Rational design of indolyl acrylamides as antibacterial agents targeting multidrug-resistant *Acinetobacter baumannii* strains

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1. EXPERIMENTAL SECTION

1.1 General Methods

All reagents and solvents used were purchased from Merck and Sigma Aldrich. Formyl-indoles **8a-d** were purified by silica gel 60 Å (230-400 mesh particle size) with Hex: EtOAc. Malonic acid was recrystallized in acetone. All reaction processes were monitored by thin layer chromatography (TLC) analysis on silica gel plates and visualized by a dual short wavelength/long wavelength UV lamp. Flash column chromatography was performed on silica gel 60 Å (230-400 mesh particle size). Melting points were determined in open capillaries using a Mel- Temp apparatus. All final products were purified by thin-layer chromatography plates, SiO_2 60 F_{254} with DCM/MeOH. ^{1}H NMR, ^{13}C NMR and 135 DEPT spectra were recorded at 25°C on a Bruker Fourier-300 MHz, Jeol Eclipse-300 MHz, Bruker Avance III-400 MHz spectrometer in hexadeuterodimethyl sulfoxide (DMSO-d_6), deuterochloroform ($CDCl_3$) or tetradeuteromethanol (MeOD-d_4), The chemical shifts are reported on the δ scale in parts per million (ppm) and calibrated to residual solvents (7.26 ppm in $CDCl_3$; 2.50 ppm in DMSO-d_6; 3.31 ppm in MeOD-d_4) for ^{1}H NMR and ^{13}C NMR (77.16 ppm in $CDCl_3$; 39.50 ppm in DMSO-d_6; 39.75 ppm in MeOD-d_4). High-resolution mass spectra (HRMS) were recorded with JEOL SX 102 A spectrometers by Electrospray ionization (ESI+). Physical and spectroscopic data of all compounds **14a-c**, **15a-c**,**16a-c**, **17a-d**, and **18a-d** are reported in supplementary material.

1.2 General procedure for synthesis of intermediates 14a-c.

1.12 mmol of the corresponding 1-*H*-indole-3-carbaldehyde was dissolved in anhydrous THF and placed under an N_2 atmosphere (0.050 mL); the solution was cooled to 0 °C. Subsequently, sodium hydride NaH (60% in mineral oil, 0.172 g, 4.3 mmol) was added, and the mixture was stirred for 1 hour. Next, a solution of di-tert-butyl dicarbonate (Boc_2O) (0.375 g, 1.72 mmol) dissolved in THF (0.010 mL) was added, and the reaction mixture was stirred for 90 min at room temperature until thin-layer chromatography (TLC) showed total consumption of the starting material, then water (6 mL) was carefully added. The mixture was diluted with ethyl acetate (30 mL), and the organic phase was washed with water (2 × 30 mL) and brine (2 × 30 mL), dried with Na_2SO_4, filtered, and concentrated. The crude product was purified by column chromatography on silica gel (hexane/EtOAc 8:2).

tert-butyl 3-formyl-5-bromo-1H-indole-1-carboxylate (14a)

14a was obtained from **13a** (0.250 g, 1.12 mmol), given as a yellow solid, 0.350 g, yield: 96%, m.p. 161-162 °C, (lit. [1] m.p.162-163°C).

tert-butyl 3-formyl-5-chloro-1H-indole-1-carboxylate (14b)

14b was obtained from **13b** (0.200 g, 1.12 mmol) given as a yellow solid, 0.300 g, yield: 96%, m.p. 157-158 °C, (lit. [2] m.p. 157-158 °C).

tert-butyl 3-formyl-1H-indole-1-carboxylate (14c)

14c was obtained from **13c** (0.162 g, 1.12 mmol) given as a yellow solid 0.245 g yield: 89%, m.p. 127-128 °C, (lit. [2], m.p. 130-132°C).

1.3 General procedure for intermediates 16a-c and 17a-d.

In a round bottom flask was placed 3.5 mmol of the corresponding 1-*H*-indole-3-carbaldehyde in anhydrous DCM (20 mL), then NaOH (10.7 mmol) and benzenetriethylammonium chloride (TEBAC) (0.07 mmol) were added; finally, *p*-toluenesulfonyl chloride (TsCl) or *p*-chlorobenzyl chloride (1.5 mmol, dissolved in 10 mL DCM) was added, and the reaction mixture was stirred for 16 h at room temperature. The reaction mixture was washed 3 times with H_2O, then dried with Na_2SO_4 and concentrated under vacuum. The resulting solid residue was triturated with diethyl ether and the precipitate was collected by filtration to give the desired compound. Compounds that did not precipitate were purified by silica gel flash chromatographic column with 7:3 Hex: EtOAc mixtures.

5-bromo-1-tosyl-1H-indole-3-carbaldehyde (16a).

16a was obtained from **13a** (0.784 g, 3.5mmol) given as a brown solid 1.08 g yield: 81%, m.p. 243-244 °C, (lit. [3] m.p. 243-244°C).

5-chloro-1-tosyl-1H-indole-3-carbaldehyde (16b).

16b was obtained from **13b** (0.628 g, 3.5mmol) given as a withe solid 1.1 g, yield: 94%, m.p. 234-236 °C. ^{1}H NMR (301 MHz, DMSO-d_6) δ 2.33 (s, 3H), 7.32 - 7.55 (m, 3H), 7.89 - 8.14 (m, 4H), 8.95 (d, J = 2.0 Hz, 1H), 10.04 (d, J = 2.2 Hz, 1H). ^{13}C NMR (76 MHz, DMSO-d_6) δ 21.67, 115.49, 121.21, 121.57, 126.84, 127.65, 127.89, 130.41, 131.27, 133.40, 133.65, 140.07, 147.36, 187.25. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{16}H_{13}ClNO_3S$ 334.03047, found: 334.03066.

1-tosyl-1H-indole-3-carbaldehyde (16c)

16c was obtained from **13c** (0.508g, 3.5 mmol) given as a withe solid, 0.99 g, yield: 94%, m.p. 147-149 °C, (lit. [4] mp 148-150°C).

5-bromo-1-(4-chlorobenzyl)-1H-indole-3-carbaldehyde (17a).

17a was obtained from **13a** (0.784 g, 3.5mmol), given as a withe solid 1.10 g, yield: 90%, m.p. 201-202 °C, (lit. [5] m.p. 200-201°C).

5-chloro-1-(4-chlorobenzyl)-1H-indole-3-carbaldehyde (17b).

17b was obtained from **13b** (0.628 g, 3.5mmol), given as a yellow solid 0.9 g, yield: 84%, m.p. 145-147 °C, (lit. [6] m.p. 146-147°C).

1-(4-chlorobenzyl)-1H-indole-3-carbaldehyde (17c).

17c was obtained from **13c** (0.508 g, 3.5mmol), given as a yellow solid 0.9 g, yield: 95%, m.p. 117-119 °C, (lit. [5] m.p. 117-119°C).

5-fluor-1-(4-chlorobenzyl)-1H-indole-3-carbaldehyde (17d).

17d was obtained from **13d** (0.570 g, 3.5mmol), given as a yellow solid 0.930 yield: 92%, m.p. 198-201°C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.32 (s, 2H), 7.02 (ddd, *J* = 10.0, 8.4, 2.5 Hz, 1H), 7.06 – 7.11 (m, 2H), 7.18 (ddd, *J* = 9.0, 4.2, 0.6 Hz, 1H), 7.30 – 7.35 (m, 2H), 7.73 (s, 1H), 7.92 – 8.03 (dd, 1H), 9.96 (s, 1H). ^{13}C NMR (76 MHz, $CDCl_3$) δ 50.76, 107.87 (d, *J* = 24.8 Hz), 111.33 (d, *J* = 9.8 Hz), 112.87 (d, *J* = 26.4 Hz), 118.60, 126.25, 126.40, 128.87 129.55, 133.64, 133.83, 134.64, 139.31, 160.02 (d, *J* = 239.6 Hz), 184.46. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{16}H_{12}ClFNO$ 288.05914, found: 288.05771.

1.4 General procedure for synthesis of intermediates 9a-c, 15a-c and 18a-d.

To 1.22 mmol of the corresponding *N*-substituted 1-*H*-indole-3-carbaldehyde, malonic acid (3.23 mmol) in pyridine anhydrous as solvent (9mL), was added two drops of piperidine and stirred for 12 hours at 100°C. It was then allowed to cool to room temperature, and 9 mL of H_2O was added. Finally, it was acidified with 6 N HCl to a pH of 2, and the precipitate obtained was isolated by vacuum filtration and washed with plenty of water.

(E)-3-(5-bromo-1-tosyl-1H-indol-3-yl)acrylic acid (9a)

9a was obtained from **16a** (1.22 mmol) given as a beige solid (0.470 g). Yield: 91%; m.p. 236-240°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.32 (s, 1H), 6.61 (d, *J* = 16.3 Hz, 1H), 7.37 – 7.43 (m, 2H), 7.72 (d, *J* = 16.2 Hz, 1H), 7.89 – 7.93 (m, 1H), 7.97 (d, *J* = 8.9 Hz, 2H), 8.00 (d, *J* = 2.1 Hz, 1H), 8.50 (s, 1H), 12.38 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ^{13}C NMR (101 MHz, DMSO-d_6) δ 21.08, 115.31, 117.24, 119.81, 123.27, 126.92, 126.96, 128.25, 129.63, 130.52, 130.64, 133.48, 133.58, 134.24, 146.24, 167.55. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{18}H_{15}BrNO_4S$ 419.99052 found: 419.99012.

(E)-3-(5-chloro-1-tosyl-1H-indol-3-yl)acrylic acid (9b)

9b was obtained from **16b** (1.22 mmol) given as a brown solid (0.405 g). Yield: 88%, m.p. 200°C decomp.; ^{1}H NMR (400 MHz, DMSO-d_6) 2.31 (s, 3H), 6.60 (d, *J* = 16.3 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.42 – 7.47 (m, 1H), 7.72 (d, *J* = 16.2 Hz, 1H), 7.88 – 7.93 (m, 2H), 7.94 – 8.02 (m, 2H), 8.50 (s, 1H), 12.37 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 21.07, 114.93, 117.32, 119.78, 120.36, 120.89, 125.56, 126.95, 129.14, 129.18, 130.50, 130.66, 133.25, 133.49, 134.25, 146.22, 167.56. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{18}H_{15}ClNO_4S$ 376.04103, found: 376.04088.

(E)-3-(1-tosyl-1H-indol-3-yl)acrylic acid (9c)

9c was obtained from **16c** (1.22 mmol) given as a brown solid (0.388g). Yield: 93%; m.p. 228-230°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.30 (s, 3H), 6.62 (d, *J* = 16.2 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.39 (dd, *J* = 8.2, 2.8 Hz, 3H), 7.64 (d, *J* = 16.2 Hz, 1H), 7.90 (dd, *J* = 8.1, 4.2 Hz, 2H), 7.96 (d, *J* = 8.3 Hz, 1H), 8.32 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 21.04, 113.42, 118.29, 120.91, 122.06, 124.26, 125.45, 126.88, 127.88, 128.88, 130.39, 132.93, 133.76, 134.84, 145.88, 168.48. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{18}H_{15}NO_4S$ 342.08000, found: 342.07944.

(E)-3-(5-bromo-1-(tert-butoxycarbonyl)-1H-indol-3-yl)acrylic acid (15a)

15a was obtained from **14a** (0.400 g, 1.23 mmol) given as a yellow solid 0.400 g, yield: 88%, m.p. 165-167°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.63 (s, 9H), 6.44 (d, *J* = 16.1 Hz, 1H), 7.42 (dt, *J* = 8.8, 2.0 Hz, 1H), 7.71 (dd, *J* = 16.1, 0.7 Hz, 1H), 7.78 (s, 1H), 7.93 (dt, *J* = 1.9, 1.0 Hz, 1H), 7.98 – 8.05 (m, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 28.09, 85.14, 116.07, 116.95, 117.05, 118.51, 121.07, 122.98, 128.06, 129.09, 129.63, 135.77, 148.77, 169.04.

(E)-3-(1-(tert-butoxycarbonyl)-5-chloro-1H-indol-3-yl)acrylic acid (15b)

15b was obtained from **14b** (0.341 g, 1.22 mmol) given as a yellow solid, 0.345 g, yield: 87%, m.p. 175-176°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 (s, 9H), 6.48 (d, J = 16.1 Hz, 1H), 7.33 (dd, J = 8.9, 2.1 Hz, 1H), 7.75 (dd, J = 16.1, 0.7 Hz, 1H), 7.78 – 7.82 (m, 1H), 7.85 (s, 1H), 8.11 (d, J = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 27.99, 85.02, 116.05, 116.46, 118.50, 119.82, 125.23, 129.03, 129.13, 129.21, 134.44, 135.53, 148.67, 168.82.

(E)-3-(1-(tert-butoxycarbonyl)-1H-indol-3-yl)acrylic acid (15c)

15c was obtained from **14c** (0.300 g, 1.22 mmol) given as a white solid 0.330g, yield: 93%, m.p. 180-182°C. ^{1}H NMR (301 MHz, DMSO-d_6) δ 1.63 (s, 9H), 6.57 (d, *J* = 16.2 Hz, 1H), 7.37 (ddd, *J* = 12.4, 7.8, 1.4 Hz, 2H), 7.79 (d, *J* = 16.2 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 8.04 – 8.14 (m, 1H), 8.26

(s, 1H). ^{13}C NMR (76 MHz, DMSO-d_6) δ 27.37, 84.39, 114.84, 115.85, 117.86, 120.13, 123.48, 124.96, 127.18, 129.45, 135.24, 135.65, 148.40, 167.64.

(E)-3-(5-bromo-1-(4-chlorobenzyl)-1H-indol-3-yl)acrylic acid (18a)

18a was obtained from **17a** (0.425 g, 1.22 mmol) given as a yellow solid 0.430 g, yield: 90%, m.p. 211-214°C. ^{1}H NMR (400 MHz, DMSO-d_6) 5.47 (s, 2H), 6.33 (d, *J* = 16.0 Hz, 1H), 7.25 (d, *J* = 8.5 Hz, 2H), 7.35 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.37 – 7.40 (m, 2H), 7.52 (d, *J* = 8.7 Hz, 1H), 7.77 (d, *J* = 16.0 Hz, 1H), 8.04 (d, *J* = 1.9 Hz, 1H), 8.15 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 48.80, 111.05, 113.18, 113.84, 114.08, 122.25, 125.29, 127.49, 128.70, 129.03, 132.35, 134.75, 135.70, 136.06, 136.82, 168.25. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{18}H_{14}BrClNO_2$ 389.98964, found: 389.98794.

(E)-3-(5-chloro-1-(4-chlorobenzyl)-1H-indol-3-yl)acrylic acid (18b)

18b was obtained from **17b** (0.371 g, 1.22 mmol) given as a yellow solid 0.380 g, yield: 89%, m.p. 200-205°C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.47 (s, 2H), 6.34 (d, *J* = 16.0 Hz, 1H), 7.26 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.41 (m, 2H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 16.0 Hz, 1H), 7.91 (d, *J* = 2.0 Hz, 1H), 8.18 (s, 1H), 12.03 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 48.81, 111.14, 112.75, 113.80, 119.29, 122.69, 126.08, 128.69, 126.86, 129.06, 132.34, 134.96, 135.45, 136.10, 136.82, 168.25. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{18}H_{14}Cl_2NO$ 346.04016, found: 346.04103.

(E)-3-(1-(4-chlorobenzyl)-1H-indol-3-yl)acrylic acid (18c)

18c was obtained from **18c** (0.329 g, 1.22 mmol) given as a beige solid 0.320 g, yield: 84%, m.p. 188-190°C decomp. (lit. [7]m.p.187-190°C decomp.).

(E)-3-(1-(4-chlorobenzyl)-5-fluor-1H-indole-3-yl)acrylic acid (18d)

18d was obtained from **17d** (0.351 g, 1.22 mmol) given as a yellow solid 0.350 g, yield: 87%, m.p. 99-102°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.31 (s, 2H), 6.33 (dd, *J* = 16.0, 1.9 Hz, 1H), 6.98 (tt, *J* = 9.0, 2.4 Hz, 1H), 7.03 – 7.13 (m, 2H), 7.19 (ddd, *J* = 8.9, 4.4, 1.9 Hz, 1H), 7.25 – 7.35 (m, 2H), 7.46 – 7.60 (m, 2H), 7.83 (d, *J* = 16.1, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 50.20, 106.06 (d, *J* = 24.4 Hz), 111.42 (d, *J* = 3.3 Hz), 111.60 (d, *J* = 20.1 Hz), 112.79, 114.11, 120.6, 127.09, 128.37, 129.28, 133.48, 134.03, 134.78, 137.48, 158.98 (d, *J* = 237.9 Hz), 169.80. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{18}H_{14}ClFNO_2$ 330.06971, found: 330.06994.

1.5 General procedure for 10a-c.

(0.273 mmol) of the corresponding 3-(1-(*tert*-butoxycarbonyl)-1*H*-indol-3-yl)acrylic acid was dissolved in 4.5 mL of DCM, and then 0.5 mL of trifluoroacetic acid (TFA) was added dropwise. The reaction was stirred for one hour at room temperature, and a precipitate was formed, which was finally separated by vacuum filtration.

(E)-3-(5-bromo-1H-indol-3-yl)acrylic acid (10a)

10a was obtained from **15a** (0.273 mmol) given as a purple solid, (0.050 g). Yield: 68%; m.p. 291-293°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.29 (d, *J* = 16.0 Hz, 1H), 7.31 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 16.0 Hz, 1H), 7.97 (dd, *J* = 10.7, 2.3 Hz, 2H), 11.91 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 111.08, 112.82, 113.25, 114.12, 121.68, 124.76, 126.59, 131.96, 135.80, 137.47, 168.17. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{11}H_9BrNO_2$ 265.98167, found: 265.98189.

(E)-3-(5-chloro-1H-indol-3-yl)acrylic acid (10b)

10b was obtained from **15b** (0.273 mmol) given as a green solid, (0.047 g). Yield: 77%; m.p. 274-277°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.29 (d, *J* = 16.0 Hz, 1H), 7.20 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.47 (d, *J* = 8. 6 Hz, 1H), 7.78 (d, *J* = 16.0 Hz, 1H), 7.84 (d, *J* = 2.1 Hz, 1H), 7.96 (d, *J* = 2.9 Hz, 1H), 11.87 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 111.19, 112.76, 113.62, 118.70, 122.16, 125.25, 125.92, 132.08, 135.54, 137.47, 168.18. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{11}H_9ClNO_2$ 222.03218, found: 222.03281.

(E)-3-(1H-indol-3-yl)acrylic acid (10c)

10c was obtained from **15c** (0.273 mmol) given as a red solid **(**0.040 g). Yield: 78%; m.p. 125°C decomp.; ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.31 (d, *J* = 16.0 Hz, 1H), 7.16 (ddd, *J* = 8.4, 7.1, 1.4 Hz, 1H), 7.21 (ddd, *J* = 7.9, 7.1, 1.4 Hz, 1H), 7.41 – 7.49 (m, 1H), 7.81 (d, *J* = 15.9 Hz, 1H), 7.85 (s, 1H), 7.90 (d, *J* = 2.9 Hz, 1H), 11.72 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 112.10, 112.57, 112.76, 120.19, 121.25, 122.85, 125.44, 131.71, 137.78, 138.96, 169.03. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{11}H_{10}NO_2$ 188.07115, found: 188.07039.

1.6 General protocol for the synthesis of 11a-h, 11a' and 12a-j.

0.500 mol of the corresponding indolylacrylic acid was dissolved in 26 mL of a DCM: DMF (3:1 v/v) mixture. Subsequently, DIPEA (0. 500 mmol) and HBTU (0.500 mmol) were added, and the mixture was stirred for 1 hour at room temperature. Finally, piperazine (2.5 mmol) was added and the reaction was stirred for 12 hours at room temperature. The DCM was evaporated, and the reaction crude was dissolved in ethyl acetate, followed by three washes with a 5% LiCl solution, and the organic phase was dried with Na_2SO_4. The crude was purified using a preparative TLC plate with a 9:1 DCM/MeOH mixture.

(E)-3-(5-bromo-1-tosyl-1H-indol-3-yl)-1-(piperazin-1-yl)prop-2-en-1-one (11a)

11a was obtained from **9a** (0.5 mmol) given as a yellow solid **(**0.06g). Yield: 24%; m.p. 106-108°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.36 (s, 3H), 2.92 – 3.09 (m, 4H), 3.63 – 3.86 (m, 4H), 6.87 (d, J = 15.5 Hz, 1H), 7.27 (s, 2H), 7.46 (dd, J = 8.8, 1.9 Hz, 1H), 7.72 (d, J = 15.5 Hz, 1H), 7.74 – 7.78 (m, 2H), 7.83 (d, J = 10.0 Hz, 2H), 7.87 (d, J = 8.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.72, 45.71, 115.36, 117.49, 117.70, 118.27, 123.26, 127.03, 128.07, 128.43, 130.27, 130.29, 133.37, 134.29, 134.59, 145.91, 165.45. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{22}H_{23}BrN_3O_3S$ 488.06435. found: 488.06594.

(E)-3-(5-chloro-1-tosyl-1H-indol-3-yl)-1-(piperazin-1-yl)prop-2-en-1-one (11b)

11b was obtained from **9b** (0.500 mmol) given as a yellow solid **(**0.058g). Yield: 26%; m.p. 102-105°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.35 (s, 3H), 3.02 (s, 4H), 3.76 (s, 4H), 6.87 (d, J = 15.5 Hz, 1H), 7.21 – 7.28 (m, 2H), 7.32 (dd, J = 8.9, 2.0 Hz, 1H), 7.63 – 7.72 (m, 2H), 7.76 (d, J = 7.8 Hz, 2H), 7.84 (s, 1H), 7.92 (d, J = 8.9 Hz, 1H). ^{13}C NMR (76 MHz, $CDCl_3$) δ 21.74, 42.39, 45.57, 115.00, 117.38, 118.38, 120.24, 125.77, 127.05, 128.35, 129.77, 130.06, 130.30, 133.47, 133.94, 134.58, 145.92, 165.46. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{22}H_{23}ClN_3O_3S$ 444.11486. found: 444.11471.

(E)-1-(piperazin-1-yl)-3-(1-tosyl-1H-indol-3-yl)prop-2-en-1-one (11c).

11c was obtained from **9c** (0.5 mmol) given as a yellow solid (0. 08g). Yield: 39%; m.p. 106-109°C; ^{1}H NMR (301 MHz, $CDCl_3$) δ 2.34 (s, 3H), 2.94 (t, *J* = 5.1 Hz, 4H), 3.69 (s, 4H), 6.94 (d, *J* = 15.5 Hz, 1H), 7.17 – 7.28 (m, 2H), 7.27 – 7.45 (m, 2H), 7.74 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.77 (d, *J* = 1.9 Hz, 1H), 7.78 – 7.83 (m, 3H), 7.94 – 8.09 (m, 1H).^{13}C NMR (75 MHz, $CDCl_3$) δ 21.70, 45.51, 113.96, 116.90, 118.92, 120.46, 124.05, 125.49, 127.05, 127.32, 128.54, 130.17, 134.15, 134.84, 135.61, 145.58, 165.67. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{22}H_{24}N_3O_3S$ 410.15384 found: 410.15296.

(E)-1-(4-methylpiperazin-1-yl)-3-(1-tosyl-1H-indol-3-yl)prop-2-en-1-one (11d)

11d was obtained from **9c** (0.500 mmol) given as a yellow solid **(**0.105g). Yield: 49%; m.p.147-150°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.34 (s, 3H), 2.37 (s, 3H), 2.51 (t, *J* = 5.1 Hz, 4H), 3.65 – 3.87 (m, 4H), 6.94 (d, *J* = 15.5 Hz, 1H), 7.24 (dd, *J* = 8.7, 0.7 Hz, 2H), 7.27 – 7.41 (m, 2H), 7.71 – 7.76 (m, 2H), 7.82 (d, *J* = 3.5 Hz, 3H), 7.97 – 8.03 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.73, 42.06, 45.65, 45.96, 54.63, 55.27, 114.01, 117.24, 119.05, 120.49, 124.06, 125.50, 127.07, 127.21, 128.64, 130.19, 133.90, 134.95, 135.68, 145.57, 165.56. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{23}H_{26}N_3O_3S$ 424.16949 found: 424.16874.

(E)-1-morpholino-3-(1-tosyl-1H-indol-3-yl)prop-2-en-1-one (11e)

11e was obtained from **9c** (0.500 mmol) given as a yellow solid **(**0.140 g). Yield: 68%; m.p.135-140°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.34 (s, 3H), 3.64 – 3.80 (m, 8H), 6.92 (d, *J* = 15.6 Hz, 1H), 7.18 – 7.26 (m, 2H), 7.27 – 7.41 (m, 2H), 7.71 – 7.78 (m, 2H), 7.78 – 7.87 (m, 3H), (d, *J* = 7.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.59, 42.58, 46.27, 66.86, 113.89, 116.64, 118.82, 120.35, 123.96, 125.40, 125.54, 126.95, 127.26, 128.45, 130.07, 134.12, 134.80, 135.55, 145.48, 165.65. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{22}H_{23}N_2O_4S$: Anal. Calcd. 411.13785, found: 411.13776.

(E)-1-thiomorpholino-3-(1-tosyl-1H-indol-3-yl)prop-2-en-1-one (11f).

11f was obtained from **9c** (0.500 mmol) given as a yellow solid **(**0.140 g). Yield: 65%; m.p. 120-124°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 3H), 2.64 - 2.71 (m, 4H), 3.97 (m, 4H). 6.91 (d, *J* = 15.5 Hz, 1H), 7.23 (d, *J* = 0.7 Hz, 2H), 7.28 - 7.41 (m, 2H), 7.73 (ddt, *J* = 7.8, 1.4, 0.7 Hz, 1H), 7.75 - 7.81 (m, 3H), 7.82 (s, 1H), 8.00 (ddt, *J* = 8.3, 1.3, 0.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.55, 27.42, 27.88, 45.10, 48.78, 113.95, 117.01, 118.85, 123.94, 125.40, 126.97, 127.18, 128.48, 130.17, 134.11, 134.78, 135.55, 145.32, 165.10. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{22}H_{23}N_2O_3S_2$: Anal. Calcd: 427.11501, found: 427.11528.

(E)-N-(2-aminoethyl)-3-(5-bromo-1-tosyl-1H-indol-3-yl)acrylamide (11g)

11g was obtained from **9a** (0.500 mmol) given as a yellow solid **(**0.05g). Yield: 21%; m.p. 123-125°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 2.32 (s, 3H), 2.71 (t, *J* = 6.3 Hz, 2H), 3.26 (q, *J* = 6.3 Hz, 2H), 6.81 (d, *J* = 16.1 Hz, 1H), 7.39 - 7. 43 (m, 2H), 7.46 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.53 (d, *J* = 16.1 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.98 - 8.01 (m, 2H), 8.34 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 21.10, 40.61, 40.84, 115.12, 117.89, 118.52, 120.46,

122.85, 125.49, 126.93, 129.02, 129.12, 129.35, 130.49, 133.53, 146.15, 165.30. HRMS (ESI+) m/z $[M+H]^+$ Calcd for $C_{20}H_{21}BrN_3O_3S$: 462.04870; found: 462.04803.

(E)-N-(2-aminoethyl)-3-(5-chloro-1-tosyl-1H-indol-3-yl)acrylamide (11h).

11h was obtained from **9b** (0.500 mmol) given as a yellow solid **(**0.055 g). Yield: 26%; m.p. 119-123°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.34 (s, 3H), 2.96 (t, *J* = 5.8 Hz, 2H), 3.49 (d, *J* = 5.8 Hz, 2H), 6.48 (d, *J* = 15.8 Hz, 1H), 7.18 – 7.26 (m, 2H), 7.41 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.59 – 7.68 (m, 1H), 7.70 – 7.79 (m, 3H), 7.80 – 7.88 (m, 2H).^{13}C NMR (75 MHz, $CDCl_3$) δ 21.64, 41.15, 41.59, 115.21, 117.61, 117.82, 121.38, 123.38, 126.95, 128.24, 130.03 130.03, 130.19, 131.25, 134.24, 134.49, 145.77, 166.13. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{20}H_{21}ClN_3O_3S$; 418.09921. found: 418.09871.

1-(piperazin-1-yl)-3-(1-tosyl-1H-indol-3-yl)propan-1-one (11a').

11a' was obtained from **20** (0.500 mmol) given as a yellow solid **(**0.090 g). Yield: 43%; m.p. 149-152°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 2.64 - 2.69 (m, 2H), 2.73 (t, 2H), 2.81 (t, *J* = 4.2 Hz, 2H), 2.94 - 3.09 (m, 2H), 3. 36 (t, 2H), 3.61 (t, 2H), 7.16 - 7.22 (m, 2H), 7.23 - 7.36 (m, 5H), 7. 50 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.97 (d, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.73, 21.68, 32.68, 42.71, 45.86, 46.21, 46.64, 113.84, 119.55, 122.27, 122.90, 123.22, 124.89, 126.89, 129.96, 130.86, 135.35, 135.41, 144.94, 170.52. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{22}H_{26}N_3O_3S$: 412.16949; found: 412.16994.

(E)-3-(5-bromo-1-(4-chlorobenzyl)-1H-indol-3-yl)-1-(piperazin-1-yl)prop-2-en-1-one (12a)

12a was obtained from **18a** (0.500 mmol) given as a yellow solid **(**0.100 g). Yield: 43%; m.p. 159-161°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 2.71 (s, 4H), 3.44 - 3.69 (m, 4H), 5.45 (s, 2H), 6.97 (d, *J* = 15.4 Hz, 1H), 7.24 (d, *J* = 8.5 Hz, 2H), 7. 33 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 15.4 Hz, 1H), 8.07 - 8.13 (m, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 45.82, 46.25, 48.74, 111.95, 112.95, 113.09, 113.50, 113.75, 122.25, 125.10, 127.61, 128.70, 129.01, 132.31, 133.51, 133.94, 135.54, 136.28, 165.25. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{22}H_{22}BrClN_3O$: 458.06348; found: 458.06246.

(E)-3-(5-chloro-1-(4-chlorobenzyl)-1H-indol-3-yl)-1-(piperazin-1-yl)prop-2-en-1-one (12b)

12b was obtained from **18b** (0.5 mmol) given as a yellow solid **(**0.096 g). Yield: 46%; m.p. 208-210°C; ^{1}H NMR (300 MHz, MeOD-d_4) δ 2.96 (t, 4H), 3.77 (t, 4H), 5.39 (s, 2H), 6.93 (d, *J* = 15.4 Hz, 1H), 7.12 – 7.17 (m, 2H), 7.20 (d, *J* = 2.0 Hz, 1H), 7.28 – 7.32 (m, 2H), 7.35 (dd, *J* = 8.8, 0.5 Hz, 2H), 7.82 – 7.85 (m, 1H), 7.87 (dd, *J* = 2.0, 0.6 Hz, 1H). ^{13}C NMR (75 MHz, CD_3OD-d_4) δ 46.28, 50.51, 112.64, 113.05, 113.73, 120.52, 124.11, 128.16, 128.78, 129.68, 129.94, 134.66, 137.03, 137.13, 137.28, 137.33, 168.74. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{22}H_{22}Cl_2N_3O$: 414.11399; found: 414.11447.

(E)-3-(1-(4-chlorobenzyl)-1H-indol-3-yl)-1-(piperazin-1-yl)prop-2-en-1-one (12c)

12c was obtained from **18c** (0.500 mmol) given as a yellow solid **(**0.09 g). Yield: 47%; m.p. 97-100°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.91 – 3.07 (m, 4H), 3.72 – 3.83 (m, 4H), 5.29 (s, 2H), 6.85 (d, *J* = 15.3 Hz, 1H), 7.01 – 7.08 (m, 2H), 7.22 – 7.31 (m, 5H), 7.40 (s, 1H), 7.86 – 7.90 (m, 1H), 7.93 (d, *J* = 15.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 45.78, 45.84, 49.91, 110.53, 111.97, 113.58, 120.69, 121.46, 123.27, 126.51, 128.31, 129.29, 131.79, 134.04, 134.99, 135.04, 136.60, 136.89, 137.58, 166.77. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{22}H_{23}ClN_3O$: 380.15296; found: 380.15150.

(E)-3-(1-(4-chlorobenzyl)-1H-indol-3-yl)-1-(4-methylpiperazin-1-yl)prop-2-en-1-one (12d)

12d was obtained from **18c** (0.500 mmol) given as a yellow solid **(**0.08 g), Yield: 40%; m.p. 97-100°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.39 (s, 3H), 2.55 (t, *J* = 5.0 Hz, 4H), 3.80 (s, 4H), 5.29 (s, 2H), 6.86 (d, *J* = 15.3 Hz, 1H), 7.05 (dd, *J* = 8.7, 0.8 Hz, 2H), 7.25 (dd, *J* = 3.3, 0.8 Hz, 3H), 7.26 – 7.30 (m, 2H), 7.39 (s, 1H), 7.85 – 7.90 (m, 1H), 7.92 – 7.97 (m, 1H).^{13}C NMR (75 MHz, $CDCl_3$) δ 45.84, 49.89, 55.06, 110.52, 112.08, 113.59, 120.68, 121.44, 123.25, 126.51, 128.29, 129.28, 131.69, 134.03, 135.04, 136.50, 137.56, 166.65. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{23}H_{25}ClN_3O$ 394.16861, found: 394.16806.

(E)-N-(2-aminoethyl)-3-(5-bromo-1-(4-chlorobenzyl)-1H-indol-3-yl)acrylamide (12e).

12e was obtained from **18a** (0.500 mmol) given as a yellow solid (0.049 g). Yield: 22%; m.p. 157-160°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 2.67 (t, *J* = 1.6 Hz, 2H), 3.21 (q, 2H), 5.43 (s, 2H), 6.60 (d, *J* = 15.9 Hz, 1H), 7. 16 - 7.29 (m, 2H), 7.29 - 7.38 (m, 3H), 7.43 - 7.57 (m, 2H), 7.89 - 8.01 (m, 2H), 8.05 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 41.21, 41.68, 48.62, 111.55, 113.11, 113.76, 117.74, 122.48, 125.06, 127.19, 128.68, 129.01, 131.38, 132.28, 134.41, 135.79, 136.28, 166.09. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{20}H_{20}BrClN_3O$; 432.04783, found: 432.04583.

(E)-N-(2-aminoethyl)-3-(5-chloro-1-(4-chlorobenzyl)-1H-indol-3-yl)acrylamide (12f).

12f was obtained from **18b** (0.500 mmol) given as a yellow solid **(**0.055 g). Yield: 28%; m.p. 168-169°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 2.66 (t, *J* = 6.4 Hz, 2H), 3.20 (q, *J* = 6.1 Hz, 2H), 5.45 (s, 2H), 6.60-6.65 (d, *J*=16.01 Hz, 1H), 7.16 - 7.25 (m, 2H), 7. 32 - 7.38 (m, 2H), 7.49 (d, *J* = 5.7 Hz, 2H), 7.54 (d, *J* = 1.4 Hz, 1H), 7.87 - 7.92 (m, 1H), 7.94 - 7.99 (m, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 41.04, 41.30, 48.68, 111.64, 112.68, 117.66, 119.52, 122.50, 125.75, 126.57, 128.69, 129.03, 131.48, 132.31, 134.56, 135.55, 136.28, 166.21. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{20}H_{20}Cl_2N_3O$; 388.09834, found: 388.09741.

(E)-N-(2-aminoethyl)-3-(1-(4-chlorobenzyl)-1H-indol-3-yl)acrylamide (12g).

12g was obtained from **18c** (0.500 mmol) given as a yellow solid **(**0.046 g). Yield: 26%; m.p. 85°C decomp.; ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.70 (t, *J* = 6.4 Hz, 2H), 3.25 (q, *J* = 6.0 Hz, 2H), 5.44 (s, 2H), 6.67 (d, *J* = 15.9 Hz, 1H), 7.15 – 7.22 (m, 2H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.37 (dd, *J* = 8.4, 1.6 Hz, 2H), 7.44 – 7.66 (m, 2H), 7.92 (s, 1H), 8.10 (t, *J* = 5.6 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 40.85, 41.20, 48.27, 110.78, 111.75, 116.97, 120.02, 120.51, 122.29, 125.46, 128.40, 128.79, 131.79, 131.96, 132.74, 136.36, 136.79, 166.14. HRMS (ESI+) m/z $[M+H]^+$ calcd $C_{20}H_{21}ClN_3O$: Calcd. for. 354.13731. found: 354.13696.

