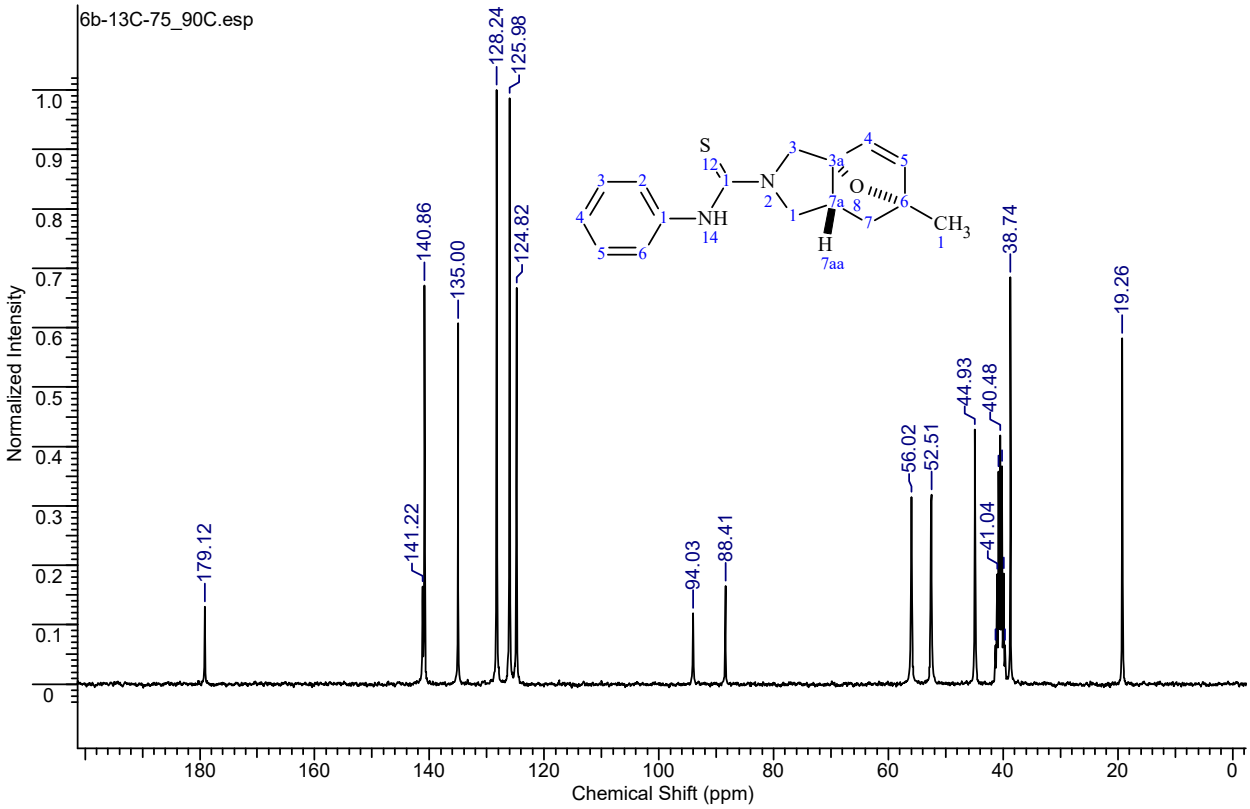


(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6b).

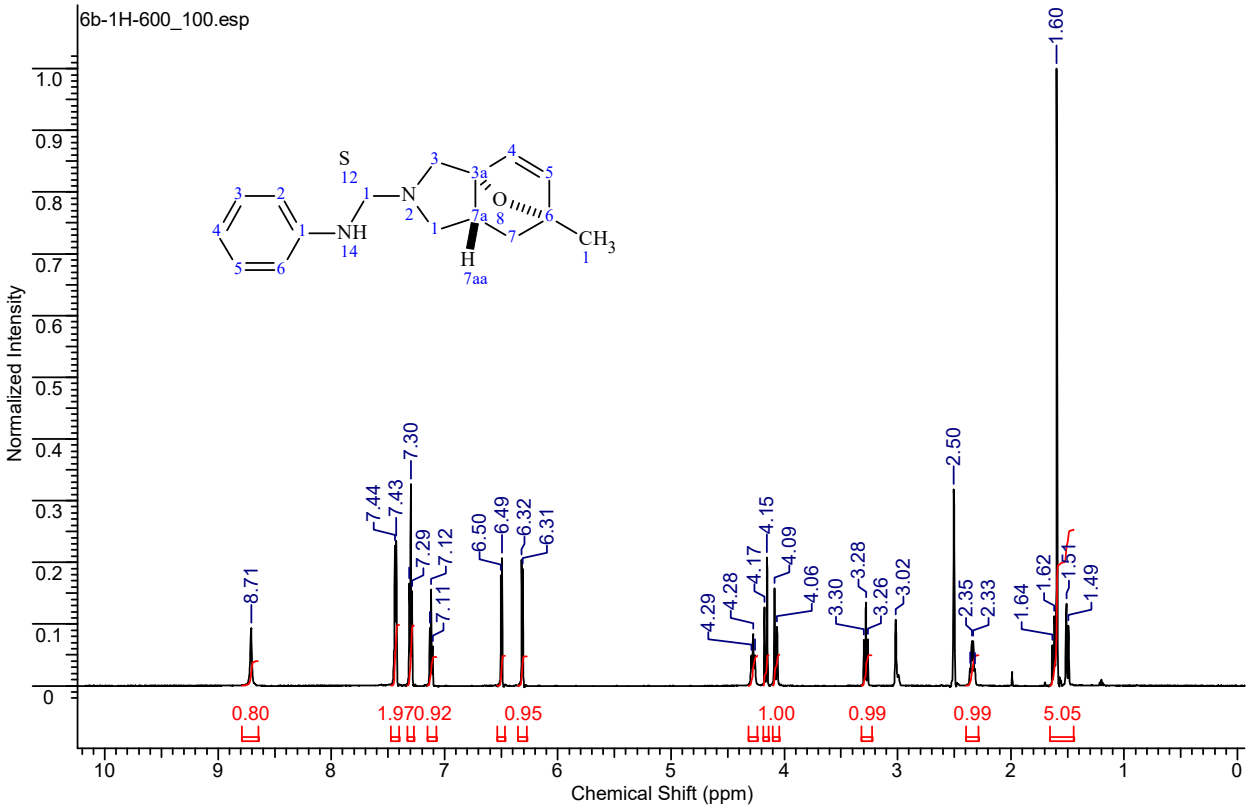
^{1}H NMR (300.1 MHz, DMSO-d_6, 90 °C)



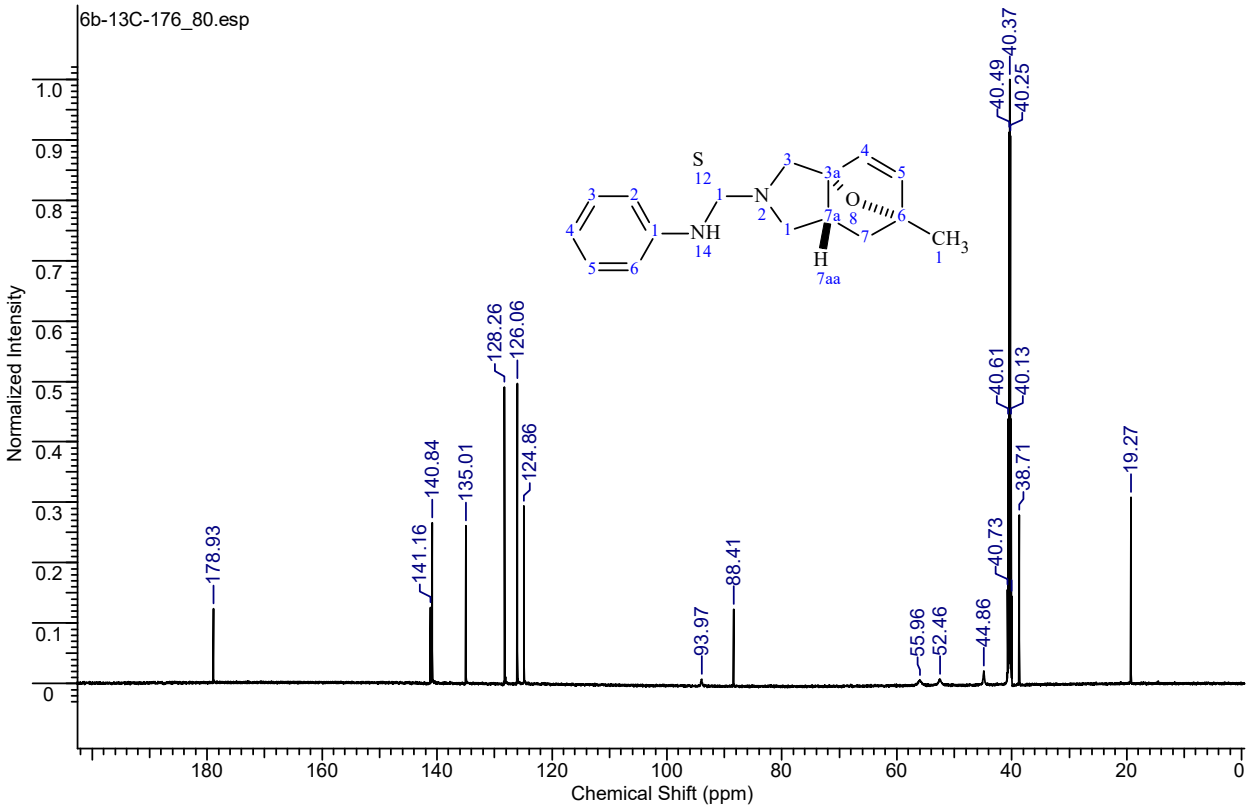
^{13}C NMR (75.5 MHz, DMSO-d_6, 90 °C)



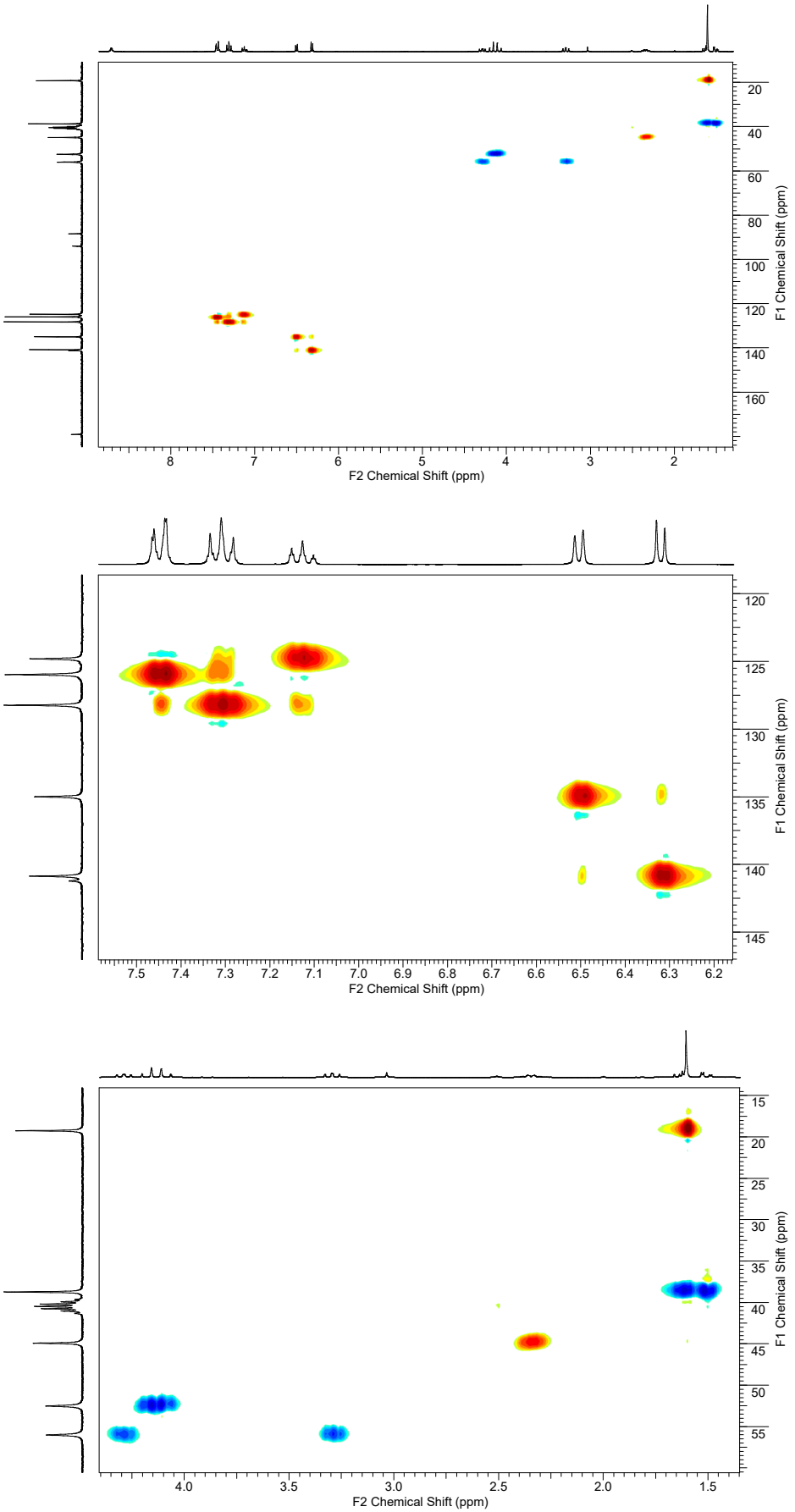
^{1}H NMR (600.2 MHz, DMSO-d_6, 100 °C)



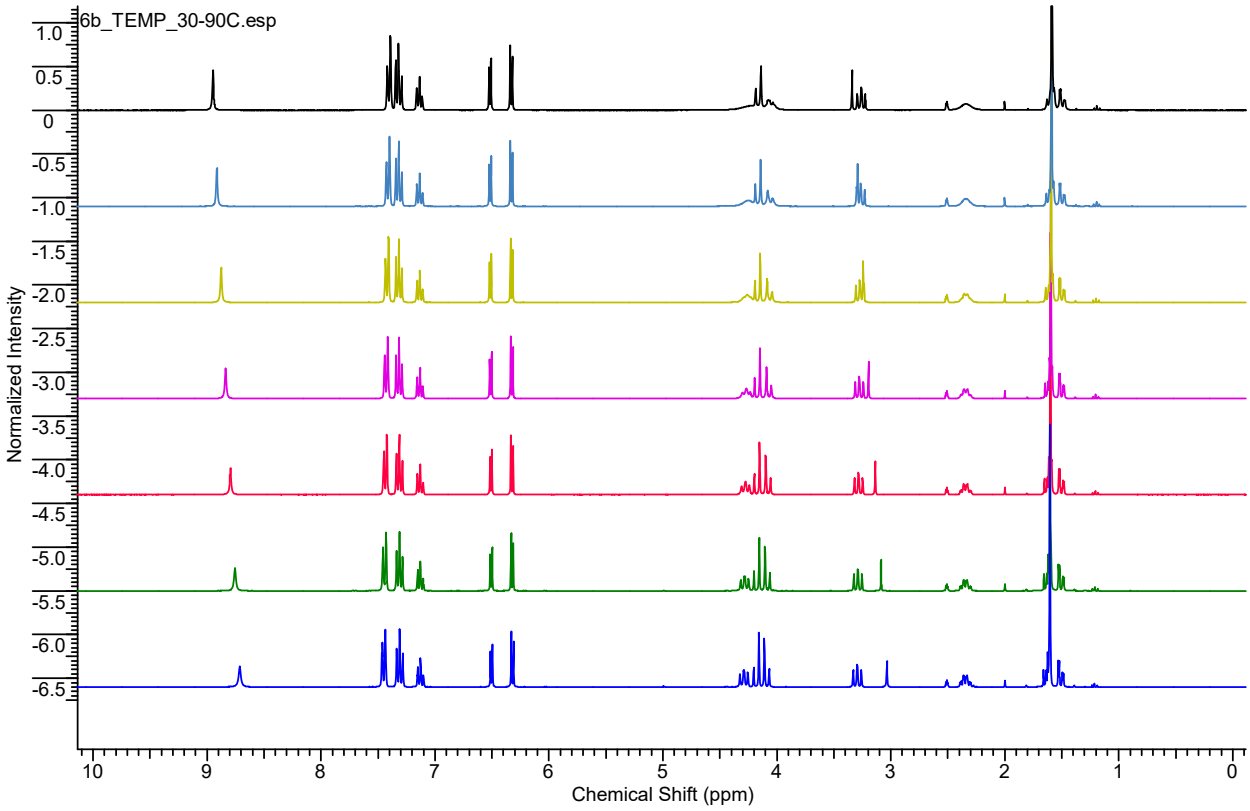
^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C)



HSQC of **6b (90 °C)**

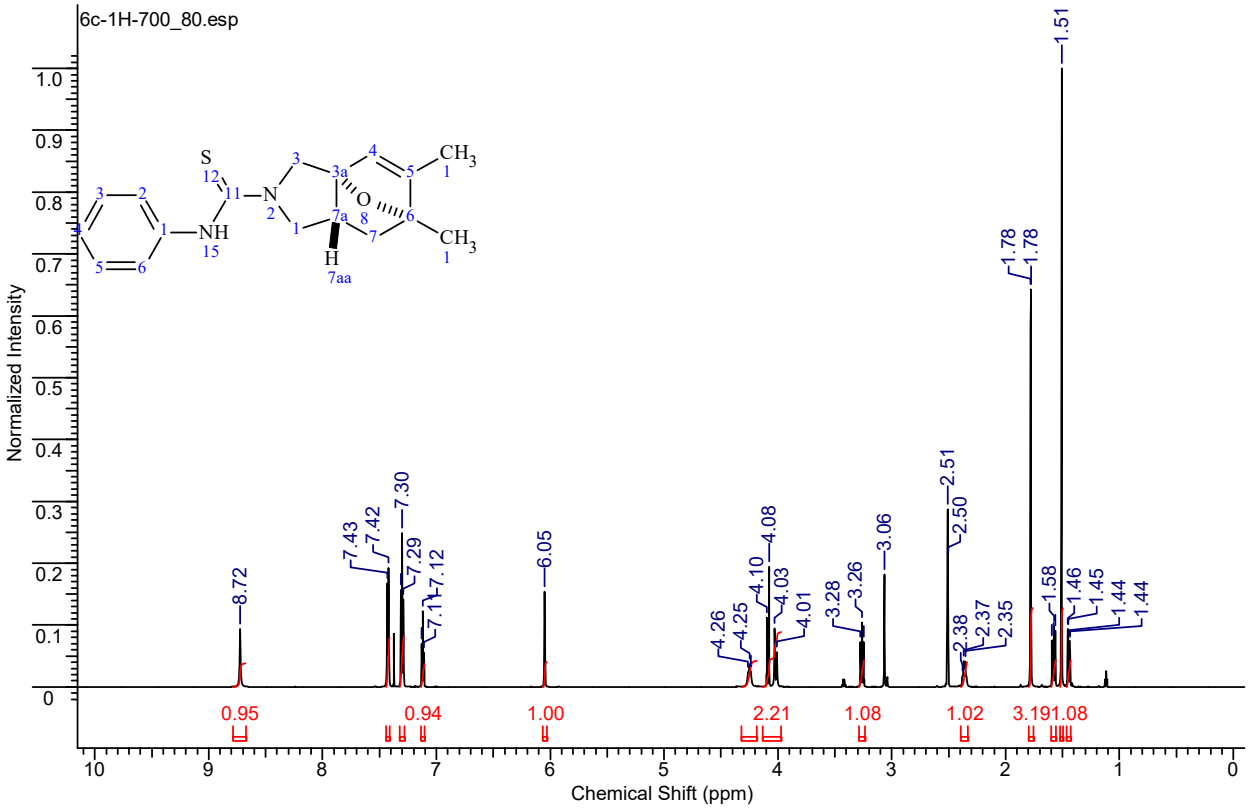


^{1}H NMR of **6b (30-90 °C)**

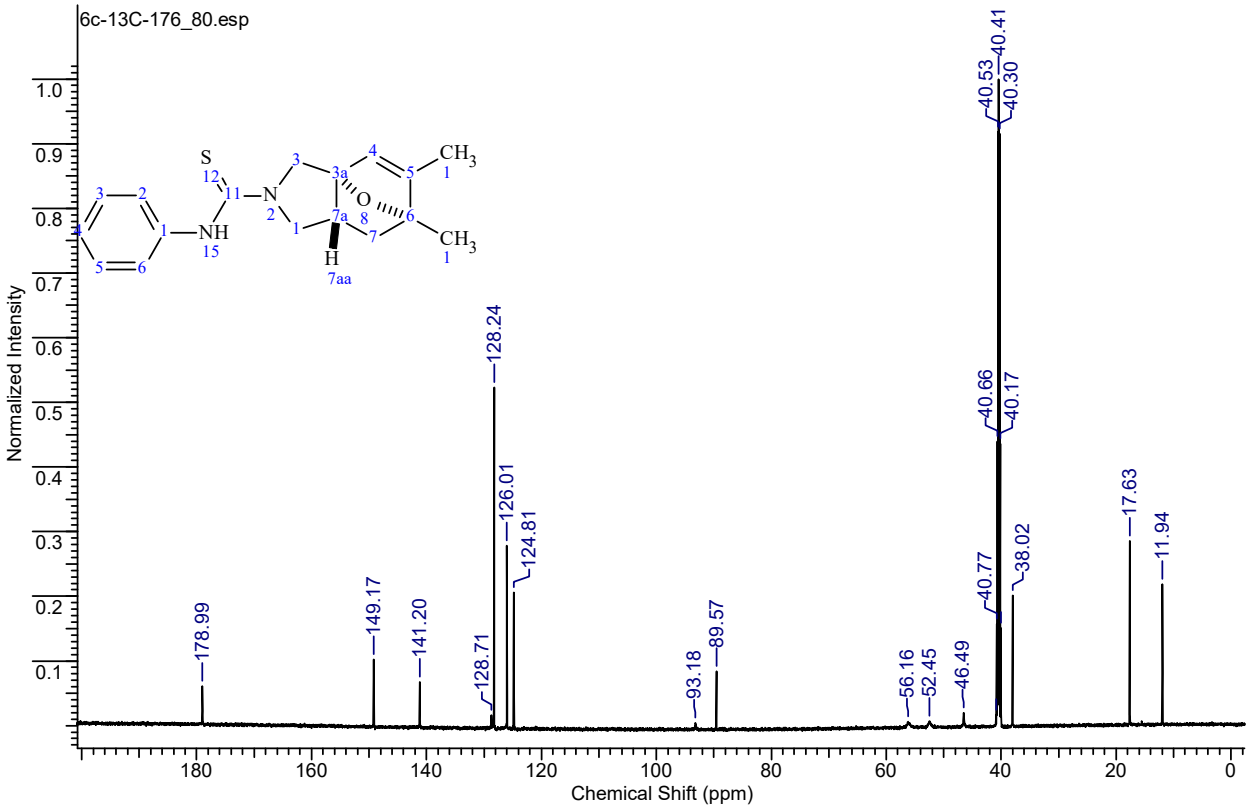


(3a*RS*,6*RS*,7a*RS*)-5,6-Dimethyl-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6c).

^{1}H NMR (700.2 MHz, DMSO-d_6, 87 °C)

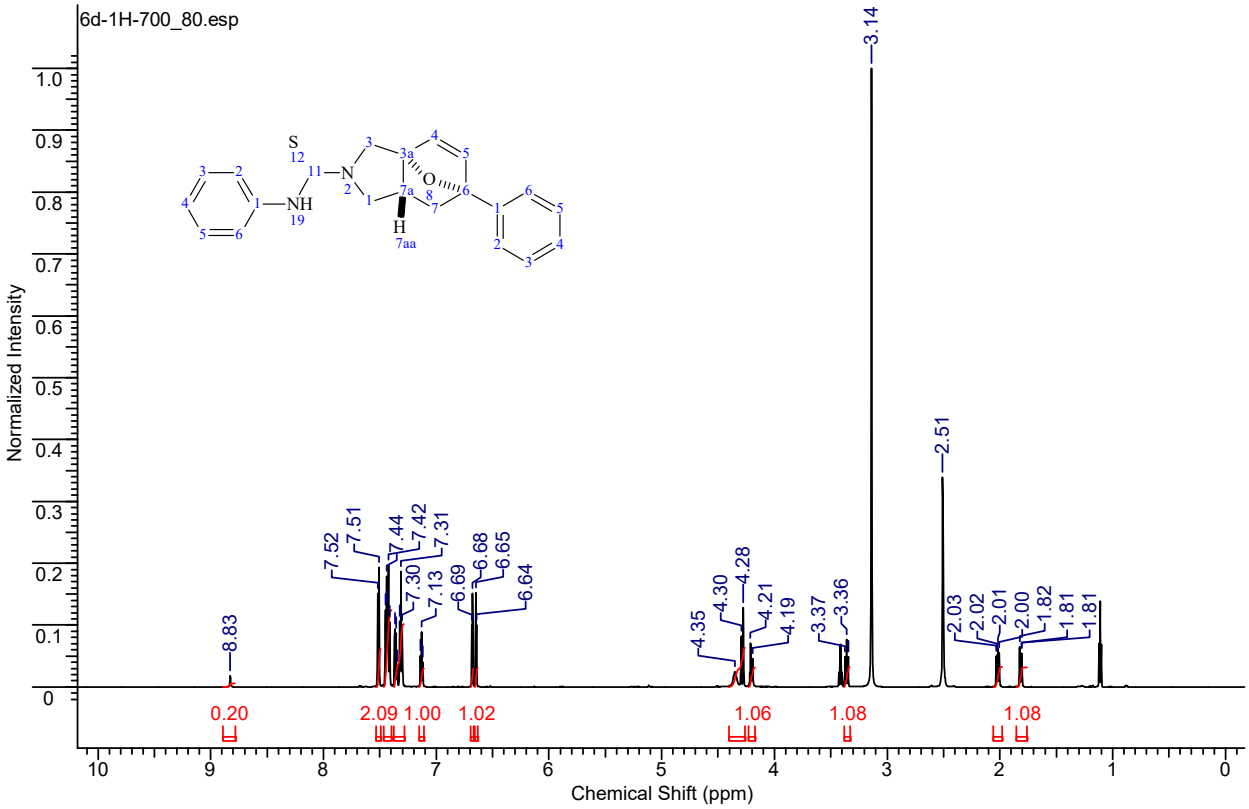


^{13}C NMR (176.1 MHz, DMSO-d_6, 87 °C)

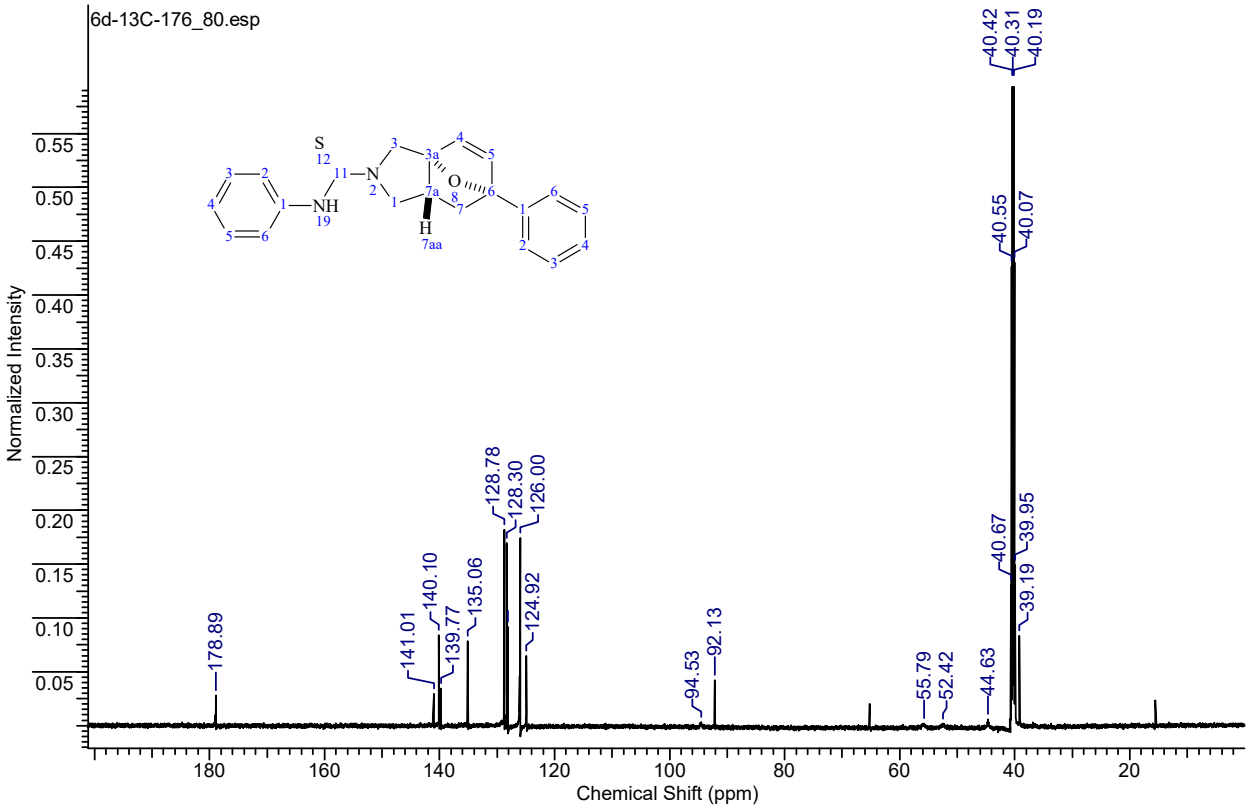


(3a*RS*,6*RS*,7a*RS*)-*N*,6-Diphenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6d). *Contains an impurity of diethyl ether*

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

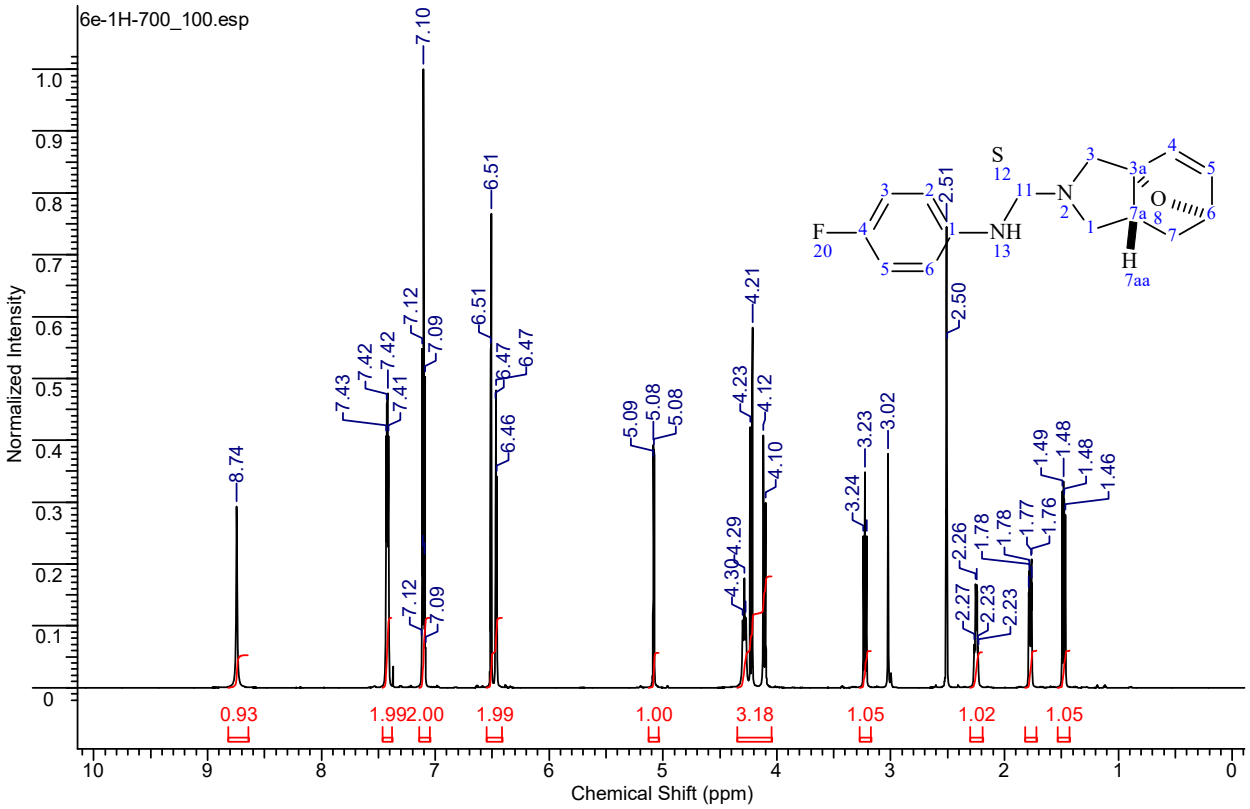


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

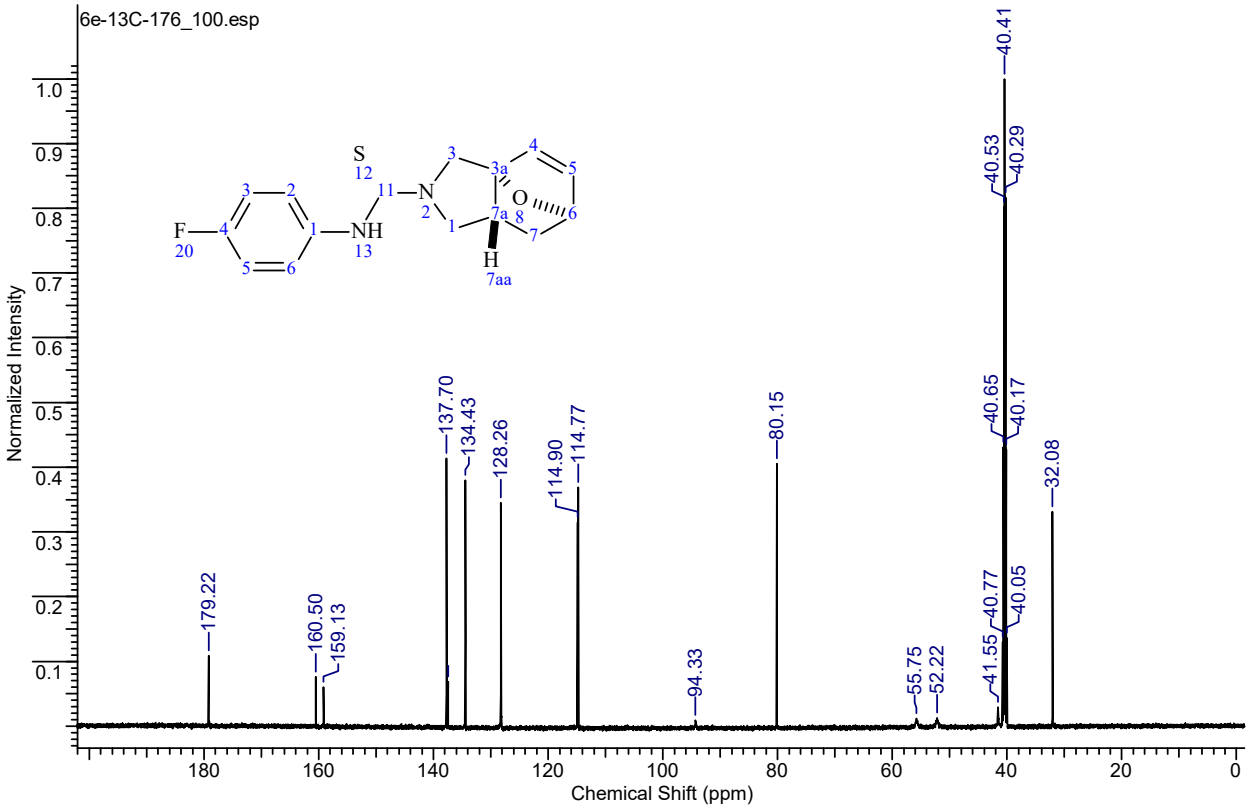


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Fluorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6e).

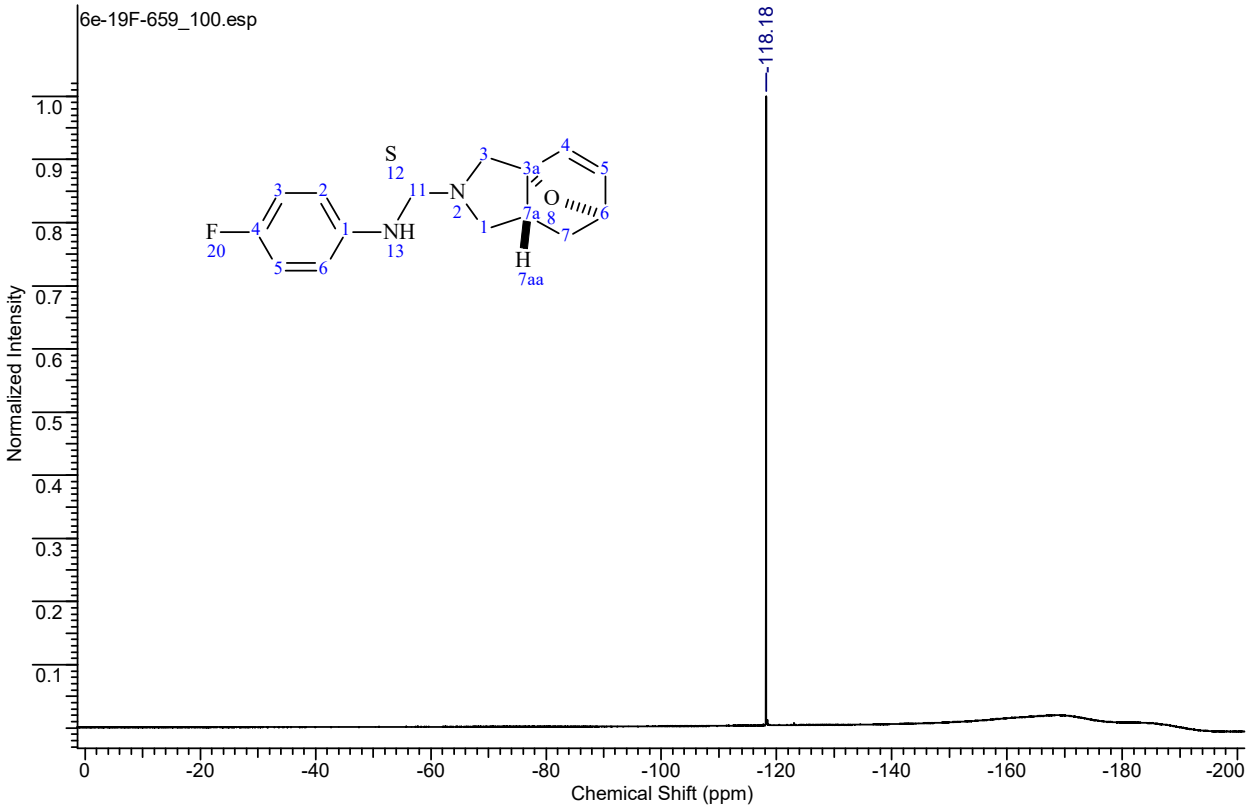
^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C)



^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C)

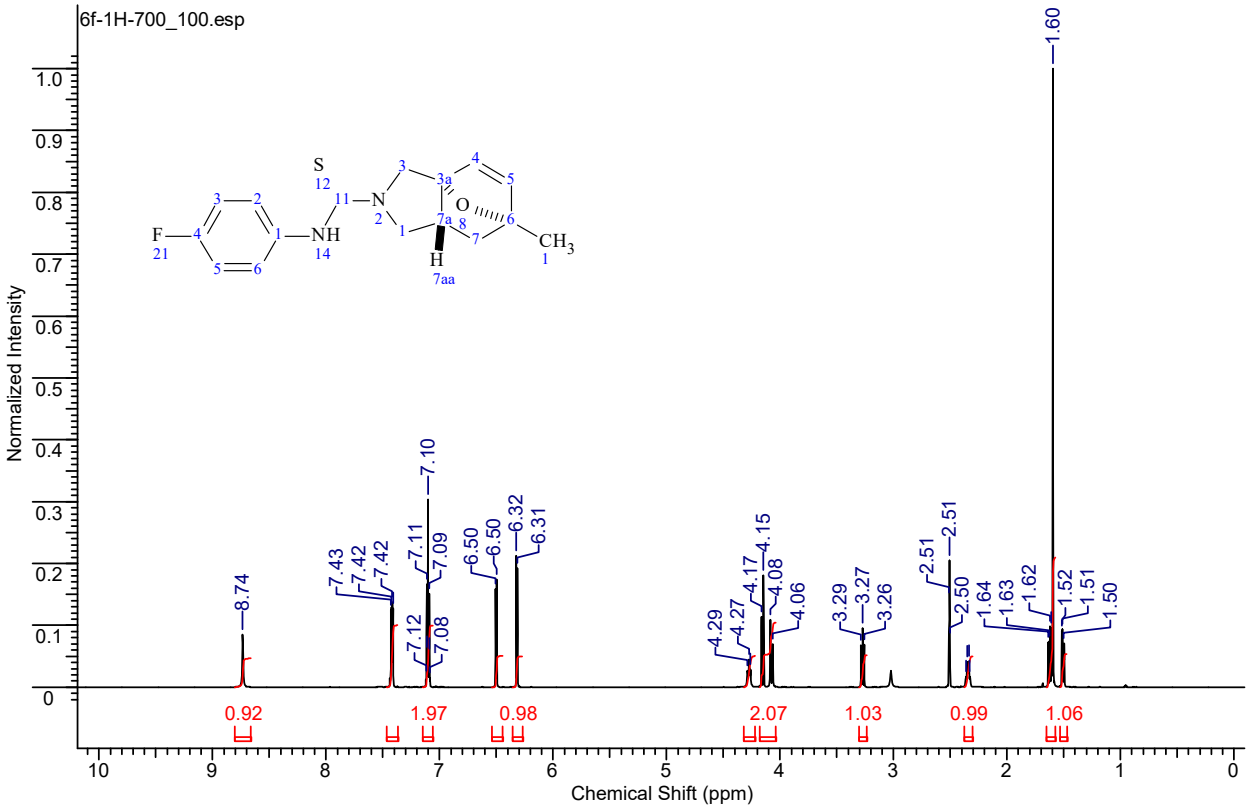


^{19}F NMR (658.8 MHz, DMSO-d_6, 97 °C)

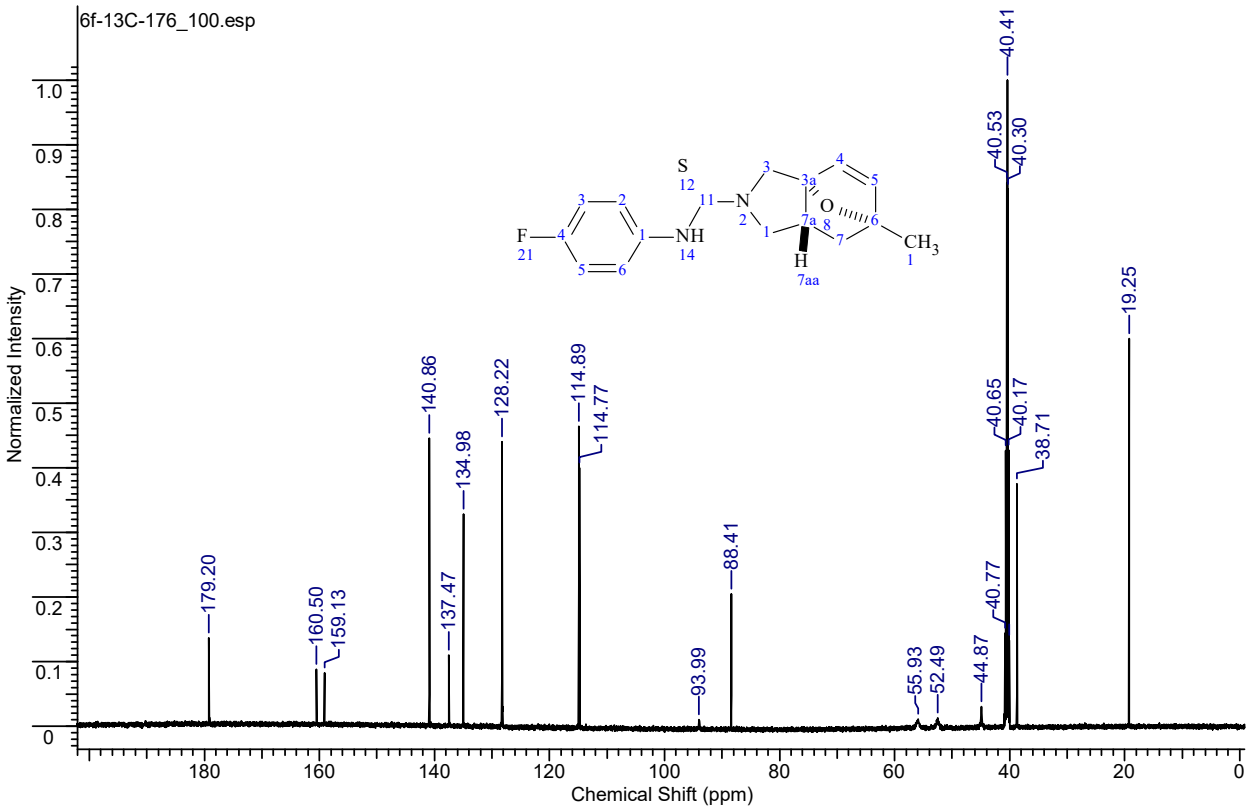


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Fluorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6f).

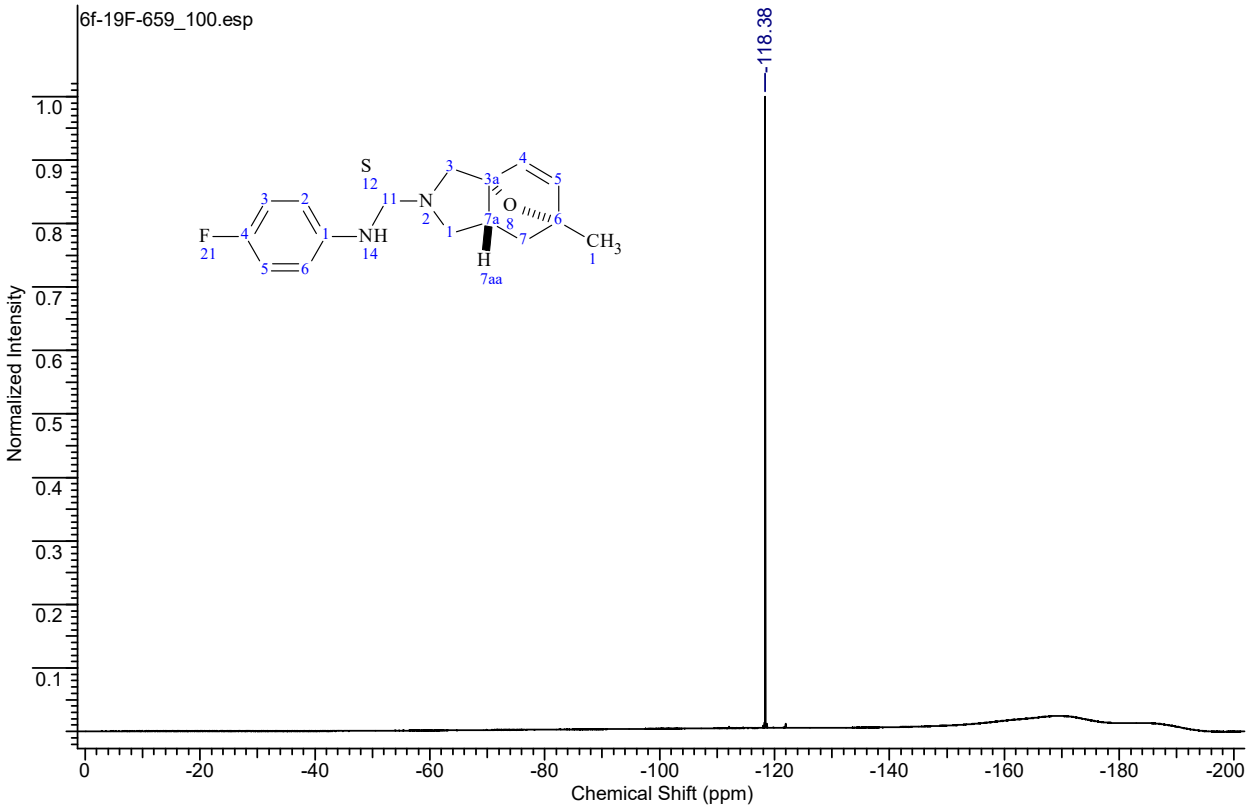
^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C)



^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C)

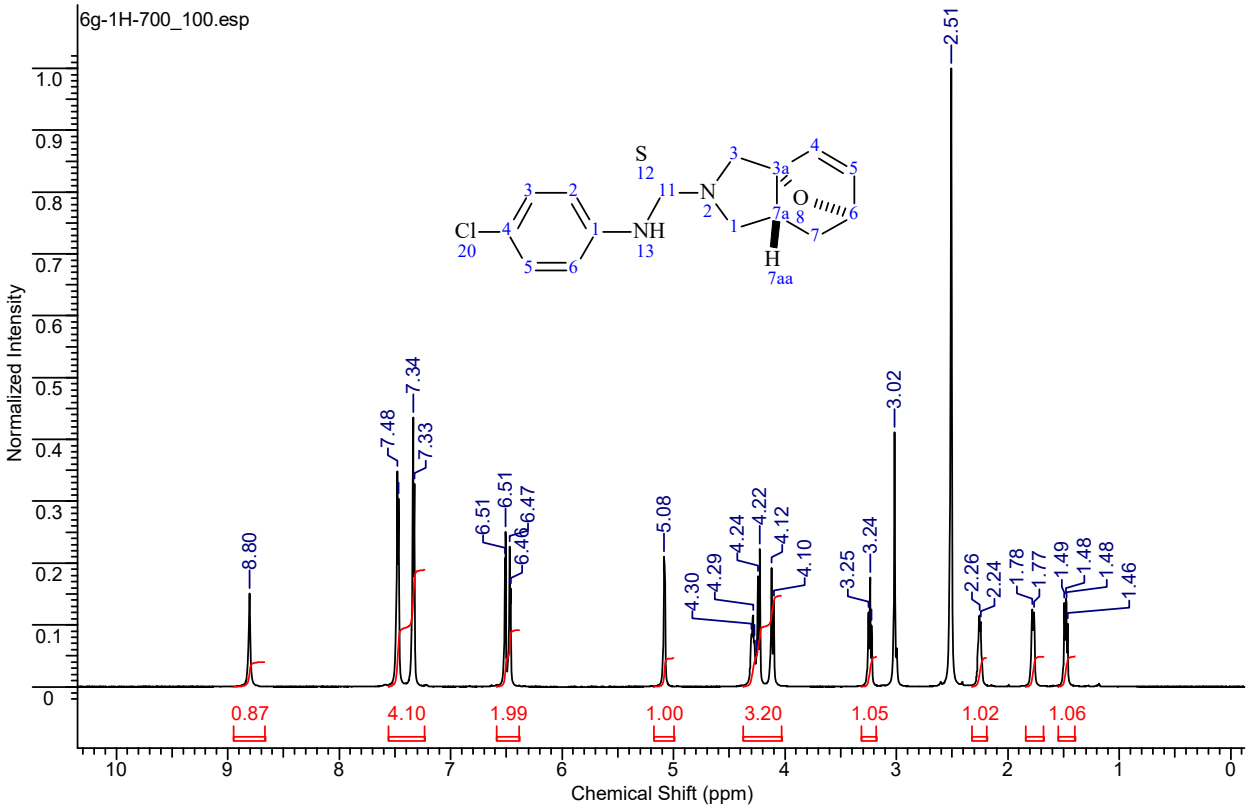


^{19}F NMR (658.8 MHz, DMSO-d_6, 97 °C)

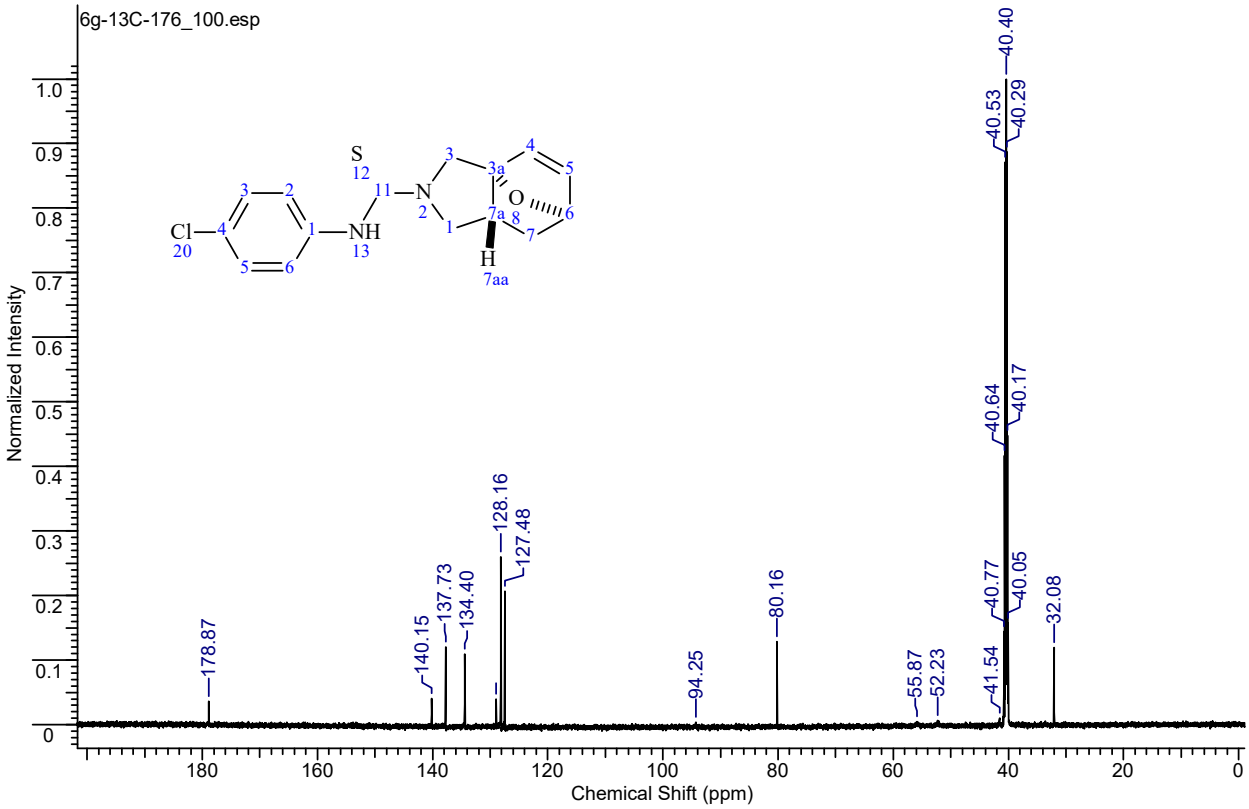


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6g).

^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C)

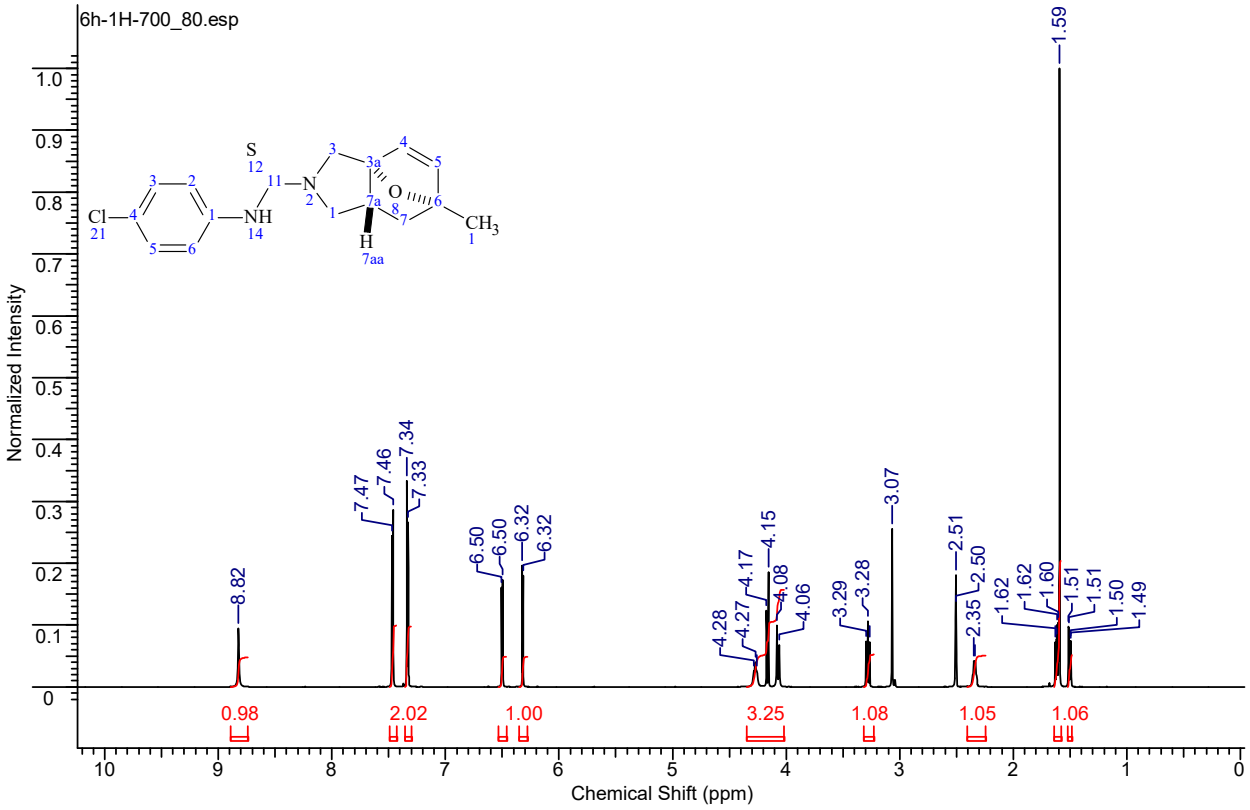


^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C)

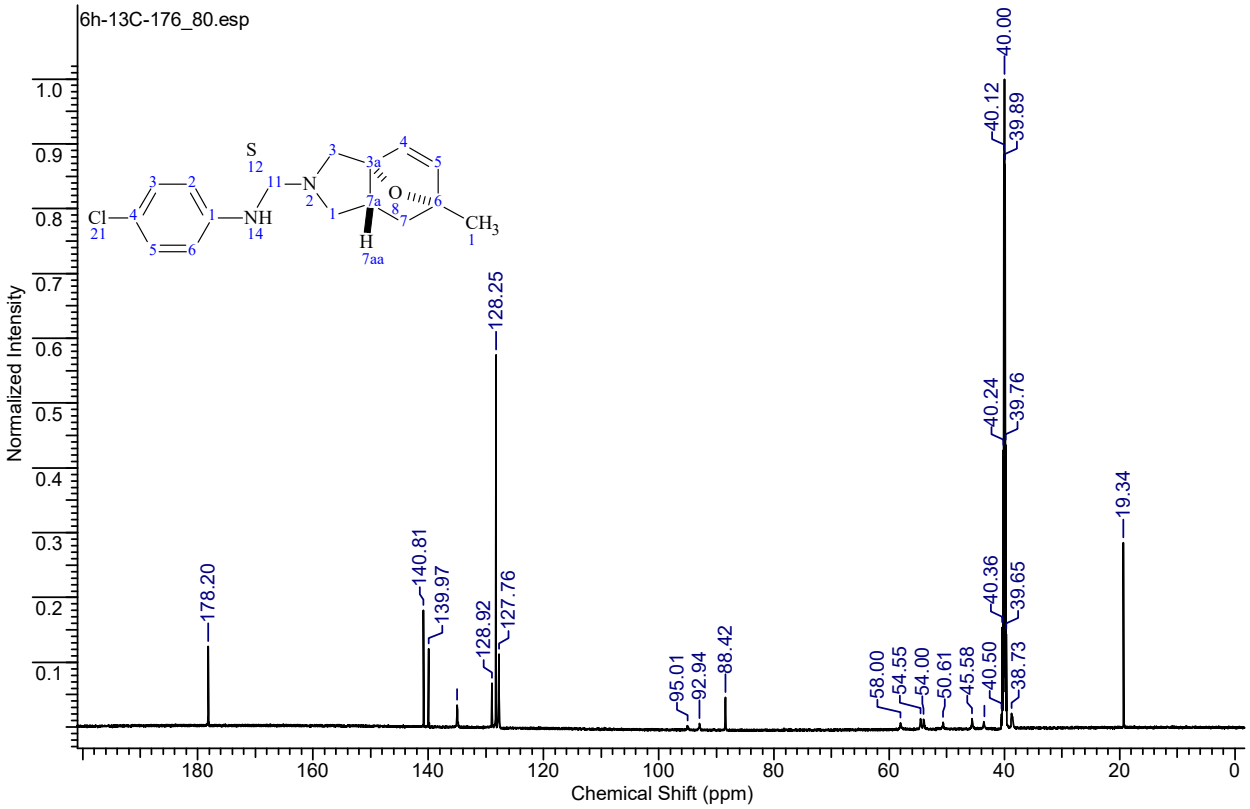


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6h).

^{1}H NMR (700.2 MHz, DMSO-d_6, 87 °C)

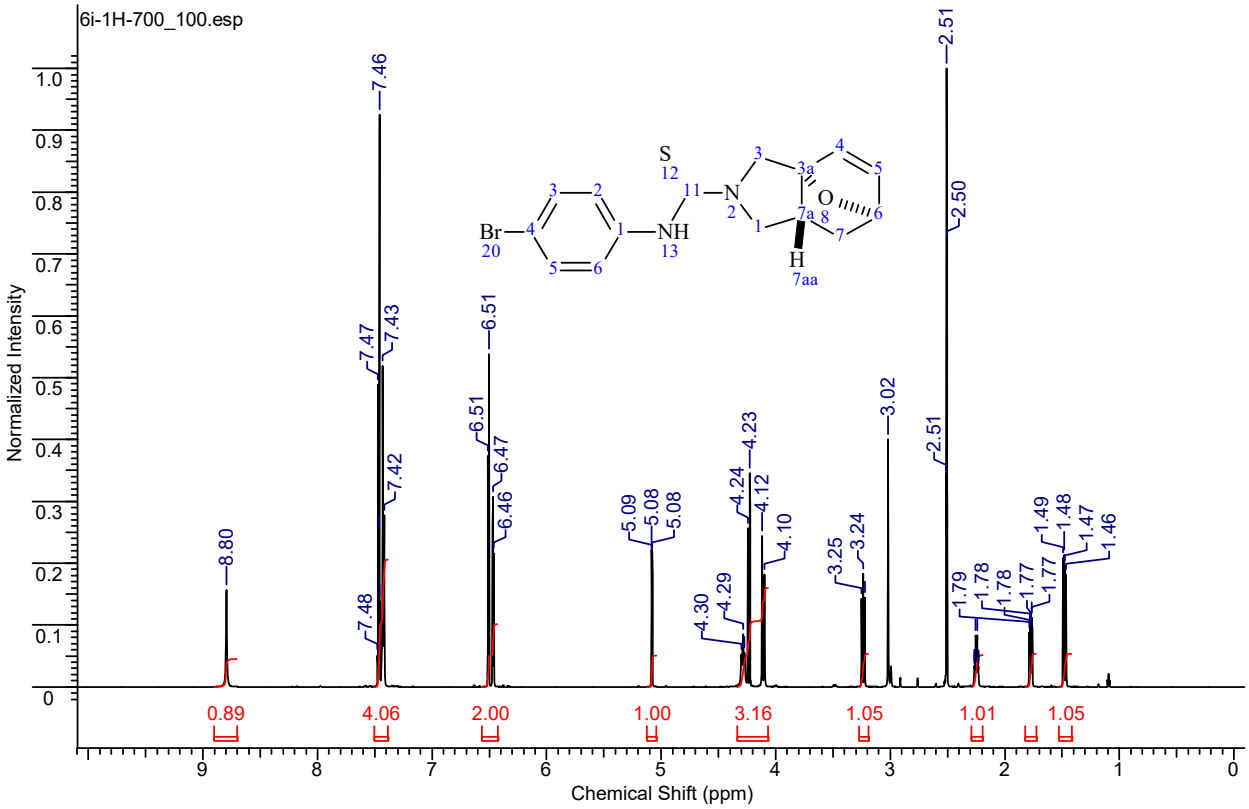


^{13}C NMR (176.1 MHz, DMSO-d_6, 87 °C)

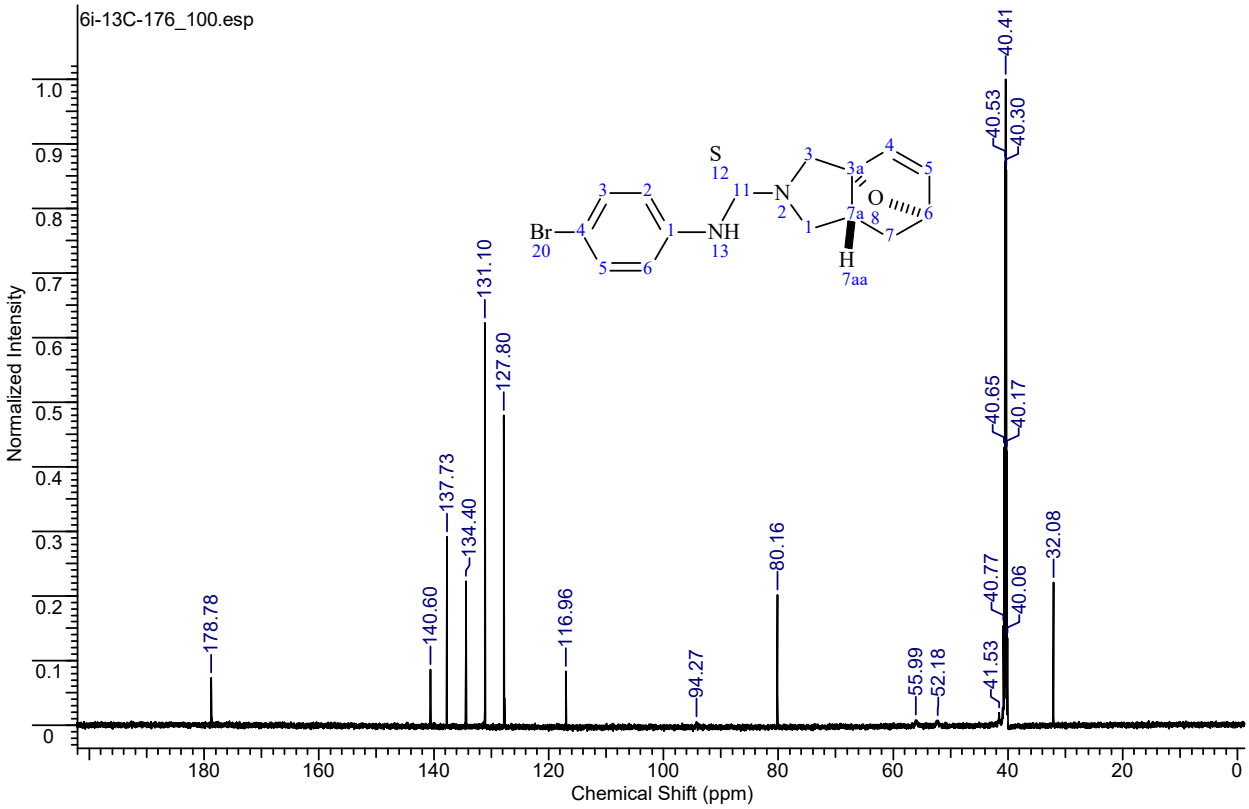


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Bromophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6i).

^{1}H NMR (700.2 MHz, DMSO-d_6, 97 °C)

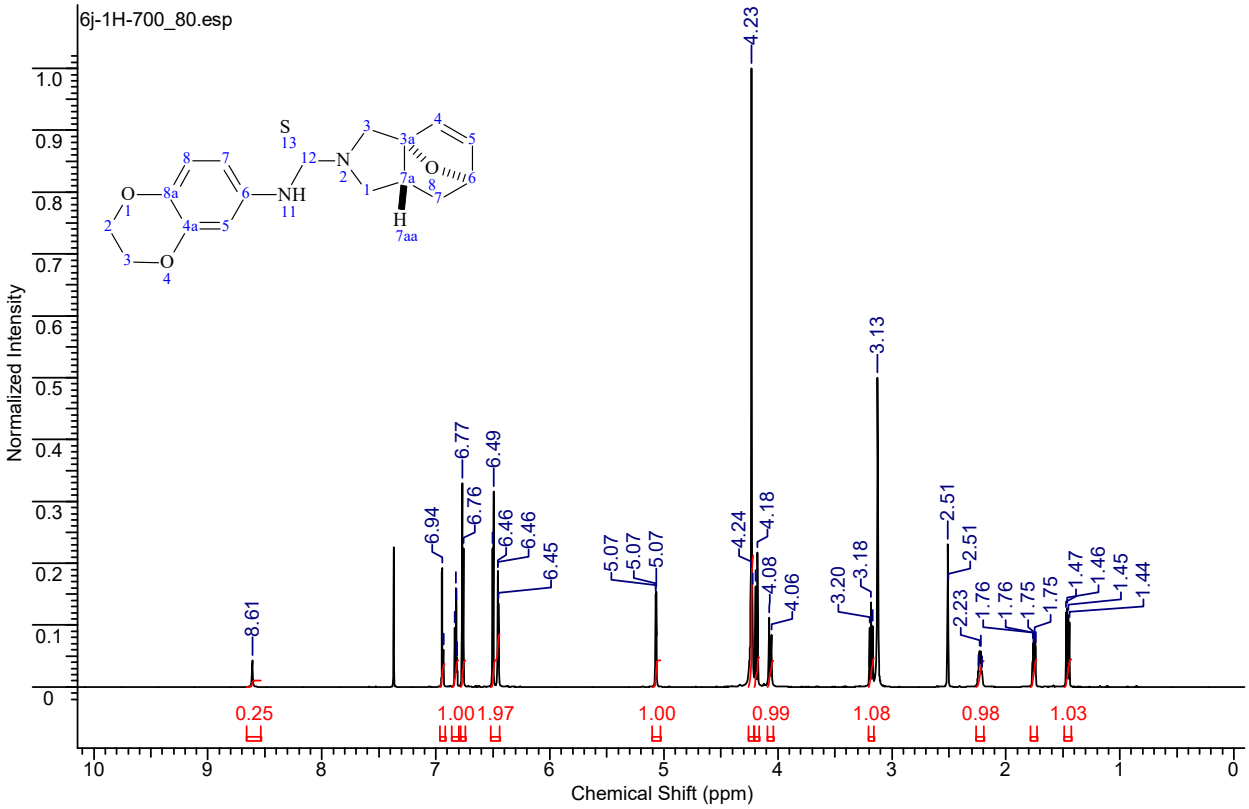


^{13}C NMR (176.1 MHz, DMSO-d_6, 97 °C)

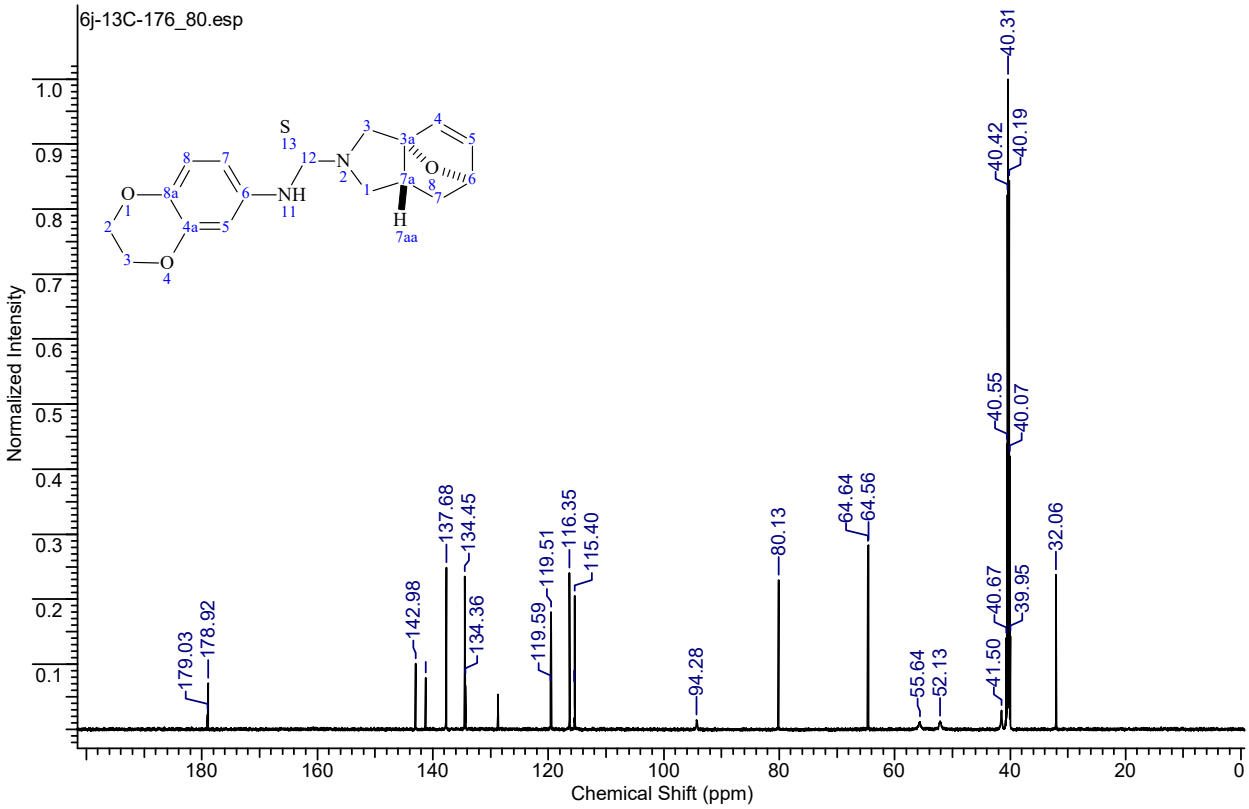


(3a*RS*,6*RS*,7a*RS*)-*N*-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6j). *Contains an impurity of benzene*

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

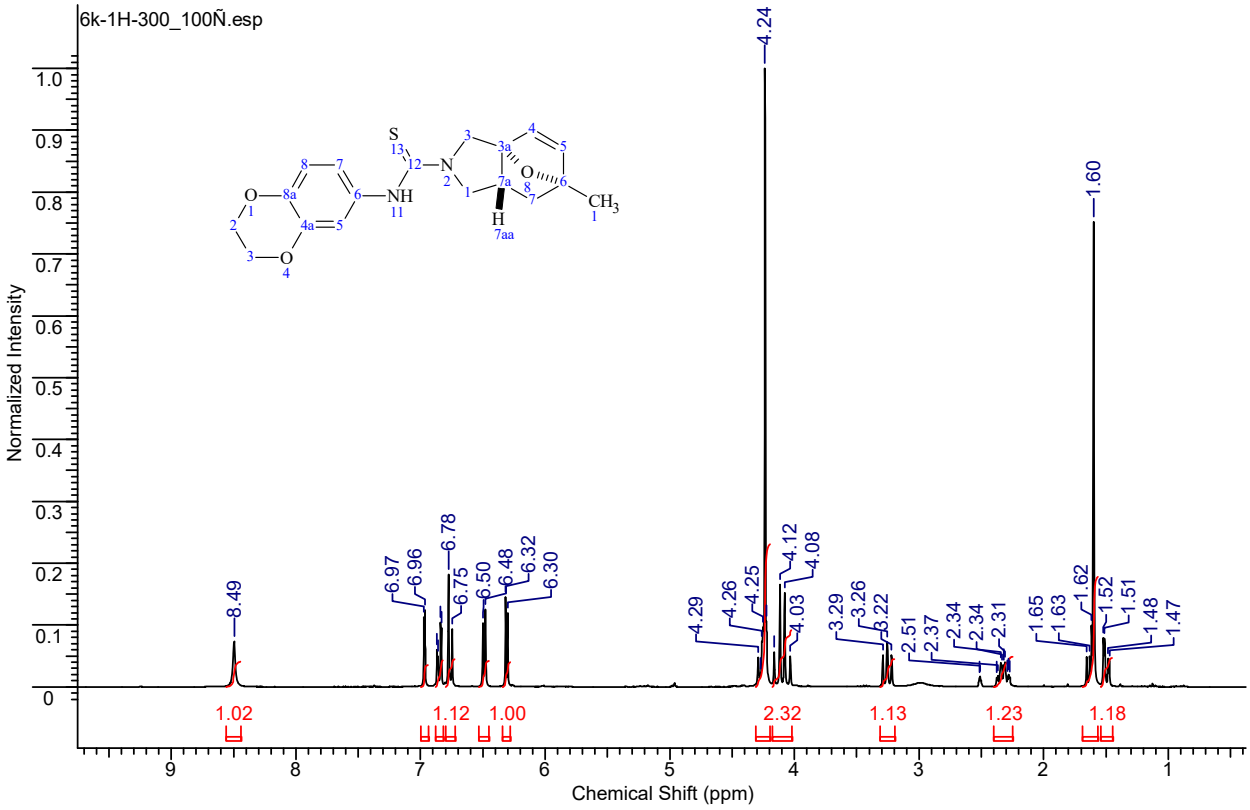


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

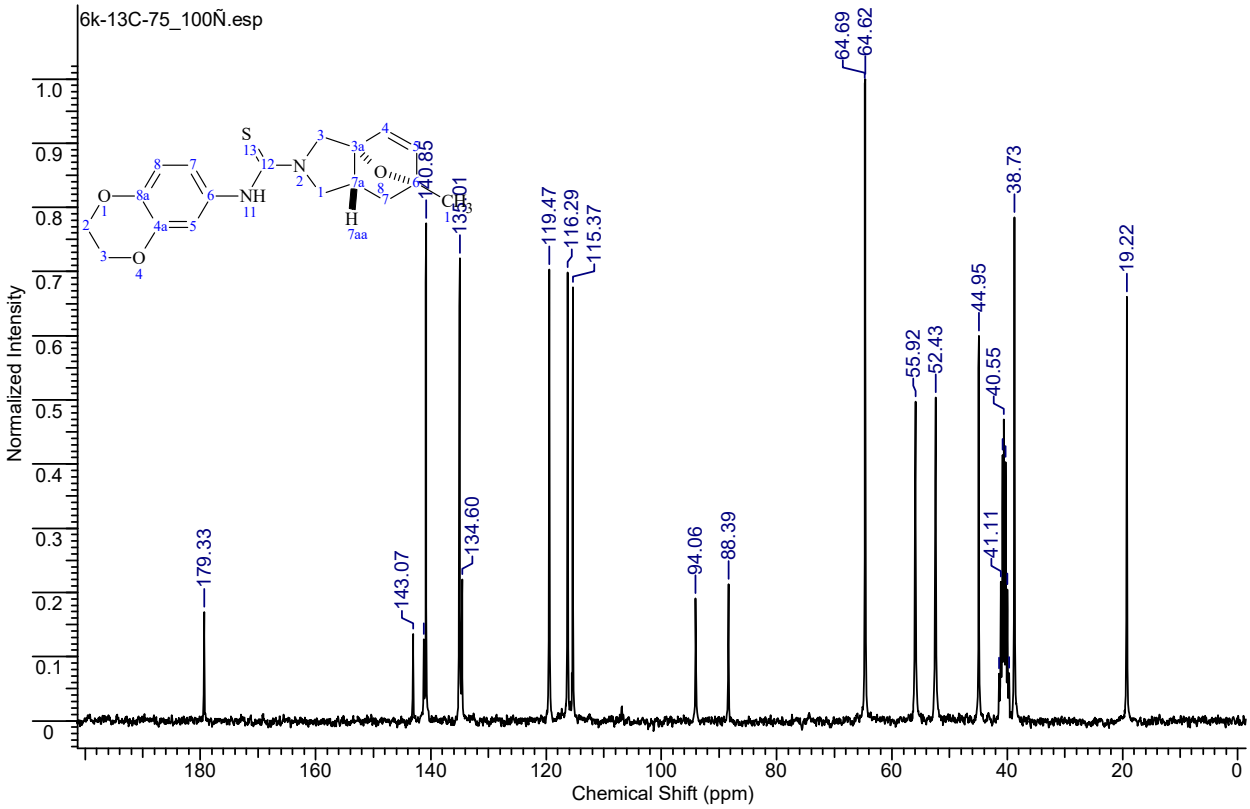


(3a*RS*,6*RS*,7a*RS*)-*N*-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6k).

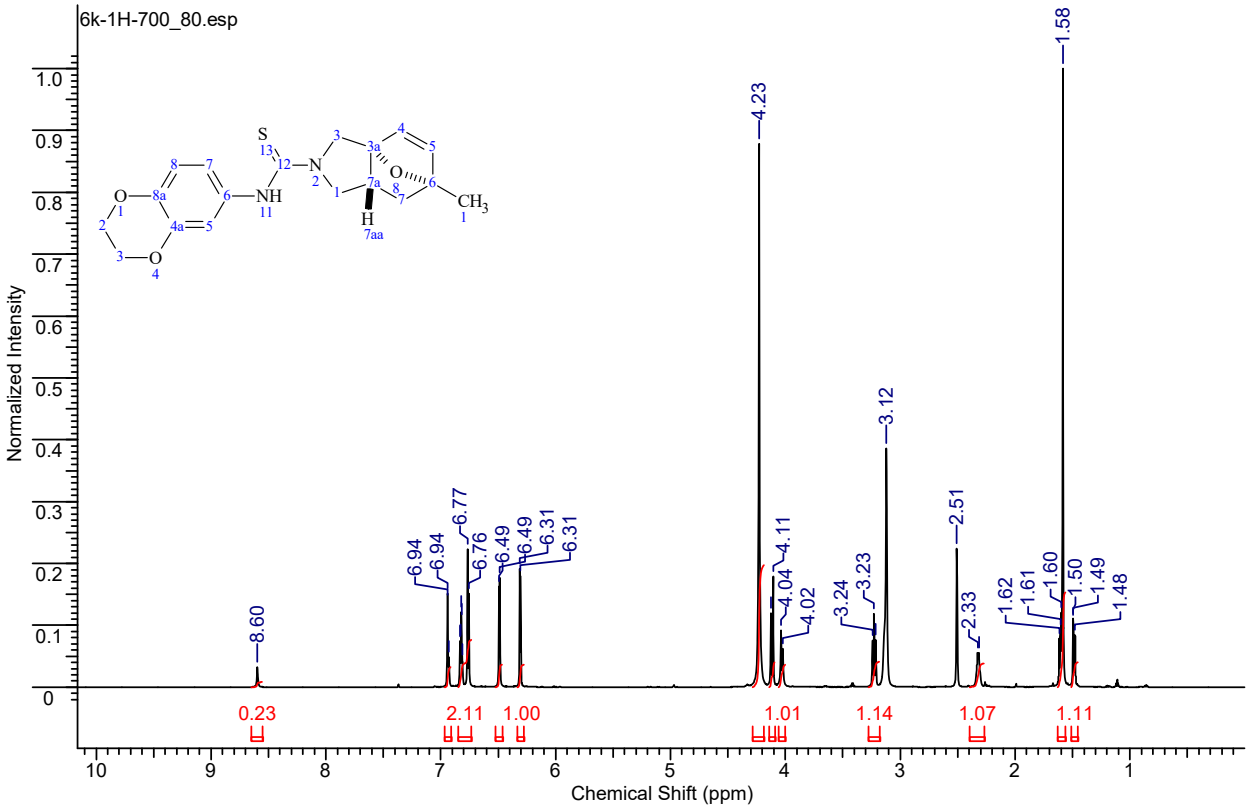
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



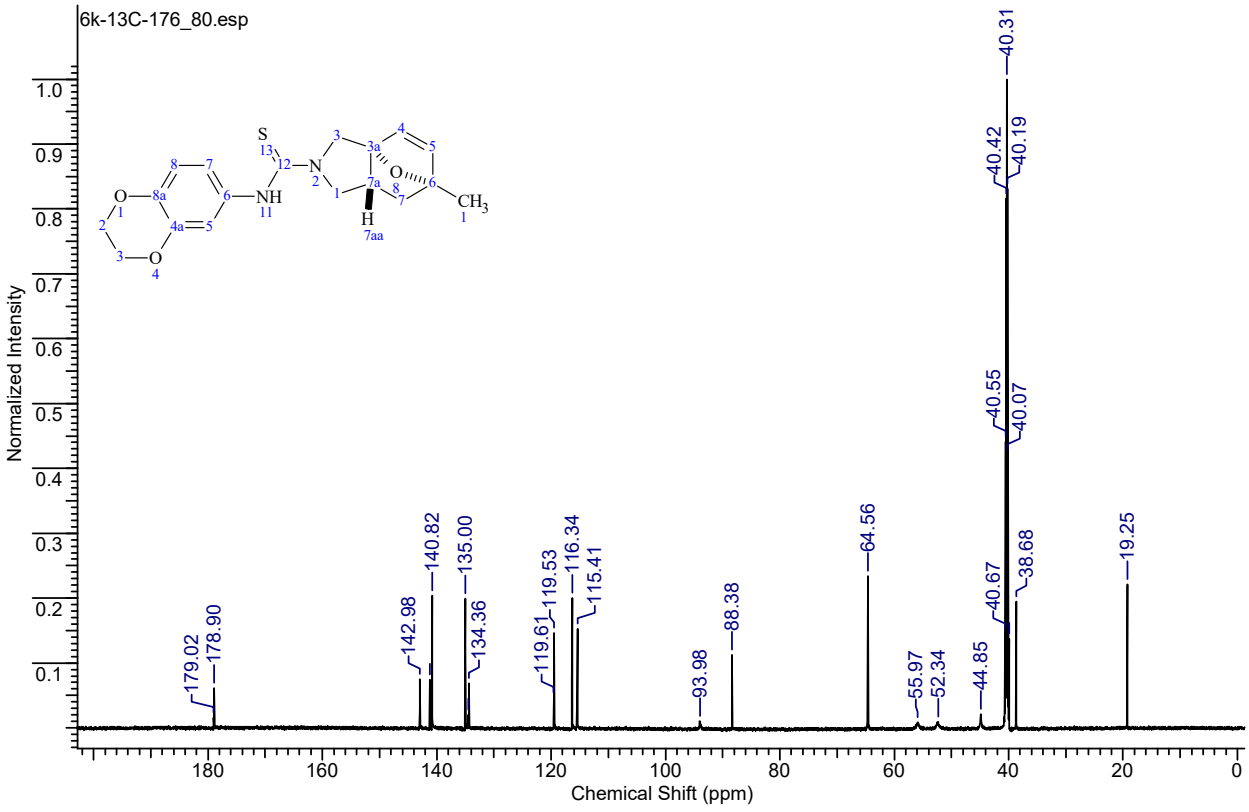
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



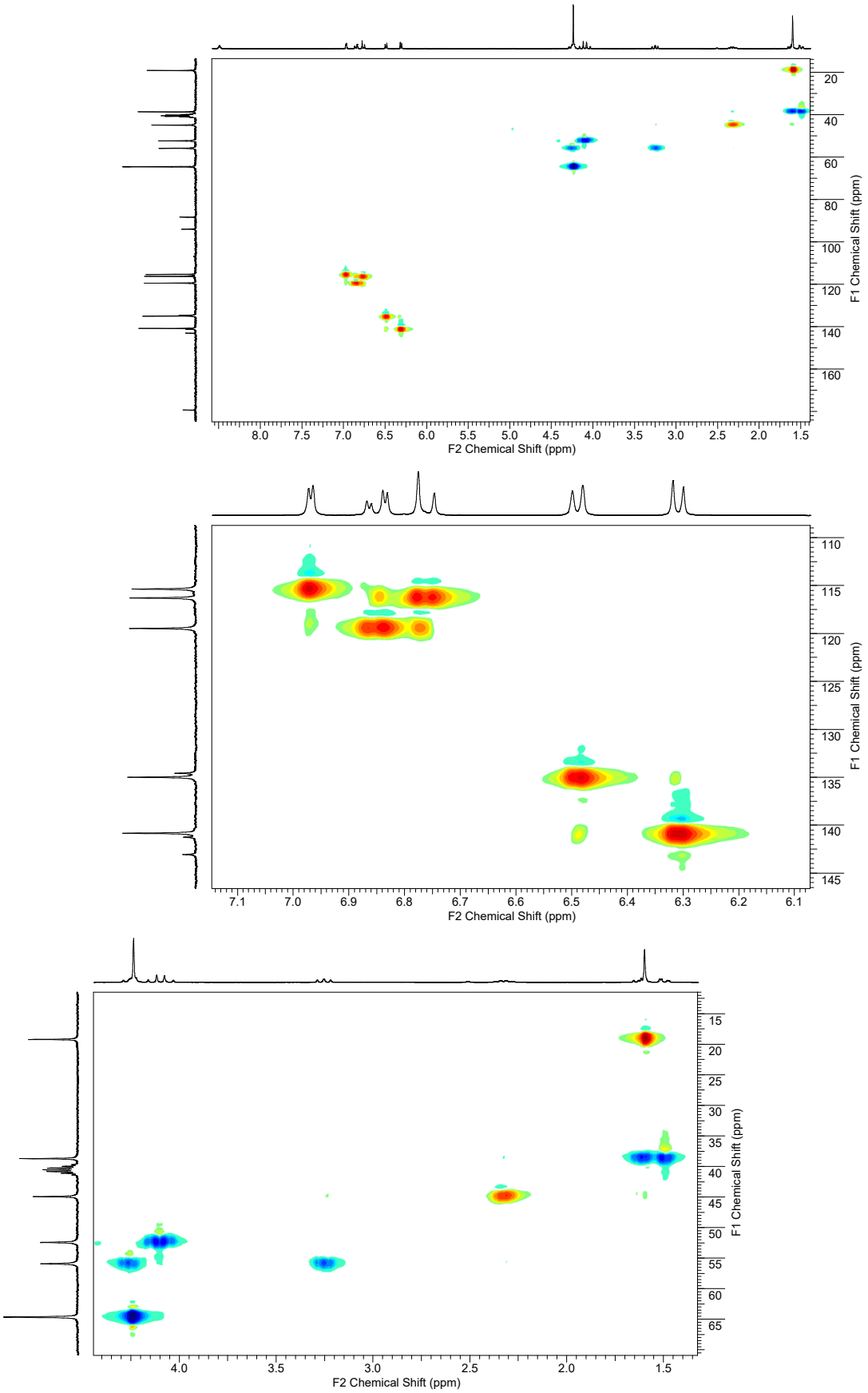
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

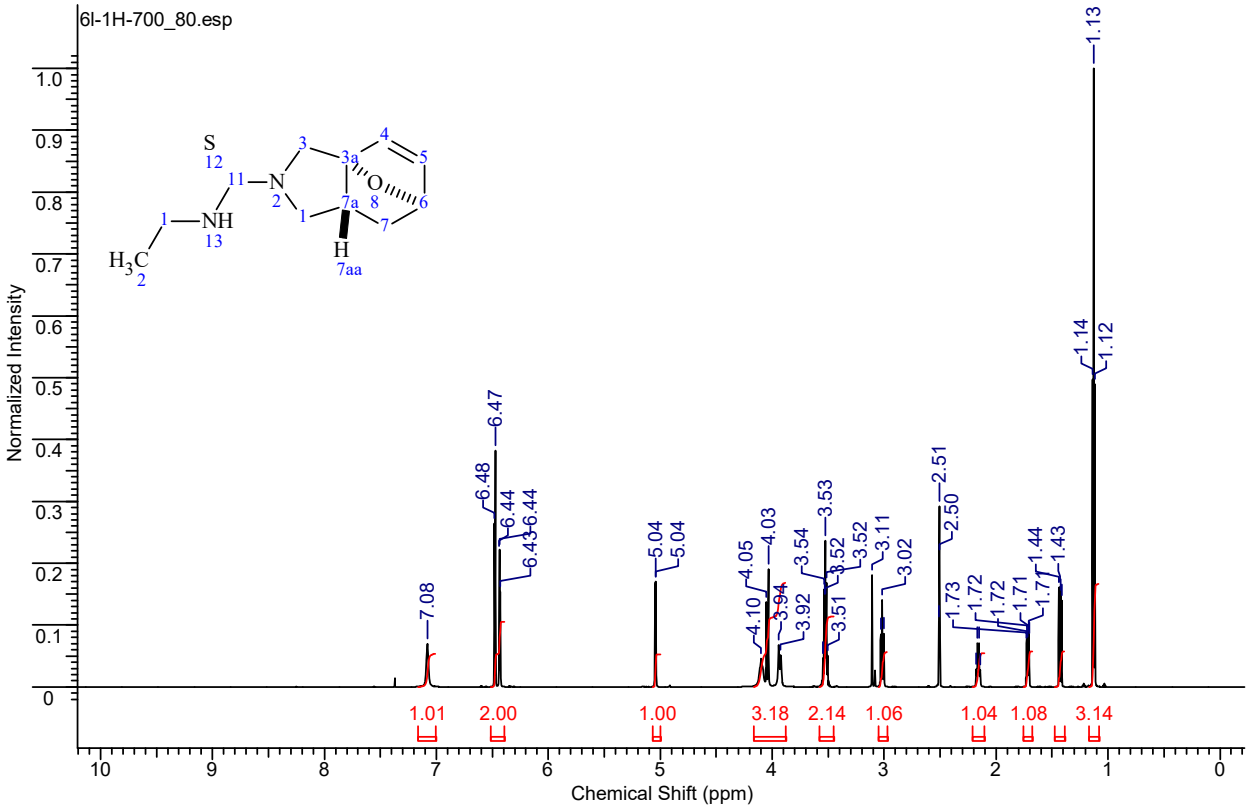


HSQC of **6k** (100 °C)

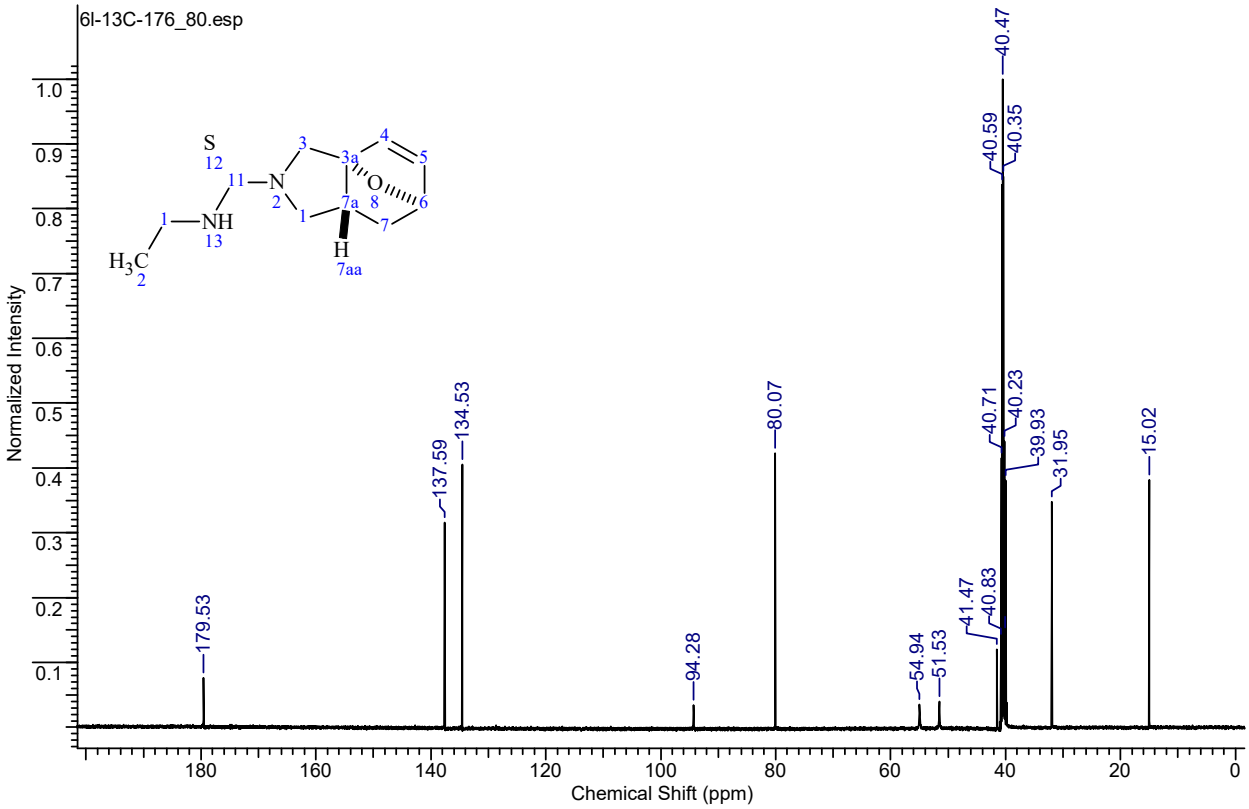


(3a*RS*,6*RS*,7a*RS*)-*N*-Ethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6l).

^{1}H NMR (700.2 MHz, DMSO-d_6, 77 °C)

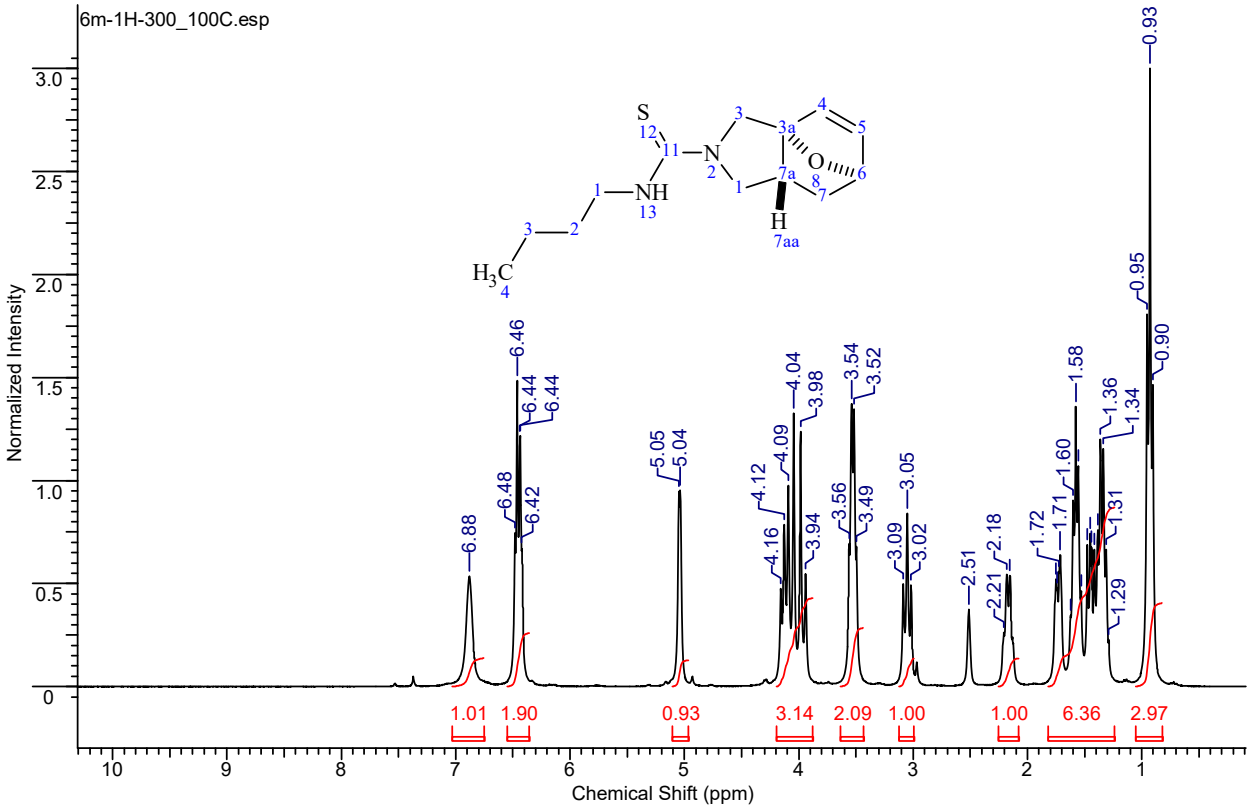


^{13}C NMR (176.1 MHz, DMSO-d_6, 77 °C)

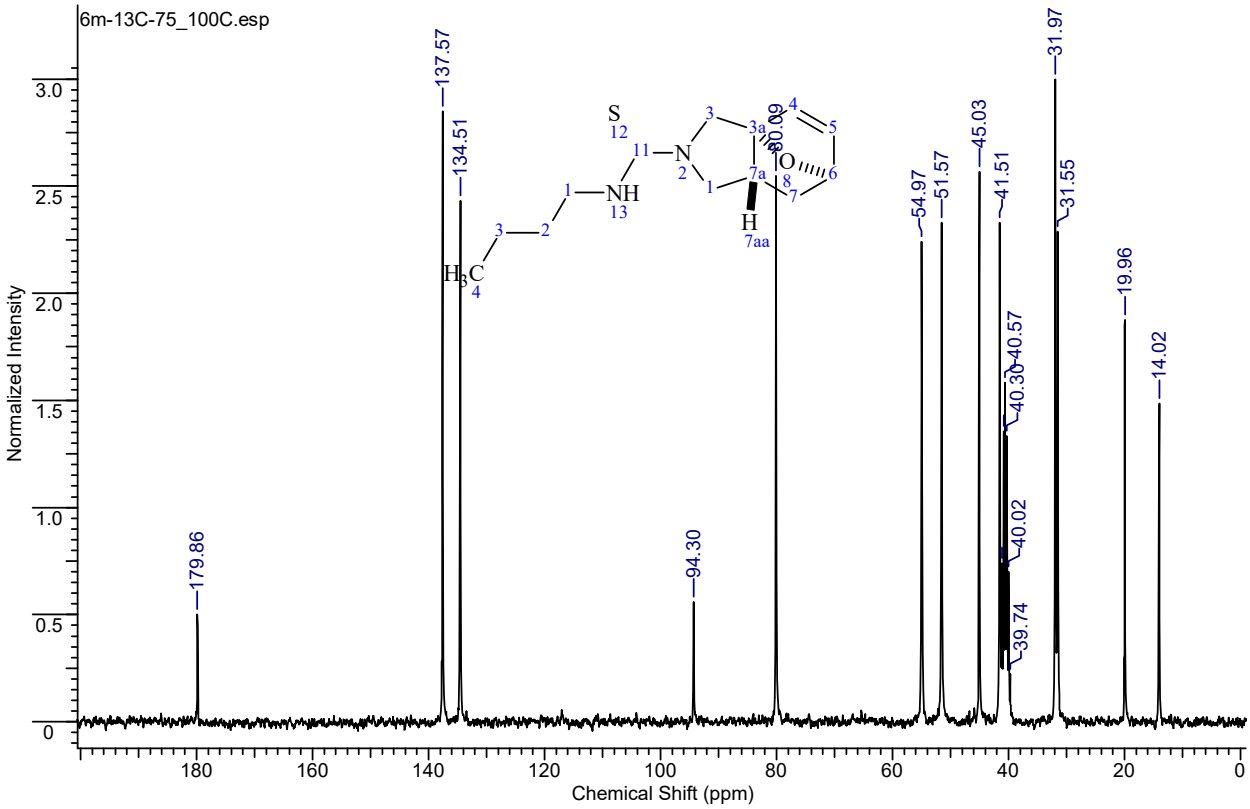


(3a*RS*,6*RS*,7a*RS*)-*N*-Butyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6m).

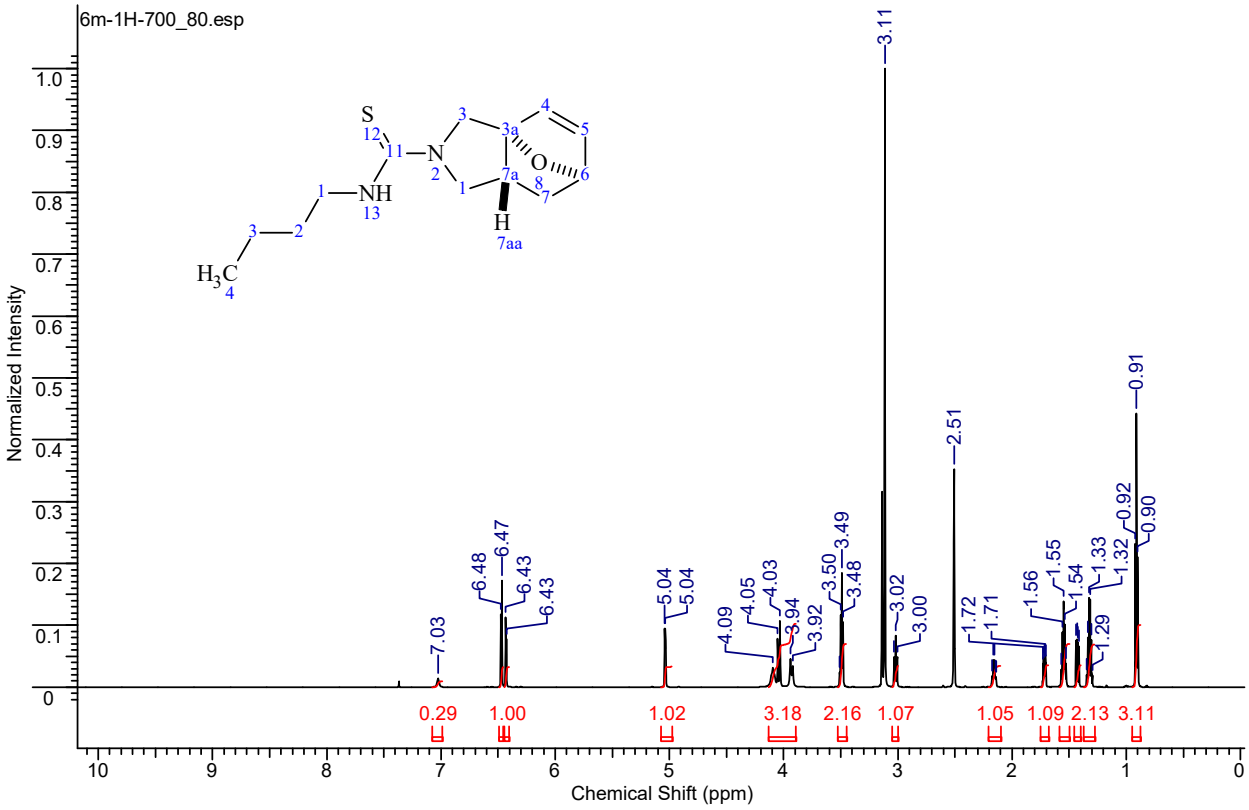
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



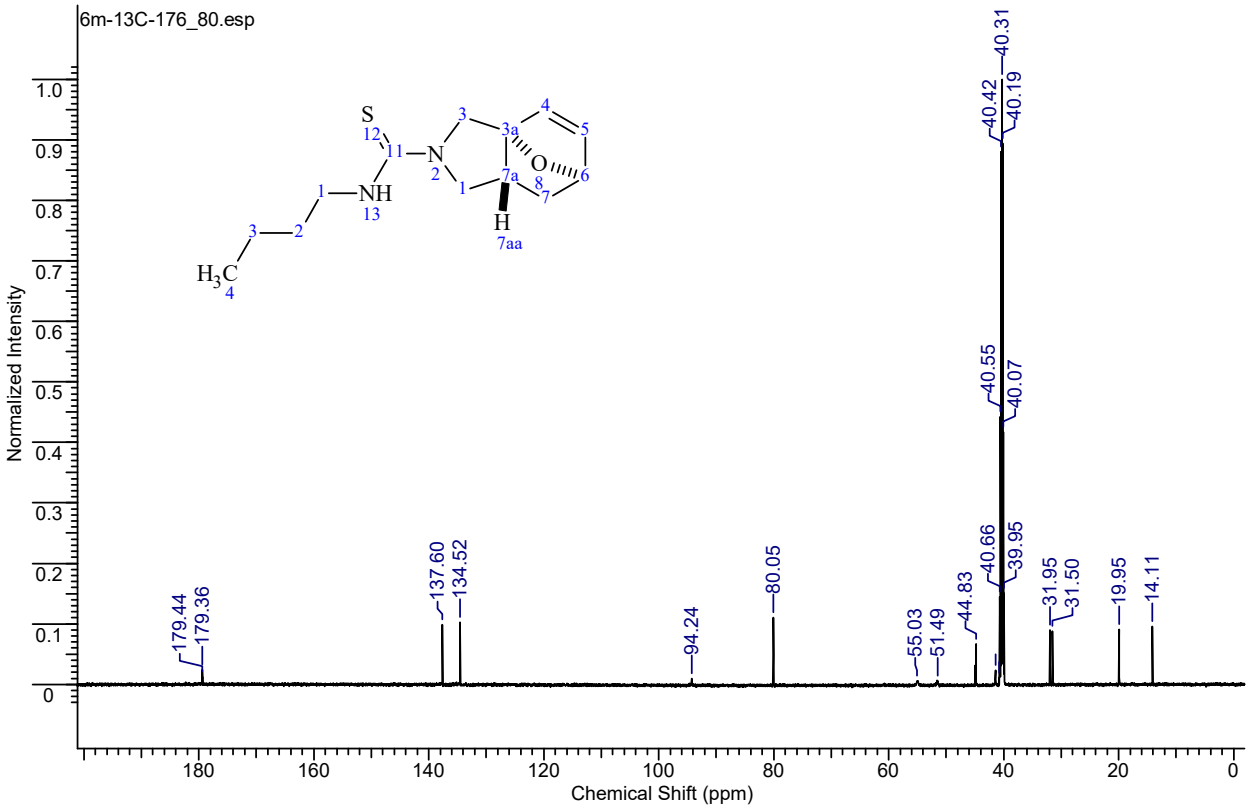
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



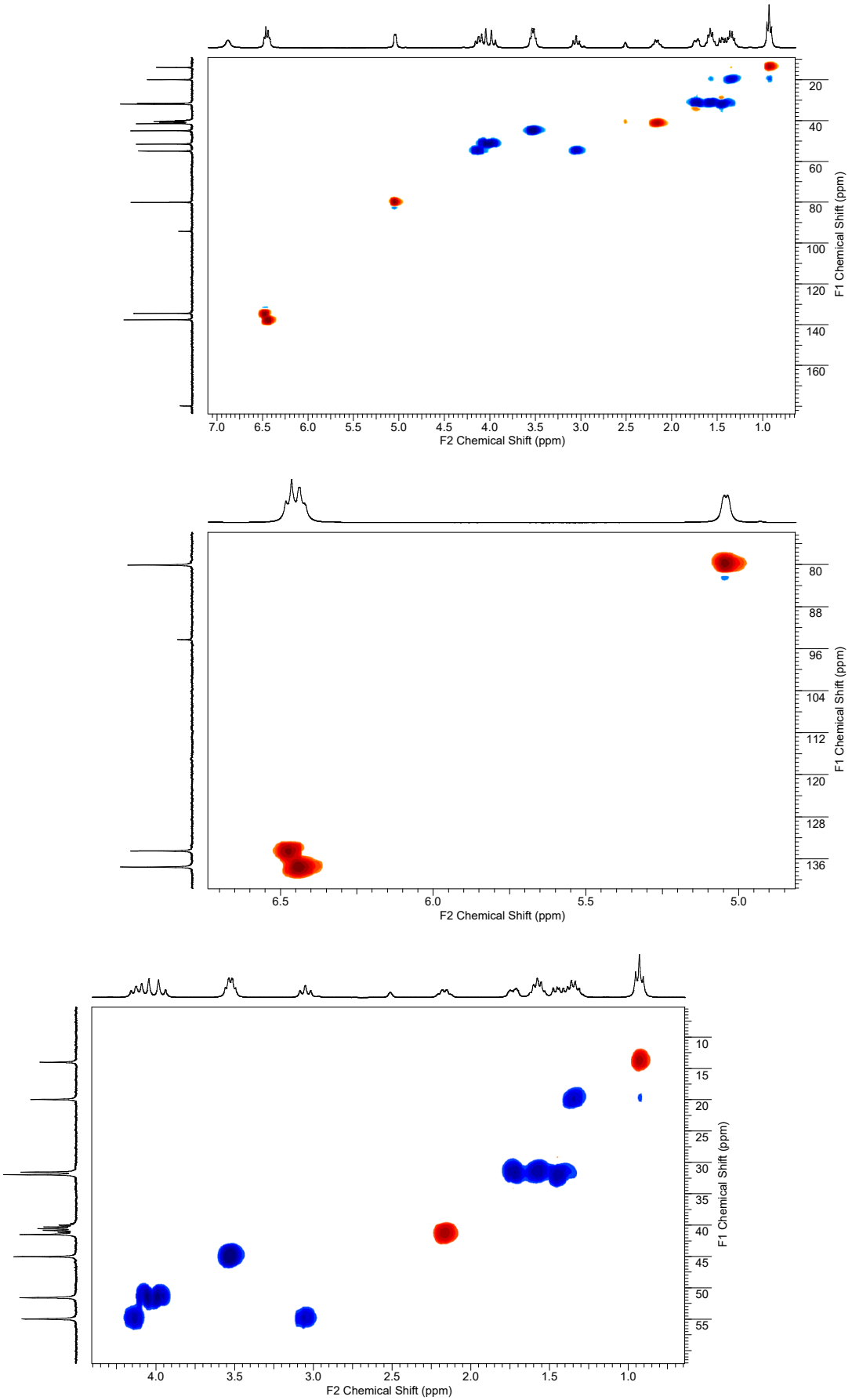
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

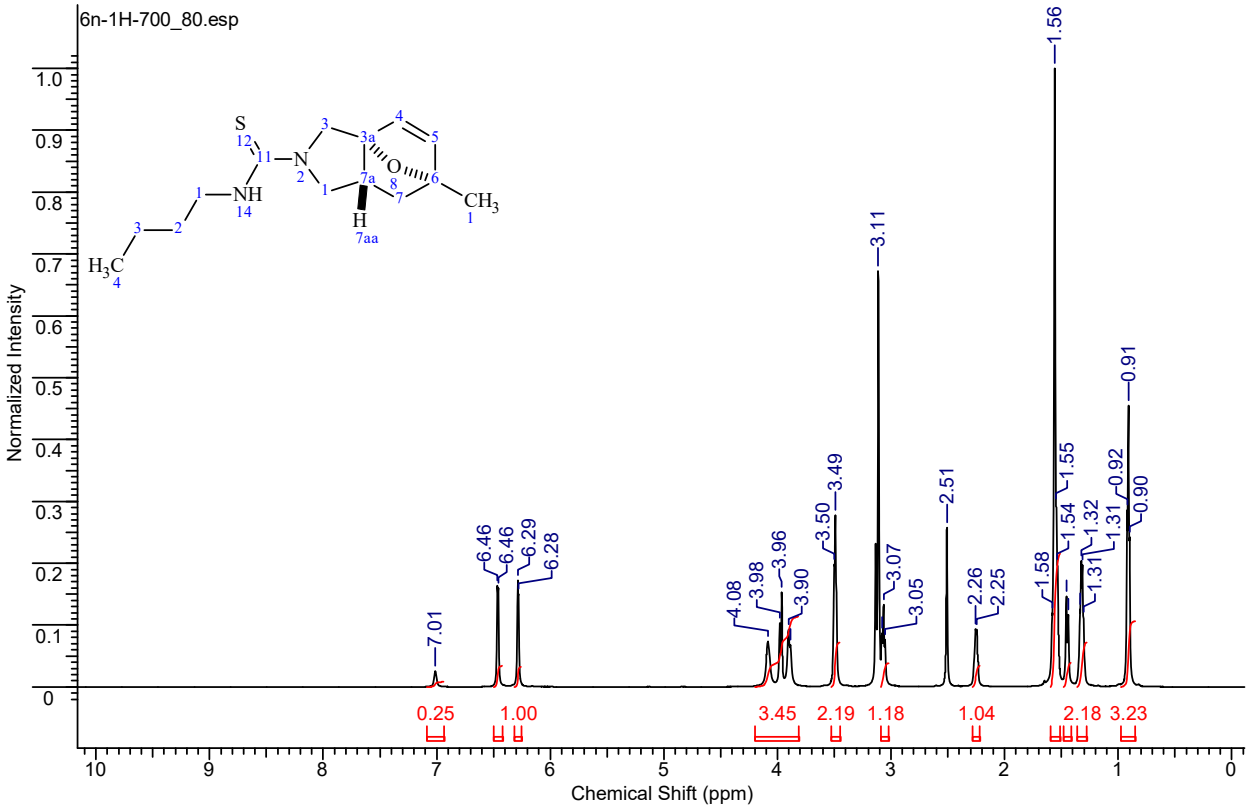


HSQC of **6m** (100 °C)

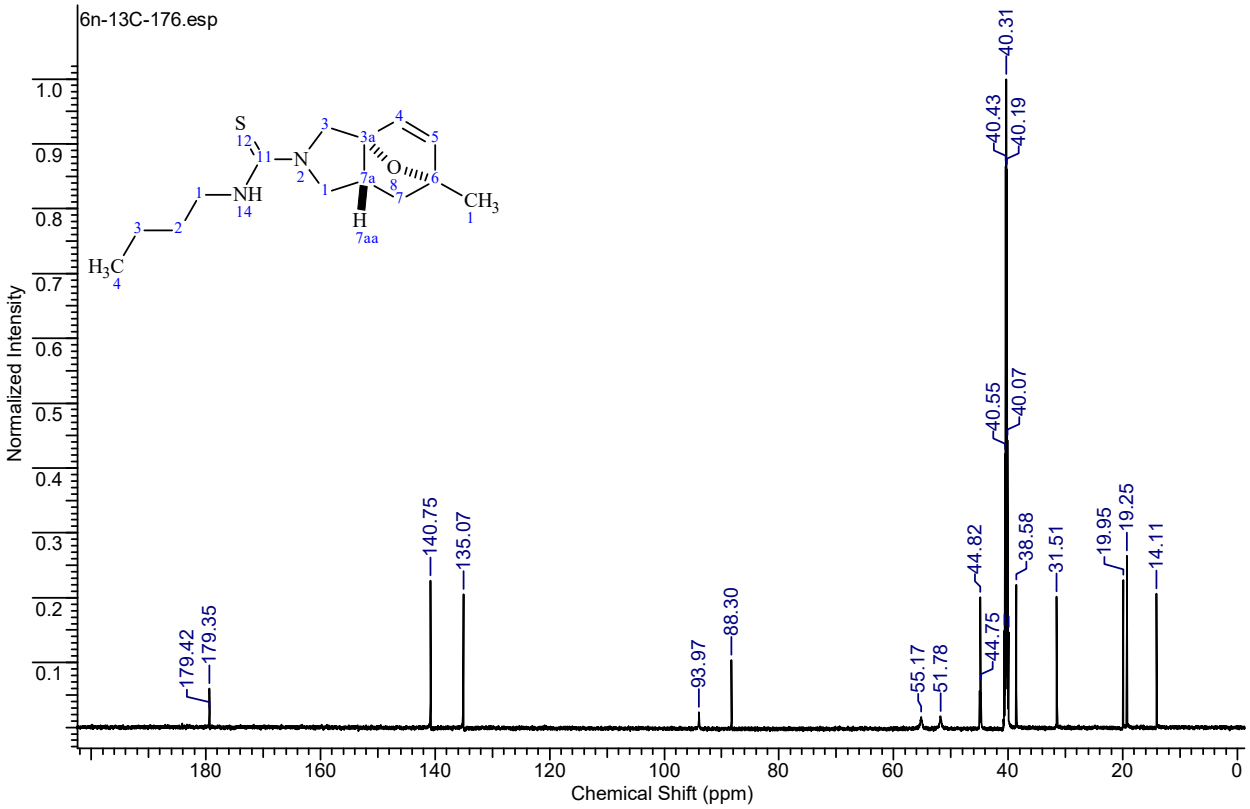


(3a*RS*,6*RS*,7a*RS*)-*N*-Butyl-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6n).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

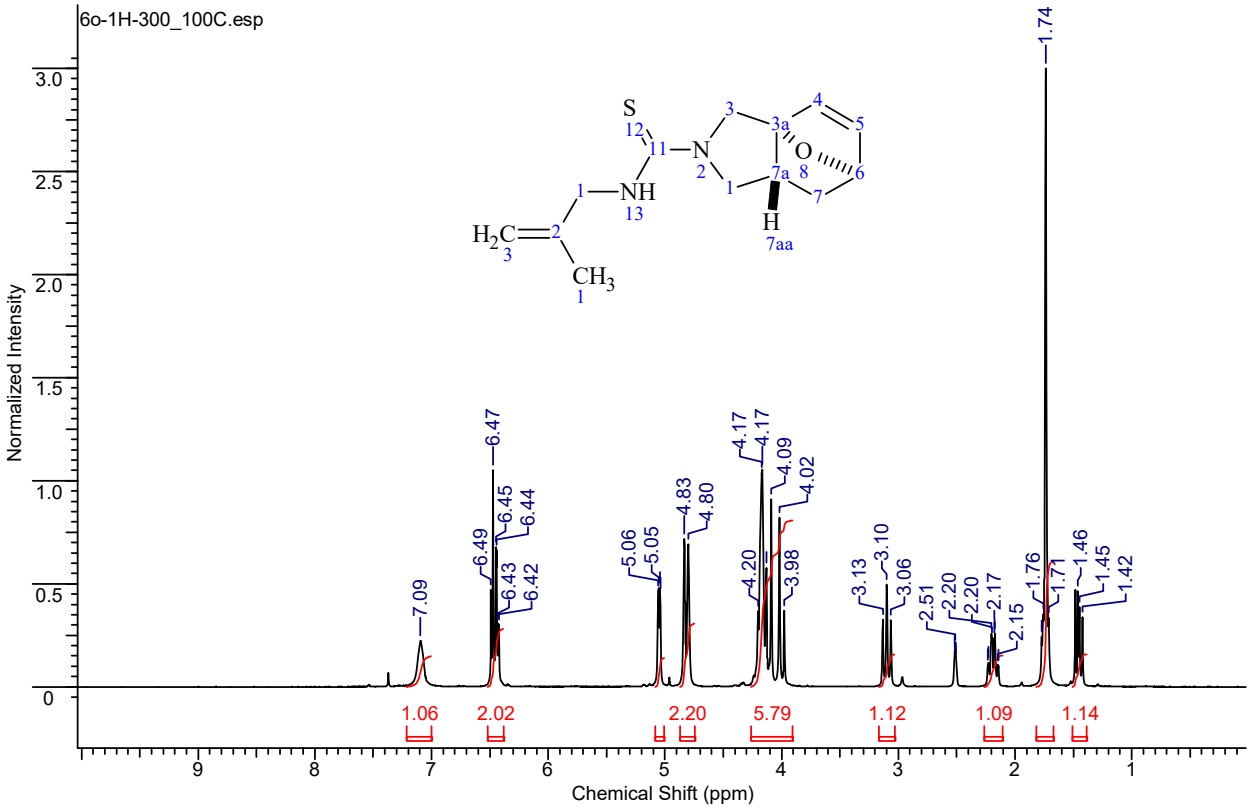


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

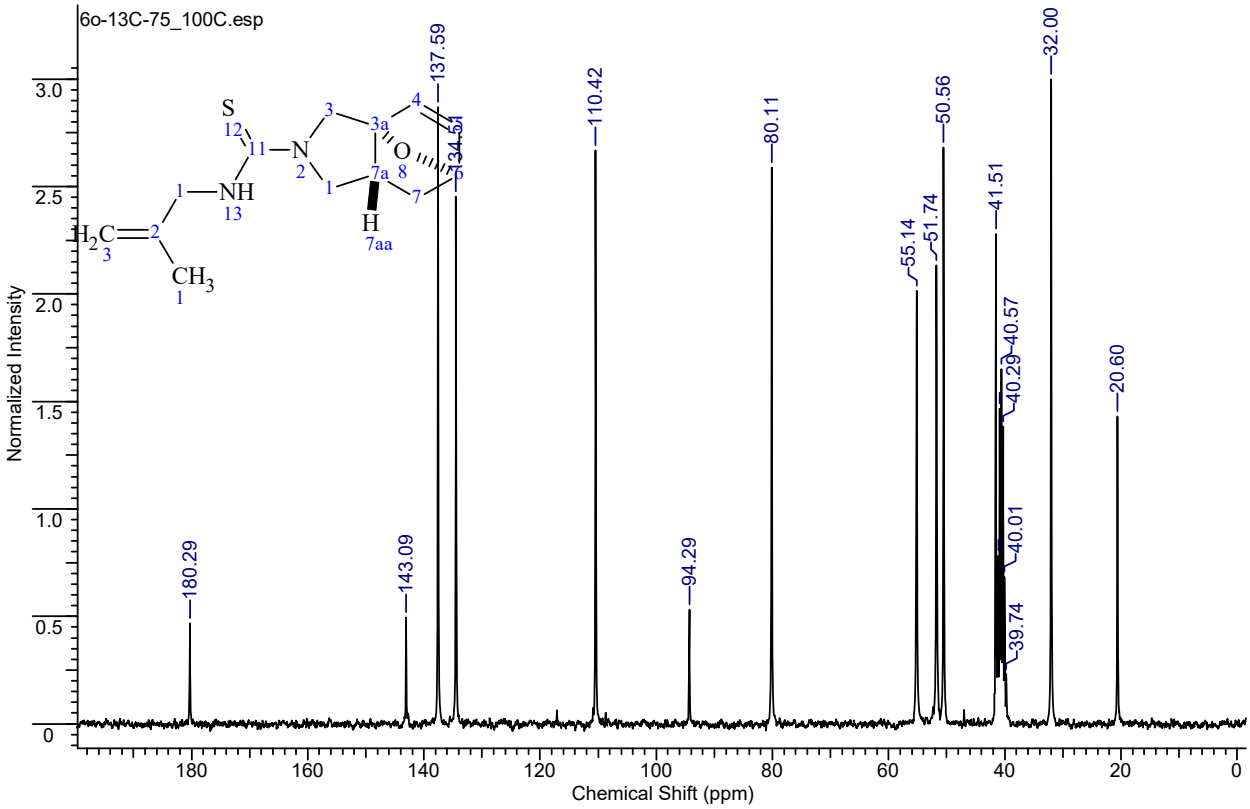


(3a*RS*,6*RS*,7a*RS*)-*N*-(2-Methylallyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6o).

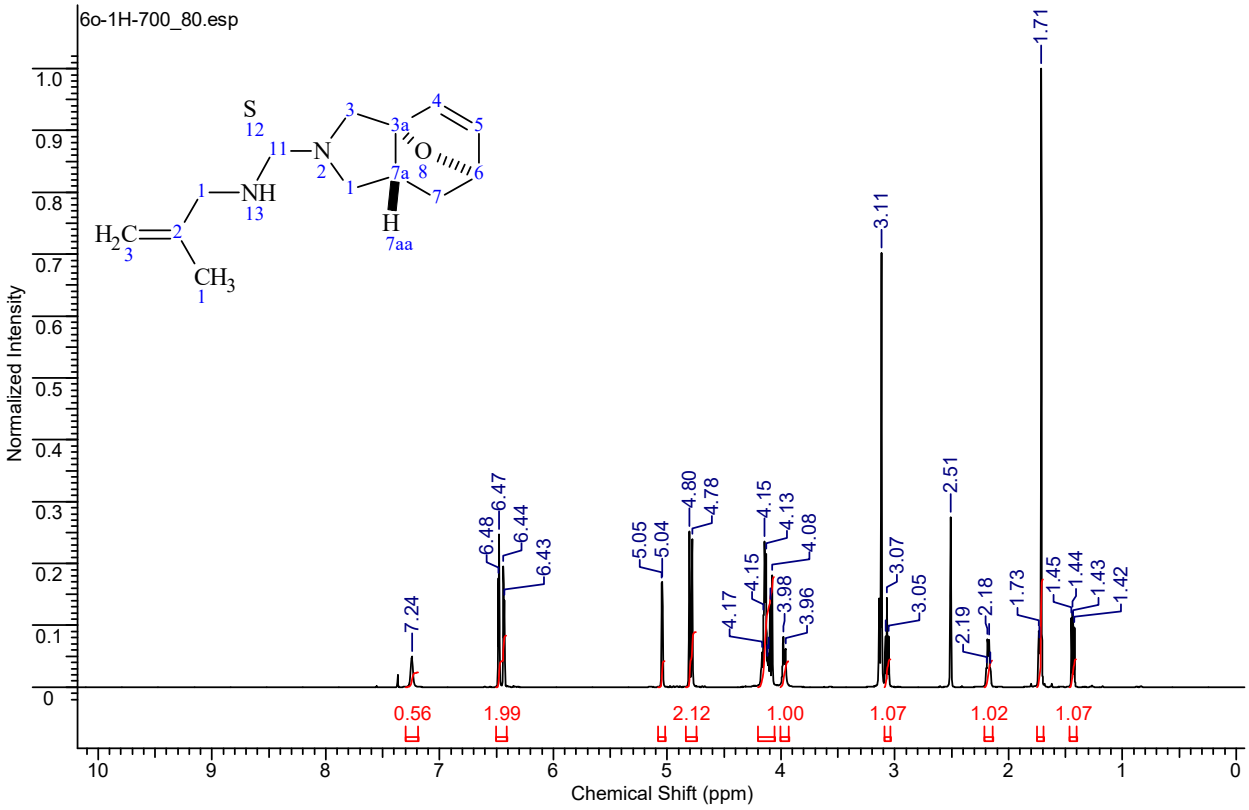
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



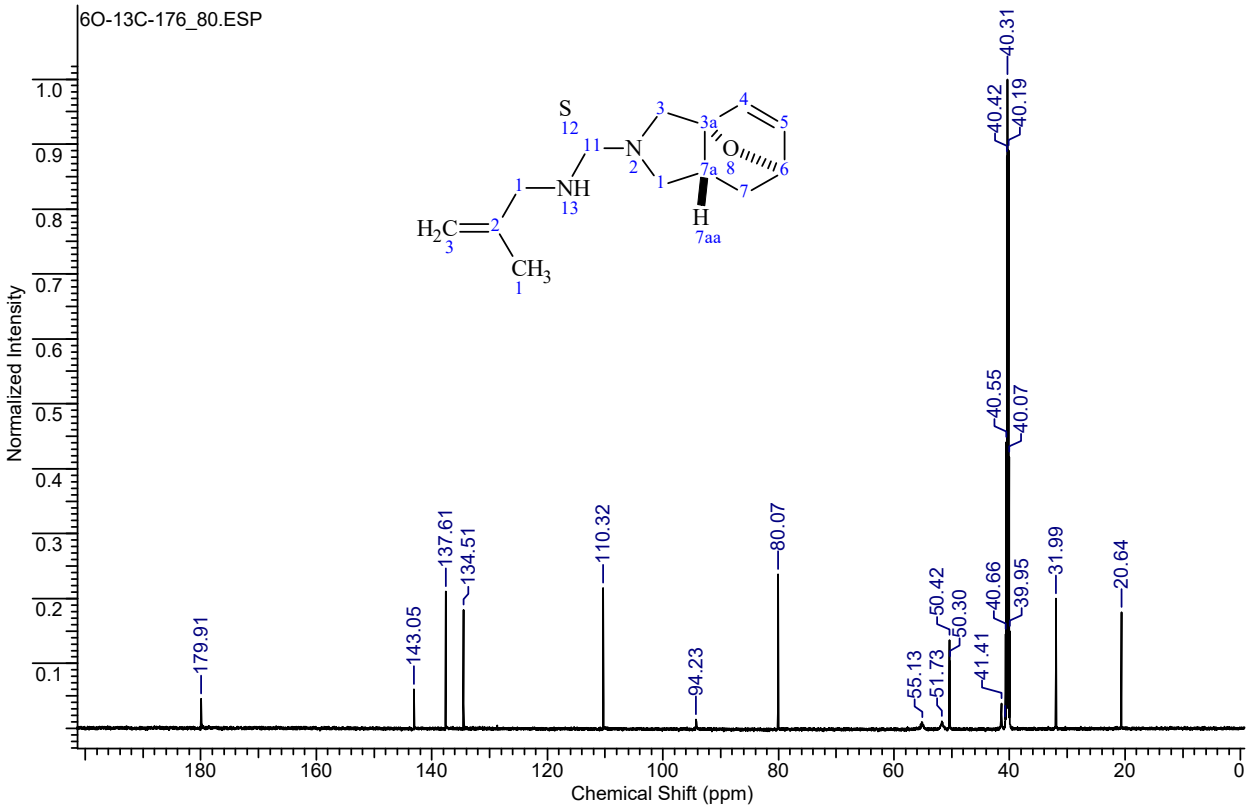
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



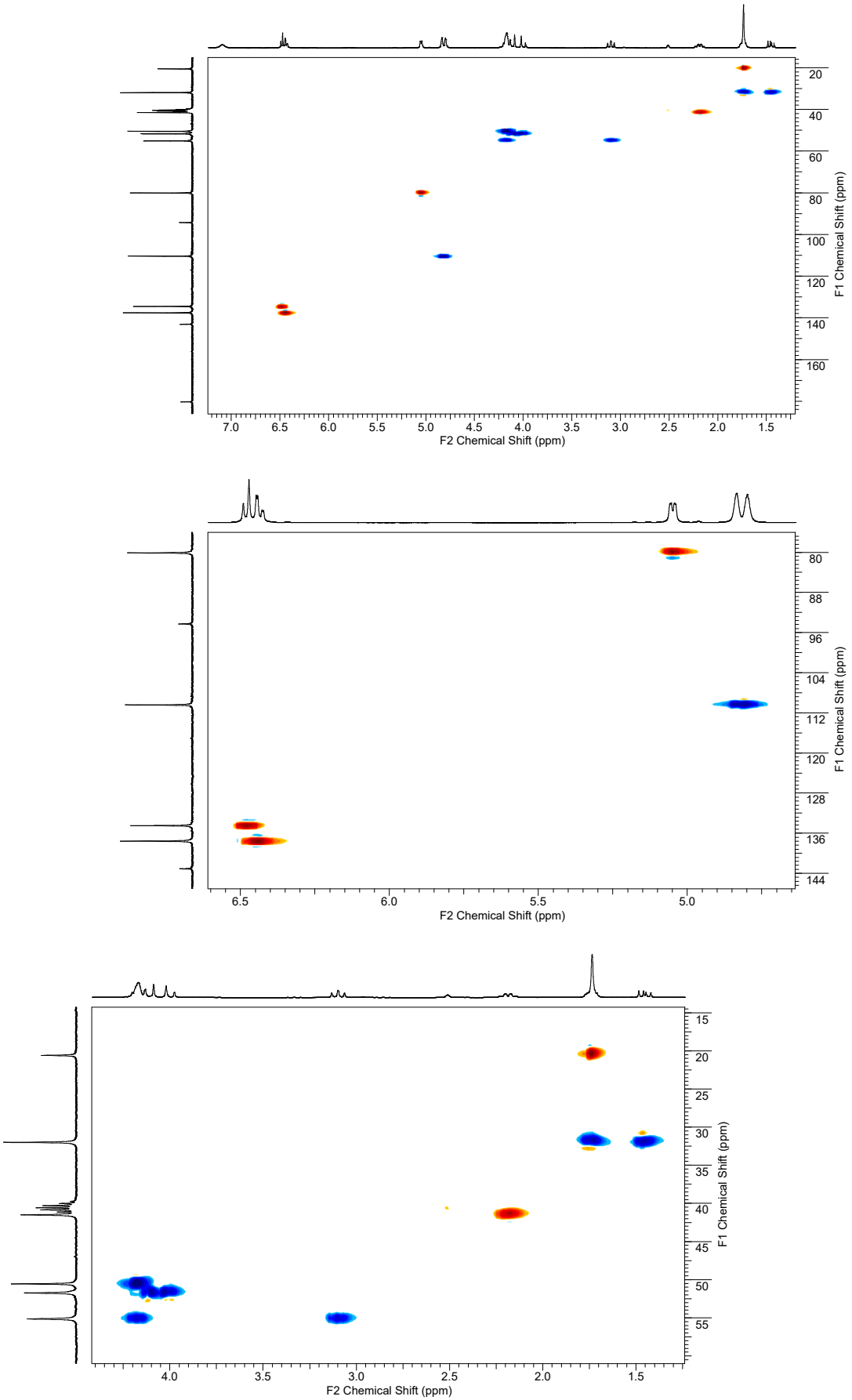
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

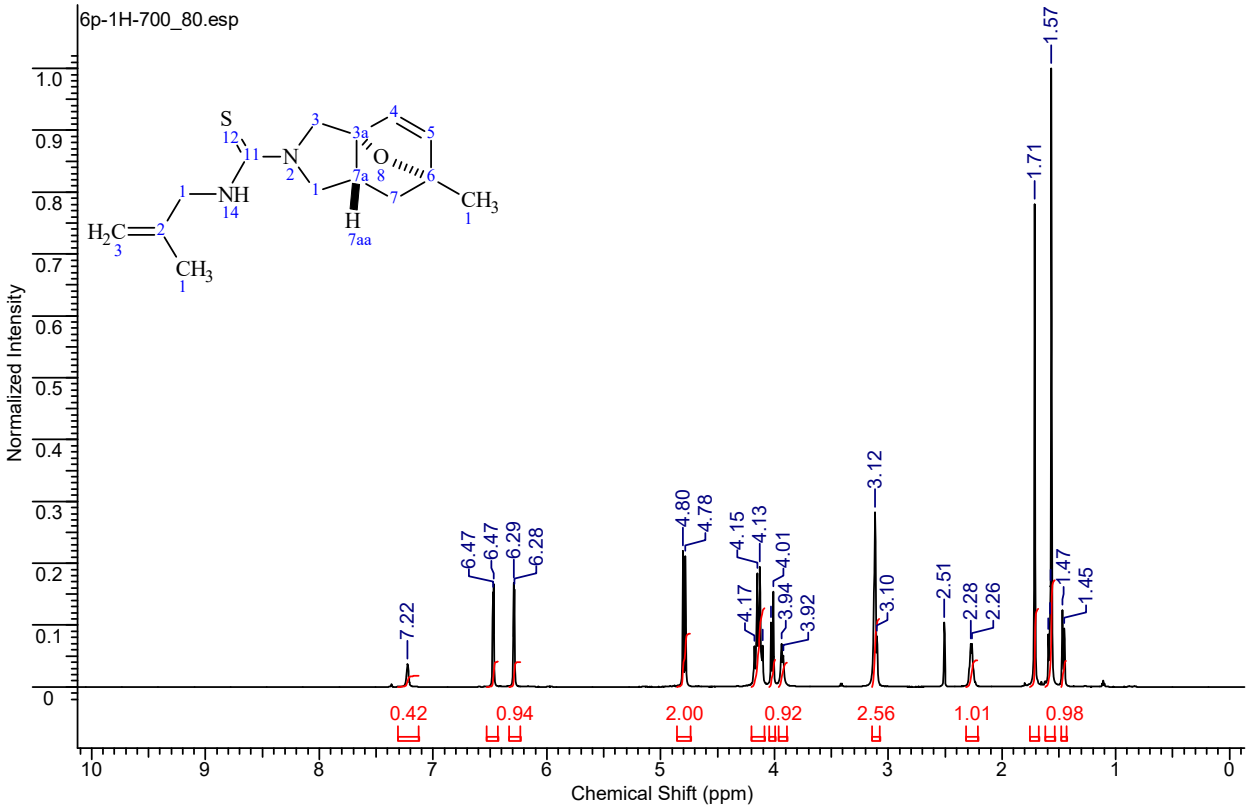


HSQC of **6o** (100 °C)

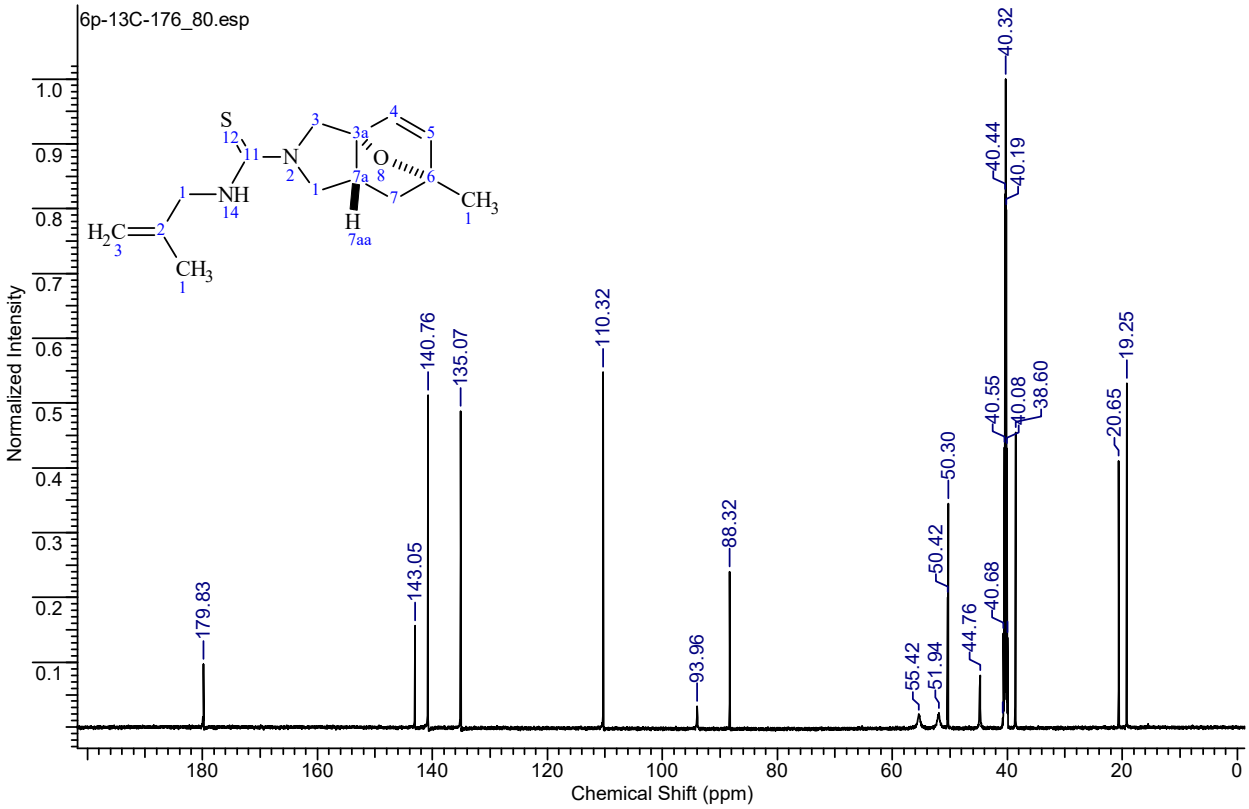


(3a*RS*,6*RS*,7a*RS*)-6-Methyl-*N*-(2-methylallyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carbothioamide (6p).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

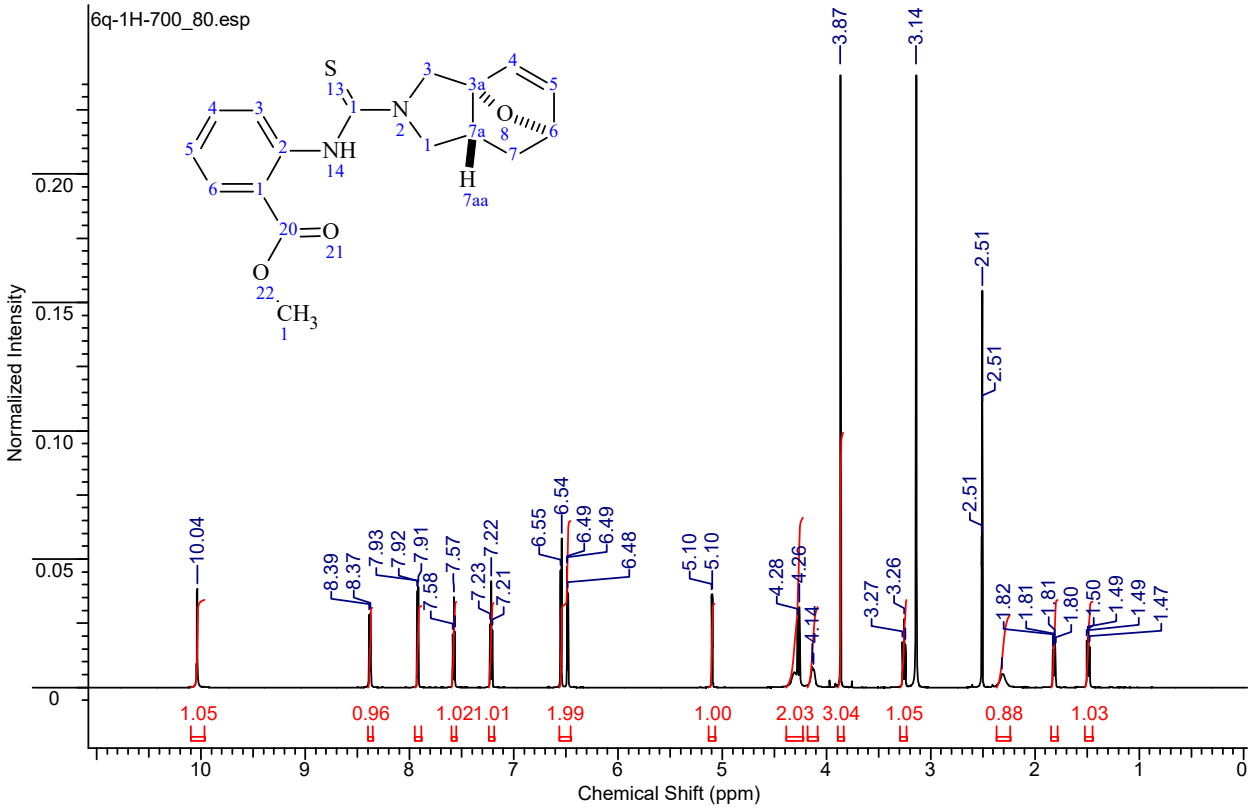


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

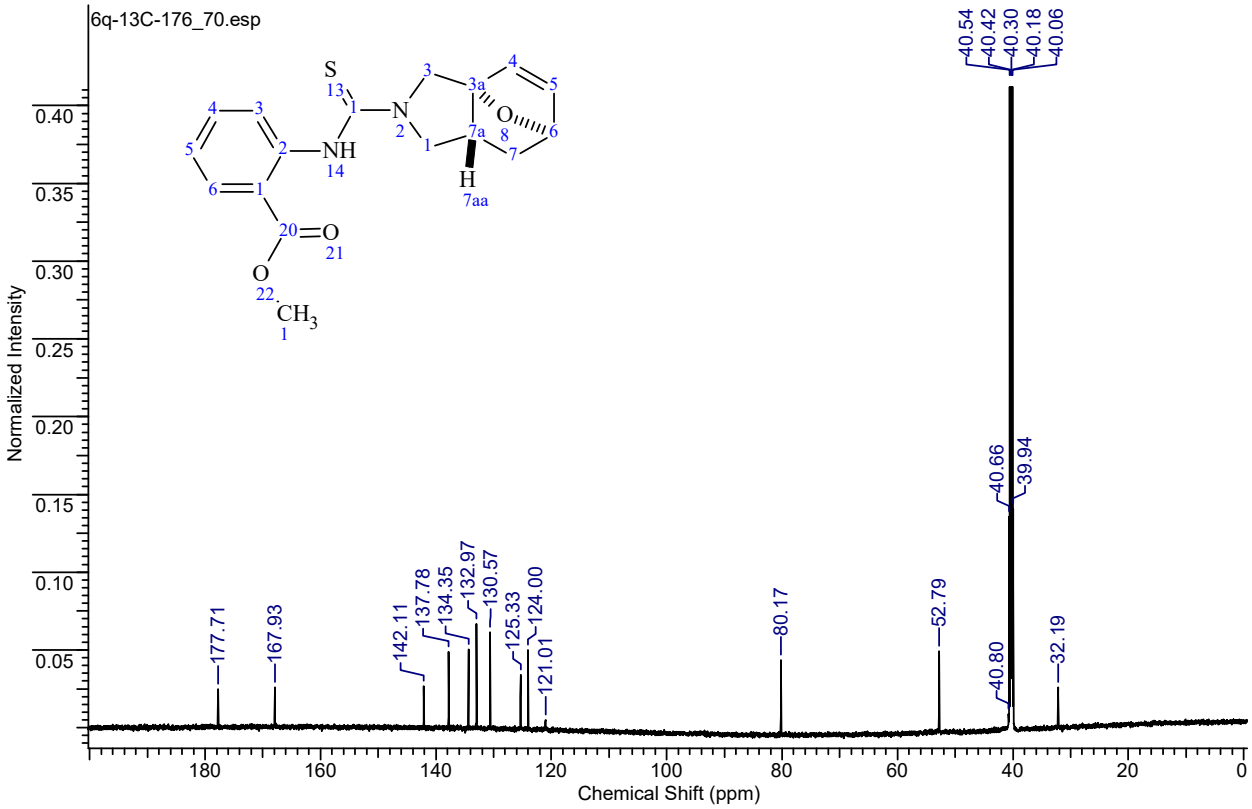


Methyl 2-{[(3a*RS*,6*RS*,7a*RS*)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindol-2-ylcarbonothioyl]amino}benzoate (6q).