(E)-N-(2-aminoethyl)-3-(1-(4-chlorobenzyl)-5-fluoro-1H-indol-3-yl)acrylamide (12h).

12h was obtained from **18d** (0.500 mmol) given as a yellow solid **(**0.08 g). Yield: 43%; m.p. 98-100°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.71 (t, *J* = 6.2 Hz, 2H), 3.25 (t, *J* = 5.9 Hz, 2H), 5.44 (s, 2H), 6.62 (d, *J* = 15.9 Hz, 1H), 7.07 (td, *J* = 9. 2, 2.5 Hz, 1H), 7.21 - 7.27 (m, 2H), 7.34 - 7.40 (m, 2H), 7.48 - 7.57 (m, 2H), 7.68 (dd, *J* = 10.2, 2.5 Hz, 1H), 7.99 (s, 1H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 40.69, 40.77, 48.74, 105.39 (d, *J* = 24.5 Hz), 110.57 (d, *J* = 25.9 Hz), 111.97 (d, *J* = 4.4 Hz), 117.39, 125.81, 125.91, 128.68, 129.04, 131.54, 132.27, 133.69, 134.63, 136.40, 158.11 (d, *J* = 234.1 Hz), 166.29. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{20}H_{20}ClFN_3O$: Anal. Calcd. 372.12789. found: 372.12604.

(E)-N-(3-aminopropyl)-3-(5-bromo-1-(4-chlorobenzyl)-1H-indol-3-yl)acrylamide (12i).

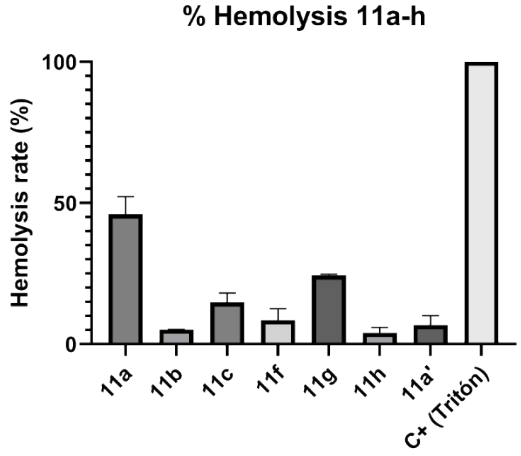
12i was obtained from **18a** (0.500 mmol) given as a yellow solid **(**0.029 g). Yield: 16%; m.p. 170°C decomp.; ^{1}H NMR (300 MHz, MeOD-d_4) δ 1.87 (q, 2H), 2.92 (t, *J* = 7.2 Hz, 2H), 3.42 (t, *J* = 6.6 Hz, 2H), 5. 39 (s, 2H), 6.58 (d, *J* = 15.8 Hz, 1H), 7.14 (d, *J* = 8.5 Hz, 2H), 7.27 - 7.35 (m, 4H), 7.63 - 7.85 (m, 2H), 8.05 (t, *J* = 1.2 Hz, 1H). ^{13}C NMR (75 MHz, MeOD-d_4) δ 30.21, 37.16, 38.65, 50.46, 113.30, 113.54, 115.62, 116.85, 123.88, 126.75,

129.15, 129.67, 129.96, 134.73, 134.86, 135.02, 137.10, 137.63, 170.44. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{21}H_{22}ClBrN_3O$; 446.06348, found: 446.06478.

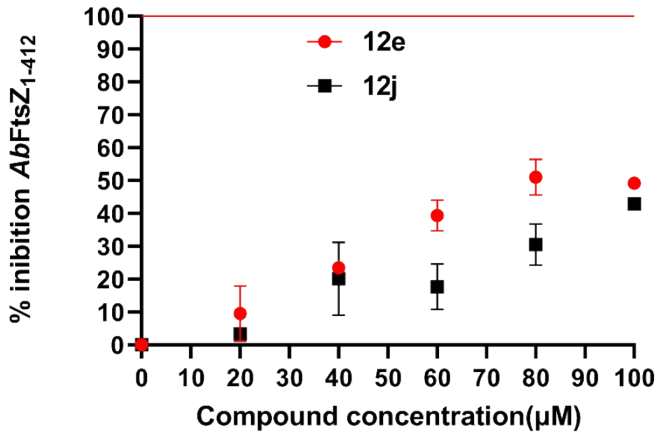
(E)-N-(4-aminobutyl)-3-(5-bromo-1-(4-chlorobenzyl)-1H-indol-3-yl)acrylamide (12j).

12j was obtained from **18a** (0.500 mmol) given as a yellow solid **(**0.025 g). Yield: 13%; m.p. 95-98°C; ^{1}H NMR (300 MHz, MeOD-d_4) δ 1.59 – 1.77 (m, 4H), 2.99 (t, *J* = 6.6 Hz, 2H), 3.37 (t, *J* = 6.5 Hz, 2H), 5.40 (s, 2H), 6.58 (d, *J* = 15.9 Hz, 1H), 7.12 – 7.20 (m, 2H), 7.26 – 7.33 (m, 4H), 7.66 – 7.75 (m, 2H), 8.06 (t, *J* = 1.2 Hz, 1H). ^{13}C NMR (75 MHz, MeOD-d_4) δ 25.92, 27.65, 39.51, 40.40, 50.45, 113.31, 113.55, 115.60, 117.14, 117.42, 123.88, 126.74, 129.12, 129.67, 129. 96, 134.64, 134.99, 137.11, 137.65, 170.03. HRMS (ESI+) m/z $[M+H]^+$ Calcd. for $C_{22}H_{24}BrClN_3O$: 460.07913; found: 460.07892.

1.7 Hemolysis of 11a-h and 11a' at 40 µg mL^{-1}



1.8 % Inhibition *Ab*FtsZ$_{1-412}$ vs concentration µM of 12e and 12j.



1.9 % Bacterial inhibition of 9a-c and 10a-c

Table S1. % Inhibition of bacterial growth (50 µg mL^{-1})

	A. baumannii BAA ATCC 747	*A. baumannii* ATCC 17978	*A. baumannii* A-564 (XDR)
10a	36.13 ± 0.092	2.654 ± 0.098	24.311 ± 0.086
10b	36.72 ± 0.127	9.710 ± 0.024	28.908 ± 0.100
10c	41.47 ± 0.061	12.21 ± 0.022	28.137 ± 0.050
9a	72.03 ± 0.093	21.10 ± 0.091	39.502 ± 0.045
9b	100 ± 0.063	13.70± 0.015	14.898 ± 0.039
9c	57.33 ± 0.020	43.19 ±.0.035	19.782 ± 0.036

1.10 Table S2. *In vitro* antimicrobial activity of indolyl acrylamides **11a-g, 12a, 12e, 12f, 12i** and **12j, MIC** (μM and μg mL^{-1}).

Table S2. *In vitro* antimicrobial activity of indolyl acrylamides 11a-g and 12a, 12e, 12f, 12i and 12j, MIC (μM and μg mL^{-1}).

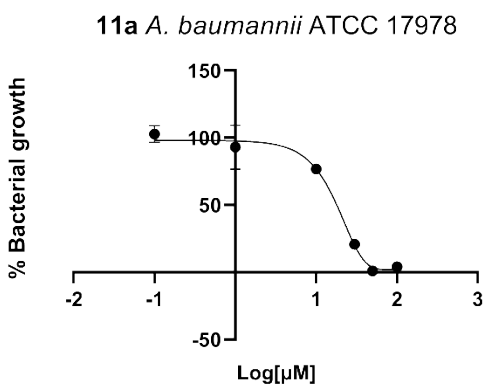
Compounds	*A. b* 17978[a]		*A. b* BAA 747[b]		*A. b* A-564 (XDR)[c]		*S. a clinic (*MRSA)[f]	
	μM	μg mL^{-1}	μM	μg mL^{-1}	μM	μg mL^{-1}	μM	μg mL^{-1}
11a	39	19.0±1.1*	**16**	**7.8±1.2***	**65**	**31.7**	100	48.8
11b	44.6	19.7±1.0*	**17**	**7.5±1.2***	**100**	**44.3**	NT	NT
11c	>150	>61.3	**50**	**20.4**	**150**	**61.3**	>150	>61
11d	**>150**	**>63.5**	**>50**	**>21.1**	**>250**	**>105.8**	>150	>63
11e	**>150**	**>61.5**	**>150**	**>61.5**	**>250**	**>102.6**	>150	>61
11f	**>150**	**>63.9**	**>150**	**>63.9**	**>250**	**>106.6**	>250	>106
11g	**18**	**8.3±1.0***	**7**	**3.2±2.3***	**22**	**10.2±1.1***	19	8.9±3.4*
11a'	**>150**	**>61.6**	**>100**	**>41.1**	**125**	**51.3**	NT	NT
12a	46	20.9±1.1*	**10**	**4.5±1.2***	**30**	**13.7±1.1***	>50	>22
12e	**16**	**7.1±1.1***	**3**	**1.2±2.6***	**10**	**4.3±1.1***	**7.6**	**3.2±1.1***
12f	19	7.4±1.0*	15	5.9±3.5*	21	8.8±1.1*	**5.5**	**2.1±2.1***
12i	22	10.23±1.0*	**21**	**9.5±1.0***	**34**	**15.4±1.1***	13	6.2±1.2*
12j	18	8.3±1.1*	**9**	**4.4±1.1***	**2.6**	**1.2±1.3***	18	8.2±1.9*
Cefepime	32	15.3	**32**	**15.3**	**>133**	**>64**	NT	NT
Meropenem	NT	NT	NT	NT	>133	>32	NT	NT
Gentamicin	2	0.95	2	0.95	>134	>64	NT	NT
Ciprofloxacin	NT	NT	NT	NT	NT	>50	NT	NT
Penicillin G	NT	NT	NT	NT	NT	NT	>250	>84

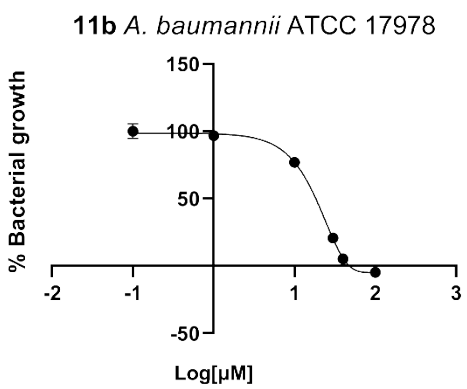
[a]*A.b*.17978, *Acinetobacter baumannii* ATCC 17978; [b]*A.b*. BAA 747, *Acinetobacter baumannii* ATCC BAA 747; [c]*A.b*. A-564 (XDR), *Acinetobacter baumannii* A-564 (XDR); [f]*S.a*. *MRSA*, penicillin-methicillin-resistant *Staphylococcus aureus*; MIC values were calculated with Gompertz equation GraphPad Prism 9.5.1, (n=3). NT= No test

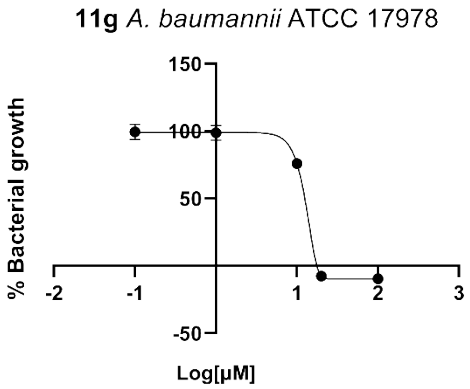
1.11 Table S3. Comparation of potency between the compounds analyzed and cefepime expressed µM and µg mL^{-1}

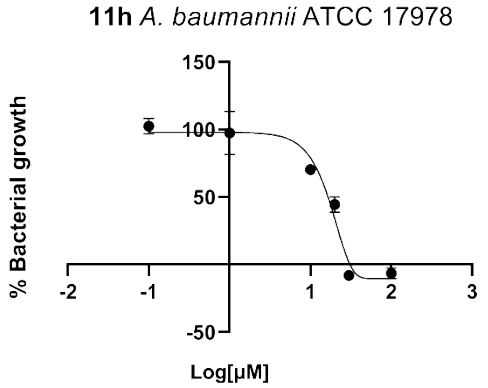
Table S3. Comparation of potency between the compounds analyzed and cefepime expressed µM and µg mL^{-1}								
Compounds	***A. b* BAA 747[b]**		**Potency**		***A. b* A-564 (XDR)**		**Potency**	
	µM	µg mL^{-1}	µM	µg mL^{-1}	µM	µg mL^{-1}	µM	µg mL^{-1}
11a	16	**7.8±1.2***	2	2	65	**31.7**	2	2
11b	17	**7.5±1.2**	1.9	2	100	**44.3**	1.3	1.4
11g	7	**3.2±2.3***	4.5	4.7	22	**10.2±1.1***	6	6.4
12a	10	**4.5±1.2***	3.2	3.4	30	**13.7±1.1***	4.4	4.6
12e	3	**1.2±2.6***	10	12	10	**4.3±1.1***	13	14.9
12j	9	**4.4±1.1***	3.5	3.4	2.6	**1.2±1.3**	51	53
Cefepime	>32	**15.3**	-	-	>133	**>64**	-	-

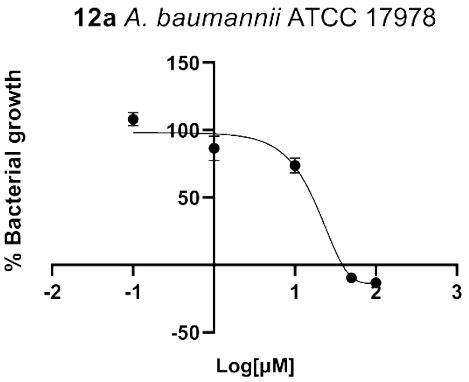
1.12 MIC´s curves

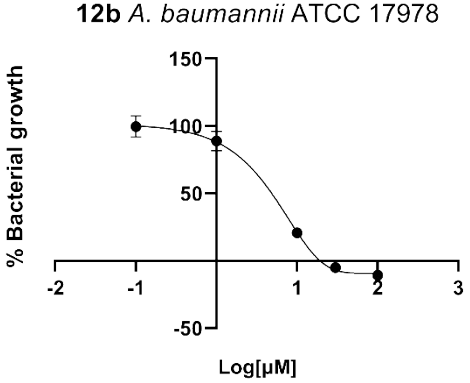




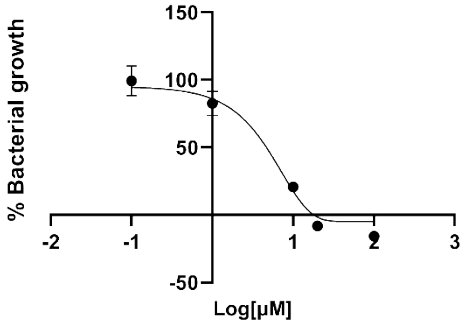




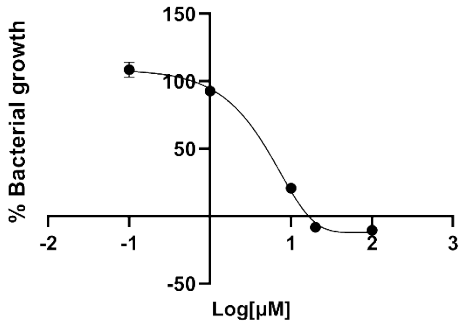




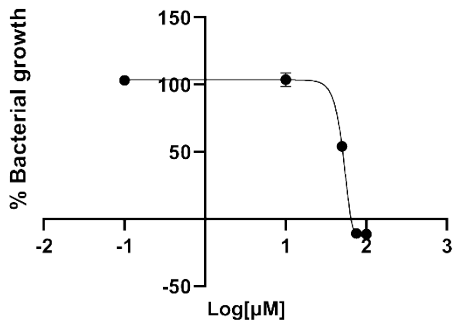
12e *A. baumannii* ATCC 17978



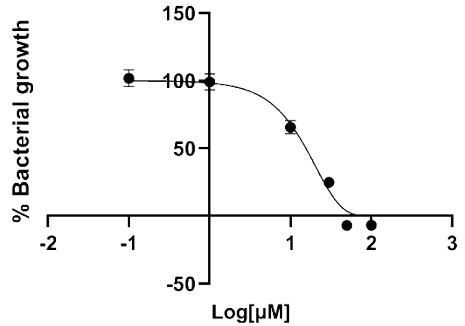
12f *A. baumannii* ATCC 17978



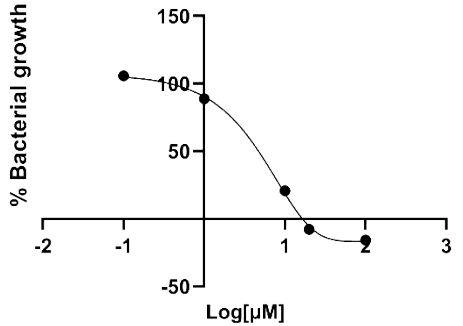
12g *A. baumannii* ATCC 17978



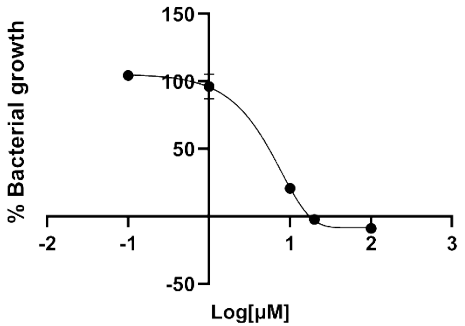
12h *A. baumannii* ATCC 17978

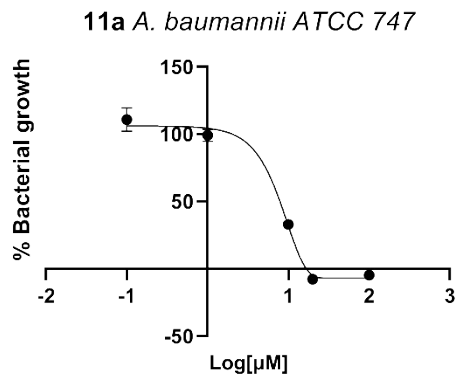


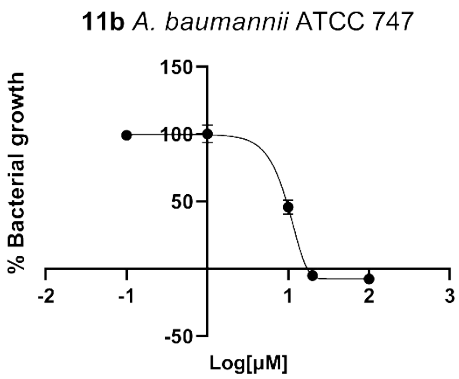
12i *A. baumannii* ATCC 17978

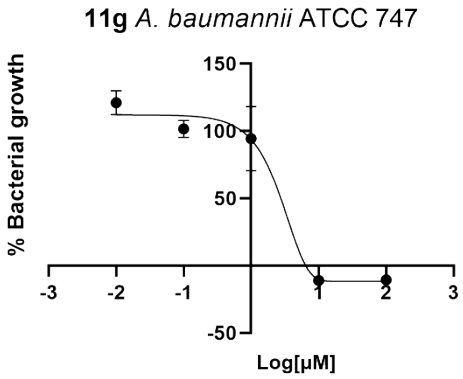


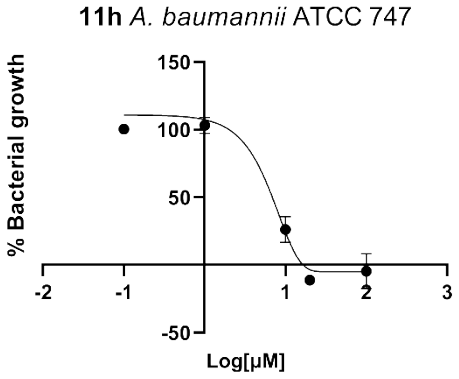
12j *A. baumannii ATCC 17978*

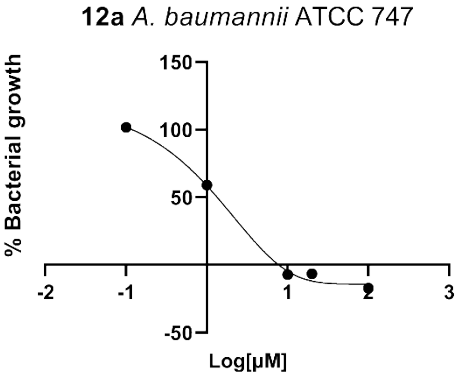


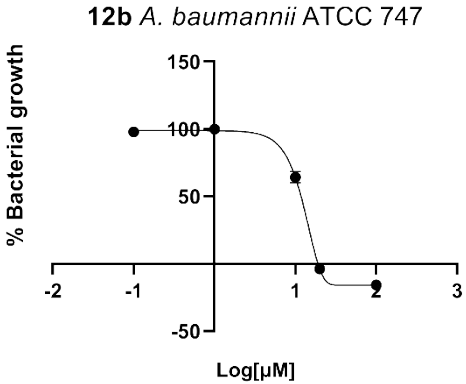

11a A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]

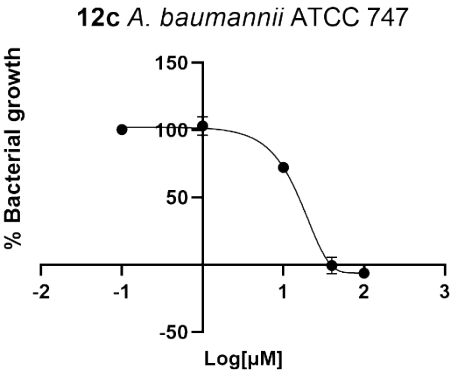

11b A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]

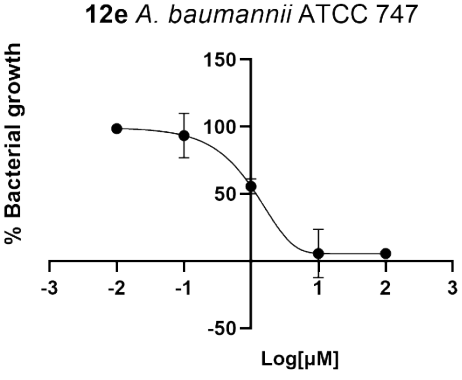

11g A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-3
-2
-1
1
2
3
Log[μM]

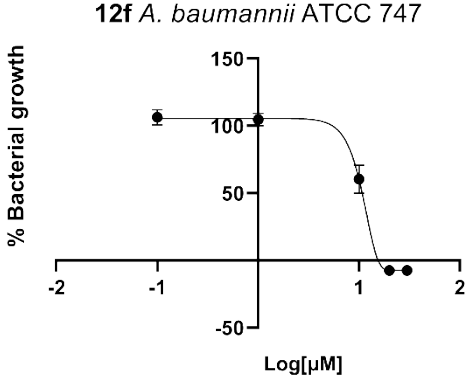

11h A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]


12a A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]

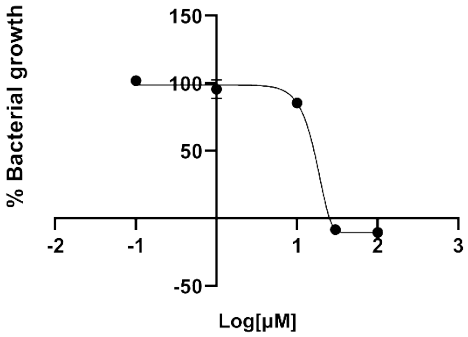

12b A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]


12c A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]

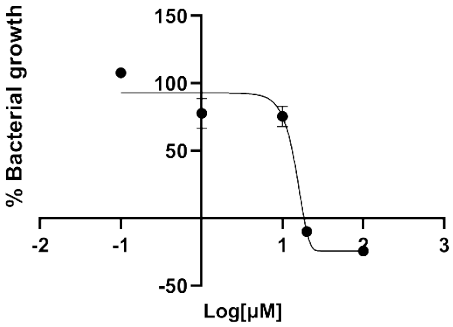

12e A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-3
-2
-1
1
2
3
Log[μM]


12f A. baumannii ATCC 747
% Bacterial growth
150
100
50
-50
-2
-1
1
2
Log[μM]

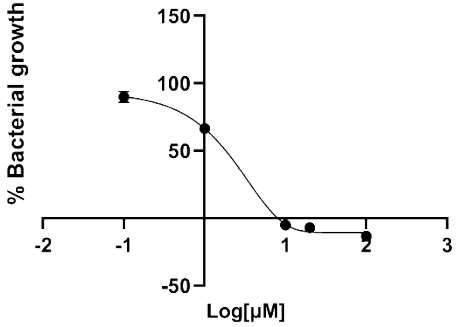
12h *A. baumannii* ATCC 747



12i *A. baumannii* ATCC 747

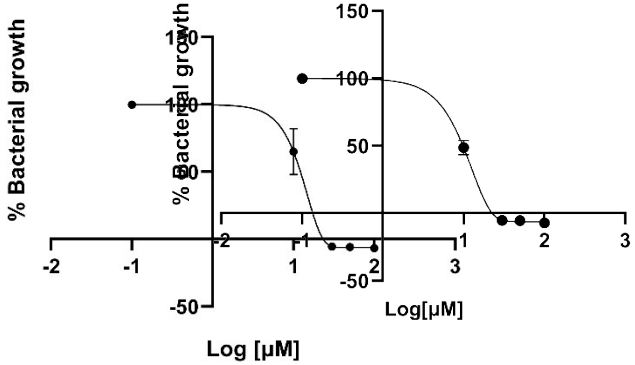


12j *A. baumannii* ATCC 747

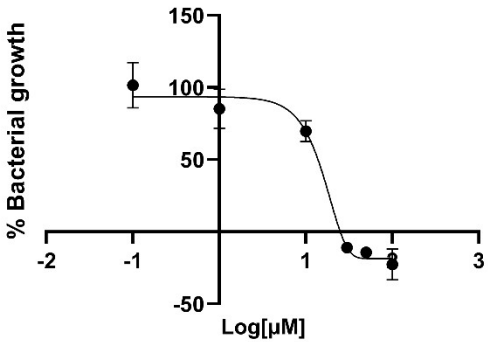


11h *A. baumannii* (XDR) A-564

11g *A. baumannii* (XDR) A-564

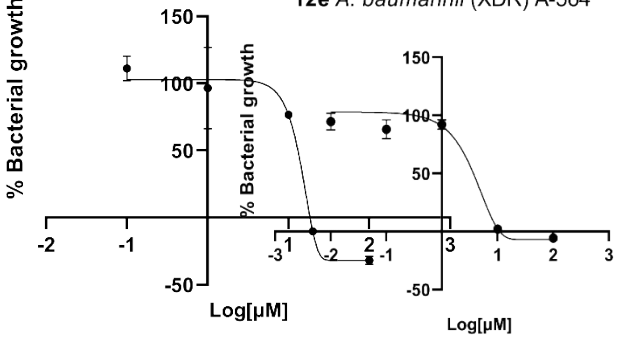


12a *A. baumannii* (XDR) A-564

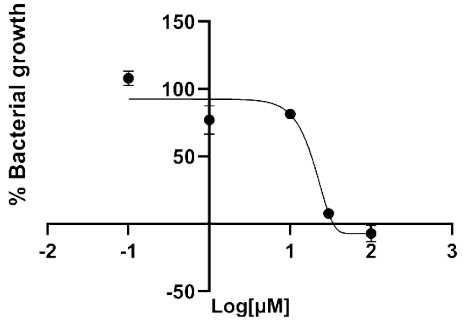


11g *A. baumannii* (XDR) A-564

12e *A. baumannii* (XDR) A-564

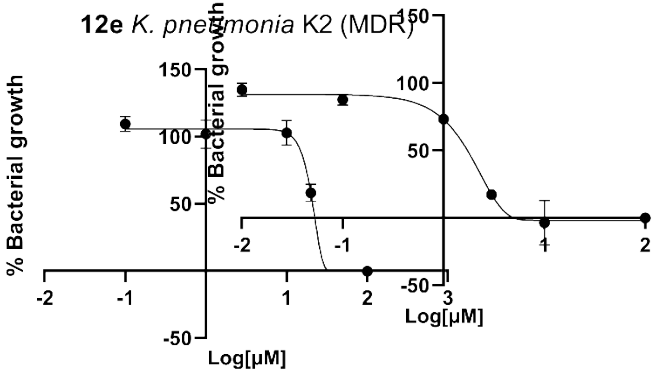


12i *A. baumannii* (XDR) A-564

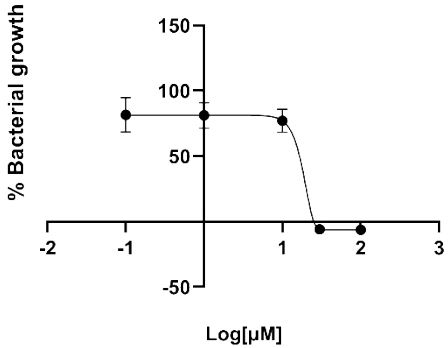


12j *A. baumannii* (XDR) A-564

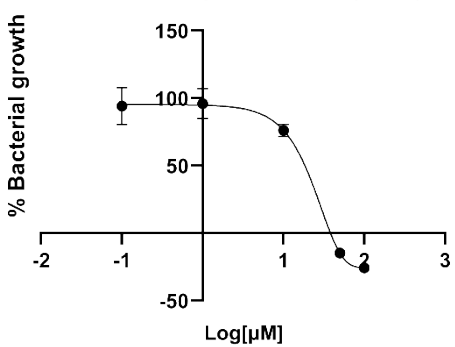
12e *K. pneumonia* K2 (MDR)



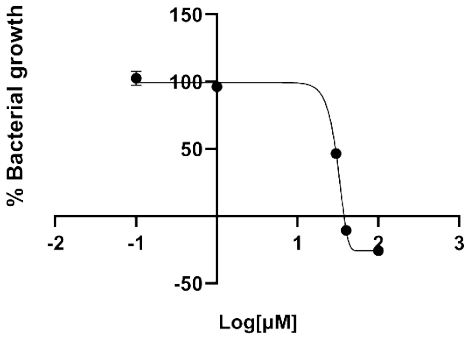
12f *K. pneumonia* K2 (MDR)



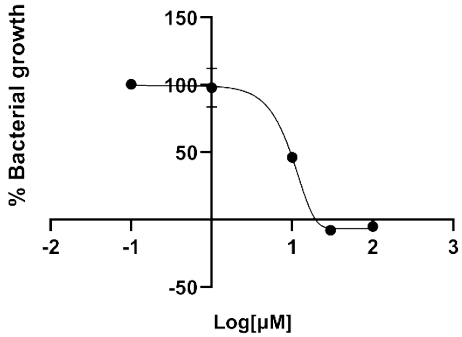
12e *P. aeruginosa* 48-M (MDR)



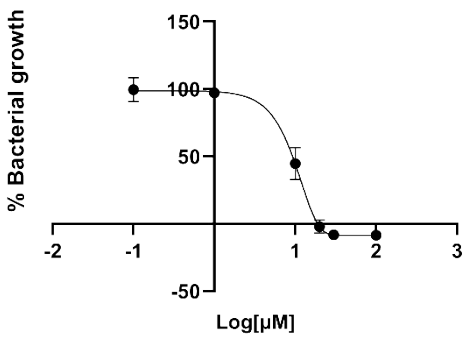
12f *P. aeruginosa* 48-M (MDR)



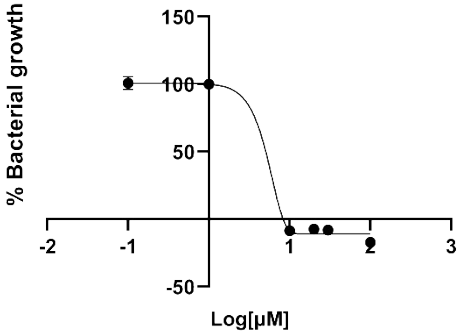
11g *S. aureus* clínico (MRSA)



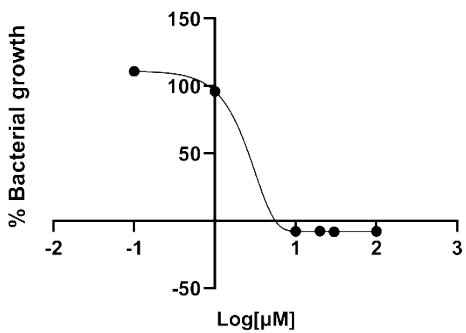
11h *S. aureus* clínico (MRSA)



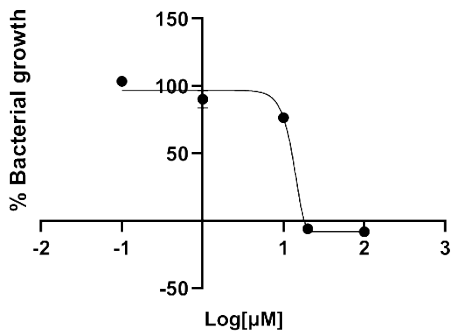
12e *S. aureus* clínico (MRSA)



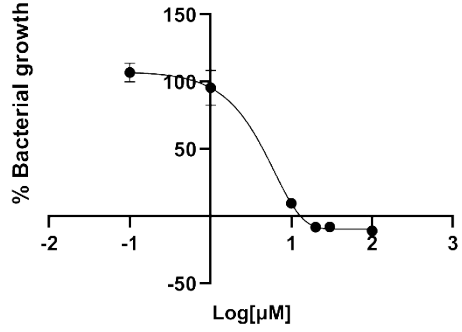
12f *S. aureus* clínico (MRSA)



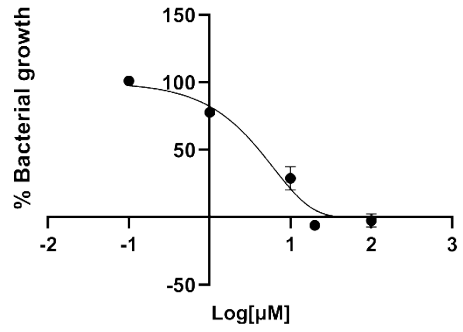
12h *S. aureus* clínico (MRSA)



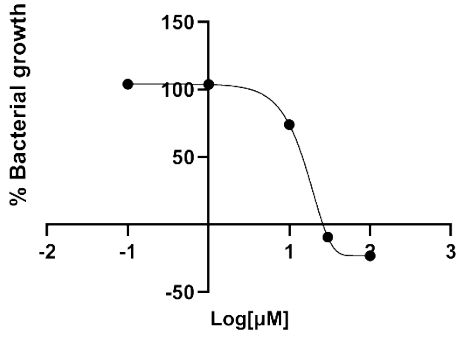
12i *S. aureus* clínico (MRSA)

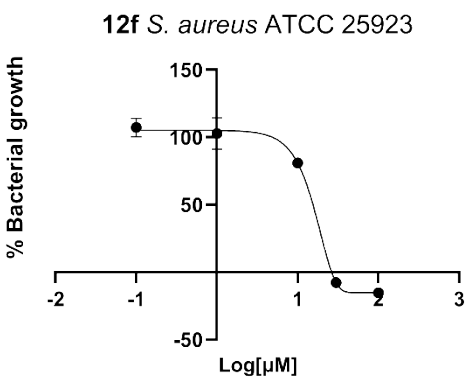


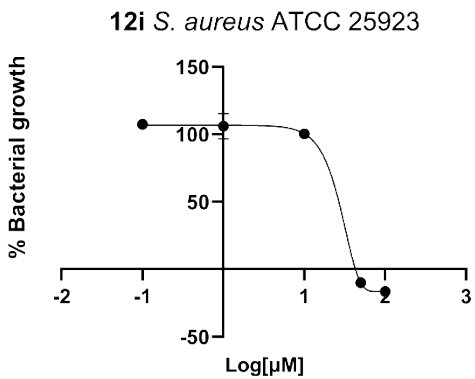
12j *S. aureus* clínico (MRSA)

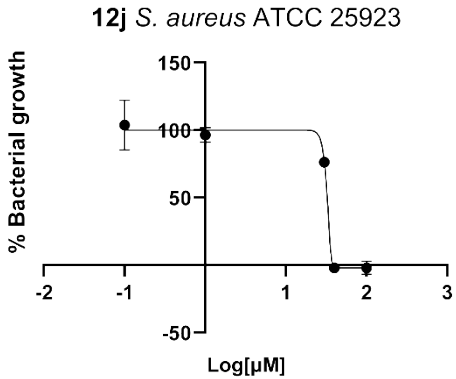


12e *S. aureus* ATCC 25923




12f S. aureus ATCC 25923
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]


12i S. aureus ATCC 25923
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]


12j S. aureus ATCC 25923
% Bacterial growth
150
100
50
-50
-2
-1
1
2
3
Log[μM]

2 ^{1}H NMR, ^{13}C NMR and HRMS spectrum of all compounds.