^{1}H NMR (700.2 MHz, DMSO-d_6, 70 °C)

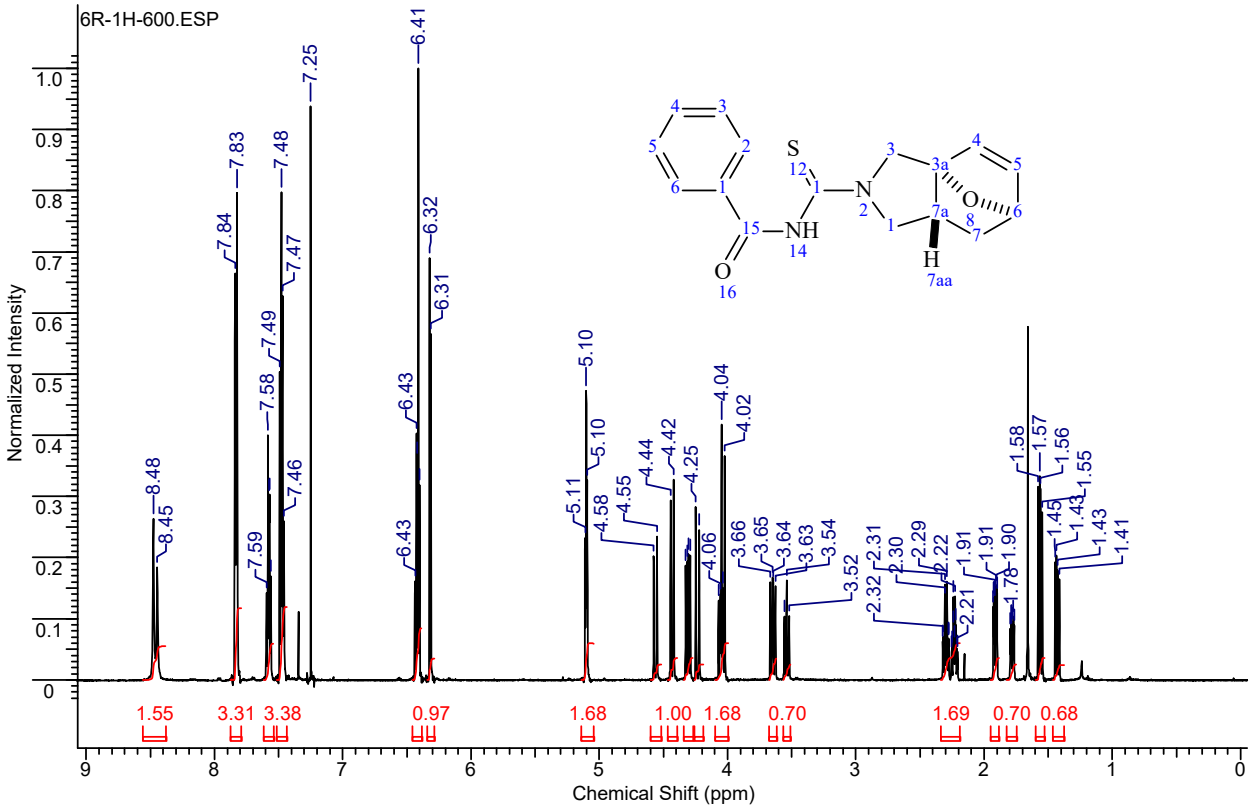


^{13}C NMR (176.1 MHz, DMSO-d_6, 70 °C)

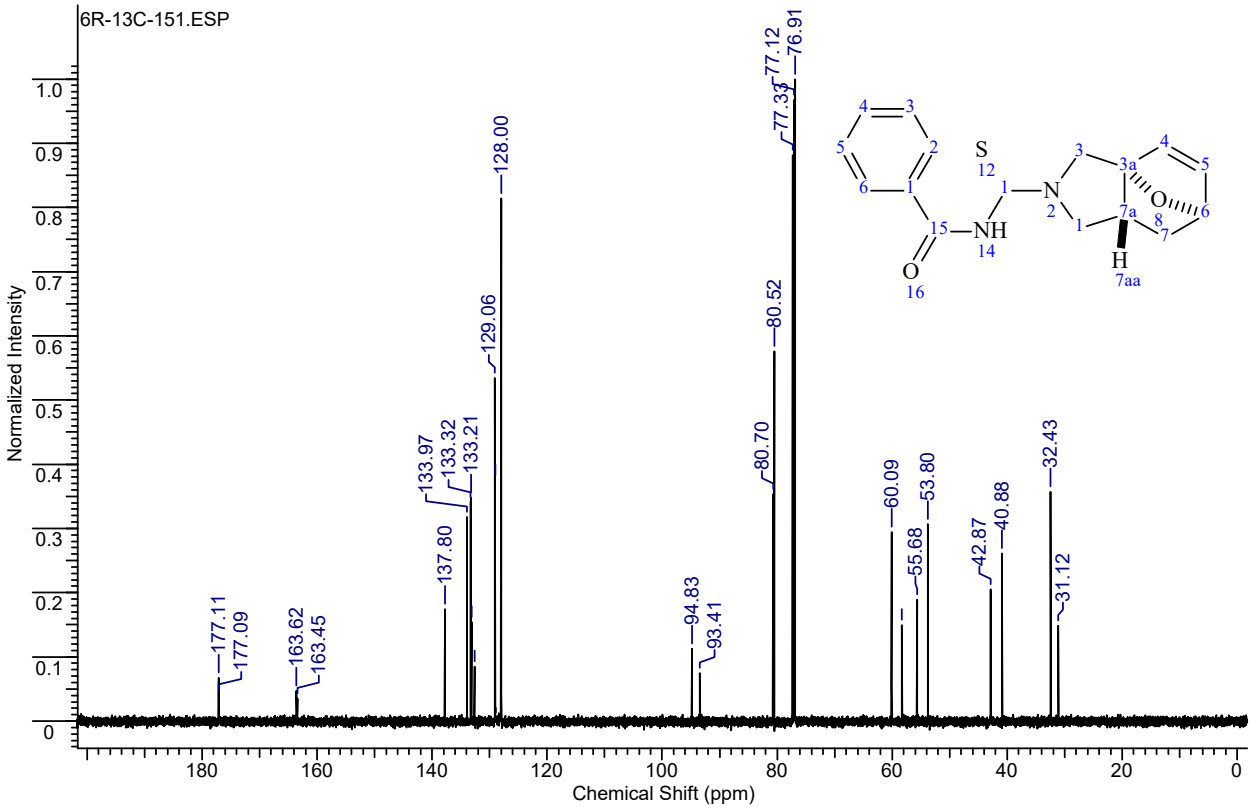


***N*-[(3a*RS*,6*RS*,7a*RS*)-1,6,7,7a-Tetrahydro-3a,6-epoxyisoindol-2-ylcarbonothioyl]benzamide (6r).**

^{1}H NMR (600.2 MHz, $CDCl_3$)

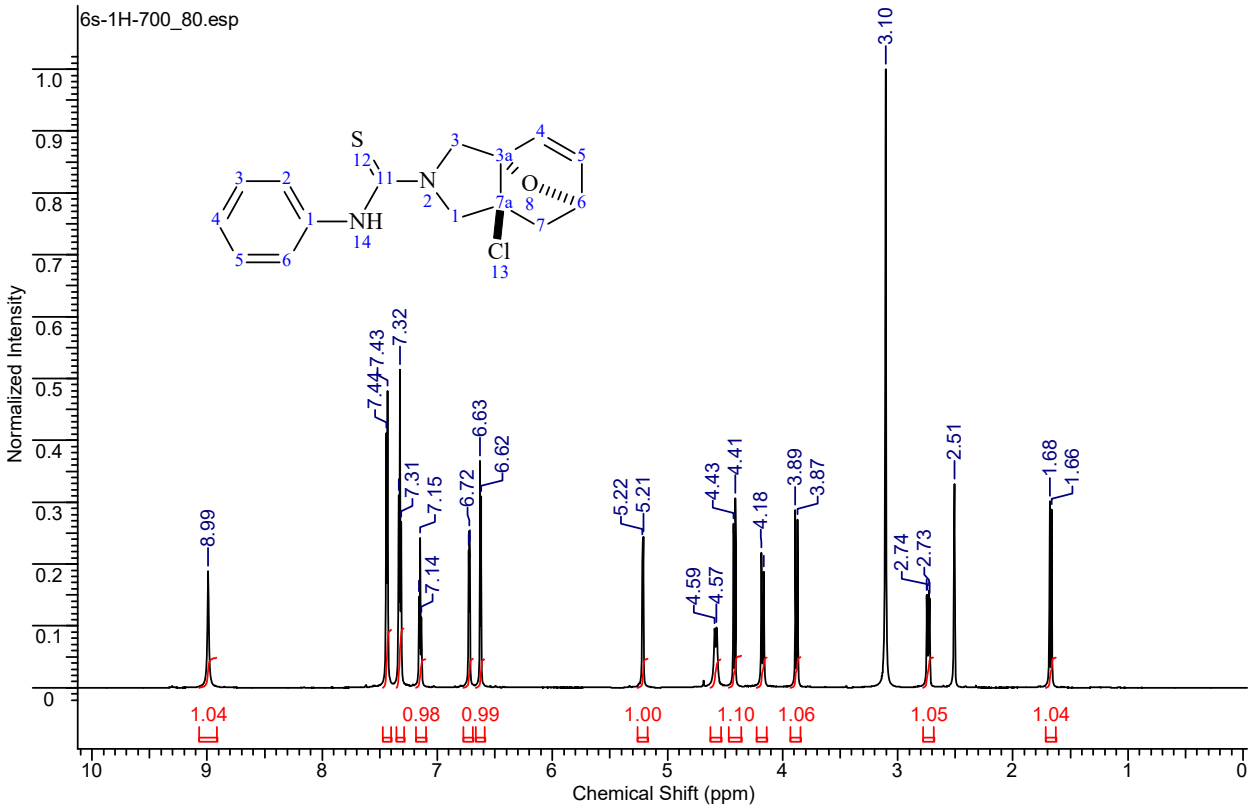


^{13}C NMR (150.9 MHz, $CDCl_3$)

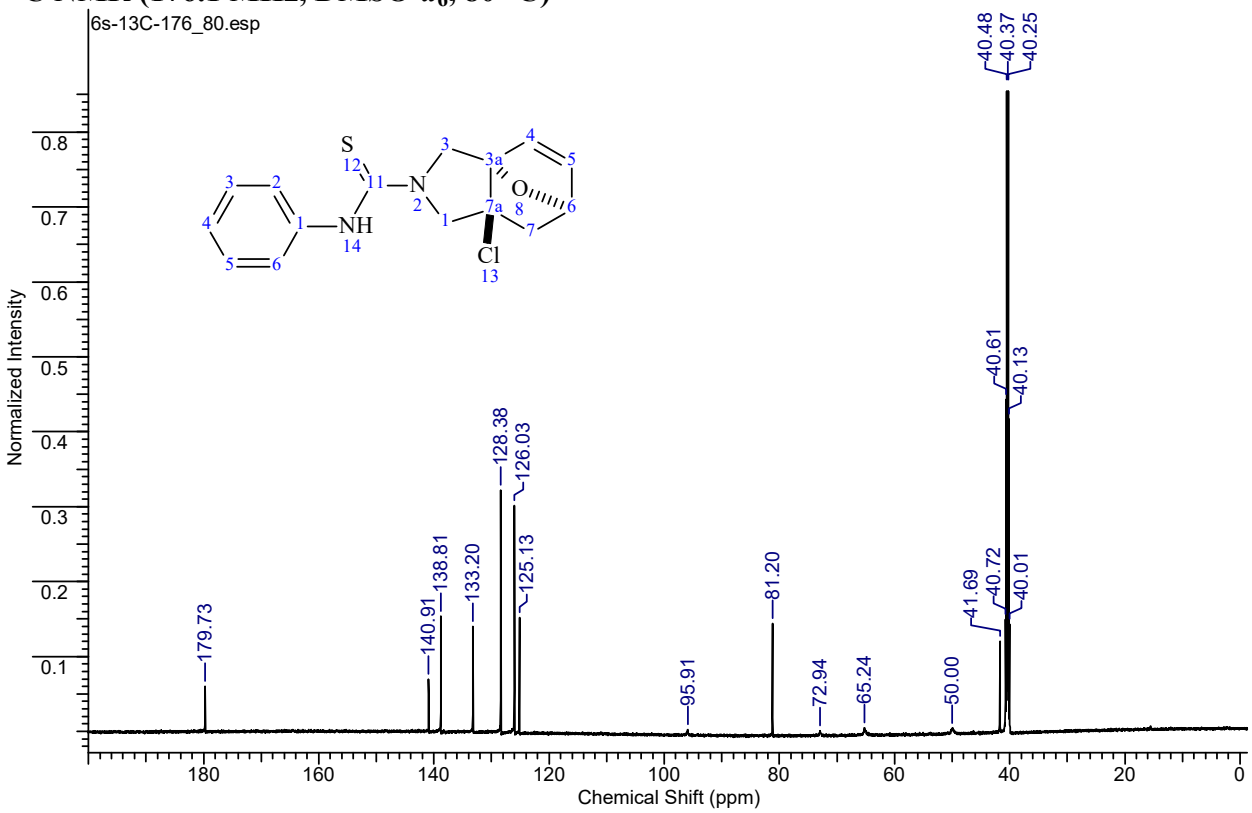


(3a*SR*,6*RS*,7a*SR*)-7a-Chloro-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carbothioamide (6s).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

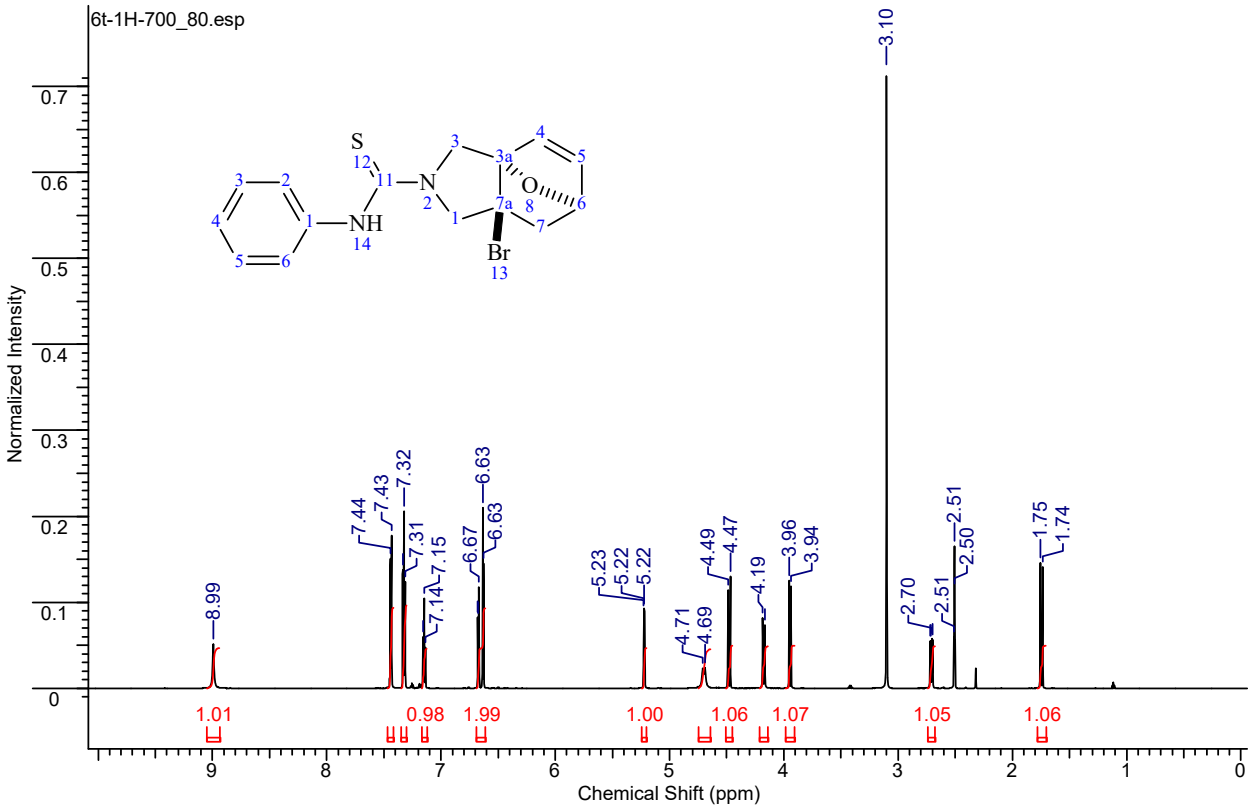


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

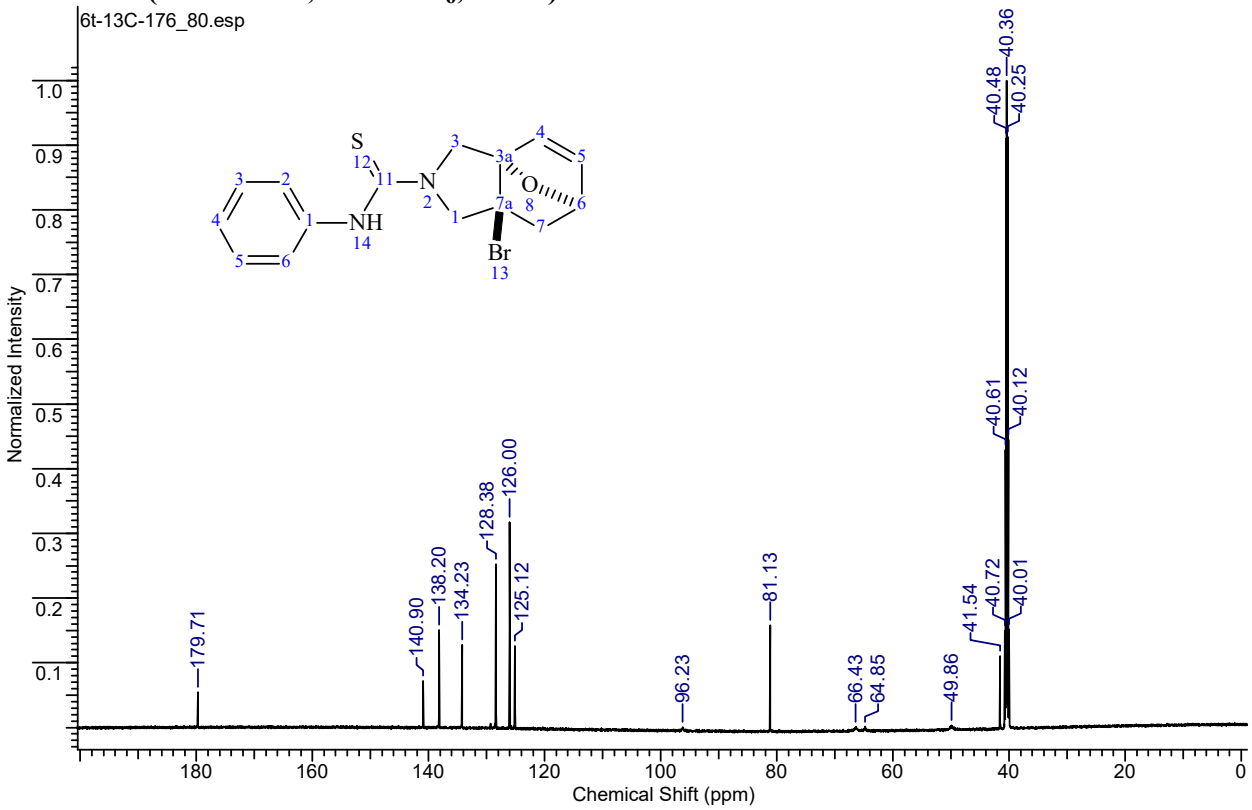


(3a*SR*,6*RS*,7a*SR*)-7a-Bromo-*N*-phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2-carbothioamide (6t).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

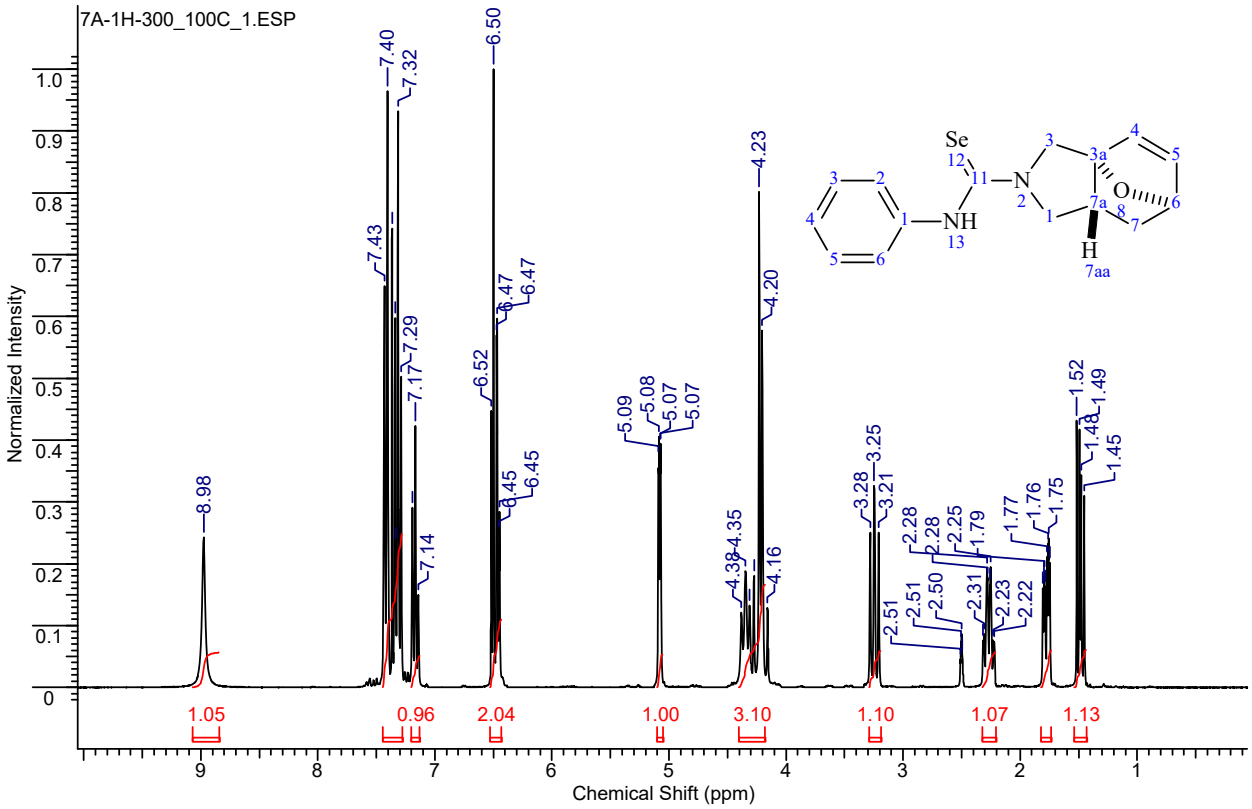


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

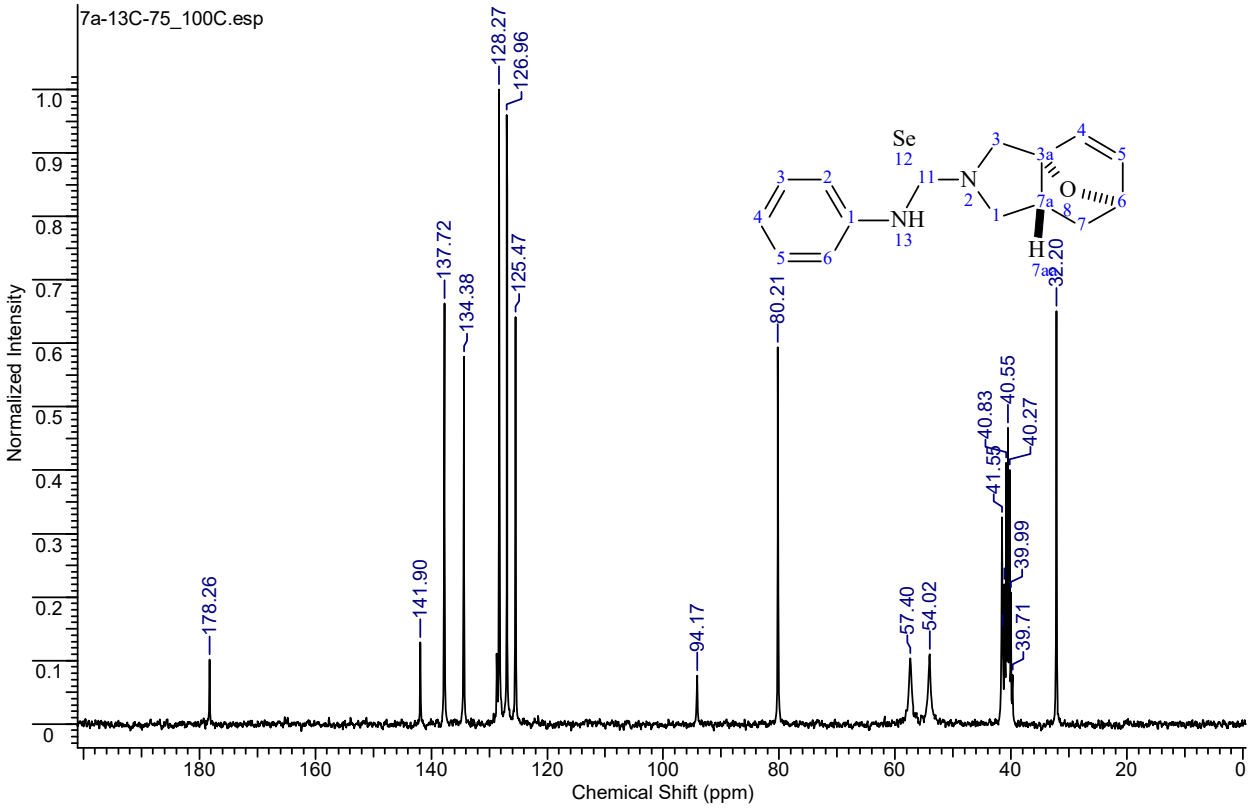


(3a*RS*,6*RS*,7a*RS*)-*N*-Phenyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7a).

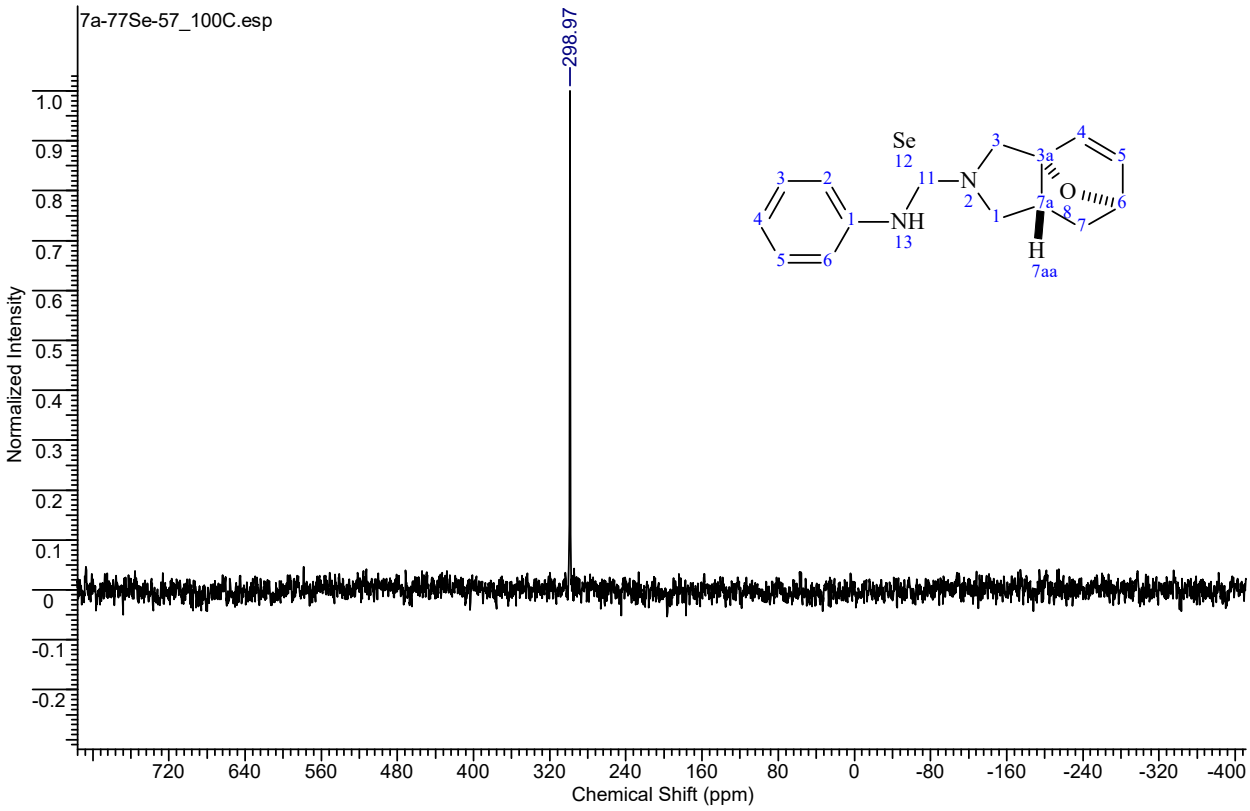
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



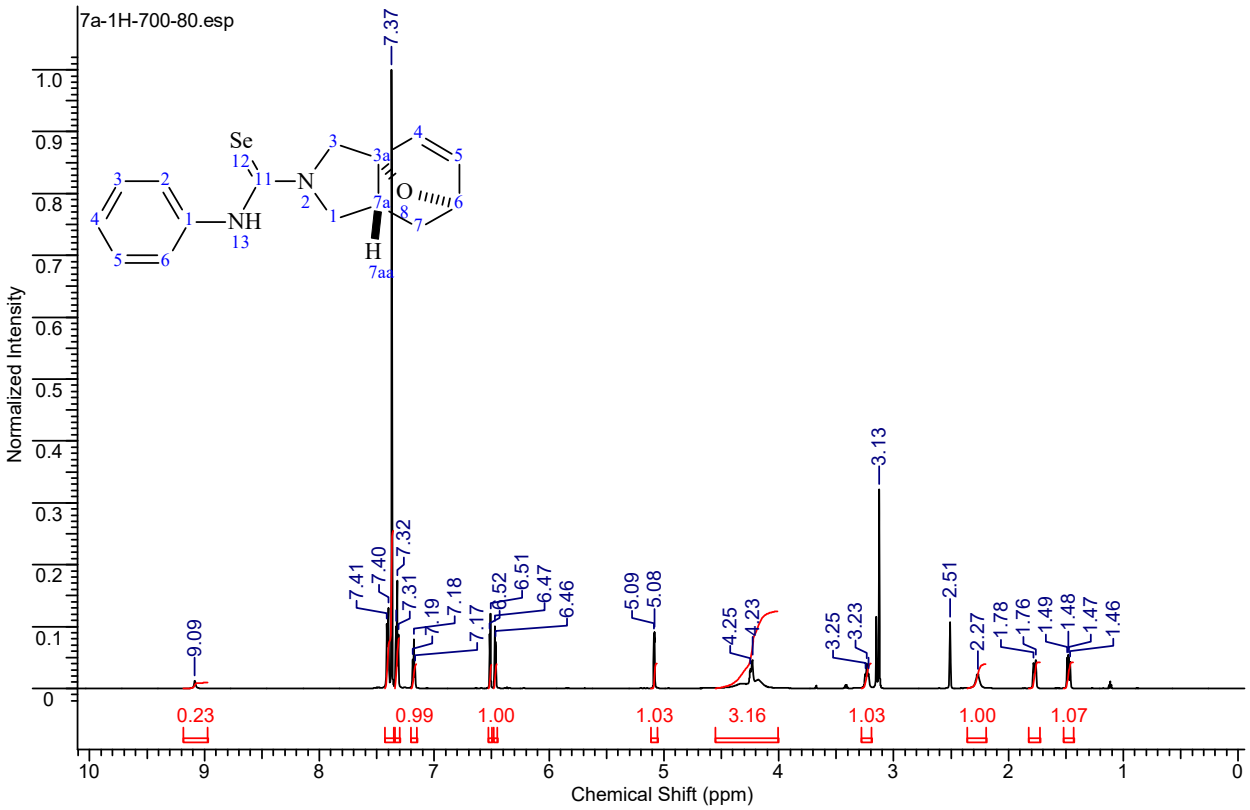
^{13}C NMR (75.5 MHz, DMSO-d_6, 80 °C)



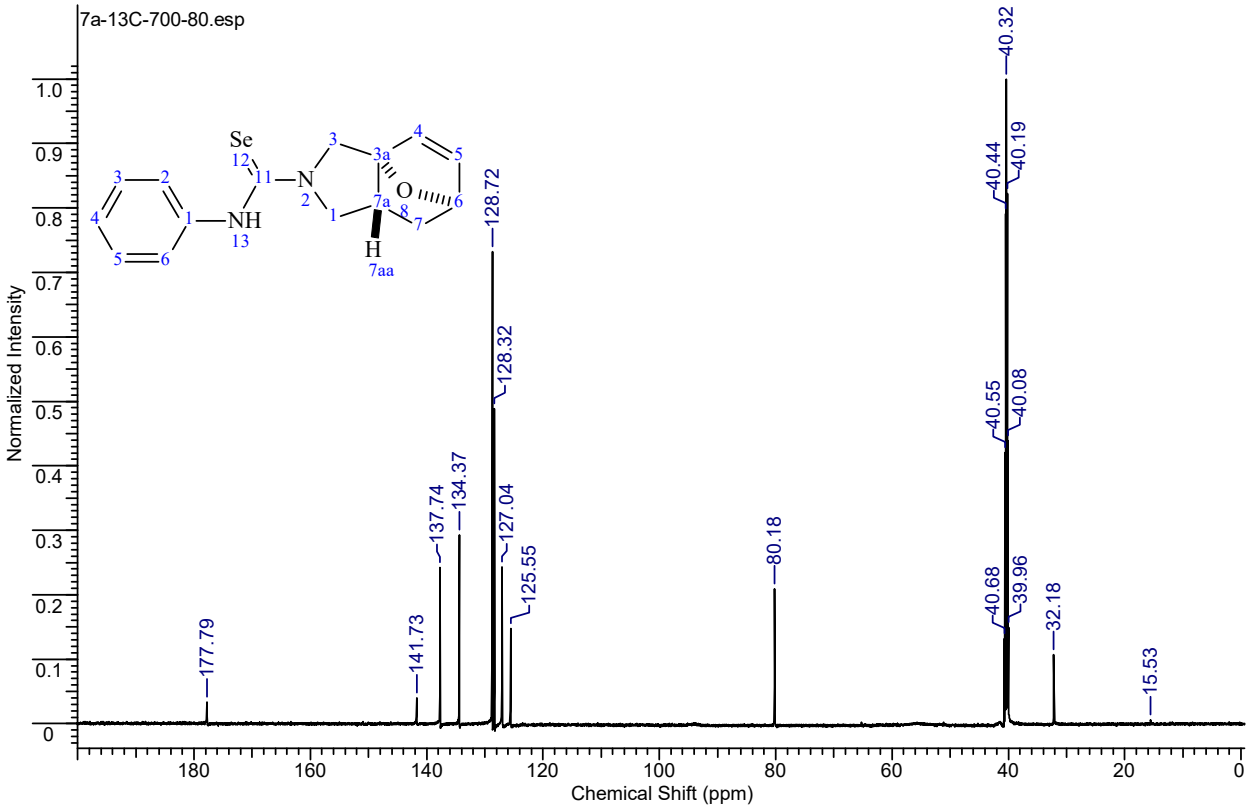
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100 °C)



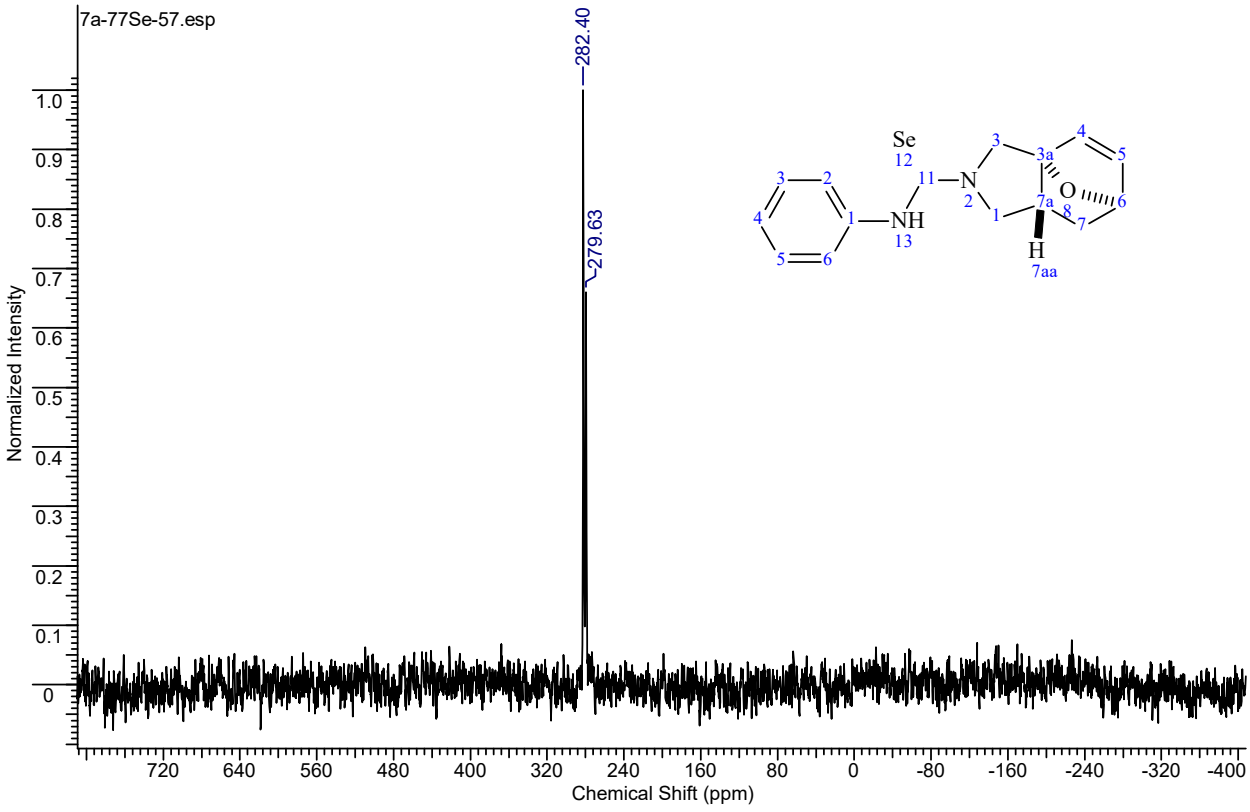
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C) *Contains an impurity of benzene*



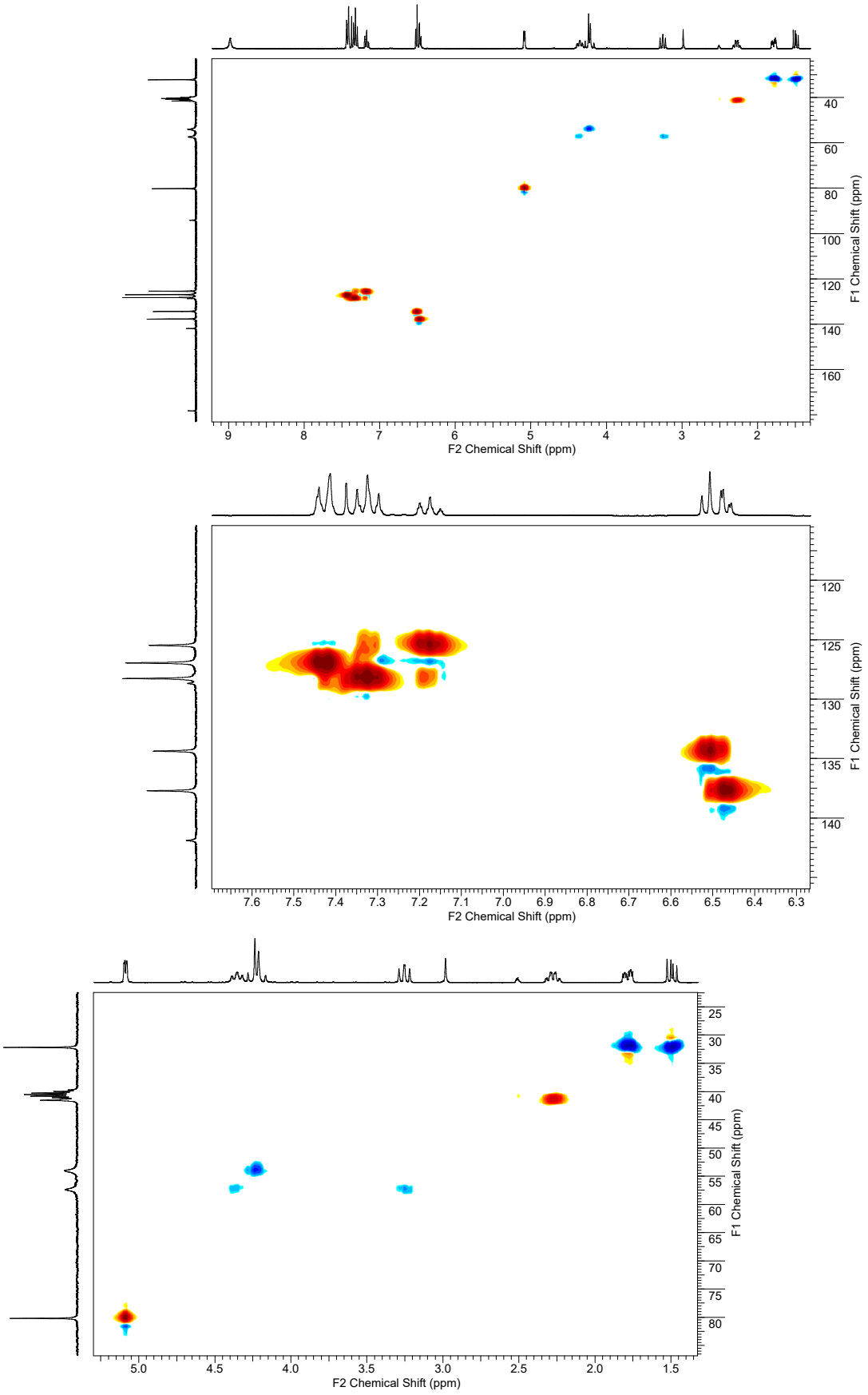
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

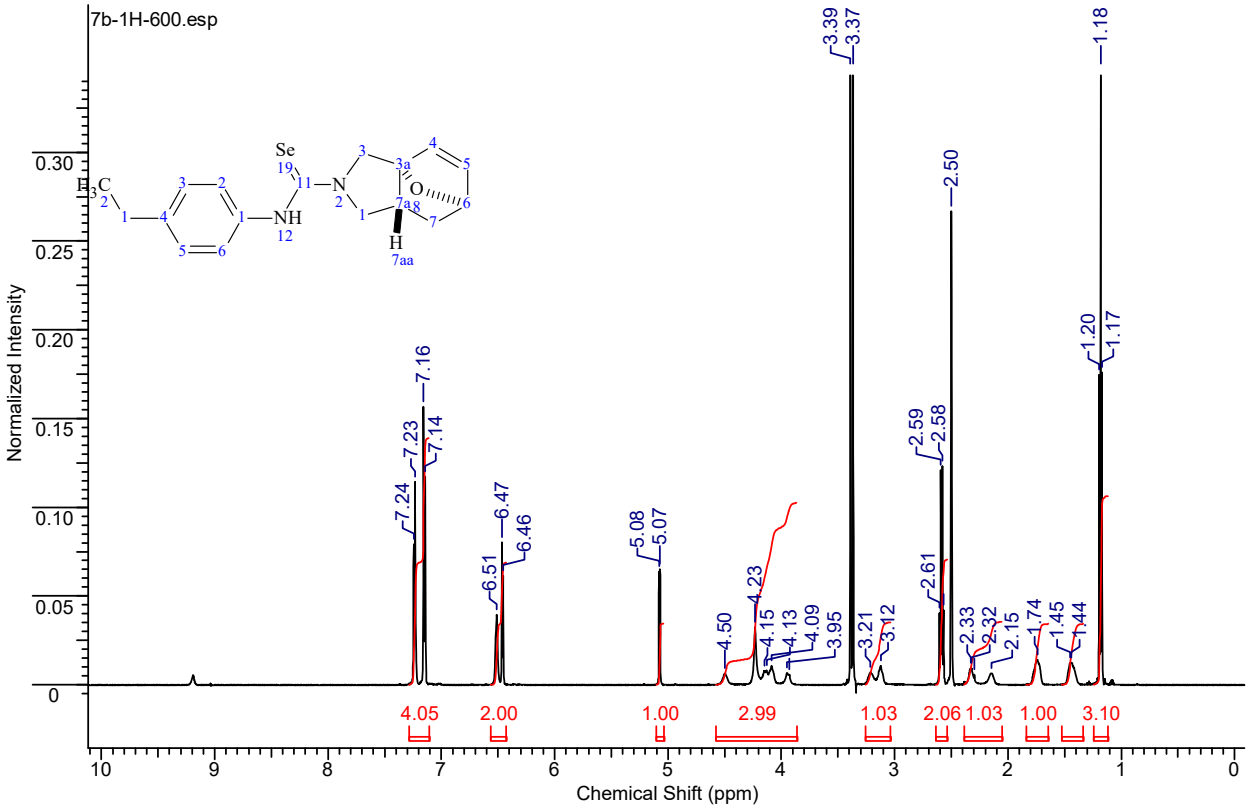


HSQC of **7a** (100 °C)

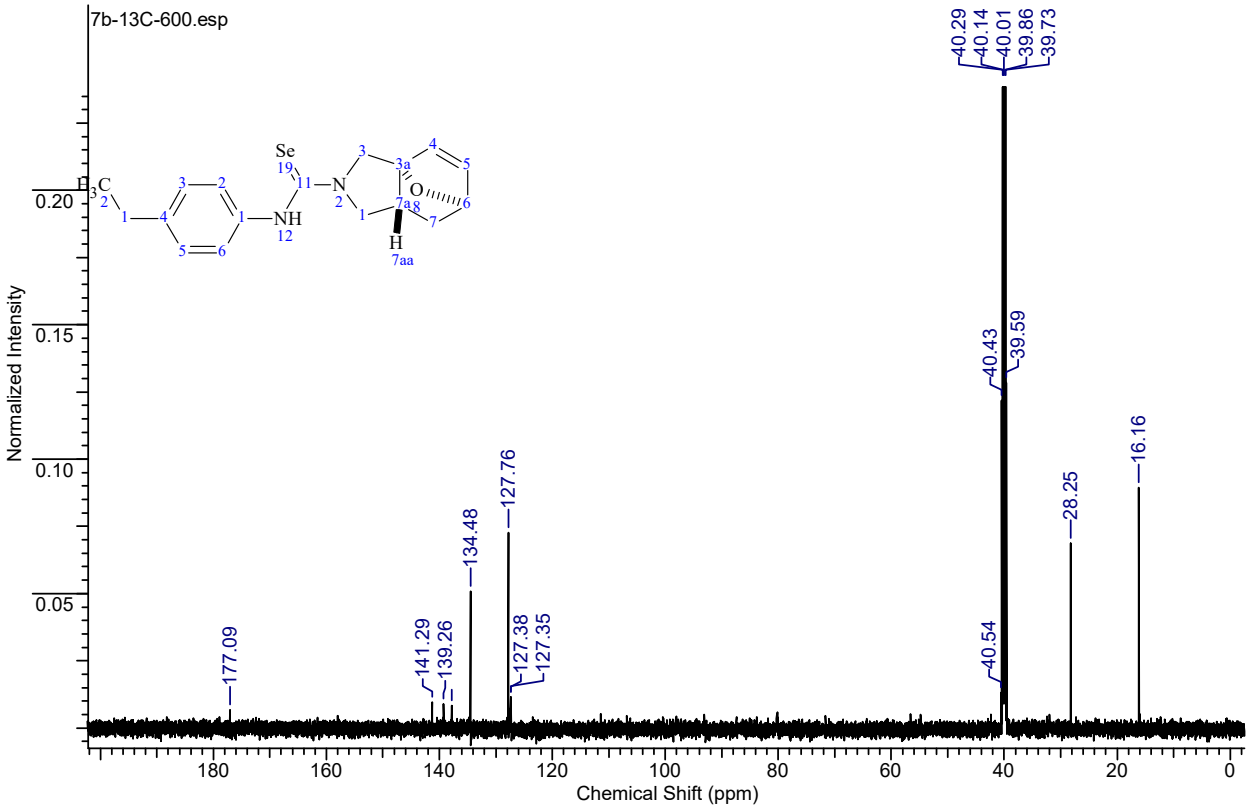


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Ethylphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7b).

^{1}H NMR (600.2 MHz, DMSO-d_6)

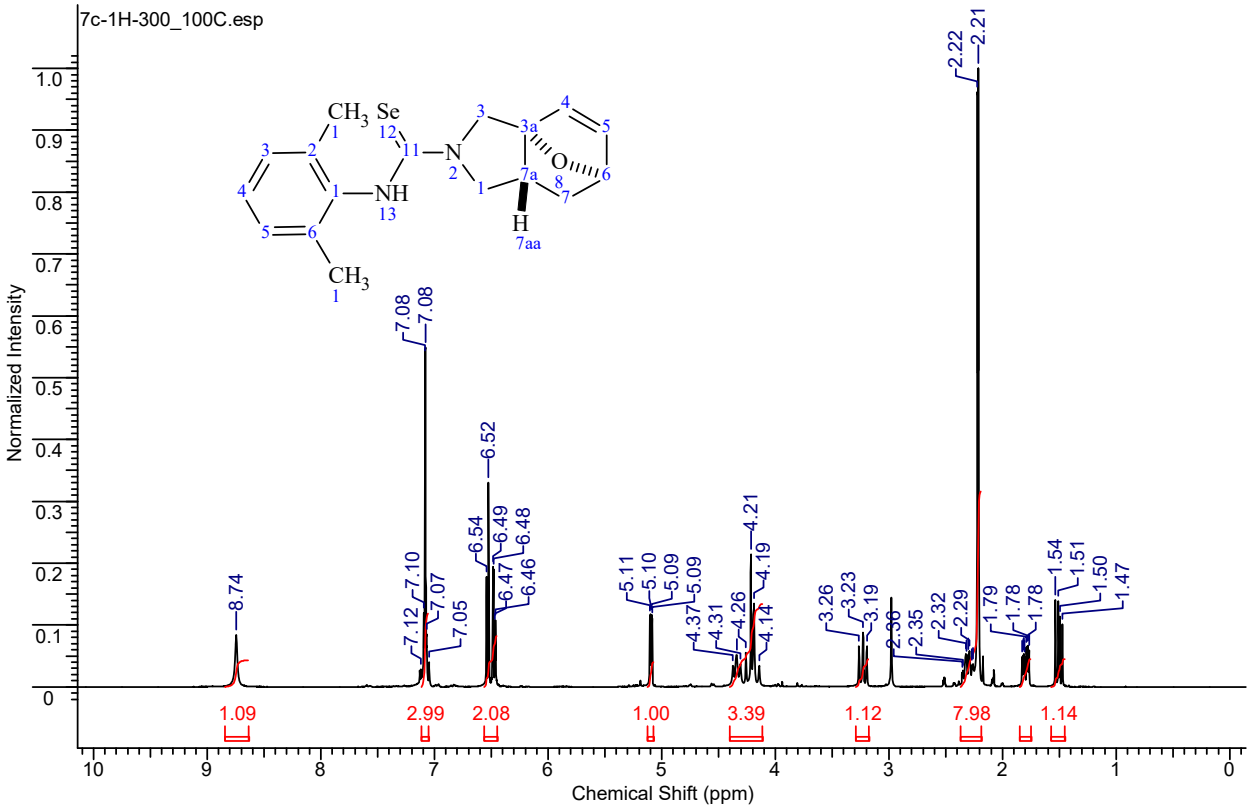


^{13}C NMR (150.9 MHz, DMSO-d_6)

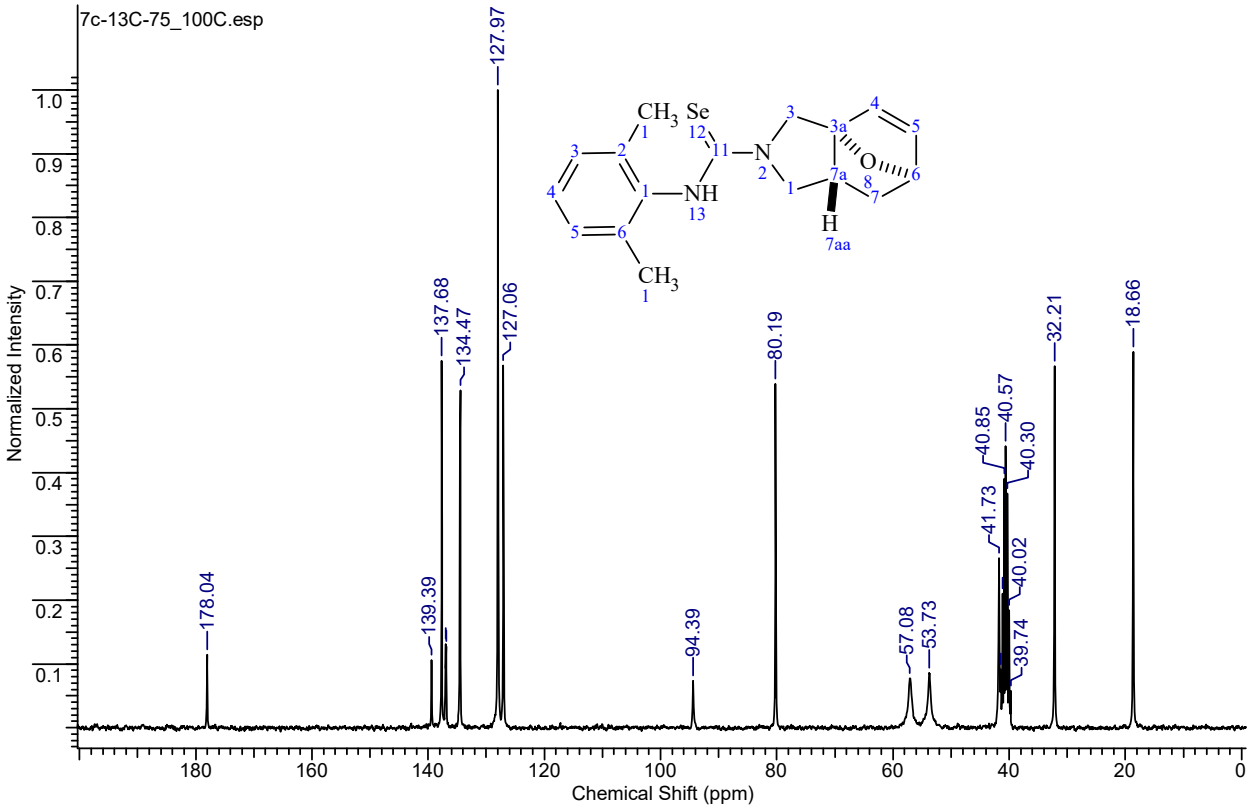


(3a*RS*,6*RS*,7a*RS*)-*N*-(2,6-Dimethylphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7c).

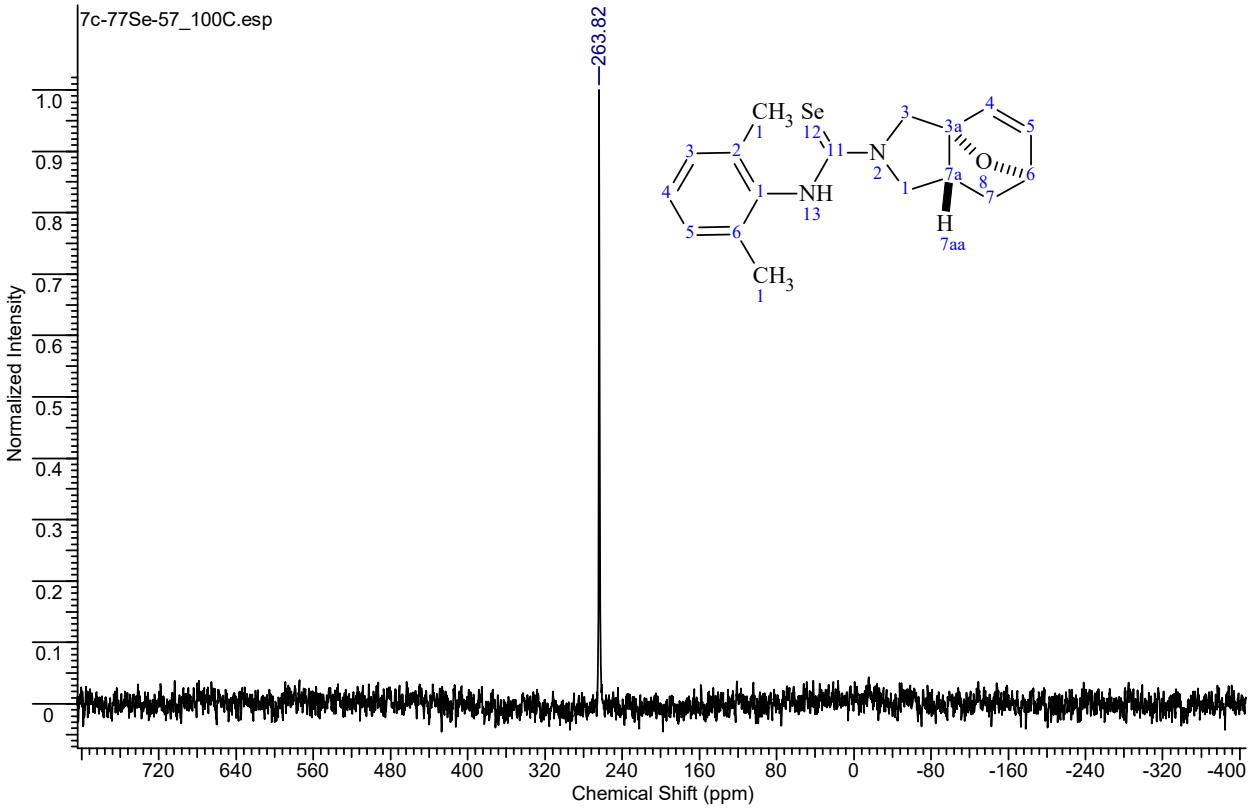
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



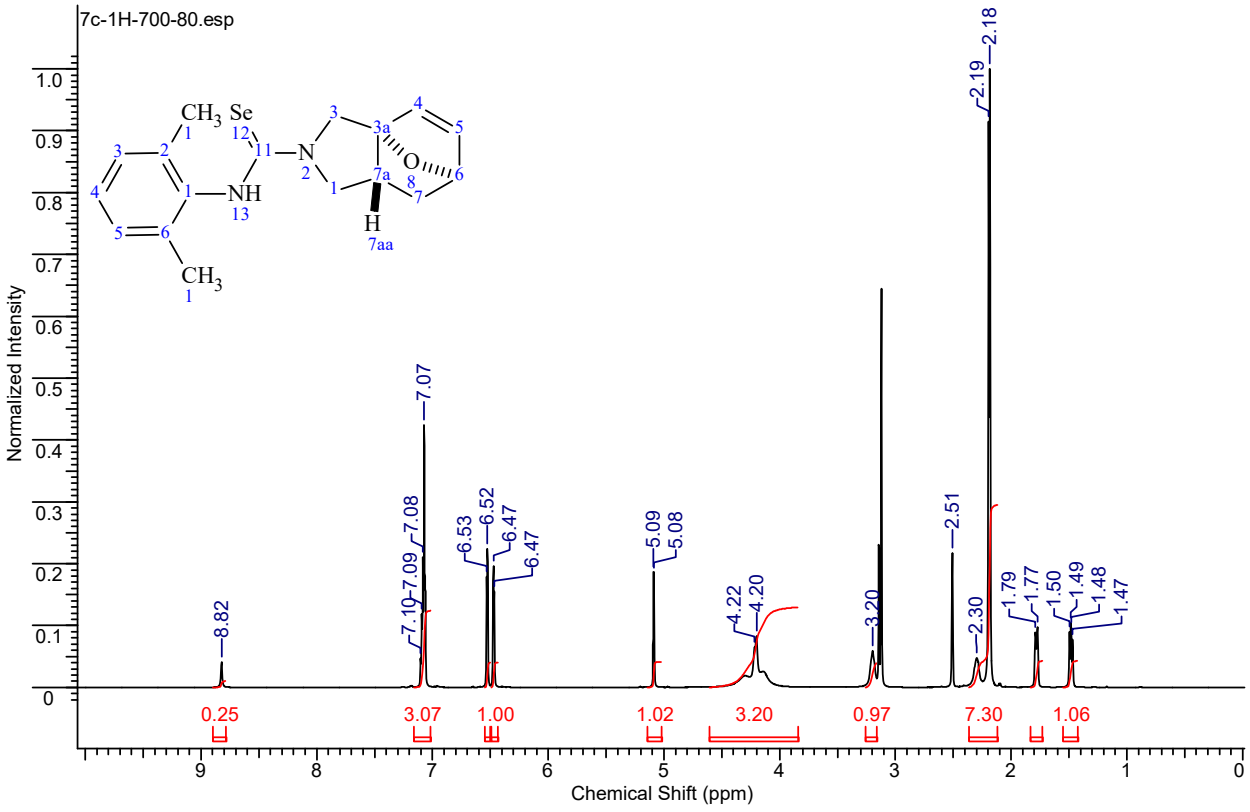
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



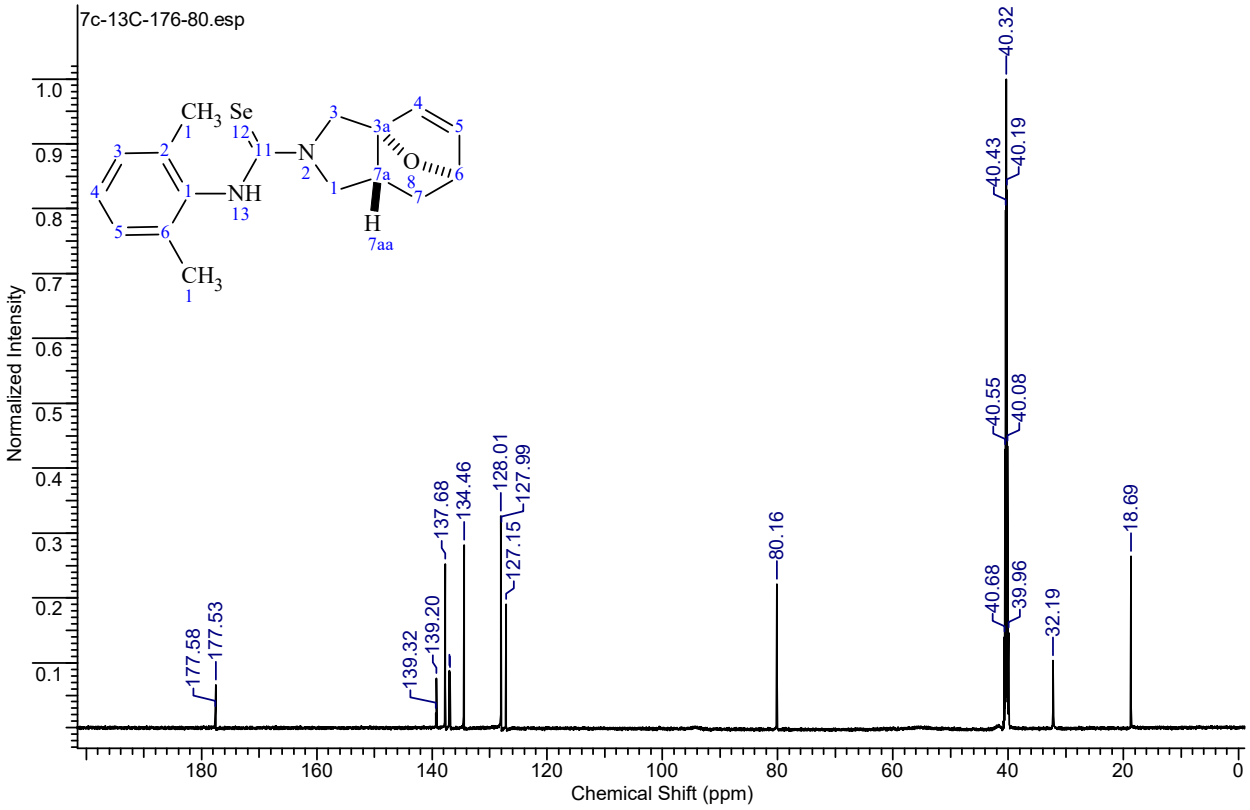
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



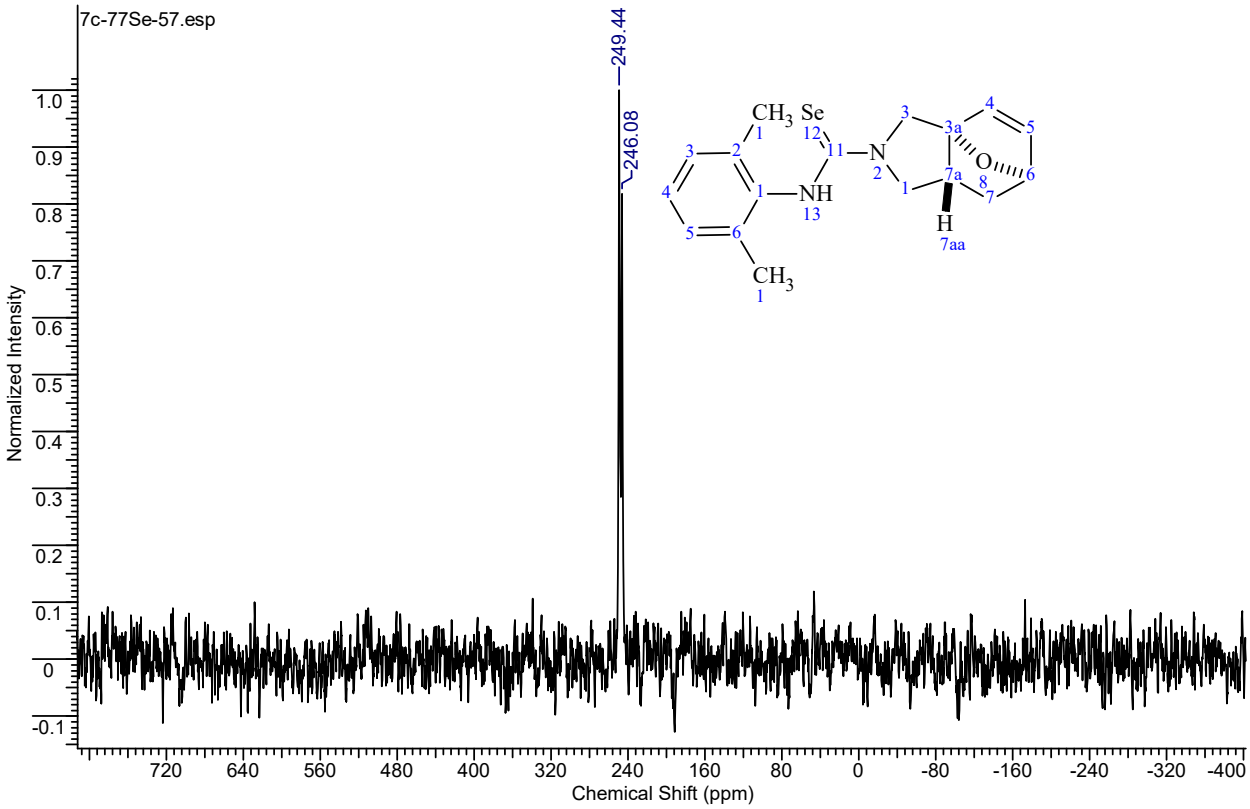
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



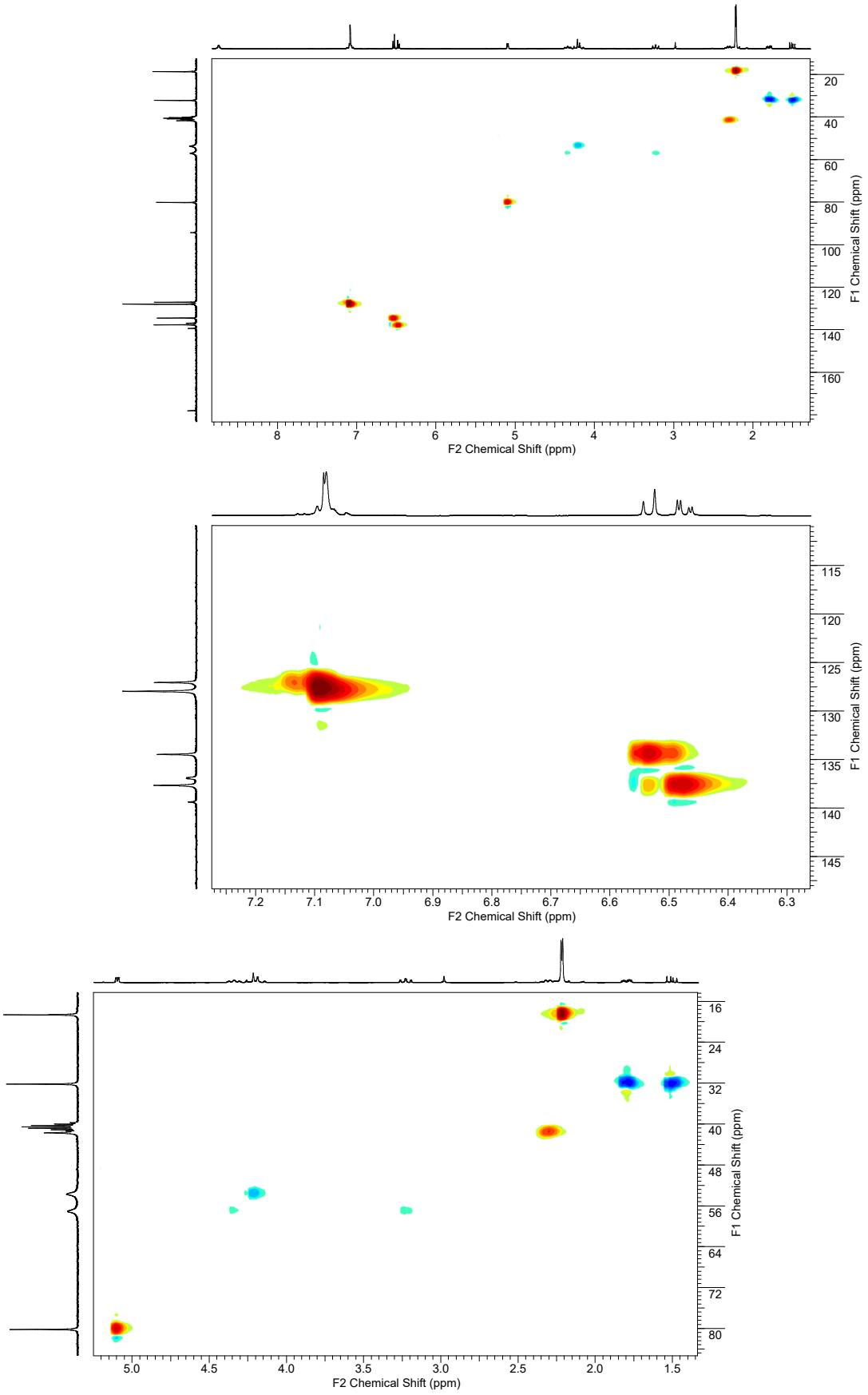
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

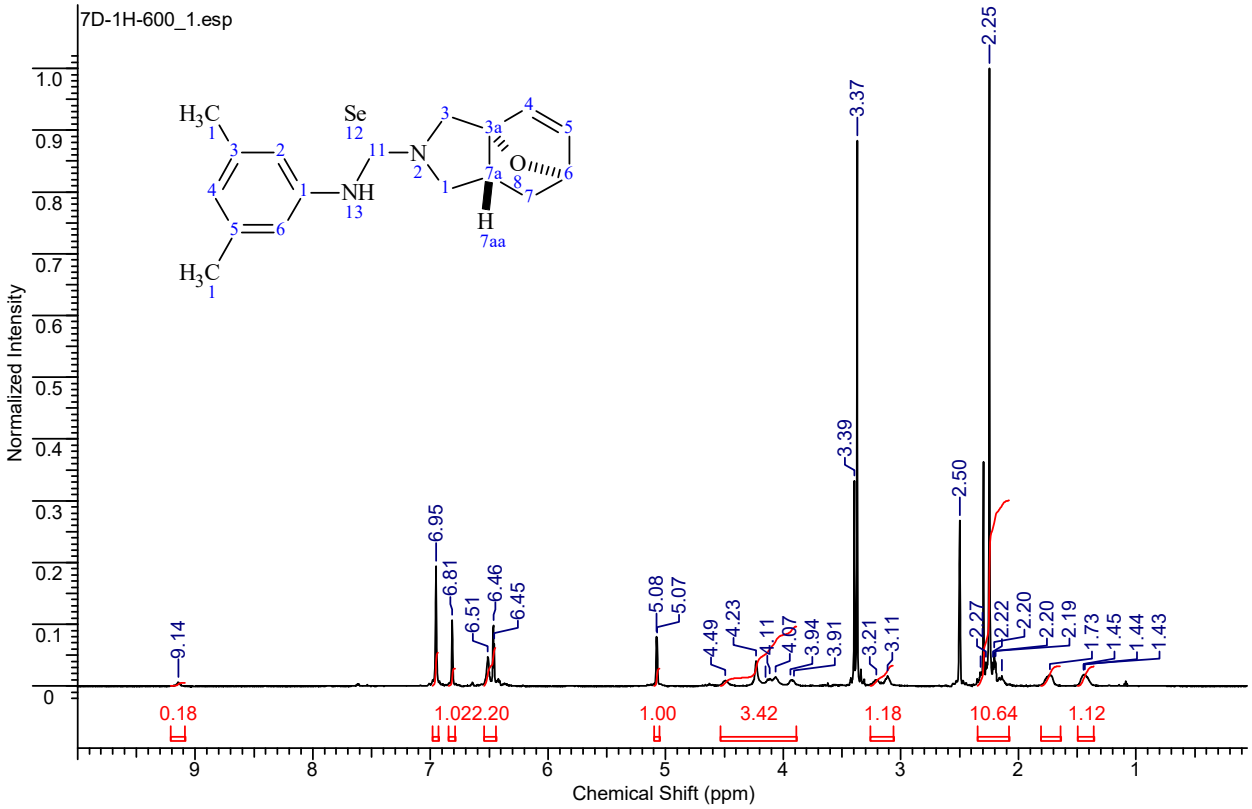


HSQC of **7c** (100 °C)

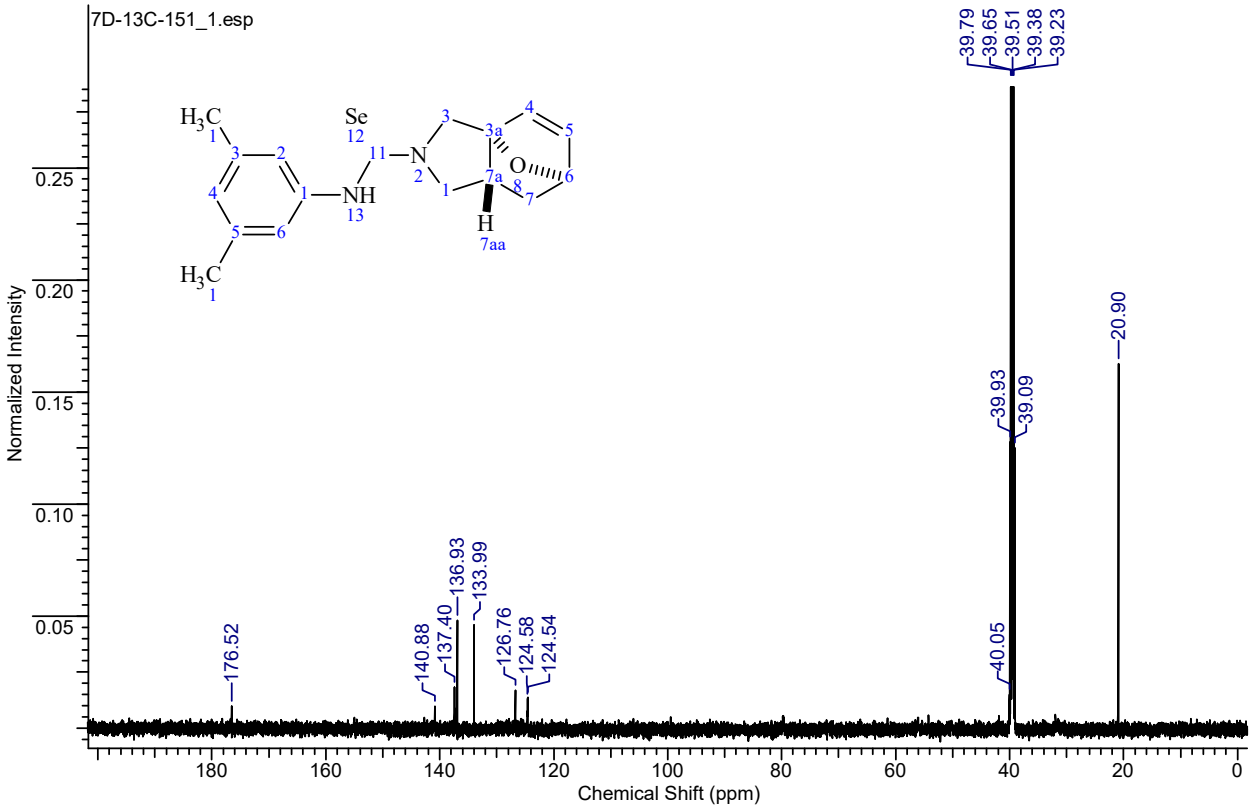


(3a*RS*,6*RS*,7a*RS*)-*N*-(3,5-Dimethylphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7d).