2.1 Compound 16b

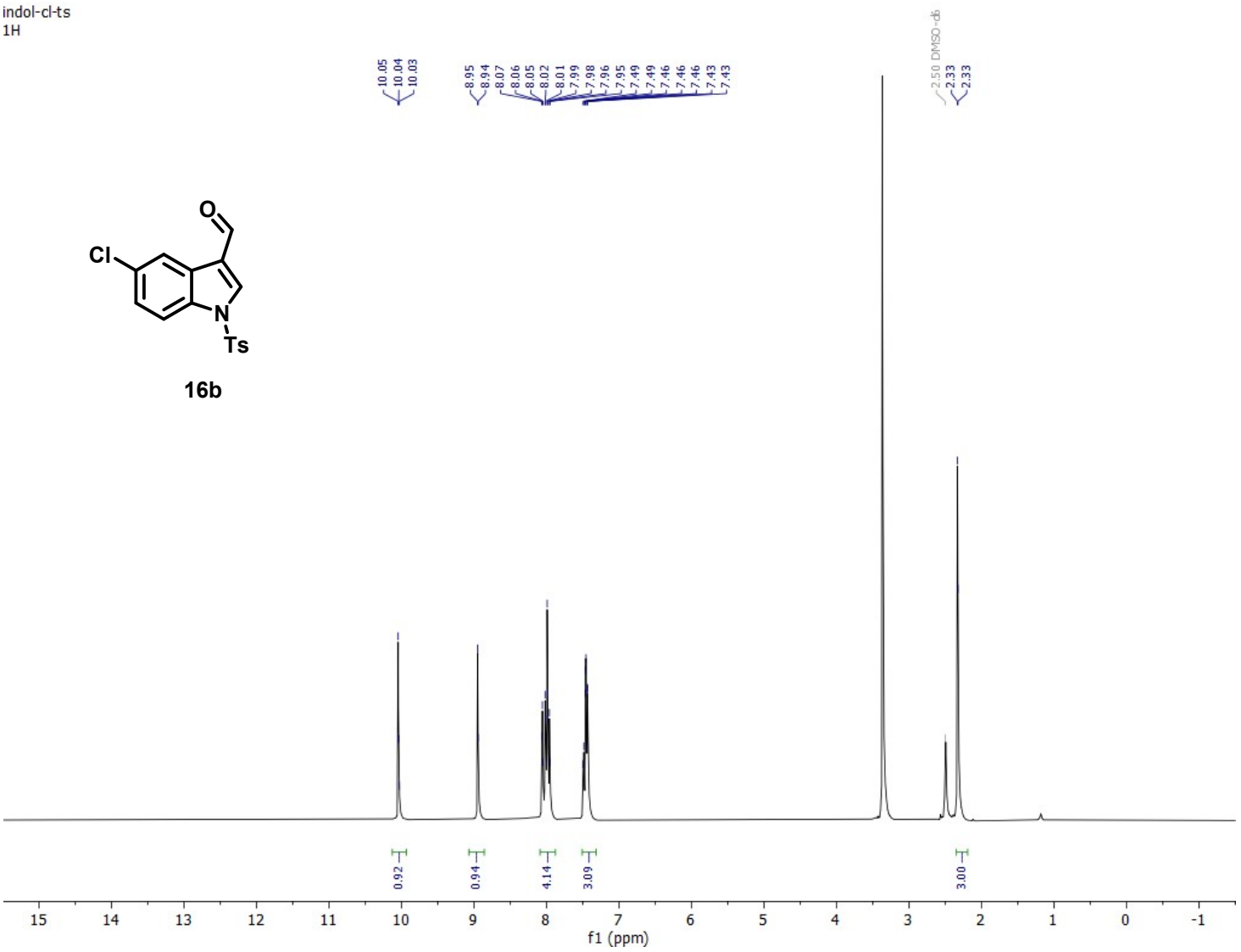


Figure 1. ^{1}H NMR spectrum of **16b** (300 MHz, DMSO-d_6).

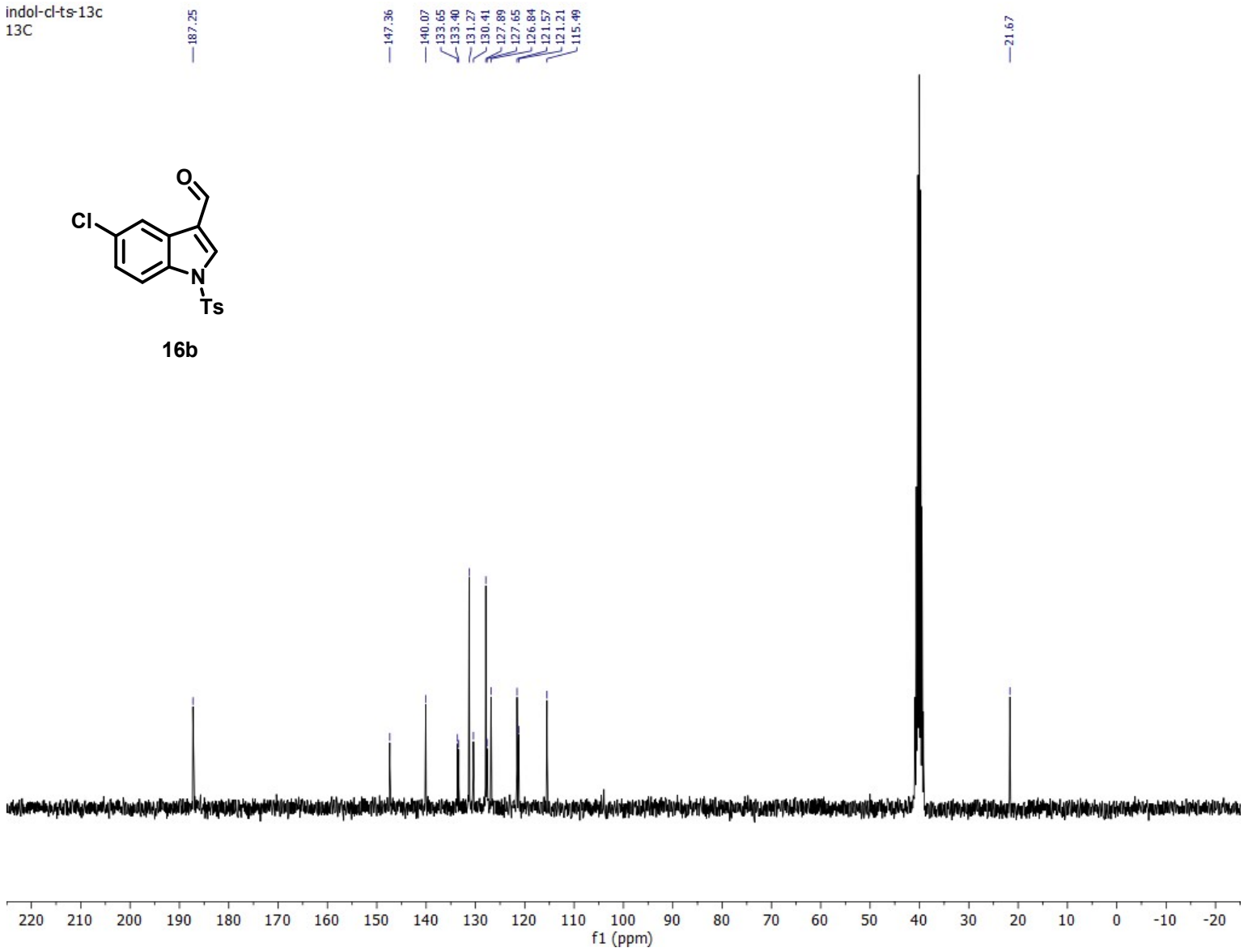
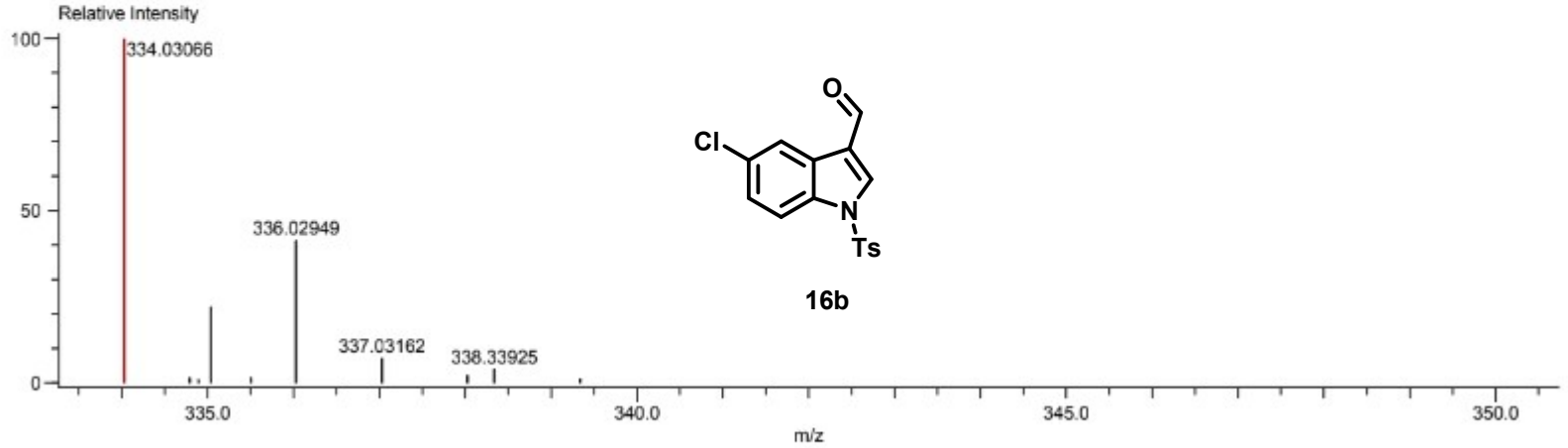


Figure 2. ^{13}C NMR spectrum of **16b** (76 MHz, DMSO-d_6).

Data:1546_4-ald
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..0)

Acquired:6/19/2024 1:02:21 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:7/1/2024 7:56:13 AM
Created by:AccuTOF

Charge number:1
Tolerance:2.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 18, ^{1}H:0 .. 50, ^{35}Cl:0 .. 2, ^{14}N:1 .. 1, ^{16}O:0 .. 4, ^{32}S:0 .. 1



16b

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
334.03066	69058.66	334.03047	0.19	0.58	$^{12}C_{16}{}^{1}H_{13}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{3}{}^{32}S_{1}$	11.5

Figure 3. ESI-HRMS spectrum of **16b**.

2.2 Compound 17d

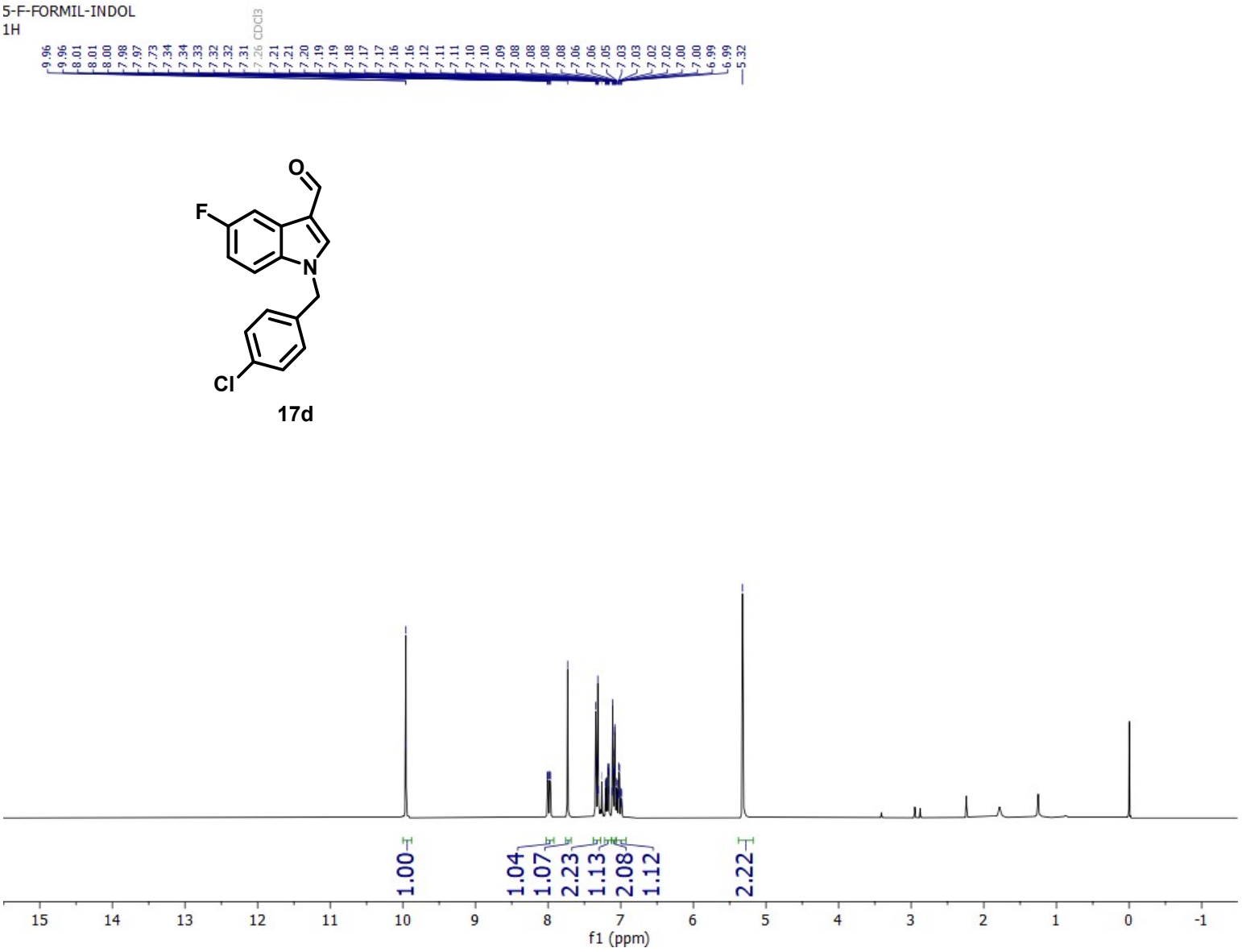


Figure 4. ^{1}H NMR spectrum of **17d** (300 MHz, $CDCl_3$).

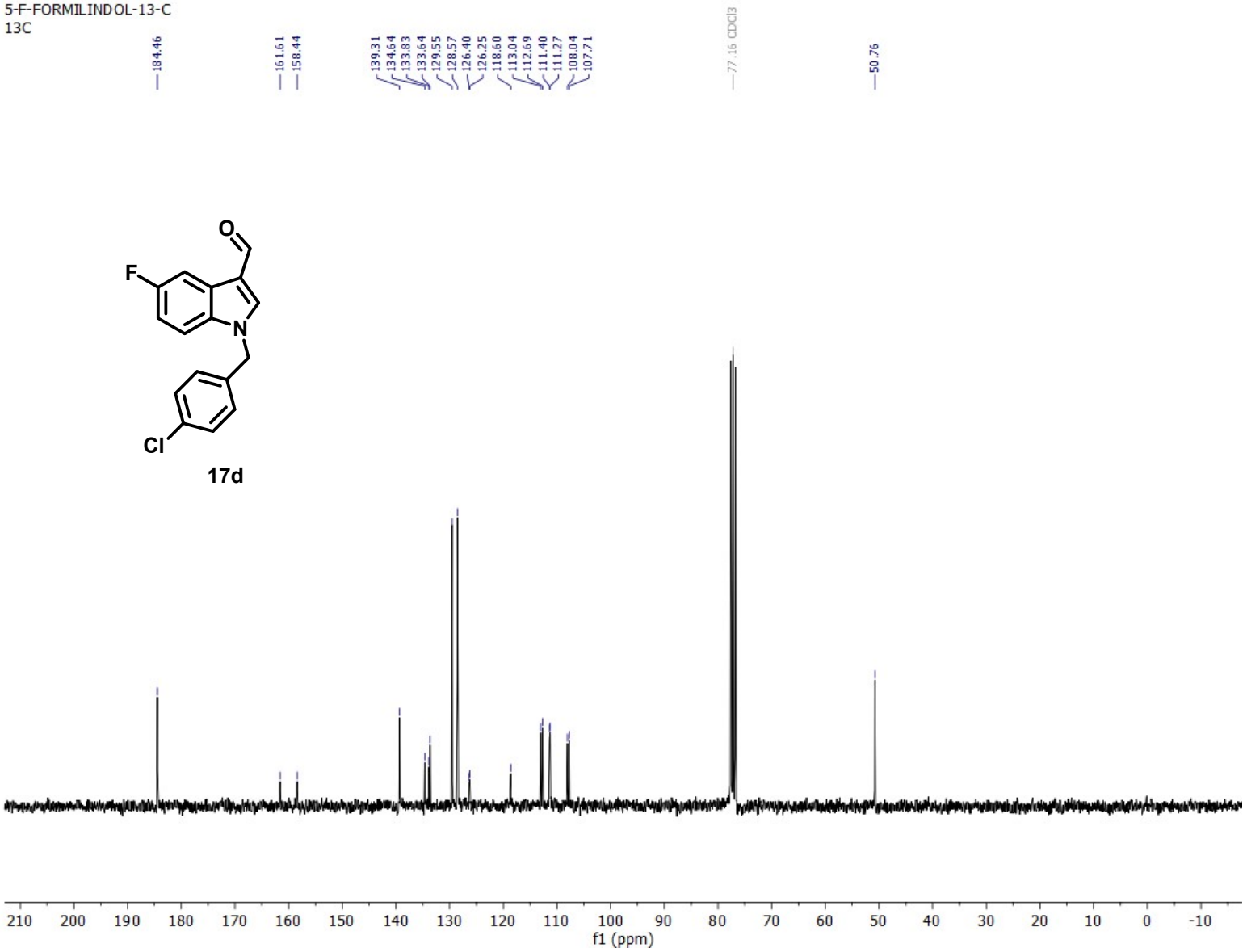
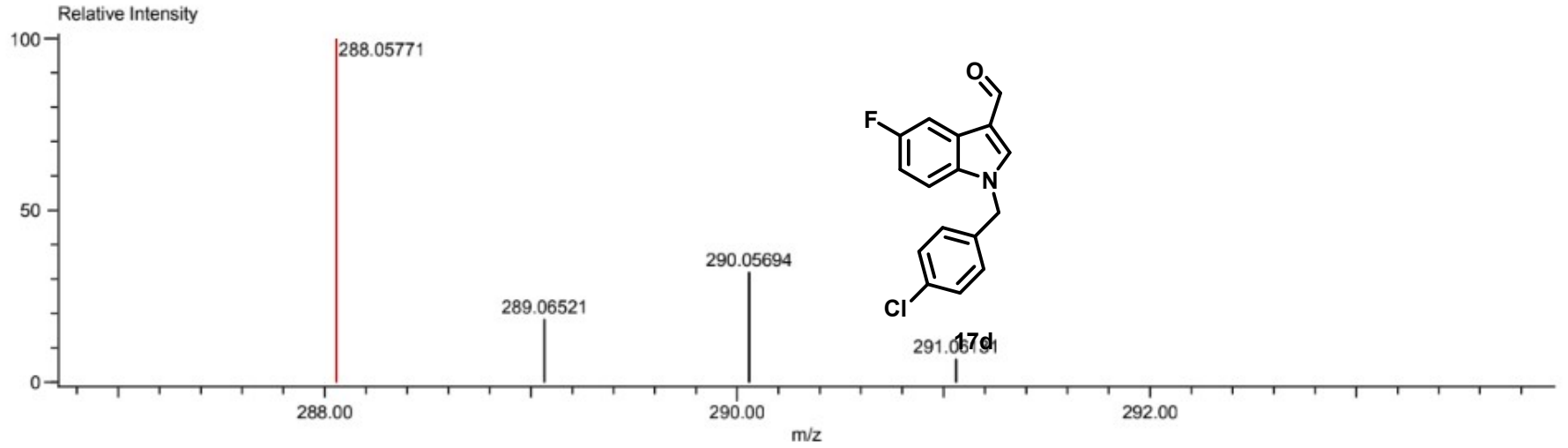


Figure 5. ^{13}C NMR spectrum of **17d** (76 MHz, $CDCl_3$).

Data:1926 5-F-Indol-3F
Sample Name:Dr Martinez Roberto / Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..1)

Acquired:7/29/2024 5:04:44 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:9/18/2024 3:23:20 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)
Element:^{12}C:0 .. 18, ^{1}H:0 .. 50, ^{35}Cl:0 .. 1, ^{19}F:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 2



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
288.05771	16273.51	288.05914	-1.43	-4.97	$^{12}C_{16}{}^{1}H_{12}{}^{35}Cl_{1}{}^{19}F_{1}{}^{14}N_{1}{}^{16}O_{1}$	10.5

Figure 6. HRMS spectrum of **17d**.

2.3 Compound 15a

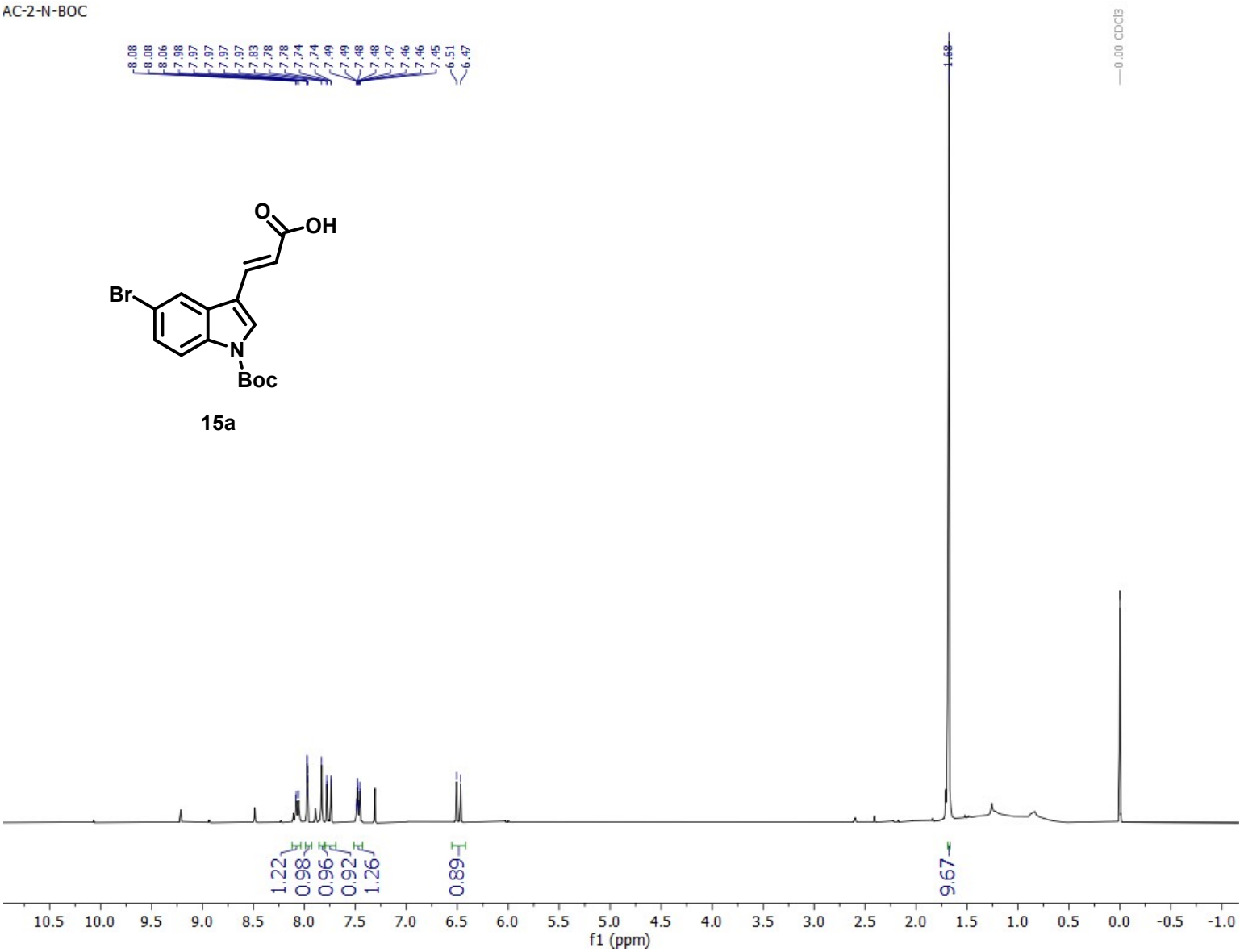


Figure 7. ^{1}H NMR spectrum of **15a** (400 MHz, $CDCl_3$).

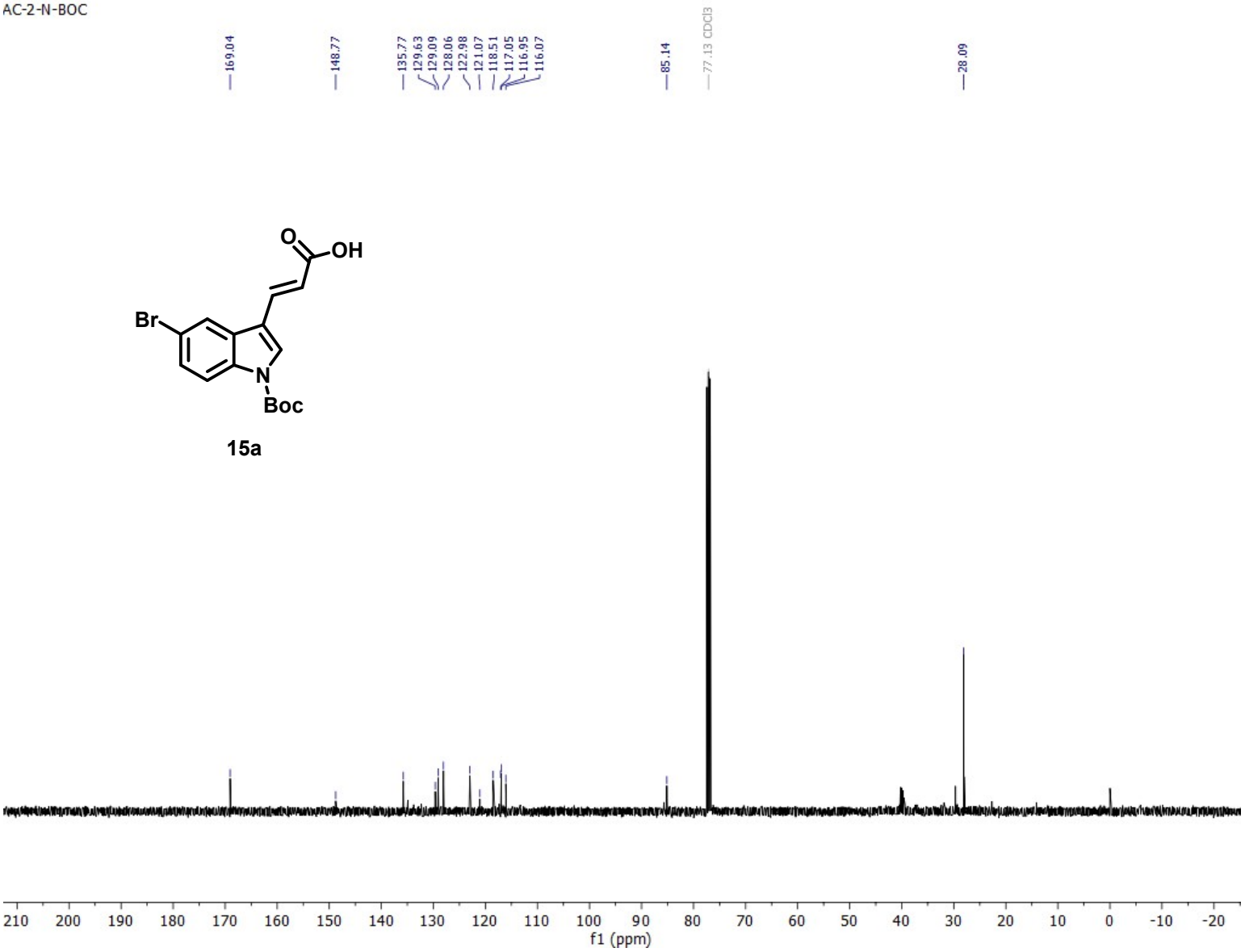


Figure 8. ^{13}C NMR spectrum of **15a** (101 MHz, $CDCl_3$).

2.4 Compound 15b

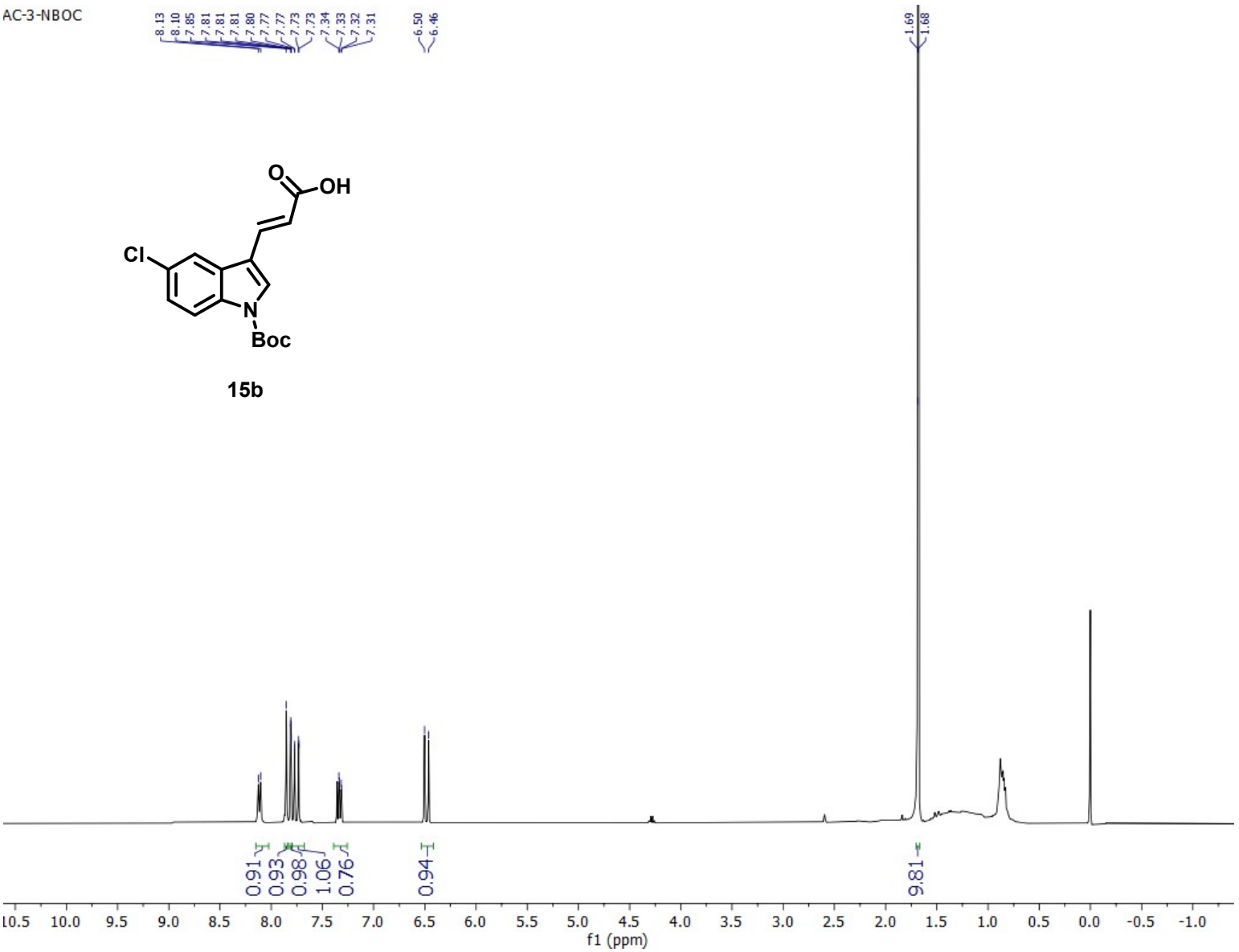


Figure 9. ^{1}H NMR spectrum of **15b** (400 MHz, $CDCl_3$).

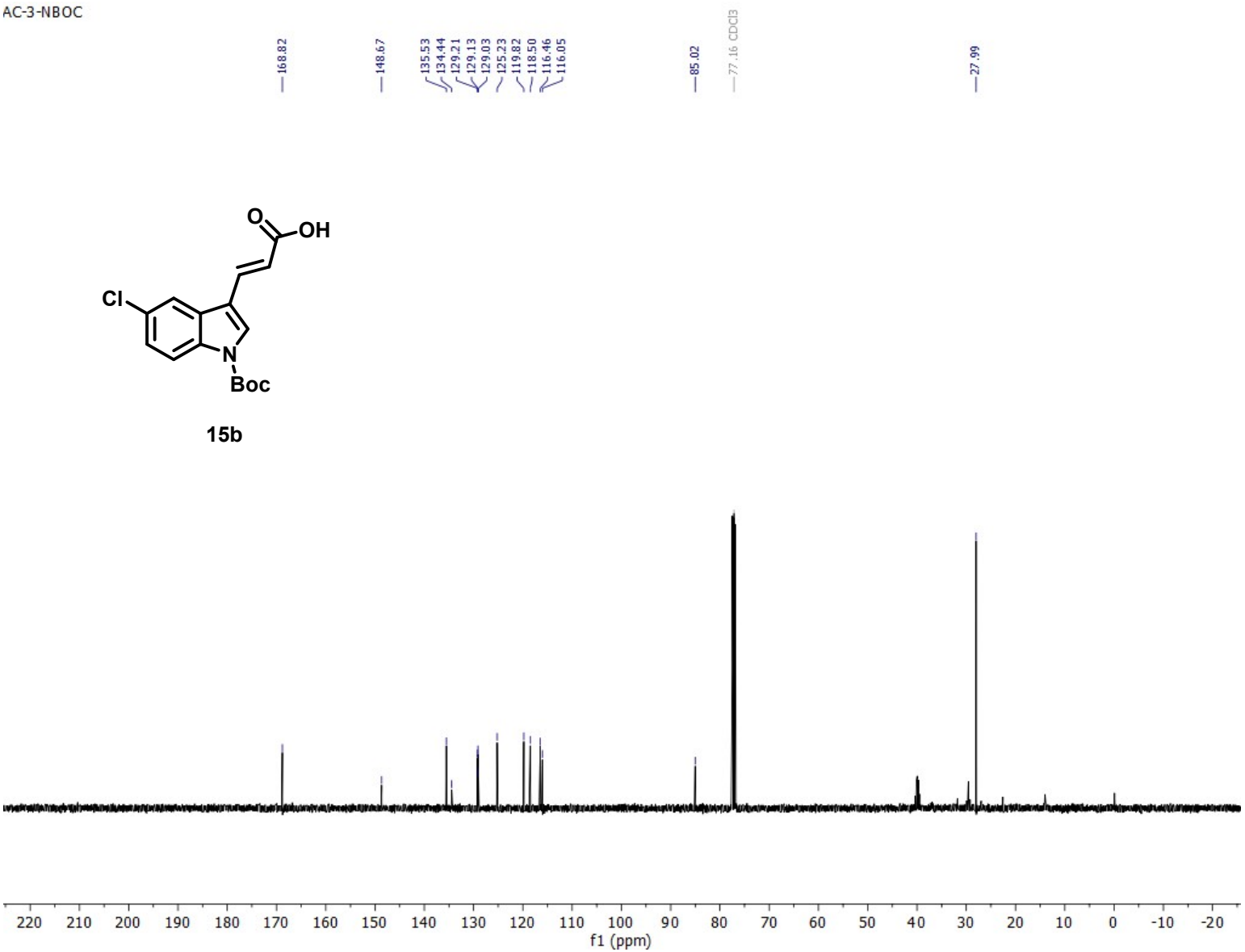


Figure 10. ^{13}C NMR spectrum of **15b** (101 MHz, $CDCl_3$).