^{1}H NMR (600.2 MHz, DMSO-d_6)

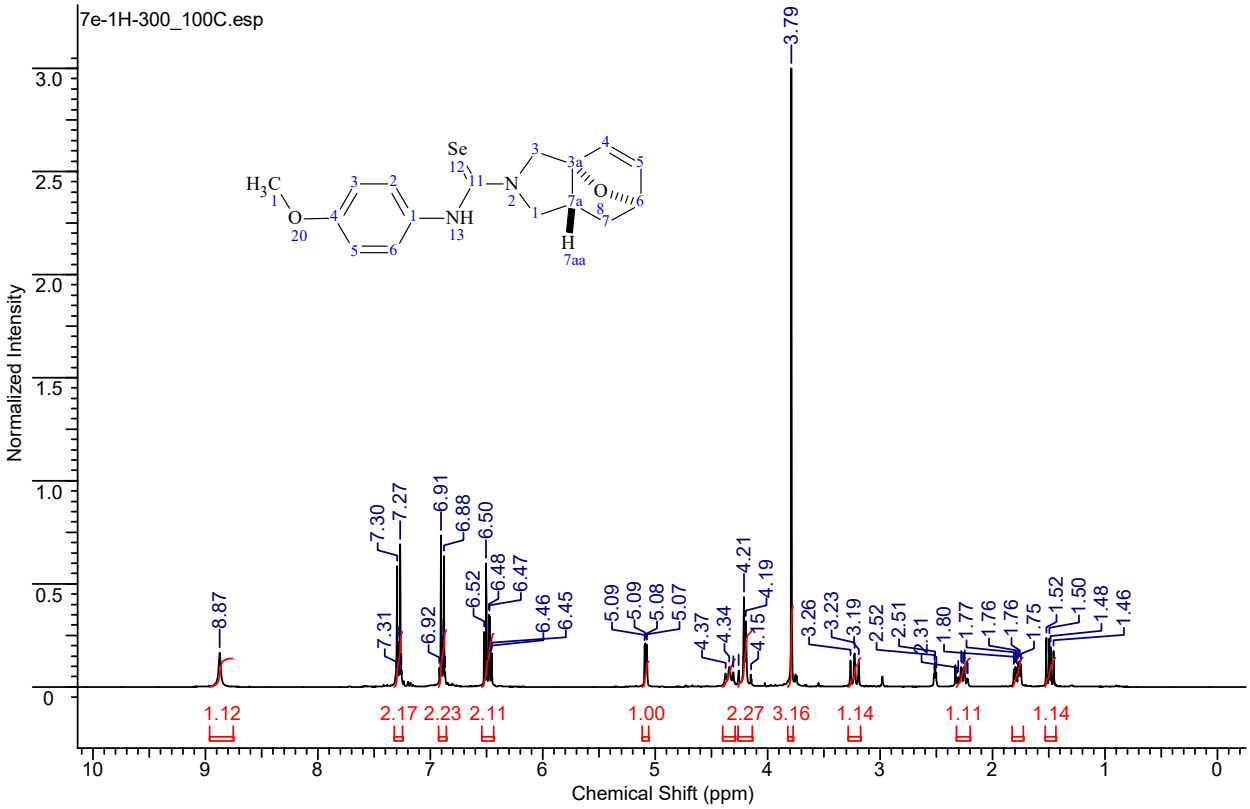


^{13}C NMR (150.9 MHz, DMSO-d_6)

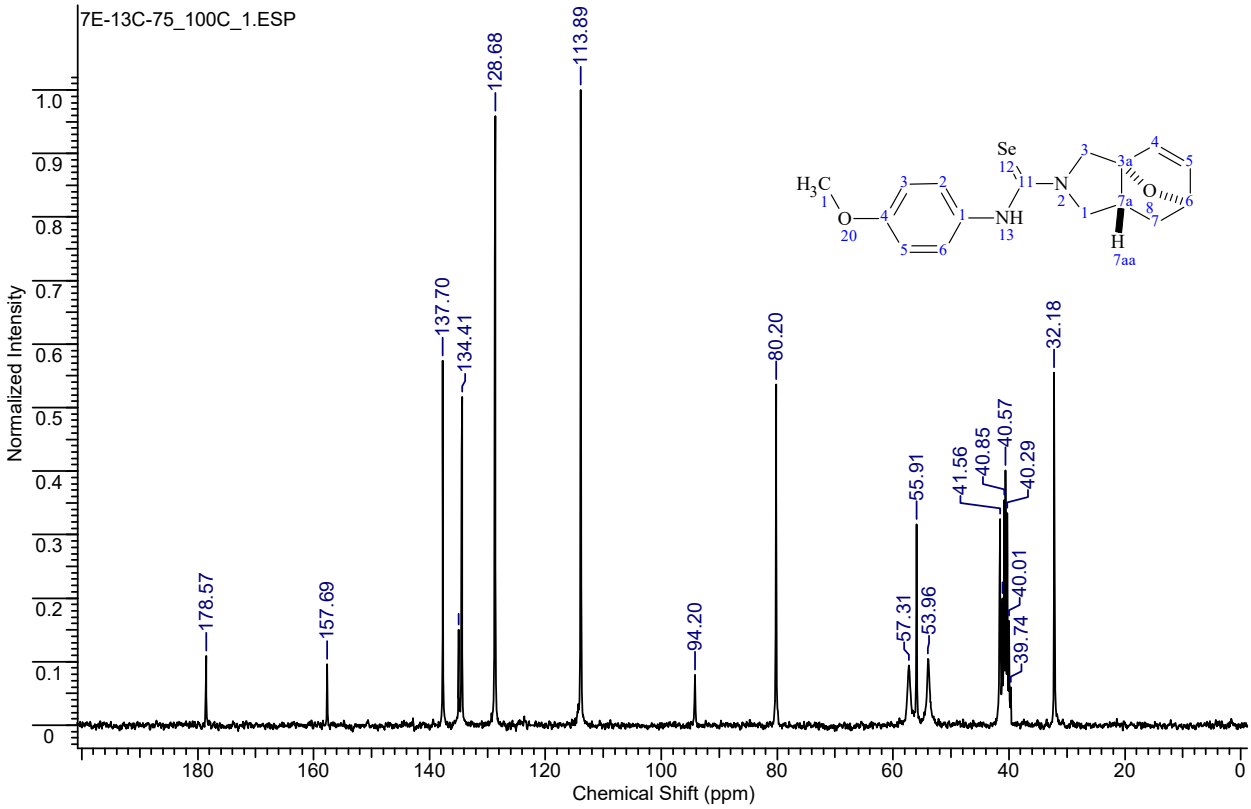


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7e).

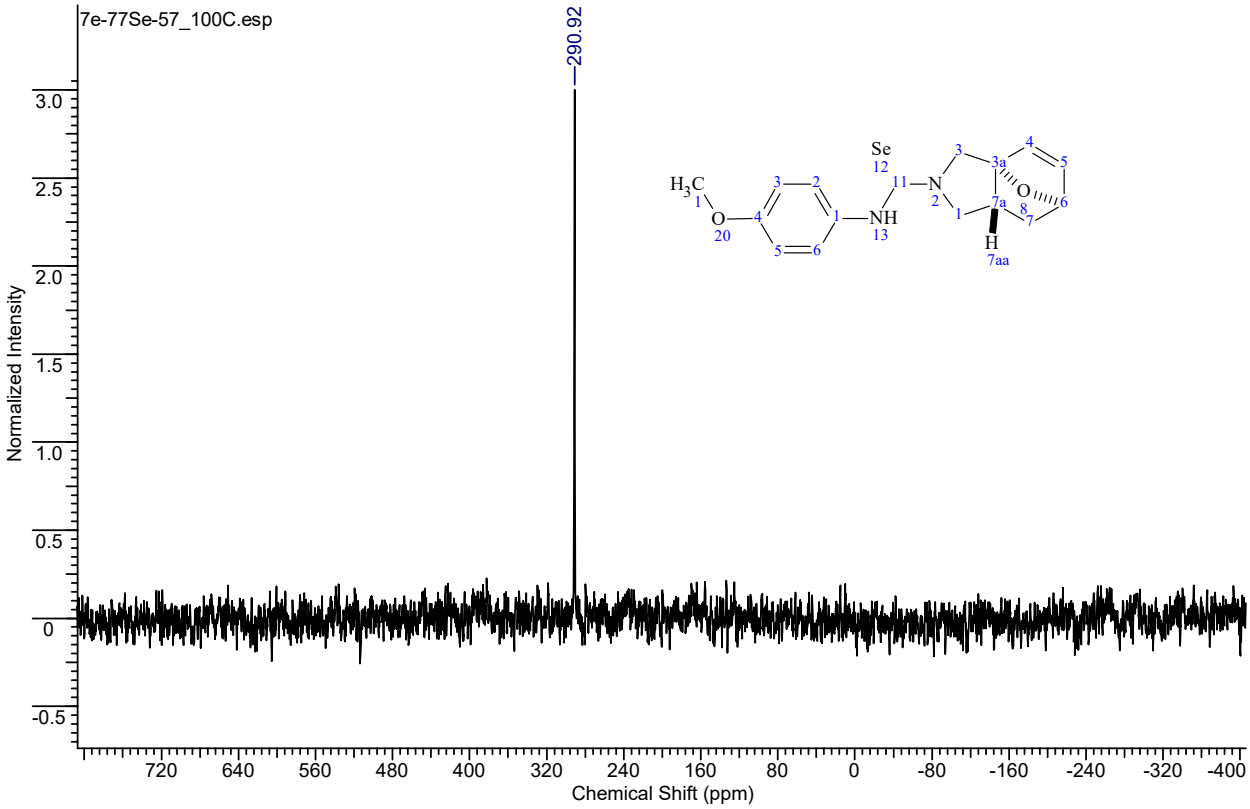
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



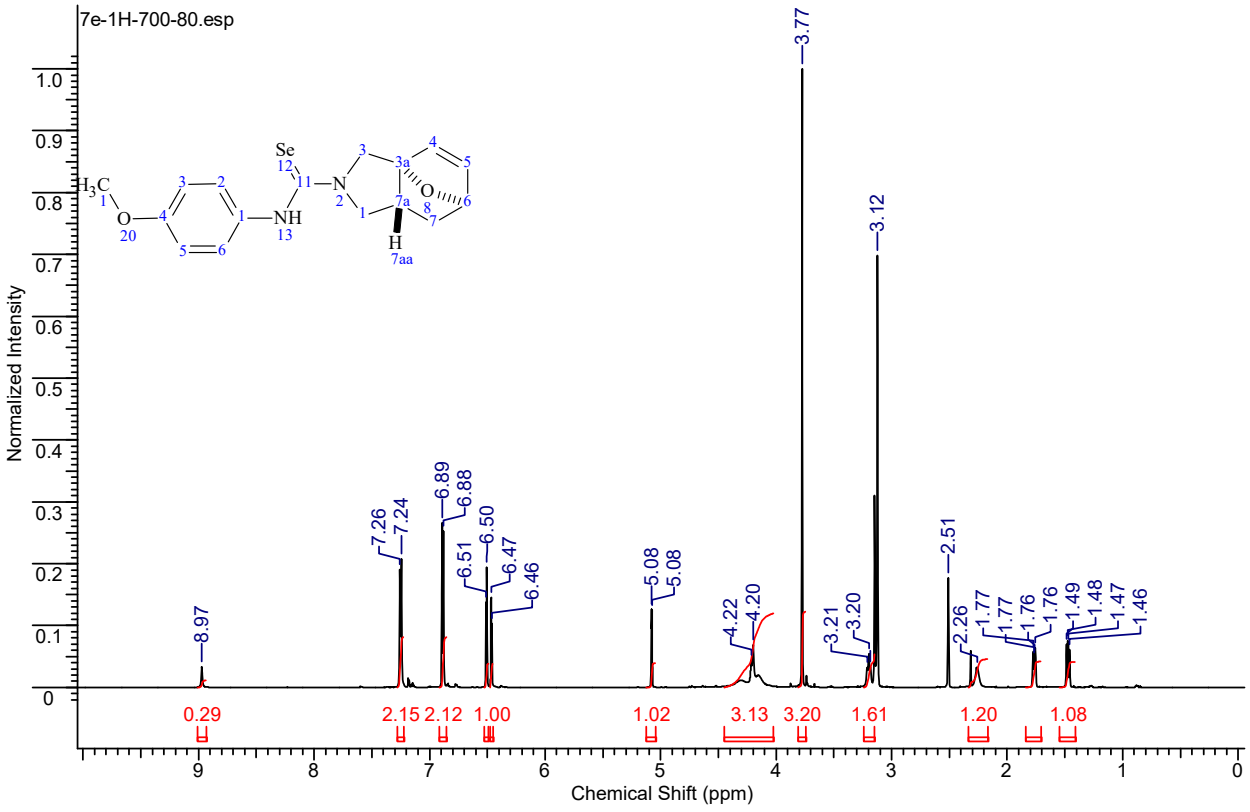
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



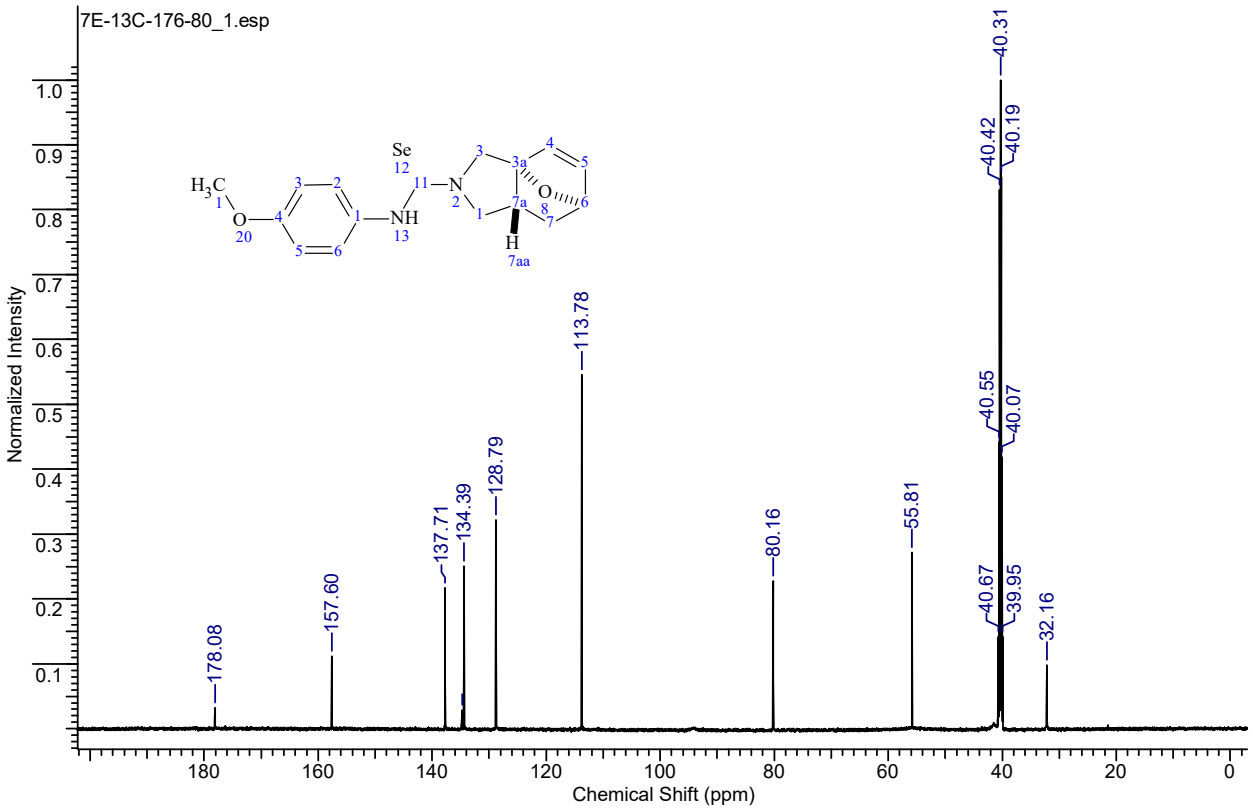
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



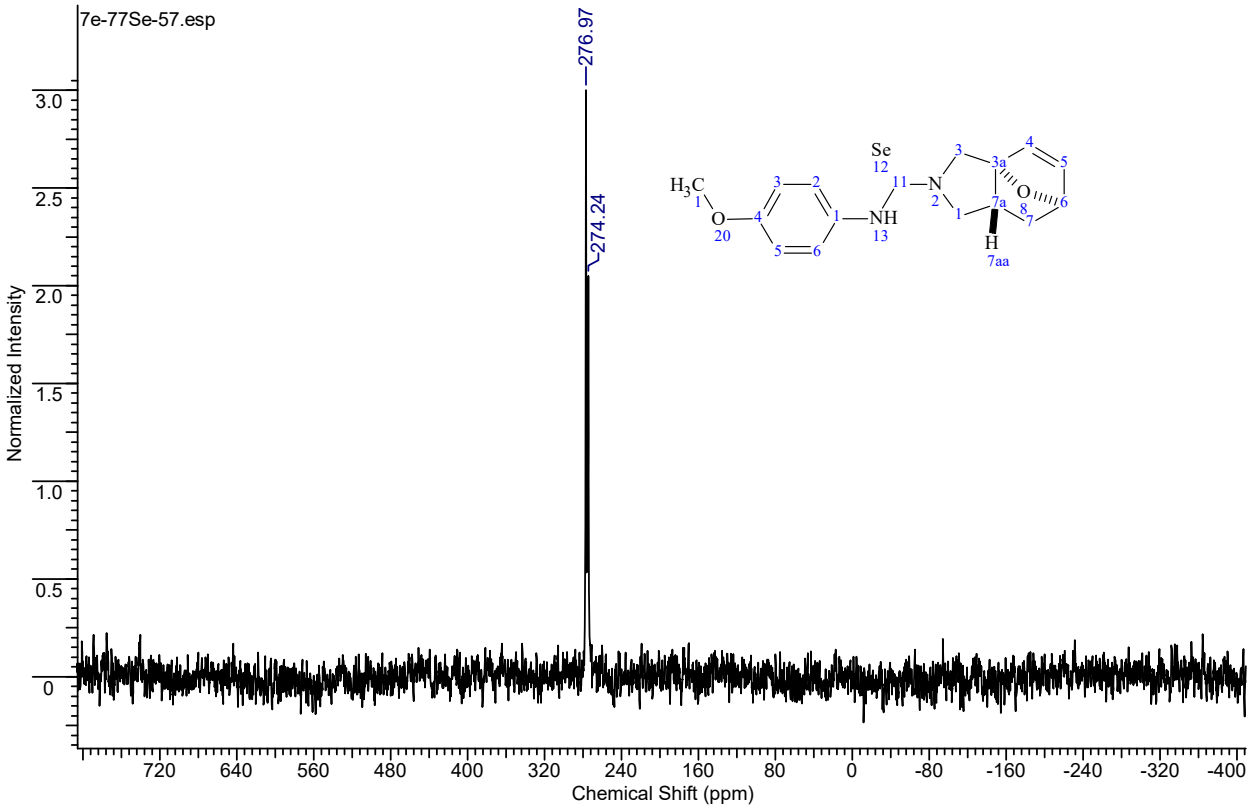
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



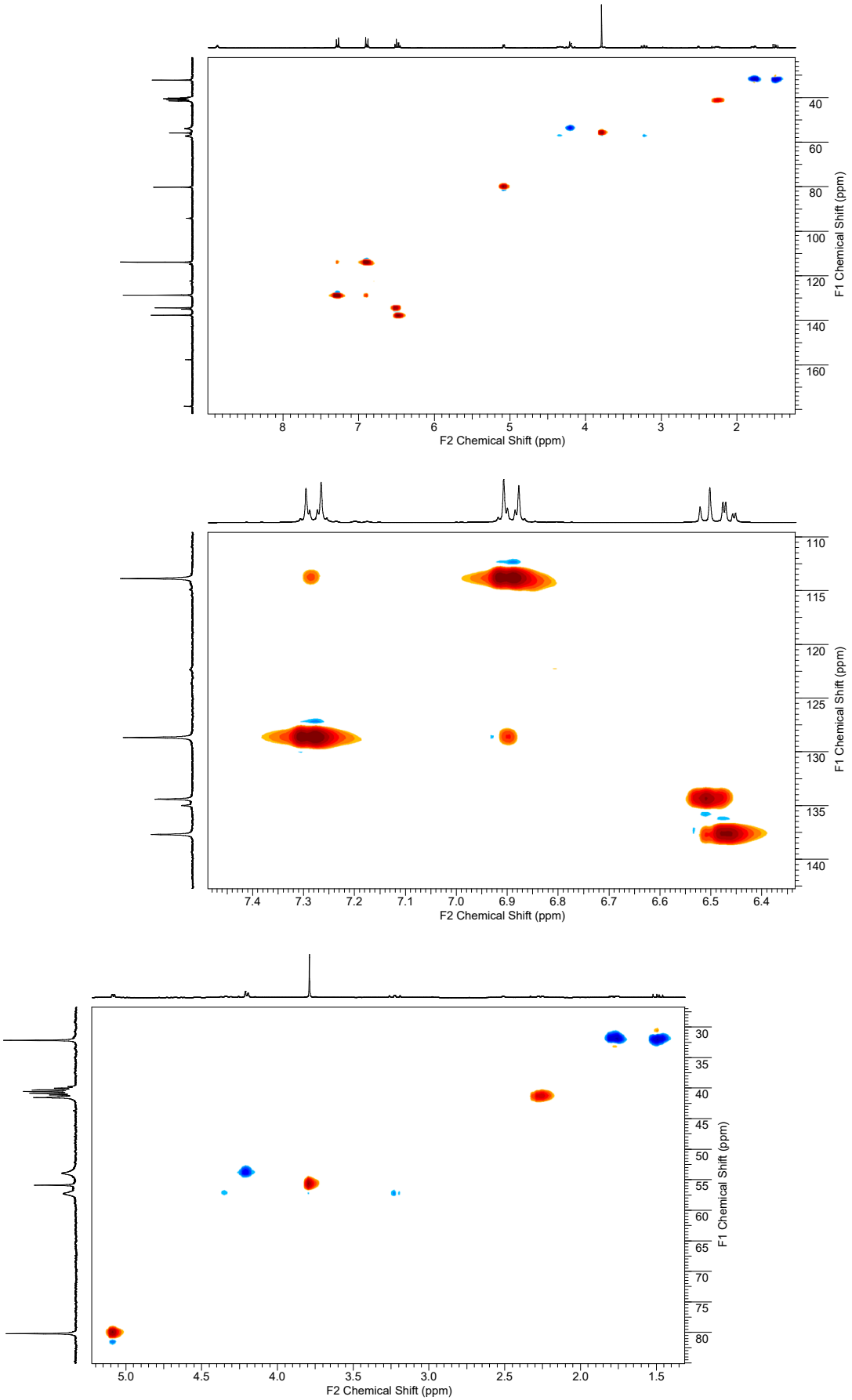
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

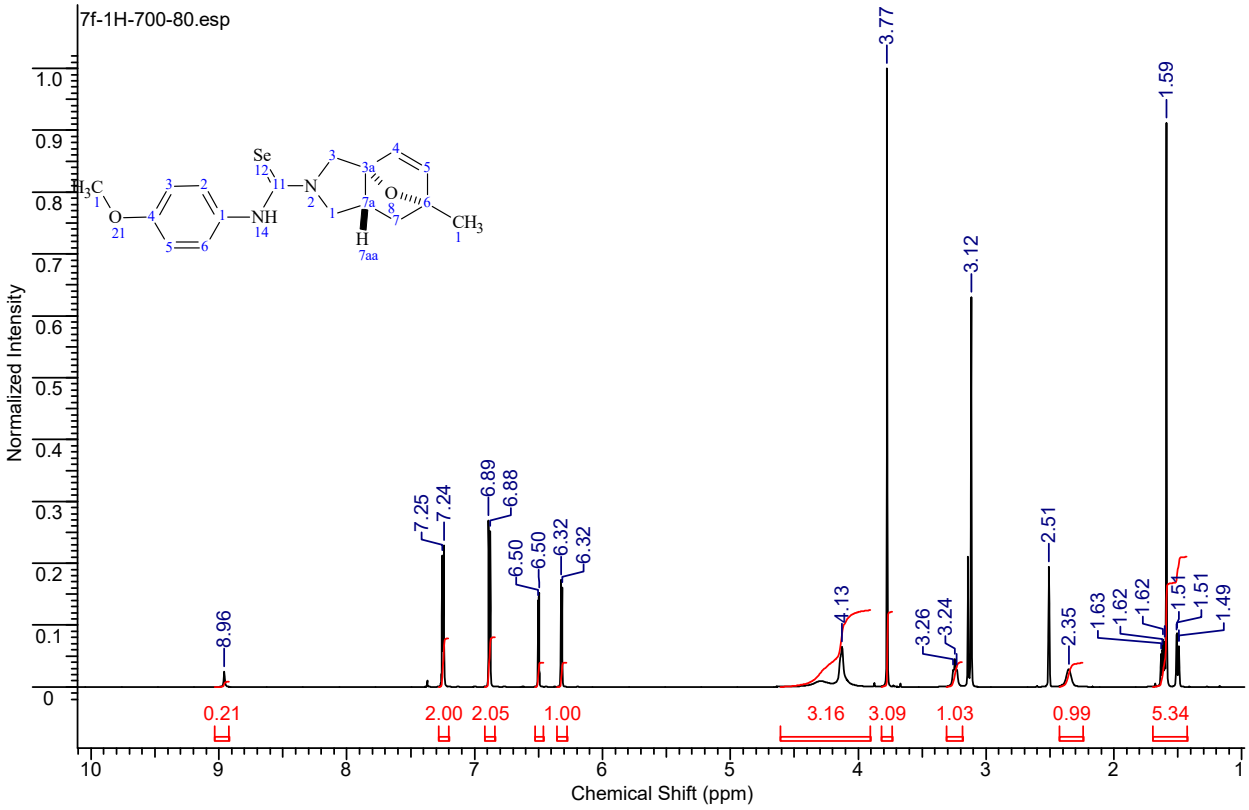


HSQC of **7e** (100 °C)

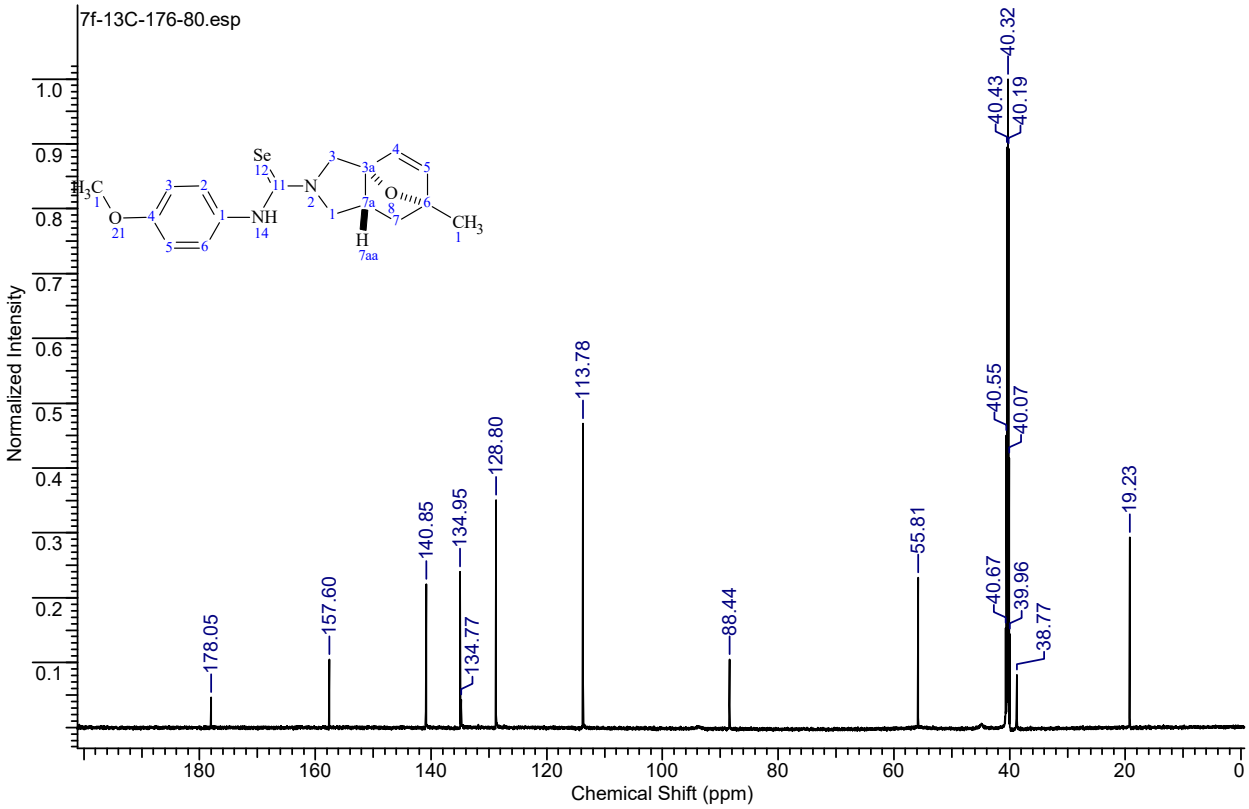


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Methoxyphenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7f).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

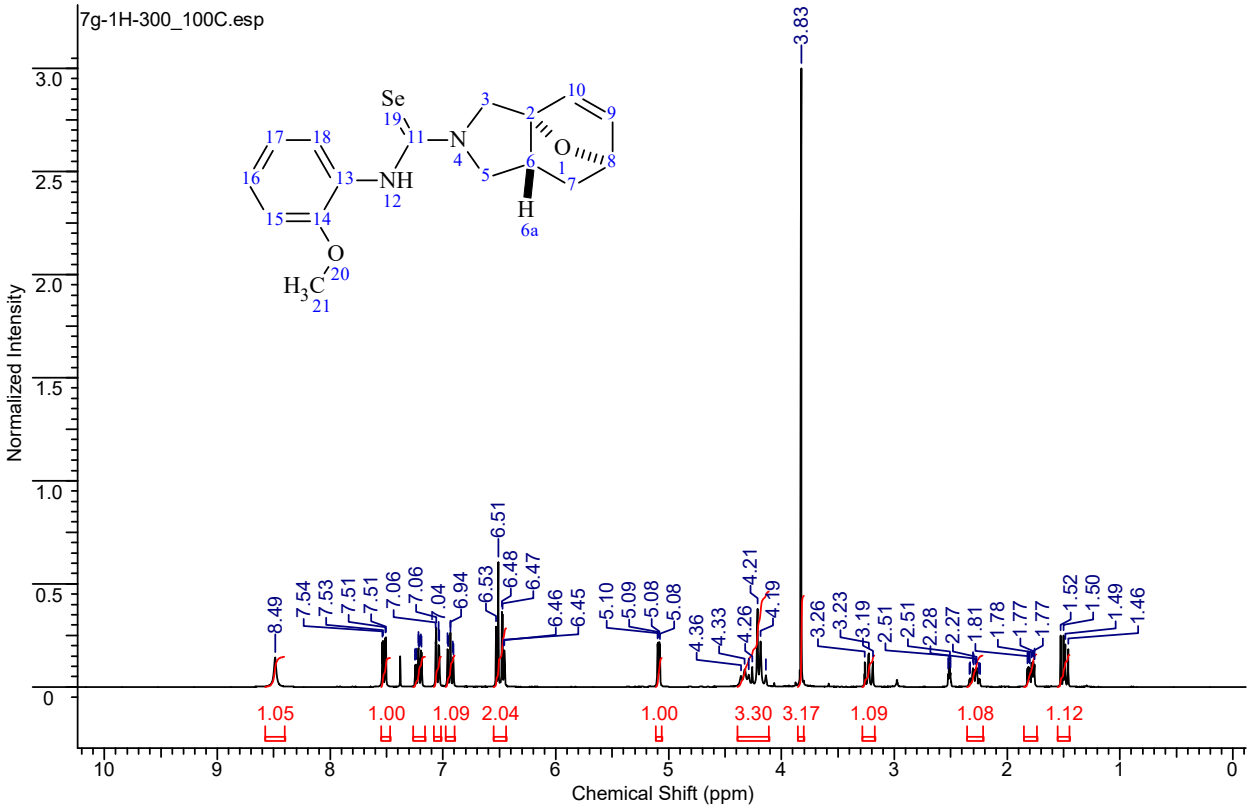


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

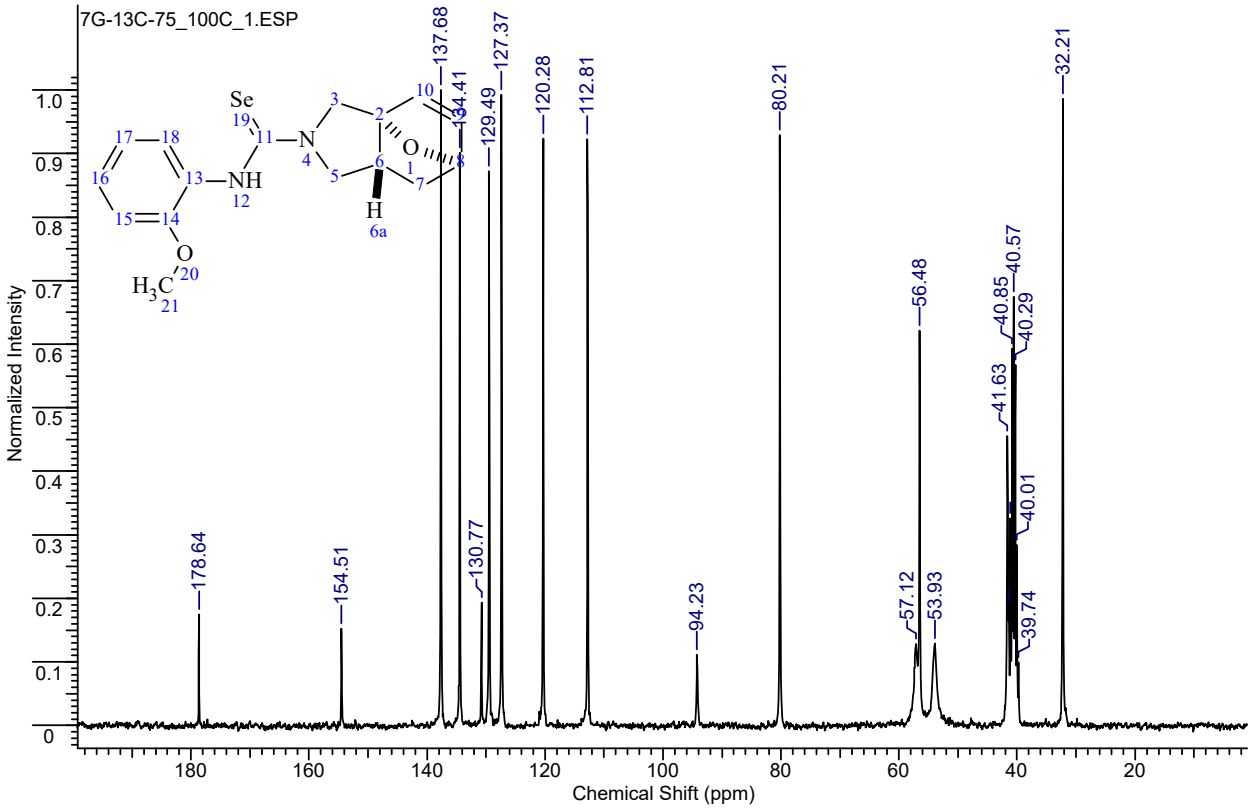


(3a*RS*,6*RS*,7a*RS*)-*N*-(2-Methoxyphenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7g).

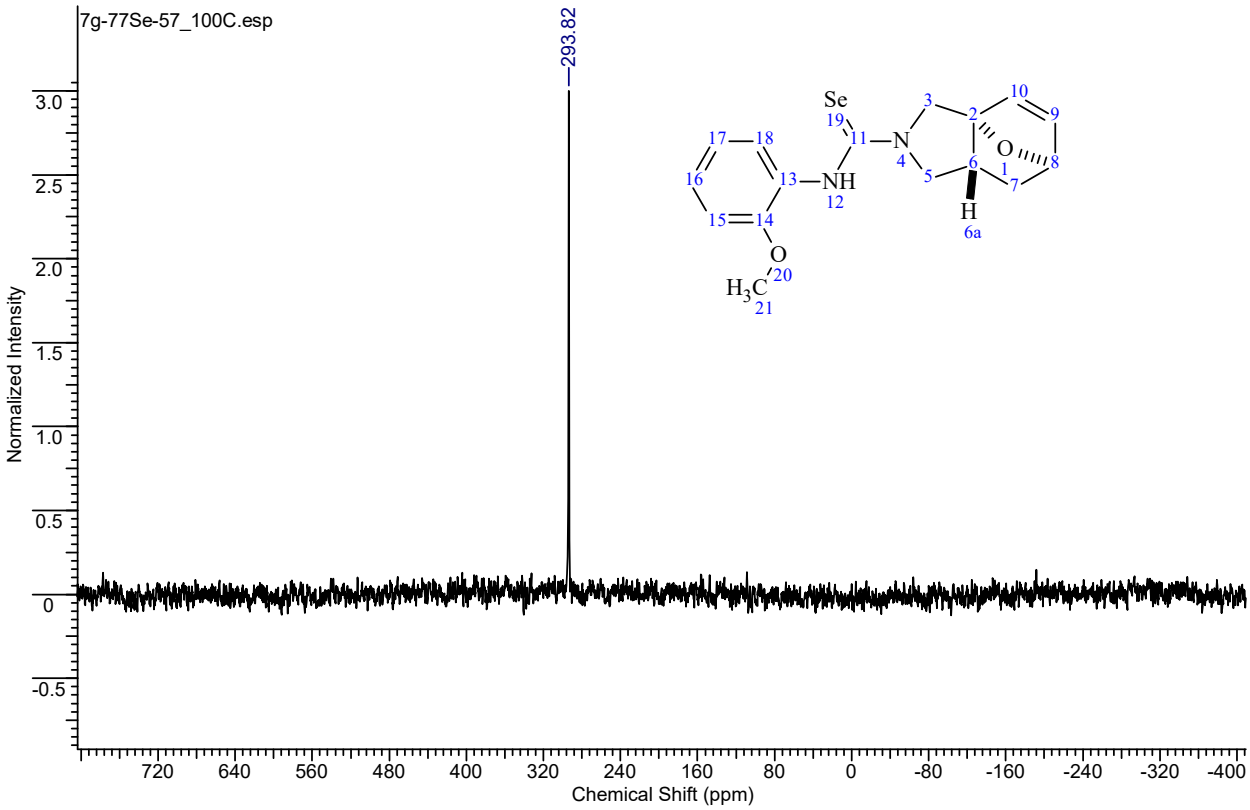
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C) *the compd.* **7g** *decomposes at 100 °C*



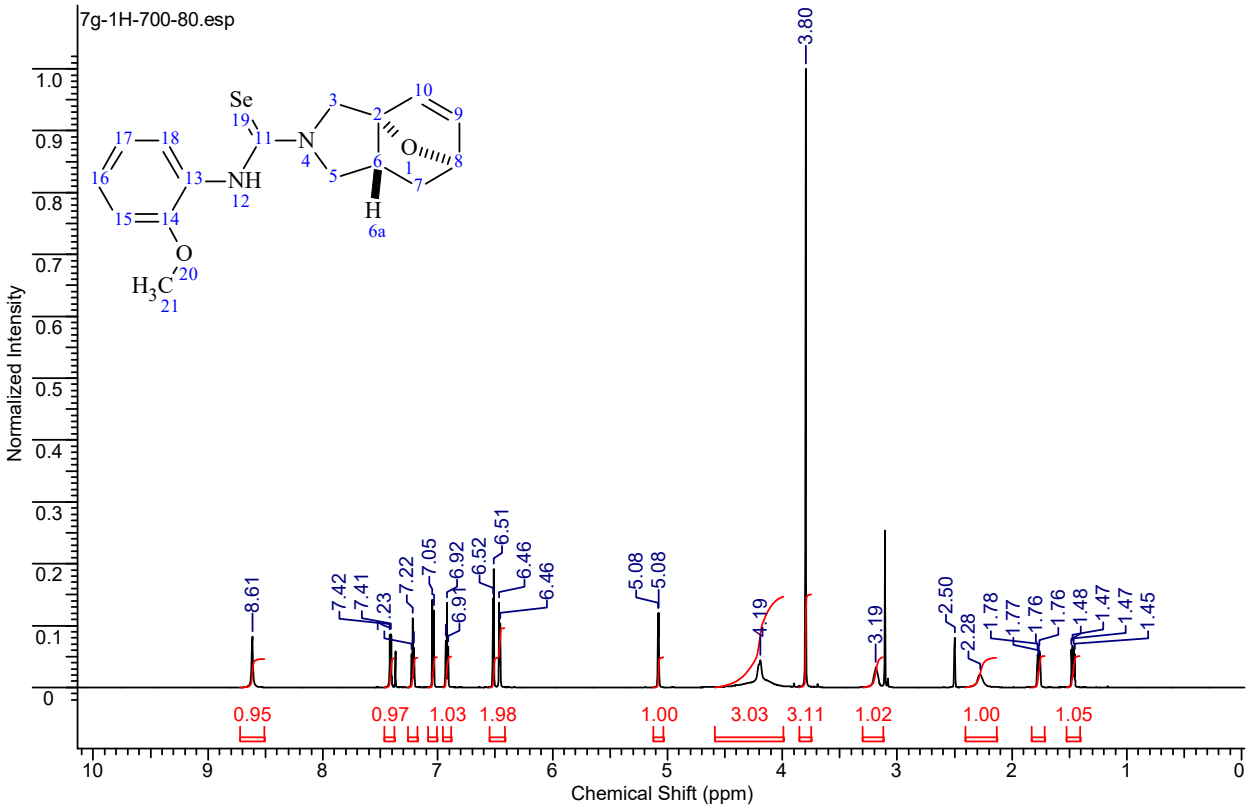
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



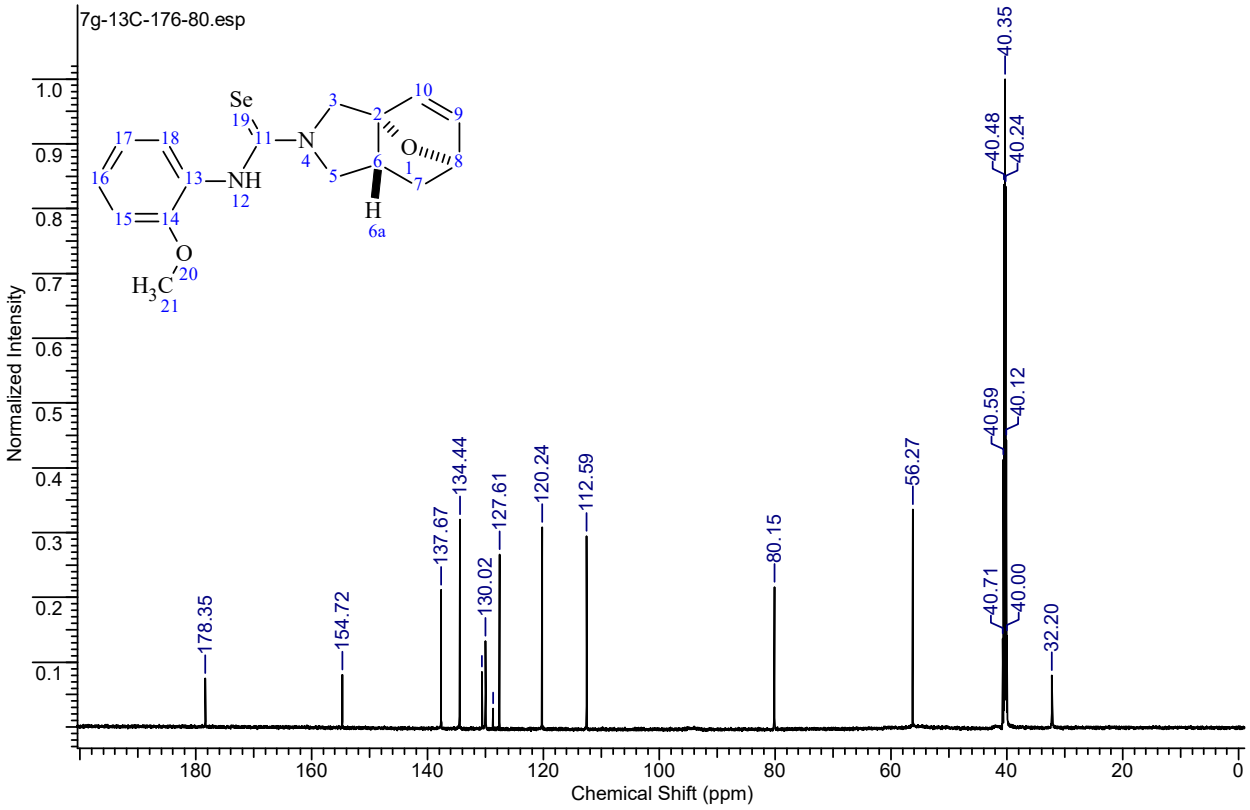
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



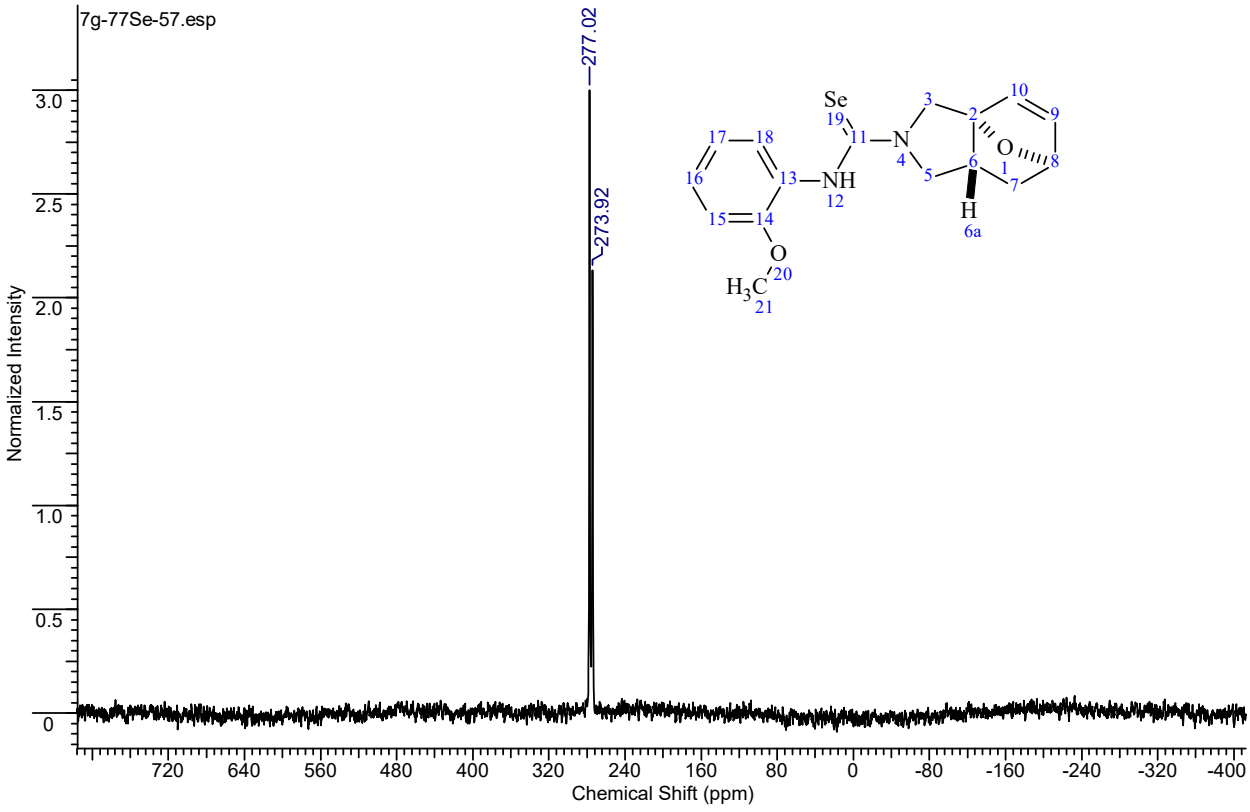
^{1}H NMR (700.2 MHz, DMSO-d_6, 77 °C)



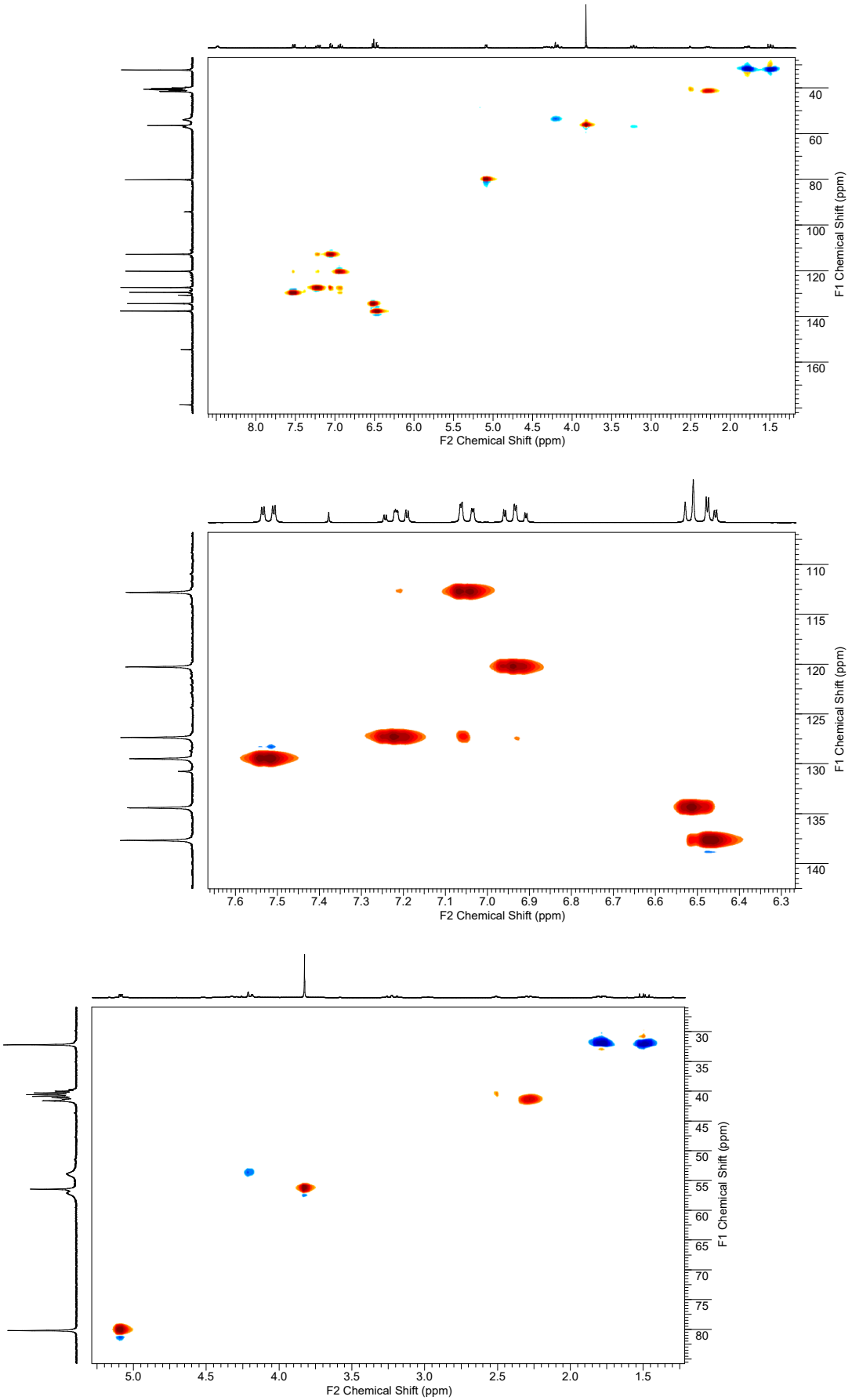
^{13}C NMR (176.1 MHz, DMSO-d_6, 77 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

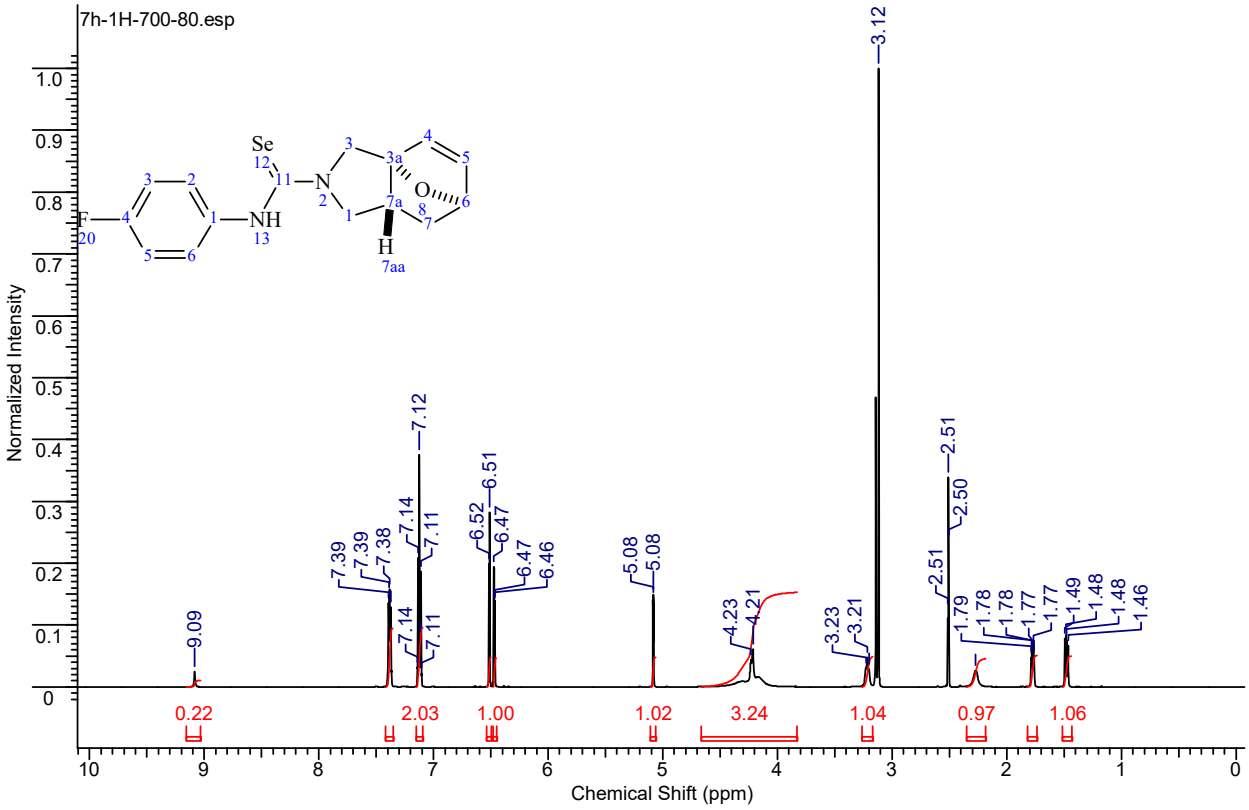


HSQC of **7g** (100 °C)

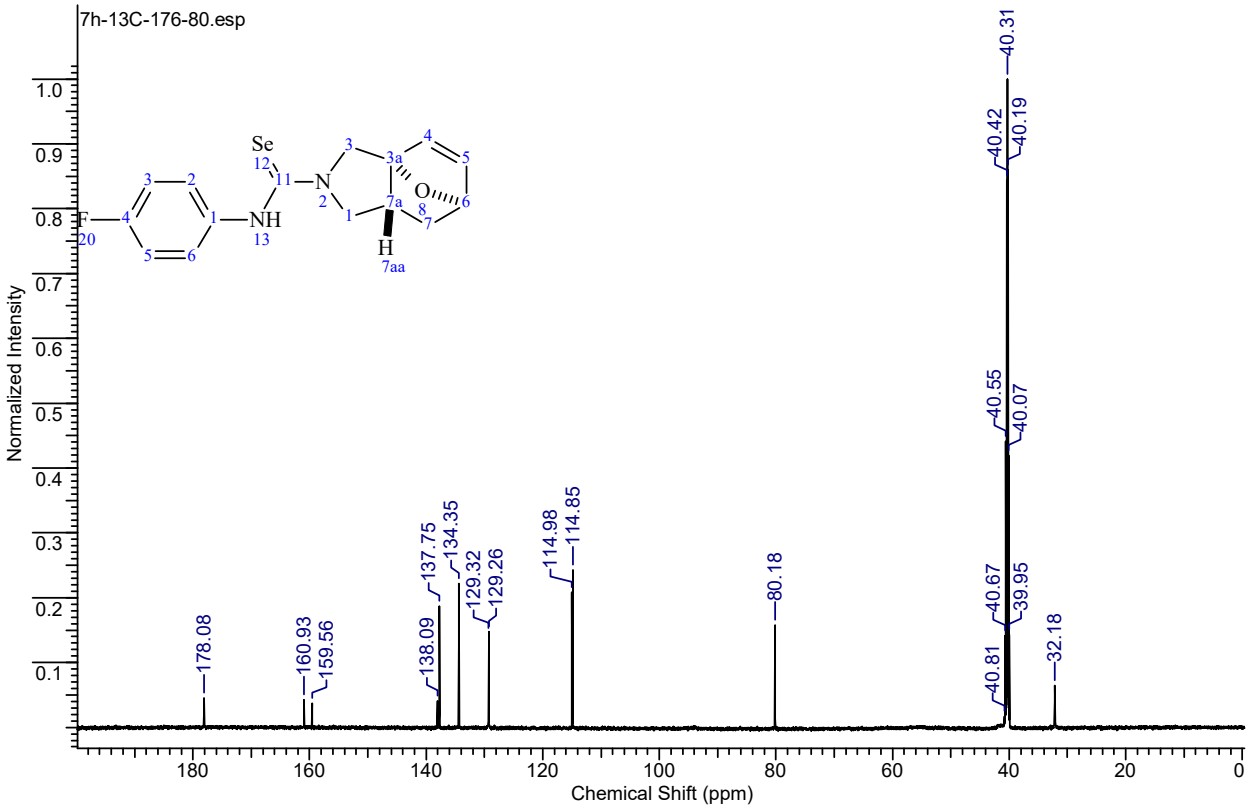


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Fluorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7h).

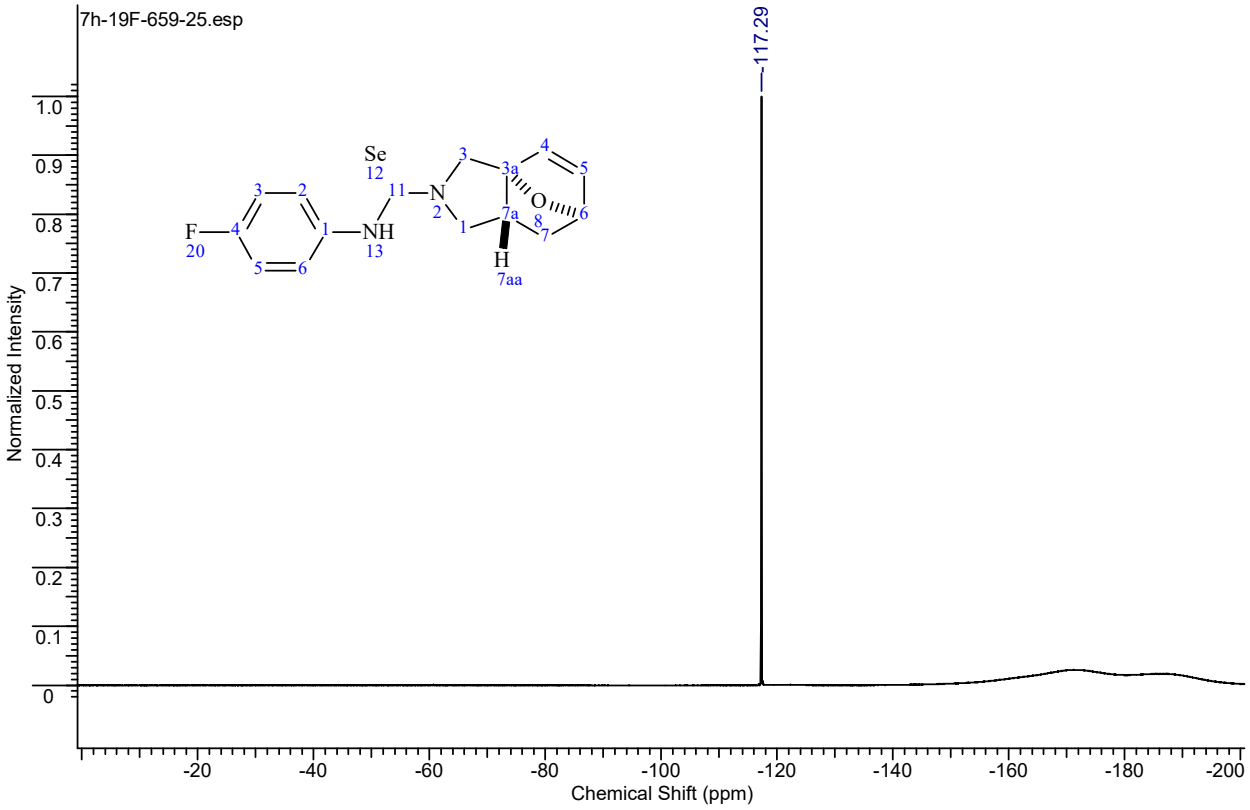
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

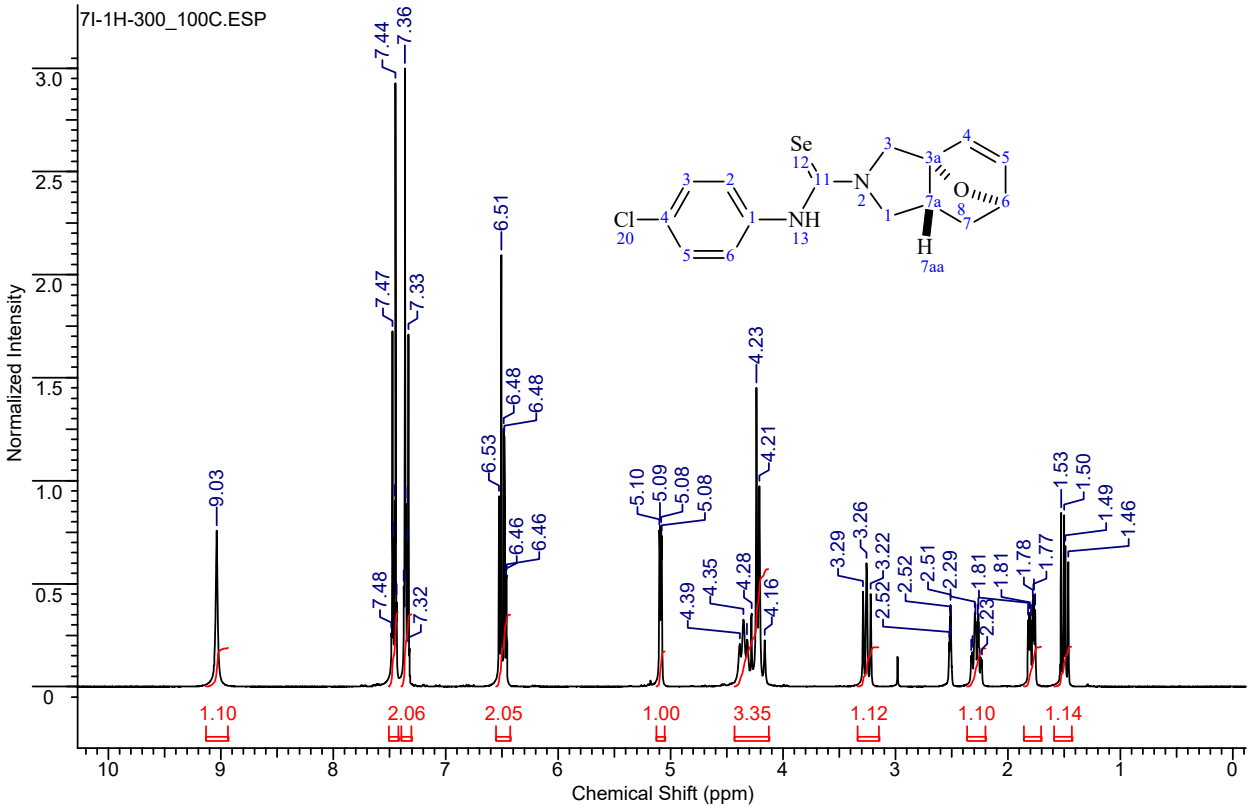


^{19}F NMR (658.8 MHz, DMSO-d_6)

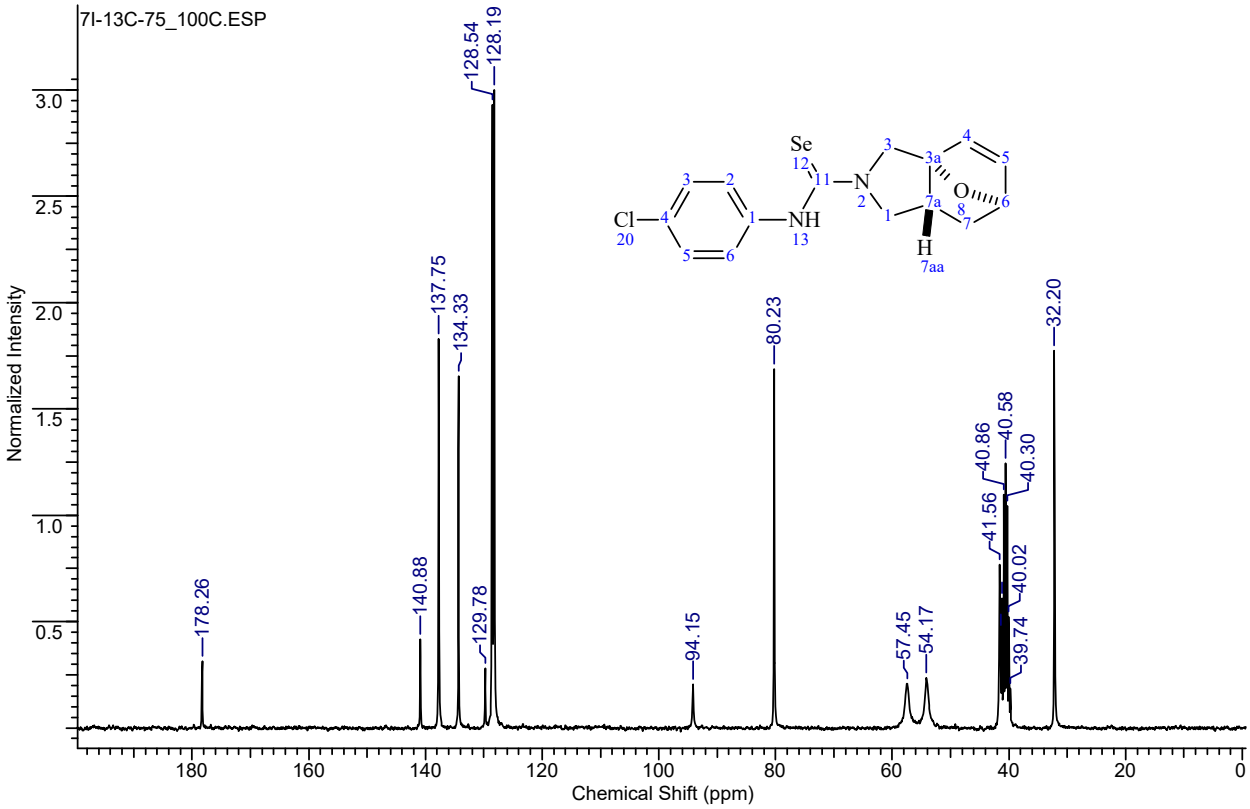


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7i).

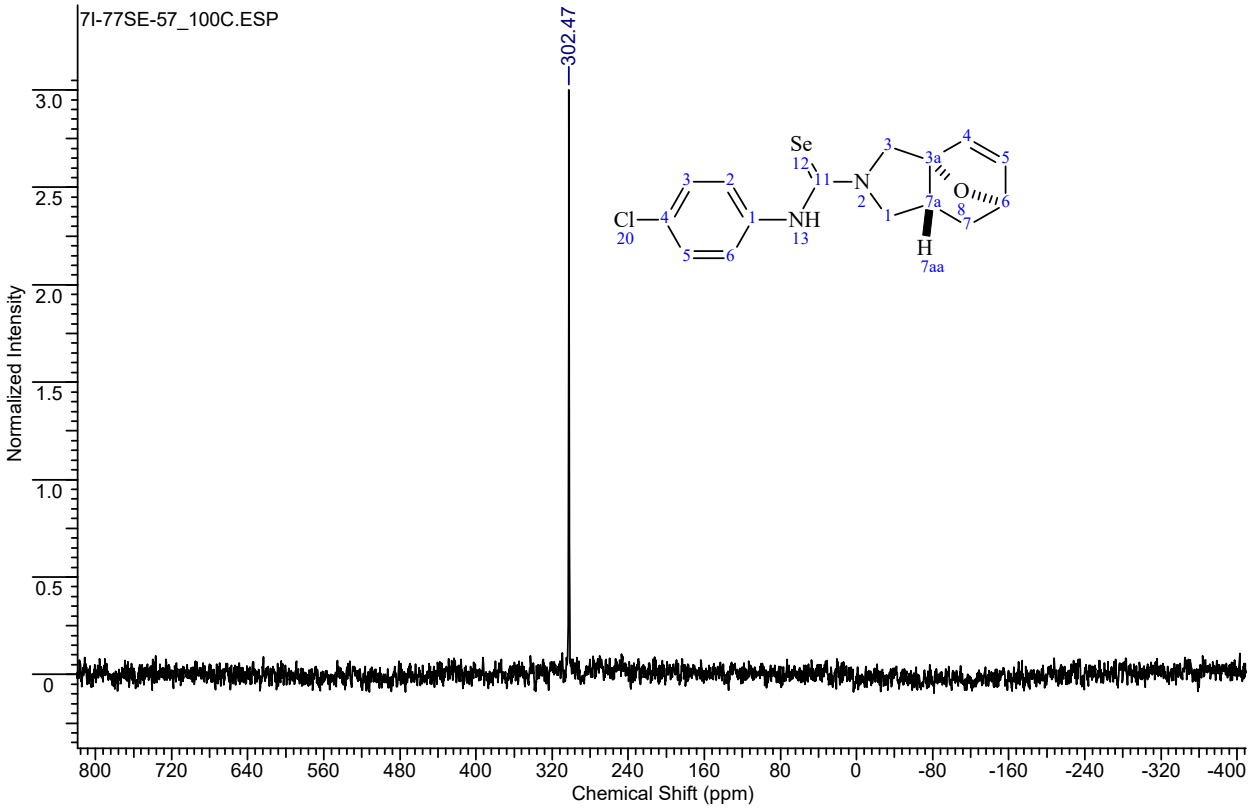
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



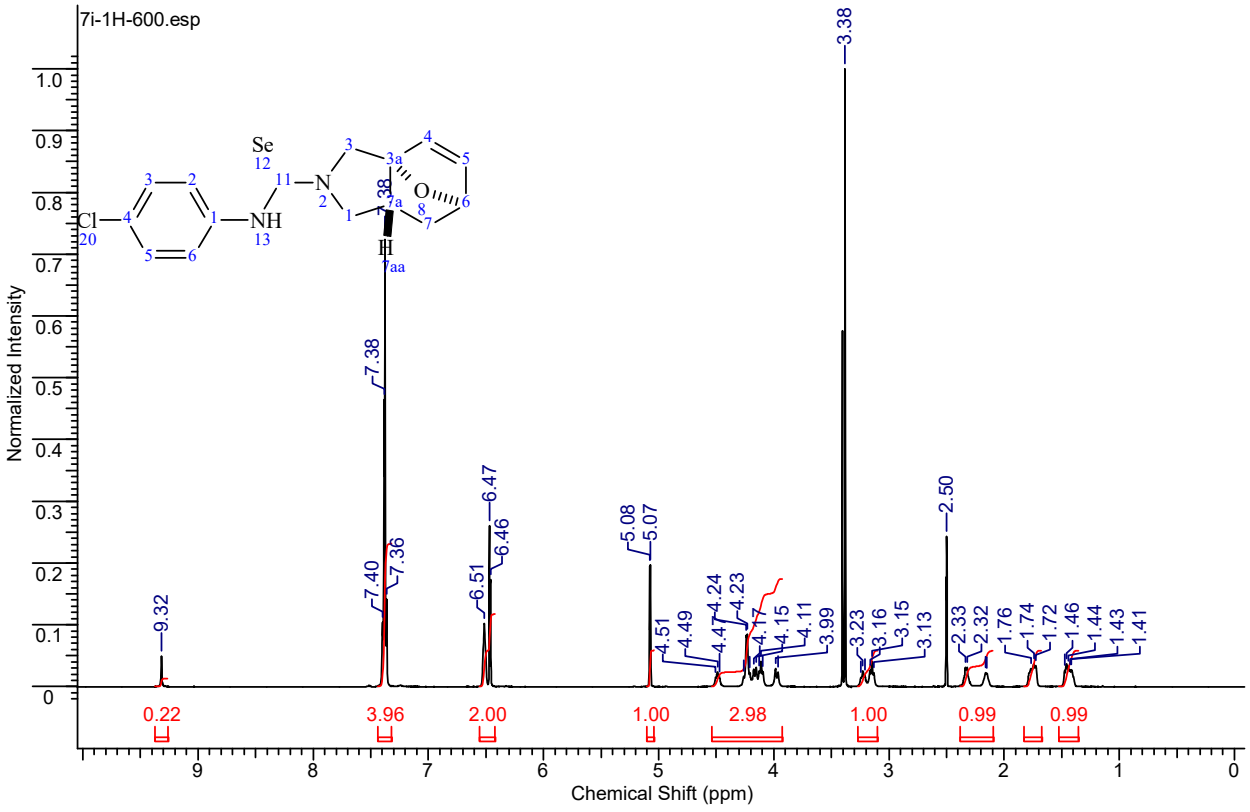
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



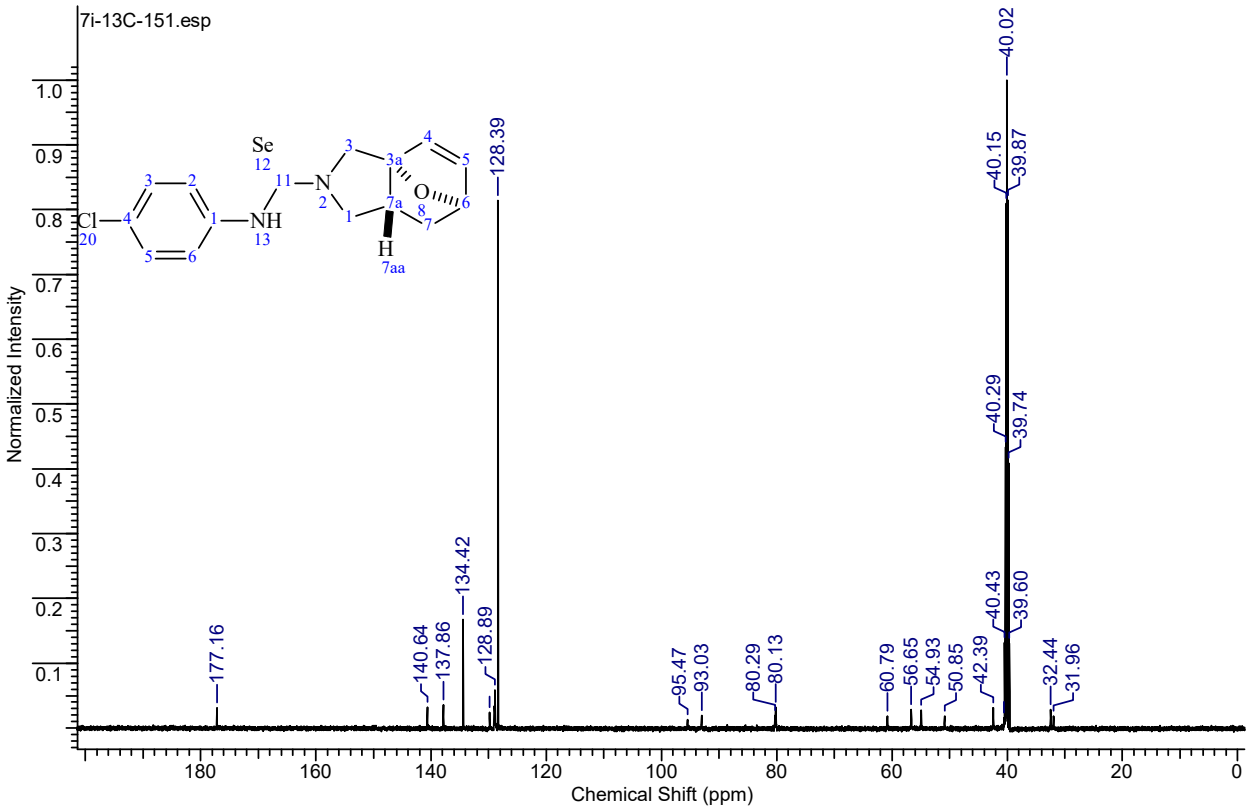
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



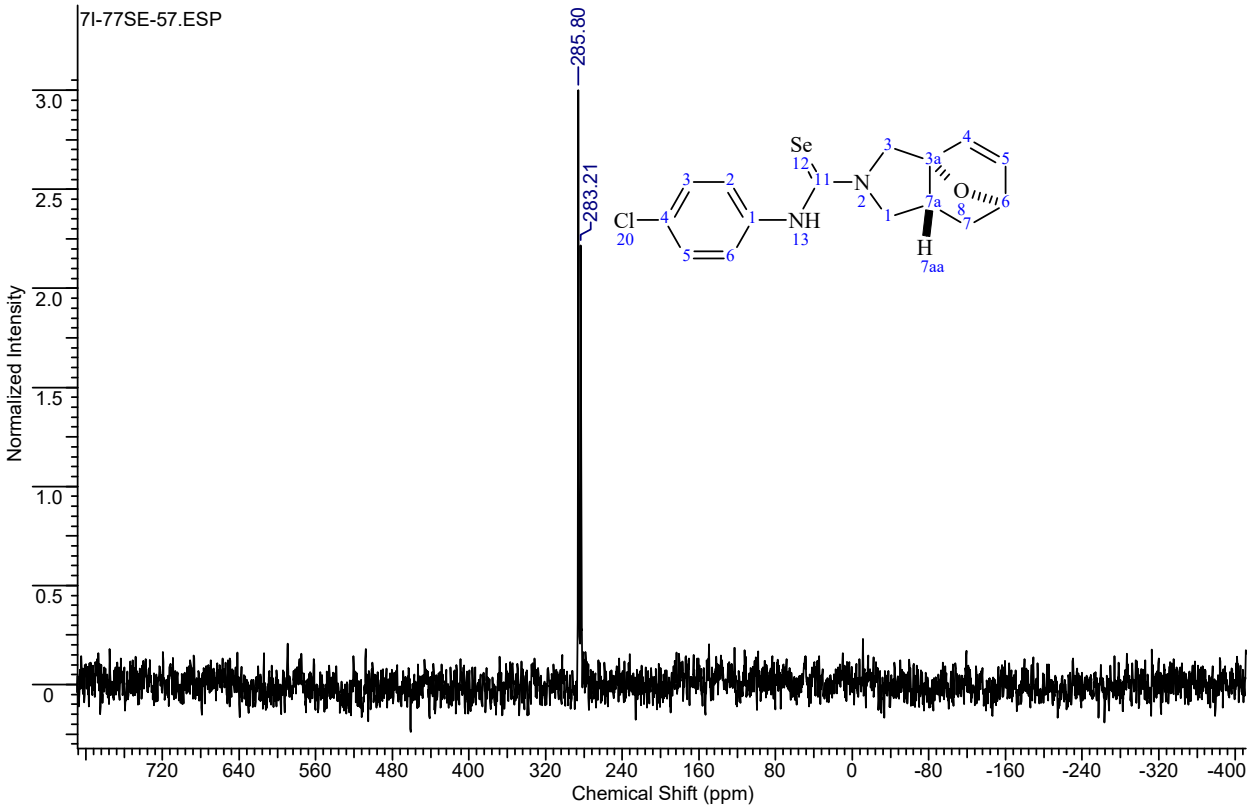
^{1}H NMR (600.2 MHz, DMSO-d_6)



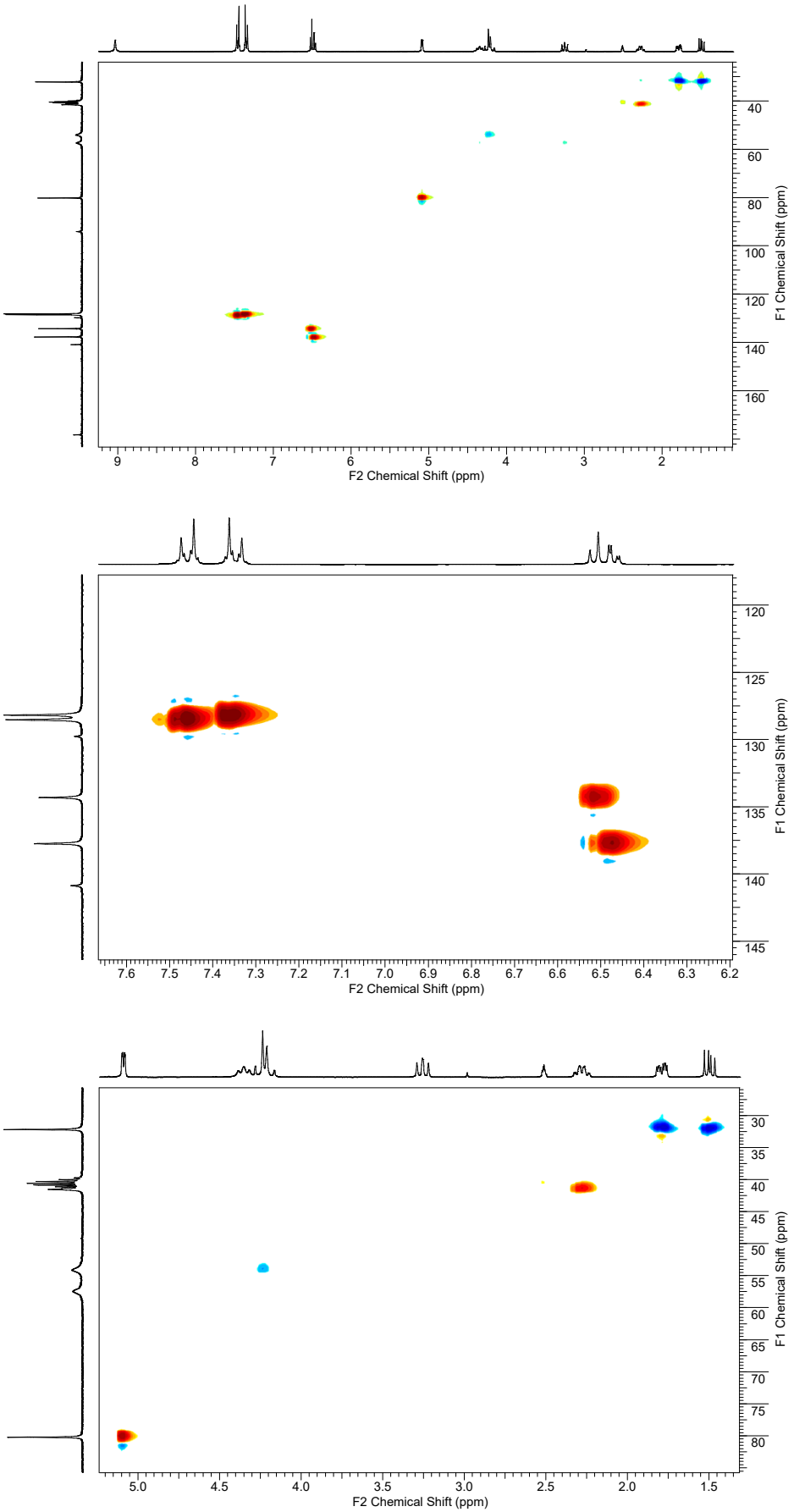
^{13}C NMR (150.9 MHz, DMSO-d_6)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

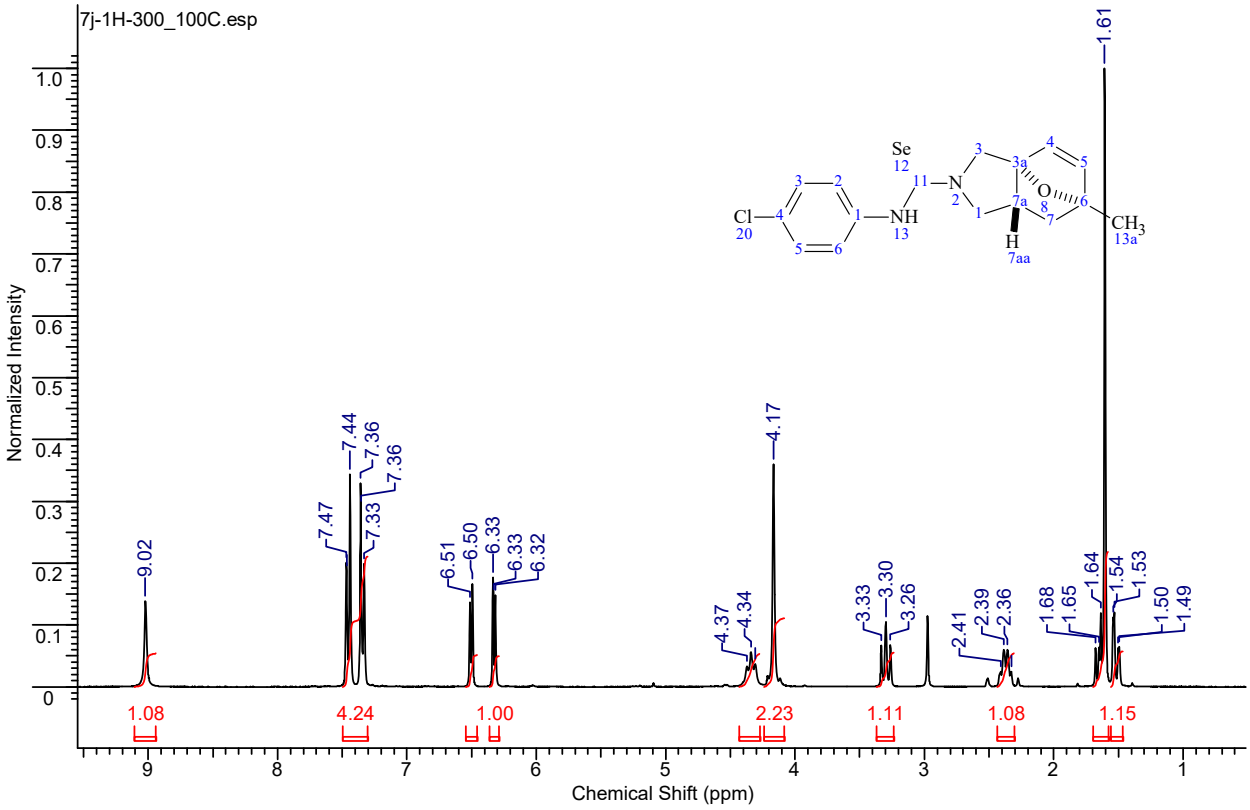


HSQC of **7i** (100 °C)

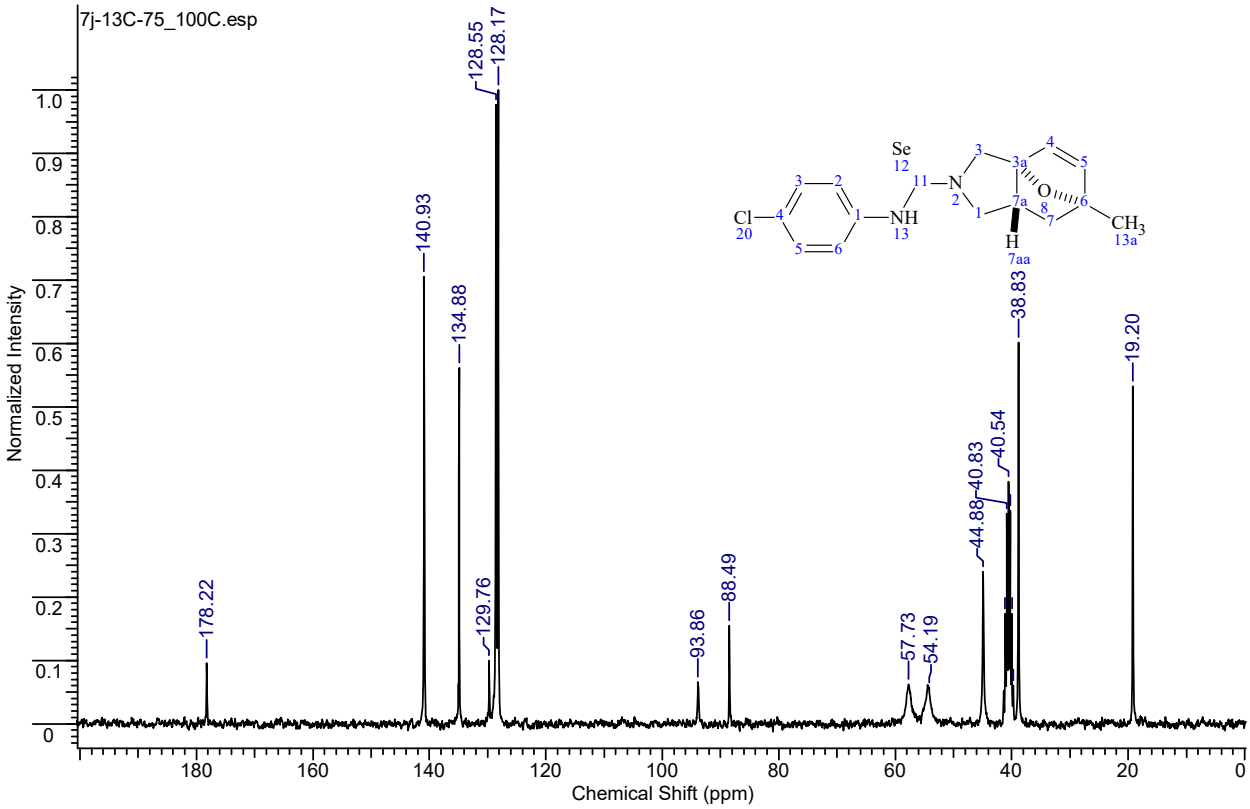


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7j).