2.5 Compound 15c

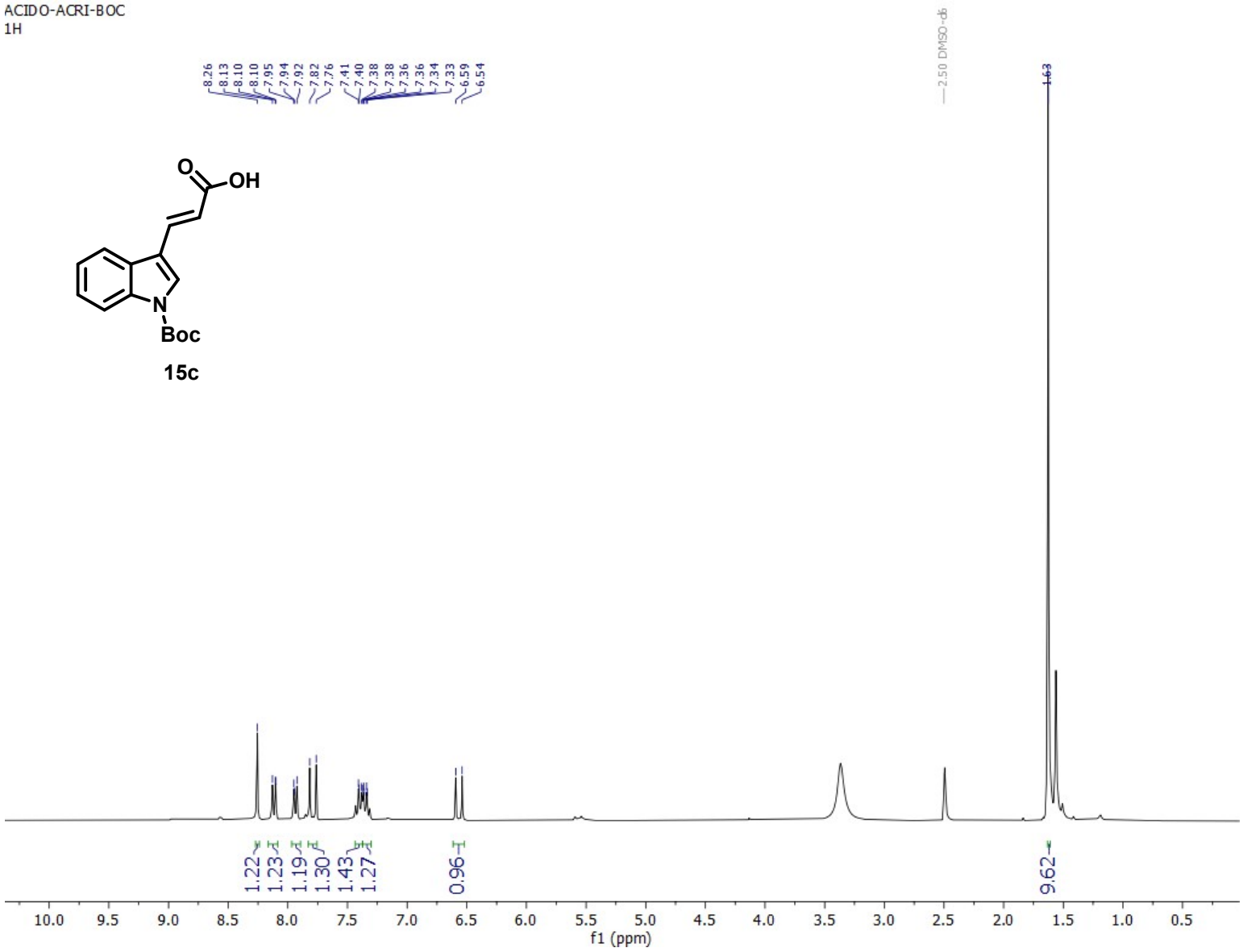


Figure 11. ^{1}H NMR spectrum of **15c** (400 MHz, $CDCl_3$).

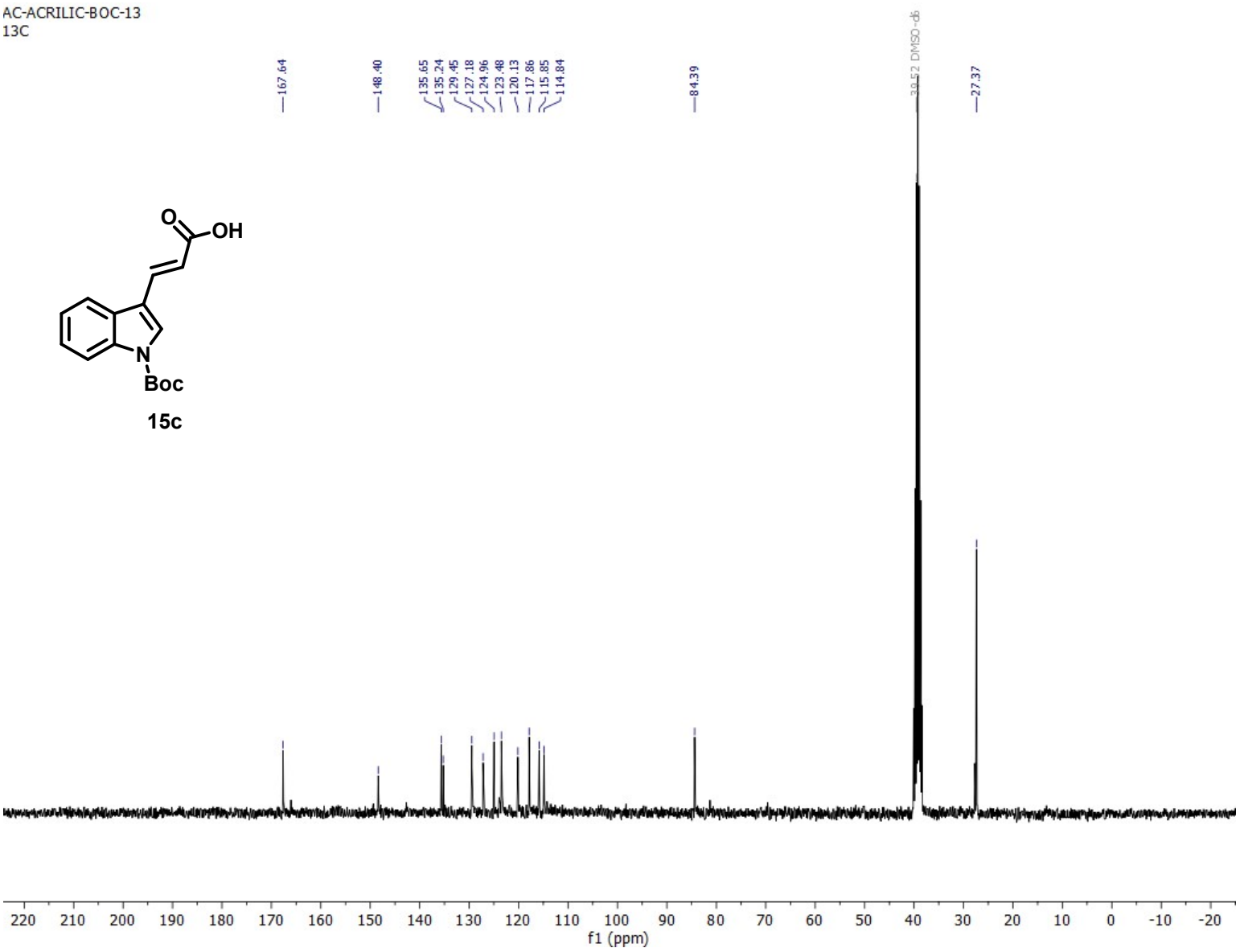


Figure 12. ^{13}C NMR spectrum of **15c** (101 MHz, DMSO-d_6).

2.6 Compound 9a

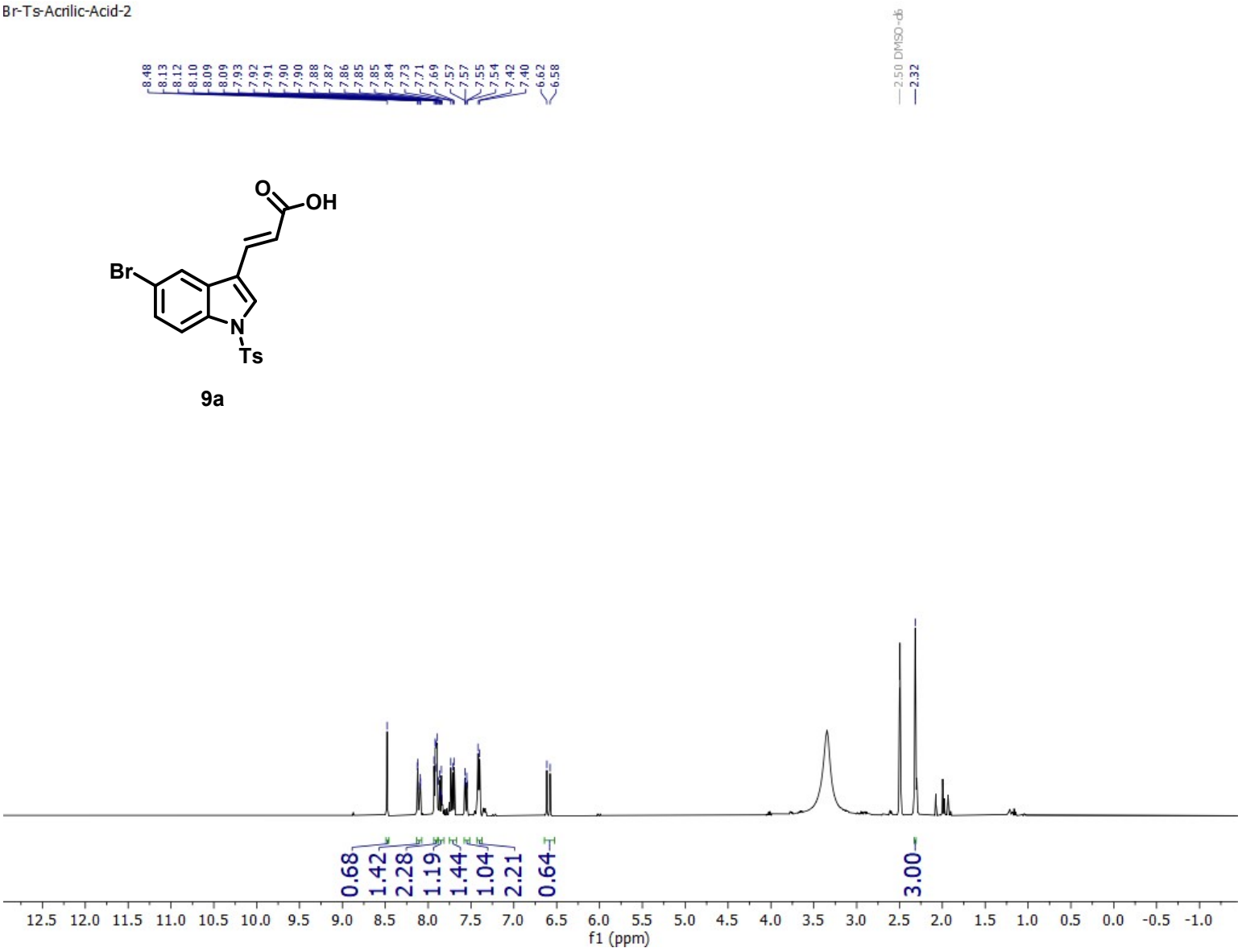


Figure 13. ^{1}H NMR spectrum of **9a** (400 MHz, DMSO-d_6).

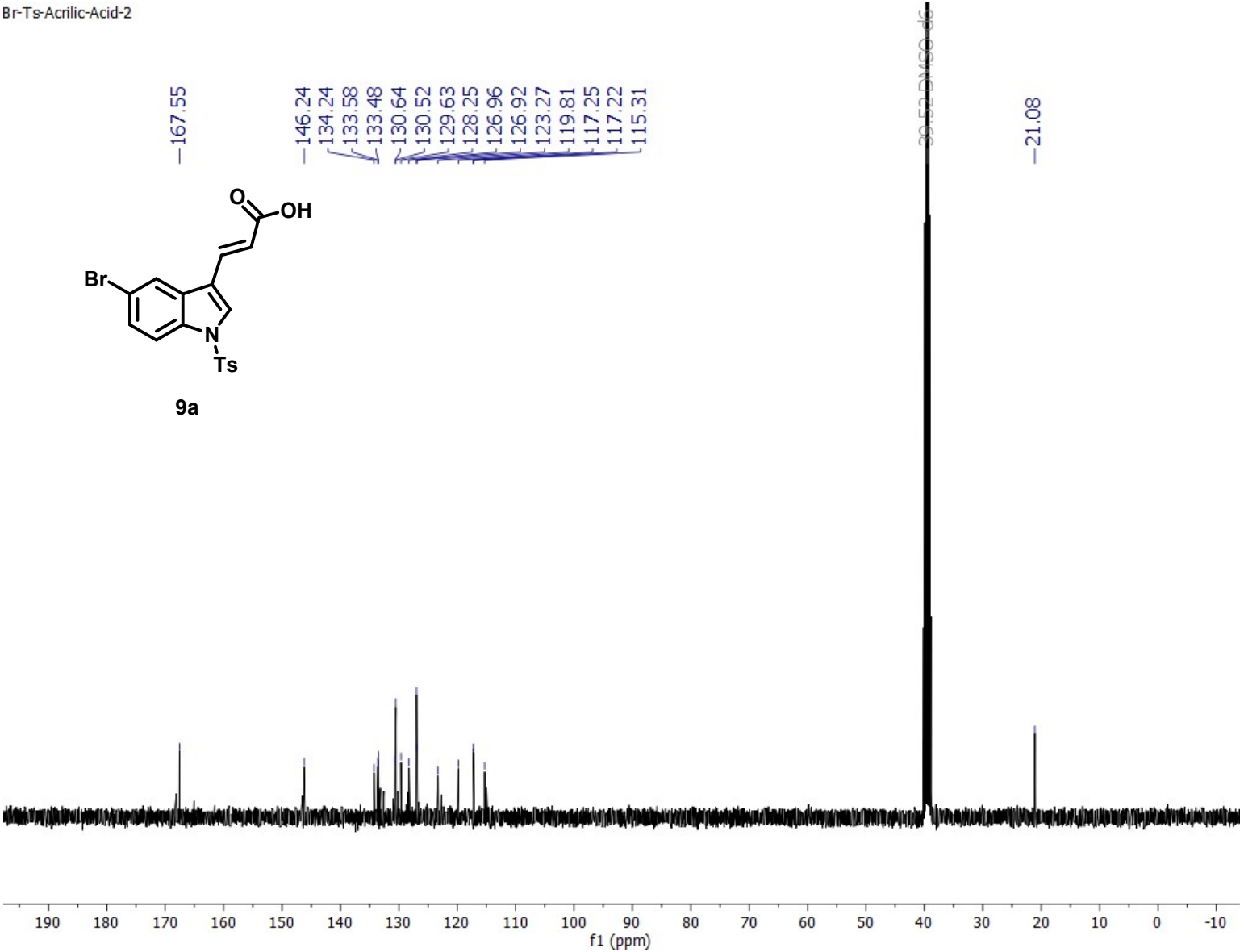
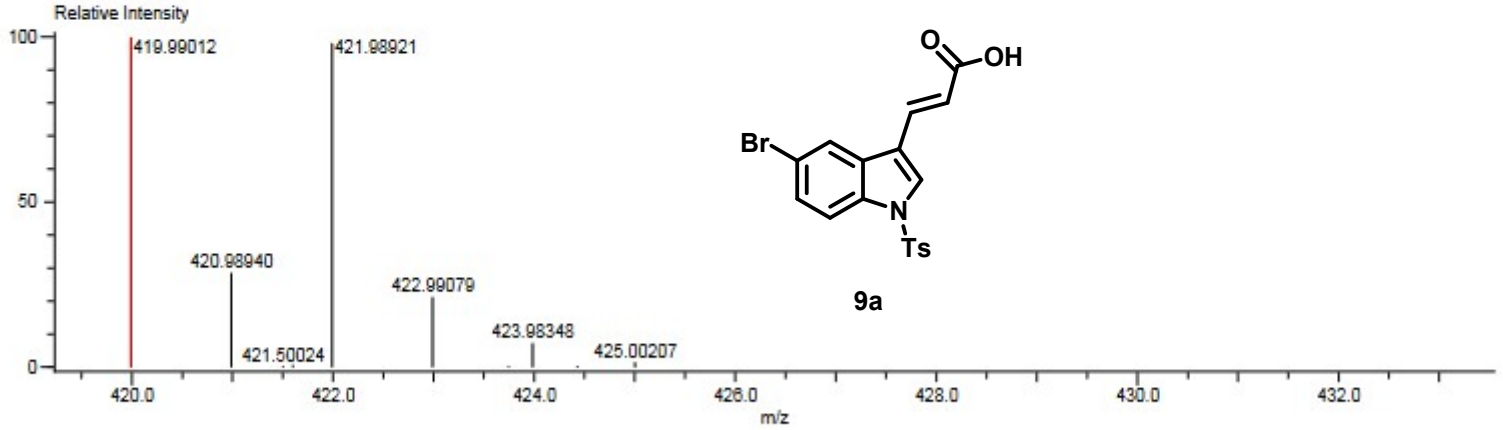


Figure 14. ^{13}C NMR spectrum of **9a** (400 MHz, DMSO-d_6).

Data:1541_3b
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:6/19/2024 12:51:11 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:7/1/2024 7:59:59 AM
Created by:AccuTOF

Charge number:1
Tolerance:2.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 18, ^{1}H:0 .. 50, ^{79}Br:0 .. 1, ^{14}N:1 .. 1, ^{16}O:0 .. 4, ^{32}S:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
419.99012	41818.25	419.99052	-0.40	-0.95	$^{12}C_{18}{}^{1}H_{15}{}^{79}Br_{1}{}^{14}N_{1}{}^{16}O_{4}{}^{32}S_{1}$	12.5

Figure 15. ESI-HRMS spectrum of **9a**.

2.7 Compound 9b

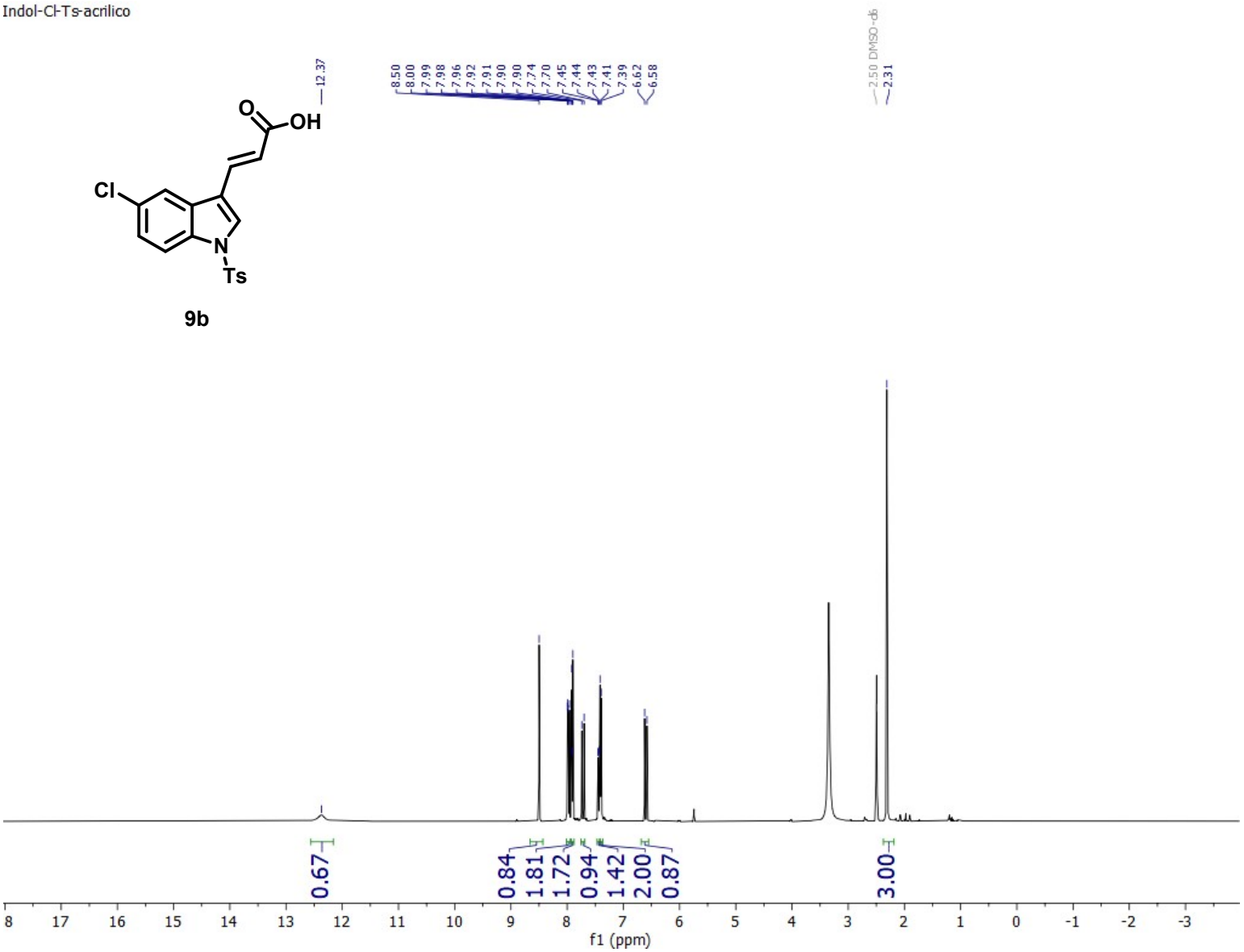


Figure 16. ^{1}H NMR spectrum of **9b** (400 MHz, DMSO-d_6).

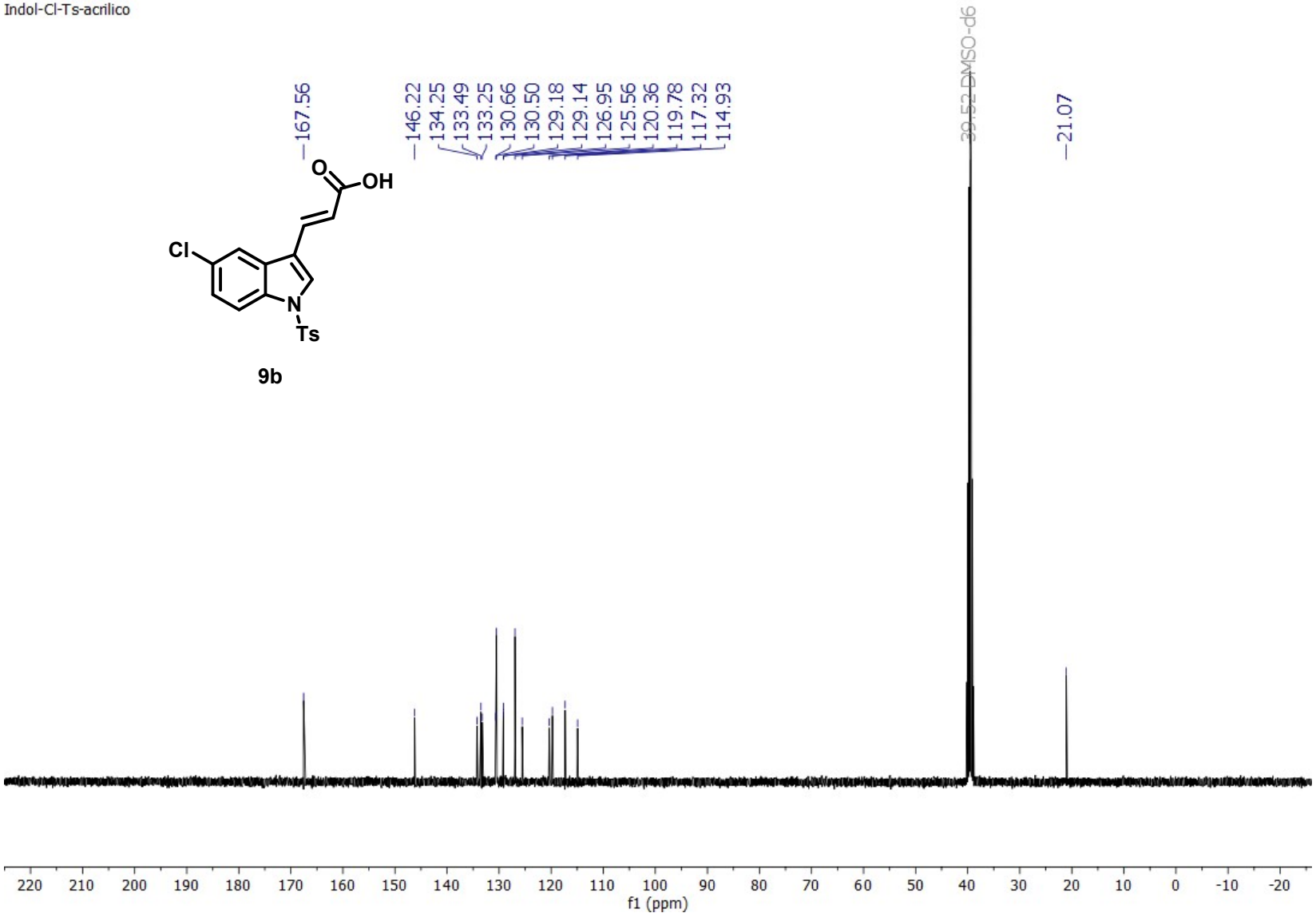
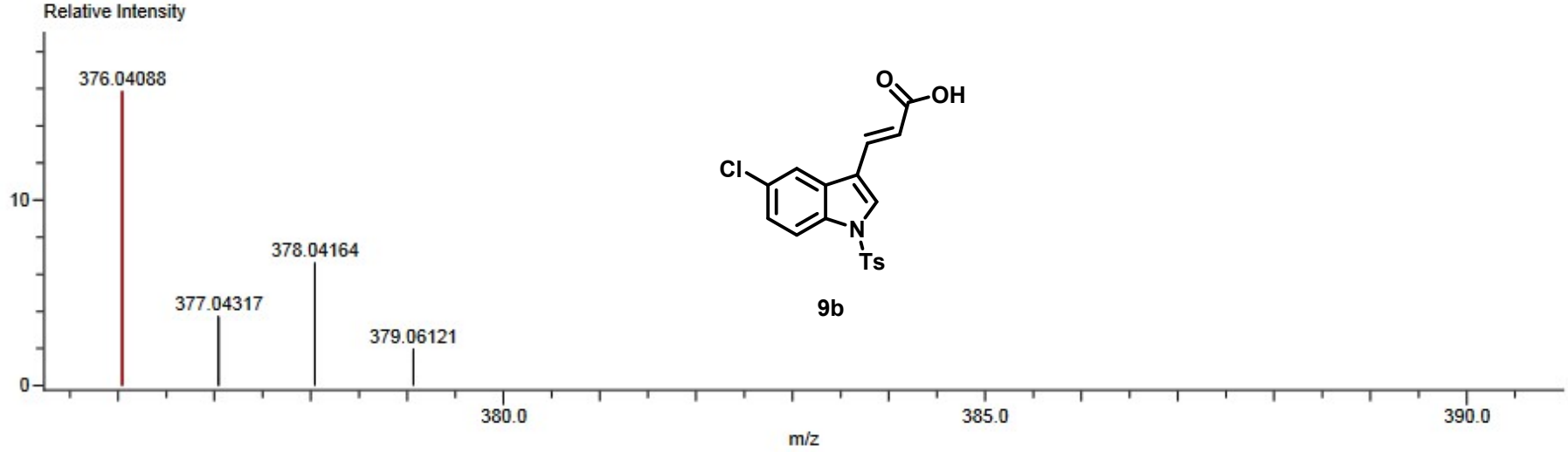


Figure 17. ^{13}C NMR spectrum of **9c** (400 MHz, DMSO-d_6).

Data:1542_4b
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:6/19/2024 12:53:21 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:7/1/2024 7:54:30 AM
Created by:AccuTOF

Charge number:1
Tolerance:2.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 18, ^{1}H:0 .. 50, ^{35}Cl:0 .. 2, ^{14}N:1 .. 1, ^{16}O:0 .. 4, ^{32}S:0 .. 1



9b

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
376.04088	16086.53	376.04103	-0.15	-0.39	$^{12}C_{18}{}^{1}H_{15}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{4}{}^{32}S_{1}$	12.5

Figure 18. ESI-HRMS spectrum of **9b**.

2.8 Compound 9c

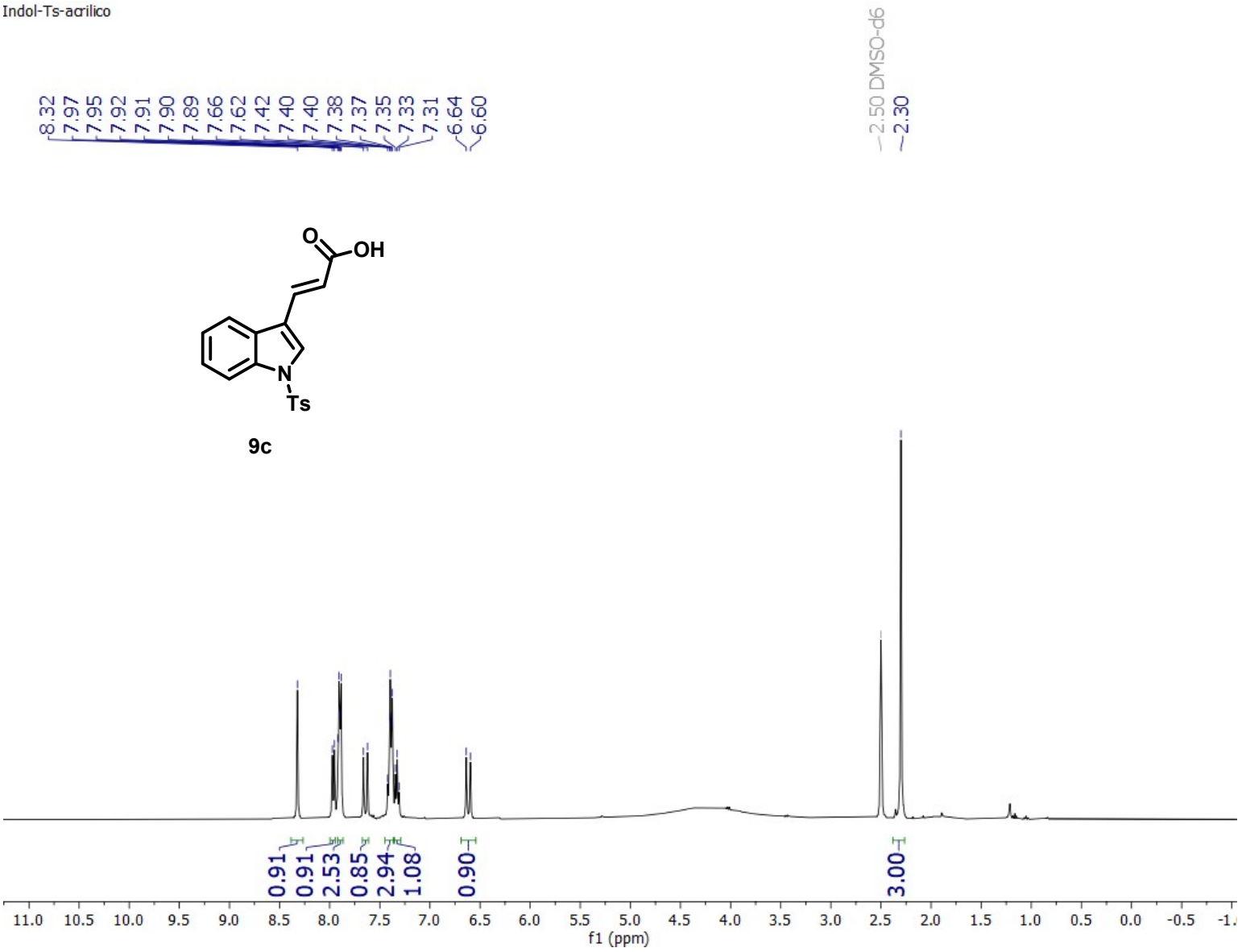


Figure 19. ^{1}H NMR spectrum of **9c** (400 MHz, DMSO-d_6).

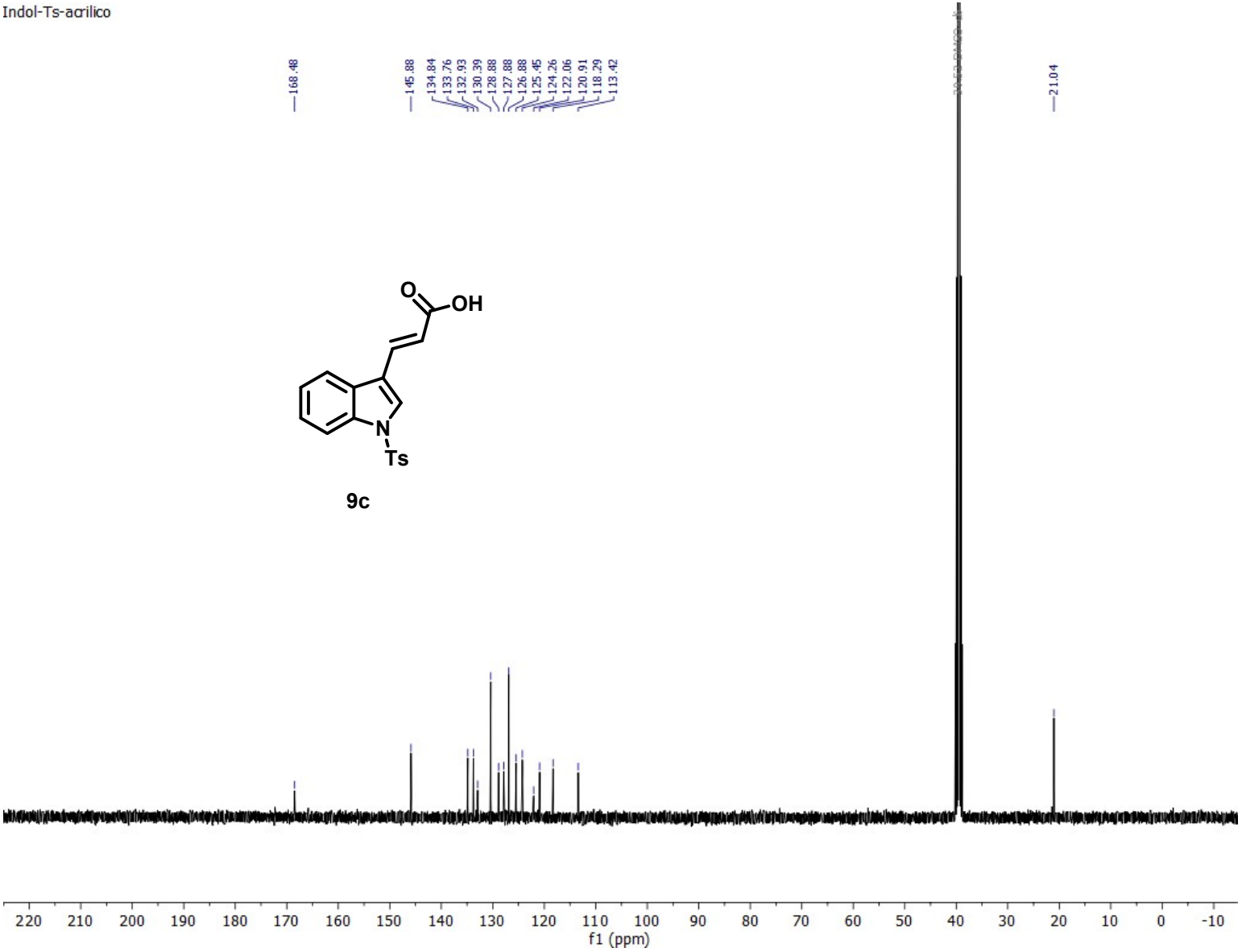
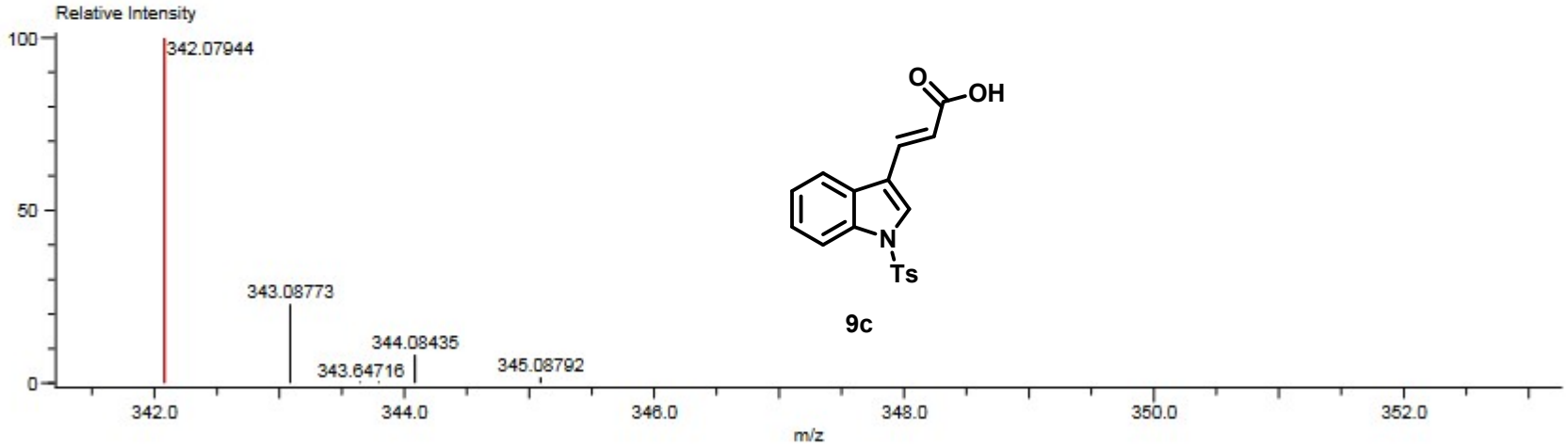


Figure 20. ^{1}H NMR spectrum of **9c** (400 MHz, DMSO-d_6).

Data:1543_8a
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..0)

Acquired:6/19/2024 12:55:49 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:7/1/2024 7:50:30 AM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{14}N:0 .. 1, ^{16}O:0 .. 4, ^{32}S:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
342.07944	23934.45	342.08000	-0.56	-1.63	$^{12}C_{18}{}^{1}H_{16}{}^{14}N_{1}{}^{16}O_{4}{}^{32}S_{1}$	12.5

Figure 21. ESI-HRMS spectrum of **9c**.

2.9 Compound 18a

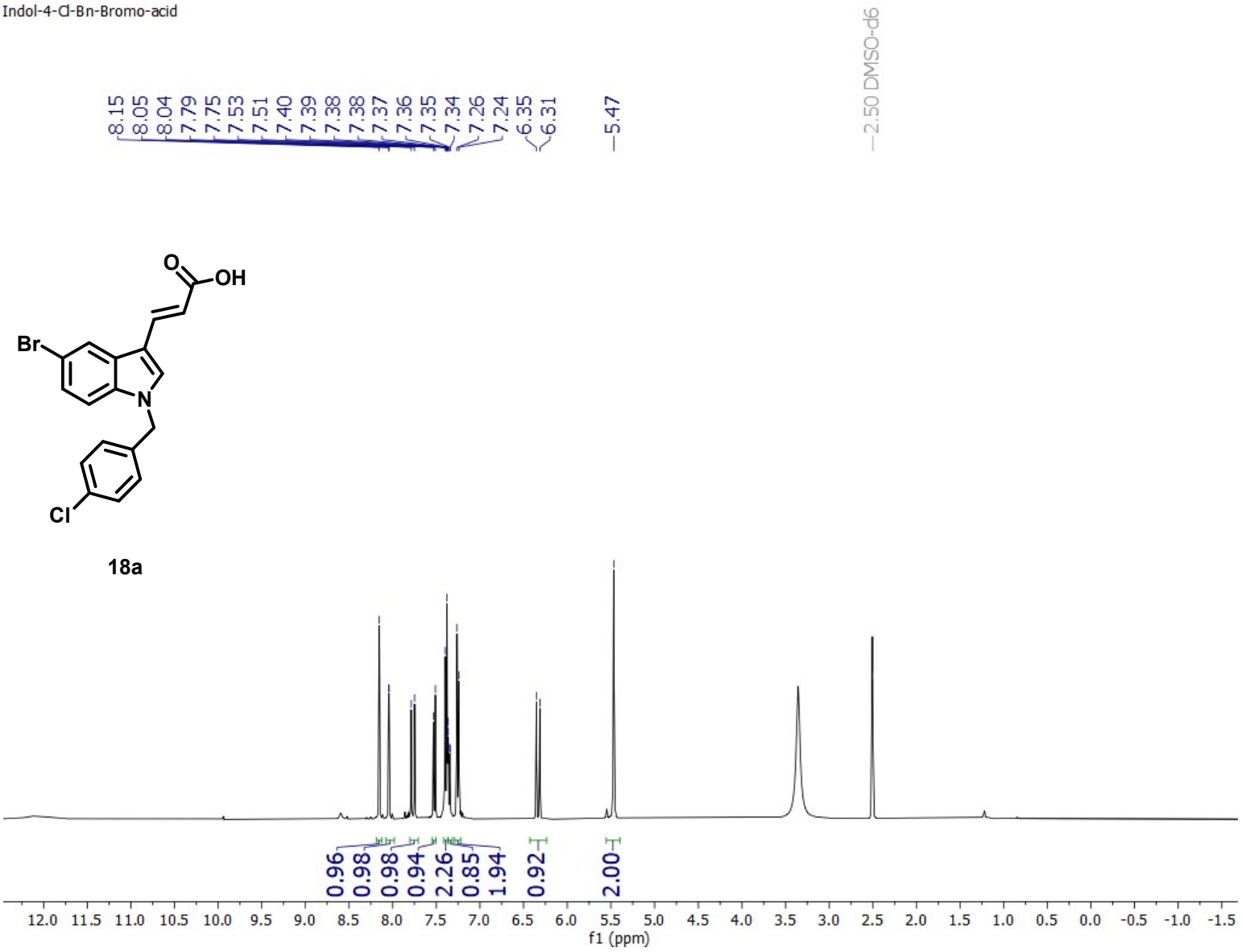


Figure 22. ^{1}H NMR spectrum of **18a** (400 MHz, DMSO-d_6).

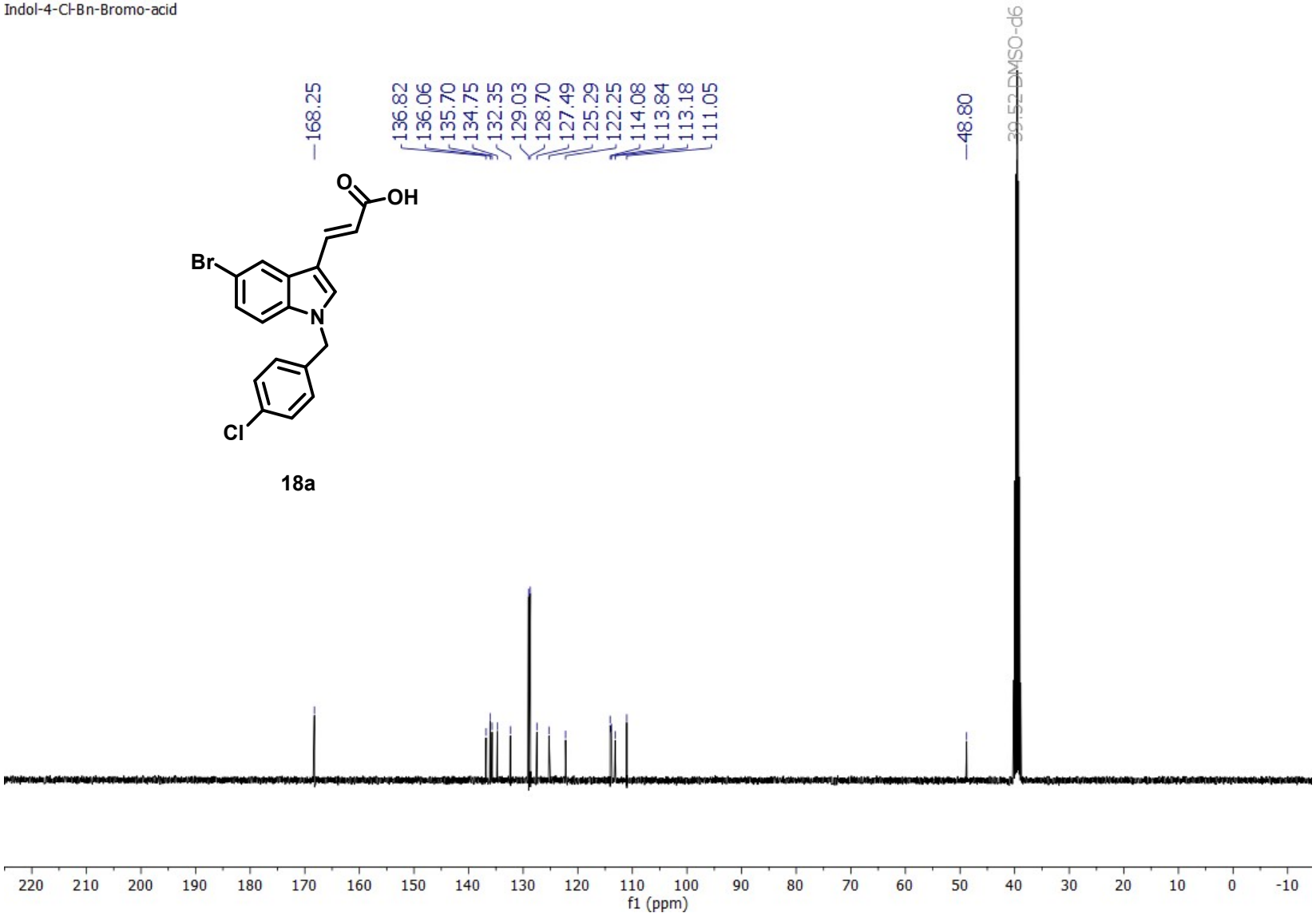
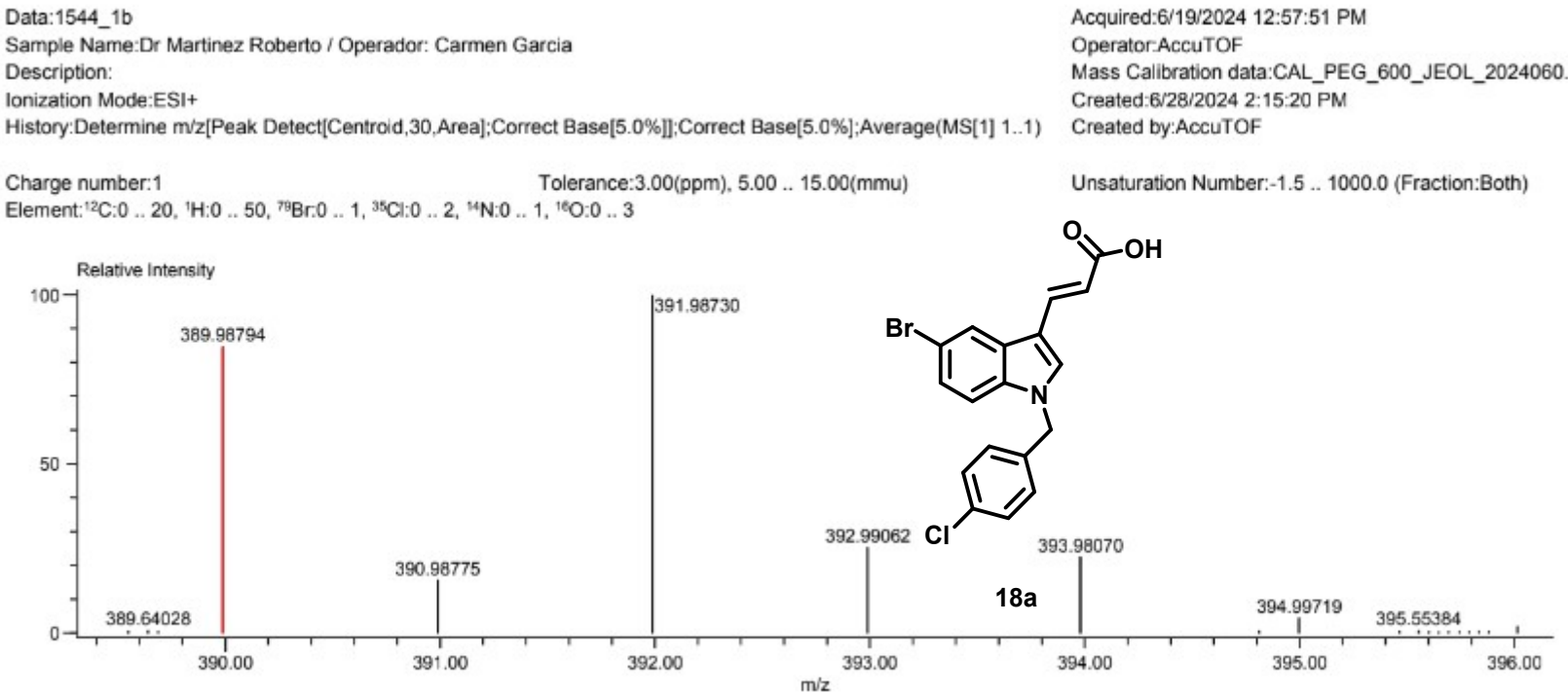


Figure 23. ^{13}C NMR spectrum of **18a** (101 MHz, DMSO-d_6).



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
389.98794	7620.68	389.98964	-1.70	-4.37	$^{12}C_{18}{}^{1}H_{14}{}^{79}Br_{1}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{2}$	11.5

Figure 24. ESI-HRMS spectrum of **18a**.

2.10 Compound 18b

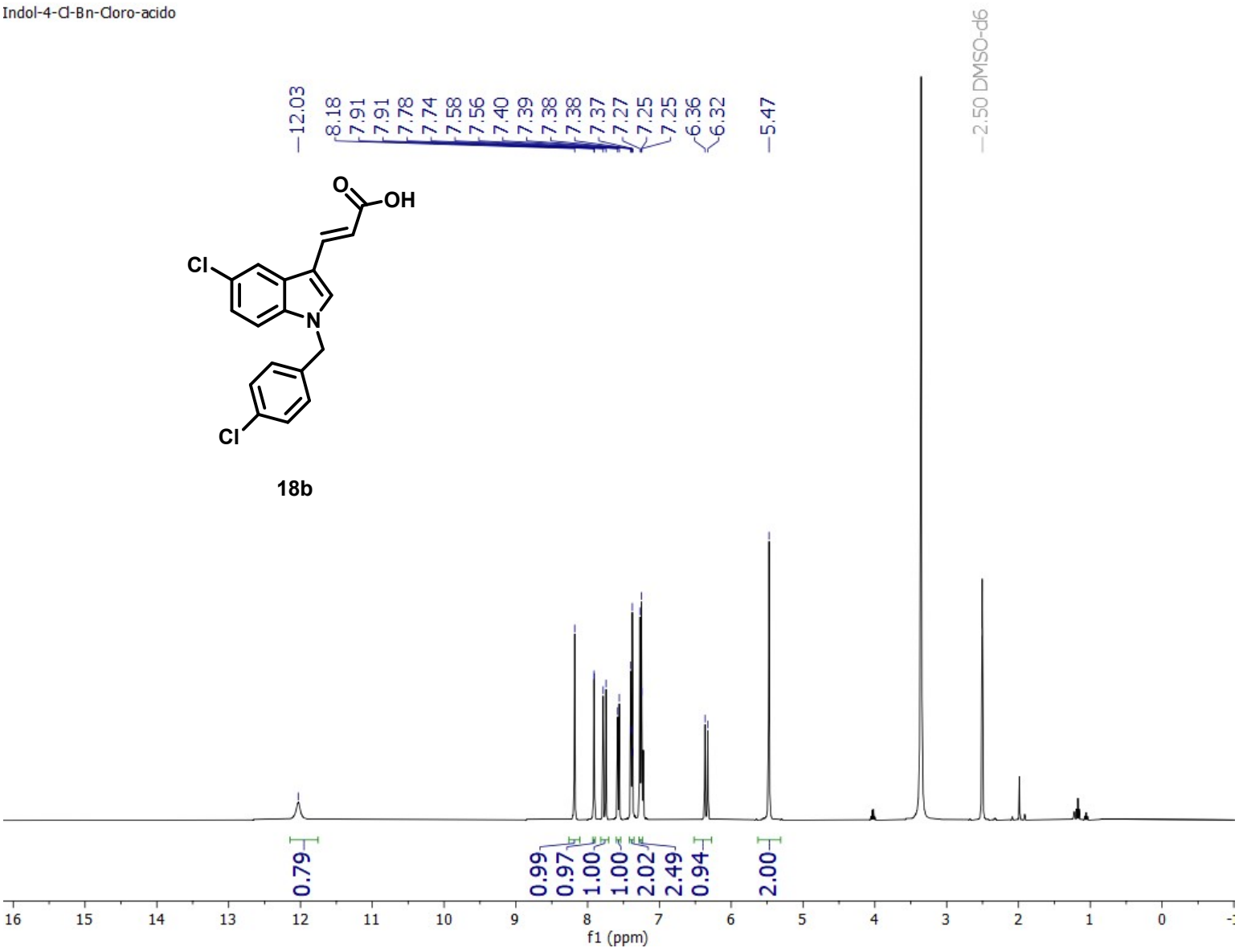


Figure 25. ^{1}H NMR spectrum of **18b** (400 MHz, DMSO-d_6).

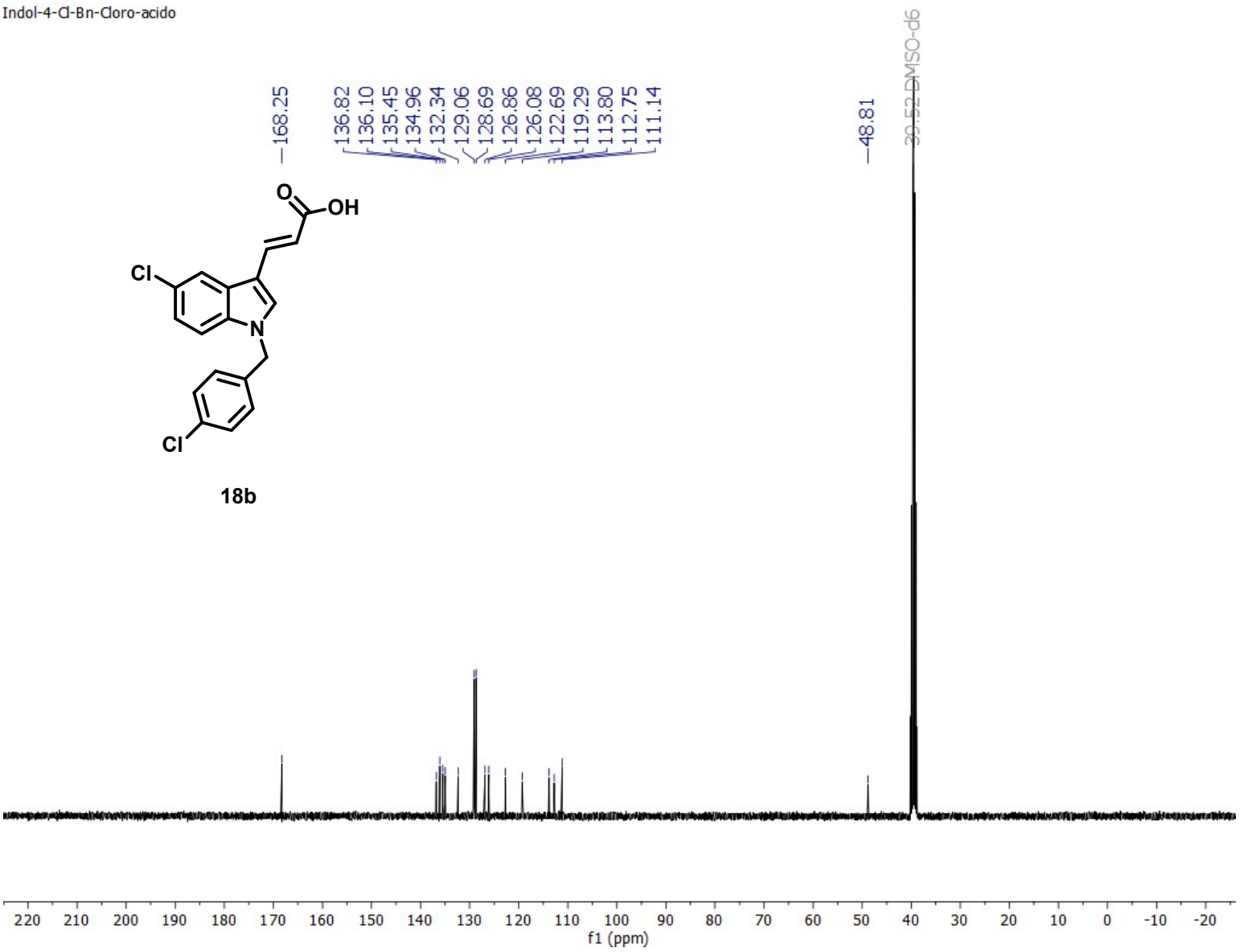
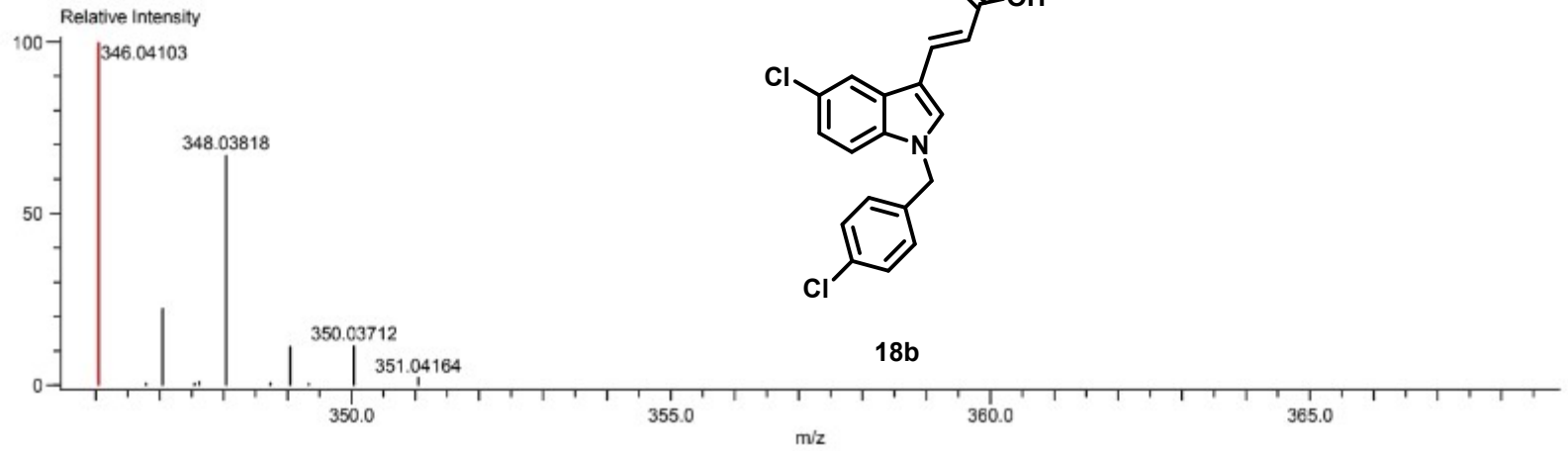


Figure 26. ^{13}C NMR spectrum of **18b** (101 MHz, DMSO-d_6).

Data:1545_9b
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:6/19/2024 1:00:00 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:6/28/2024 2:12:24 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{35}Cl:0 .. 2, ^{14}N:0 .. 1, ^{16}O:0 .. 3



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
346.04103	61588.50	346.04016	0.87	2.52	$^{12}C_{18}{}^{1}H_{14}{}^{35}Cl_{2}{}^{14}N_{1}{}^{16}O_{2}$	11.5

Figure 27. ESI-HRMS spectrum of **18b**.

2.11 Compound 18d

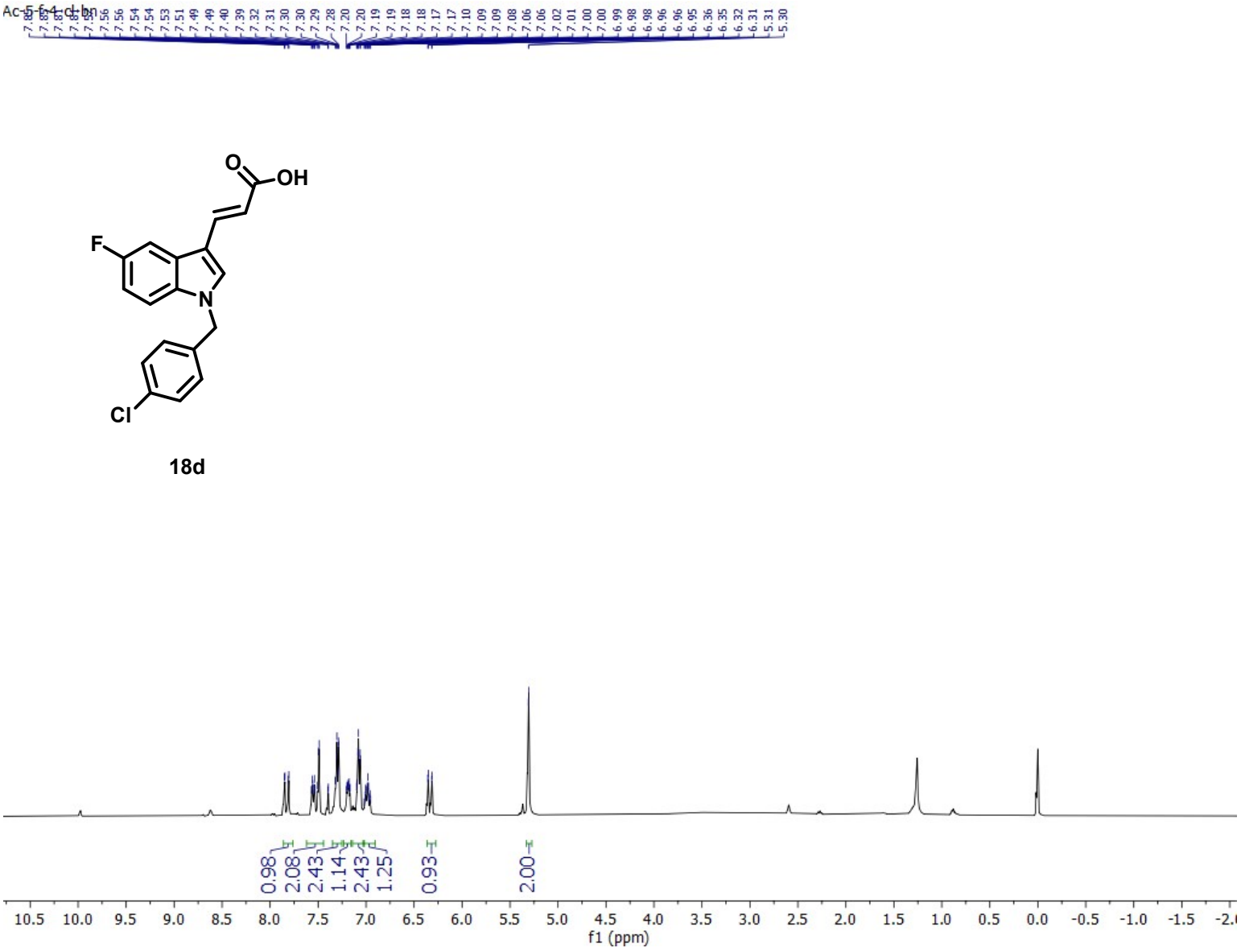


Figure 28. ^{1}H NMR spectrum of **18d** (400 MHz, $CDCl_3$).

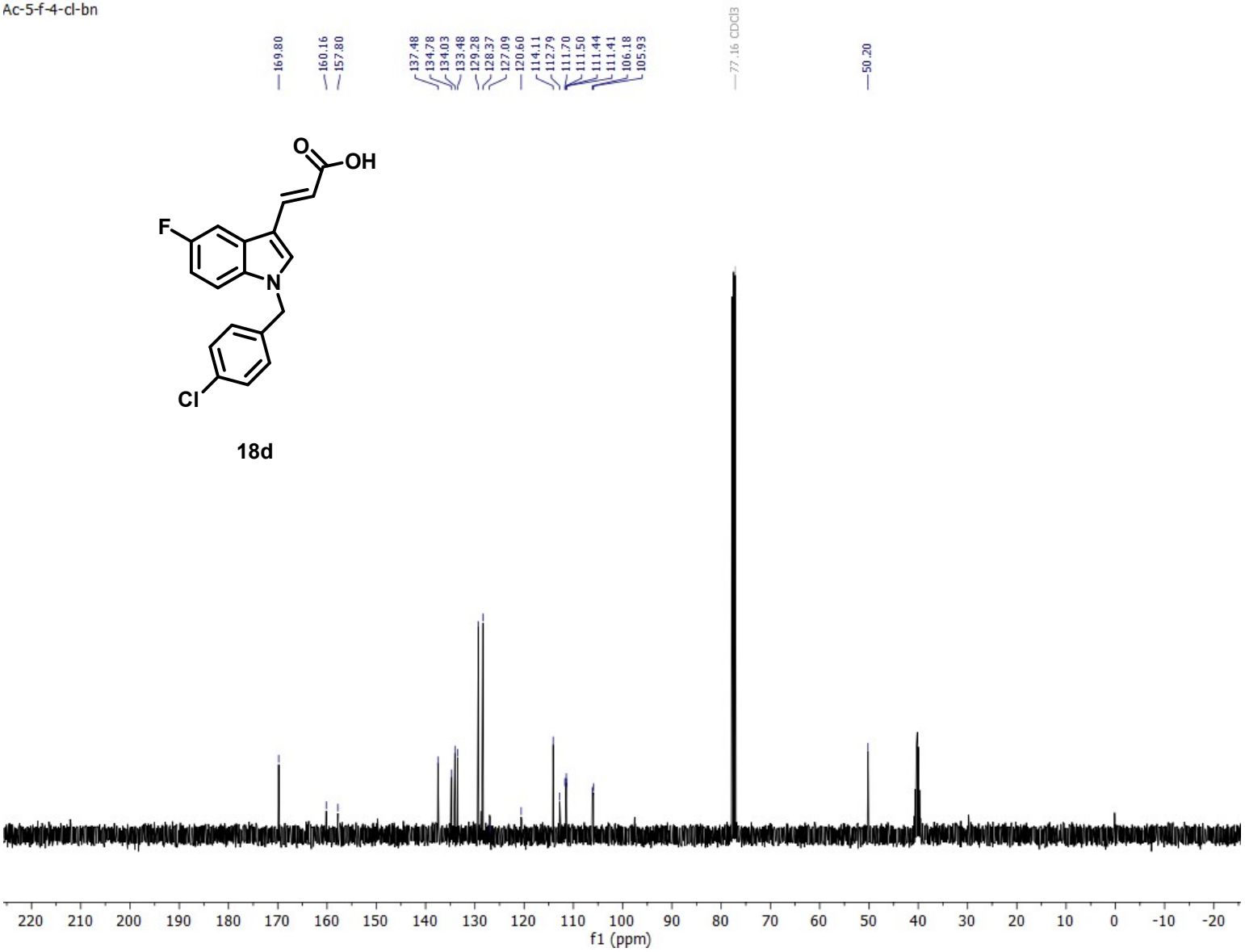
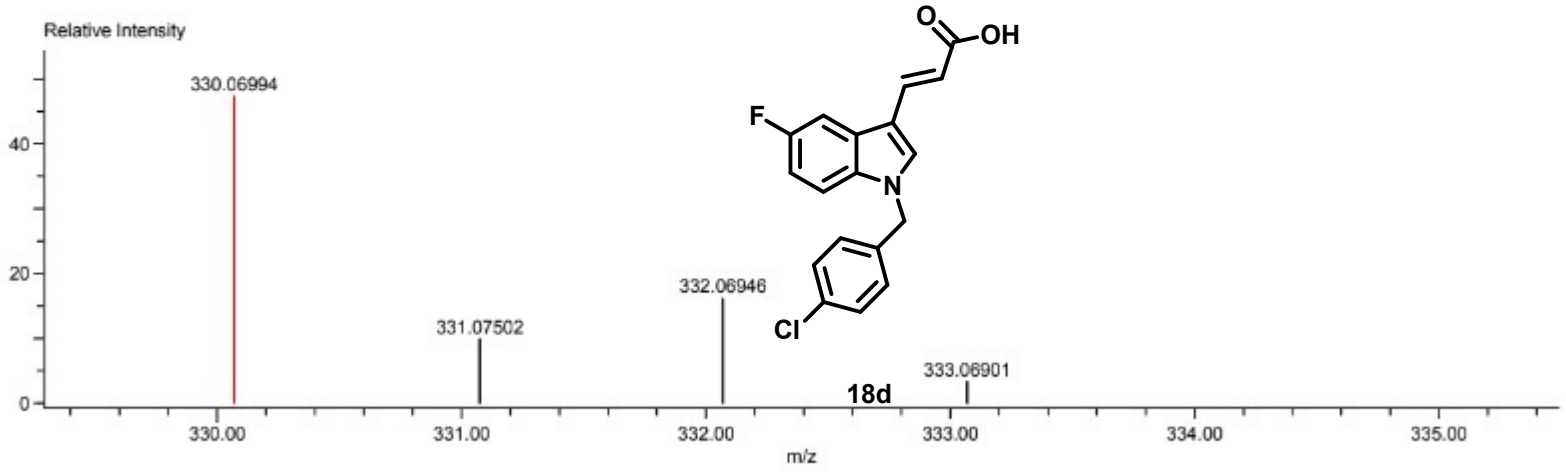


Figure 29. ^{13}C NMR spectrum of **18d** (101 MHz, $CDCl_3$).

Data:1927 5-F-4-9-bn
Sample Name:Dr Martinez Roberto / Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:7/29/2024 5:09:15 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:9/18/2024 3:17:26 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)
Element:^{12}C:0 .. 18, ^{1}H:0 .. 50, ^{35}Cl:0 .. 1, ^{19}F:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 2



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
330.06994	106669.72	330.06971	0.23	0.71	$^{12}C_{18}{}^{1}H_{14}{}^{35}Cl_{1}{}^{19}F_{1}{}^{14}N_{1}{}^{16}O_{2}$	11.5

Figure 30. ESI-HRMS spectrum of **18d**.