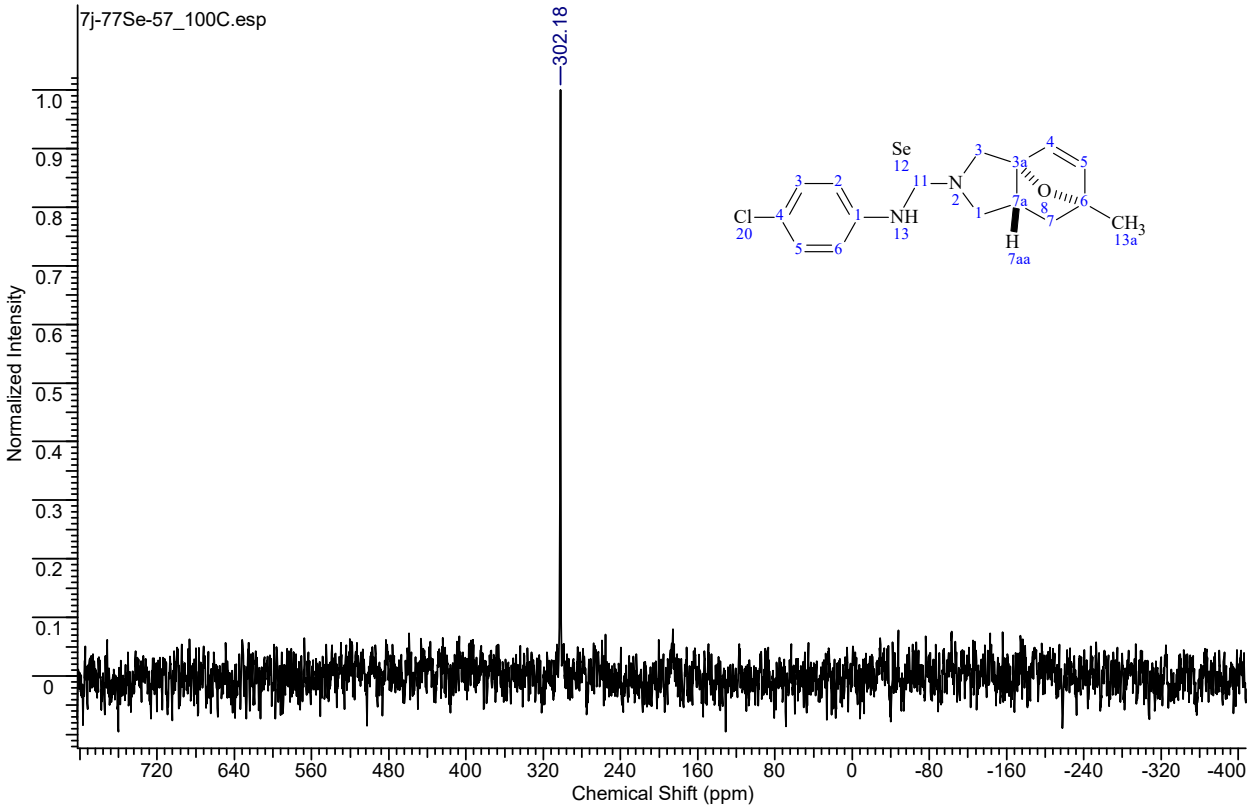
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



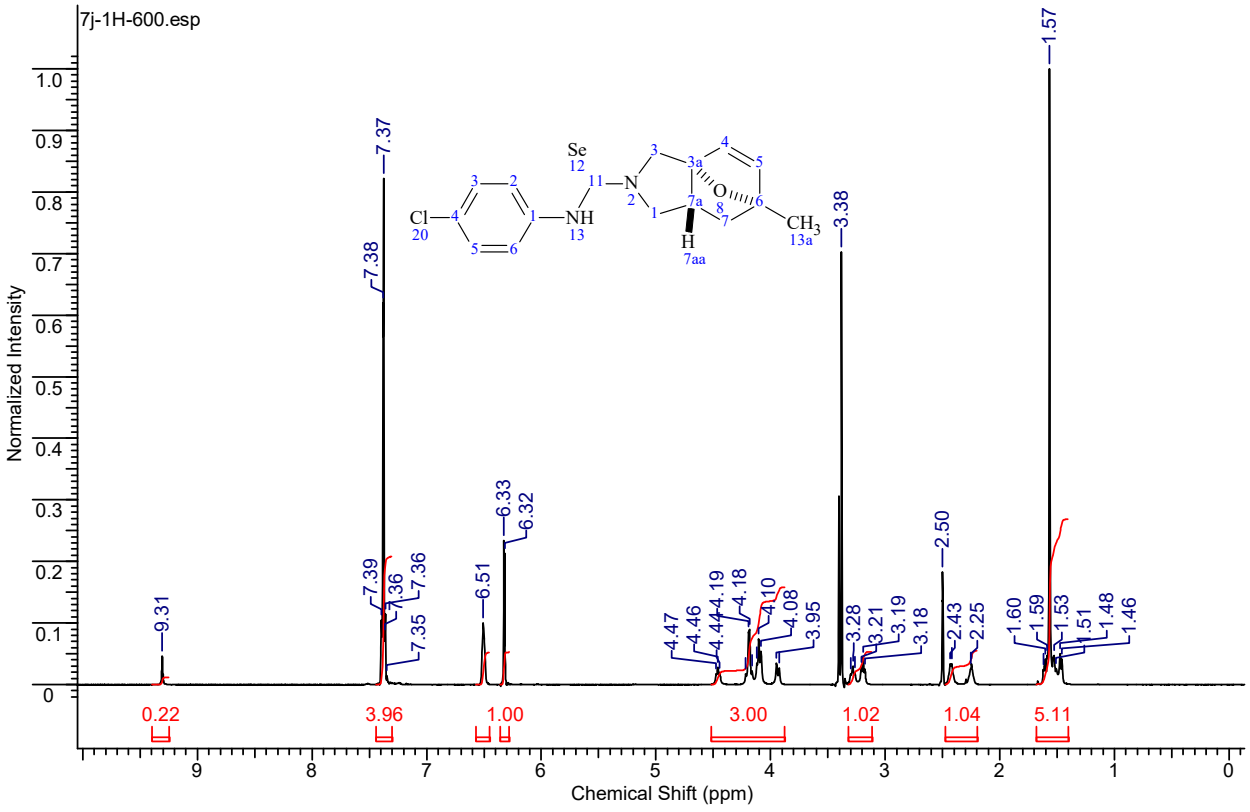
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



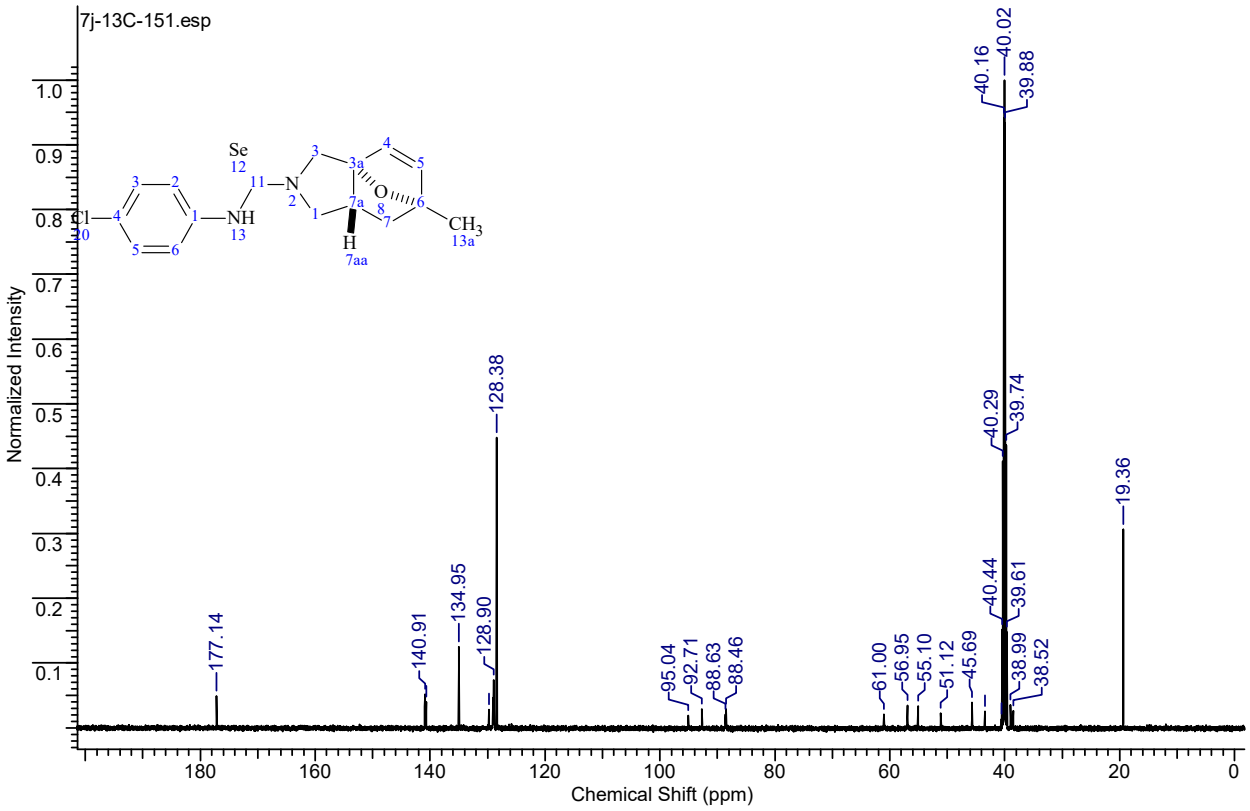
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



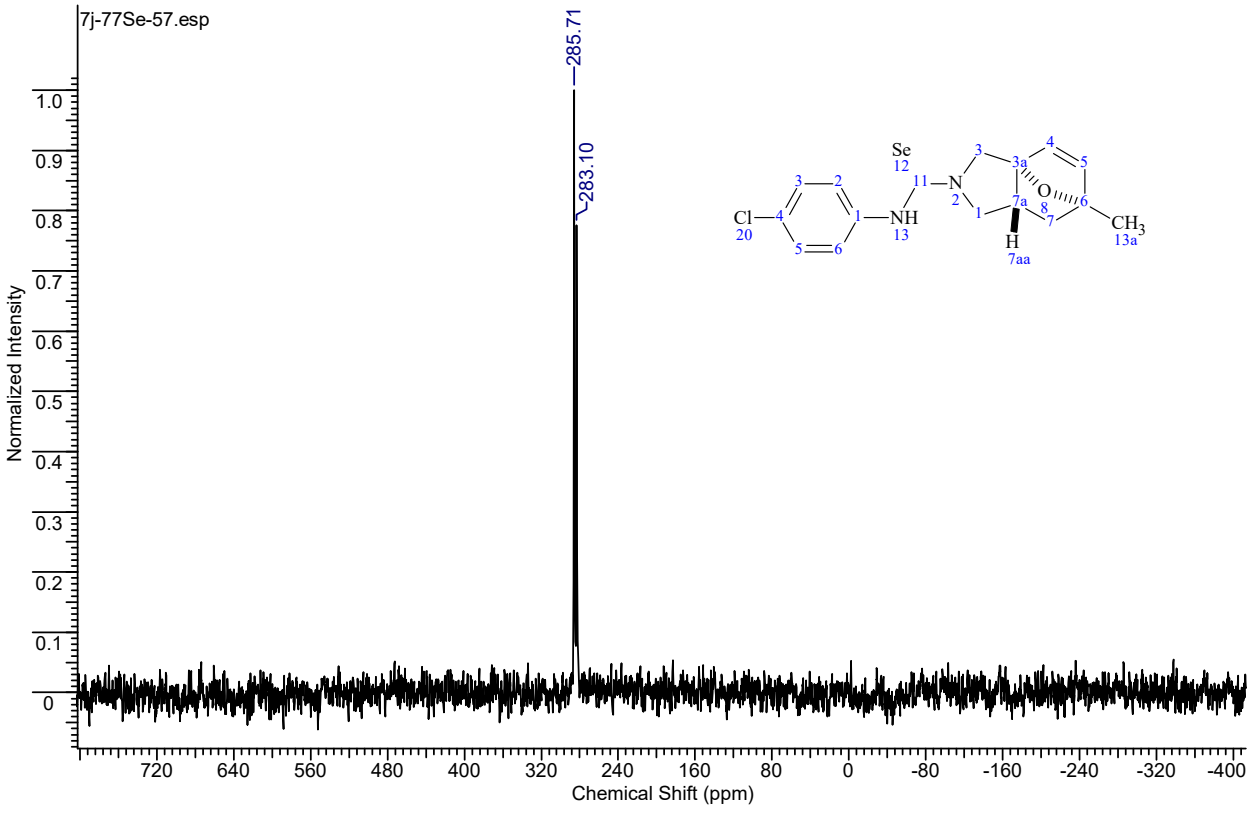
^{1}H NMR (600.2 MHz, DMSO-d_6)



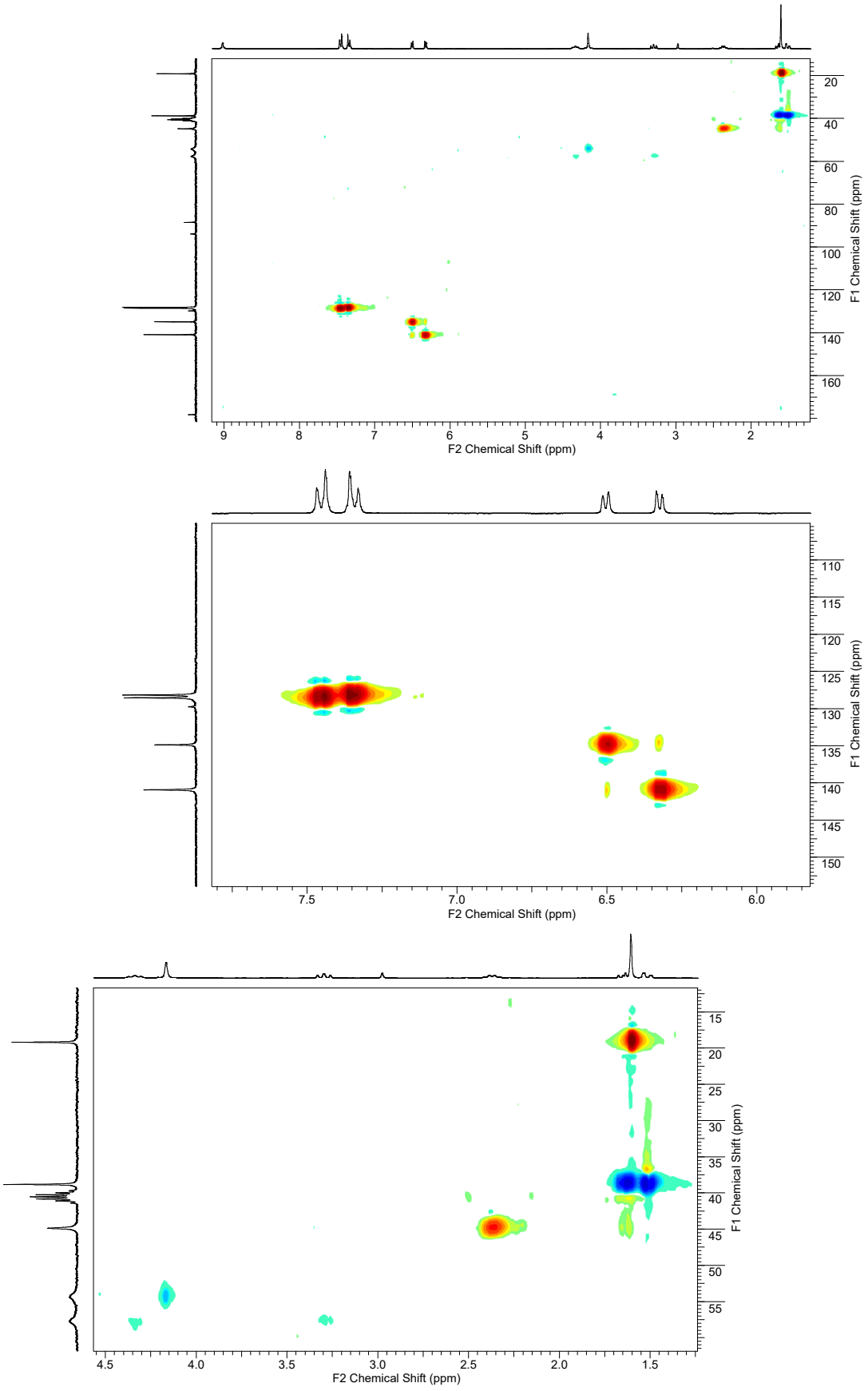
^{13}C NMR (150.9 MHz, DMSO-d_6)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

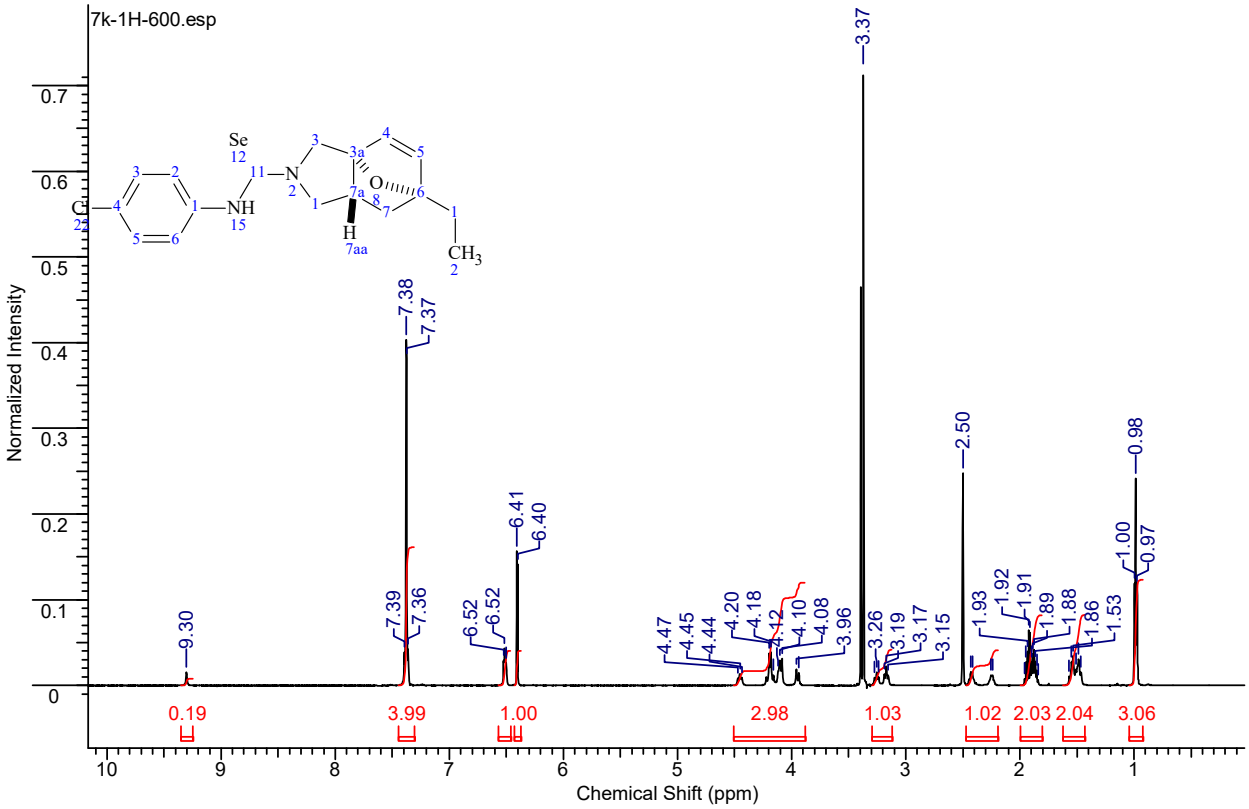


HSQC of **7j (100 °C)**

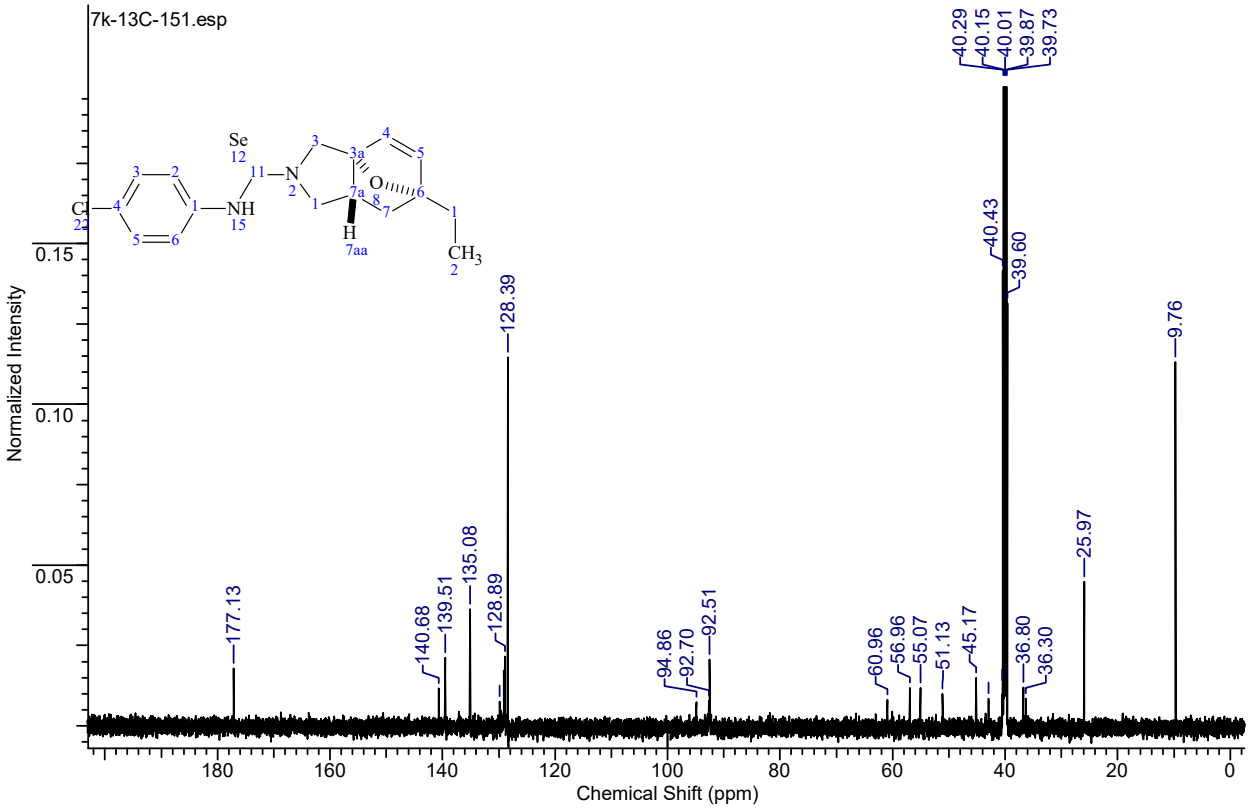


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-ethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7k).

^{1}H NMR (600.2 MHz, DMSO-d_6)

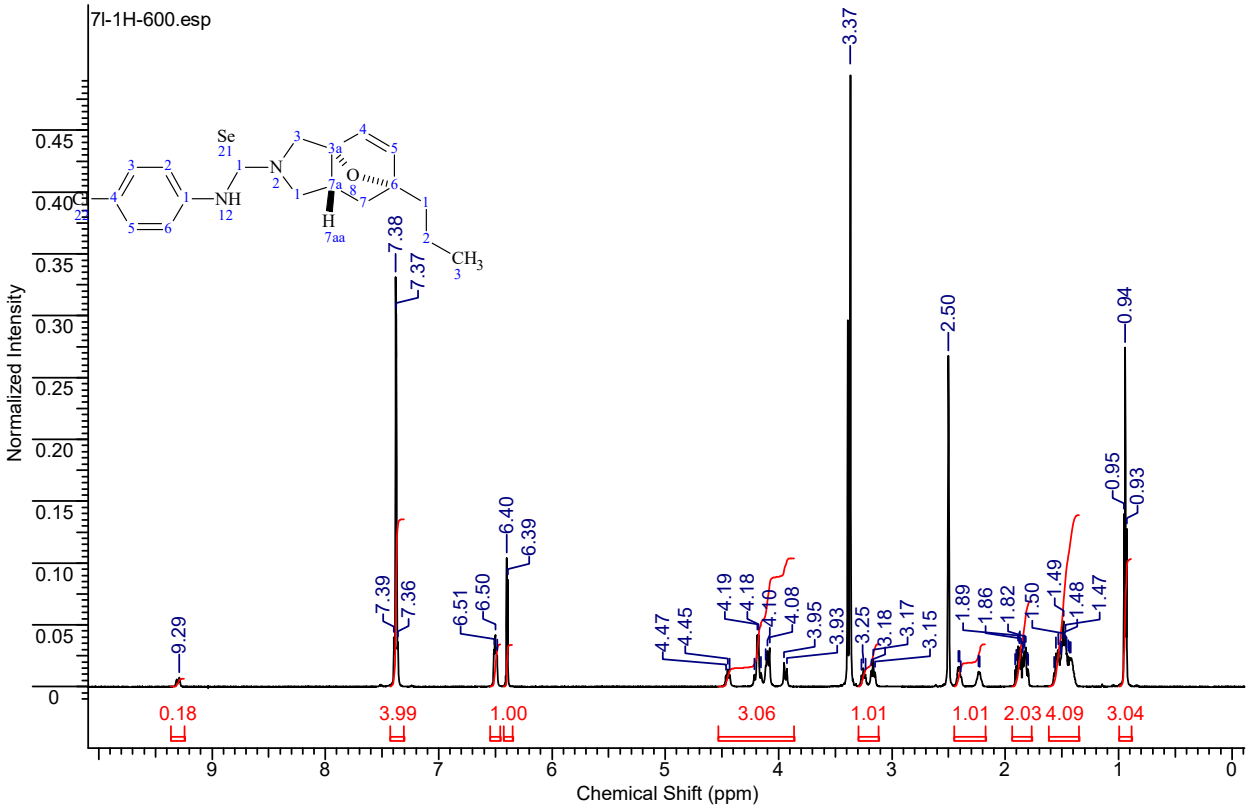


^{13}C NMR (150.9 MHz, DMSO-d_6)

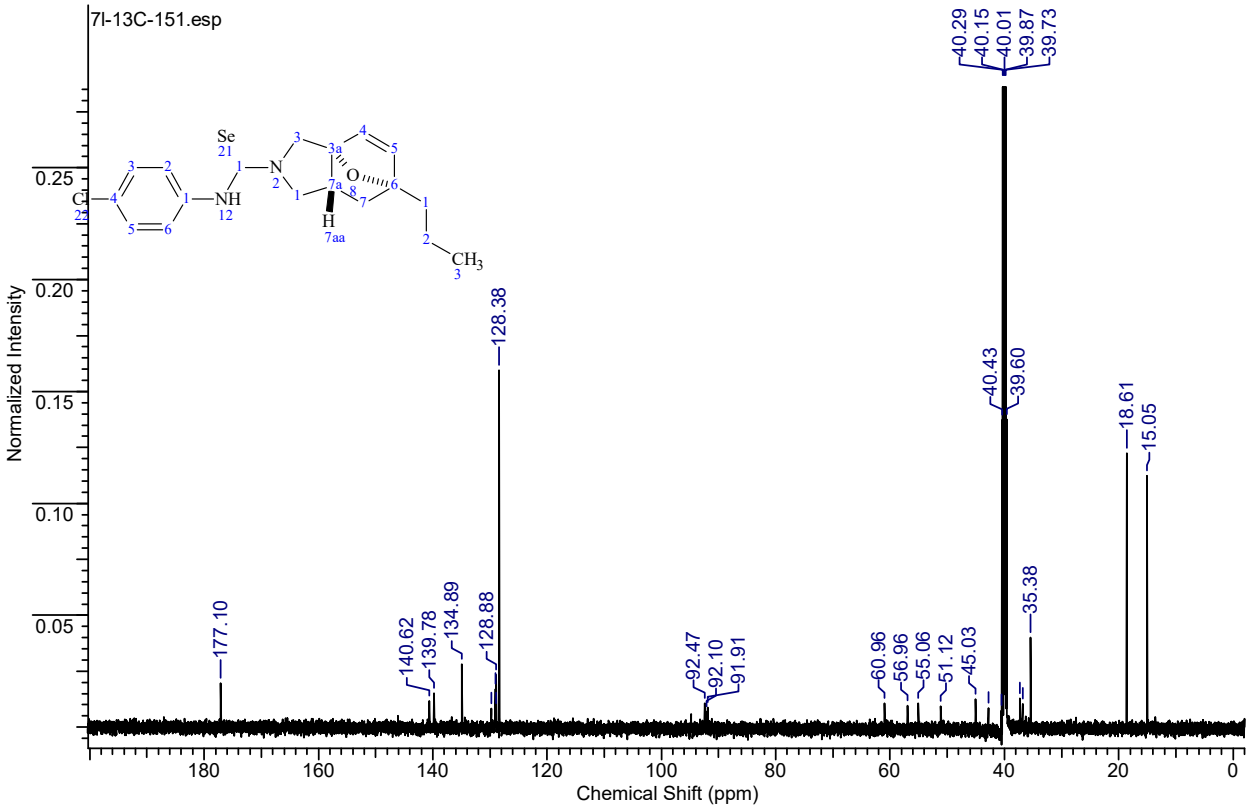


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-6-propyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7l).

^{1}H NMR (600.2 MHz, DMSO-d_6)

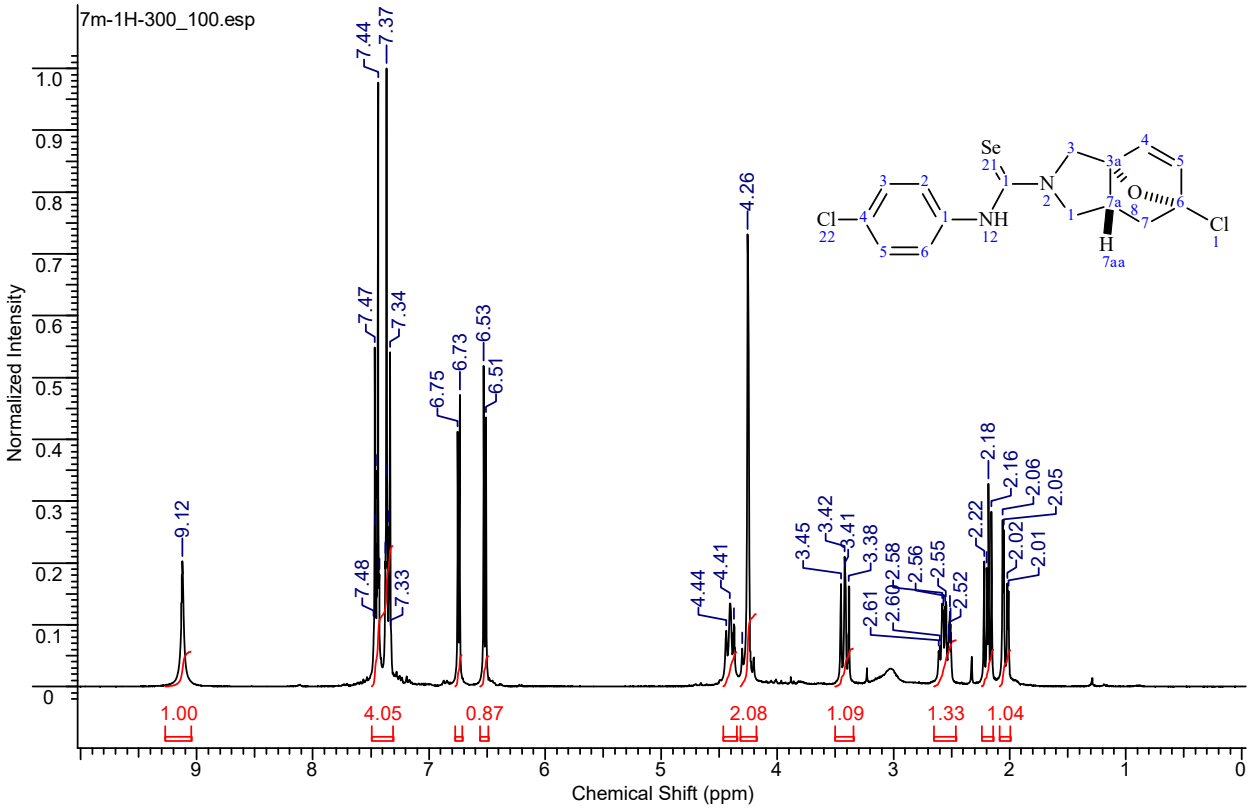


^{13}C NMR (150.9 MHz, DMSO-d_6)

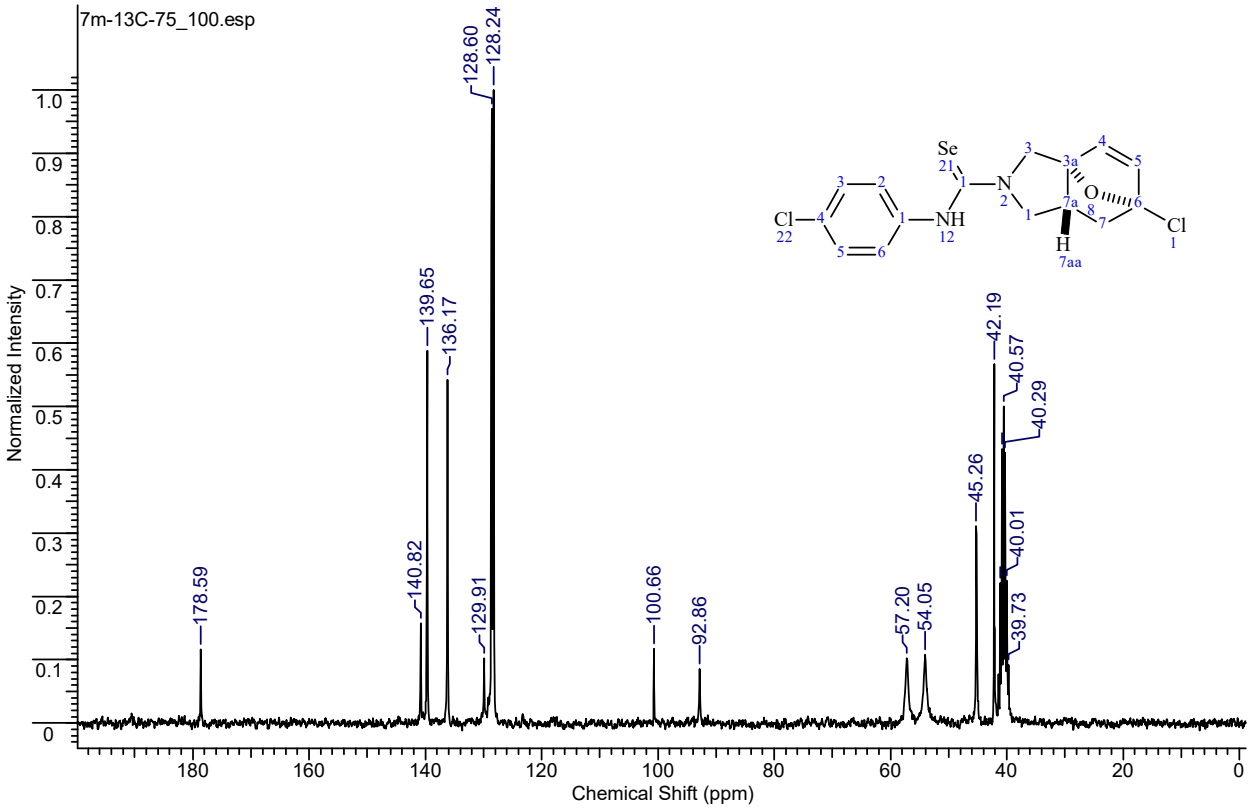


(3a*RS*,6*SR*,7a*RS*)-6-Chloro-*N*-(4-chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7m).

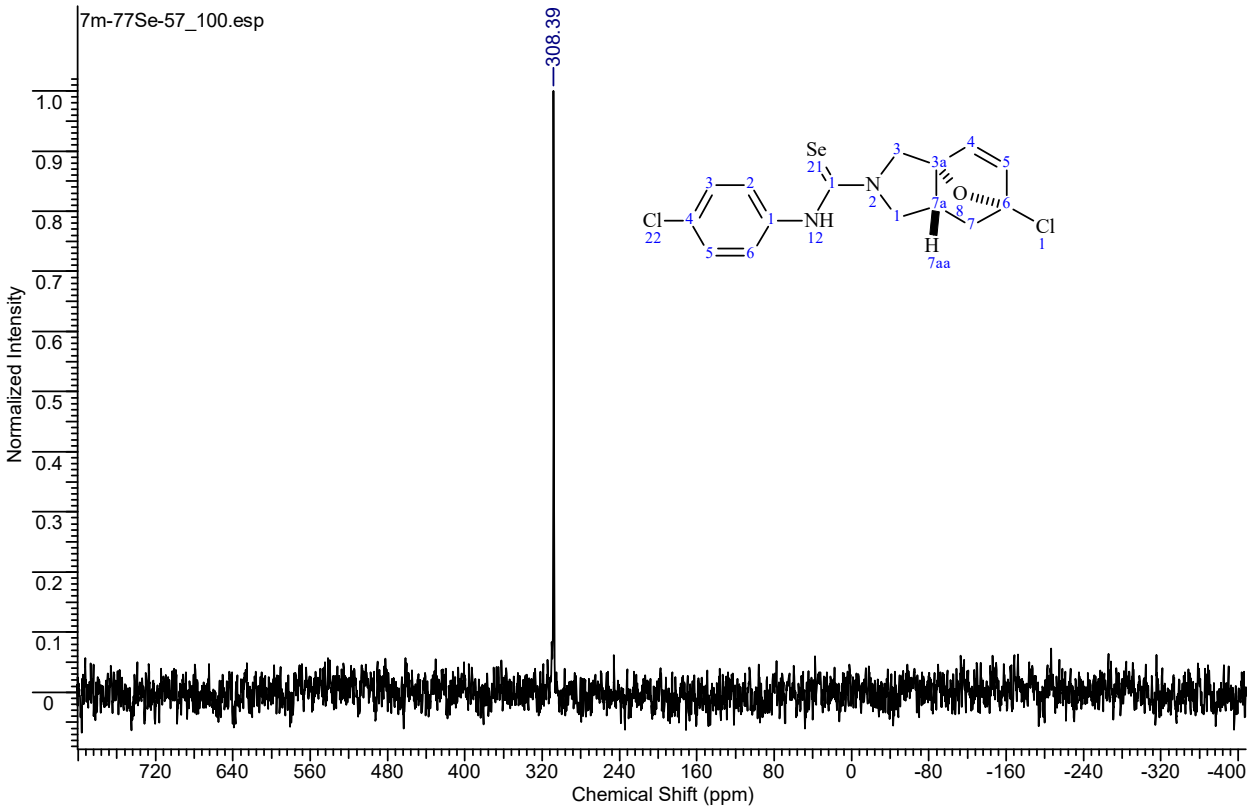
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



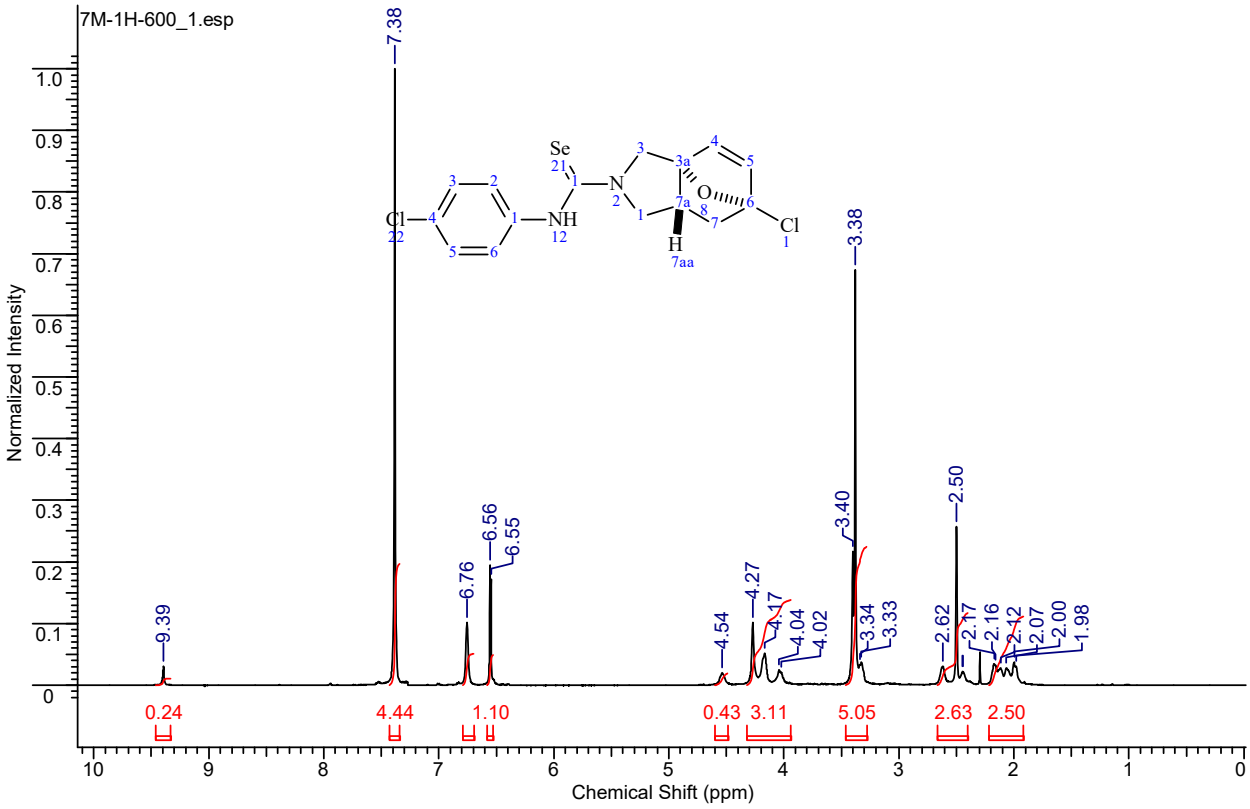
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



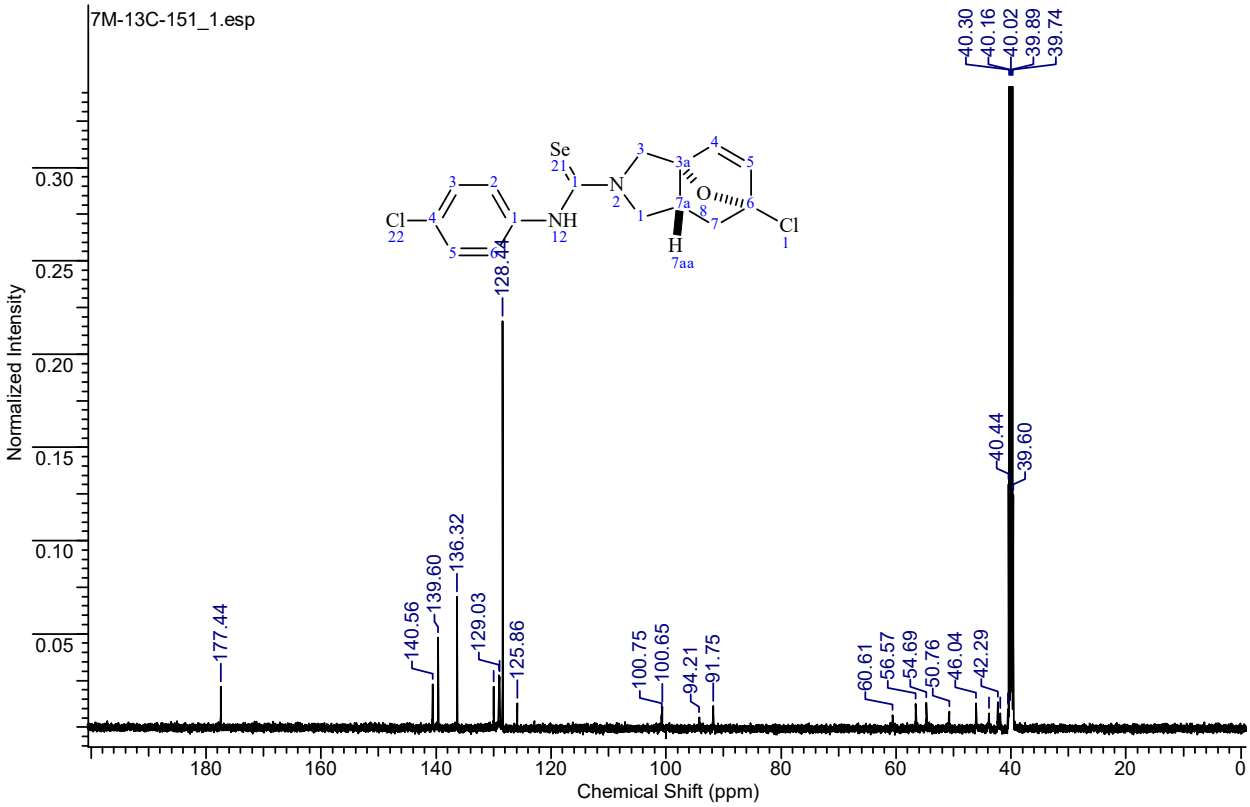
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



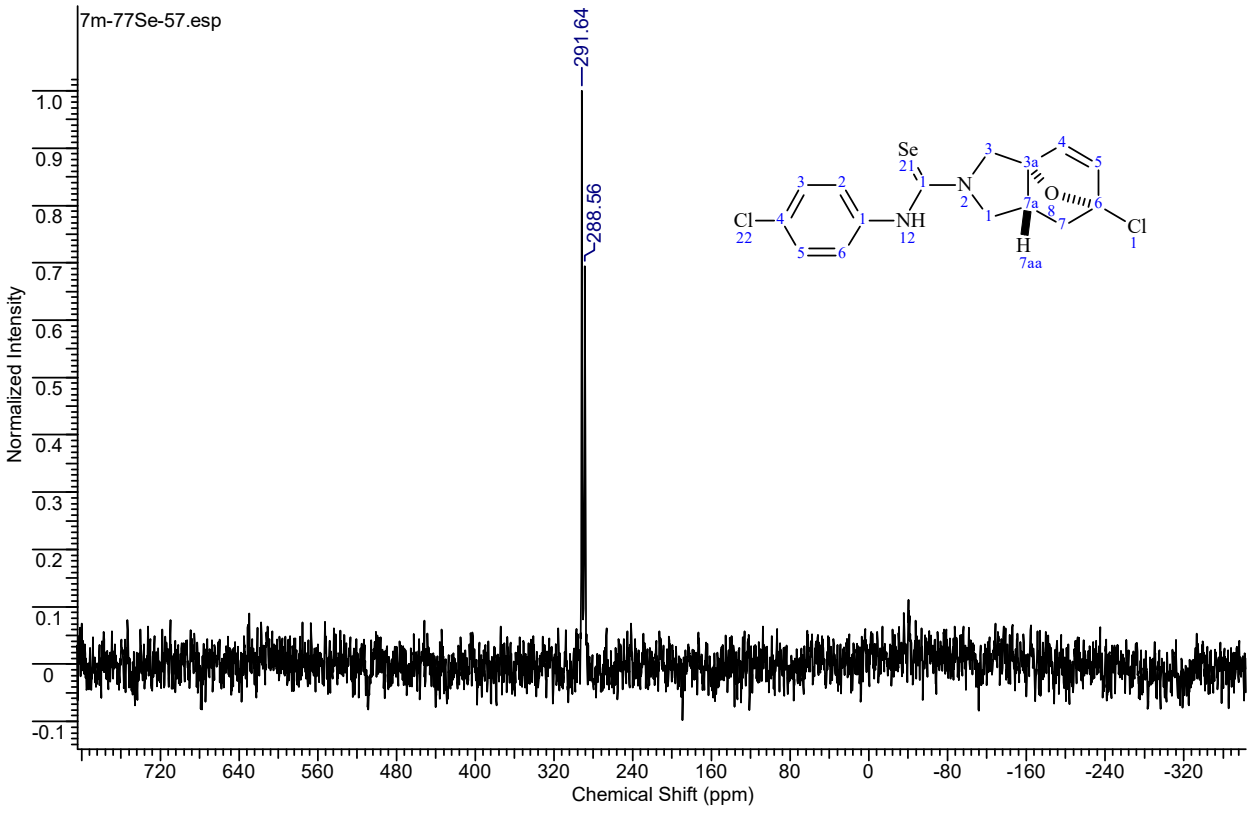
^{1}H NMR (600.2 MHz, DMSO-d_6)



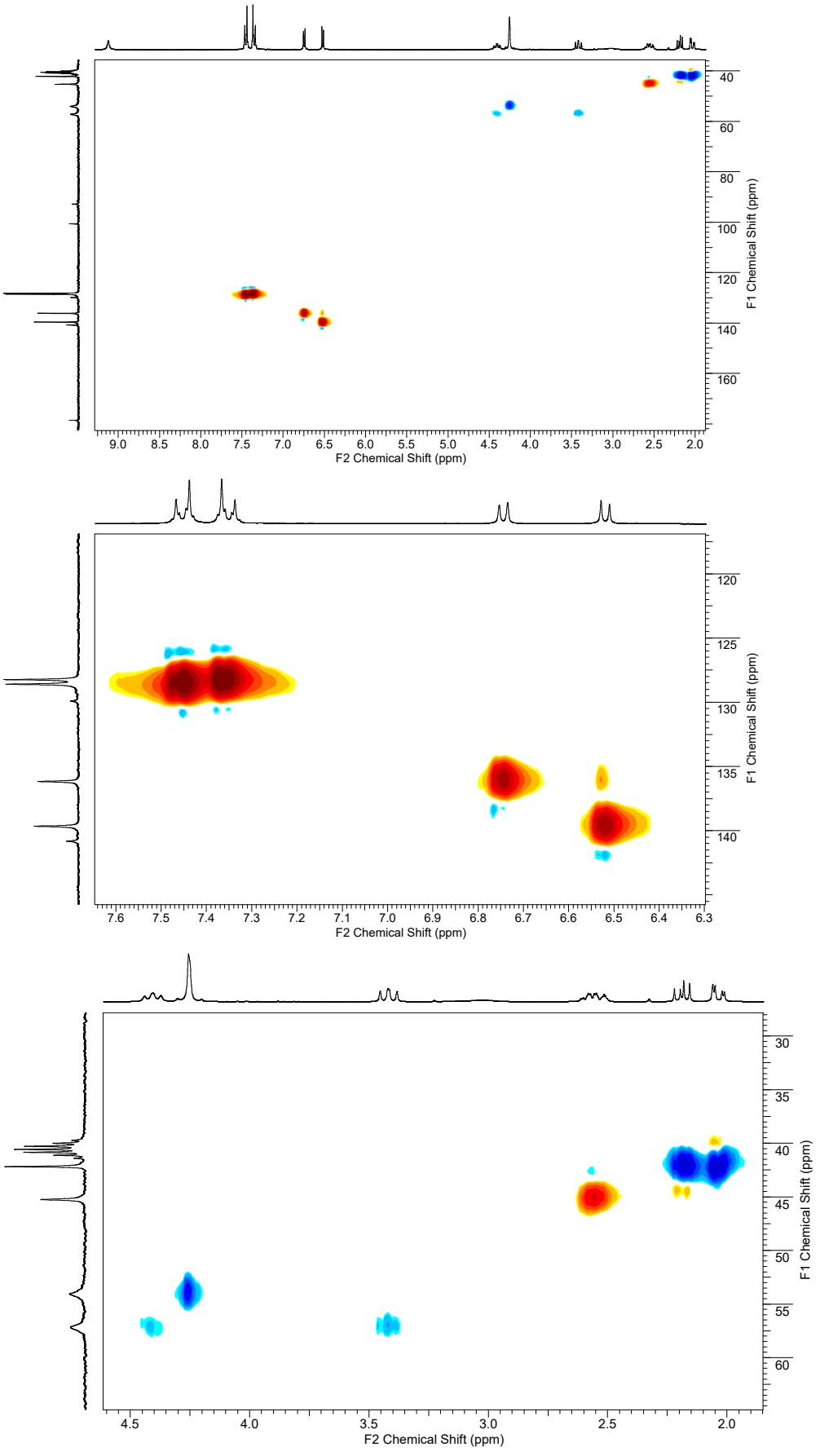
^{13}C NMR (150.9 MHz, DMSO-d_6)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

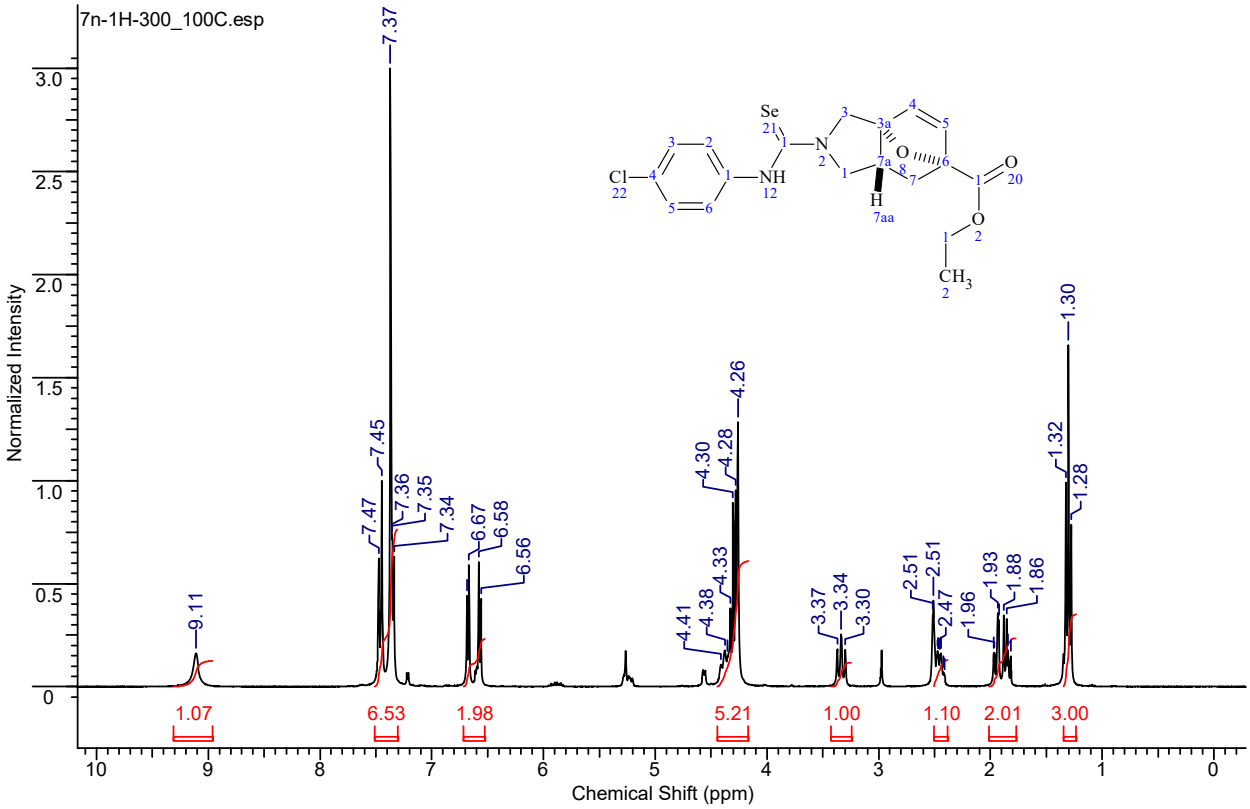


HSQC of **7m** (100 °C)

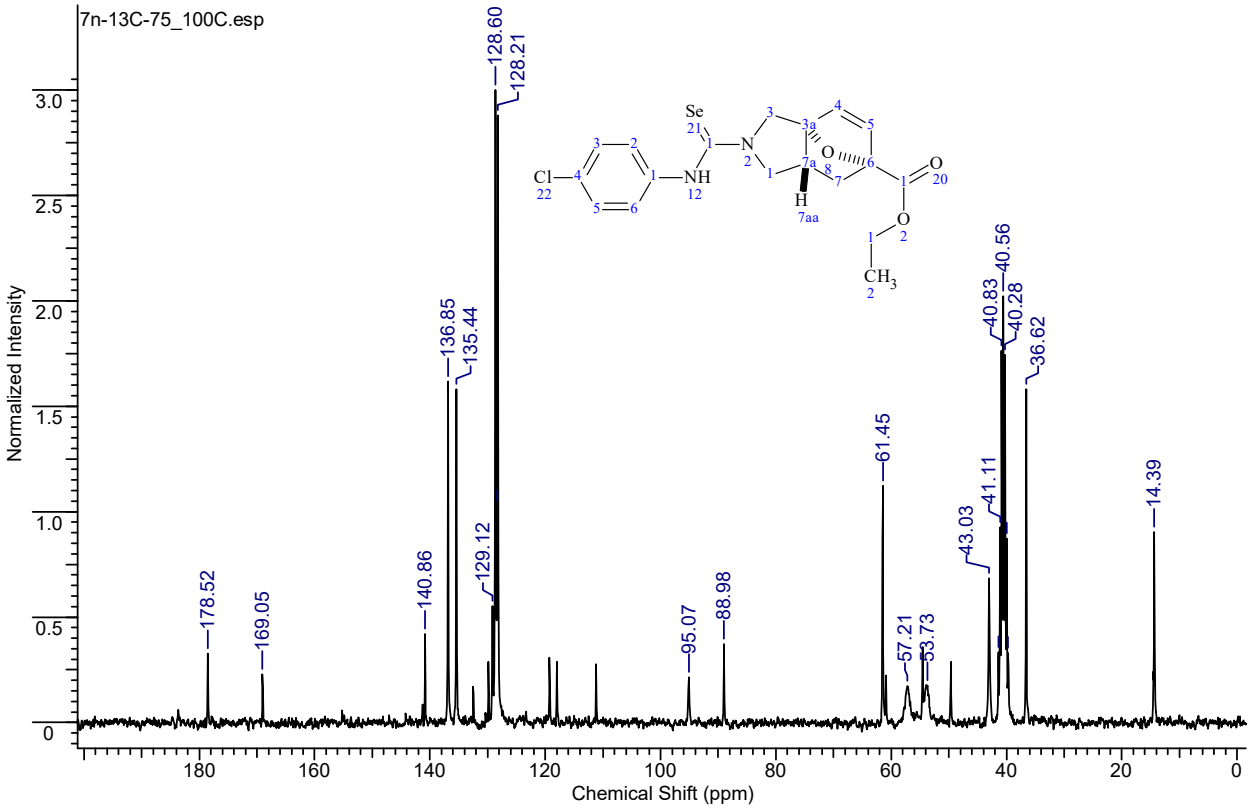


Ethyl (3a*RS*,6*RS*,7a*RS*)-2-((4-chlorophenyl)carbamoselenoyl)-2,3,7,7a-tetrahydro-3a,6-epoxyisoindole-6(1*H*)-carboxylate (7n).