2.12 Compound 10a

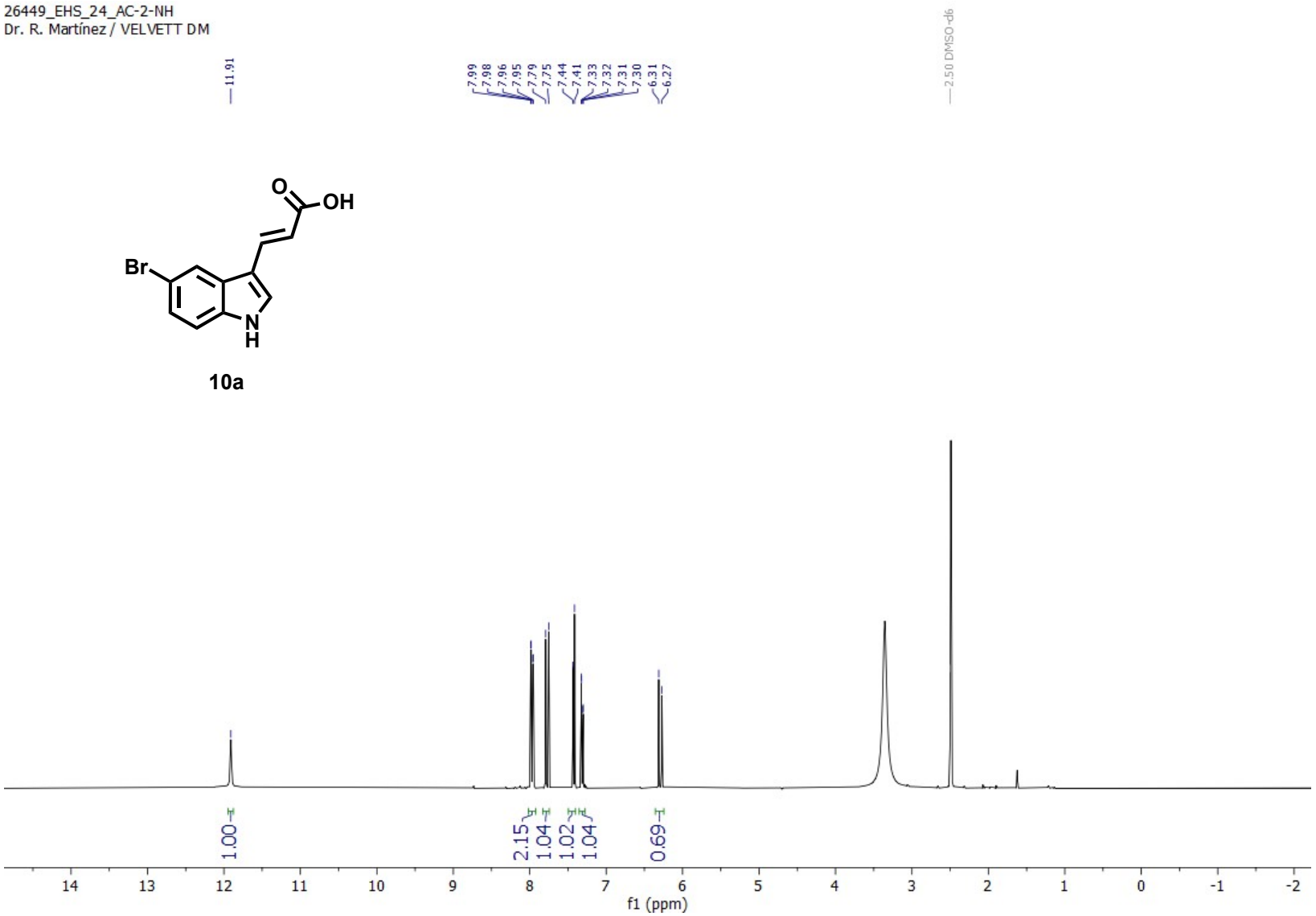


Figure 31. ^{1}H NMR spectrum of **10a** (400 MHz, DMSO-d_6).

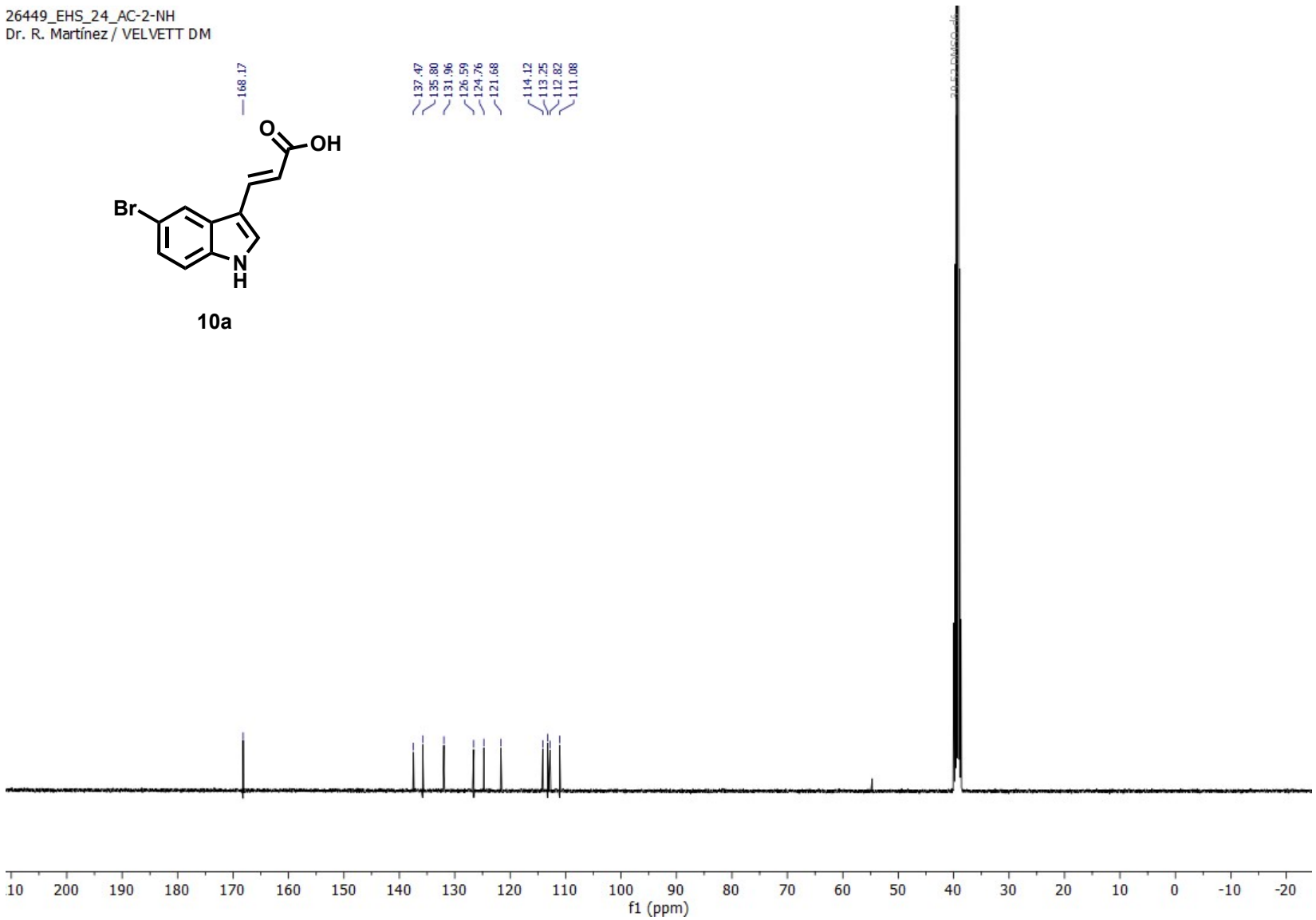
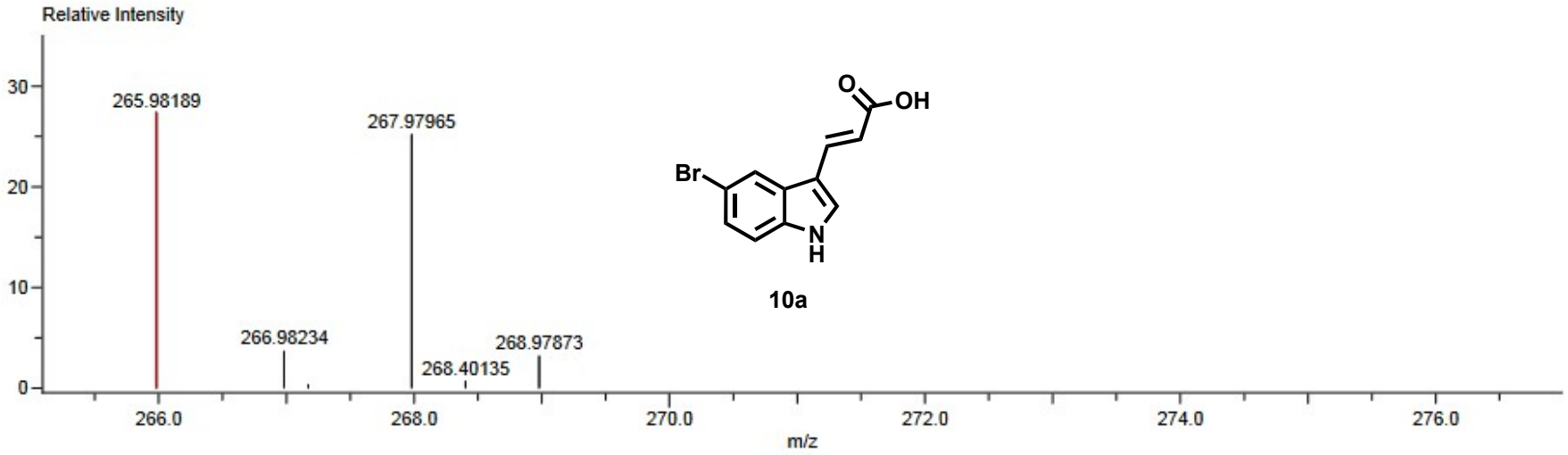


Figure 32. ^{13}C NMR spectrum of **10a** (400 MHz, DMSO-d_6).

Data:1550_AC-2-NH
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:6/19/2024 1:04:34 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:6/28/2024 2:07:00 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{79}Br:0 .. 1, ^{14}N:0 .. 2, ^{16}O:0 .. 3



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
265.98189	12238.85	265.98167	0.22	0.84	$^{12}C_{11}{}^{1}H_{9}{}^{79}Br_{1}{}^{14}N_{1}{}^{16}O_{2}$	7.5

Figure 33. ESI-HRMS spectrum of **10a**.

2.13 Compound 10b

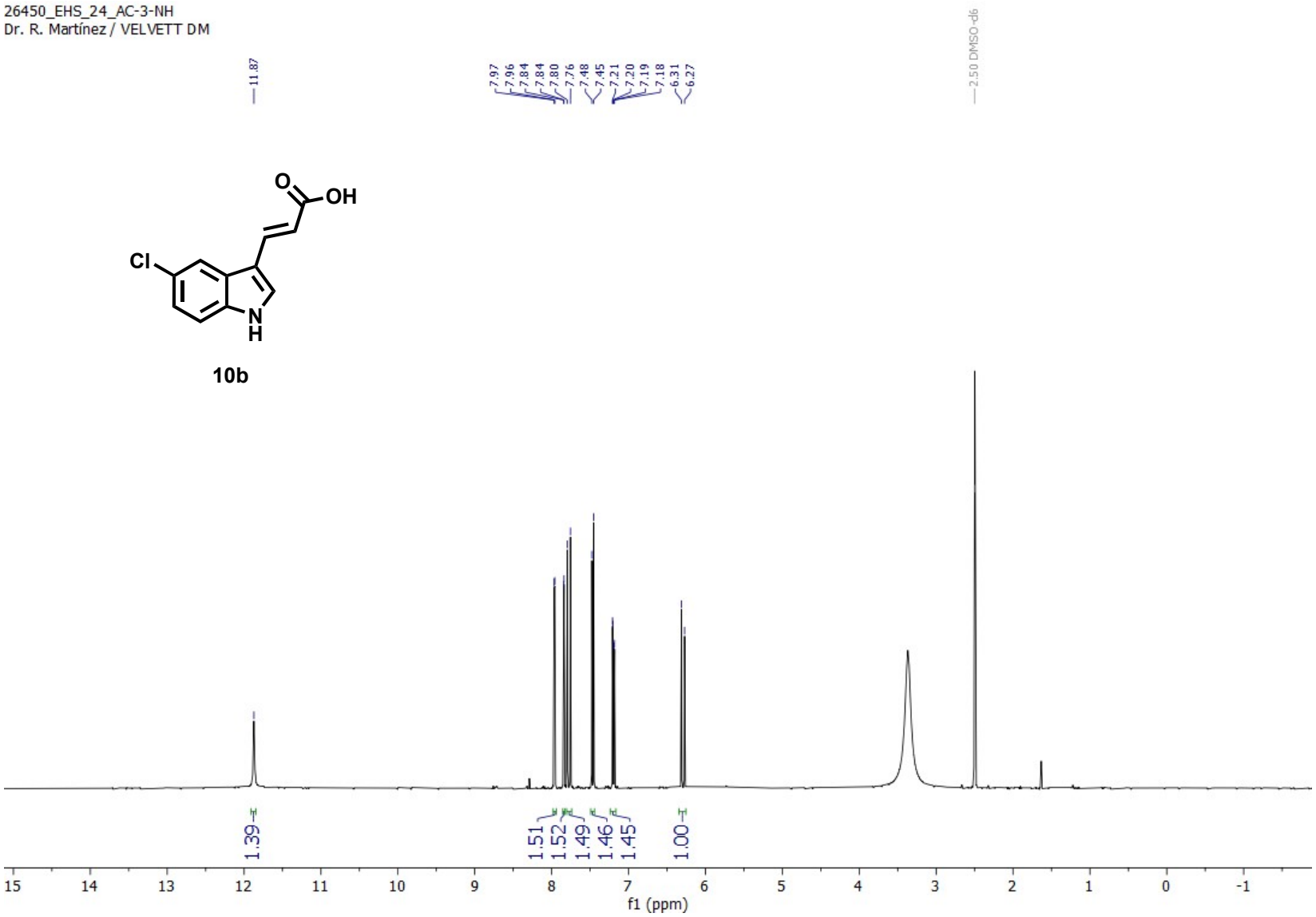


Figure 34. ^{1}H NMR spectrum of **10b** (400 MHz, DMSO-d_6).

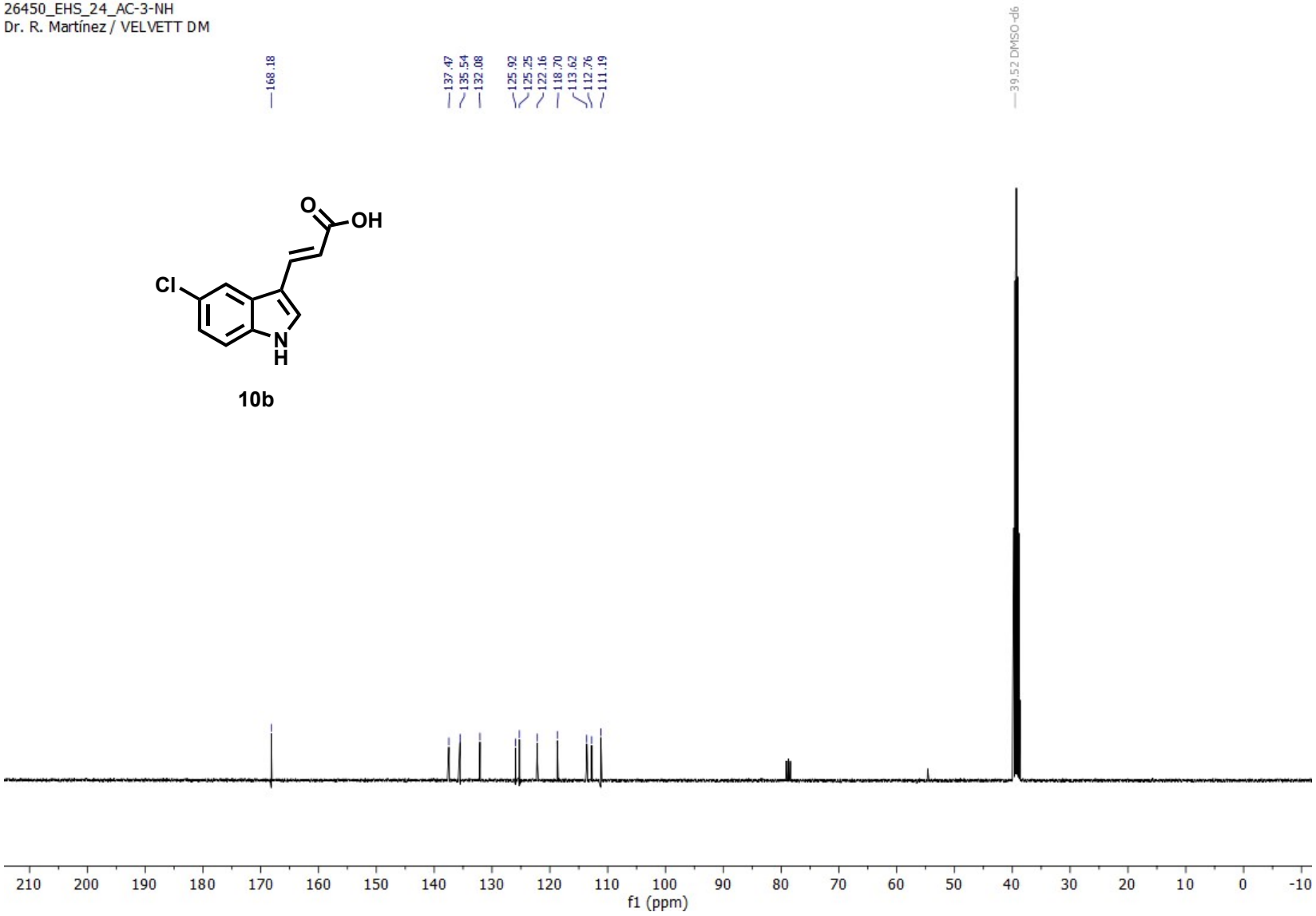
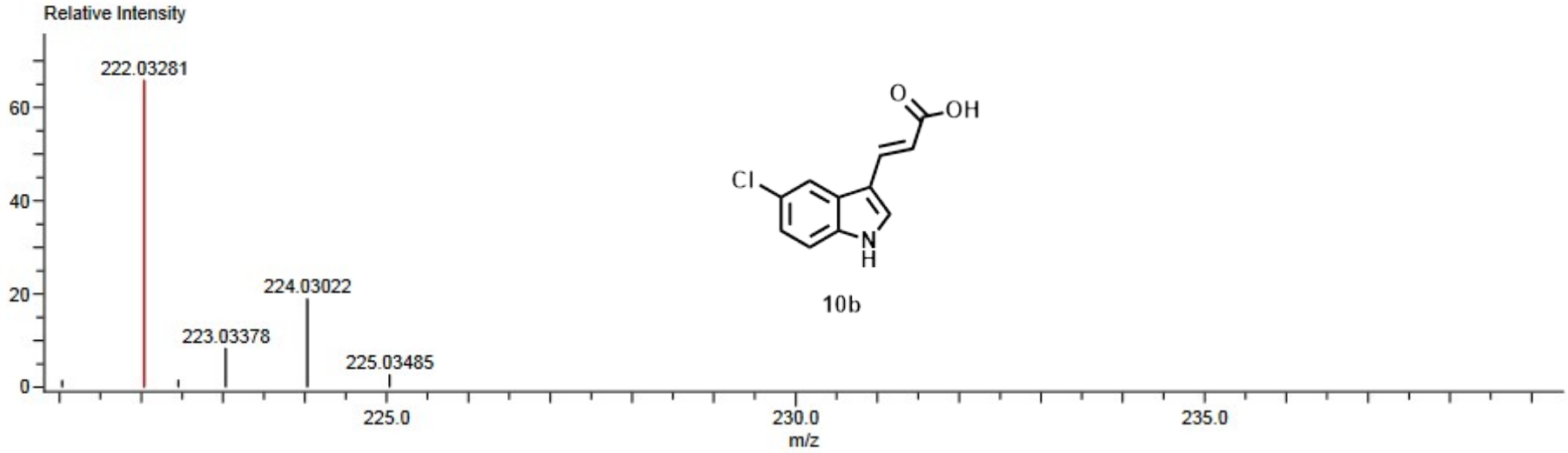


Figure 35. ^{1}H NMR spectrum of **10b** (400 MHz, DMSO-d_6).

Data:1551_AC-3-NH
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..0)

Acquired:6/19/2024 1:06:31 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:6/28/2024 2:10:30 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 1000.0 (Fraction:Both)
Element:^{12}C:0 .. 11, ^{1}H:0 .. 50, ^{35}Cl:0 .. 2, ^{14}N:0 .. 1, ^{16}O:0 .. 3



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
222.03281	120114.97	222.03218	0.62	2.81	$^{12}C_{11}{}^{1}H_{9}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{2}$	7.5

Figure 36. ESI-HRMS spectrum of **10b**.

2.14 Compound 10c

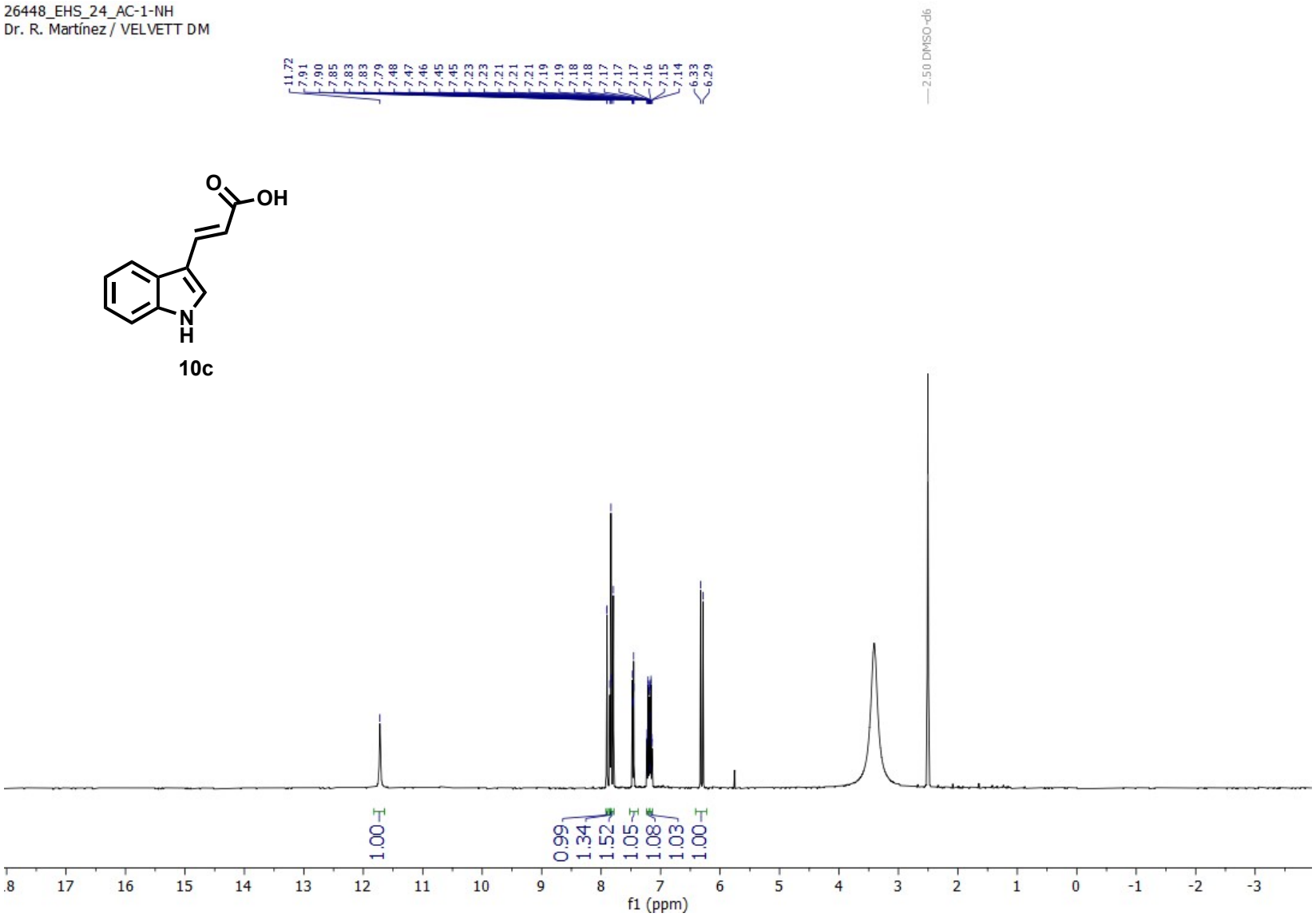


Figure 37. ^{1}H NMR spectrum of **10c** (400 MHz, DMSO-d_6).

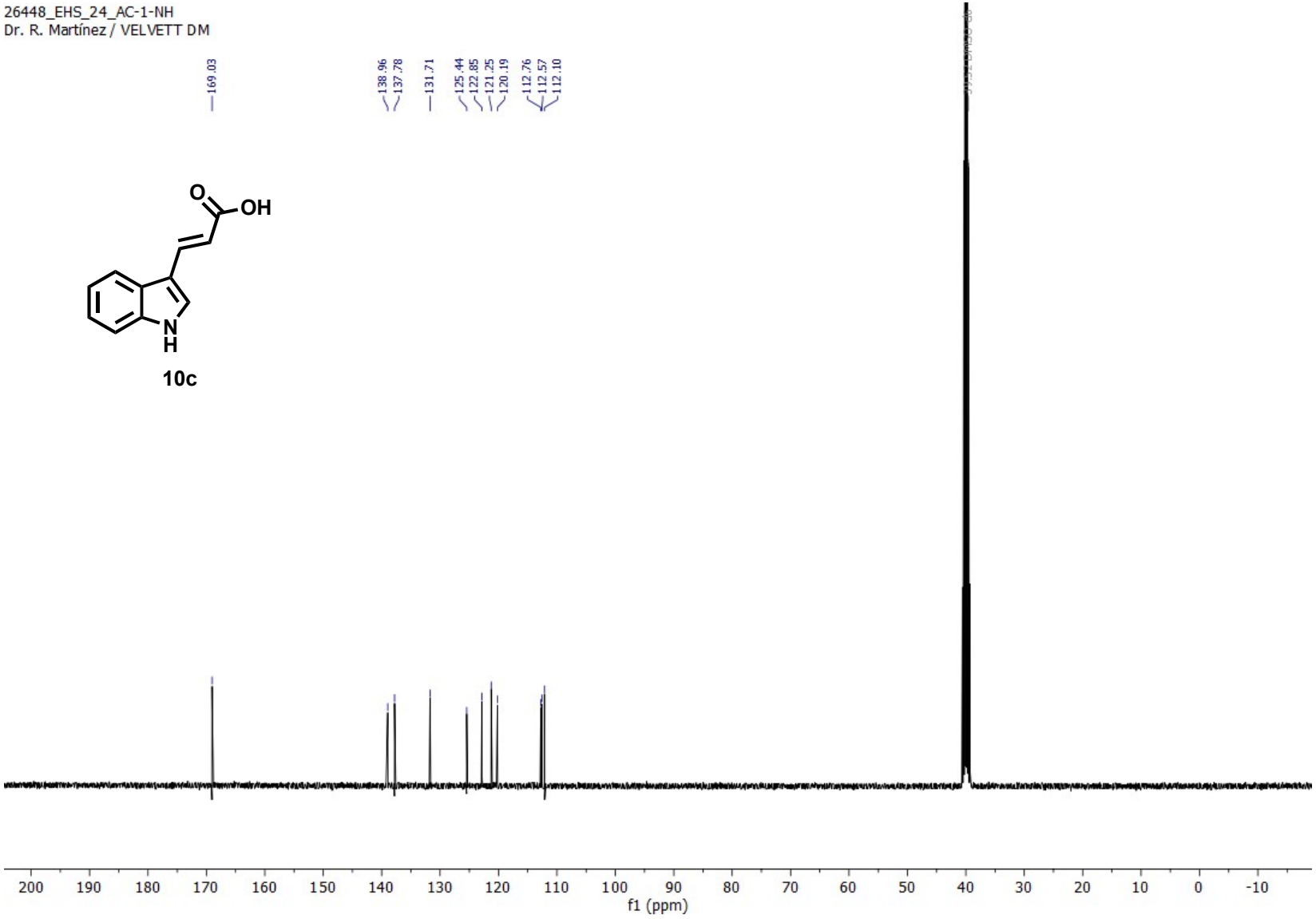


Figure 38. ^{13}C NMR spectrum of **10c** (101 MHz, DMSO-d_6).

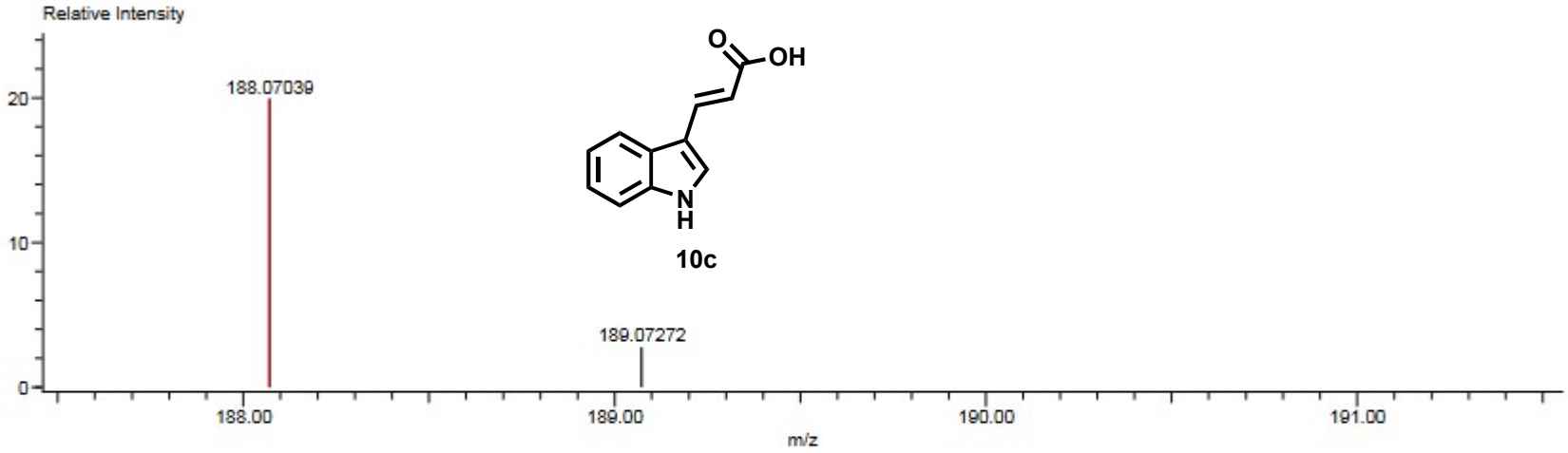
Data:1693 AC-1-NH-2
Sample Name:Dr Martinez Roberto Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..0)

Acquired:6/27/2024 12:47:59 PM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_JEOL_2024060...
Created:7/26/2024 12:16:26 PM
Created by:AccuTOF

Charge number:1
Element:^{12}C:0 .. 11, ^{1}H:0 .. 50, ^{14}N:0 .. 1, ^{16}O:0 .. 4

Tolerance:2.00(ppm), 5.00 .. 15.00(mmu)

Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
188.07039	13300.70	188.07115	-0.76	-4.06	$^{12}C_{11}{}^{1}H_{10}{}^{14}N_{1}{}^{16}O_{2}$	7.5

Figure 39. ESI-HRMS spectrum of **10c**.

2.15 Compound 11a

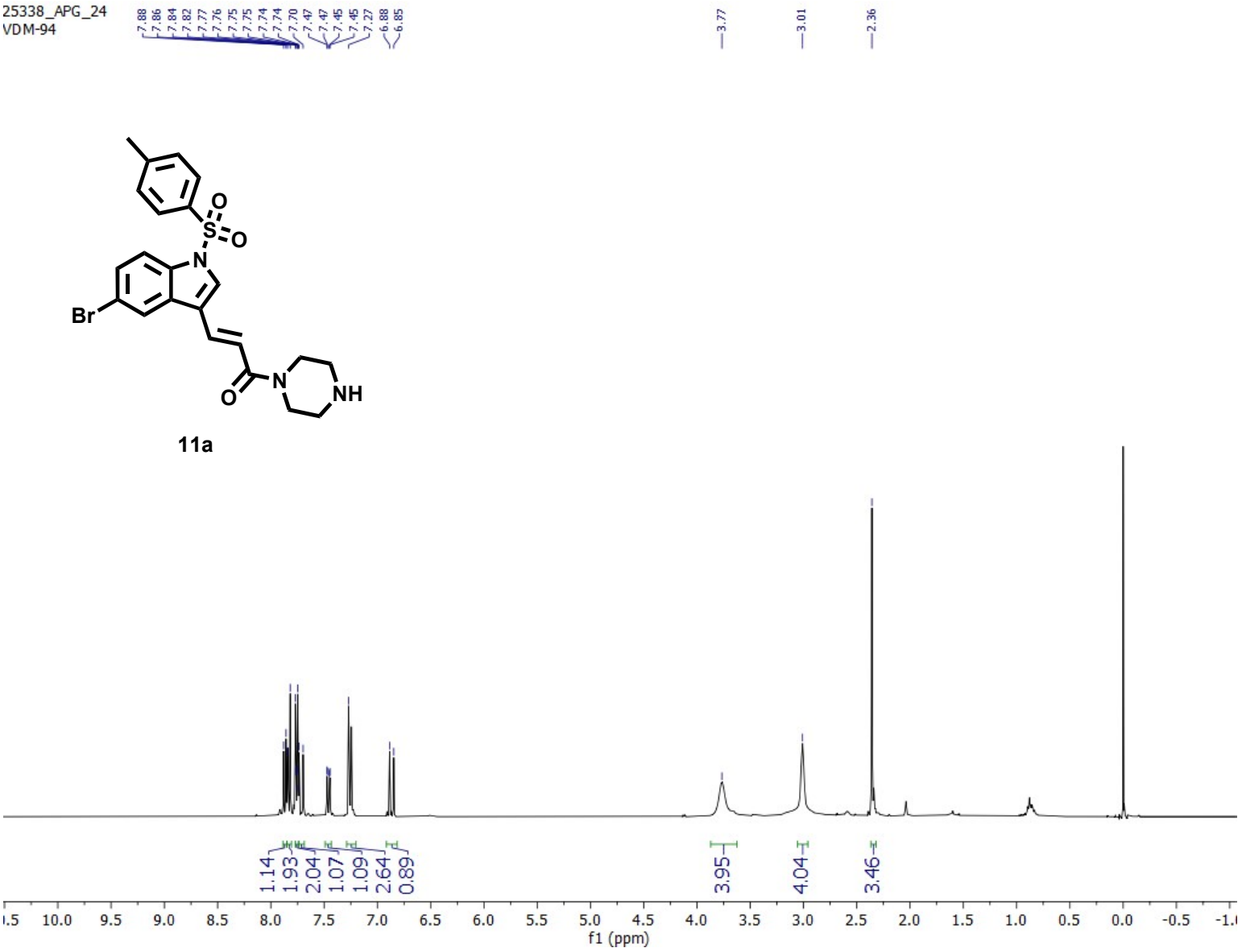


Figure 40. ^{1}H NMR spectrum of **11a** (400 MHz, $CDCl_3$).