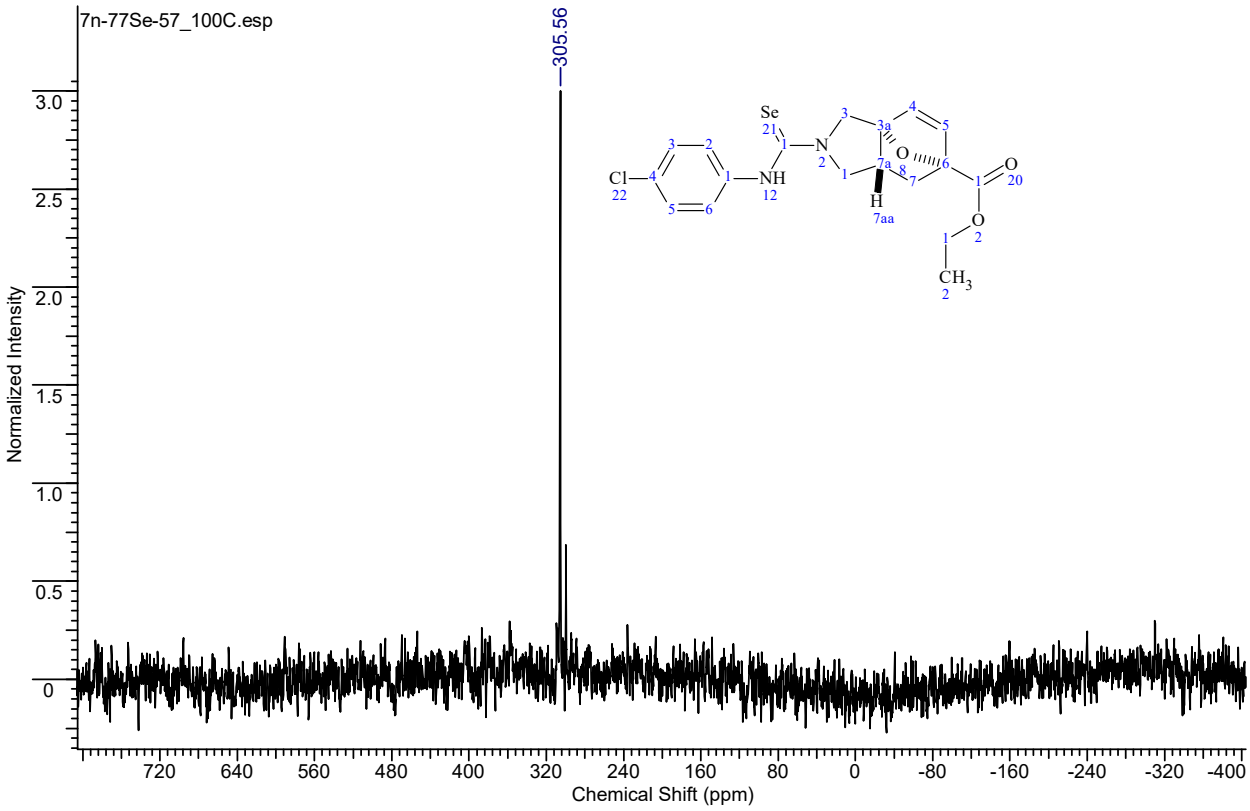
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C) *the compd.* **7n** *decomposes at 100 °C*



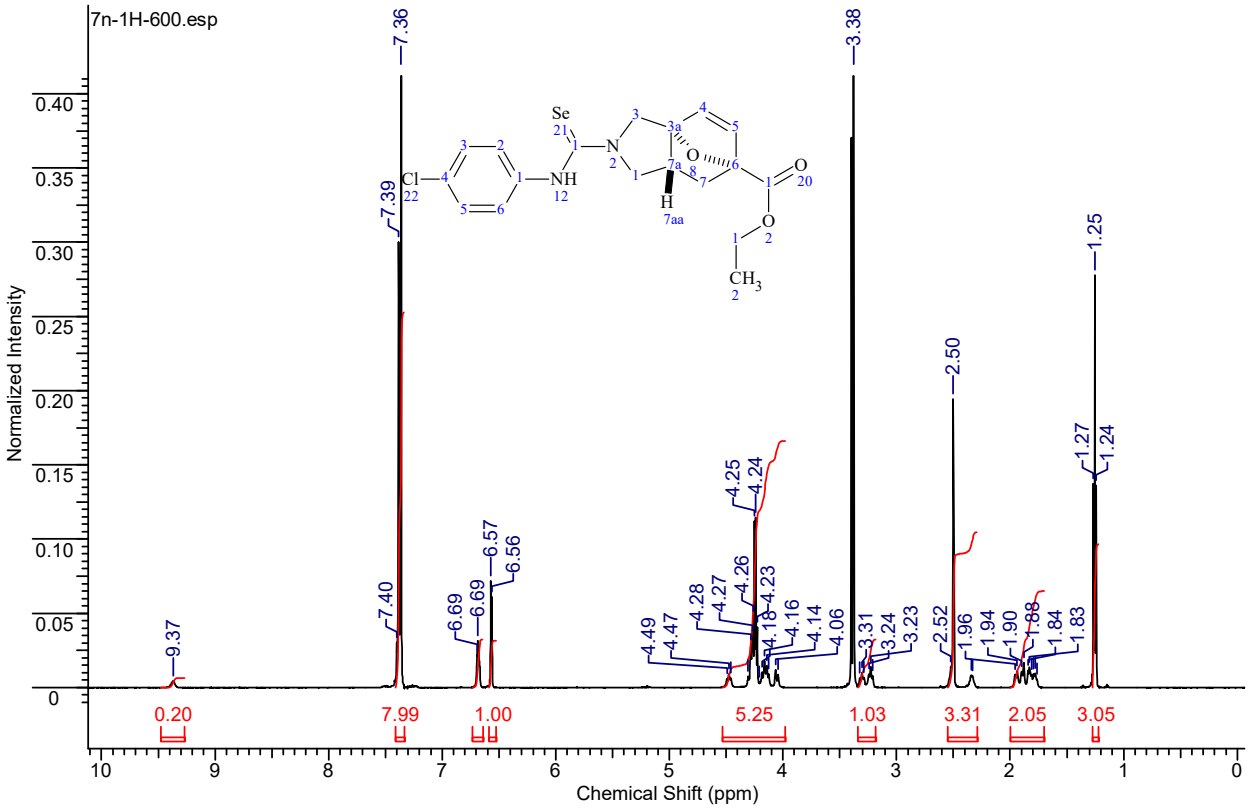
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



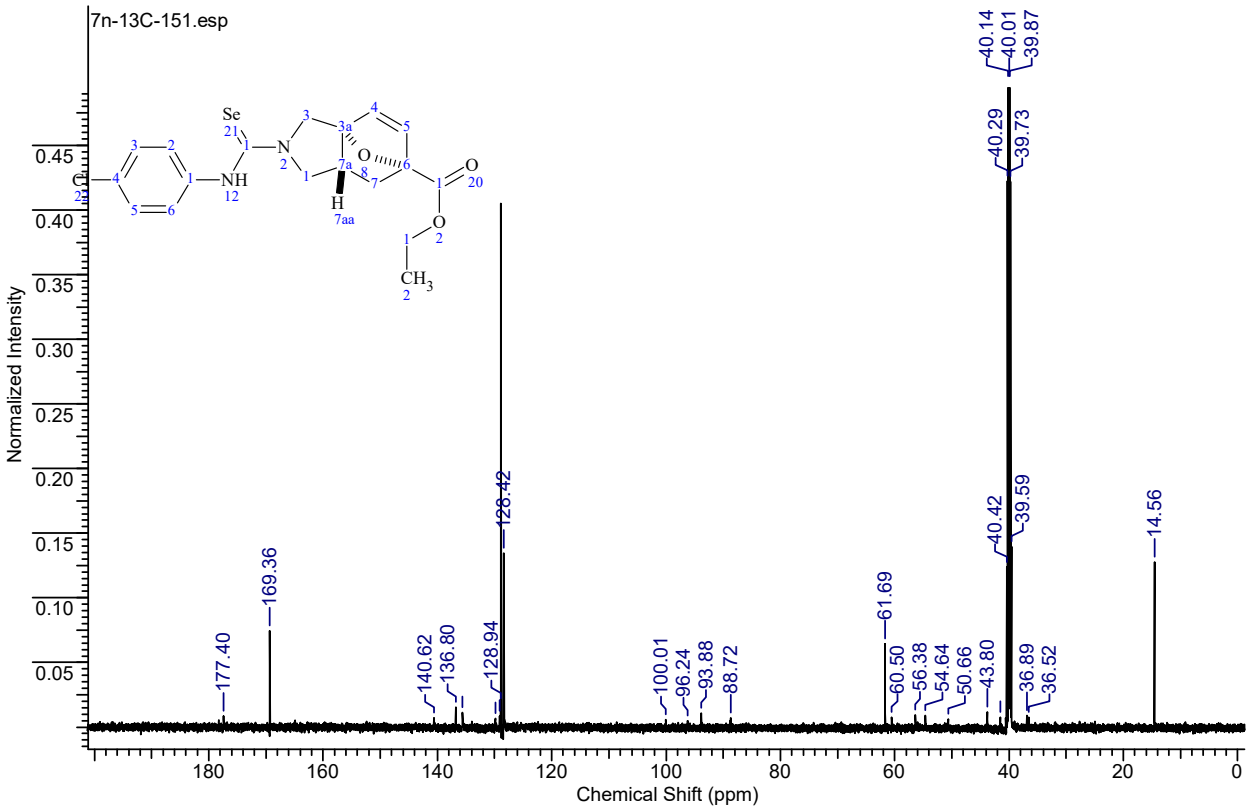
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



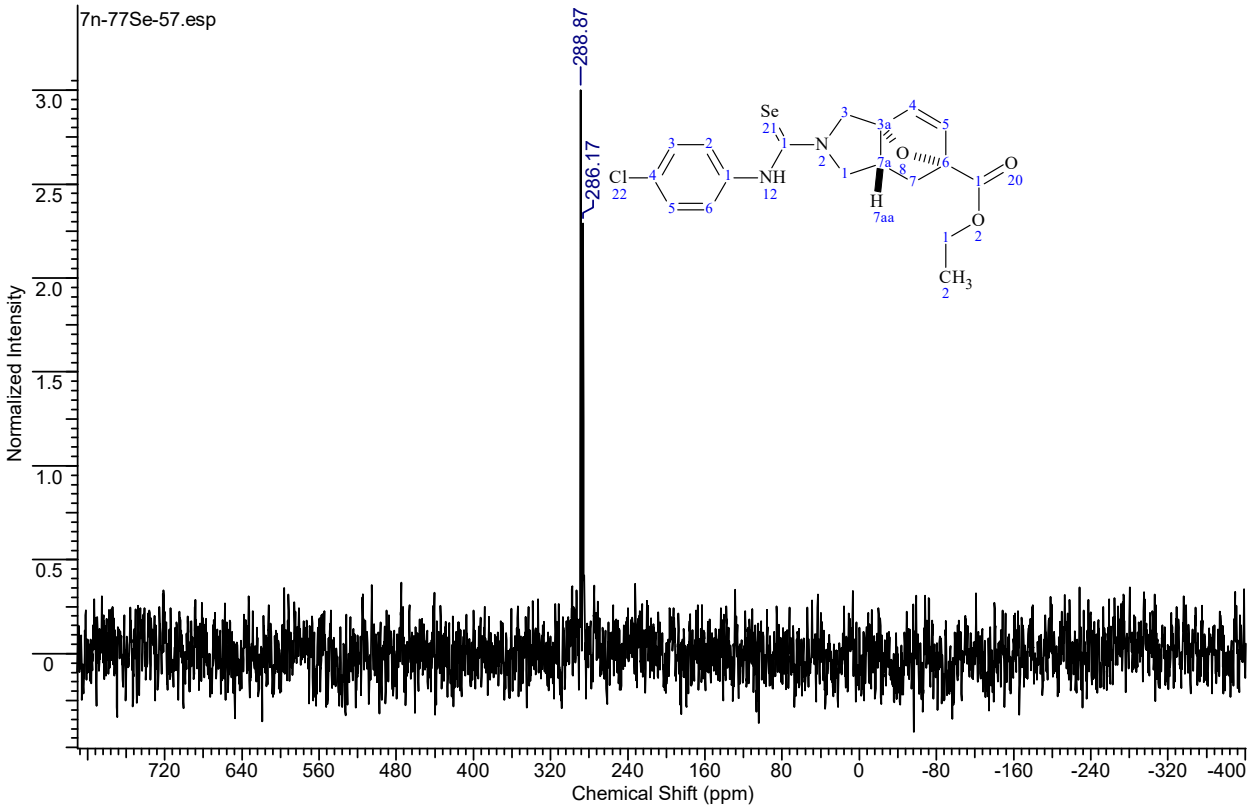
^{1}H NMR (600.2 MHz, DMSO-d_6) *Contains an impurity of benzene*



^{13}C NMR (150.9 MHz, DMSO-d_6)

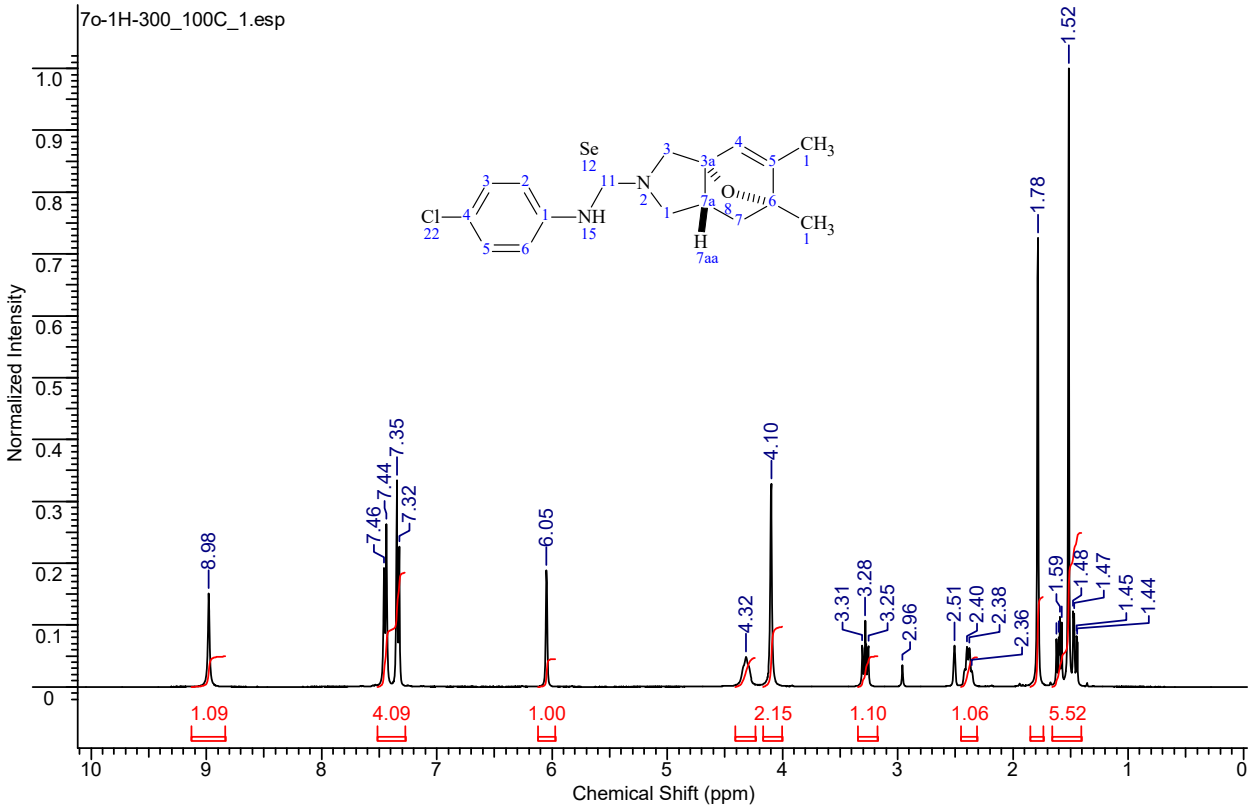


^{77}Se NMR (57.2 MHz, DMSO-d_6)

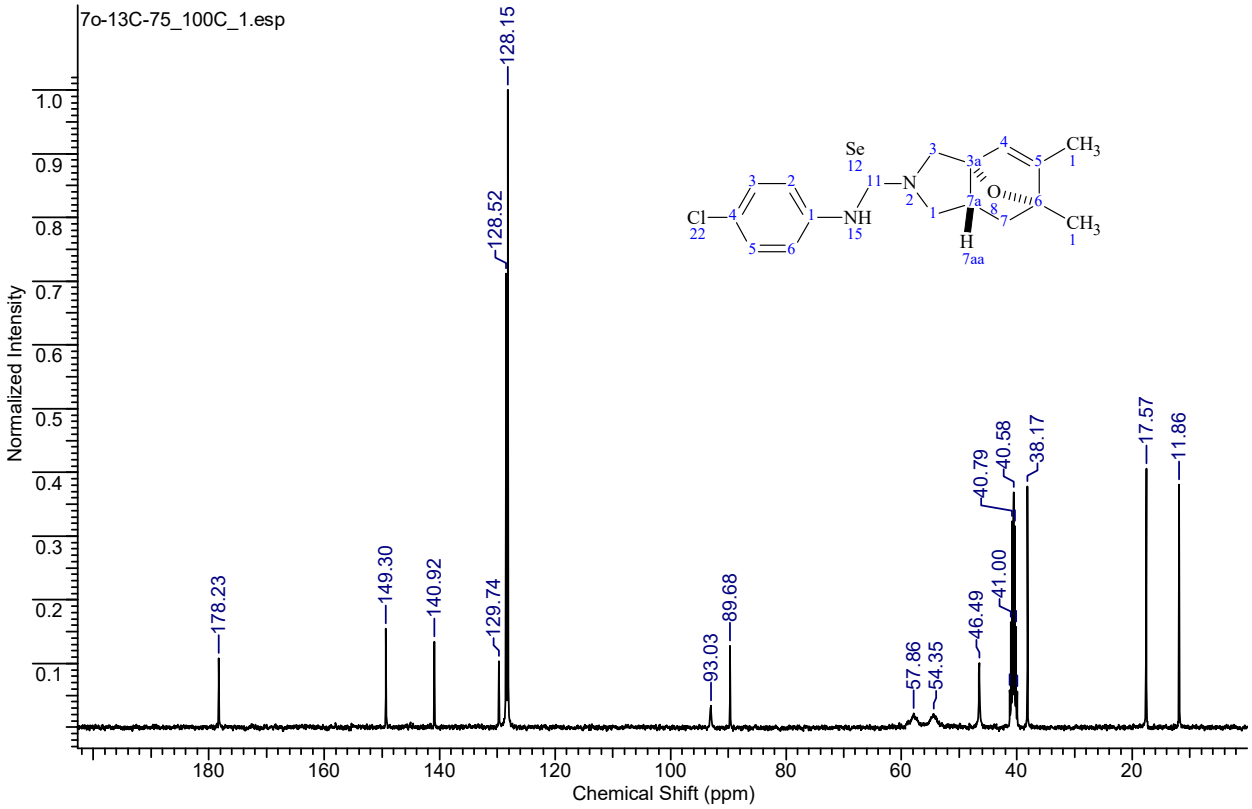


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Chlorophenyl)-5,6-dimethyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7o).

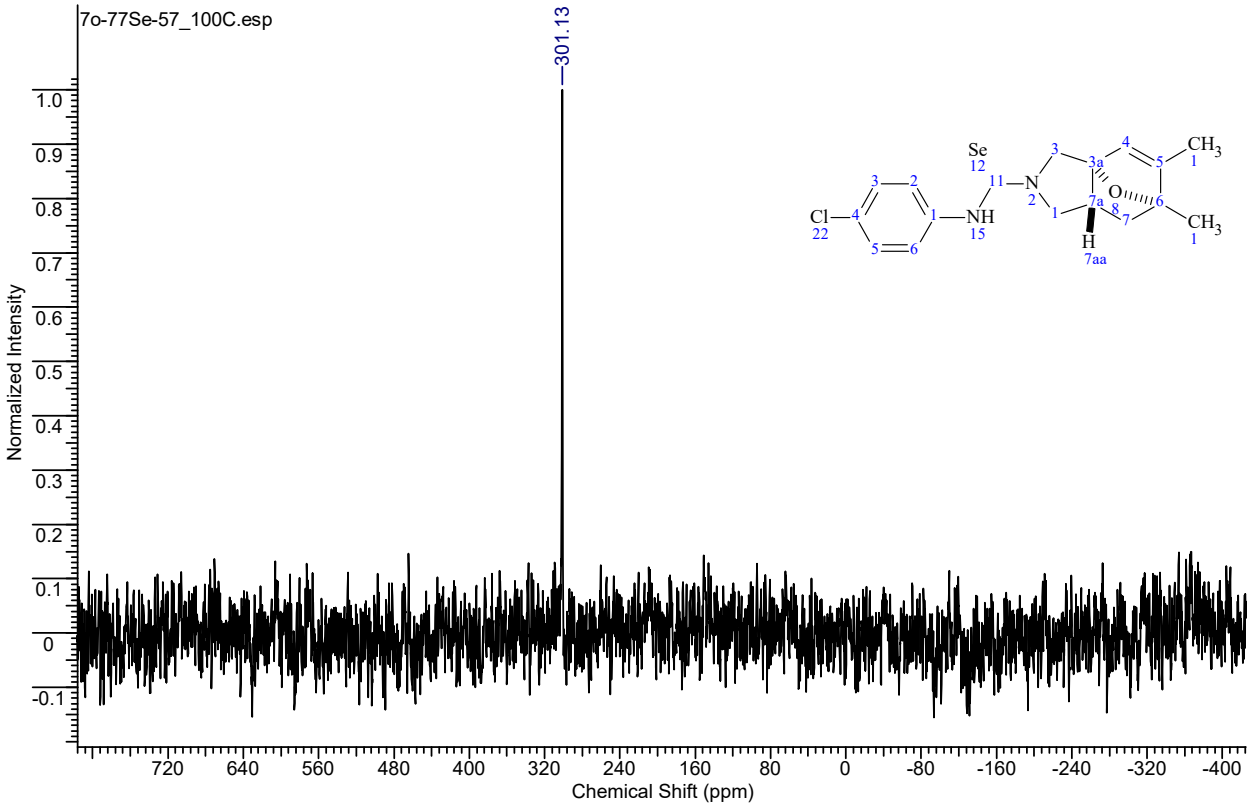
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



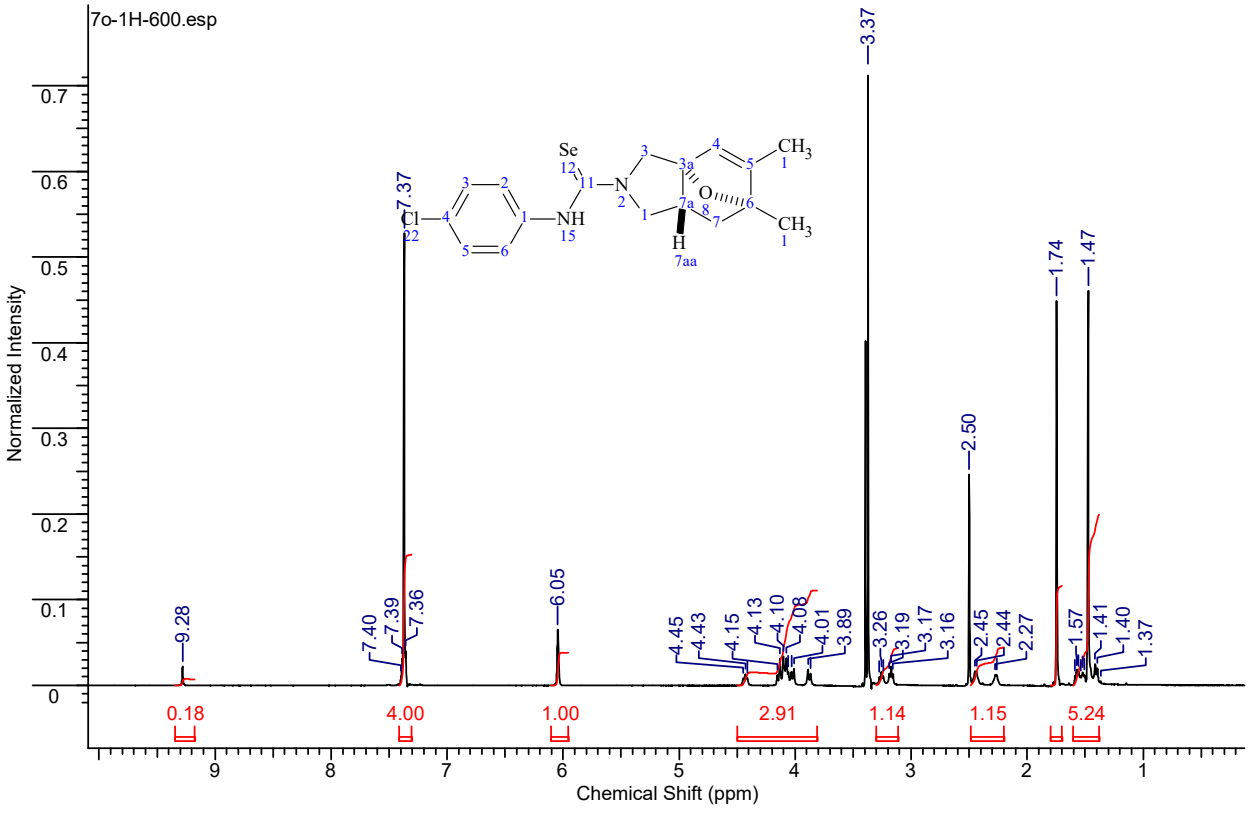
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



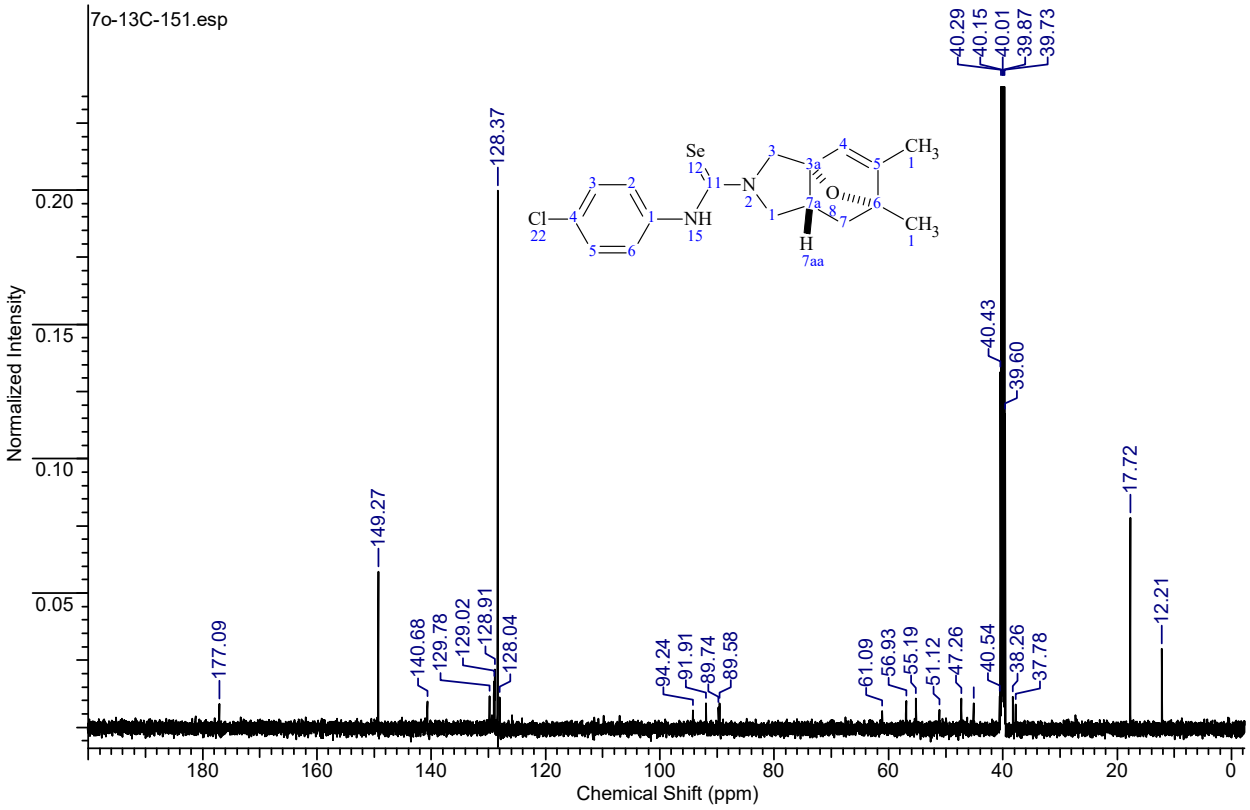
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



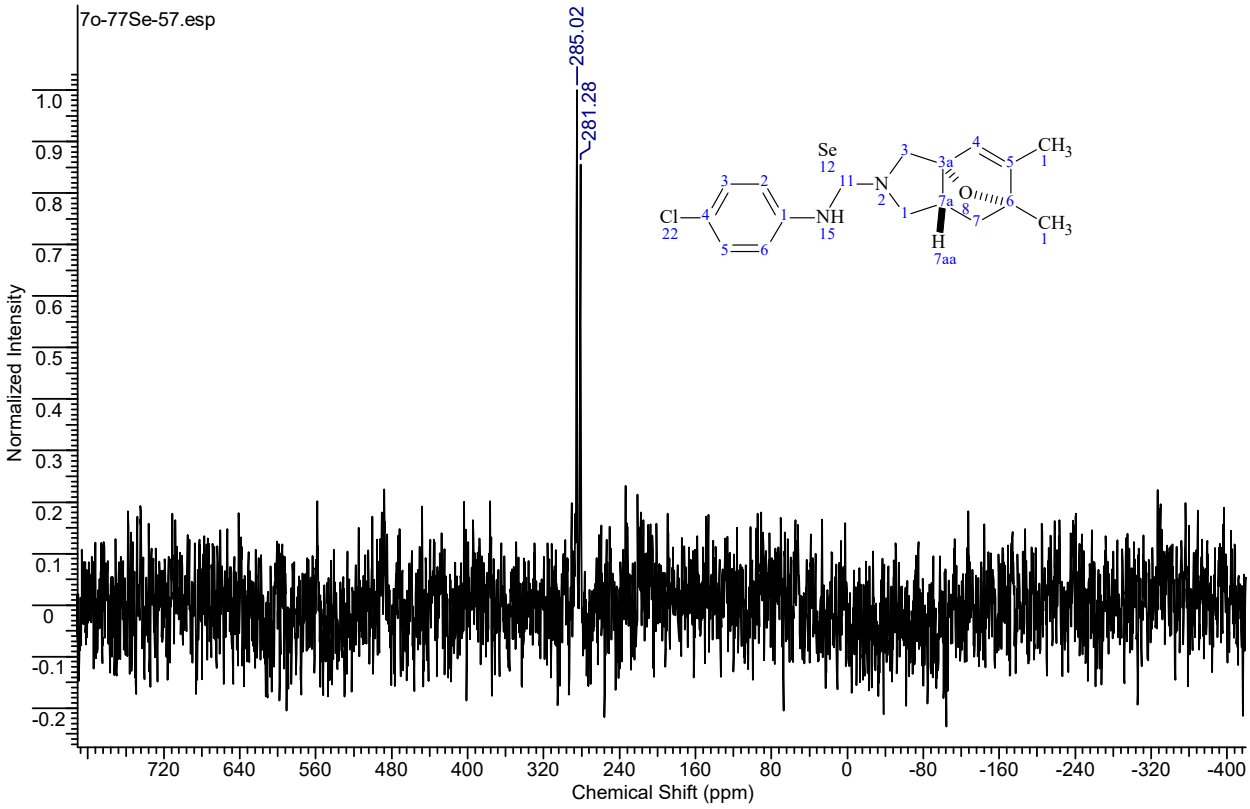
^{1}H NMR (600.2 MHz, DMSO-d_6)



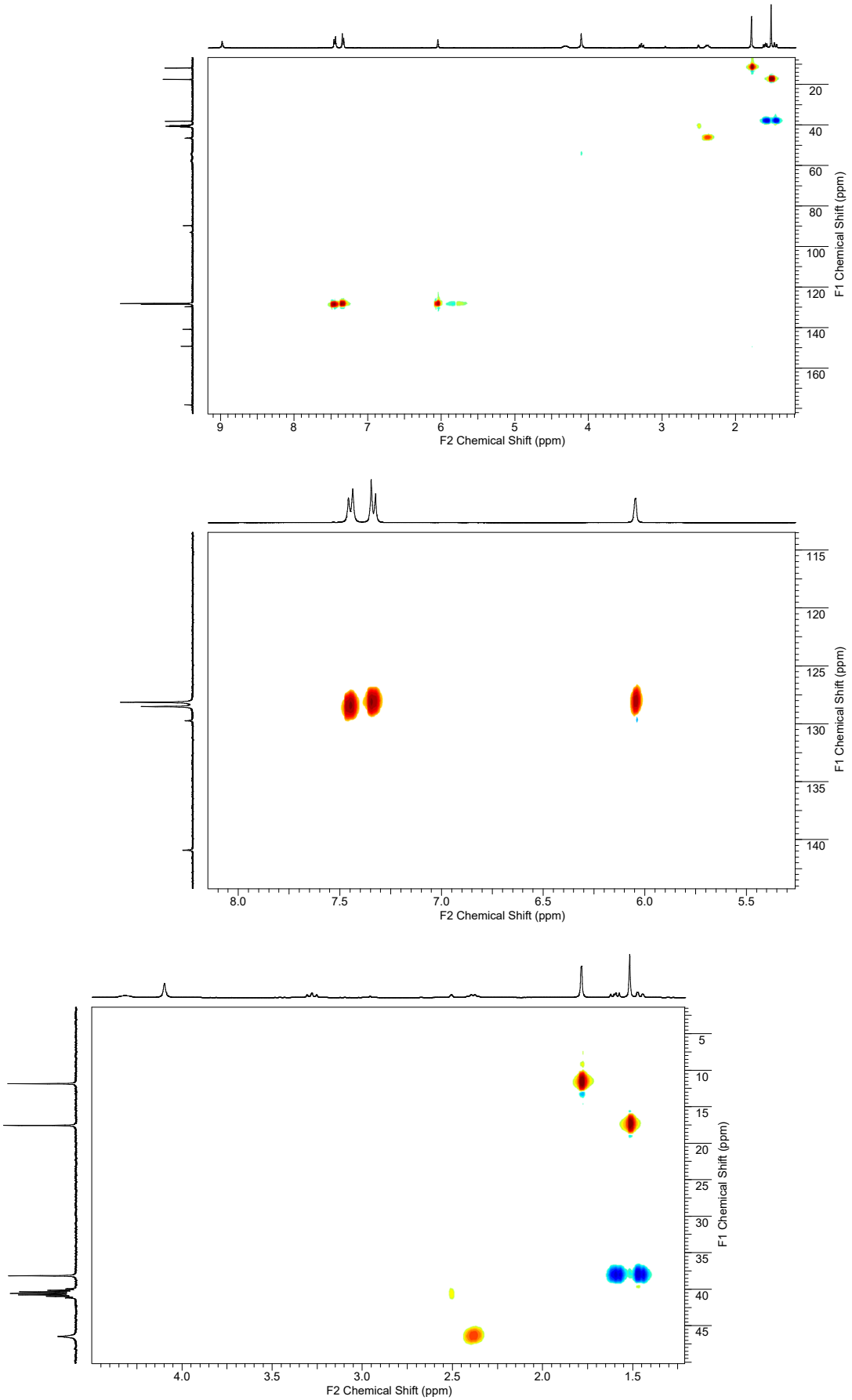
^{13}C NMR (150.9 MHz, DMSO-d_6)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

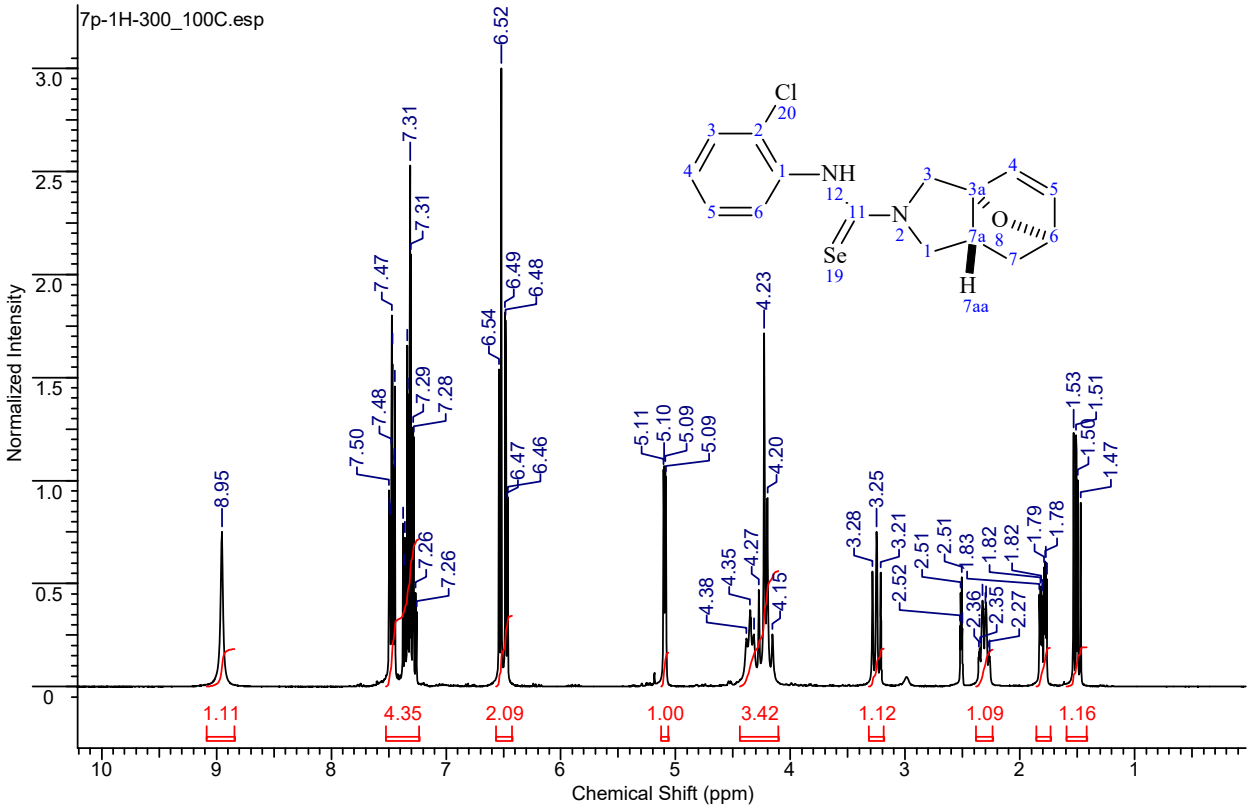


HSQC of **7o** (100 °C)

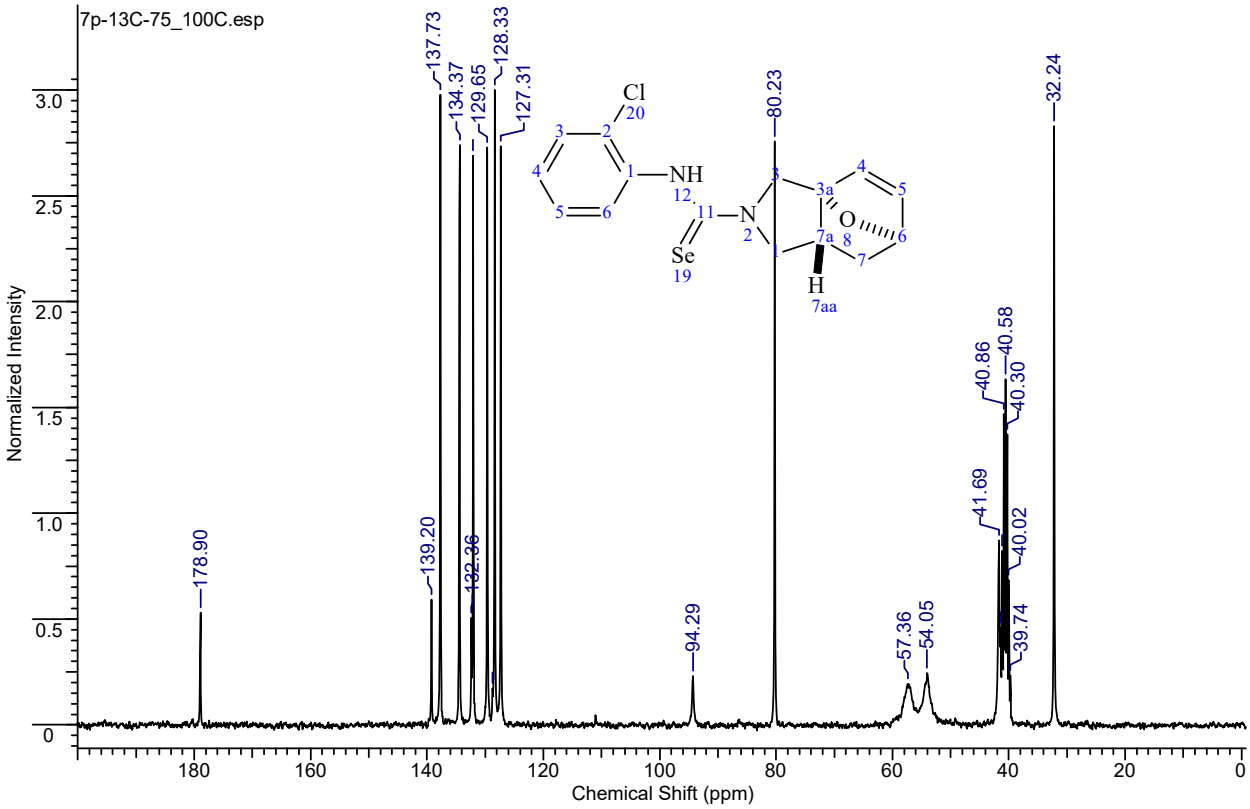


(3a*RS*,6*RS*,7a*RS*)-*N*-(2-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7p).

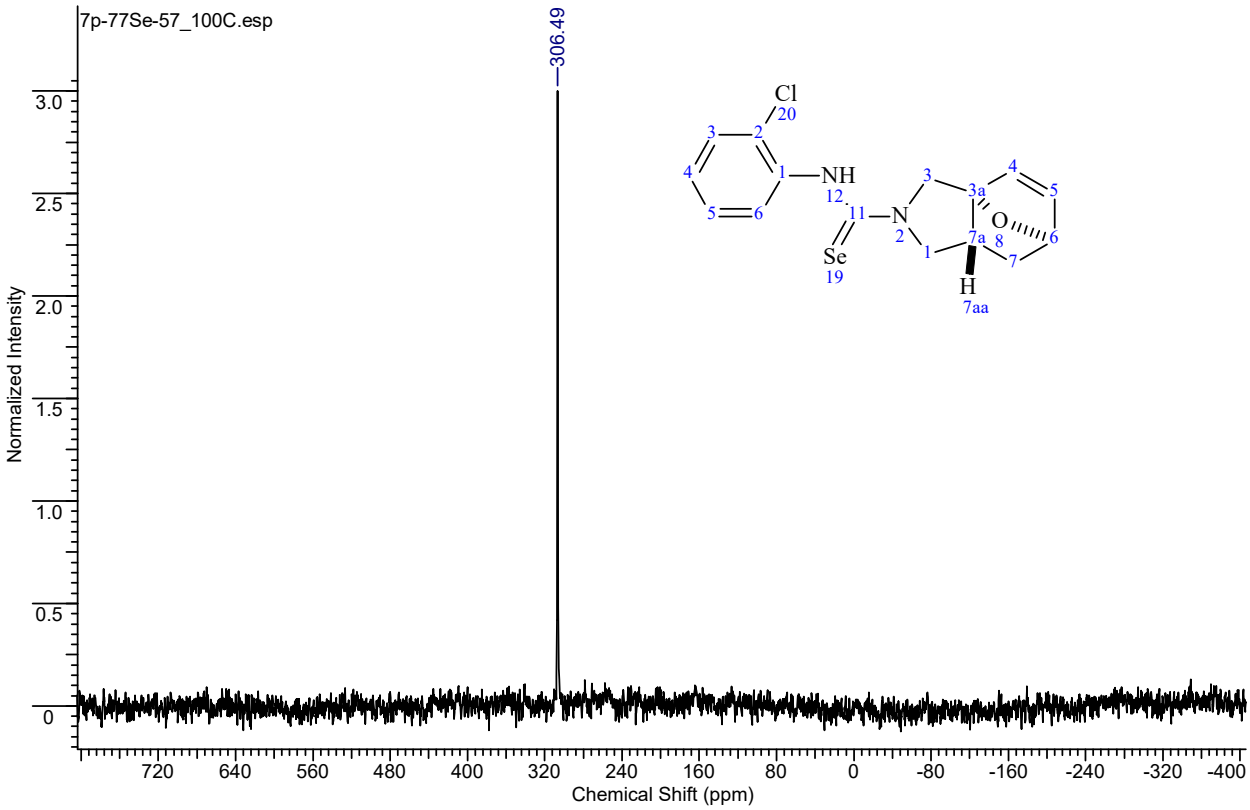
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



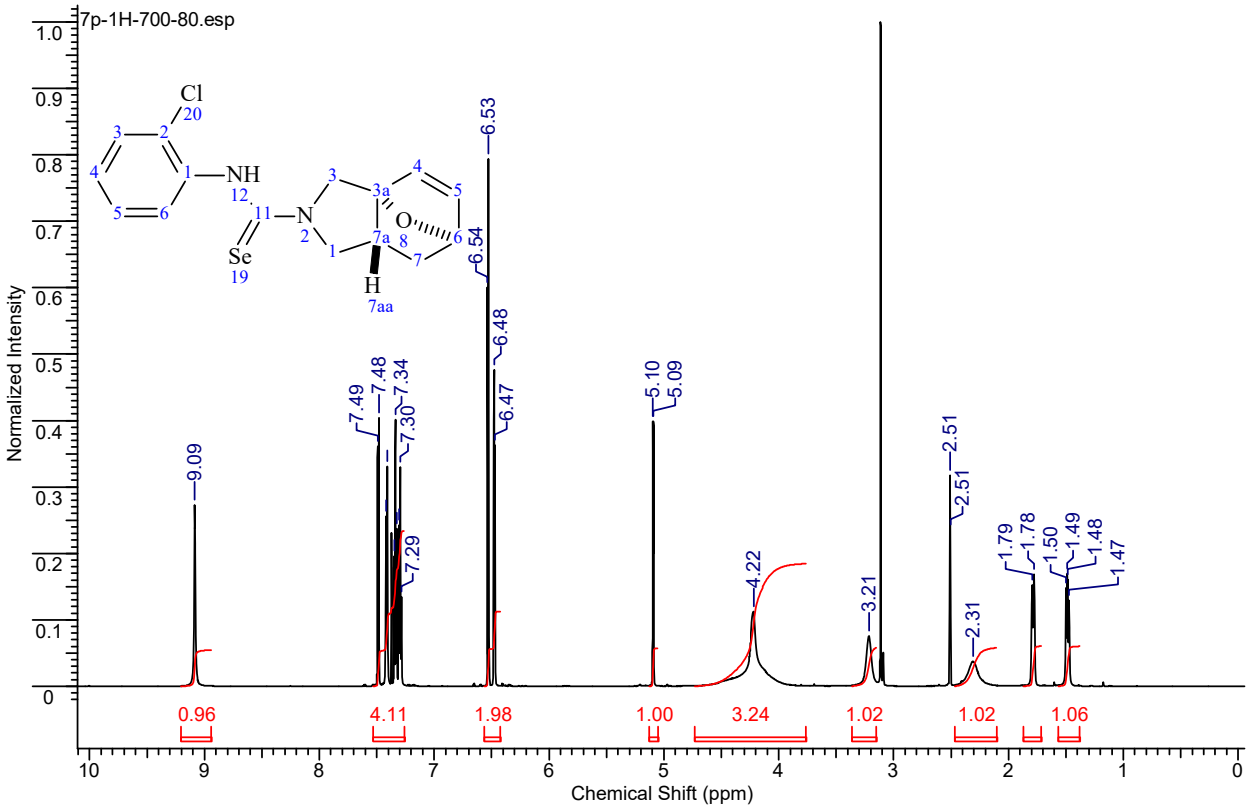
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



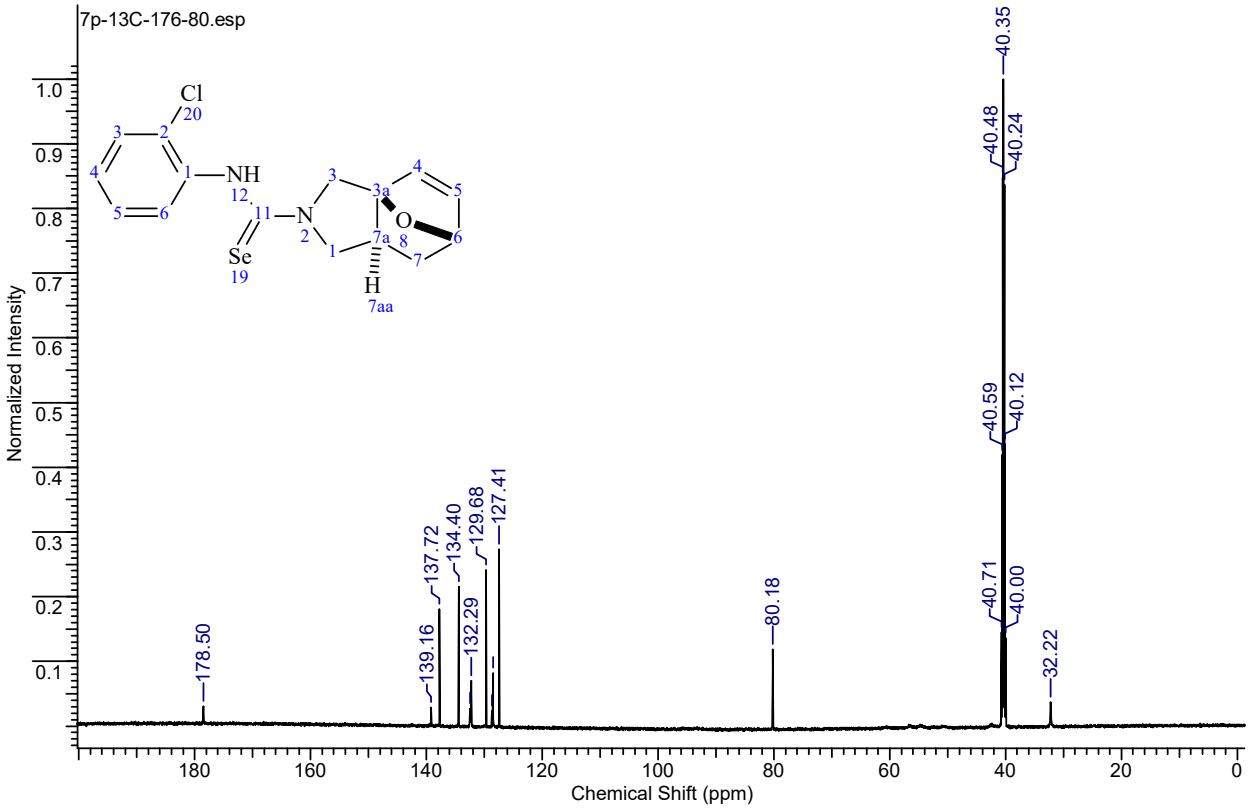
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



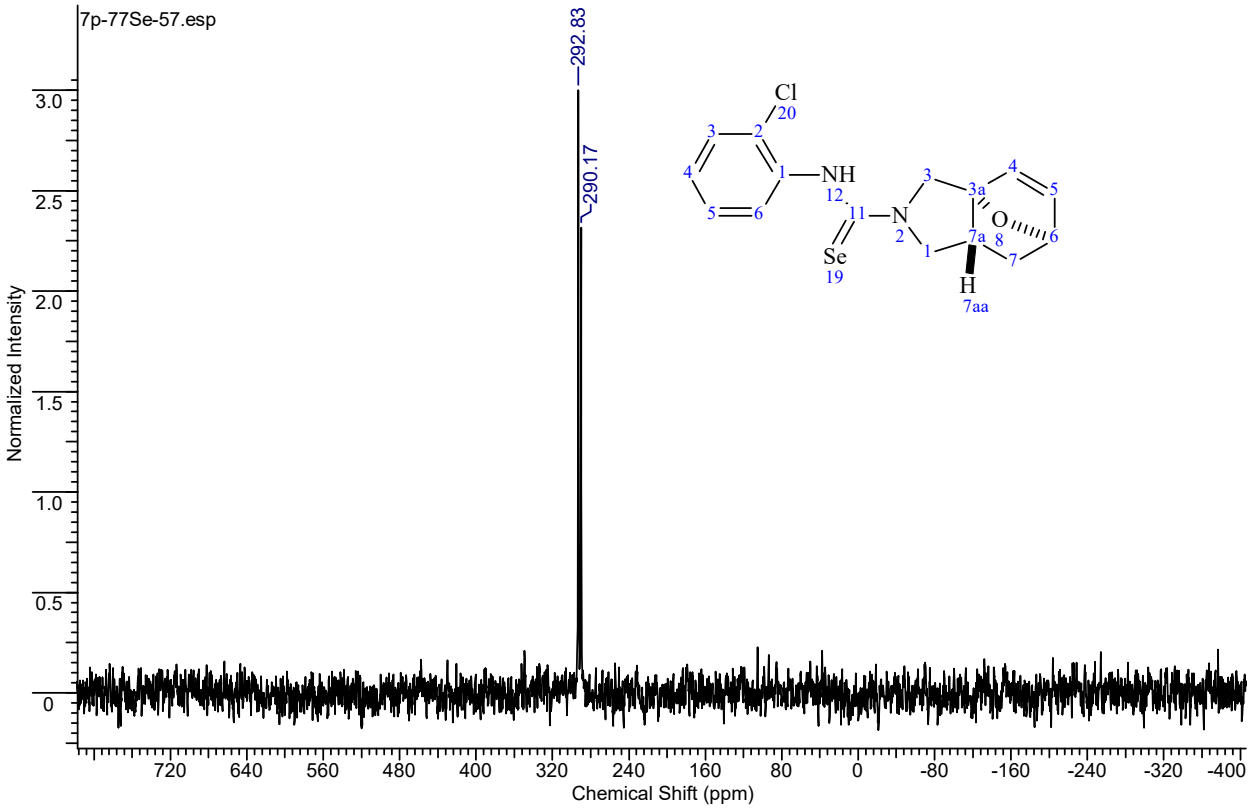
^{1}H NMR (700.2 MHz, DMSO-d_6, 77 °C)



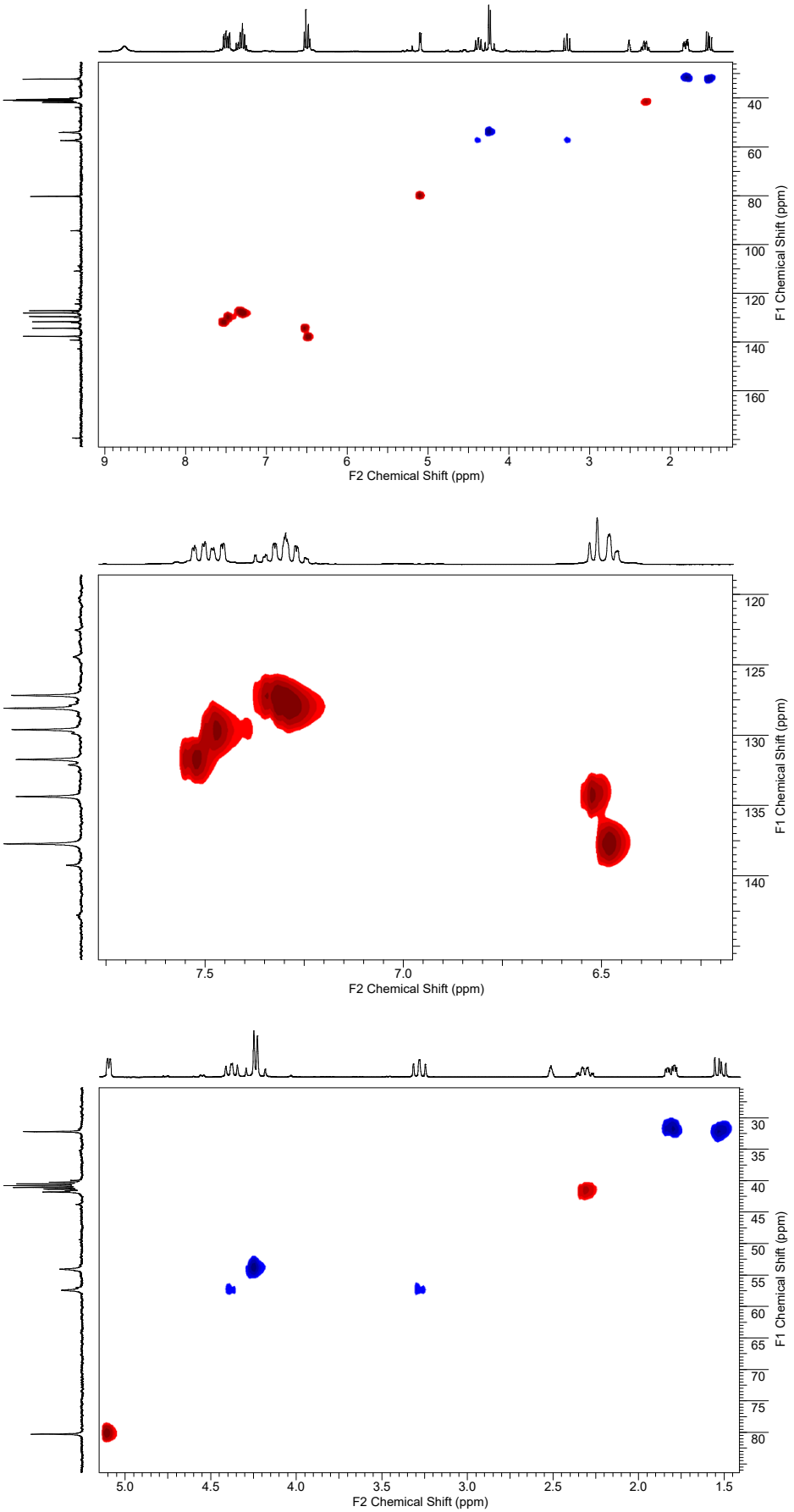
^{13}C NMR (176.1 MHz, DMSO-d_6, 77 °C)



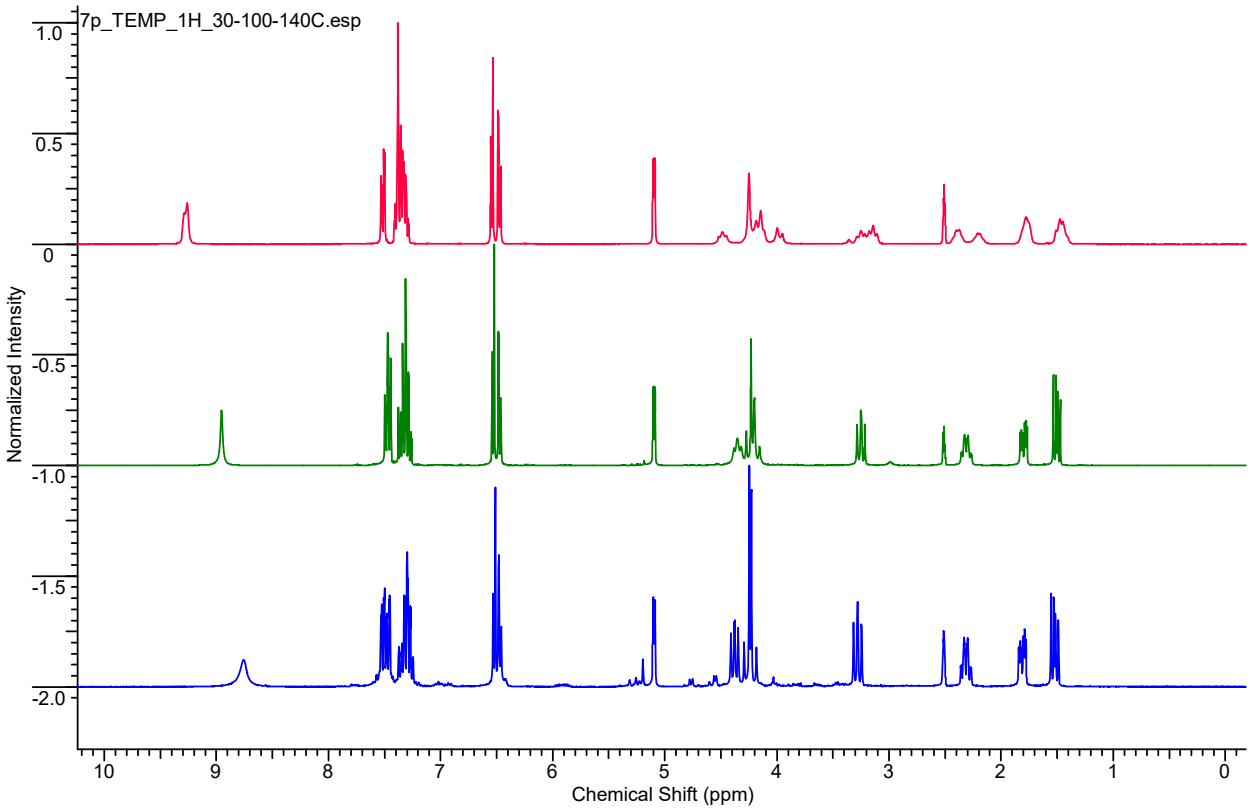
^{77}Se NMR (57.2 MHz, DMSO-d_6)



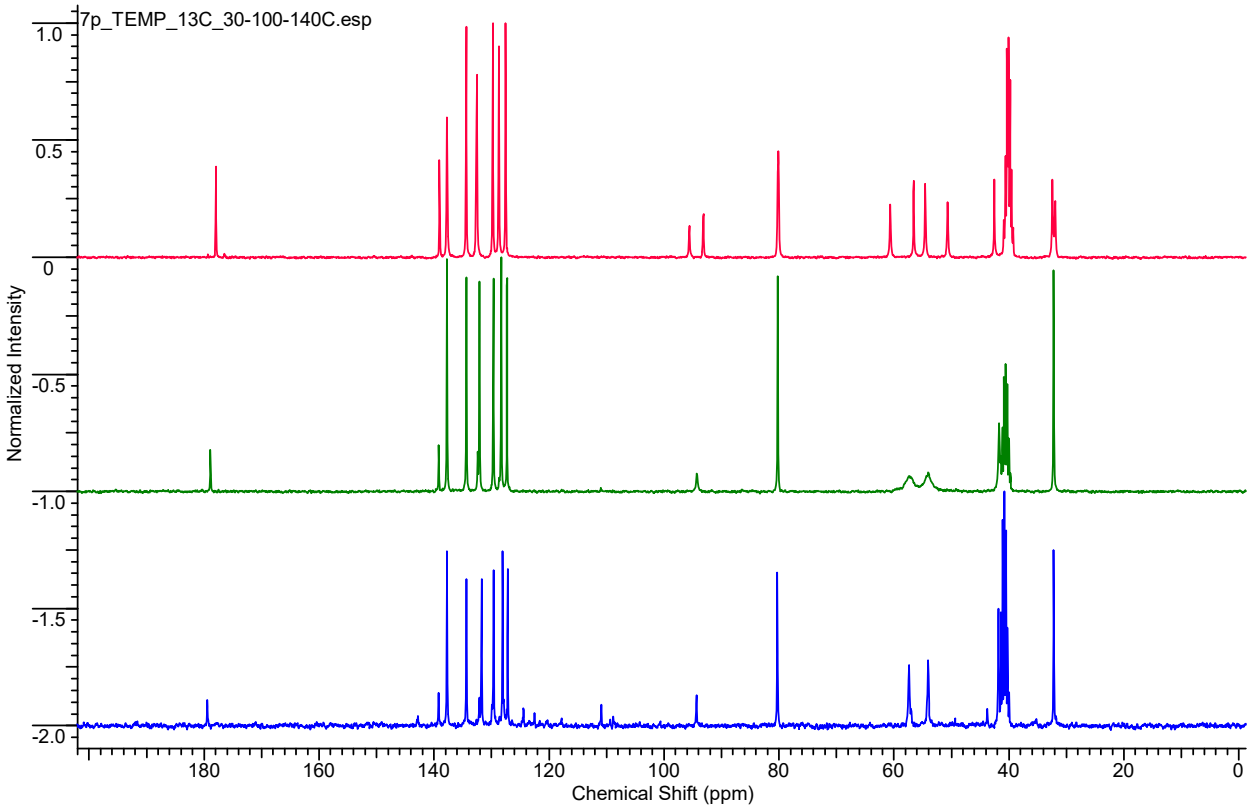
HSQC of **7p** (140 °C)



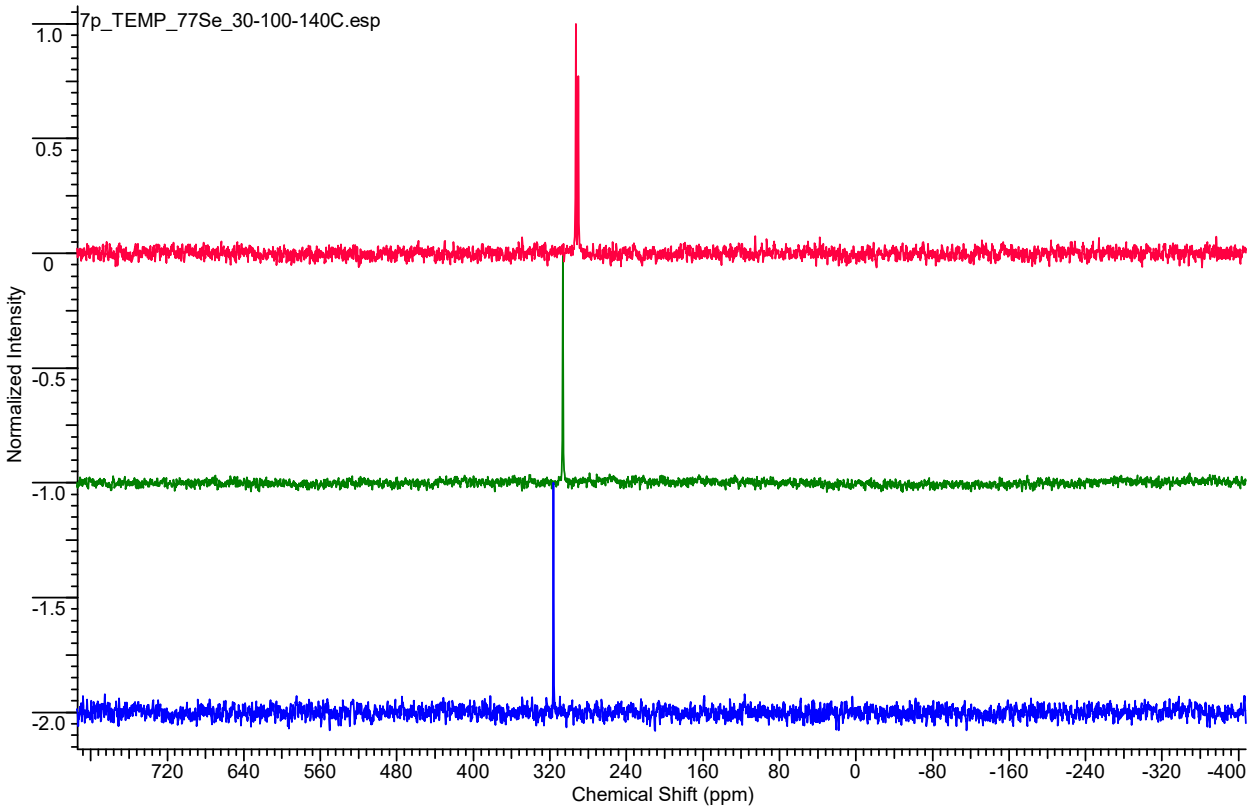
^{1}H NMR of **7p** (30-100-140 °C)



^{13}C NMR of **7p** (30-100-140 °C)

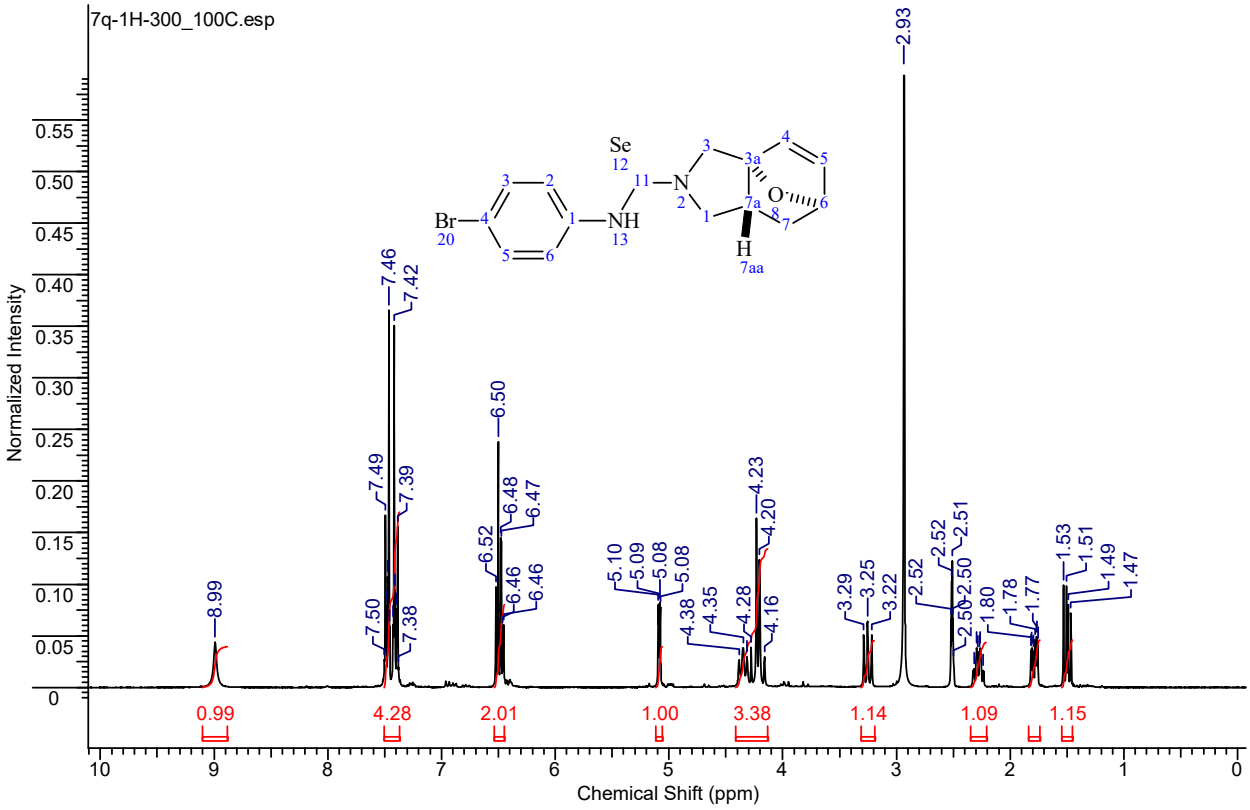


^{77}Se NMR of **7p** (30-100-140 °C)

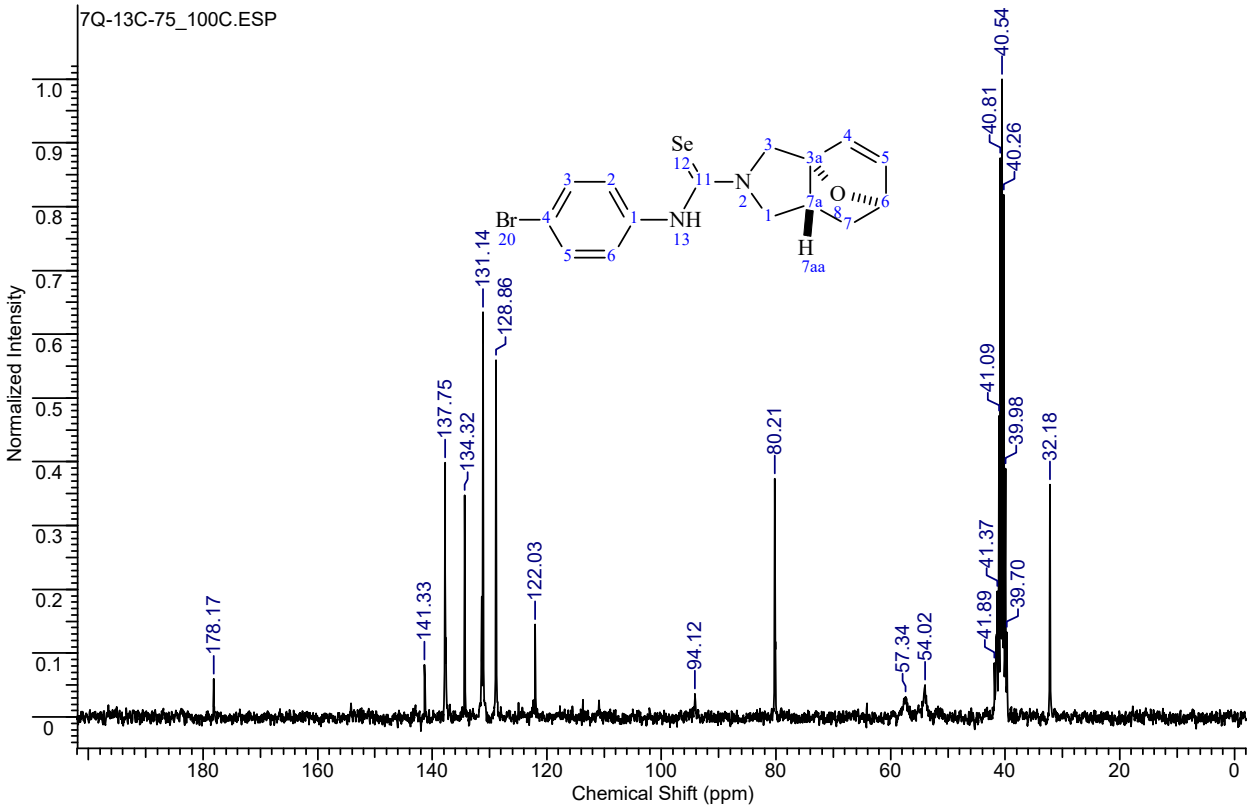


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Bromophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7q).

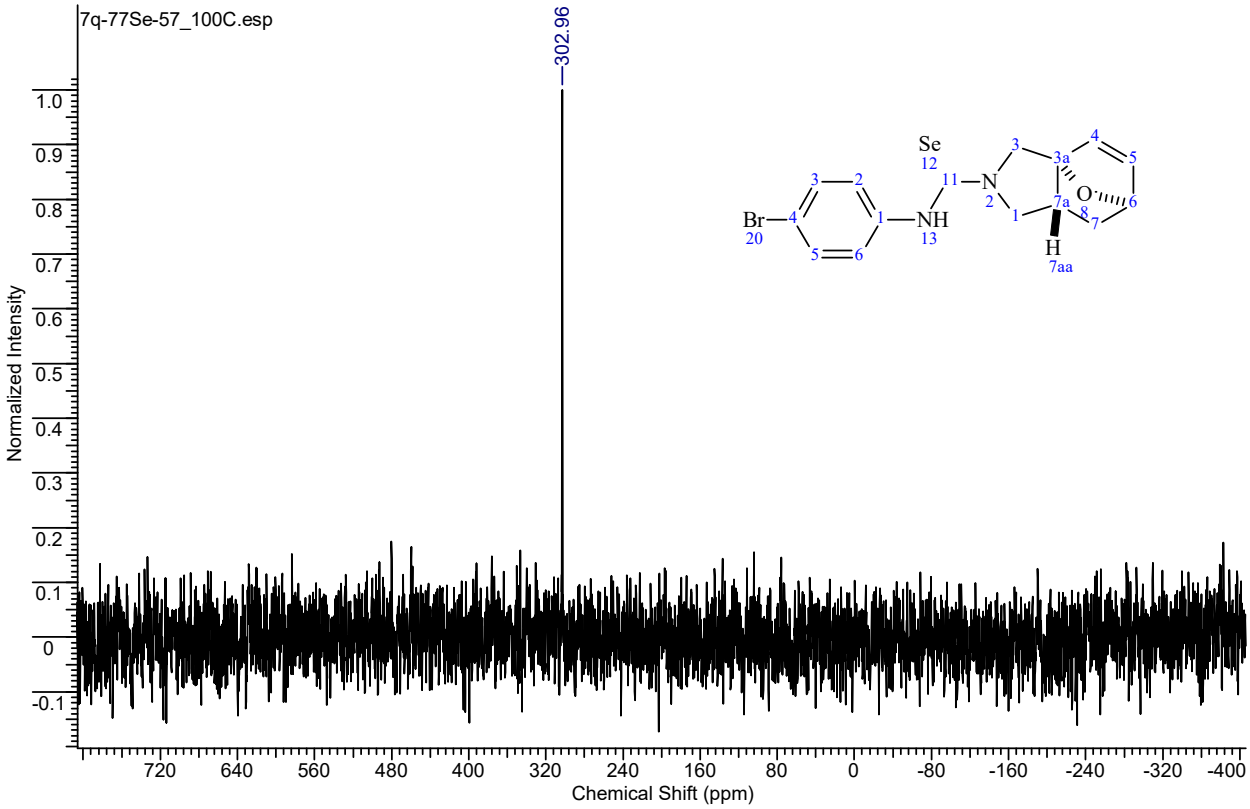
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



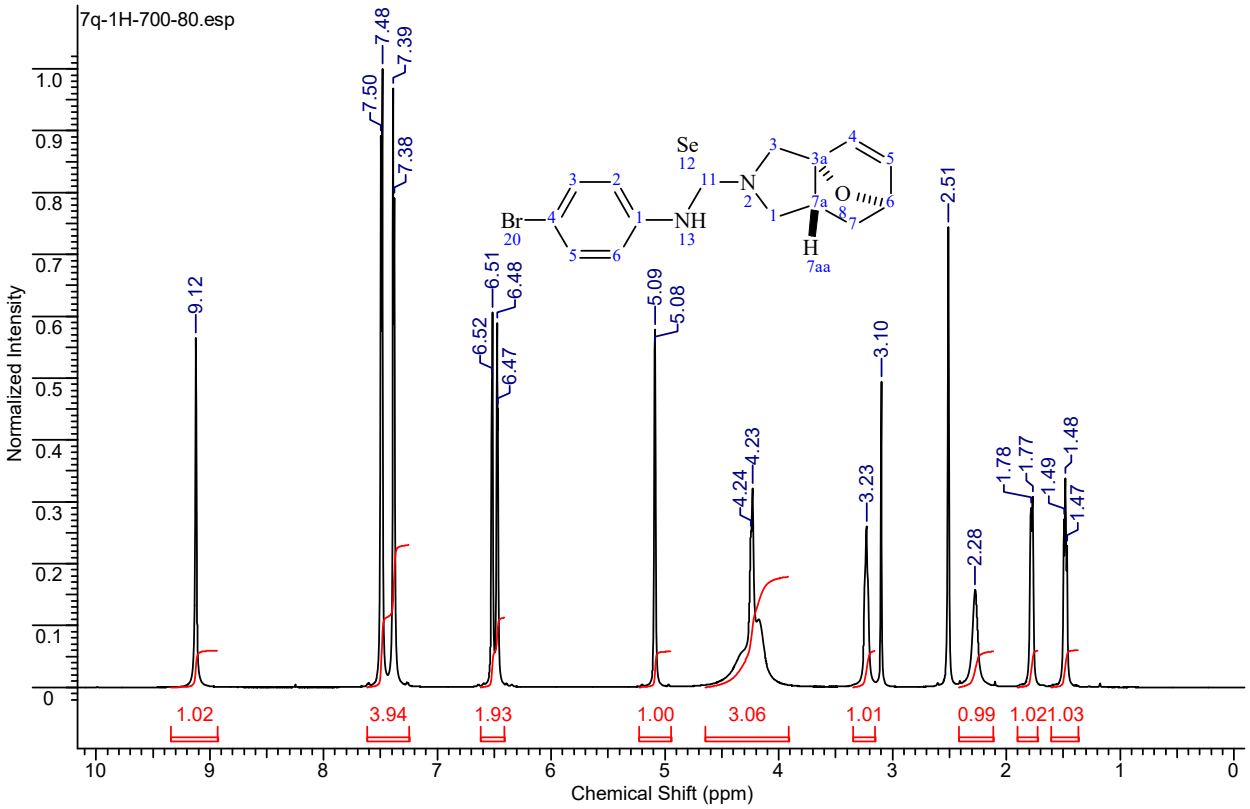
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



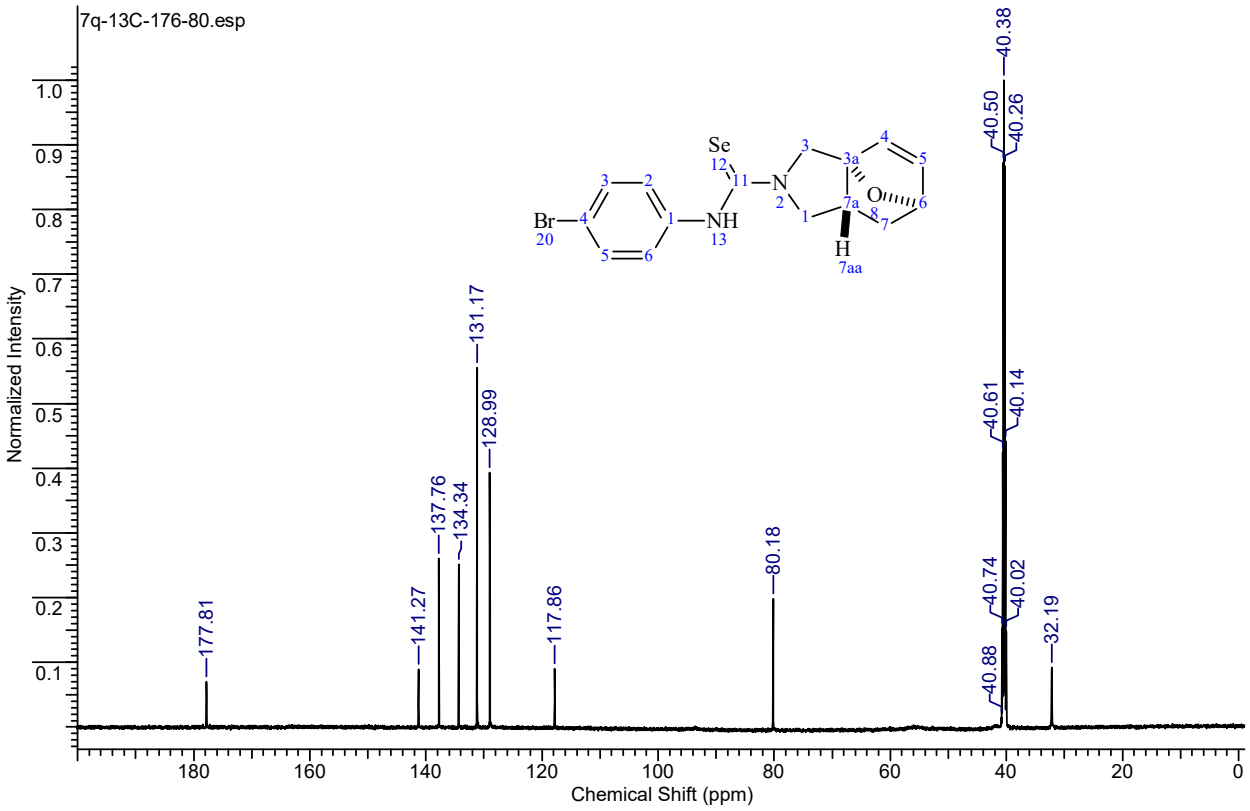
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



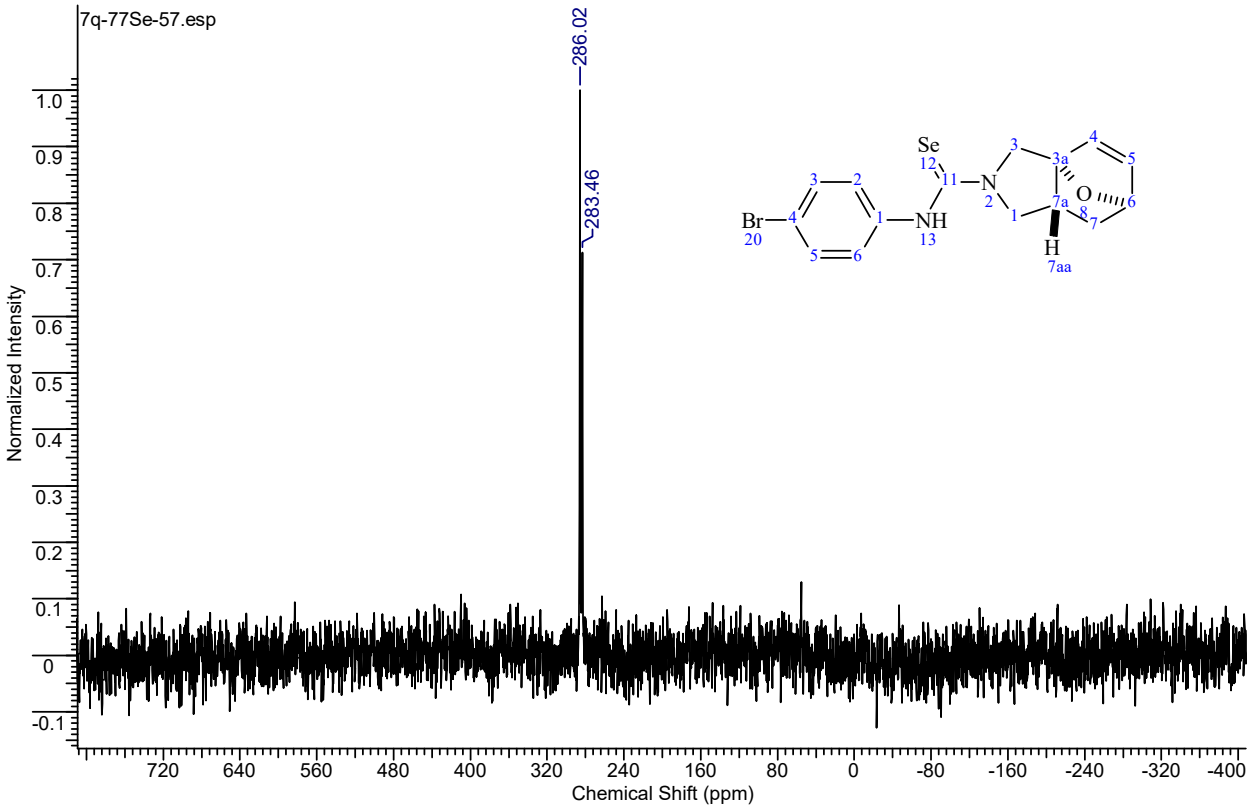
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



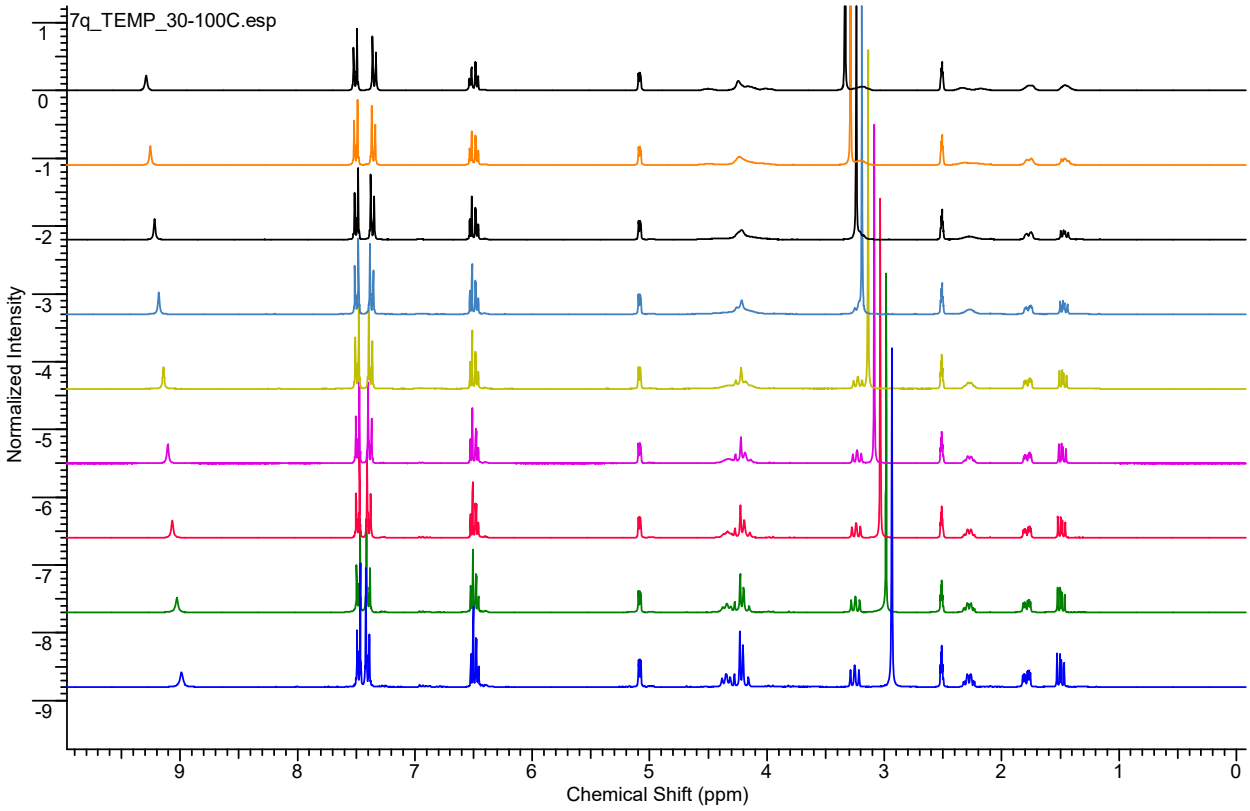
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

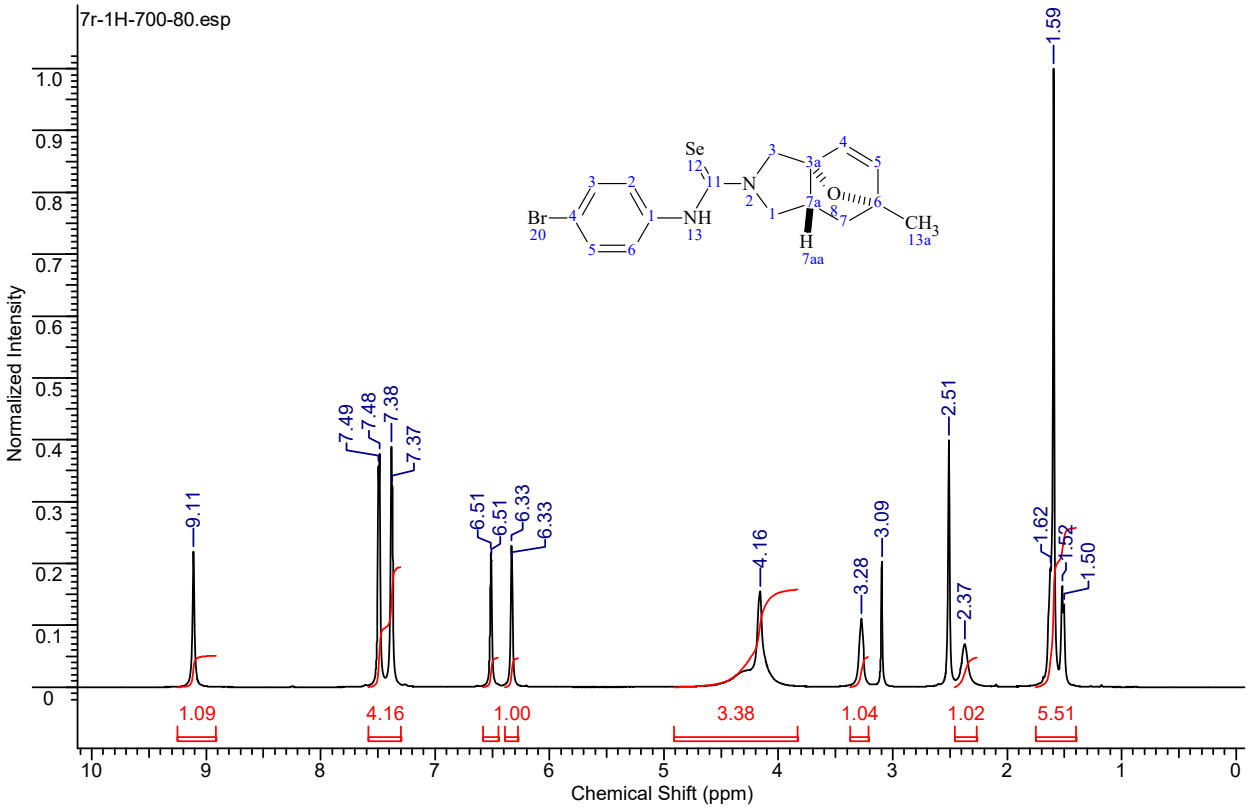


^{1}H NMR of **7q (30-100 °C)**

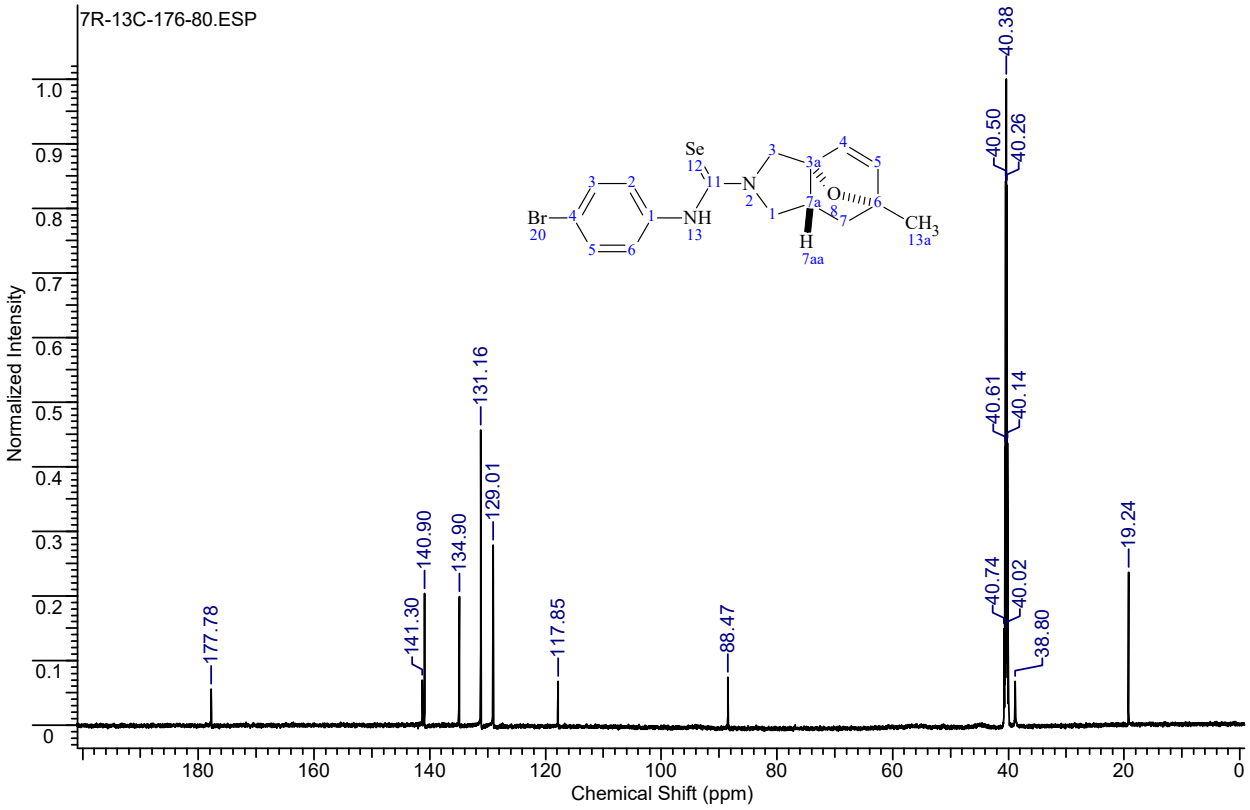


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Bromophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7r).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

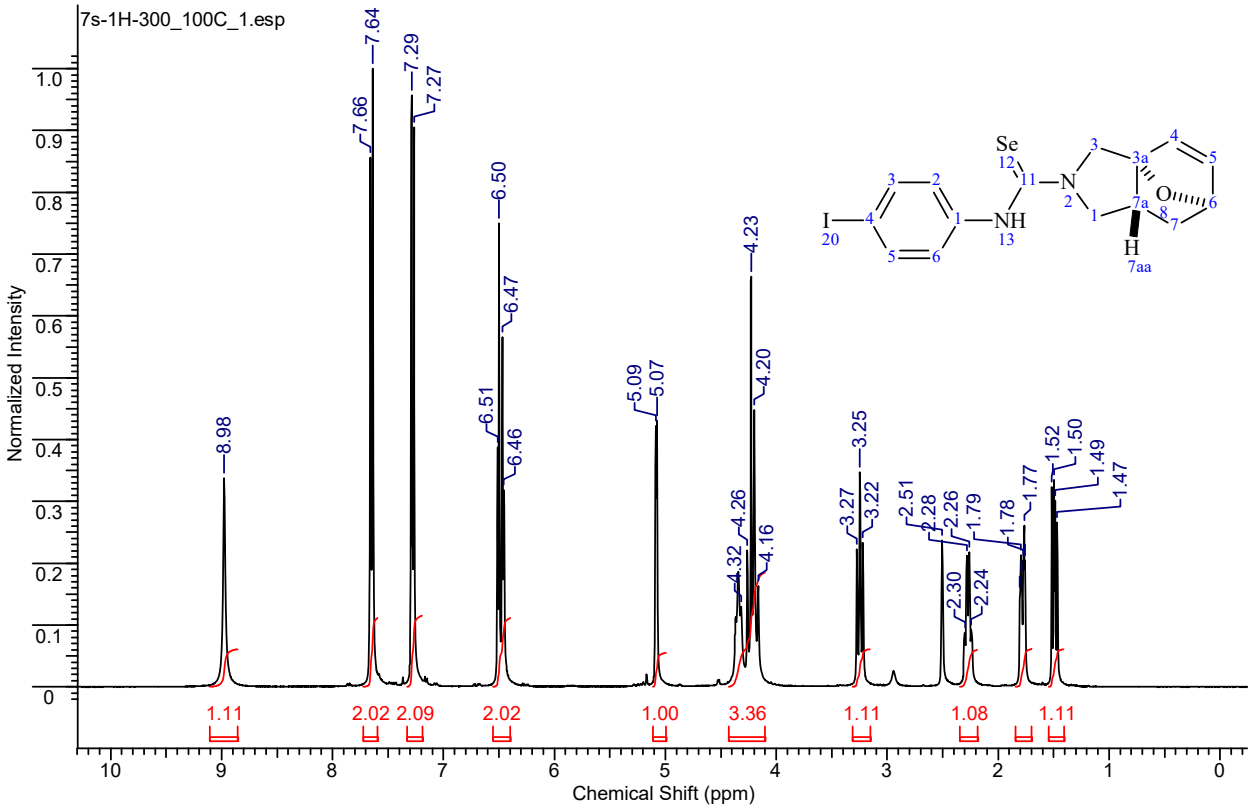


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

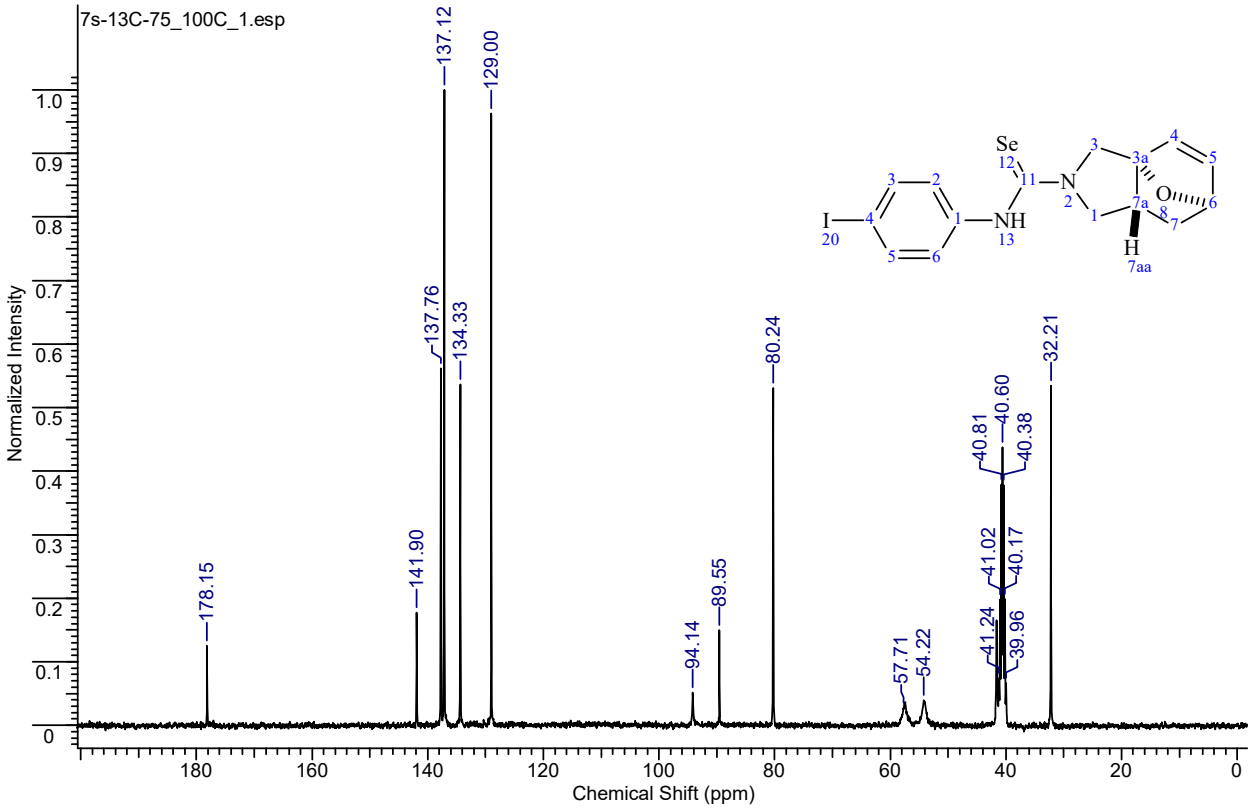


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Iodophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7s).

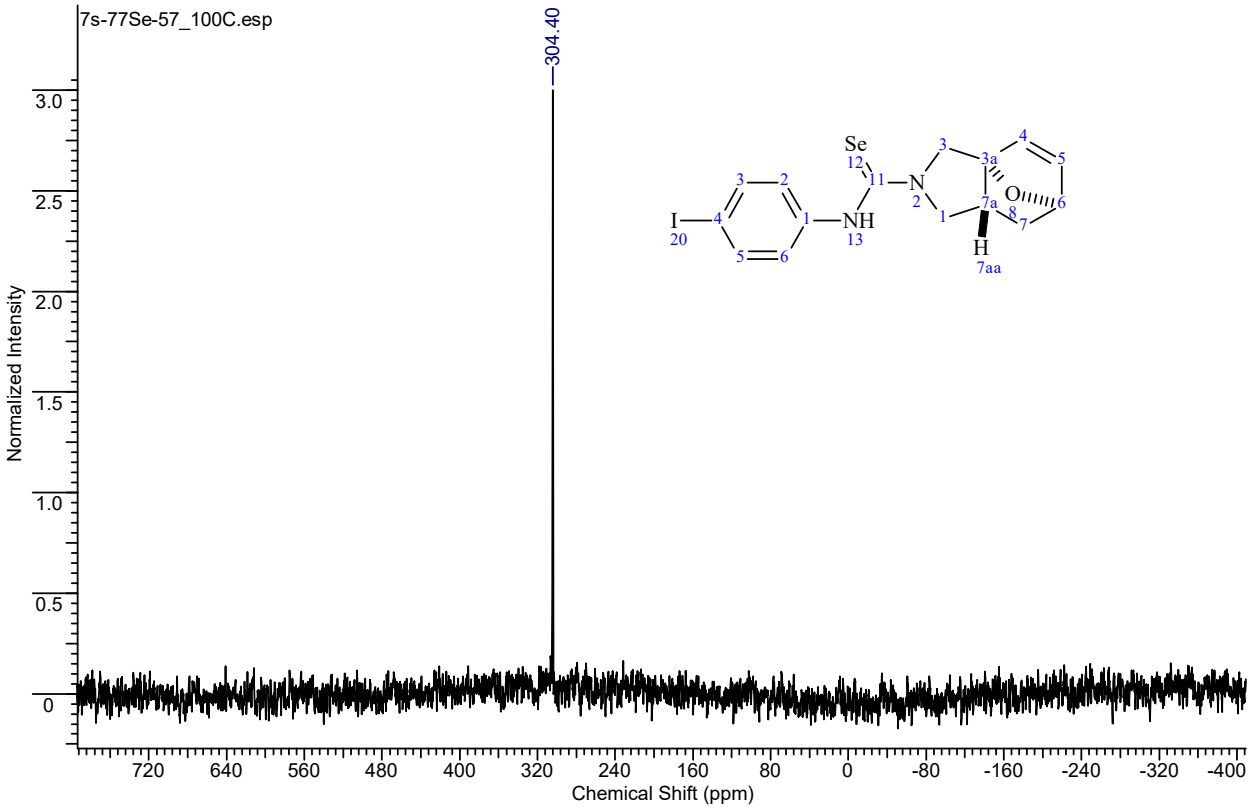
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



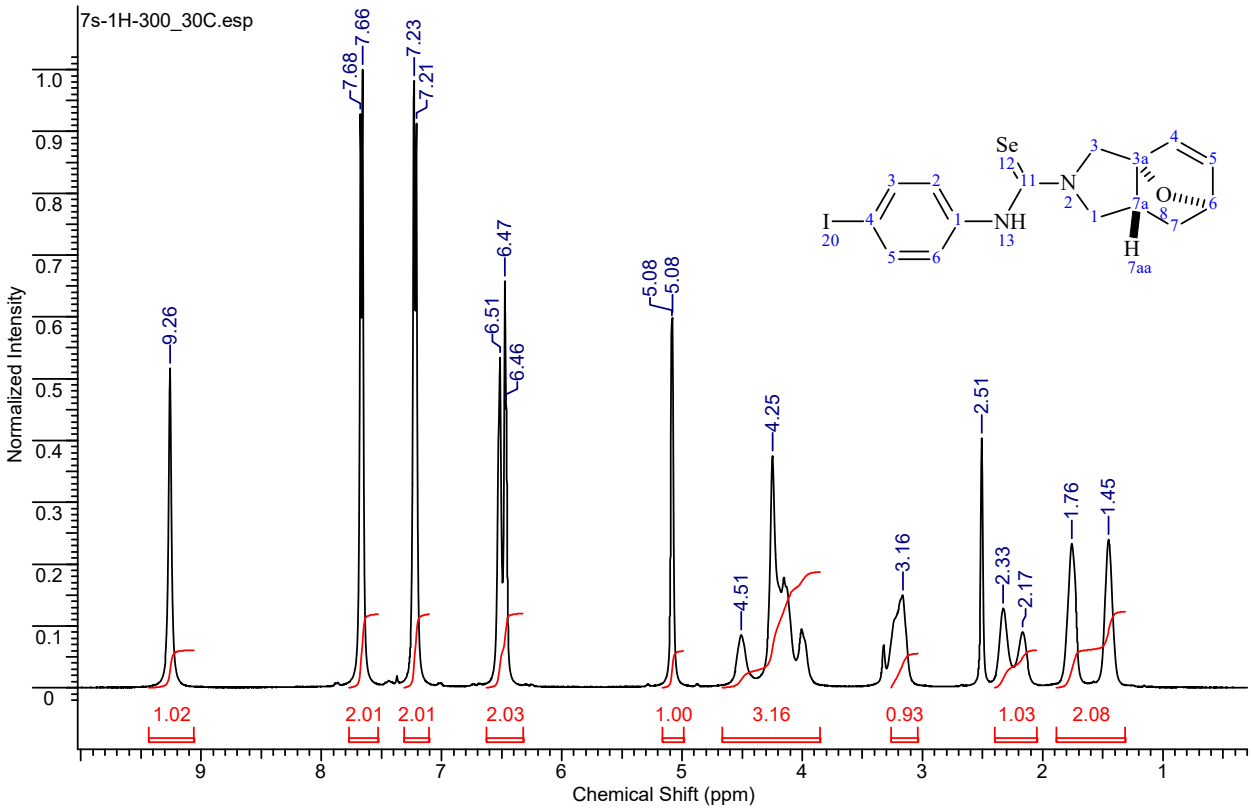
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



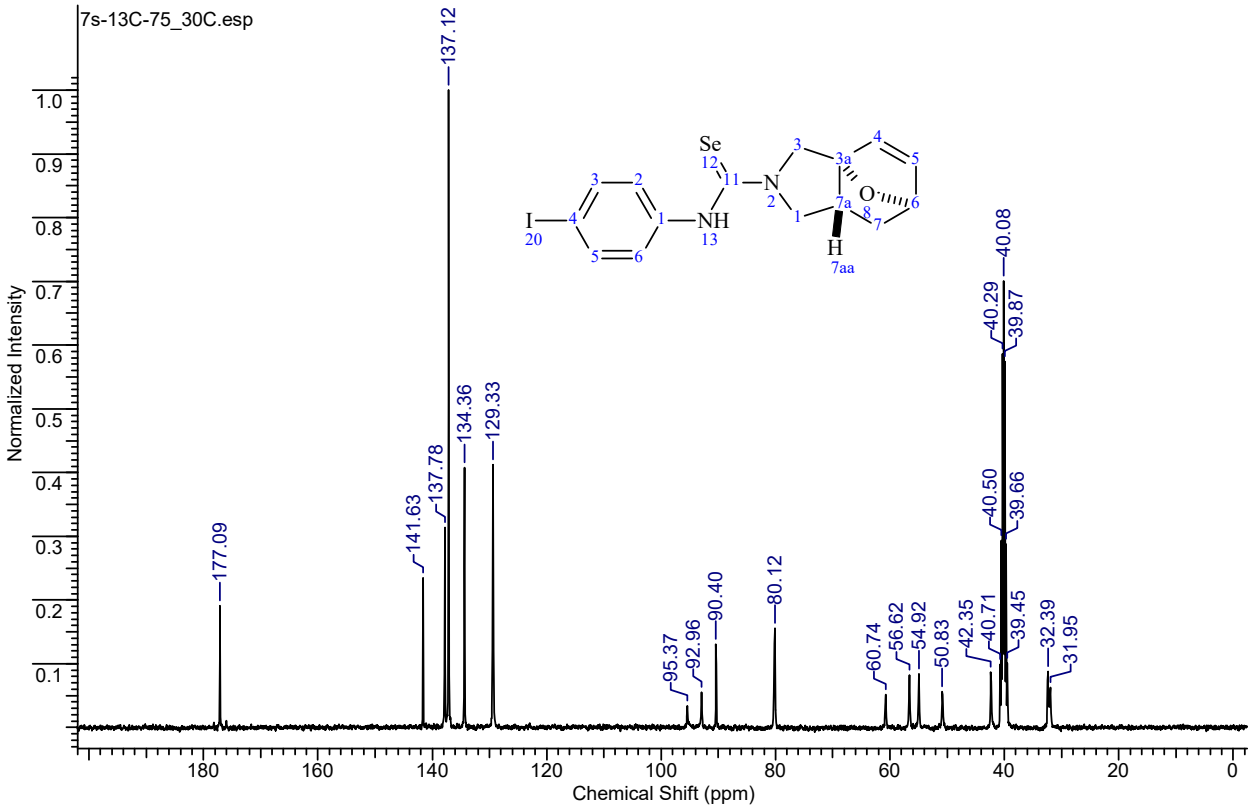
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100 °C)



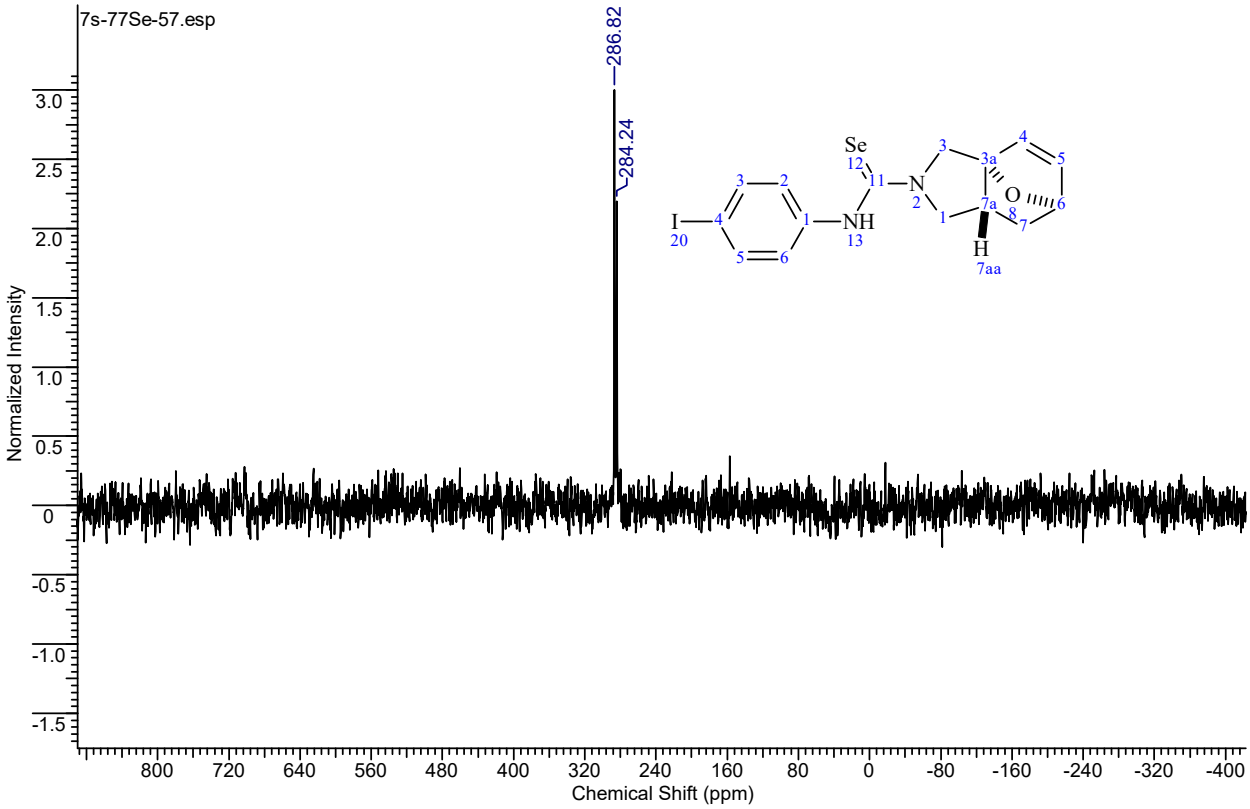
^{1}H NMR (300.1 MHz, DMSO-d_6, 30 °C)



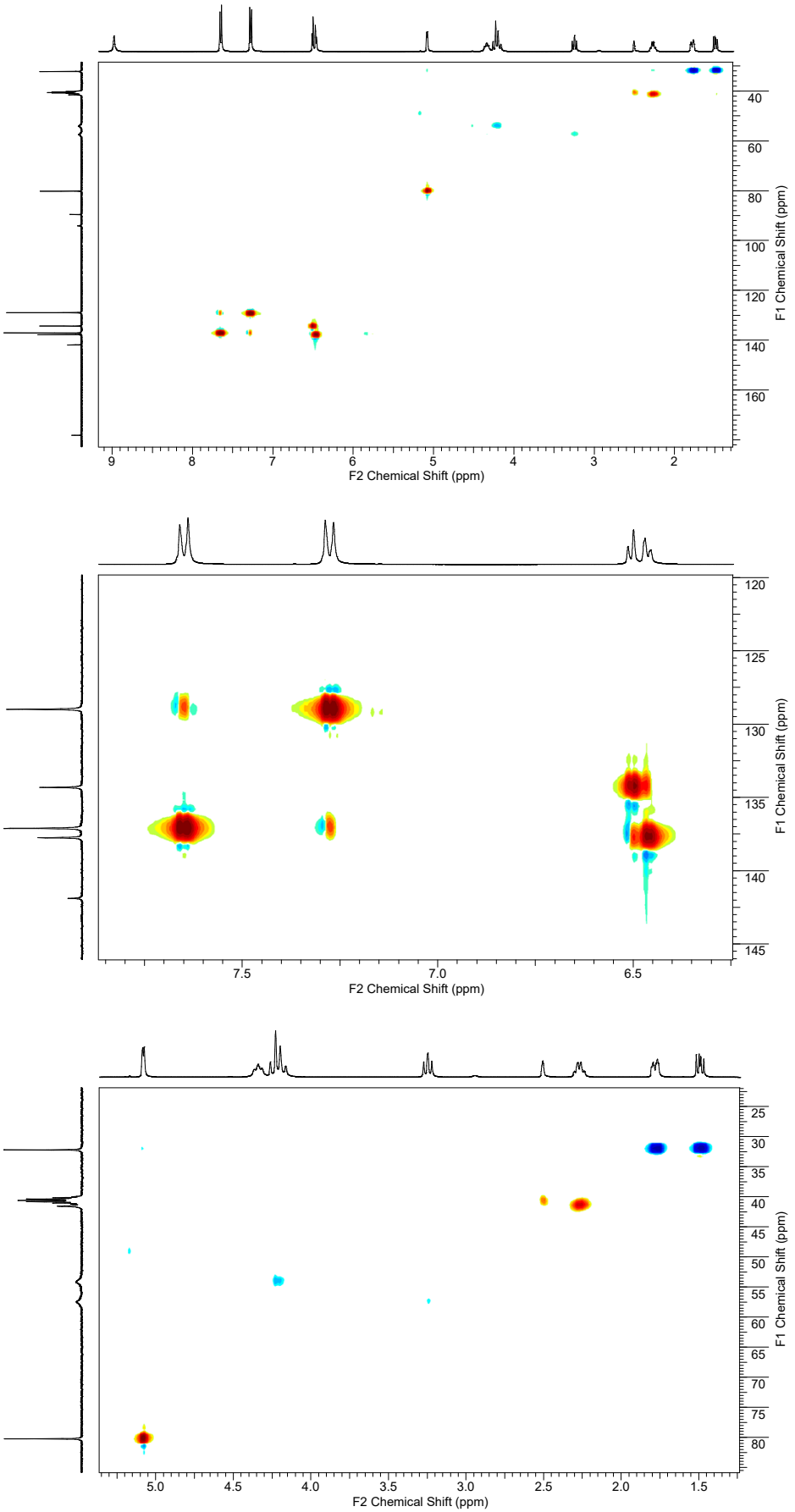
^{13}C NMR (75.5 MHz, DMSO-d_6, 30 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

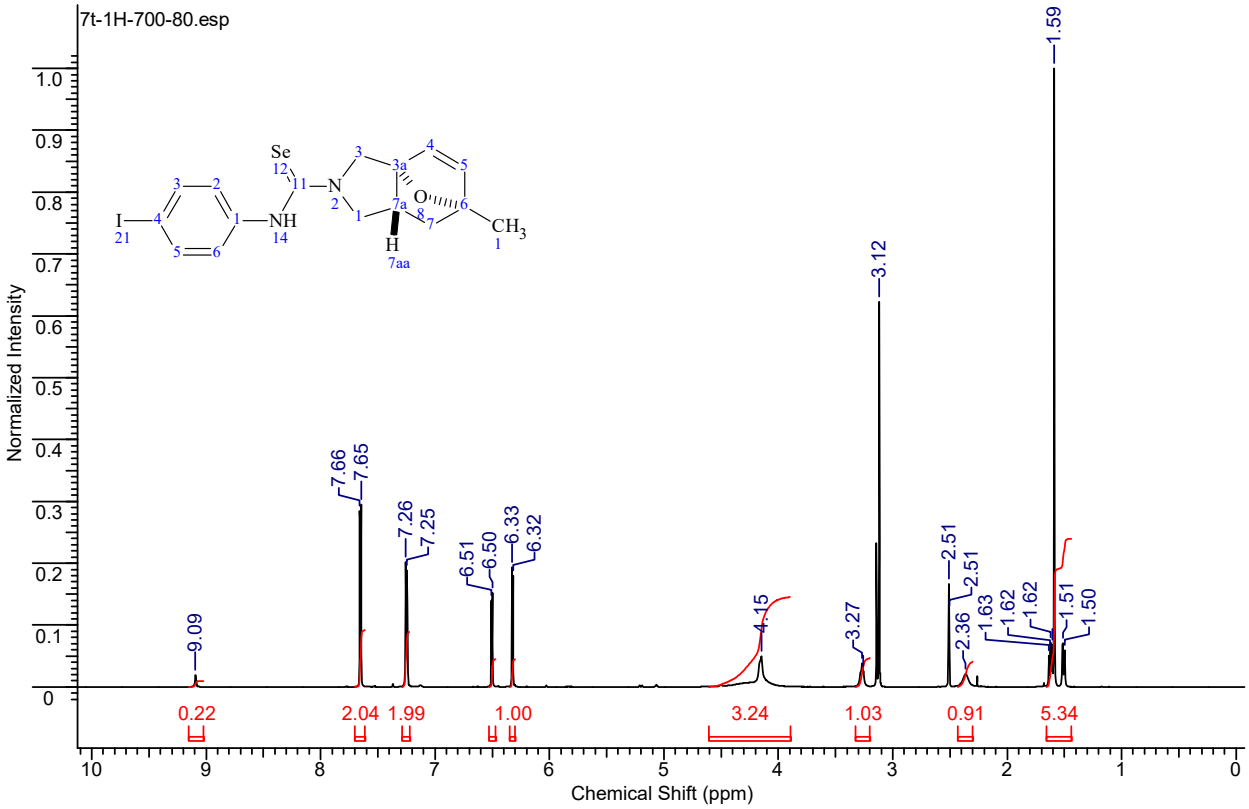


HSQC of **7s** (100 °C)

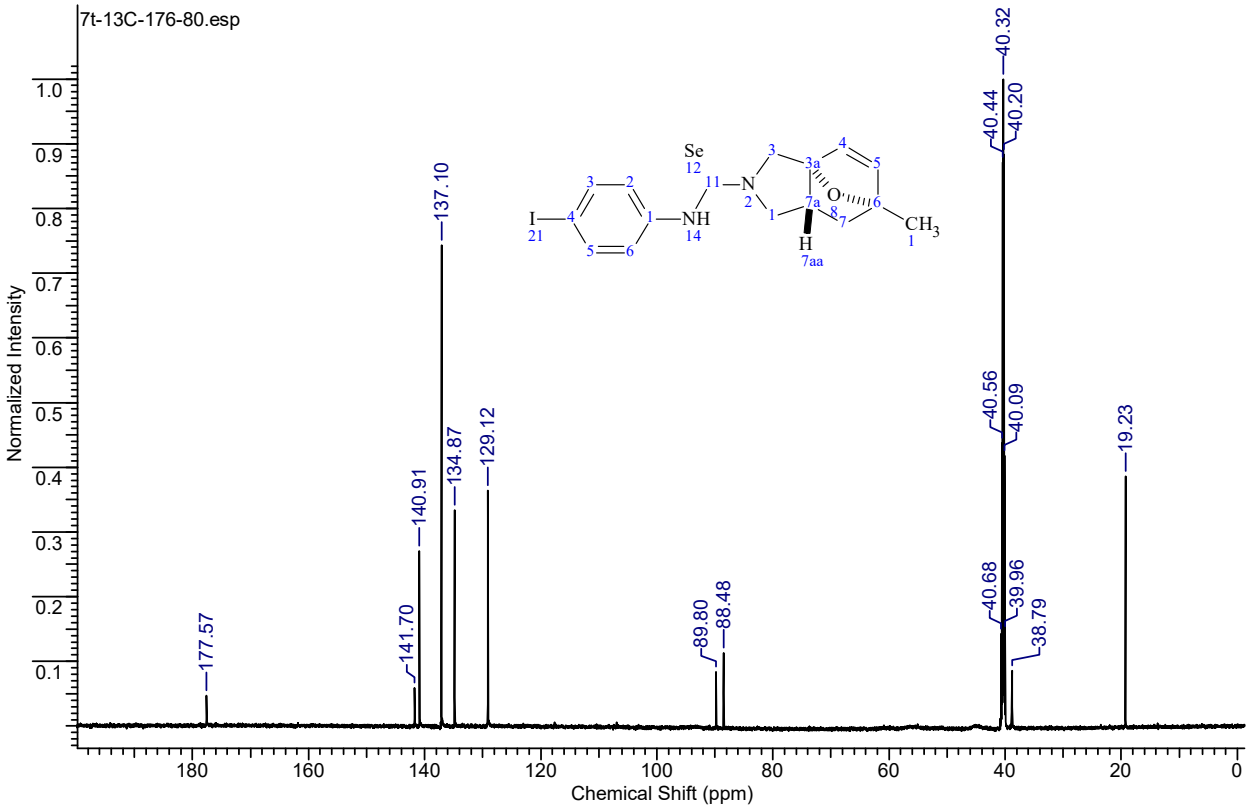


(3a*RS*,6*RS*,7a*RS*)-*N*-(4-Iodophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7t).

^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)

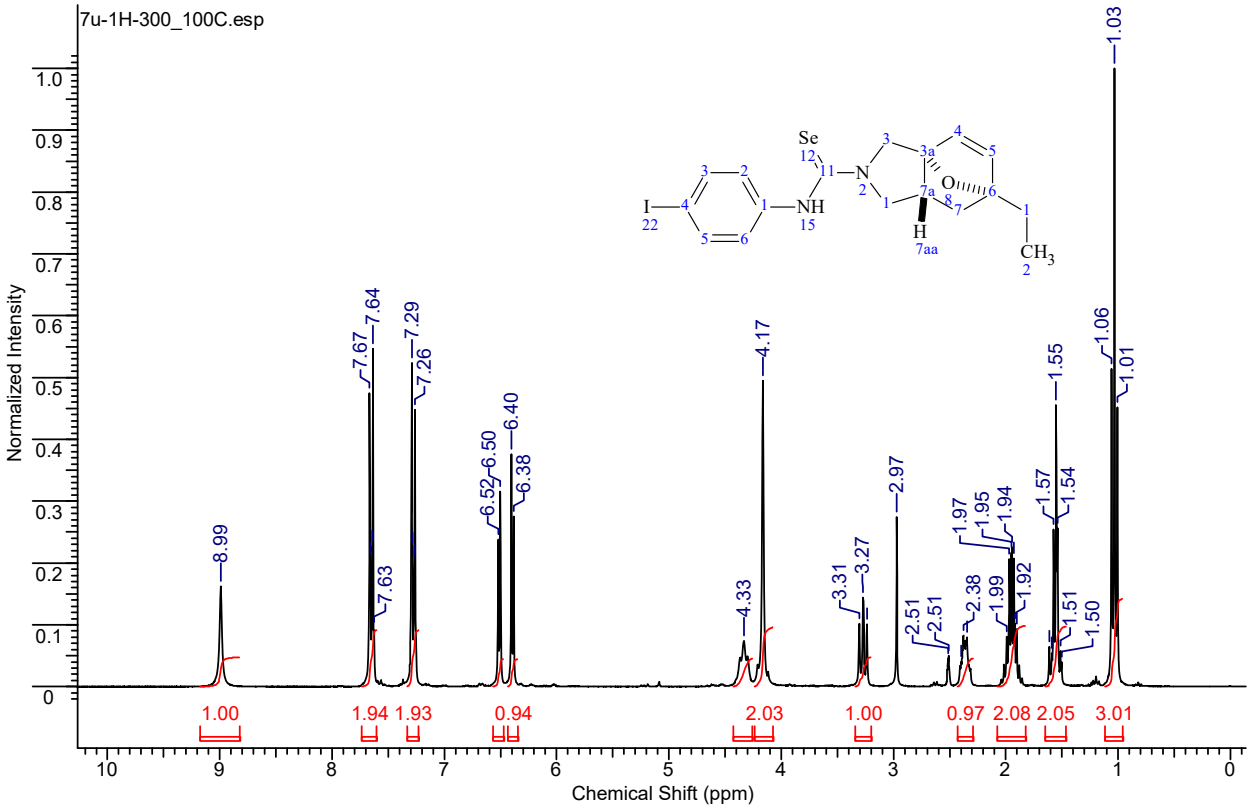


^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)

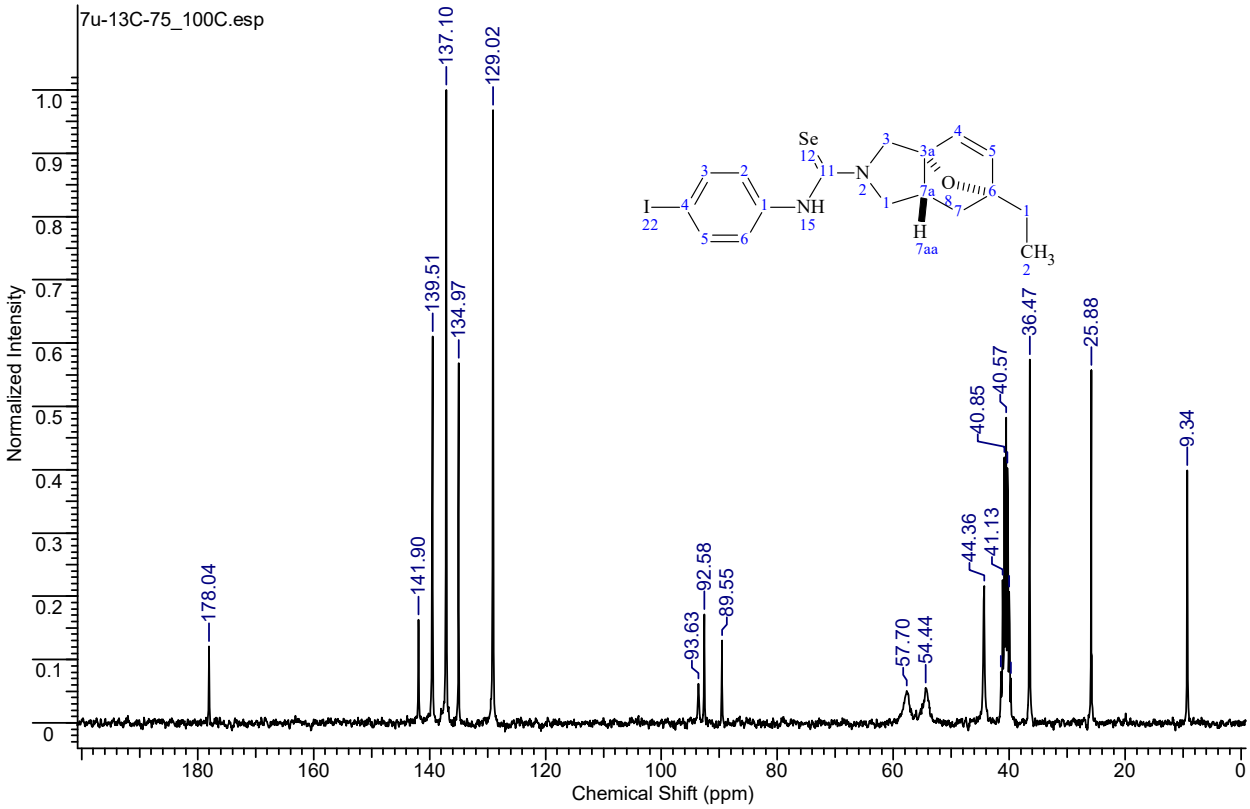


(3a*RS*,6*RS*,7a*RS*)-6-Ethyl-*N*-(4-iodophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7u).

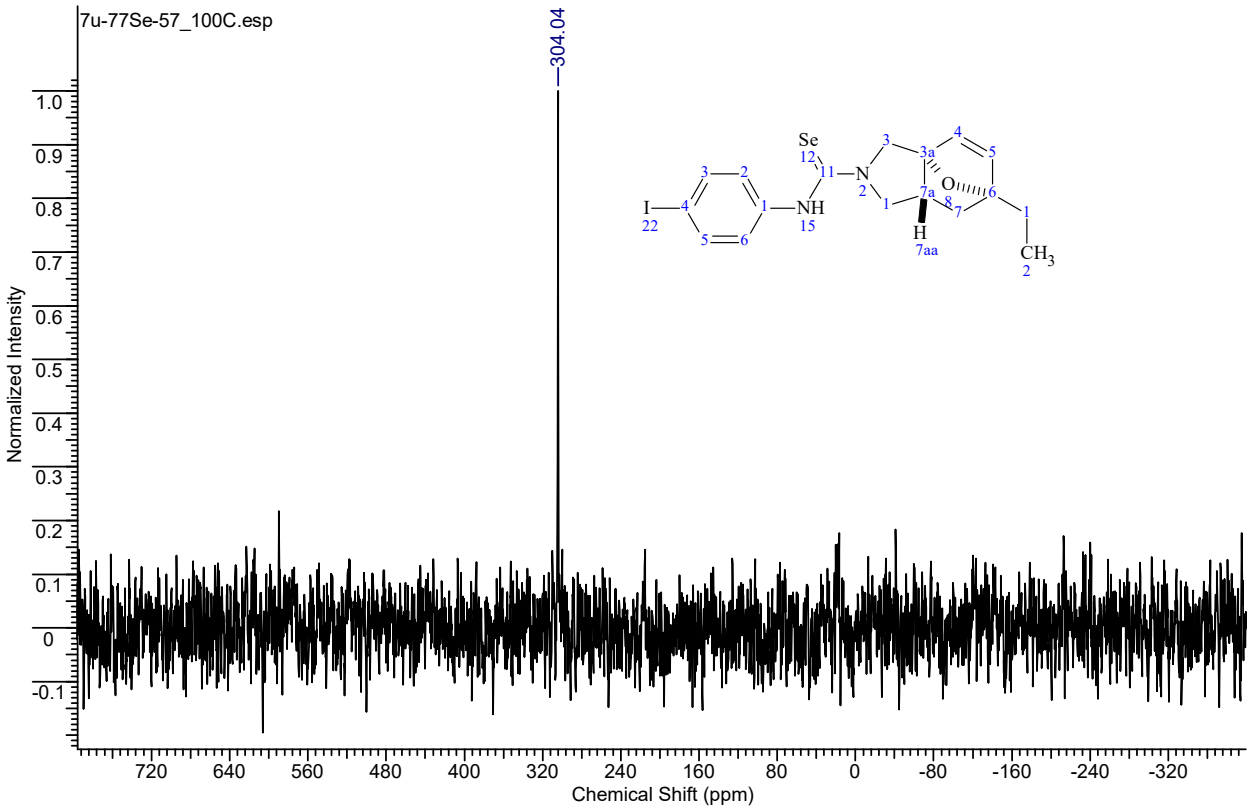
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



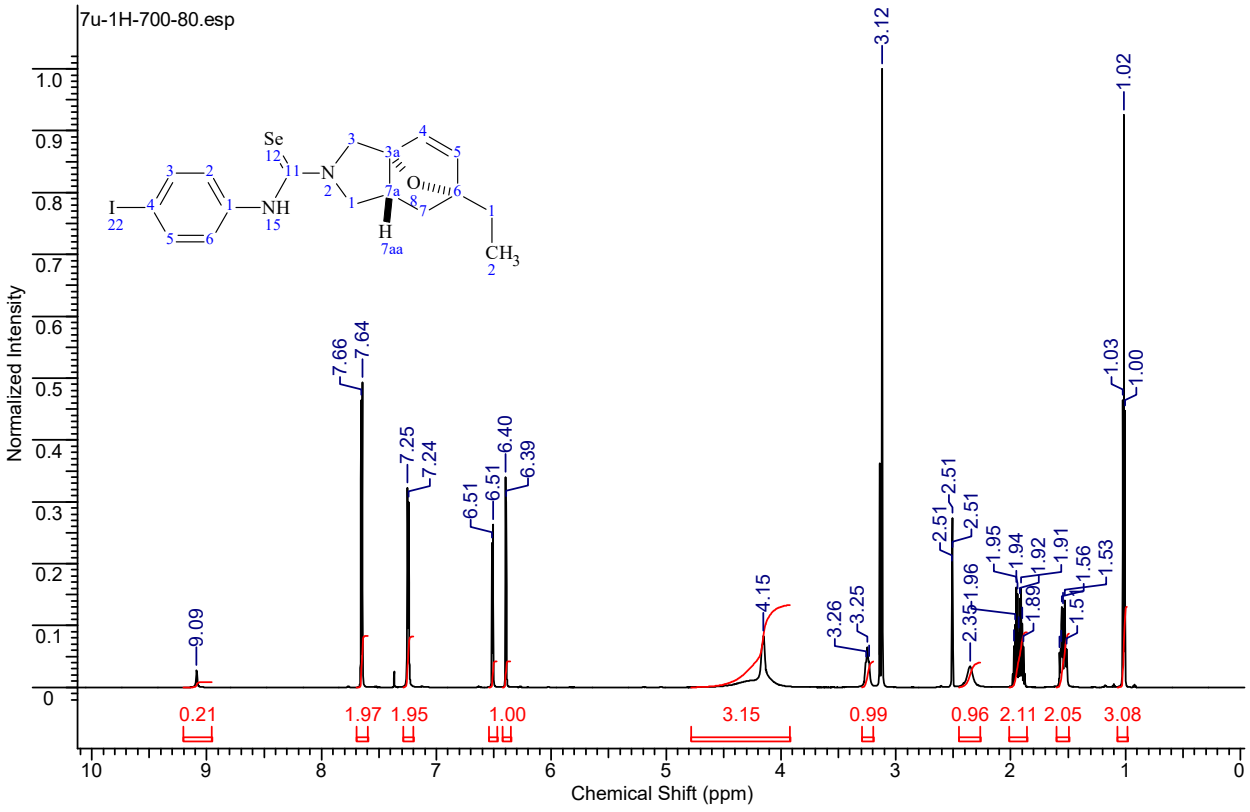
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



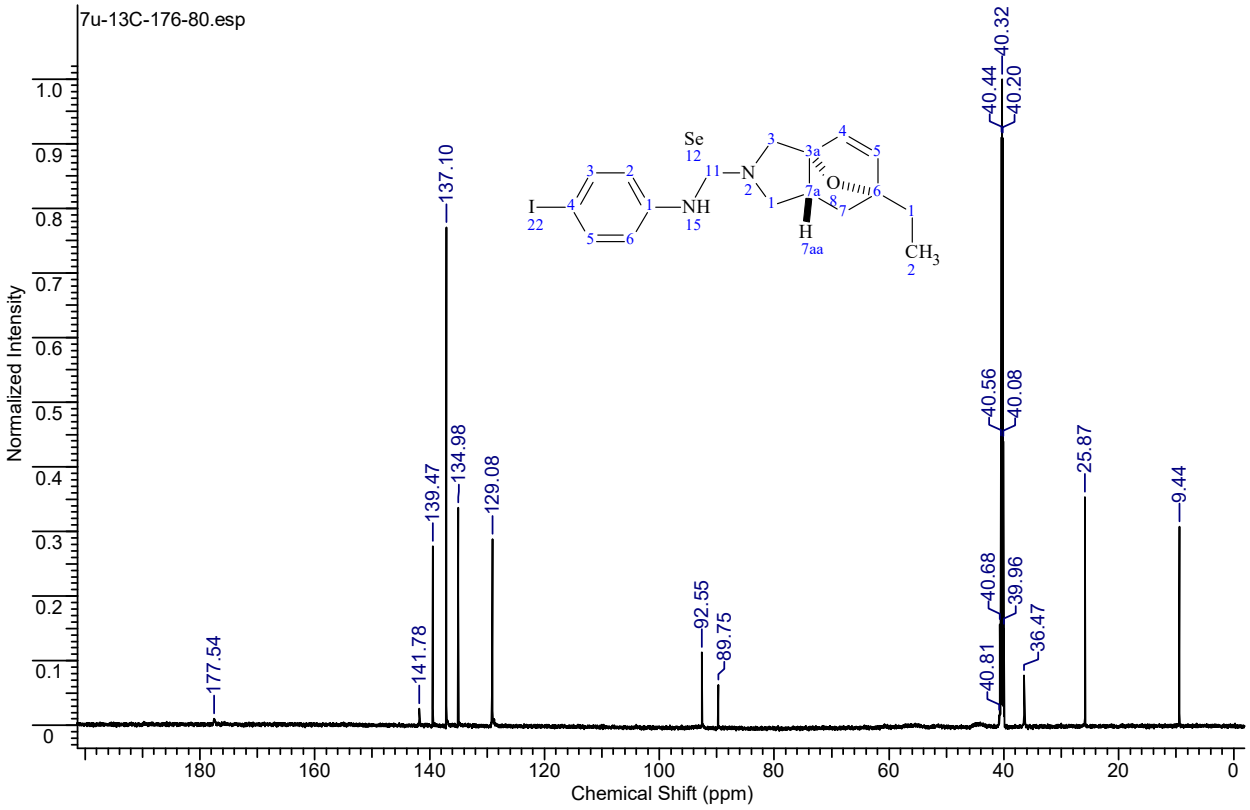
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100 °C)



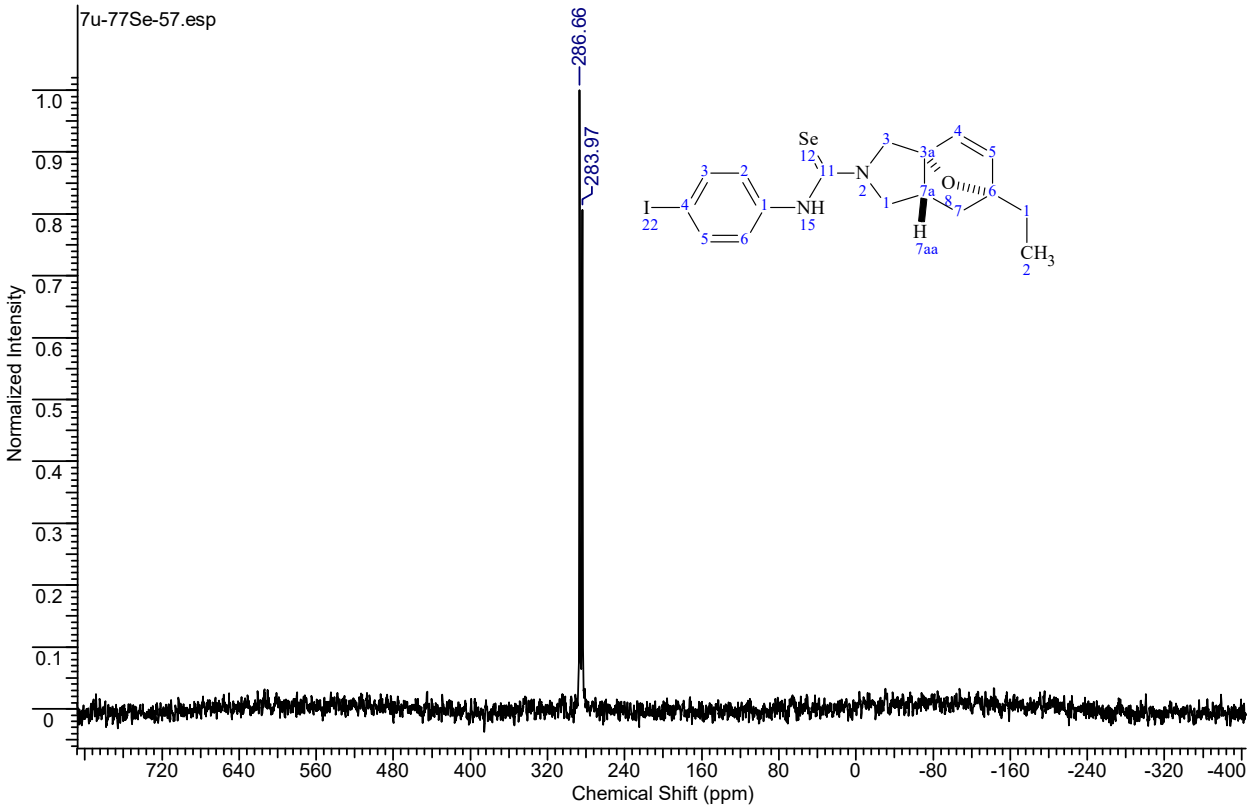
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



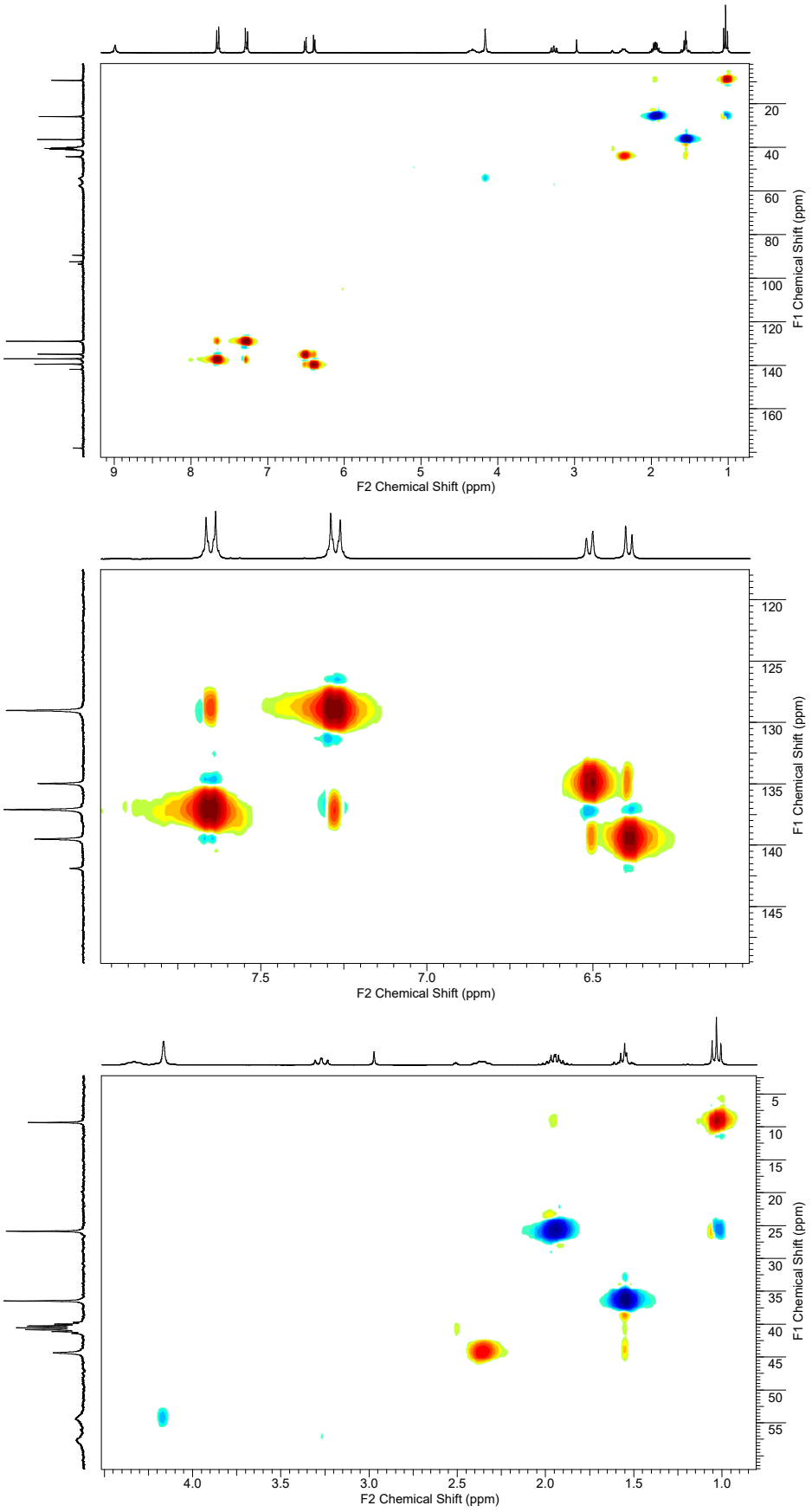
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



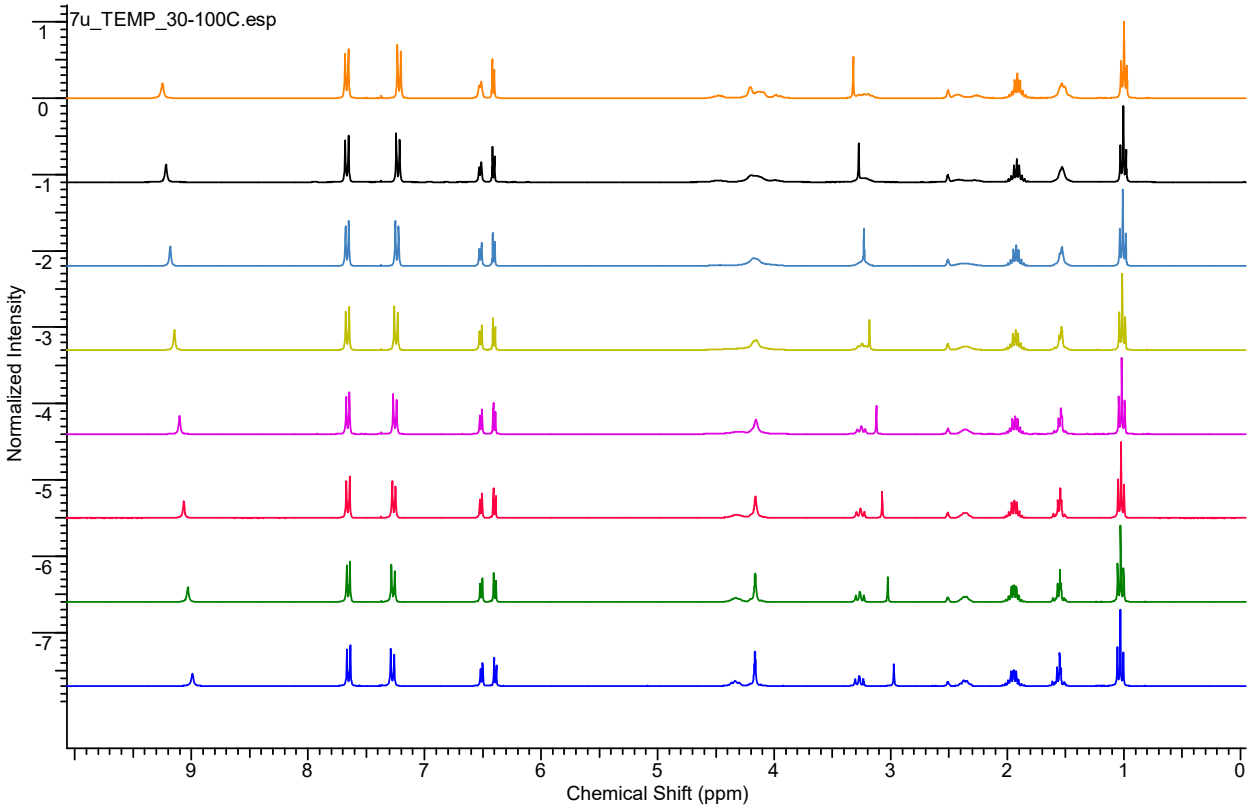
^{77}Se NMR (57.2 MHz, DMSO-d_6)



HSQC of **7u** (100 °C)

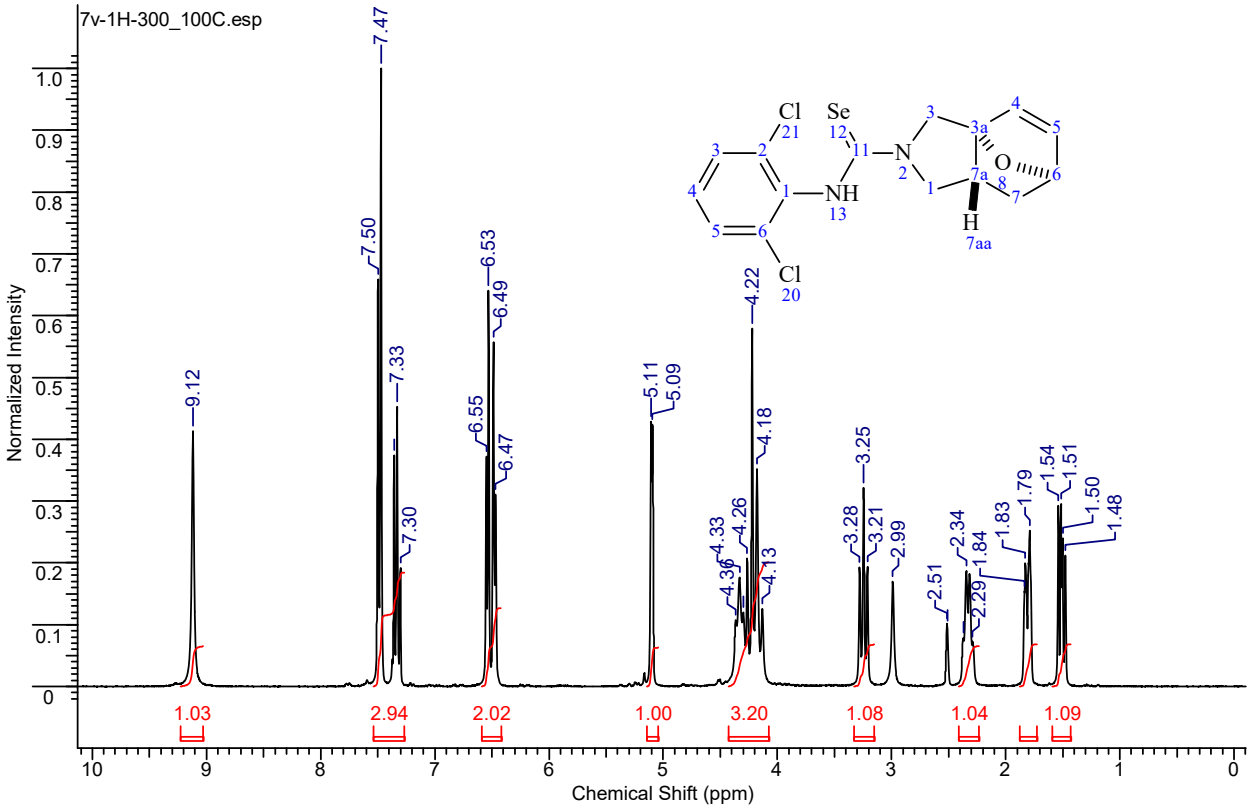


^{1}H NMR of **7u** (30-100 °C)

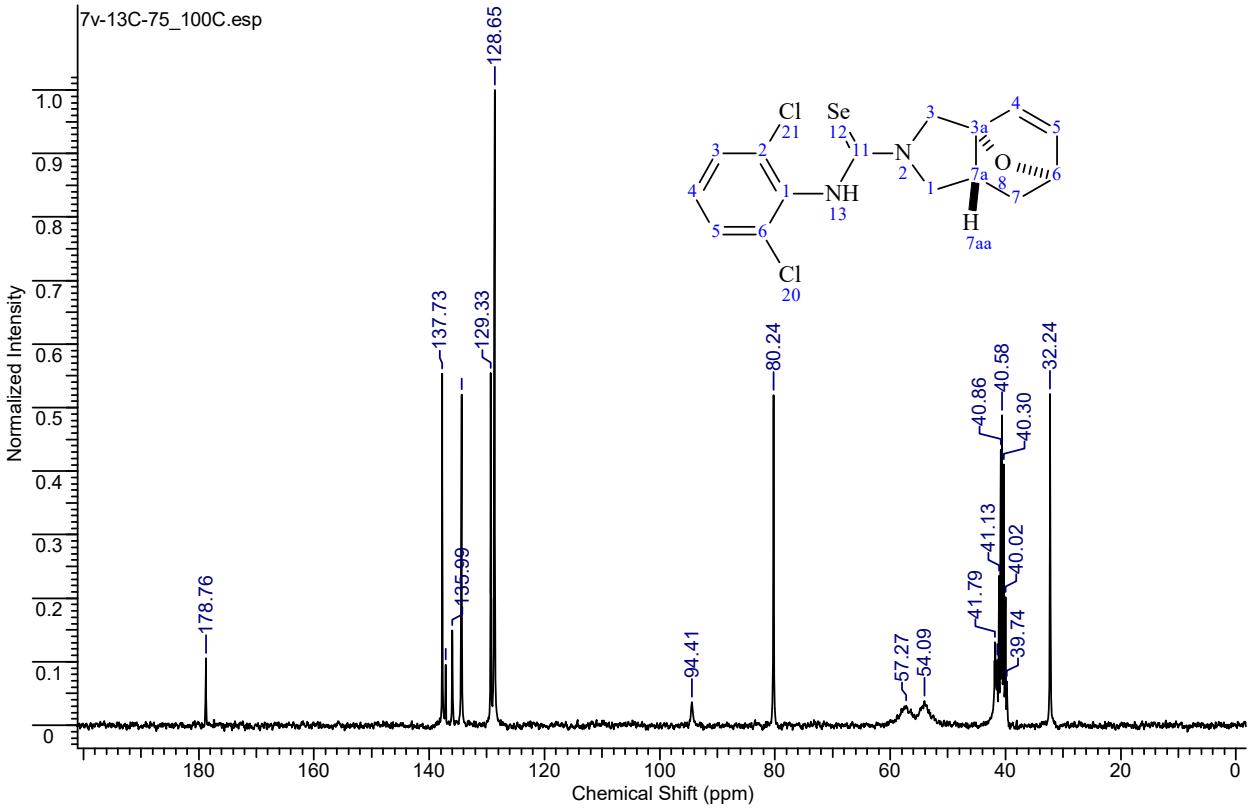


(3a*RS*,6*RS*,7a*RS*)-*N*-(2,6-Dichlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7v).