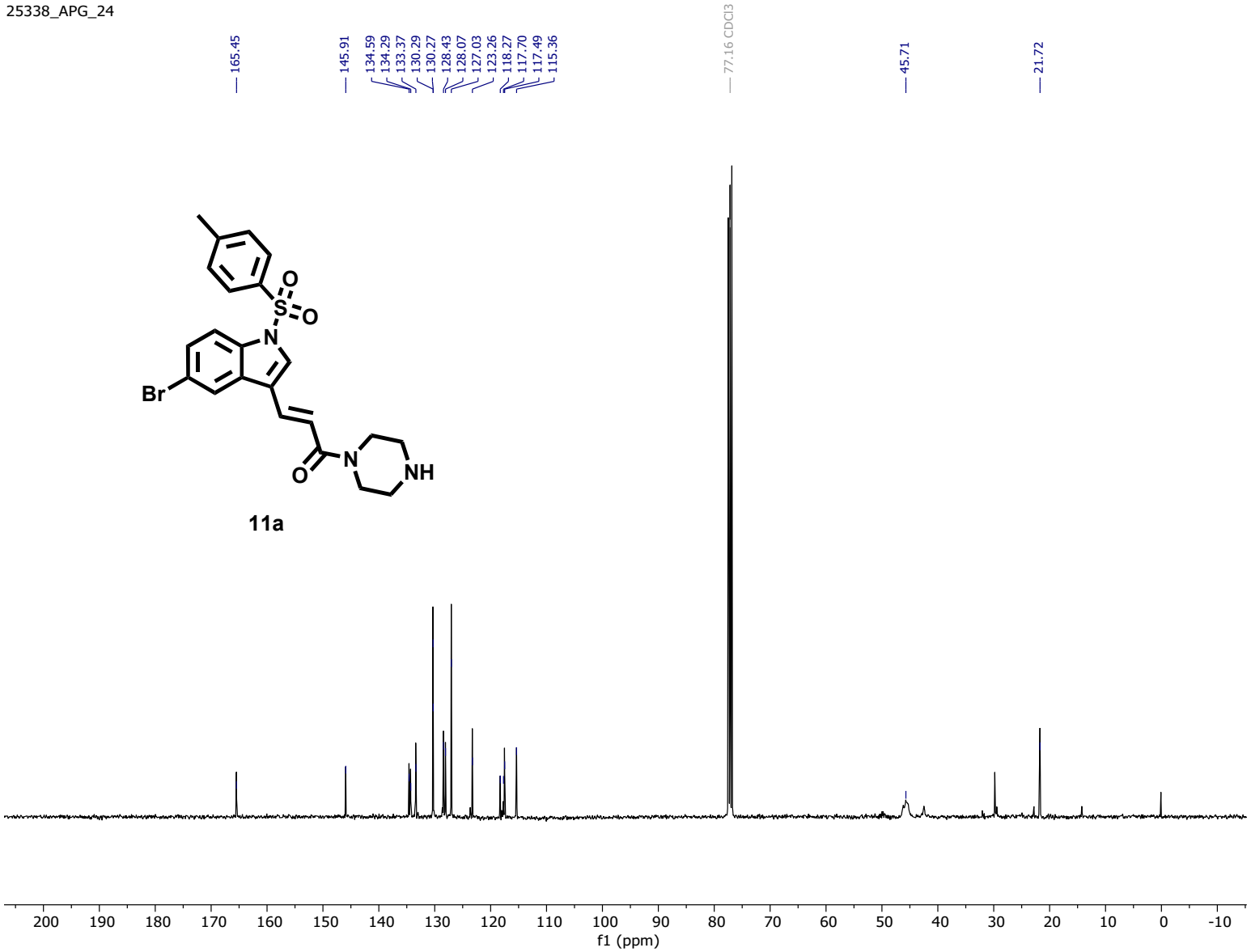


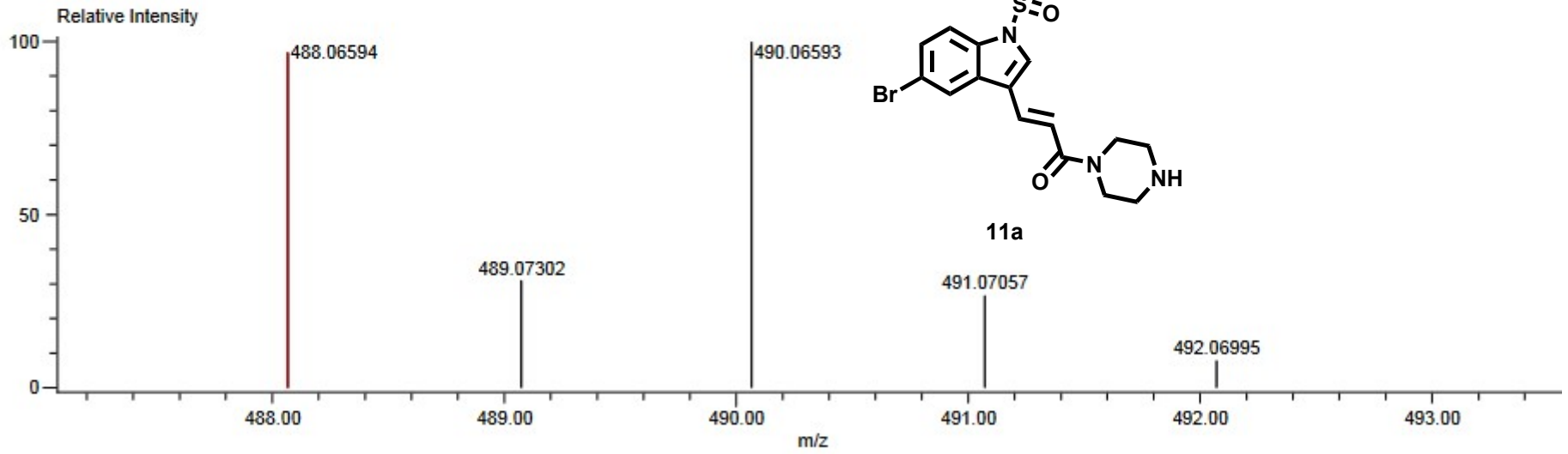
Figure 41. ^{13}C NMR spectrum of **11a** (101 MHz $CDCl_3$).

Data:808 VDM-94
Sample Name:Dr. Martinez Roberto/ Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:3/16/2023 5:36:37 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:3/28/2023 4:31:54 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(mmu)
Element:^{12}C:0 .. 24, ^{1}H:0 .. 60, ^{79}Br:0 .. 1, ^{14}N:0 .. 4, ^{16}O:0 .. 3, ^{32}S:1 .. 1

Unsaturation Number:-1.0 .. 50.0 (Fraction:.5)



11a

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
488.06594	32612.95	488.06435	1.59	3.26	$^{12}C_{22}{}^{1}H_{23}{}^{79}Br_{1}{}^{14}N_{3}{}^{16}O_{3}{}^{32}S_{1}$	13.5

Figure 42. ESI-HRMS spectrum of **11a.**

2.16 Compound 11b

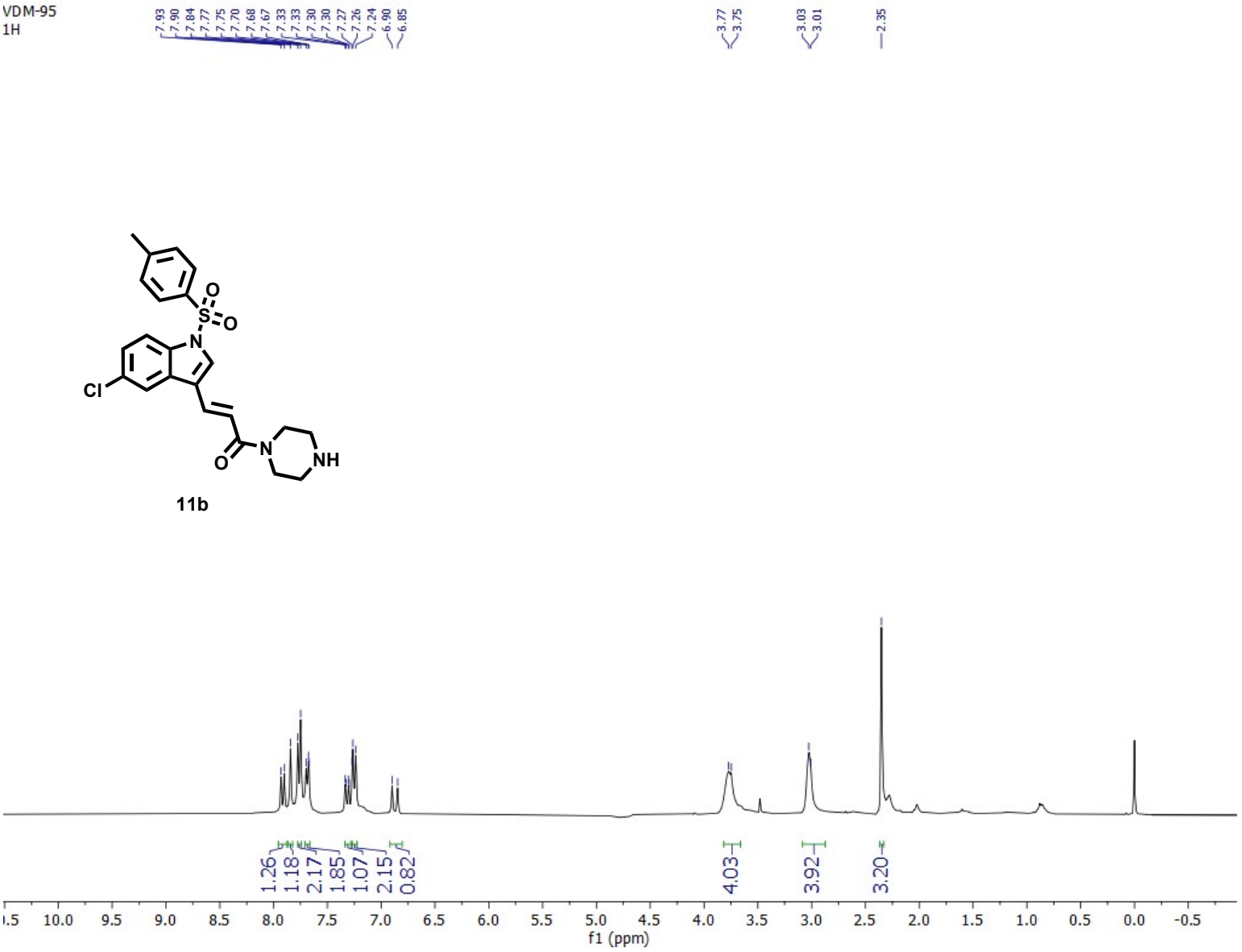


Figure 43. ^{1}H NMR spectrum of **11b** (300 MHz, $CDCl_3$).

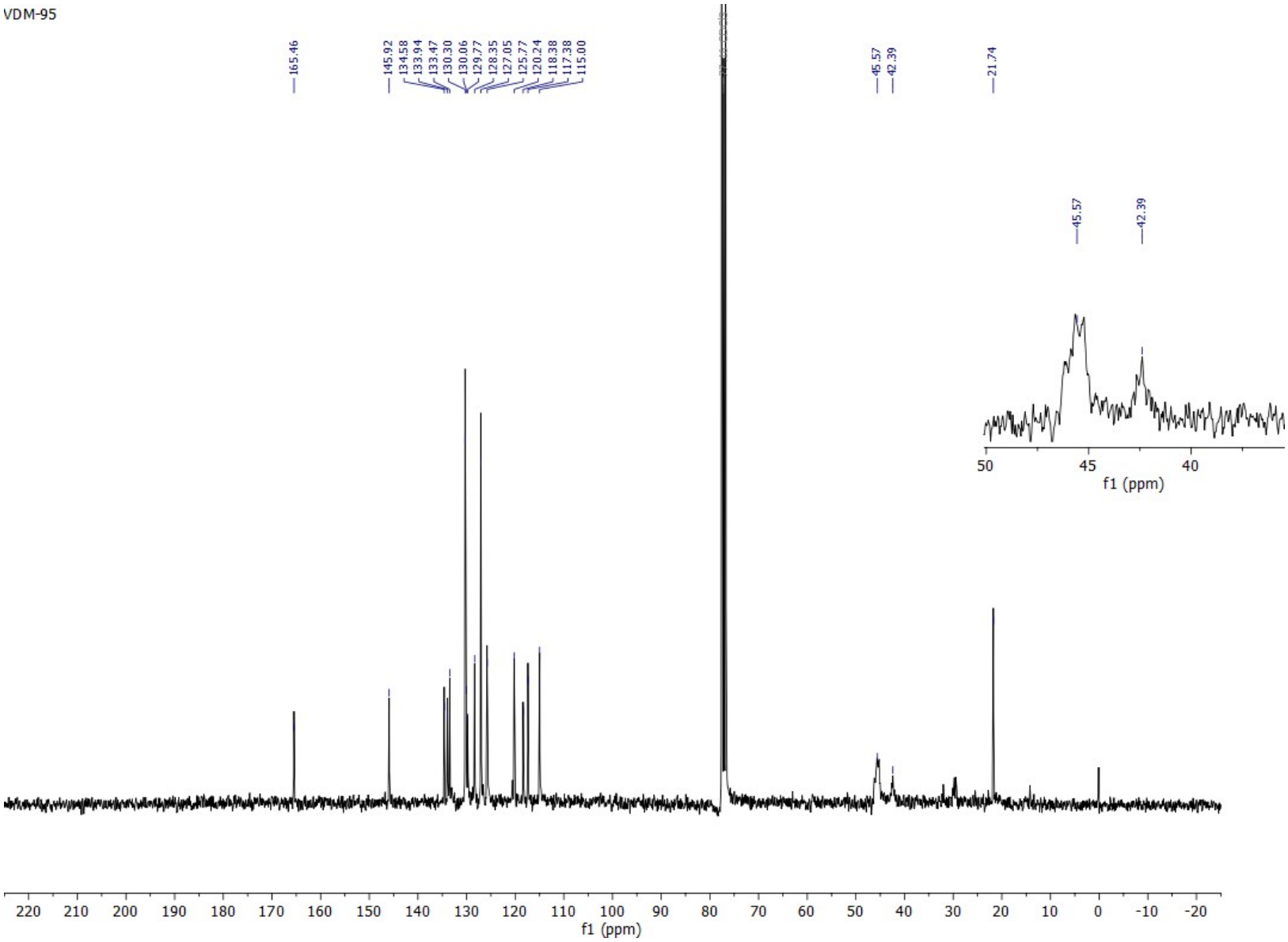
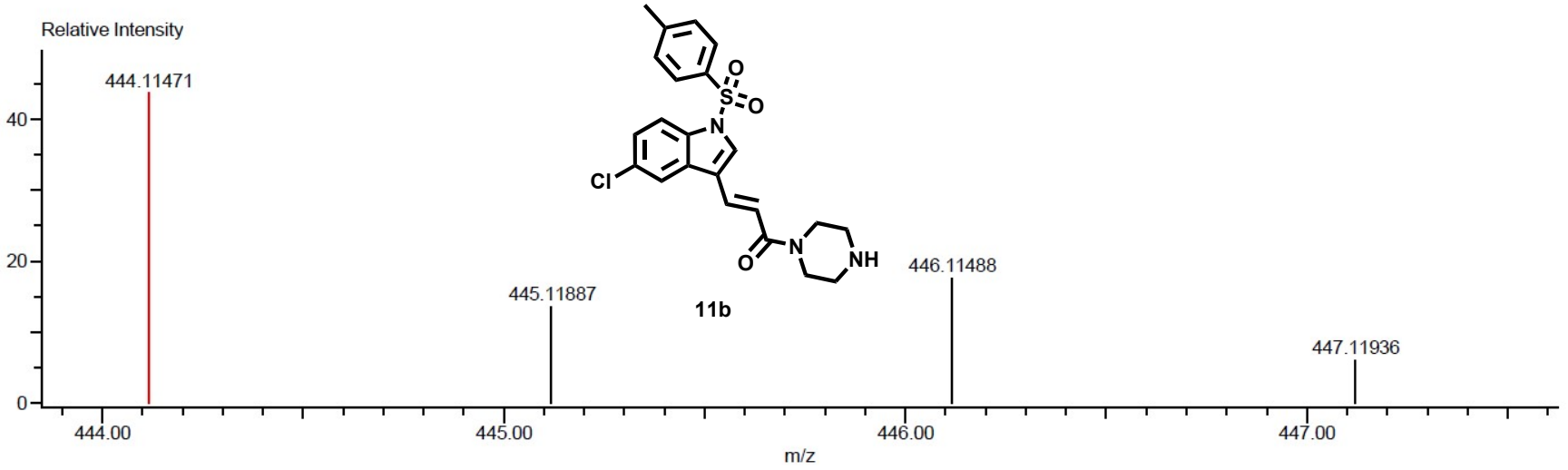


Figure 44. ^{13}C NMR spectrum of **11b** (101 MHz, $CDCl_3$).

Data:1418 VDM-95
Sample Name:DR. MARTINEZ ROBERTO / OPERADORA CARMEN GARCIA - PAULA BERNARDO
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:5/24/2023 1:04:28 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:6/26/2023 1:35:44 PM
Created by:AccuTOF

Charge number:1
Tolerance:2.00(mmu)
Unsaturation Number:-1.0 .. 20.0 (Fraction:Both)
Element:^{12}C:0 .. 35, ^{1}H:0 .. 70, ^{35}Cl:1 .. 1, ^{14}N:1 .. 3, ^{16}O:0 .. 4, ^{32}S:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
444.11471	198012.67	444.11486	-0.15	-0.34	$^{12}C_{22}{}^{1}H_{23}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{3}{}^{32}S_{1}$	13.5

Figure 45. ESI-HRMS spectrum of **11b.**

2.17 Compound 11c

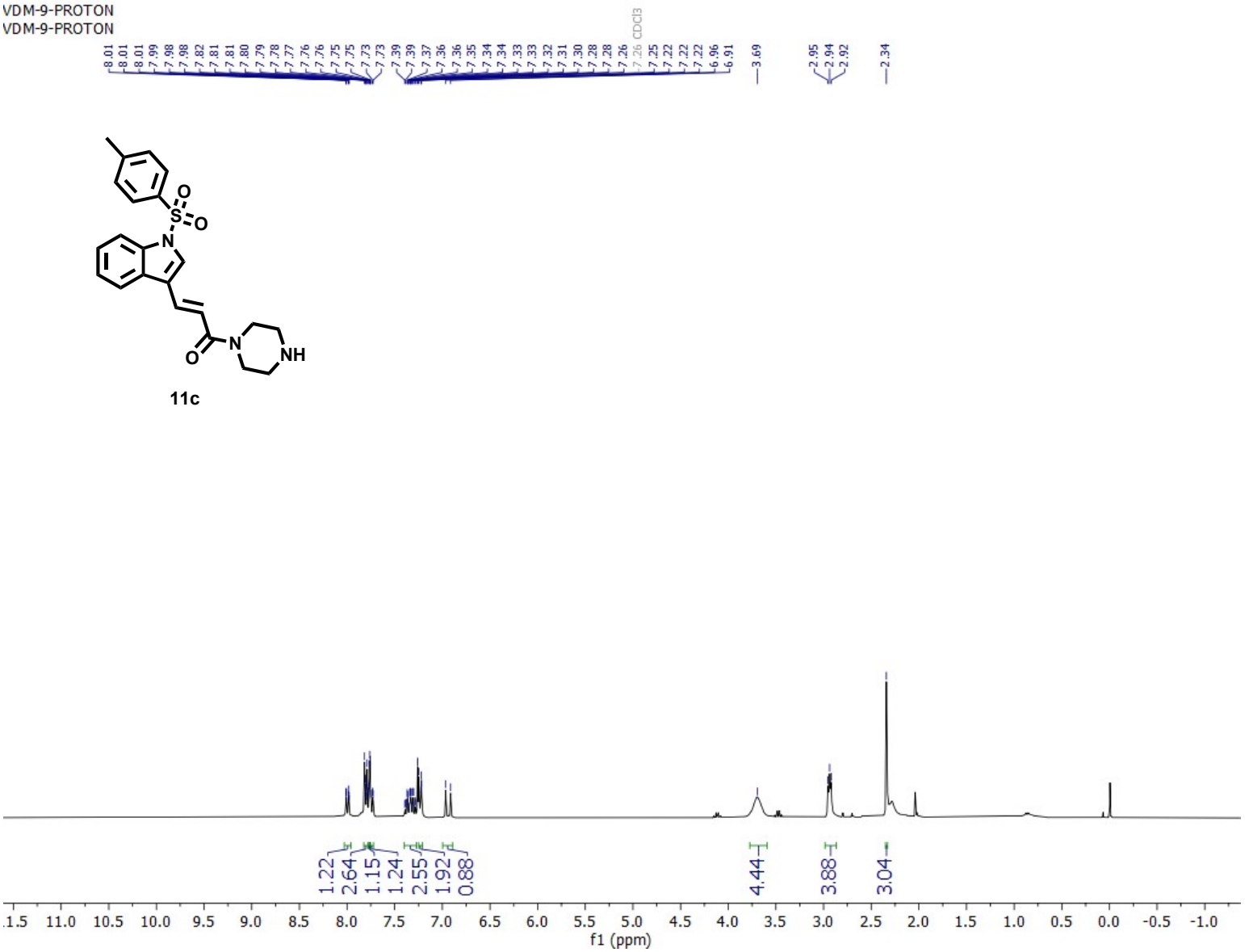


Figure 46. ^{1}H NMR spectrum of **11c** (300 MHz, $CDCl_3$).

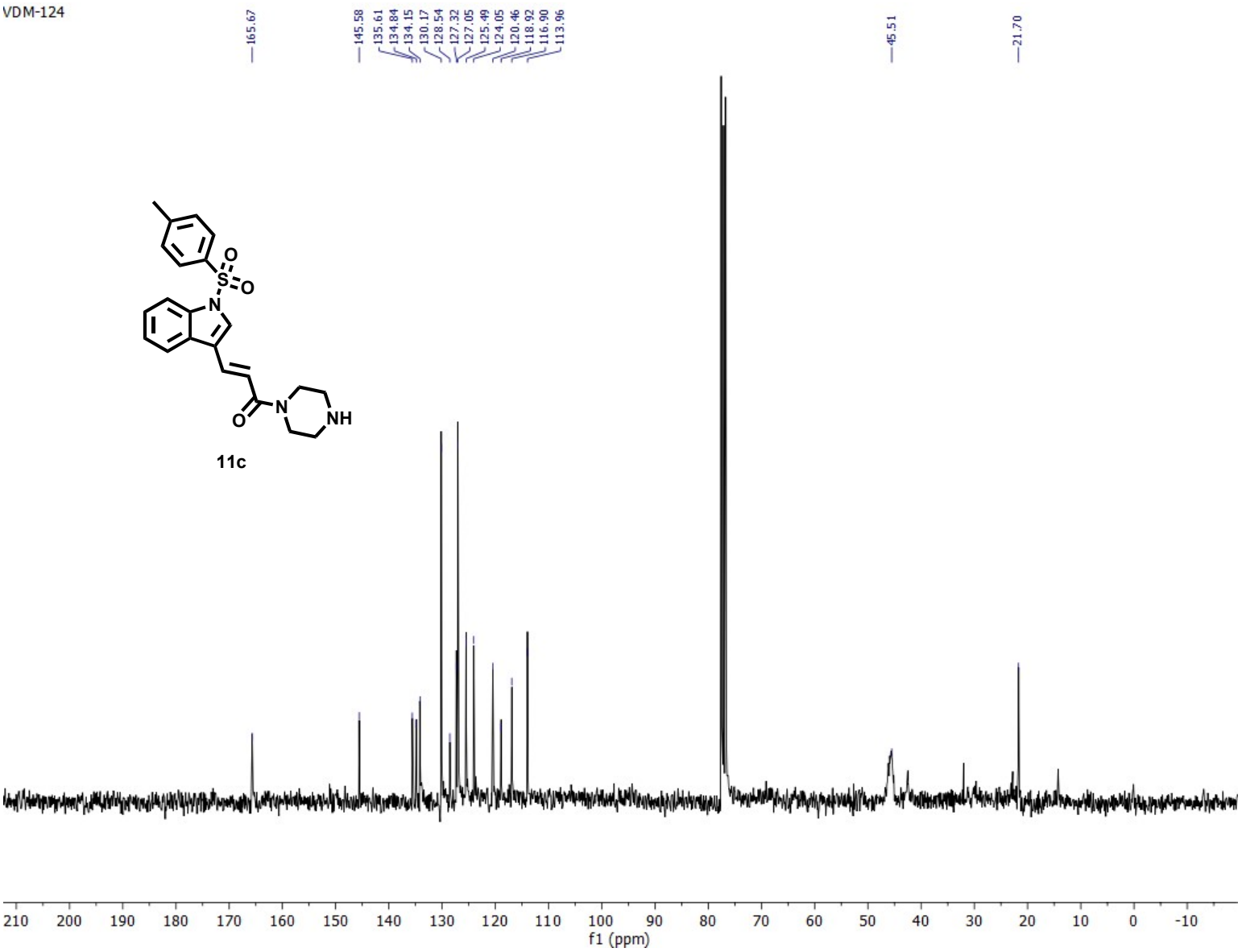
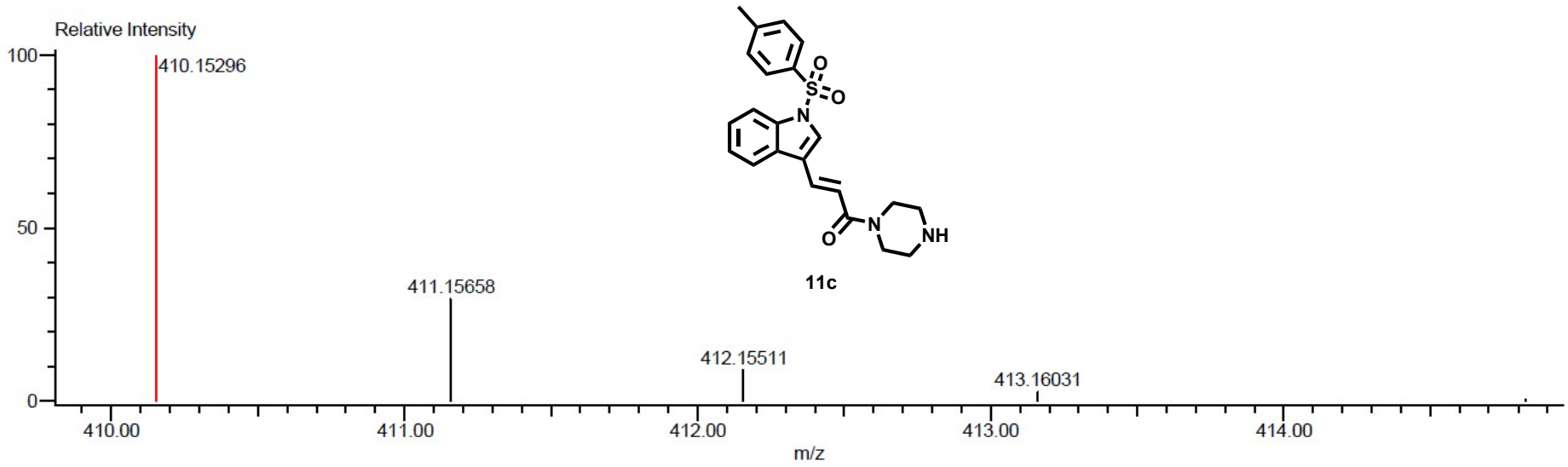


Figure 47. ^{13}C NMR spectrum of **11c** (75 MHz, $CDCl_3$).

Data:804 VDM-9
Sample Name:Dr. Martinez Roberto/ Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:3/16/2023 5:24:02 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:3/28/2023 4:20:10 PM
Created by:AccuTOF

Charge number:1
Tolerance:4.00(mmu)
Unsaturation Number:-1.0 .. 50.0 (Fraction:.5)
Element:^{12}C:0 .. 24, ^{1}H:0 .. 60, ^{14}N:0 .. 4, ^{16}O:0 .. 3, ^{32}S:1 .. 1



11c

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
410.15296	166221.63	410.15384	-0.88	-2.13	$^{12}C_{22}{}^{1}H_{24}{}^{14}N_{3}{}^{16}O_{3}{}^{32}S_{1}$	13.5

Figure 48. ESI-HRMS spectrum of **11c.**

2.18 Compound 11d

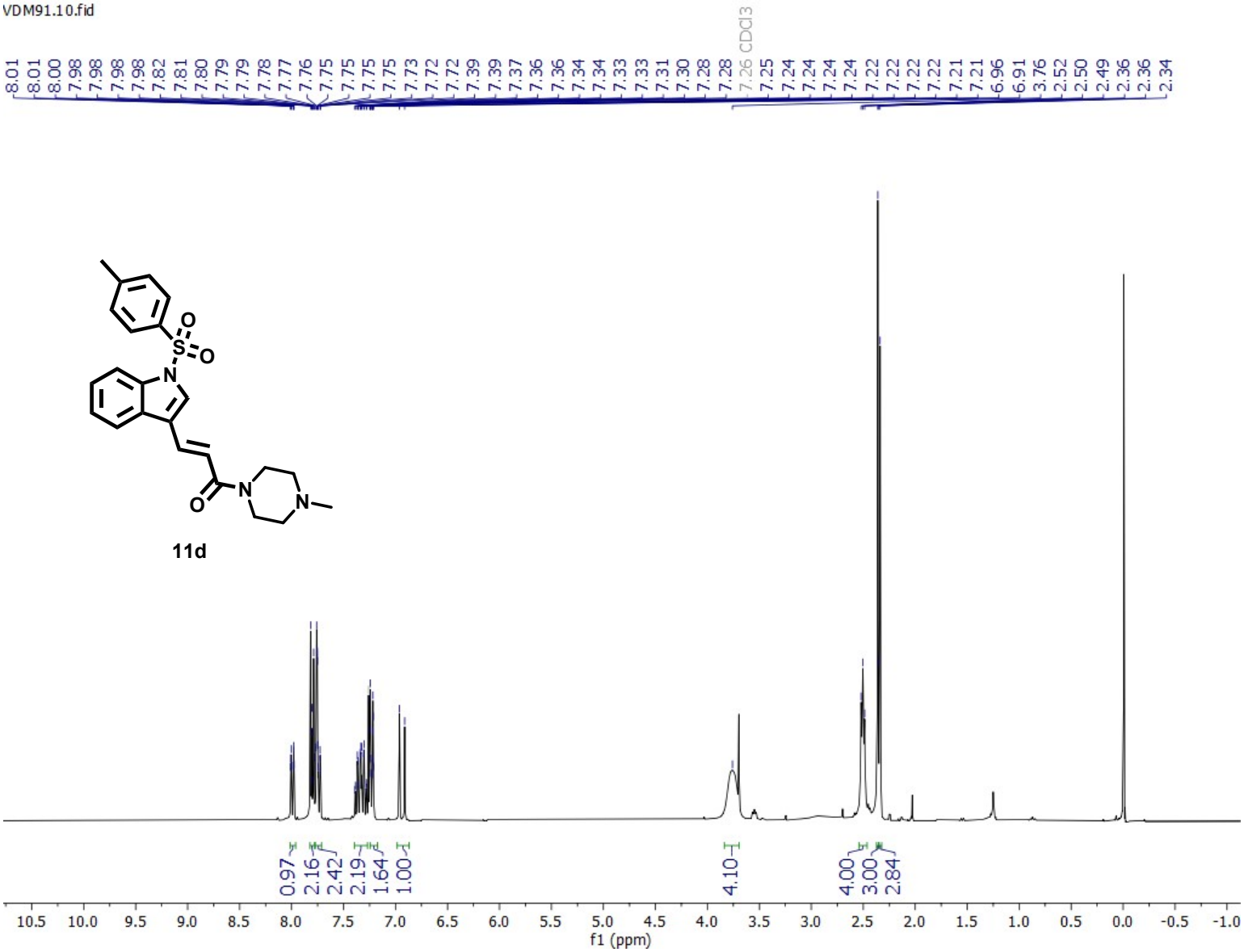


Figure 49. ^{1}H NMR spectrum of **11d** (300 MHz, $CDCl_3$).

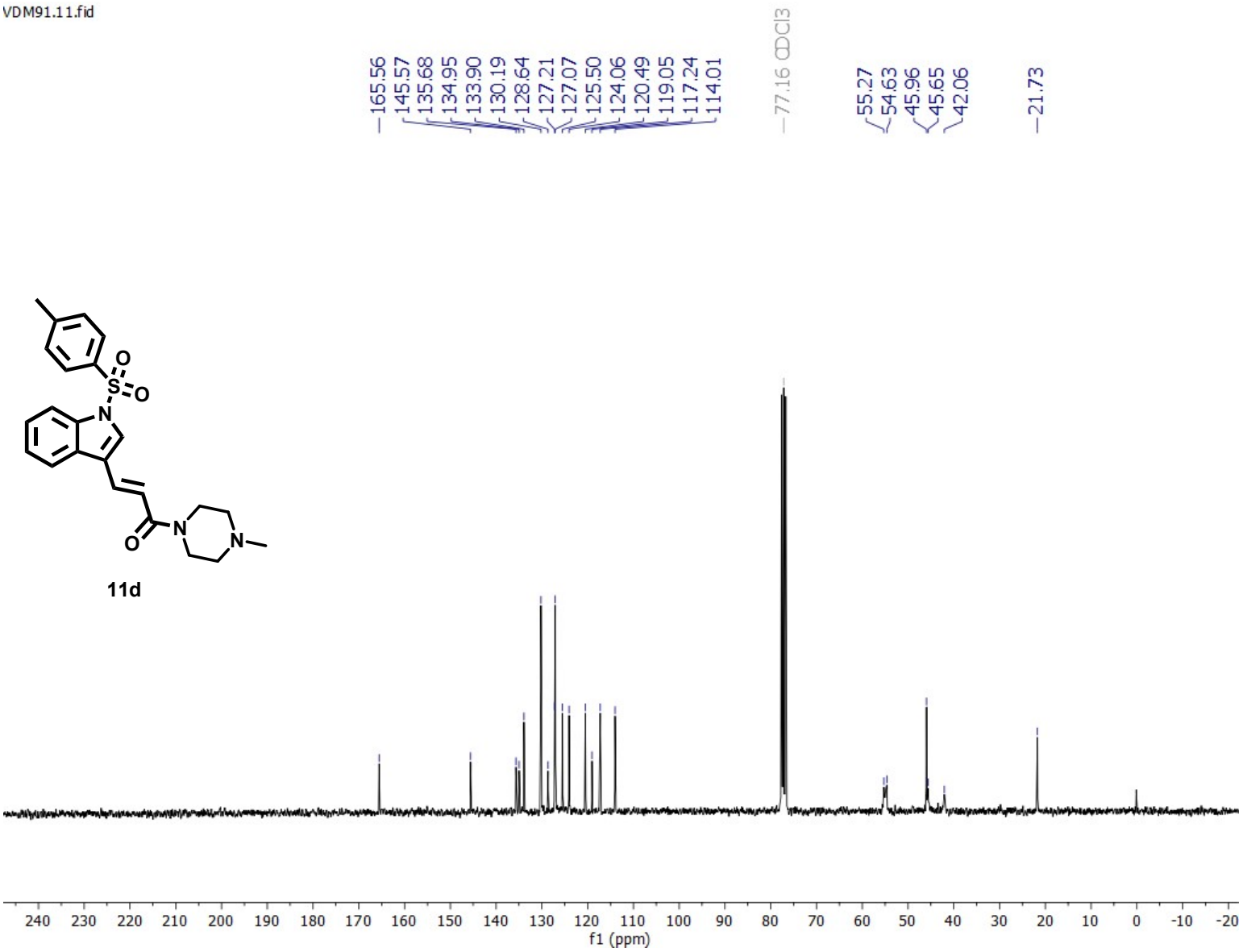
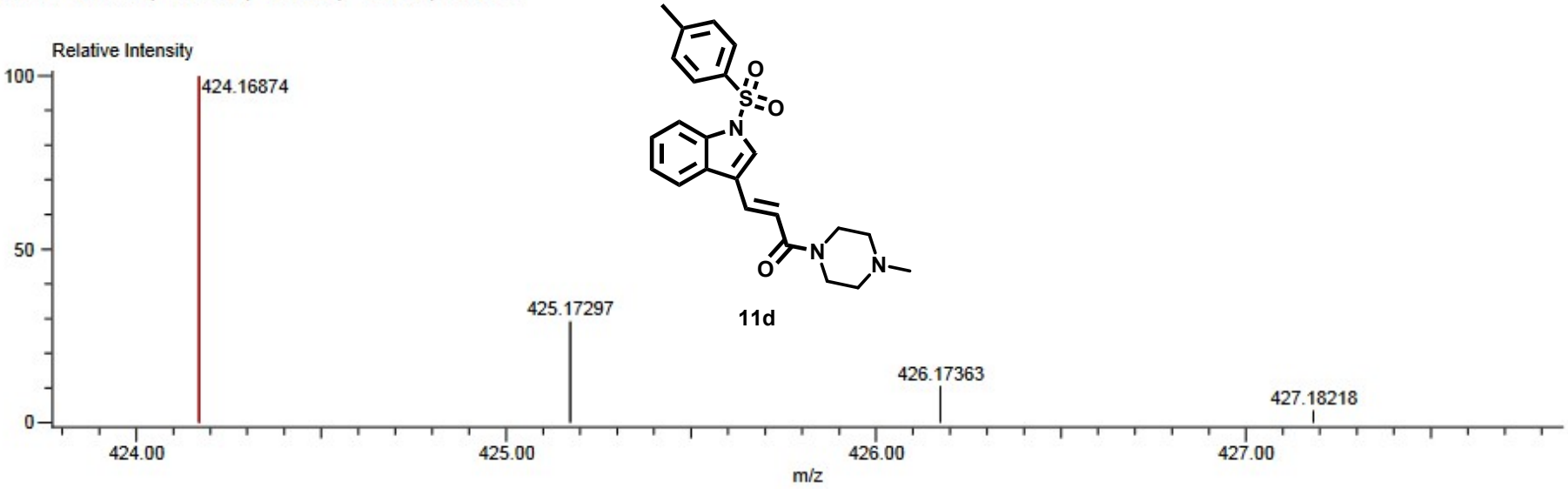


Figure 50. ^{13}C NMR spectrum of **11c** (75 MHz, $CDCl_3$).