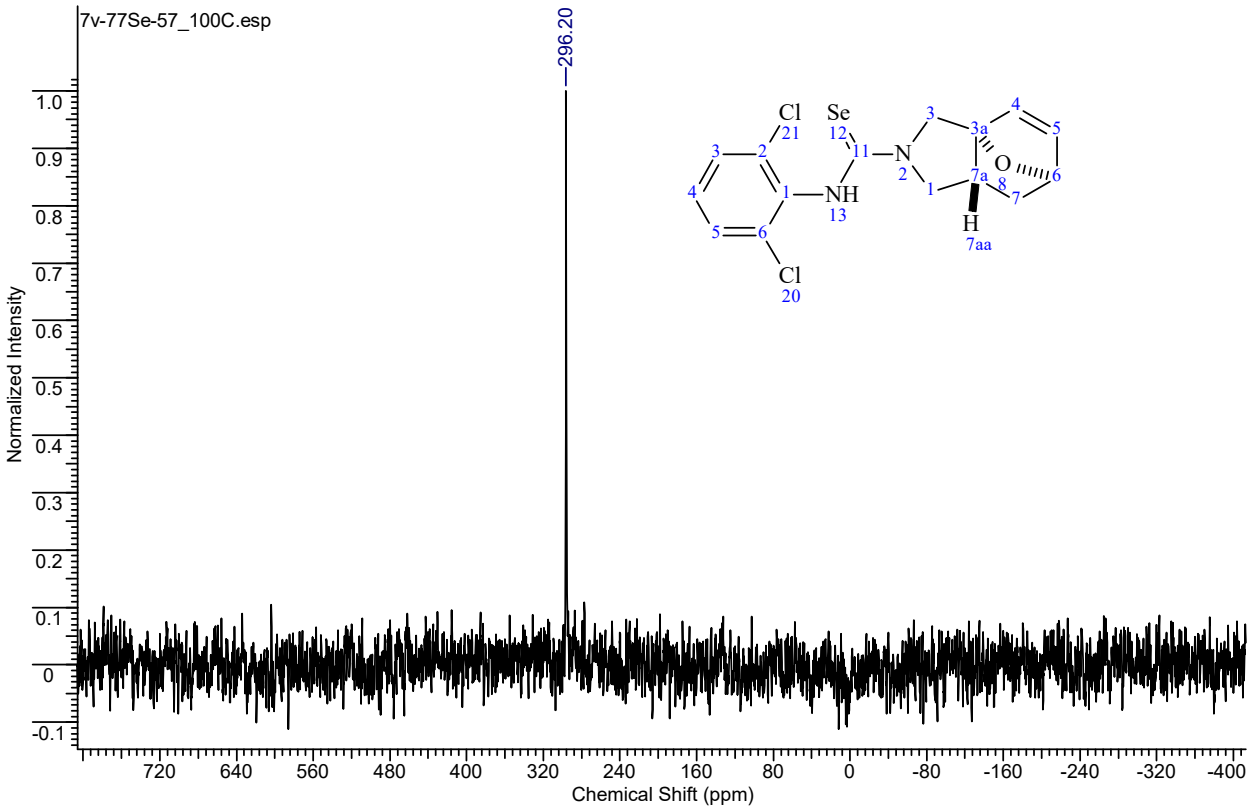
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



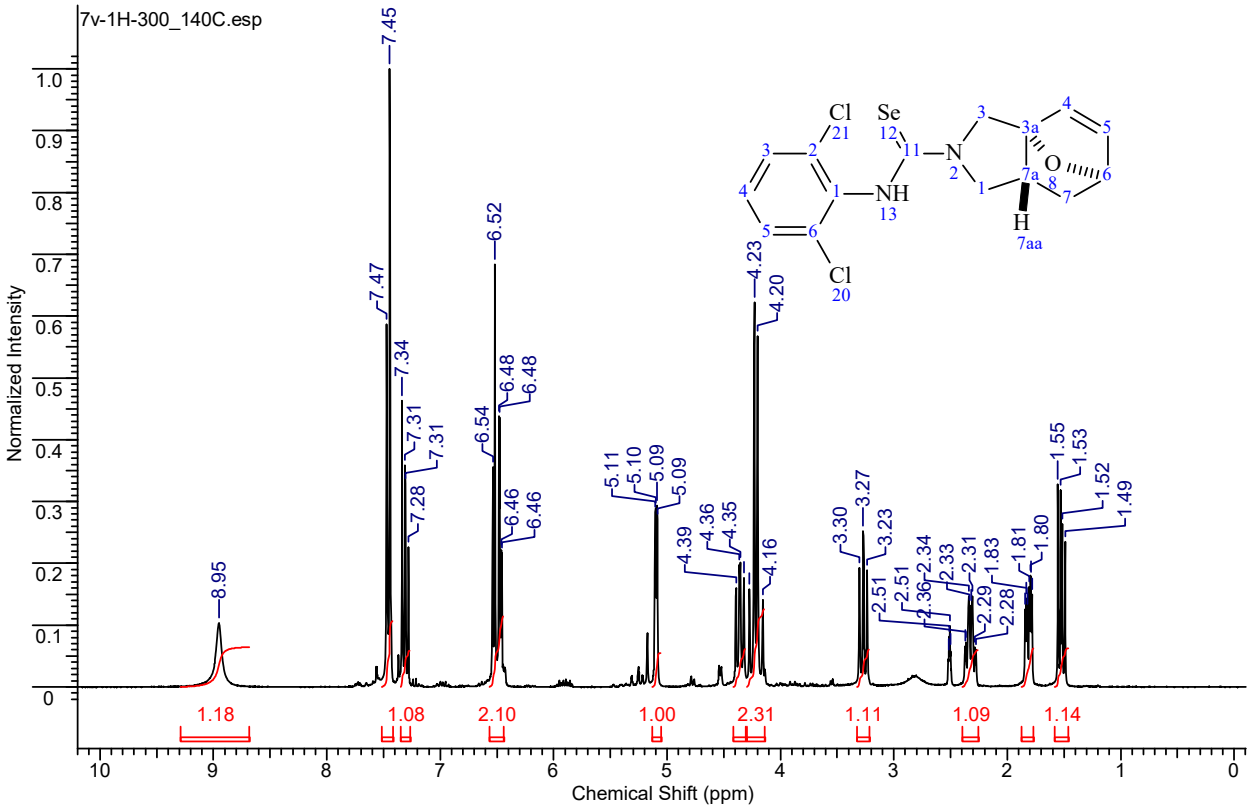
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



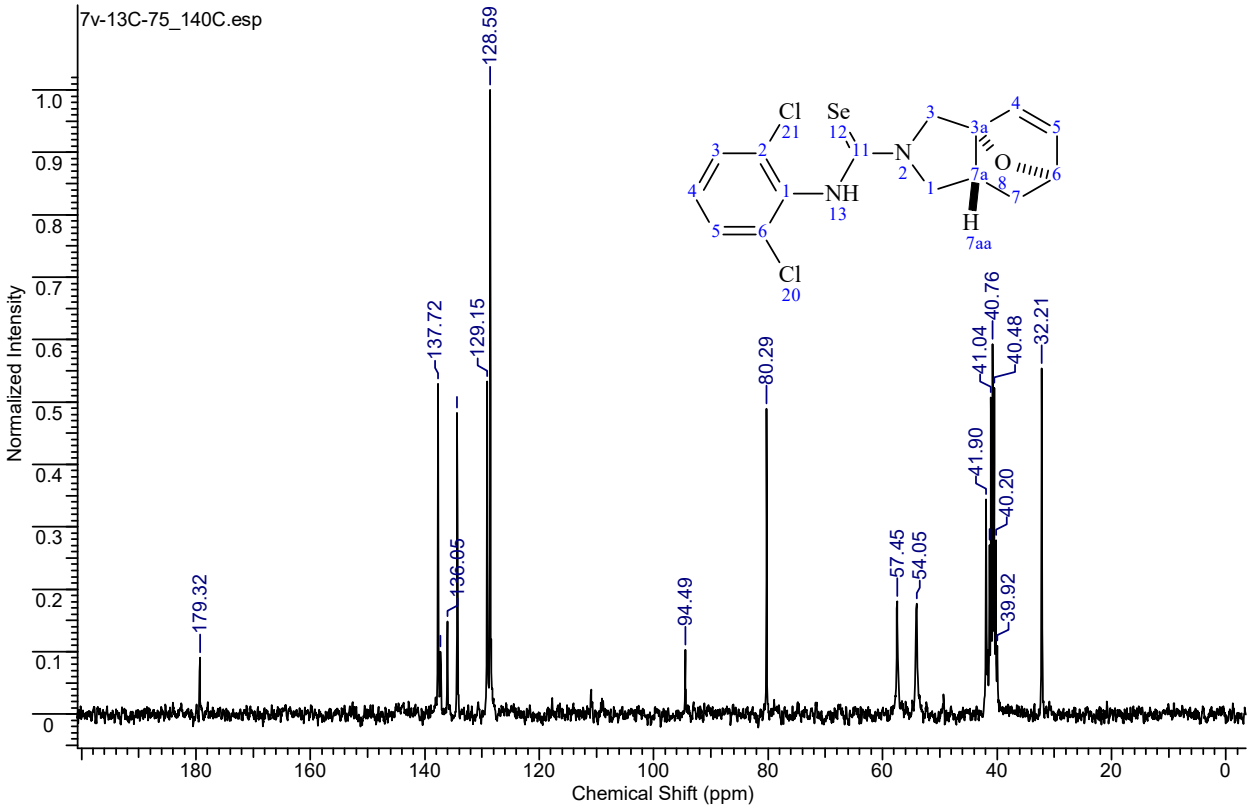
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100°C)



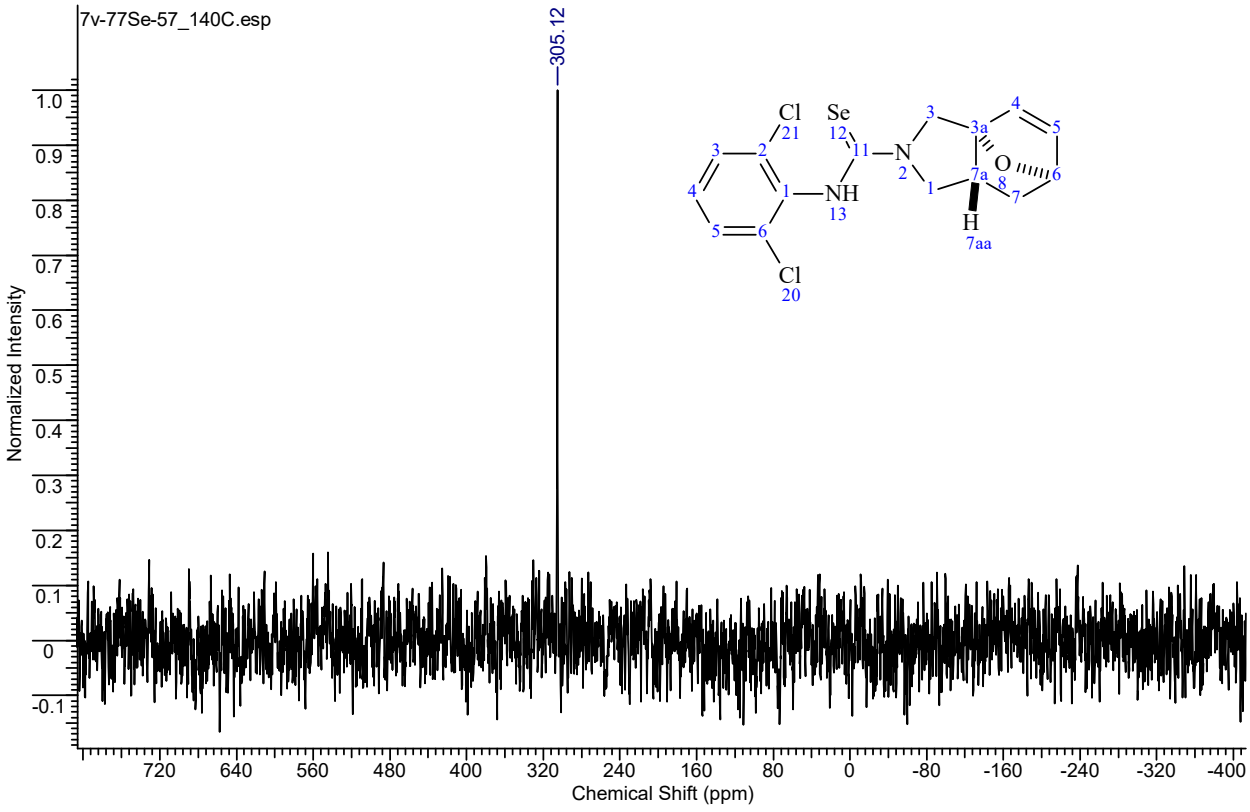
^{1}H NMR (300.1 MHz, DMSO-d_6, 140 °C) *the compd.* **7v** *decomposes at 140 °C*



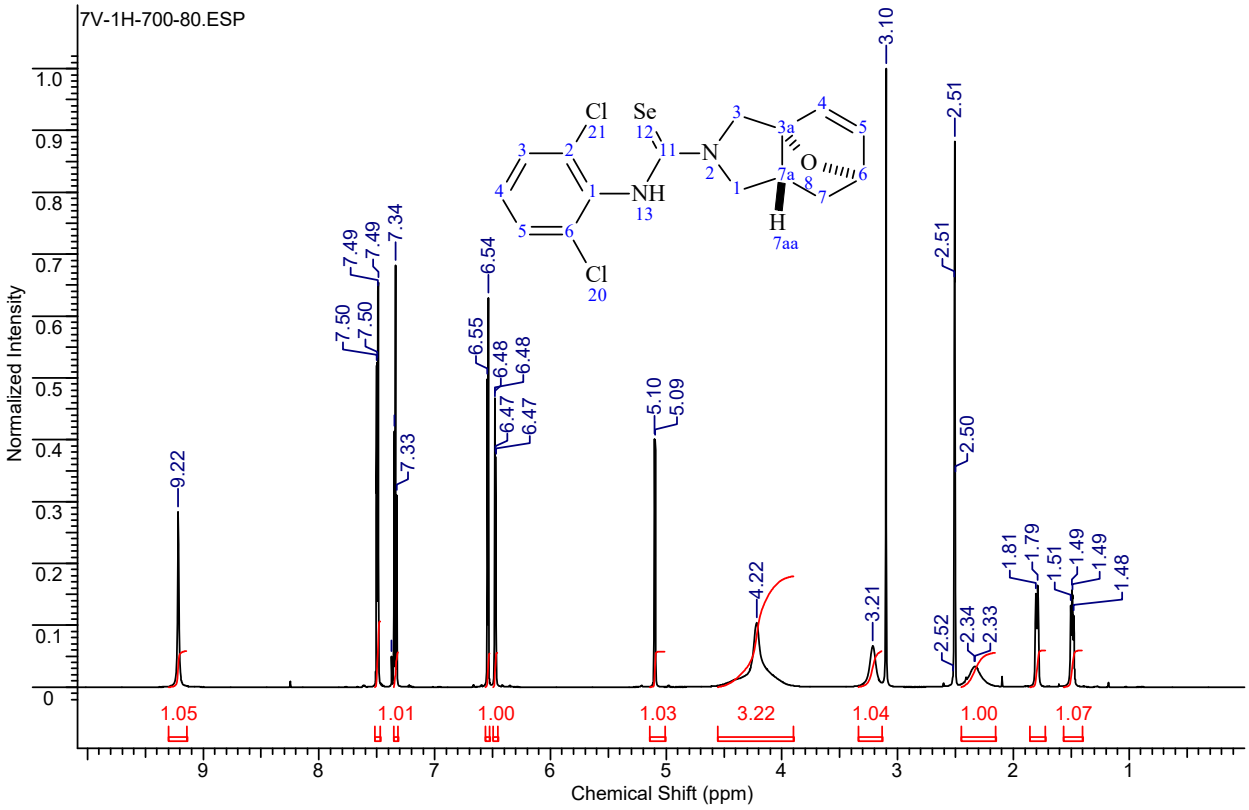
^{13}C NMR (75.5 MHz, DMSO-d_6, 140 °C)



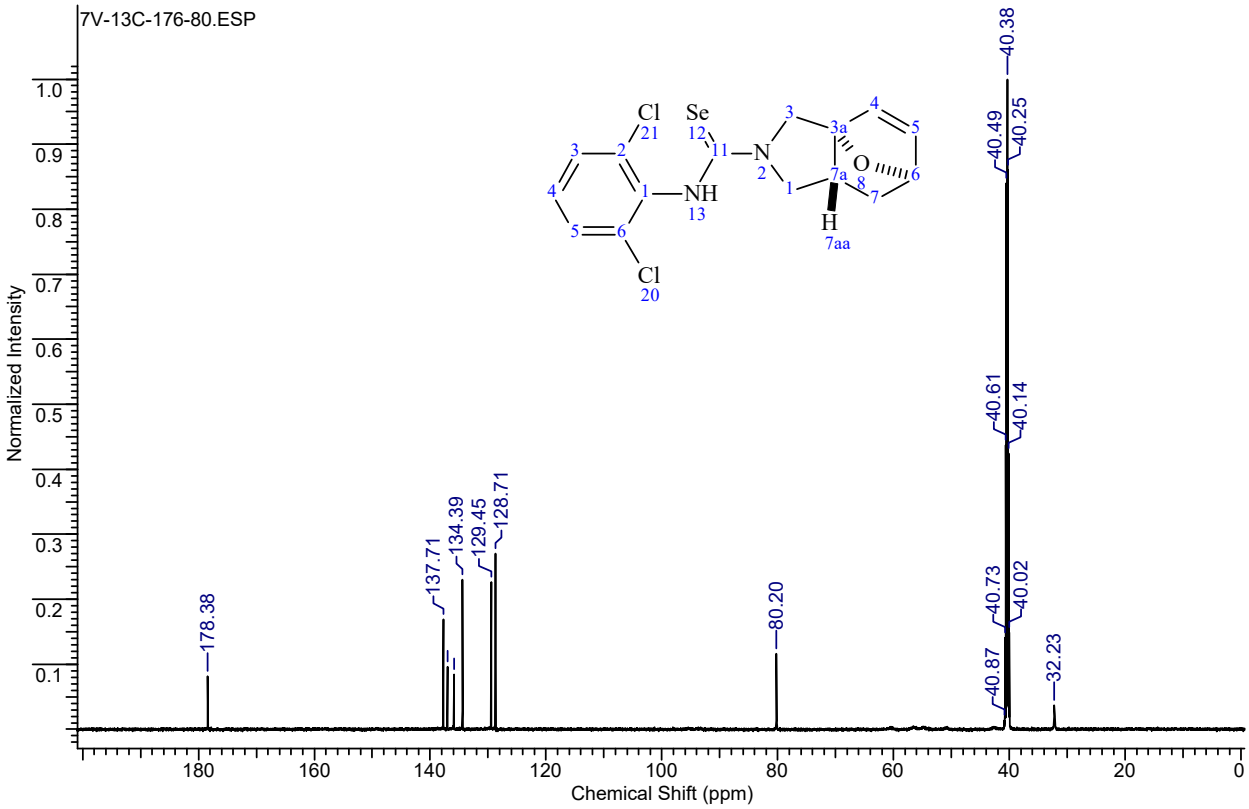
^{77}Se NMR (57.2 MHz, DMSO-d_6, 140°C)



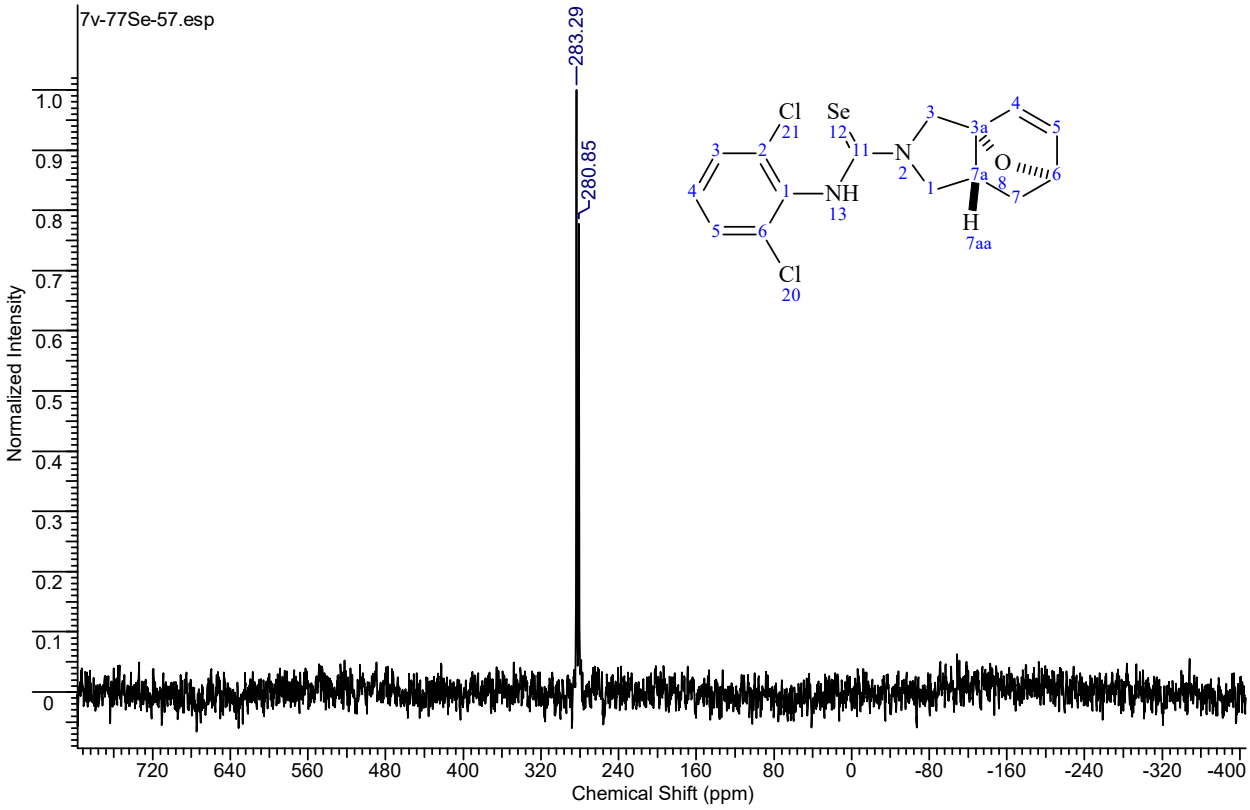
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



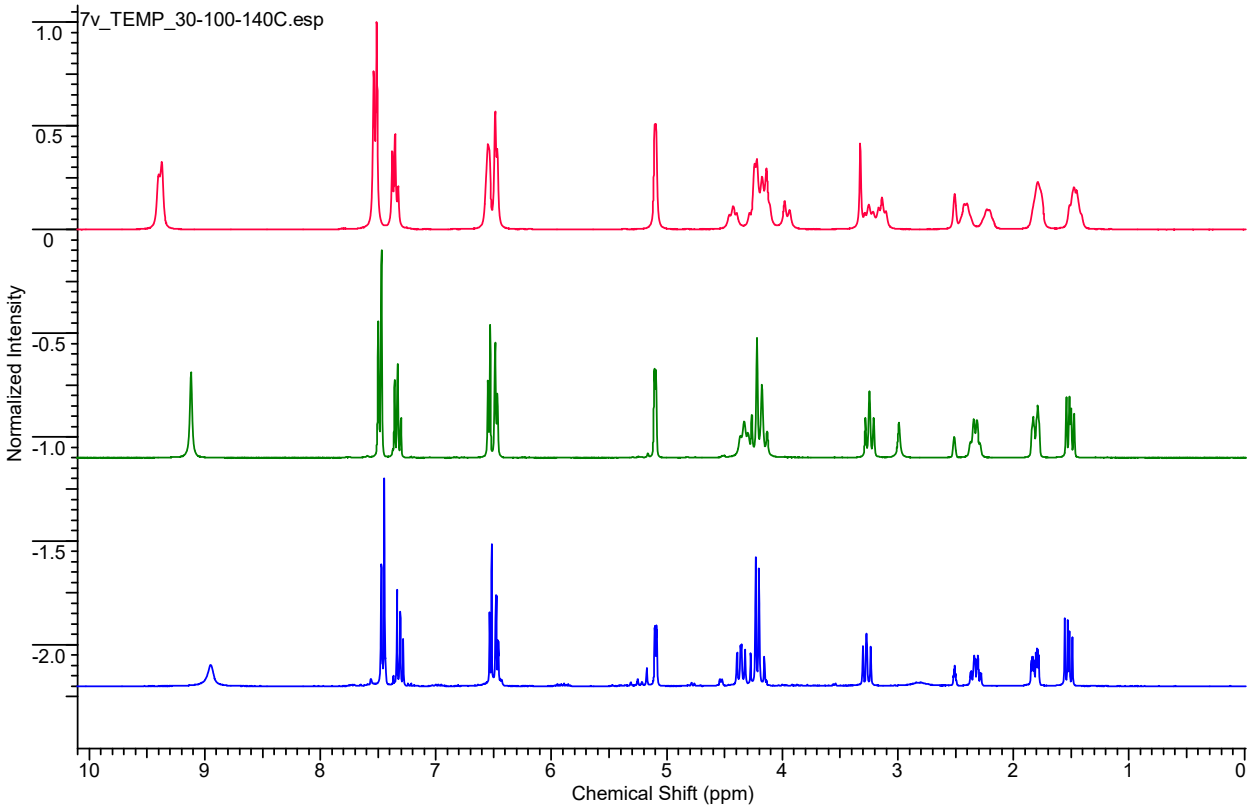
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



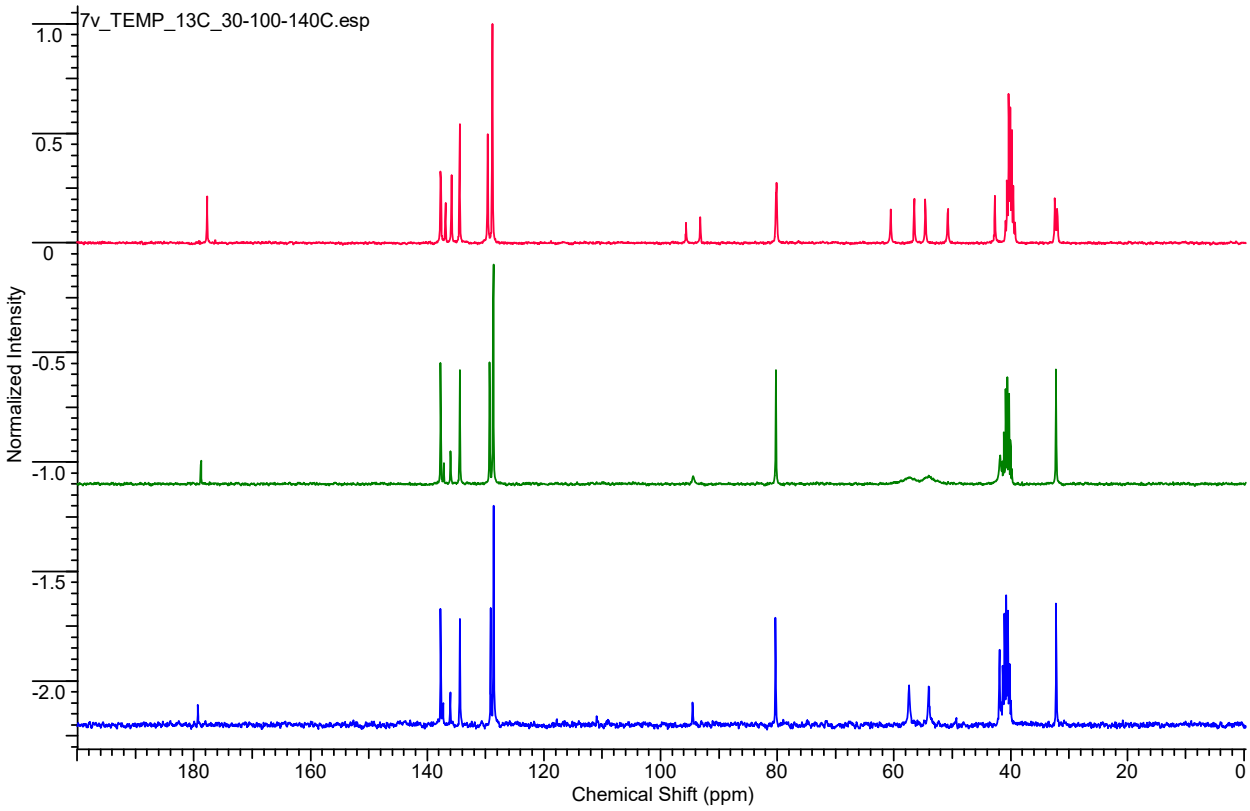
^{77}Se NMR (57.2 MHz, DMSO-d_6)



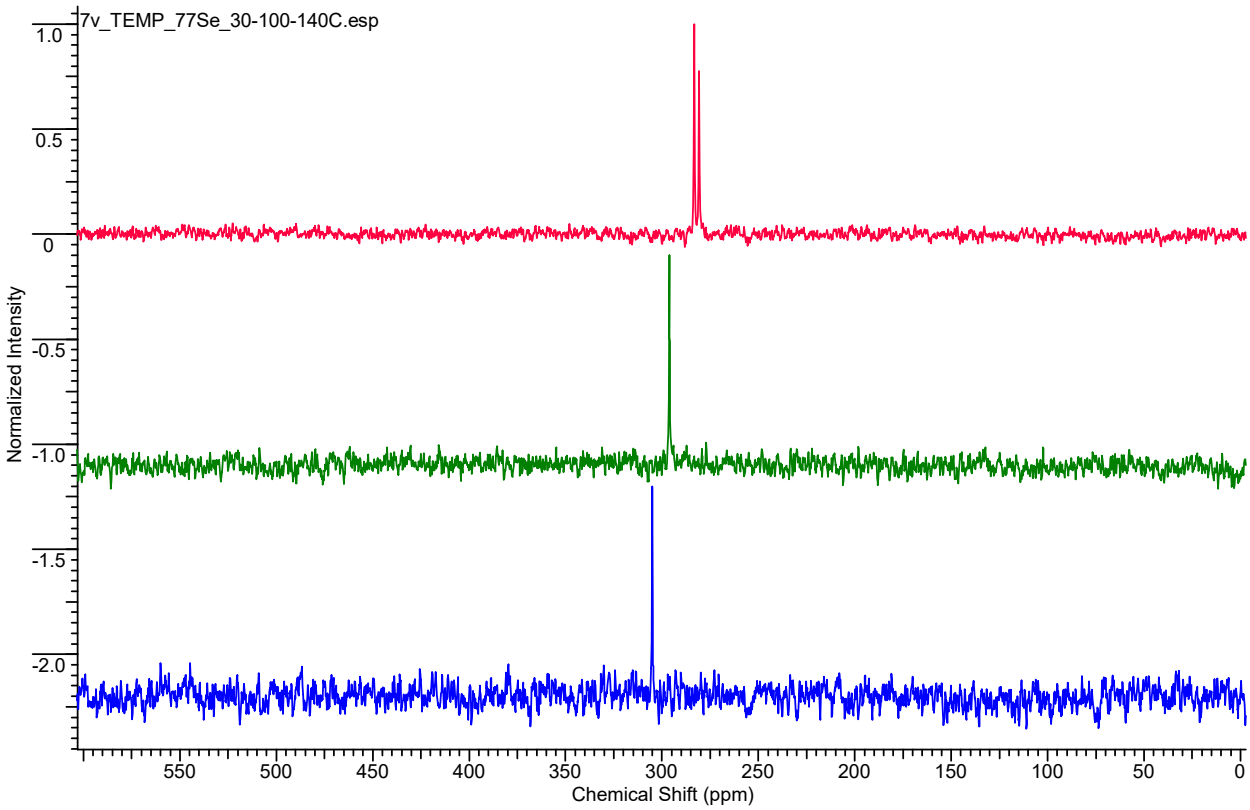
^{1}H NMR of **7v** (30-100-140 °C)



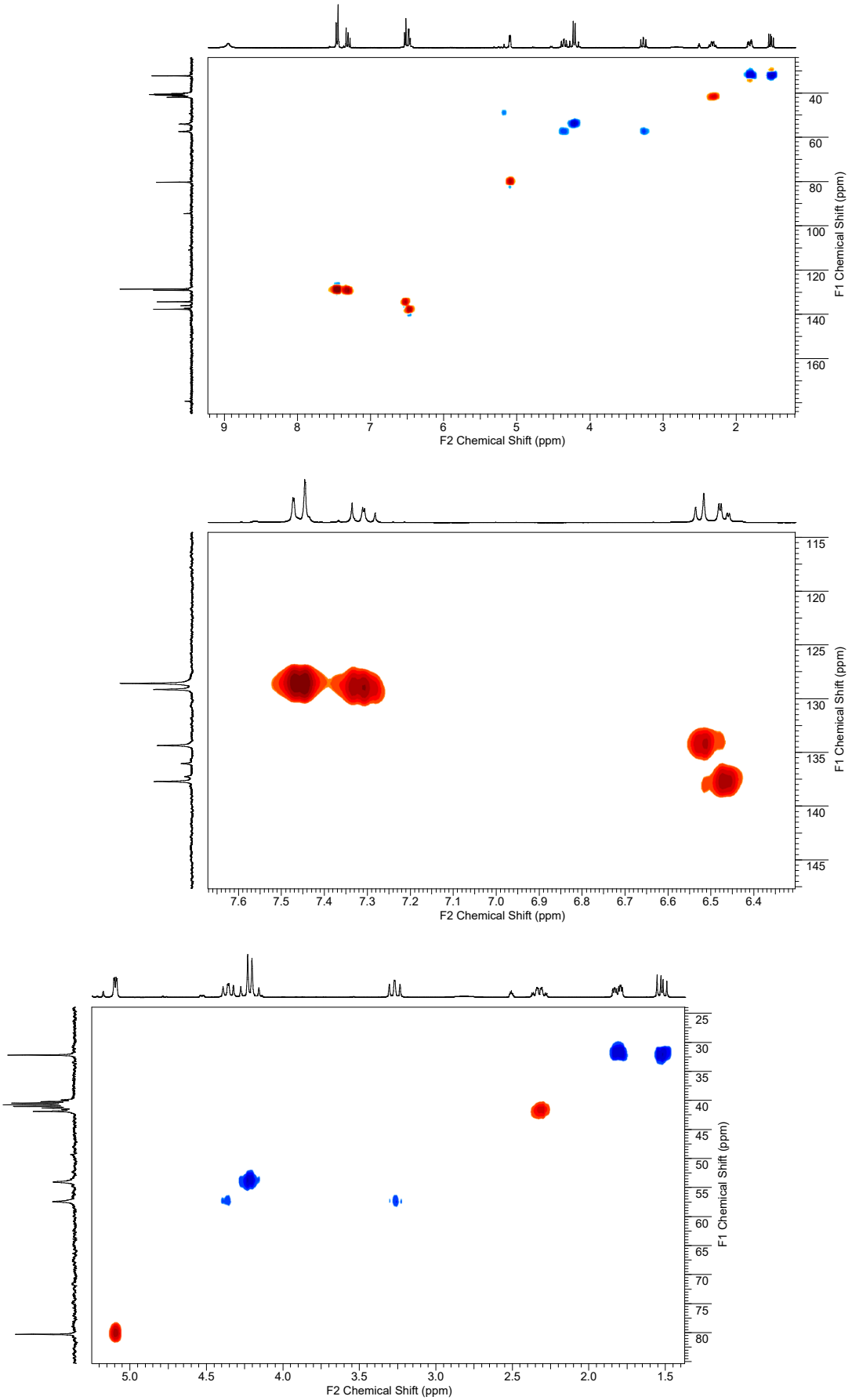
^{13}C NMR of **7v** (30-100-140 °C)



^{77}Se NMR of **7v** (30-100-140 °C)

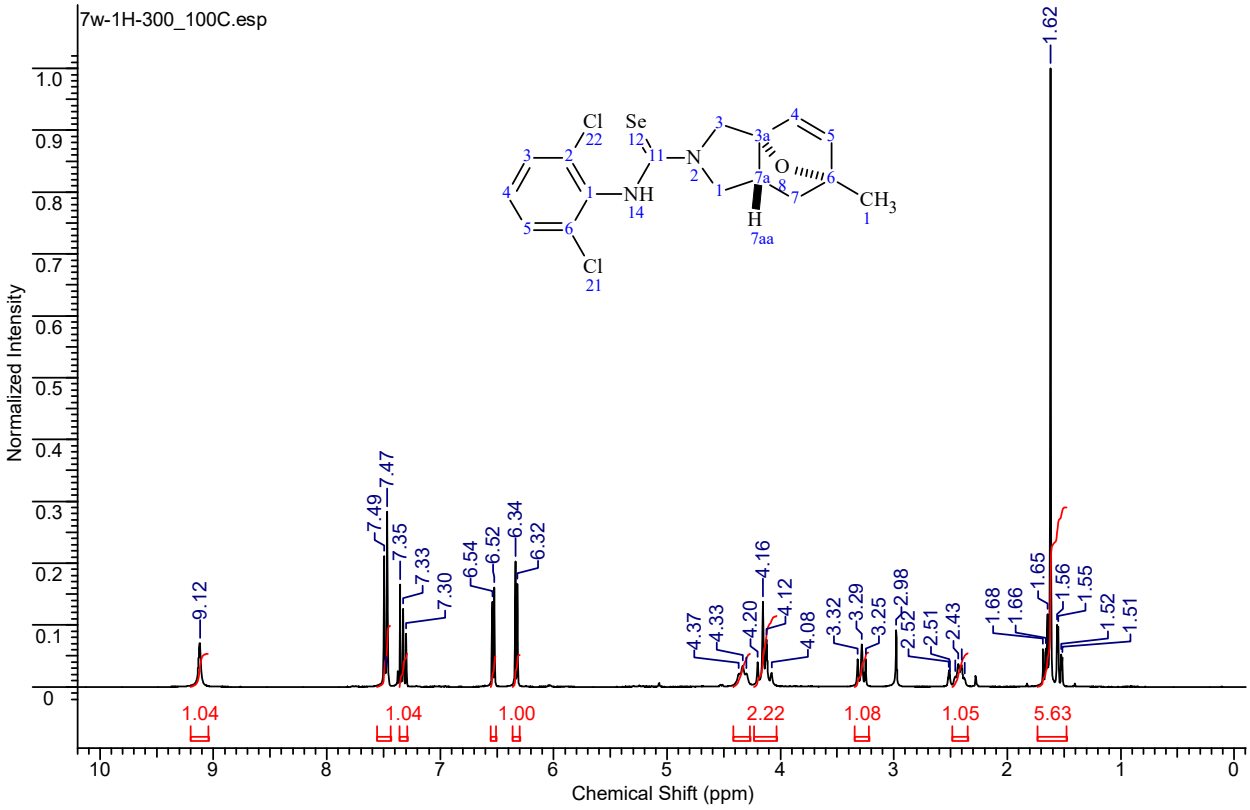


HSQC of **7v** (140 °C)

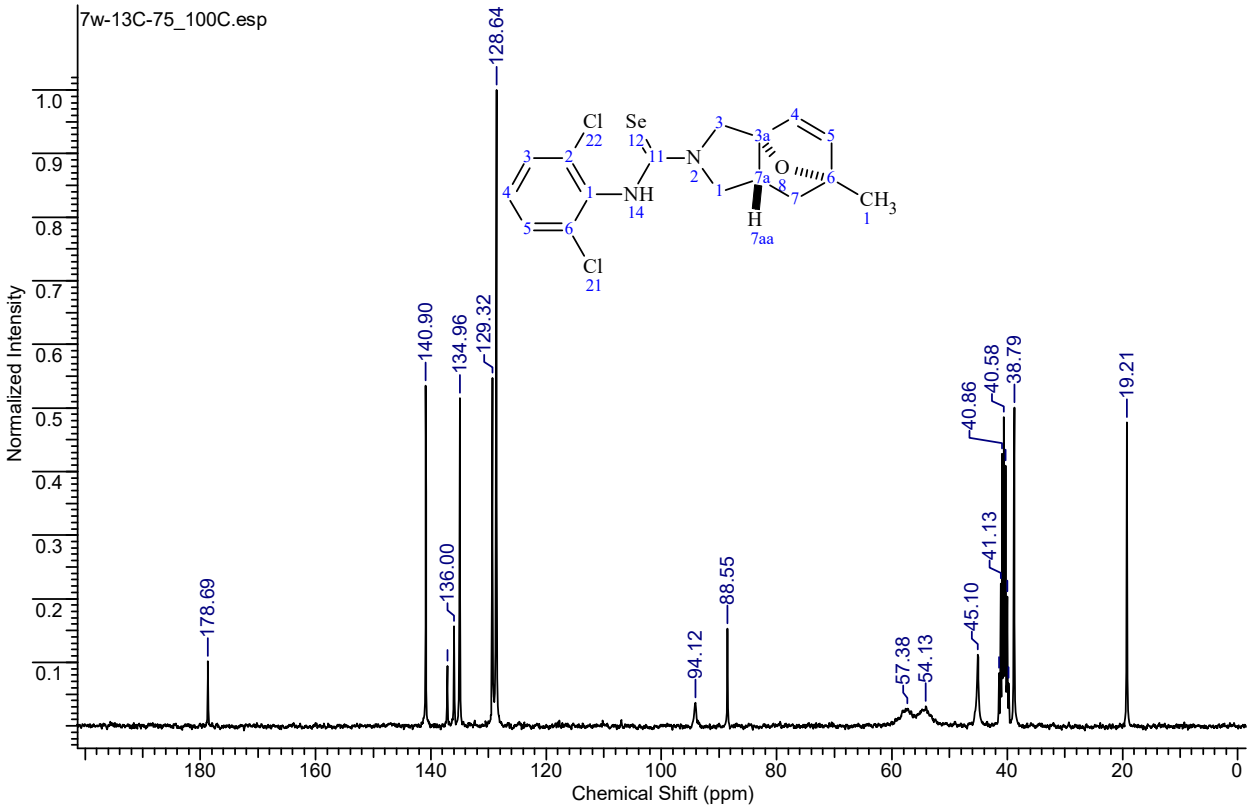


(3a*RS*,6*RS*,7a*RS*)-*N*-(2,6-Dichlorophenyl)-6-methyl-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7w).

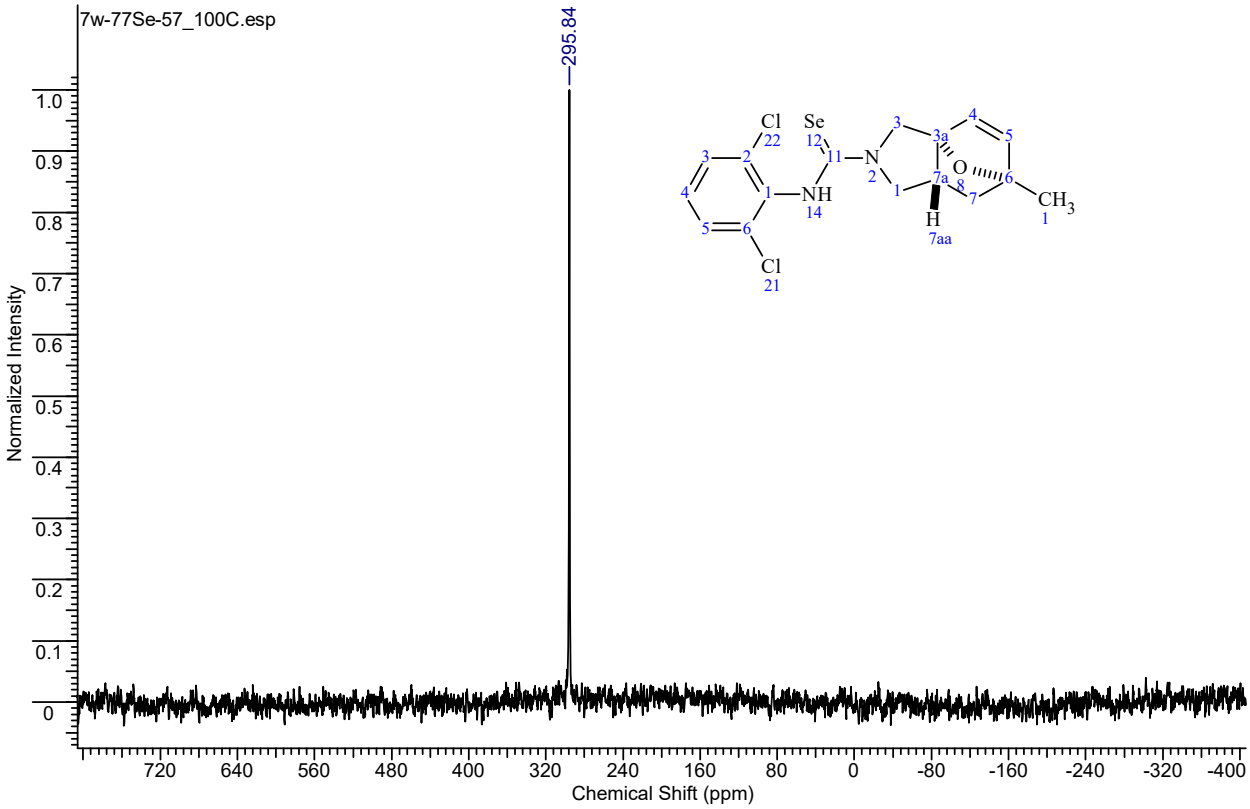
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



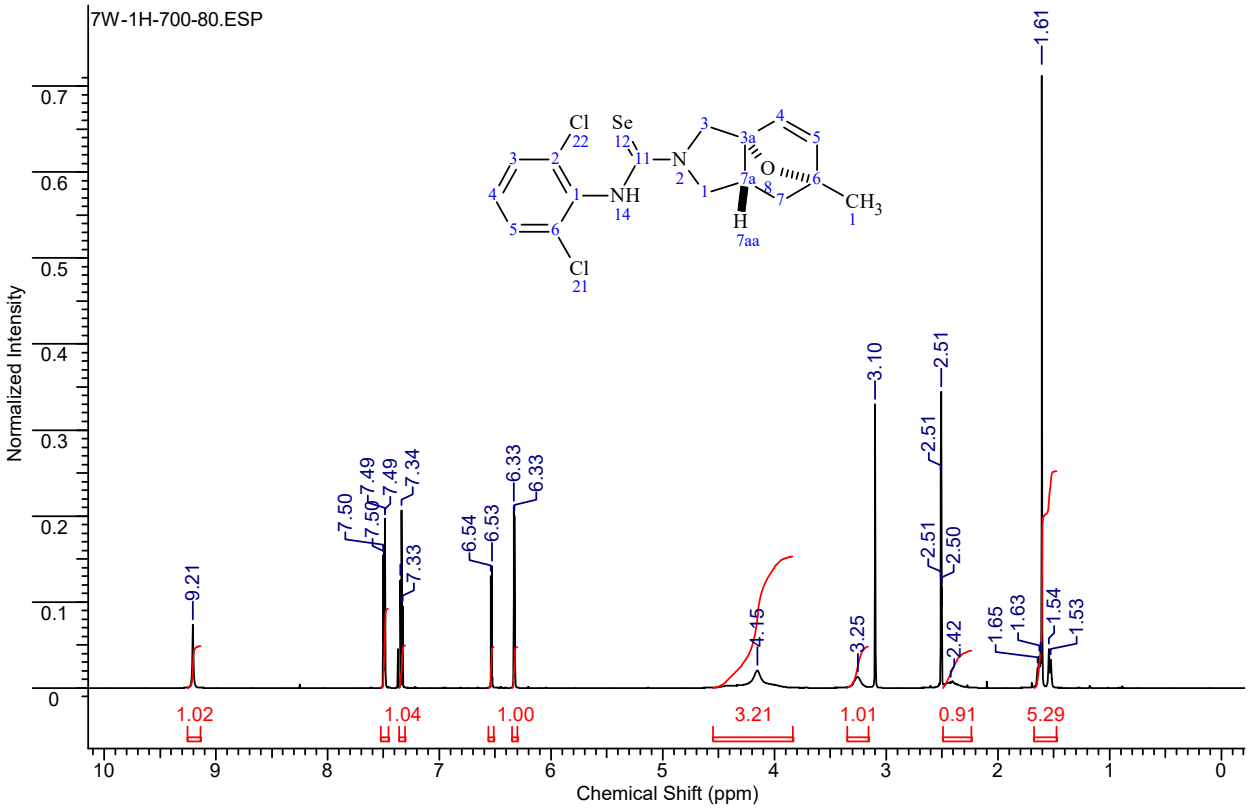
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



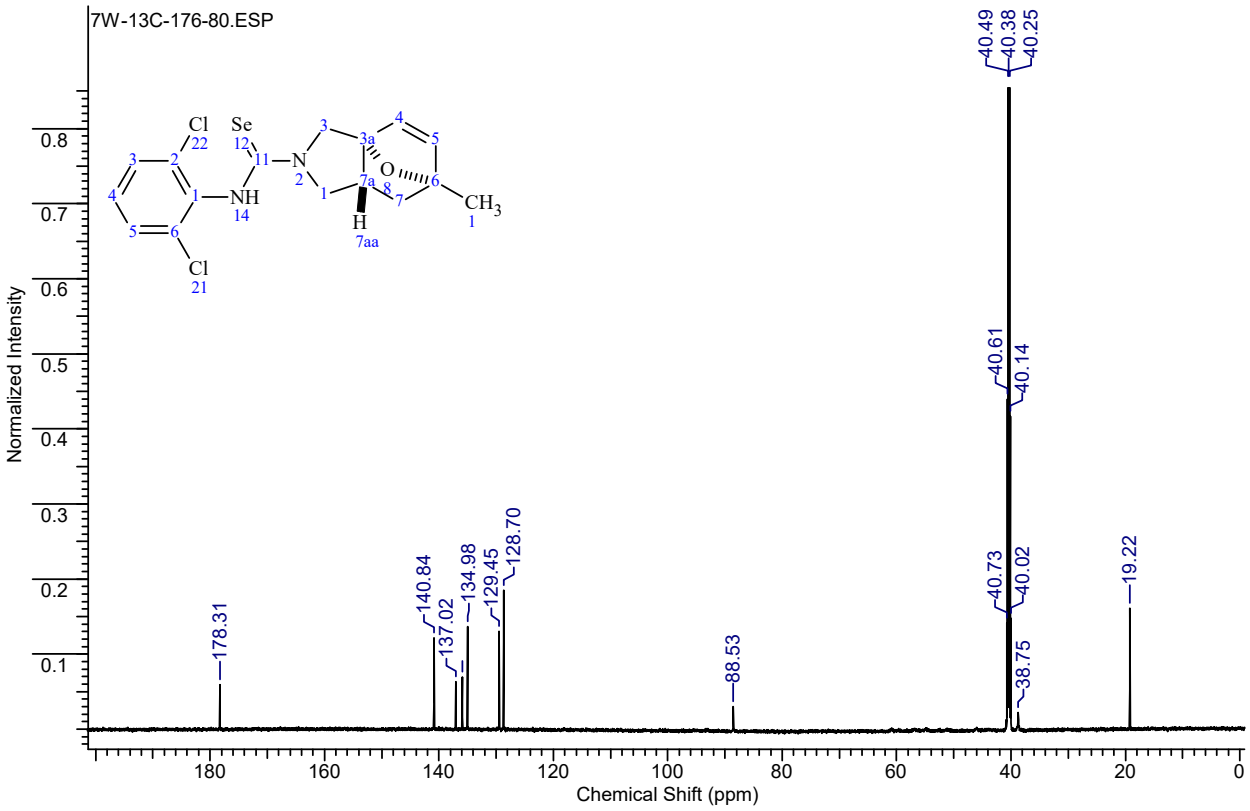
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100 °C)



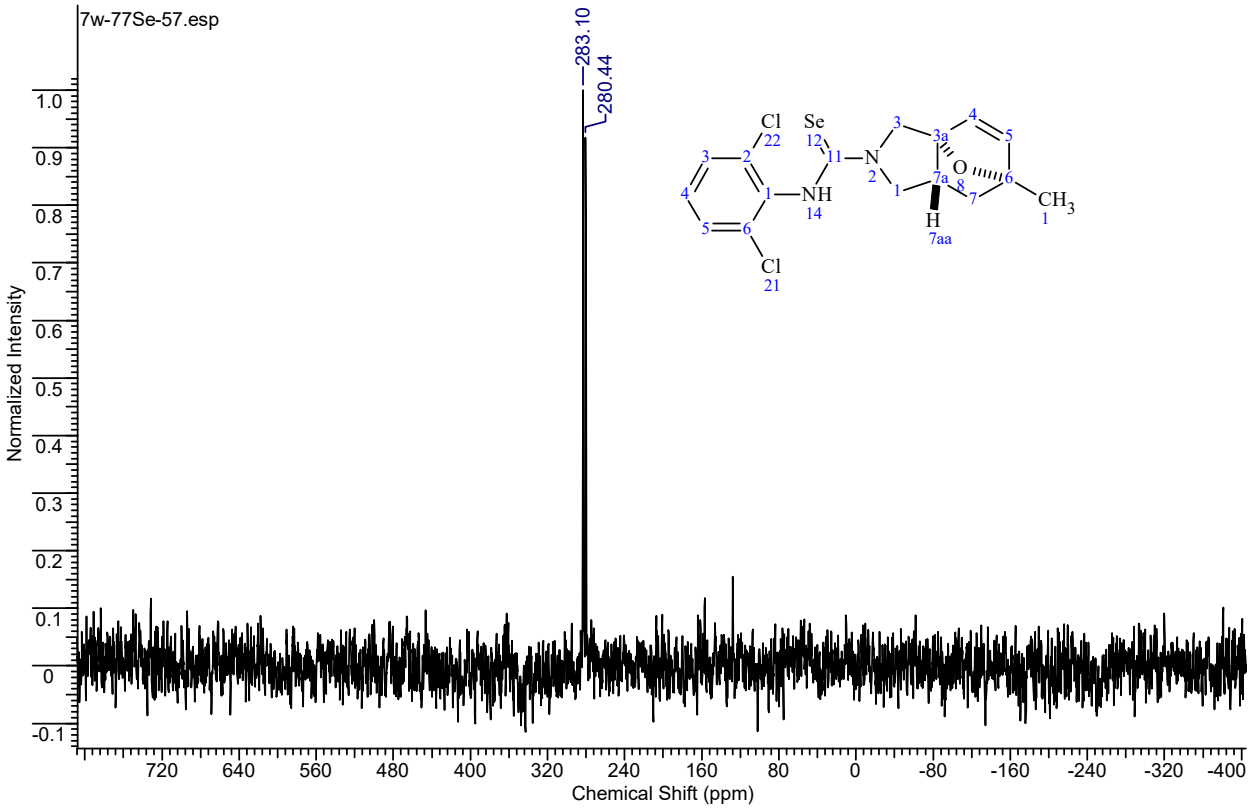
^{1}H NMR (700.2 MHz, DMSO-d_6, 80 °C)



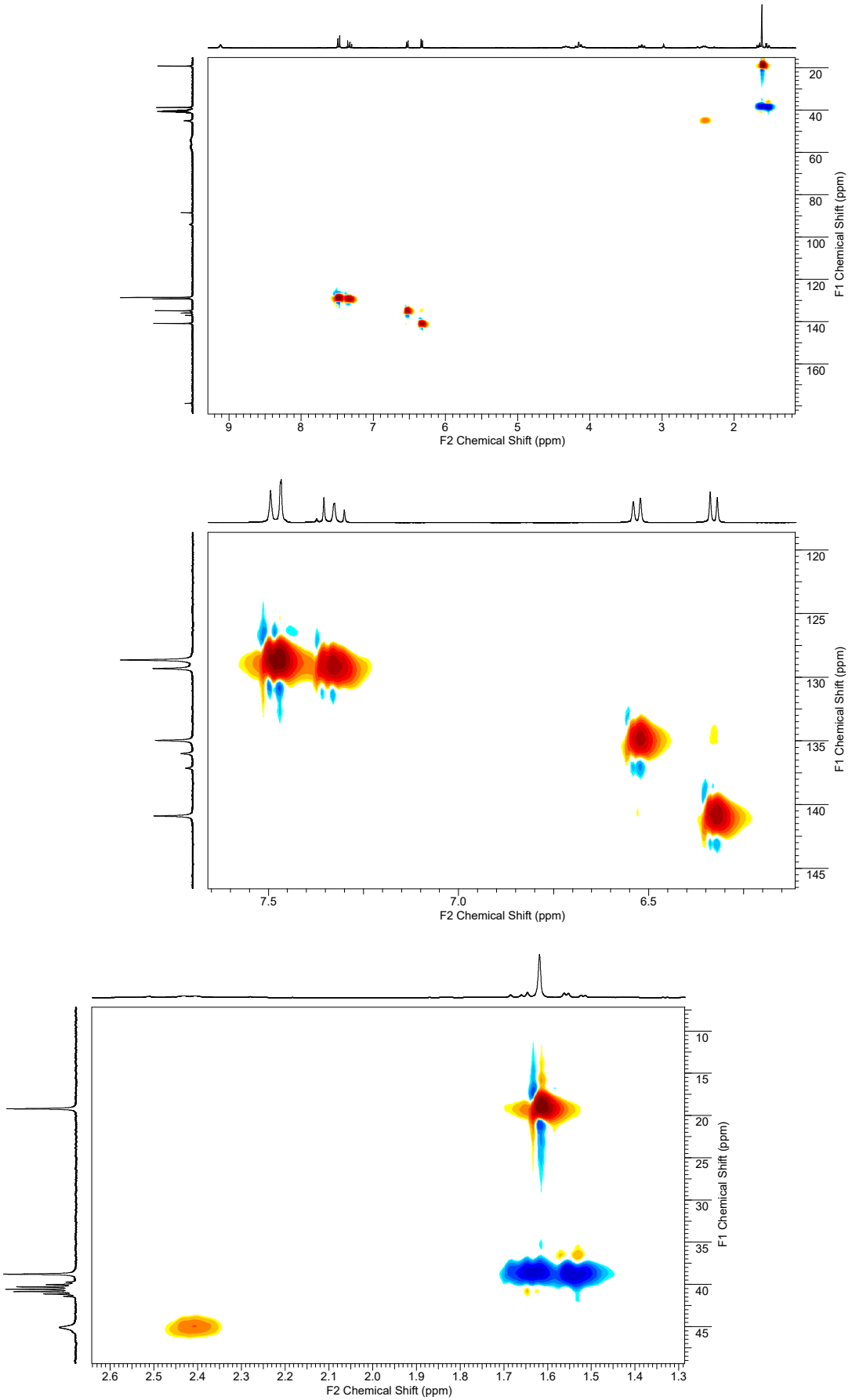
^{13}C NMR (176.1 MHz, DMSO-d_6, 80 °C)



^{77}Se NMR (57.2 MHz, DMSO-d_6)

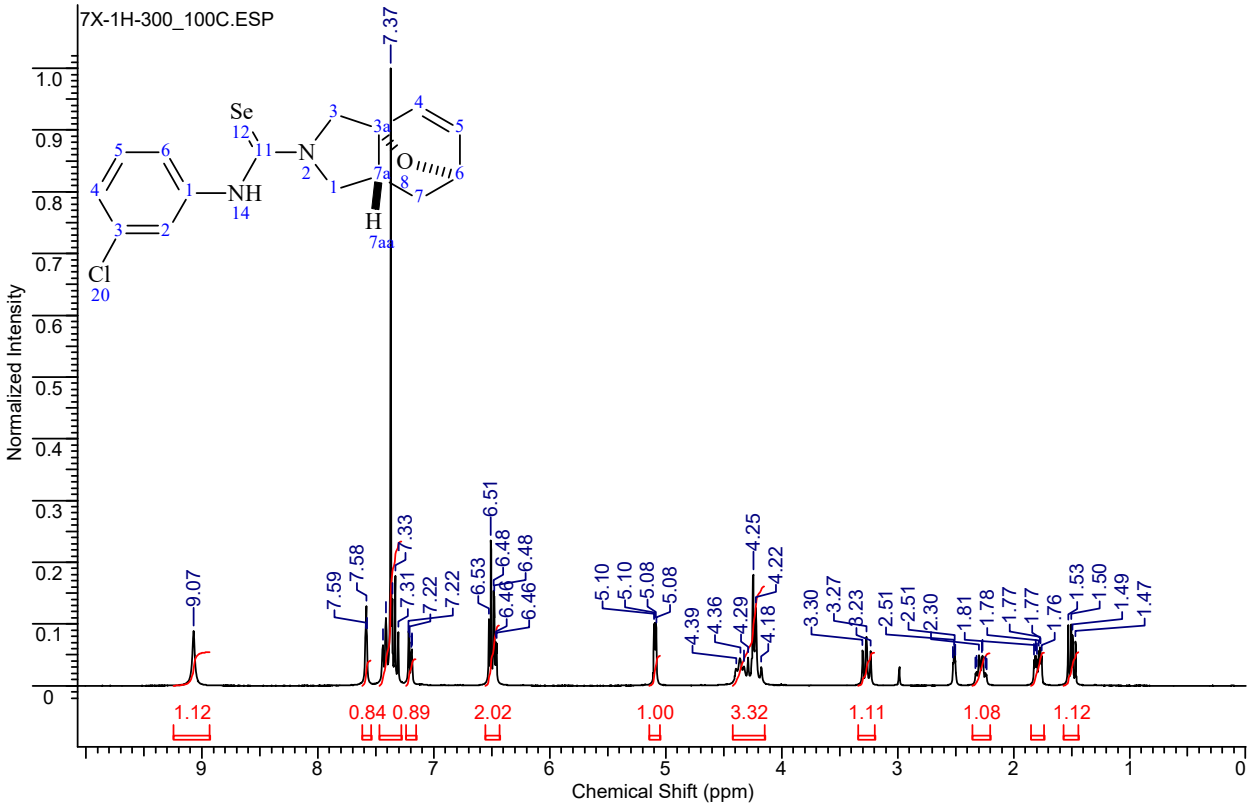


HSQC of **7w** (100 °C)

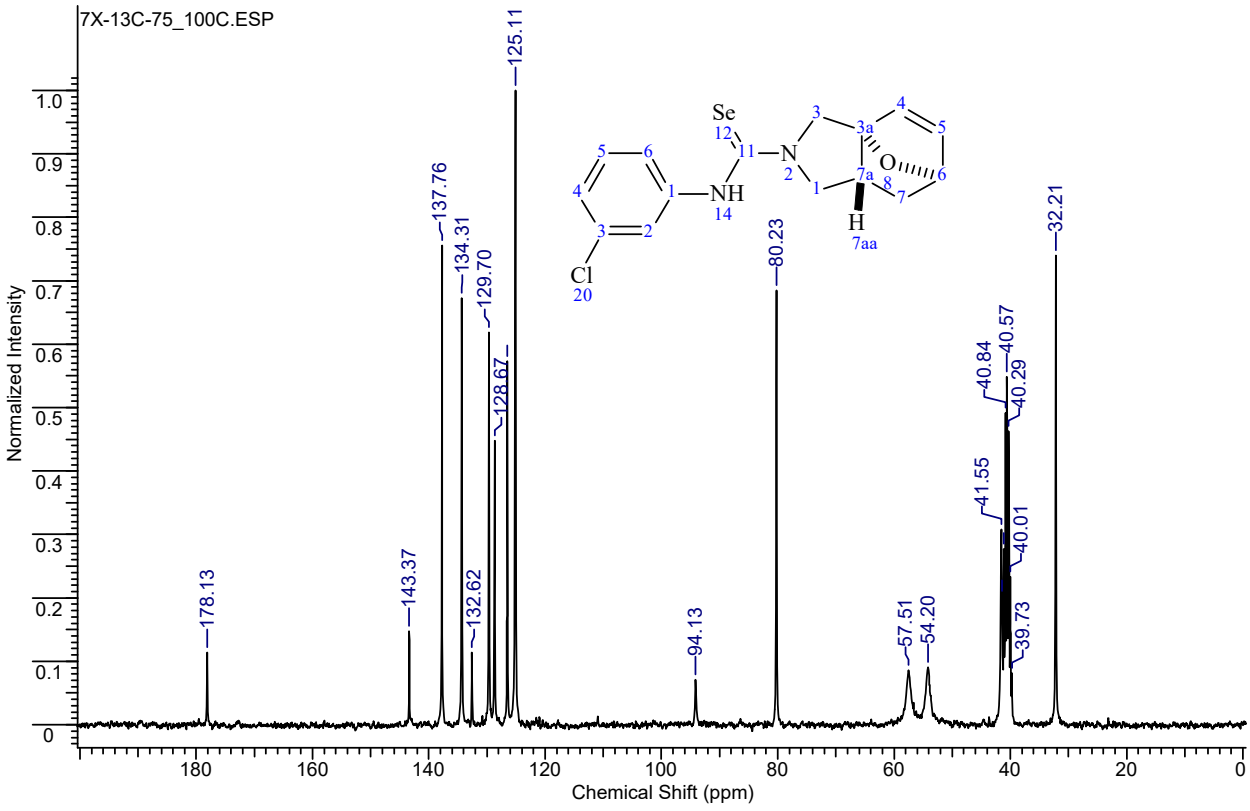


(3a*RS*,6*RS*,7a*RS*)-*N*-(3-Chlorophenyl)-1,6,7,7a-tetrahydro-3a,6-epoxyisoindole-2(3*H*)-carboselenoamide (7x).

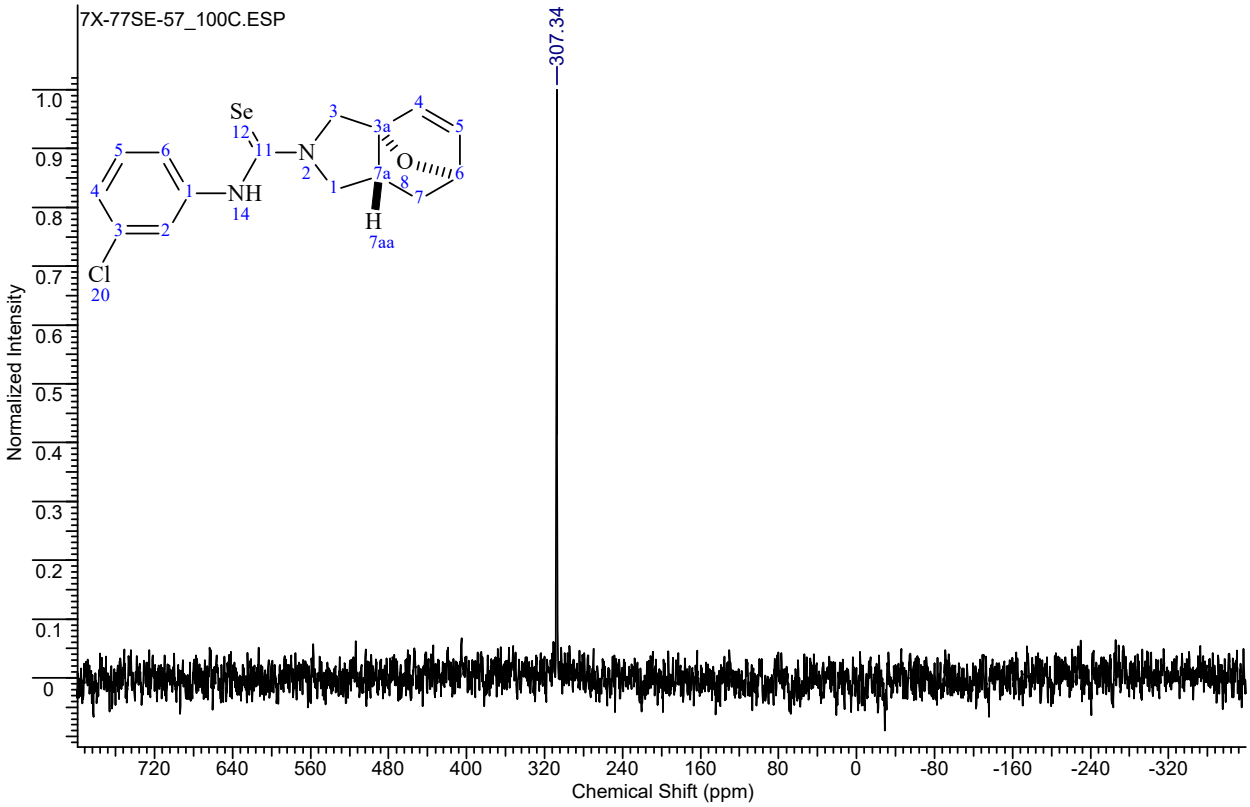
^{1}H NMR (300.1 MHz, DMSO-d_6, 100 °C)



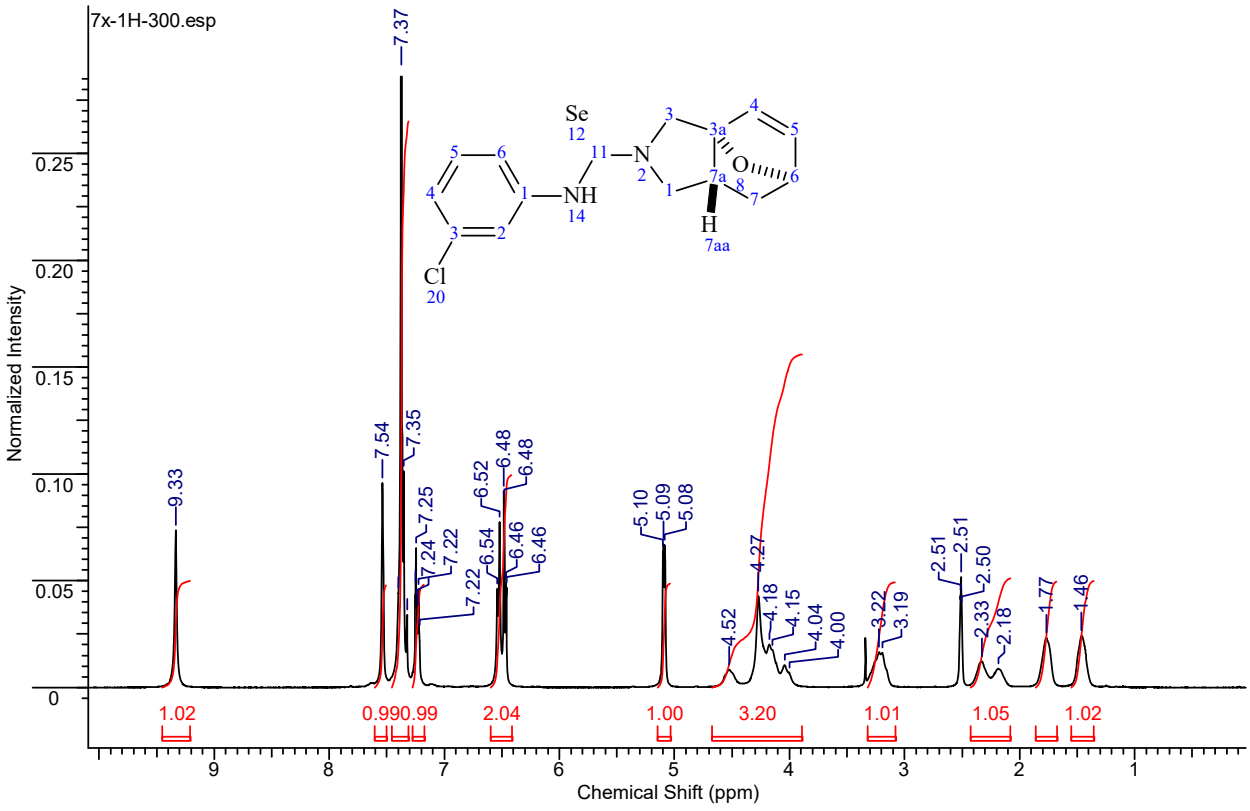
^{13}C NMR (75.5 MHz, DMSO-d_6, 100 °C)



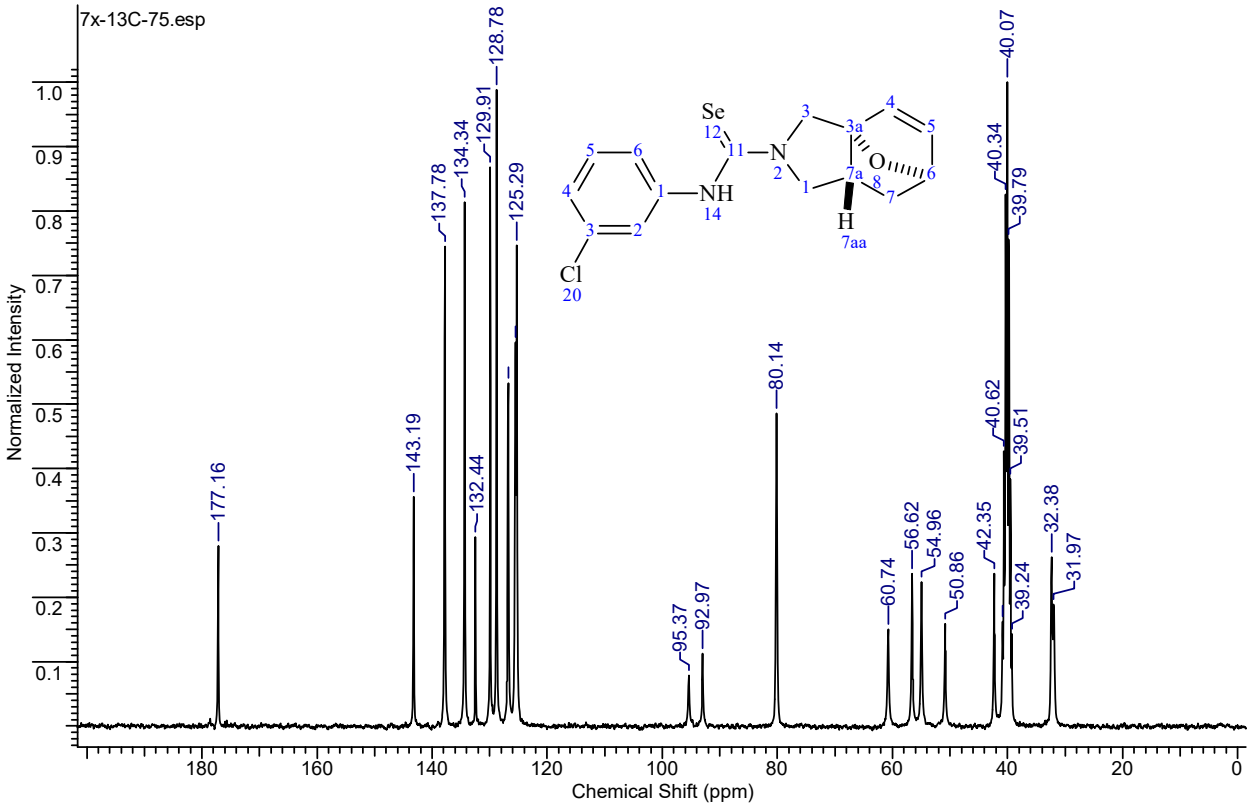
^{77}Se NMR (57.2 MHz, DMSO-d_6, 100 °C)



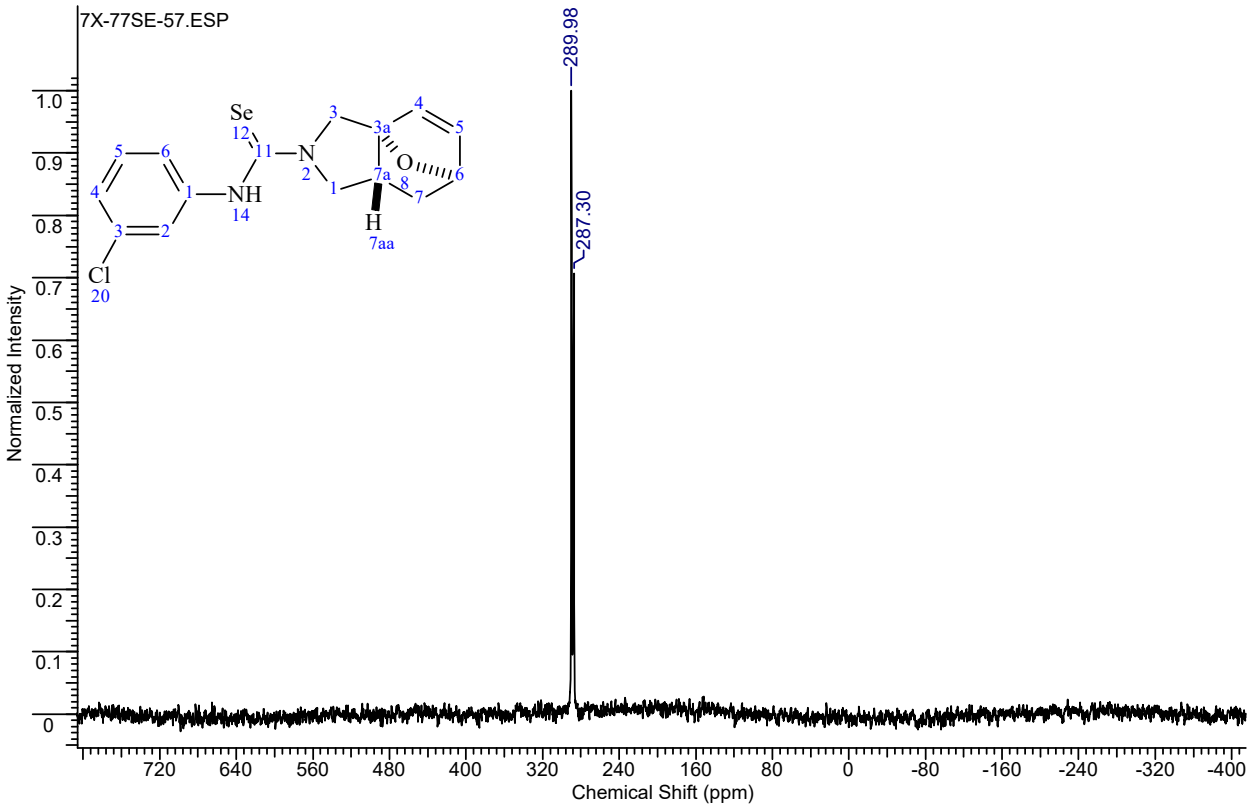
^{1}H NMR (300.1 MHz, DMSO-d_6)



^{13}C NMR (75.5 MHz, DMSO-d_6)



^{77}Se NMR (57.2 MHz, DMSO-d_6)



HSQC of **7x** (100 °C)