Data:806 VDM-91
Sample Name:Dr. Martinez Roberto/ Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:3/16/2023 5:30:18 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:3/28/2023 4:26:25 PM
Created by:AccuTOF

Charge number:1
Tolerance:10.00(mmu)
Unsaturation Number:-1.0 .. 50.0 (Fraction:.5)
Element:^{12}C:0 .. 24, ^{1}H:0 .. 60, ^{14}N:0 .. 4, ^{16}O:0 .. 3, ^{32}S:1 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
424.16874	303110.05	424.16949	-0.75	-1.76	$^{12}C_{23}{}^{1}H_{26}{}^{14}N_{3}{}^{16}O_{3}{}^{32}S_{1}$	13.5

Figure 51. ESI-HRMS spectrum of **11d.**

2.19 Compound 11e

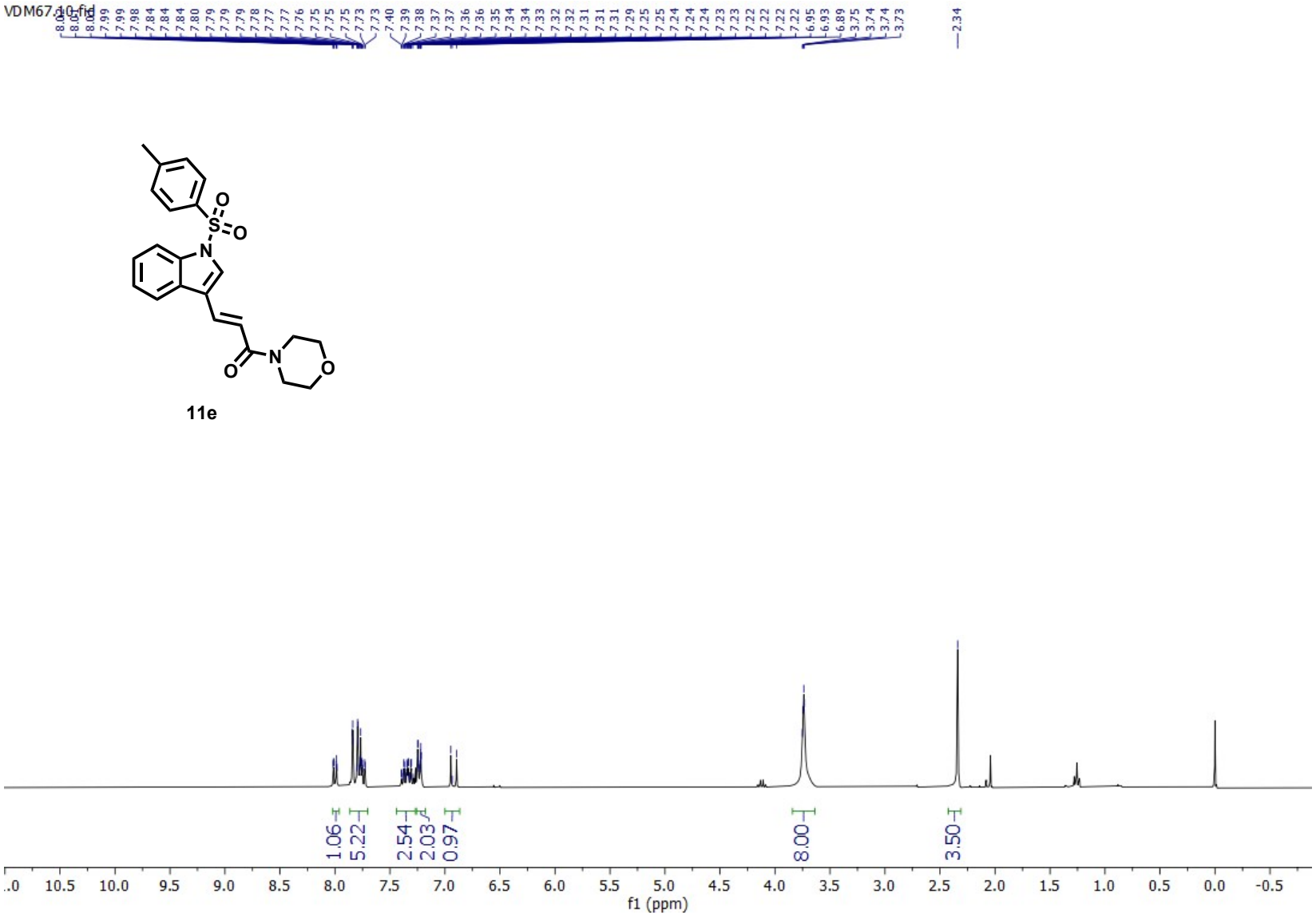


Figure 52. ^{1}H NMR spectrum of **11e** (300 MHz, $CDCl_3$).

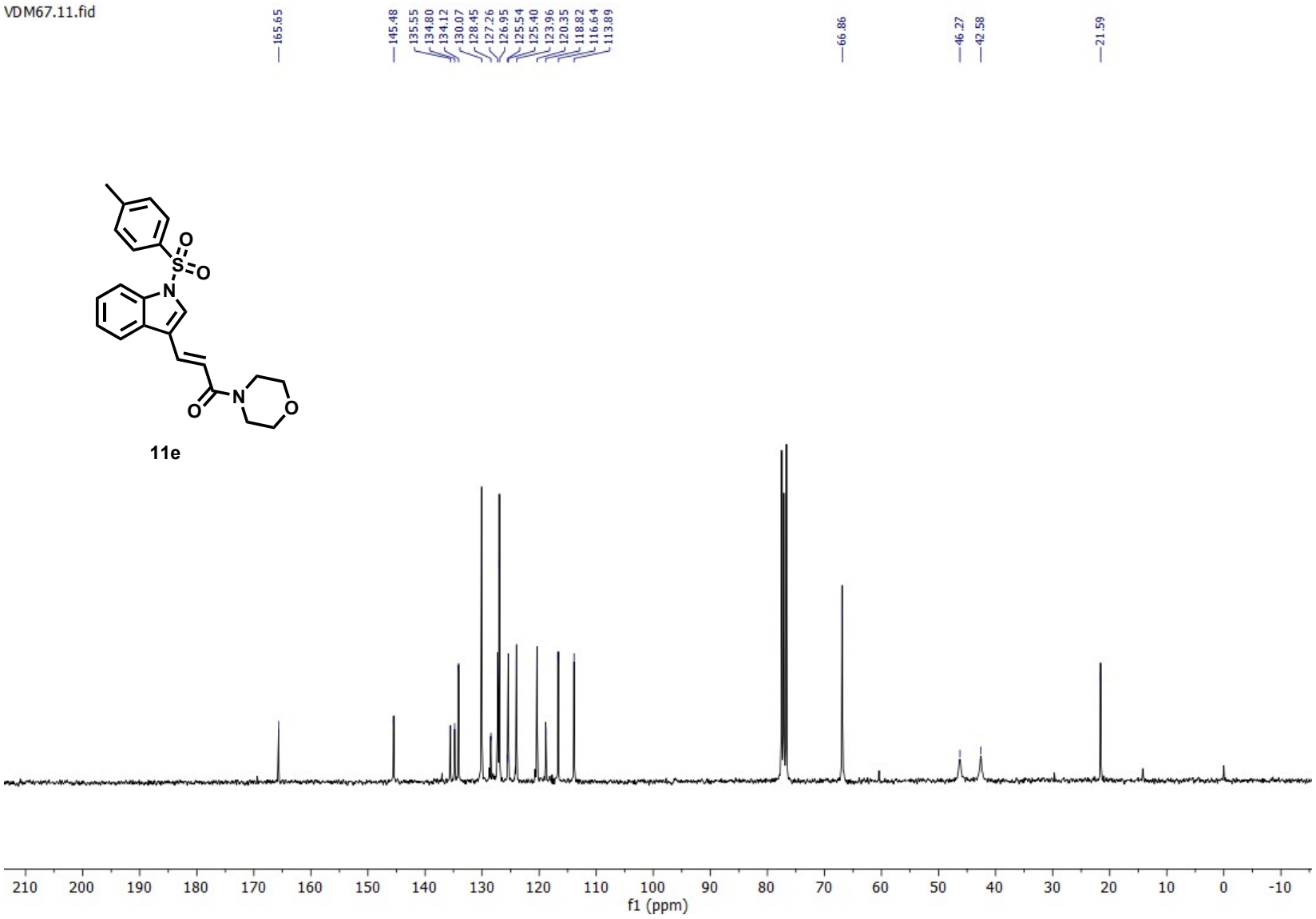
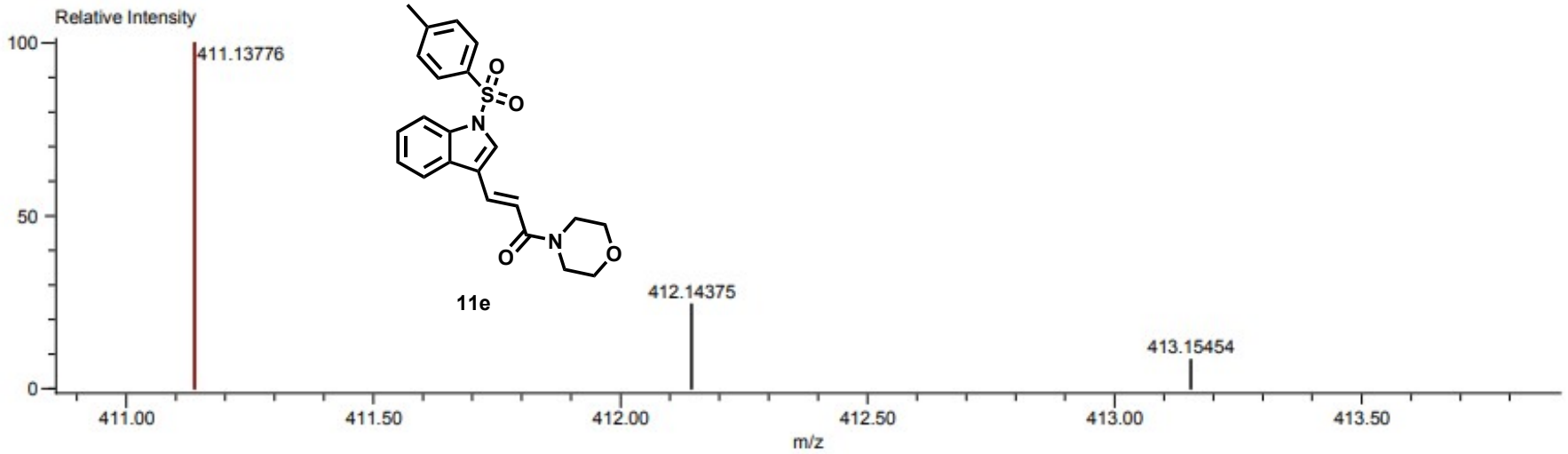


Figure 53. ^{13}C NMR spectrum of **11e** (75 MHz, $CDCl_3$).

Data:927_VDM-67
Sample Name:Dr Martinez Roberto /Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..0)

Acquired:4/16/2024 9:34:04 AM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_ok
Created:4/29/2024 4:07:41 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)
Element:^{12}C:20 .. 22, ^{1}H:0 .. 30, ^{14}N:0 .. 4, ^{16}O:0 .. 4, ^{32}S:1 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
411.13776	24079.17	411.13785	-0.10	-0.24	$^{12}C_{22}{}^{1}H_{23}{}^{14}N_{2}{}^{16}O_{4}{}^{32}S_{1}$	13.5

Figure 54. ESI-HRMS spectrum of **11e.**

2.20 Compound 11f

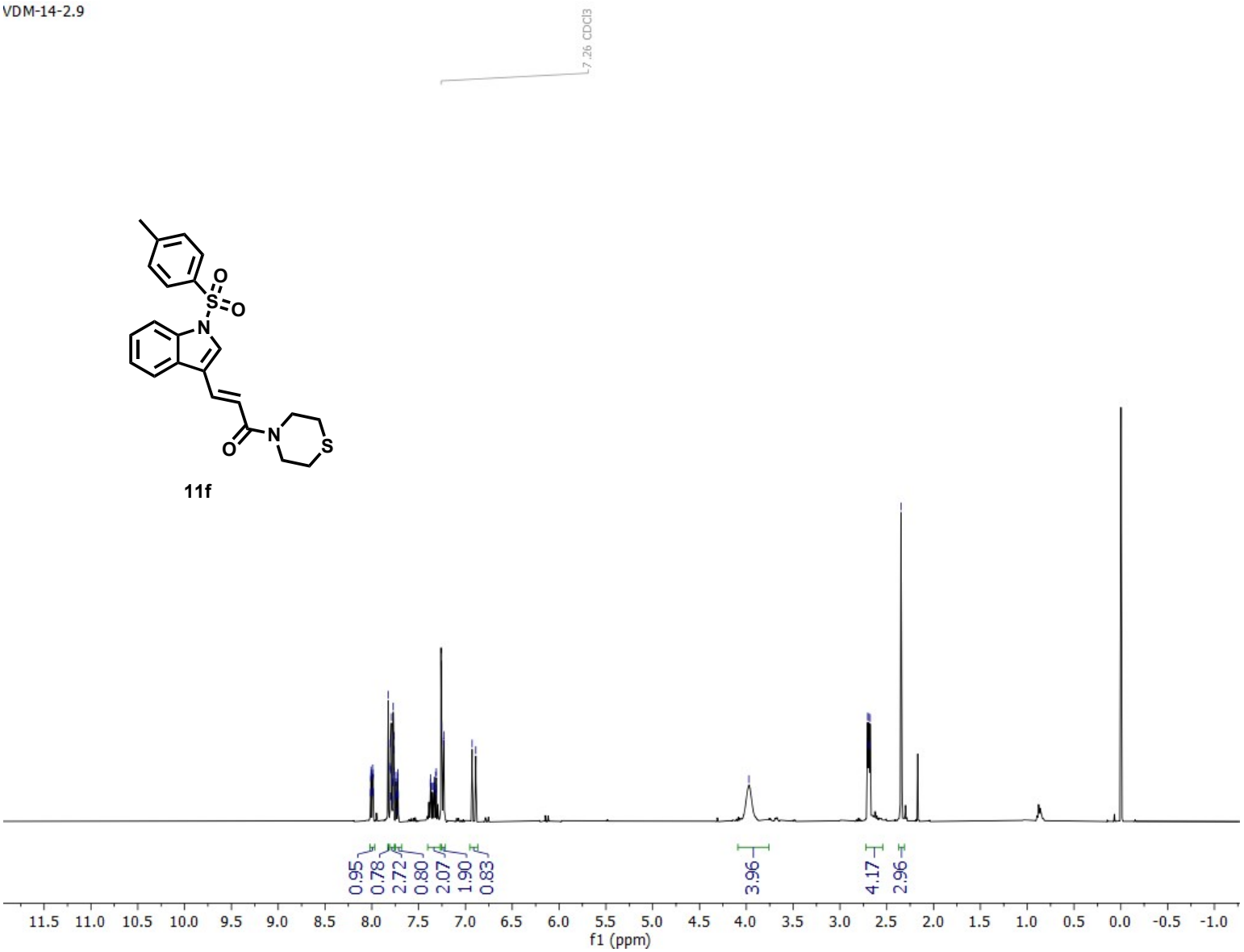


Figure 55. ^{1}H NMR spectrum of **11f** (400 MHz, $CDCl_3$).

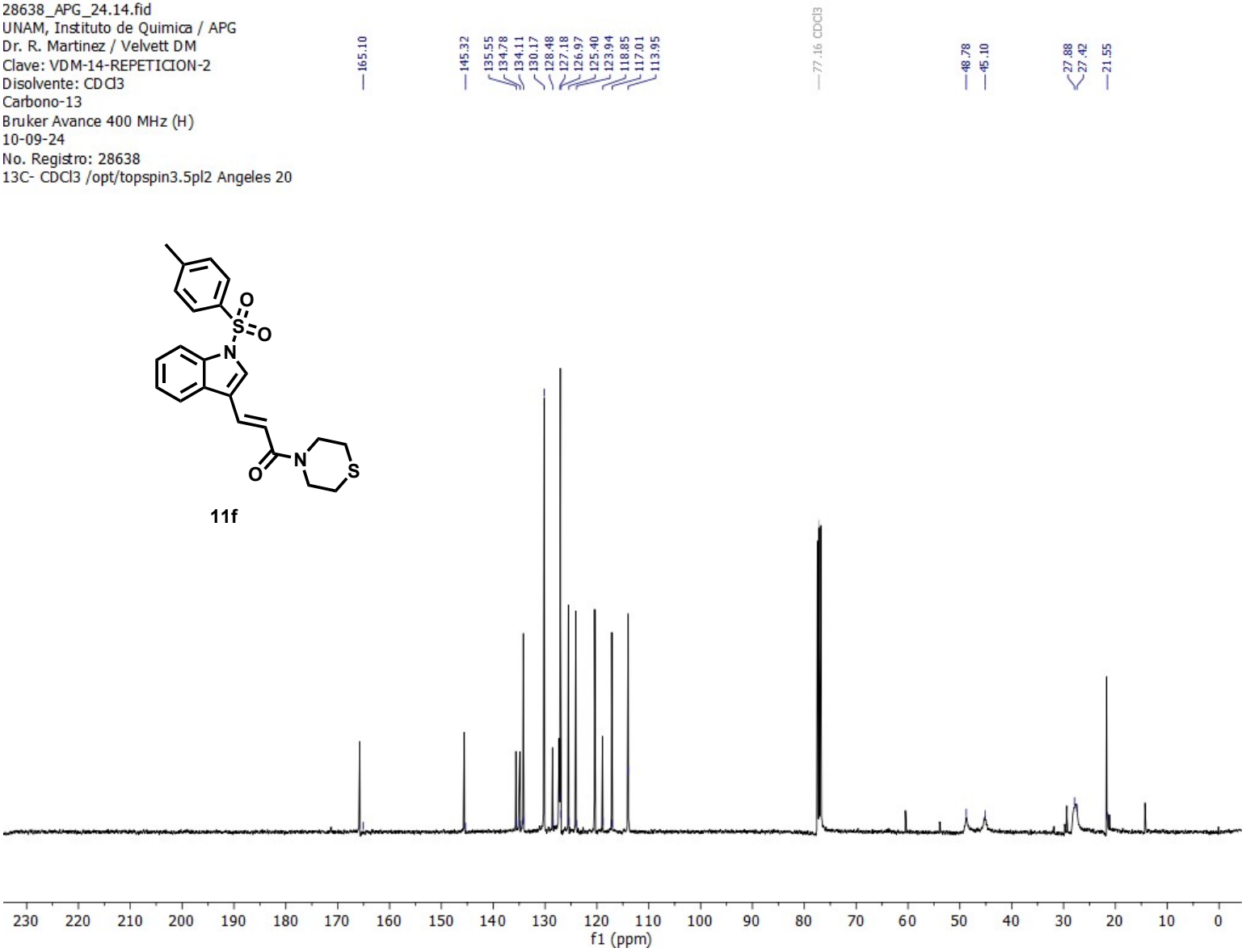
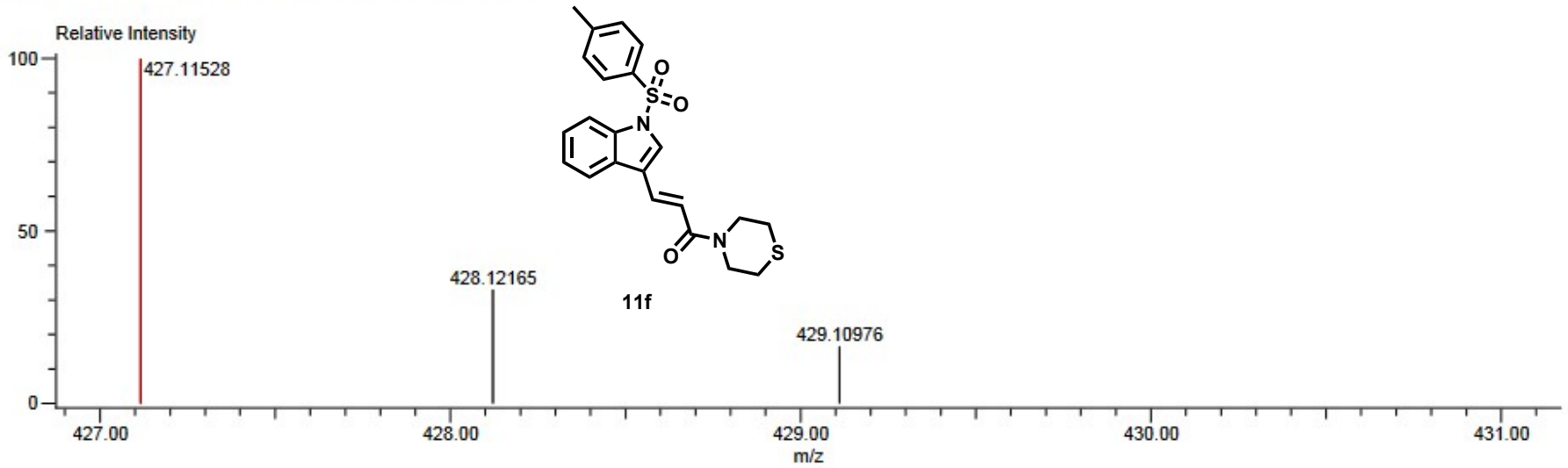


Figure 56. ^{13}C NMR spectrum of **11f** (101 MHz, $CDCl_3$).

Data:926_VDM-14
Sample Name:Dr Martinez Roberto /Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0..0)

Acquired:4/16/2024 9:32:08 AM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_ok
Created:4/29/2024 4:11:46 PM
Created by:AccuTOF

Charge number:1
Tolerance:1.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)
Element:^{12}C:20 .. 22, ^{1}H:0 .. 30, ^{14}N:0 .. 4, ^{16}O:0 .. 4, ^{32}S:1 .. 2



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
427.11528	8664.81	427.11501	0.27	0.64	$^{12}C_{22}{}^{1}H_{23}{}^{14}N_{2}{}^{16}O_{3}{}^{32}S_{2}$	14.5

Figure 57. ESI-HRMS spectrum of **11f**

2.21 Compound 11g

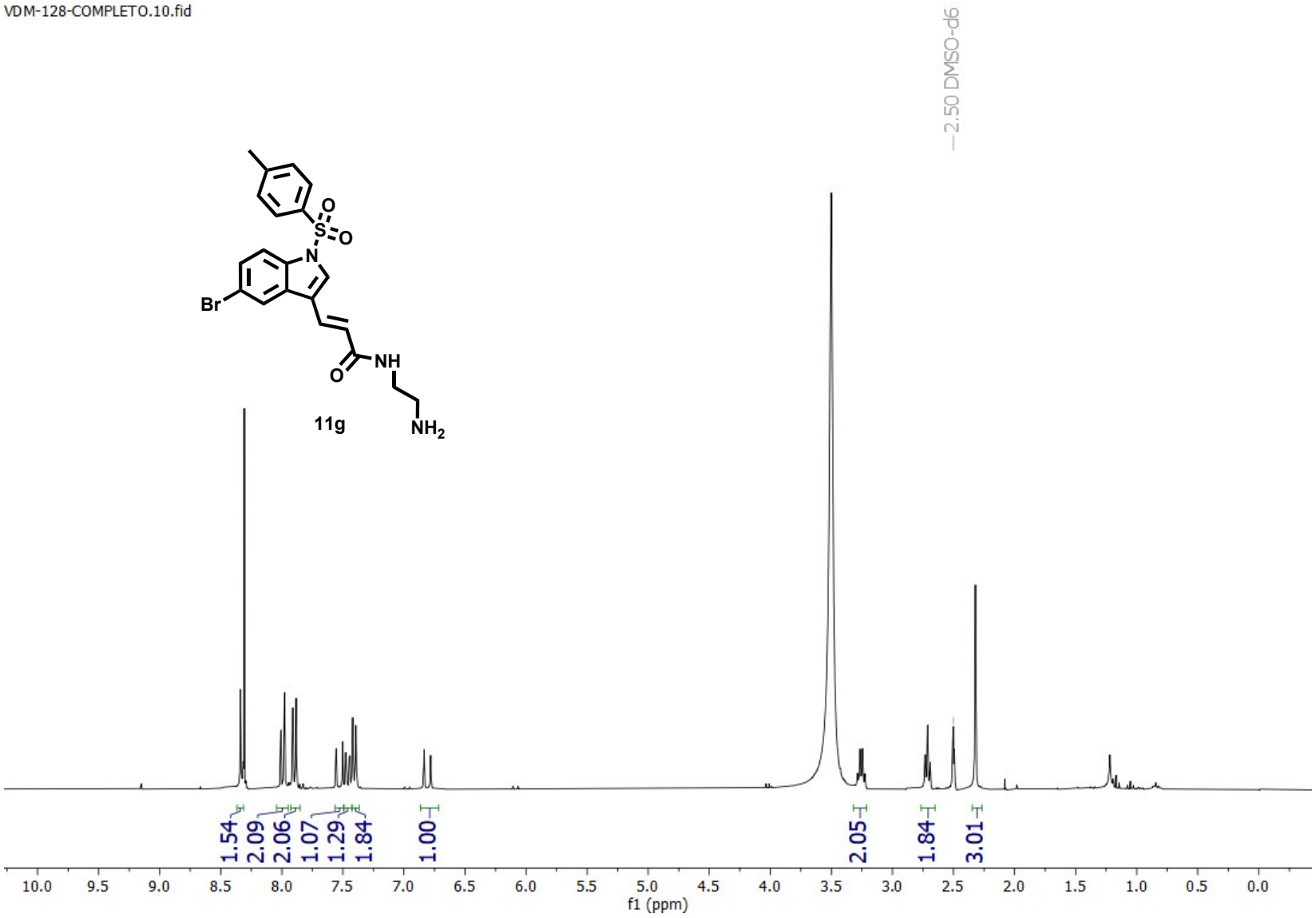


Figure 58. ^{1}H NMR spectrum of **11g** (300 MHz, DMSO-d_6).

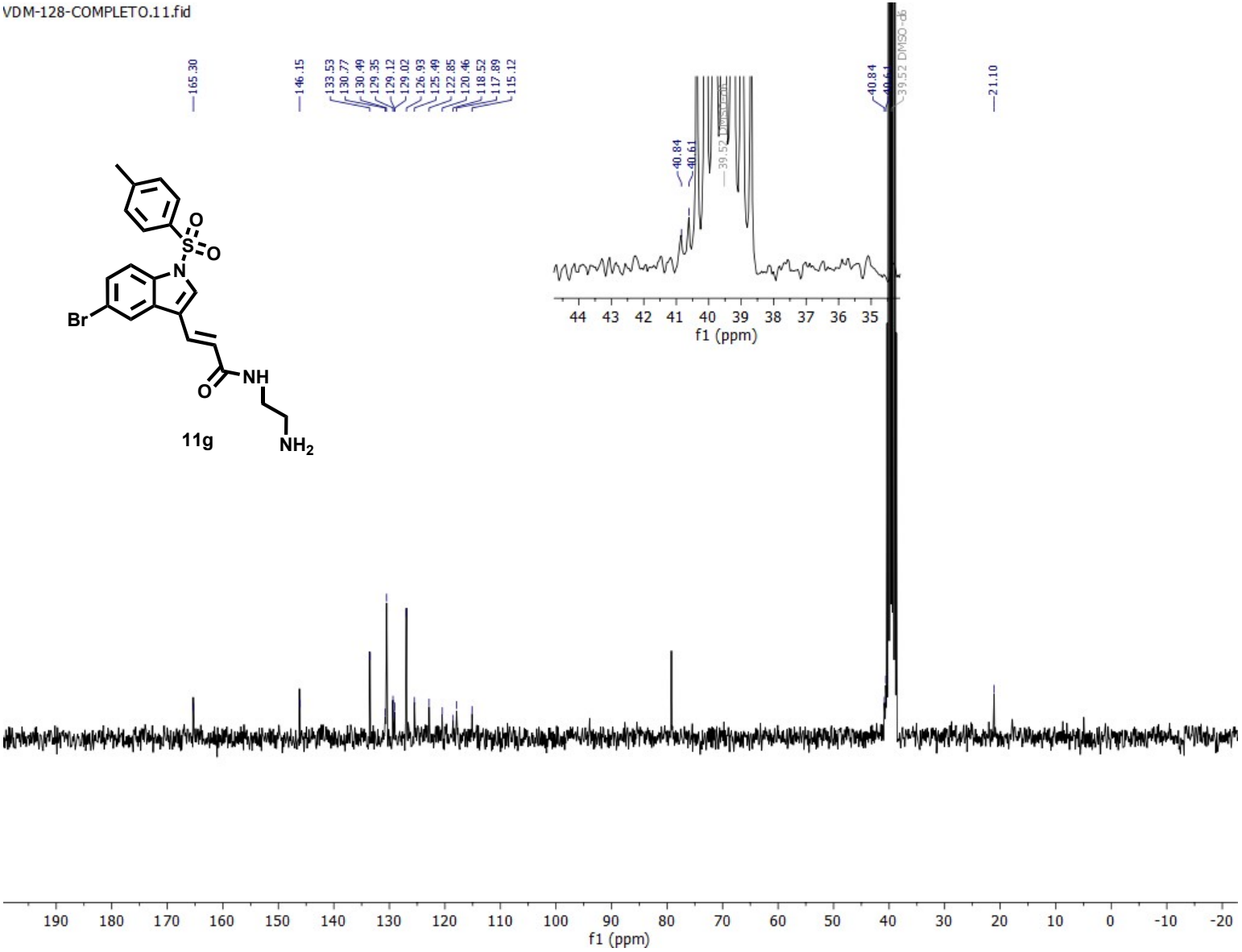


Figure 59. ^{13}C NMR spectrum of **11g** (75 MHz, DMSO-d_6).

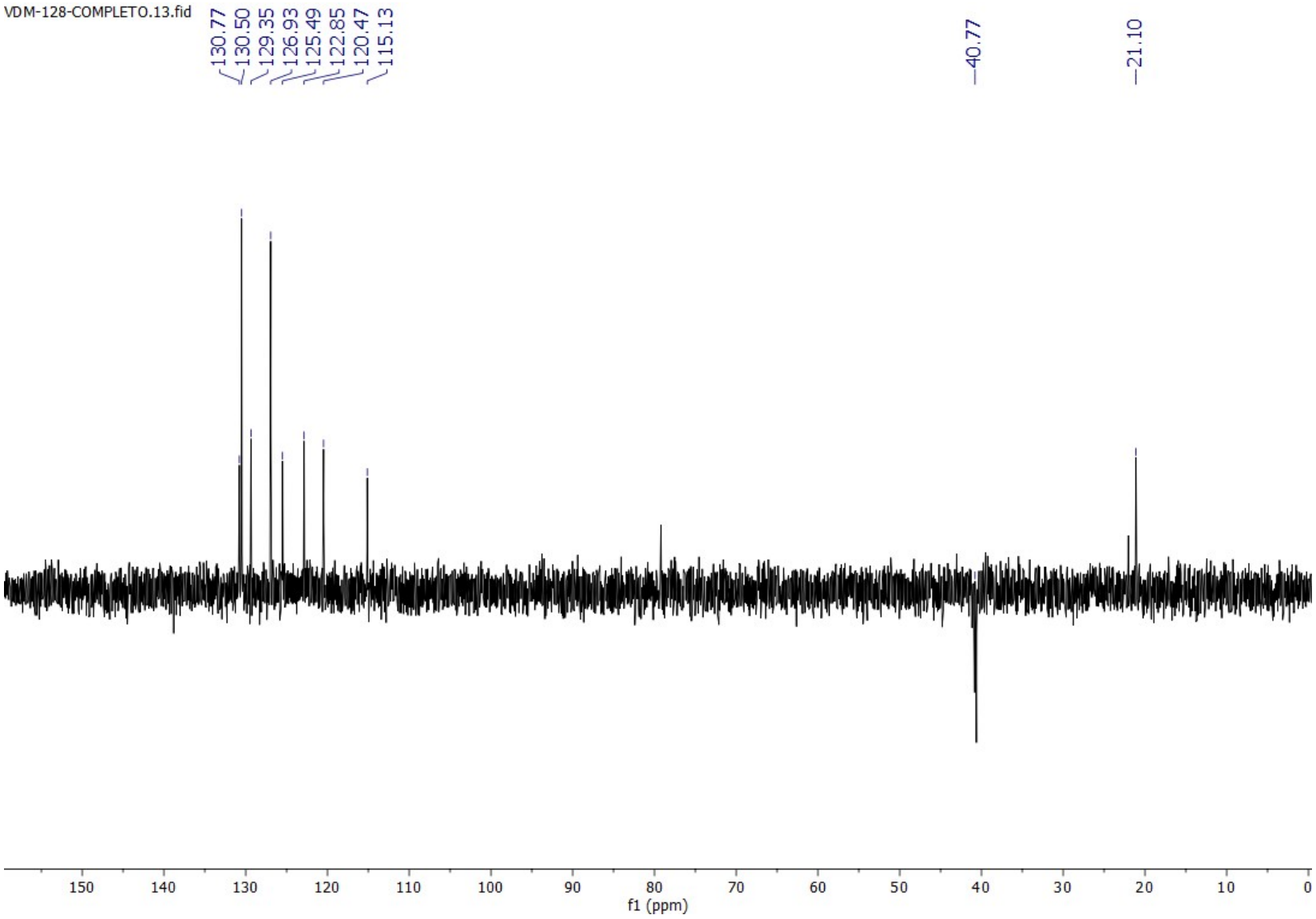
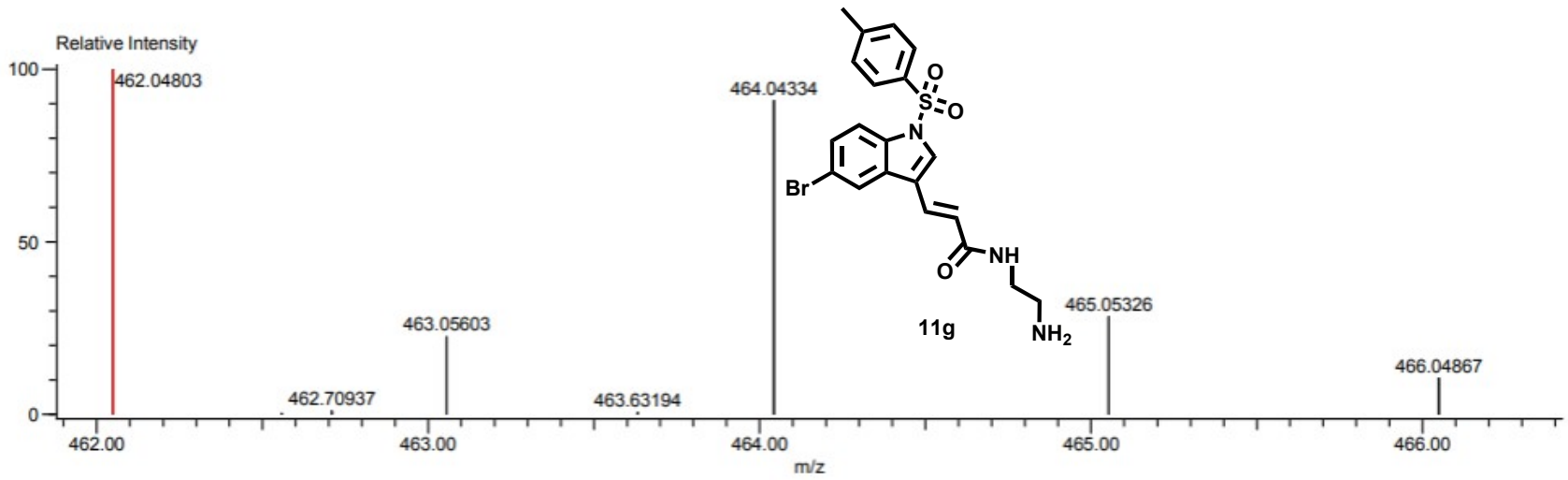


Figure 60. ^{13}C DEPT-135 NMR spectrum of **11g** (75 MHz, DMSO-d_6).

Data:1710_VDM-128
Sample Name:DR. Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:6/20/2023 1:21:51 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:8/2/2023 4:29:54 PM
Created by:AccuTOF

Charge number:1
Tolerance:40.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.0 .. 54.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{79}Br:0 .. 2, ^{14}N:3 .. 3, ^{16}O:3 .. 3, ^{32}S:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
462.04803	3784.37	462.04870	-0.67	-1.45	$^{12}C_{20}{}^{1}H_{21}{}^{79}Br_{1}{}^{14}N_{3}{}^{16}O_{3}{}^{32}S_{1}$	12.5

Figure 61. ESI-HRMS spectrum of **11g.**

2.22 Compound 11h

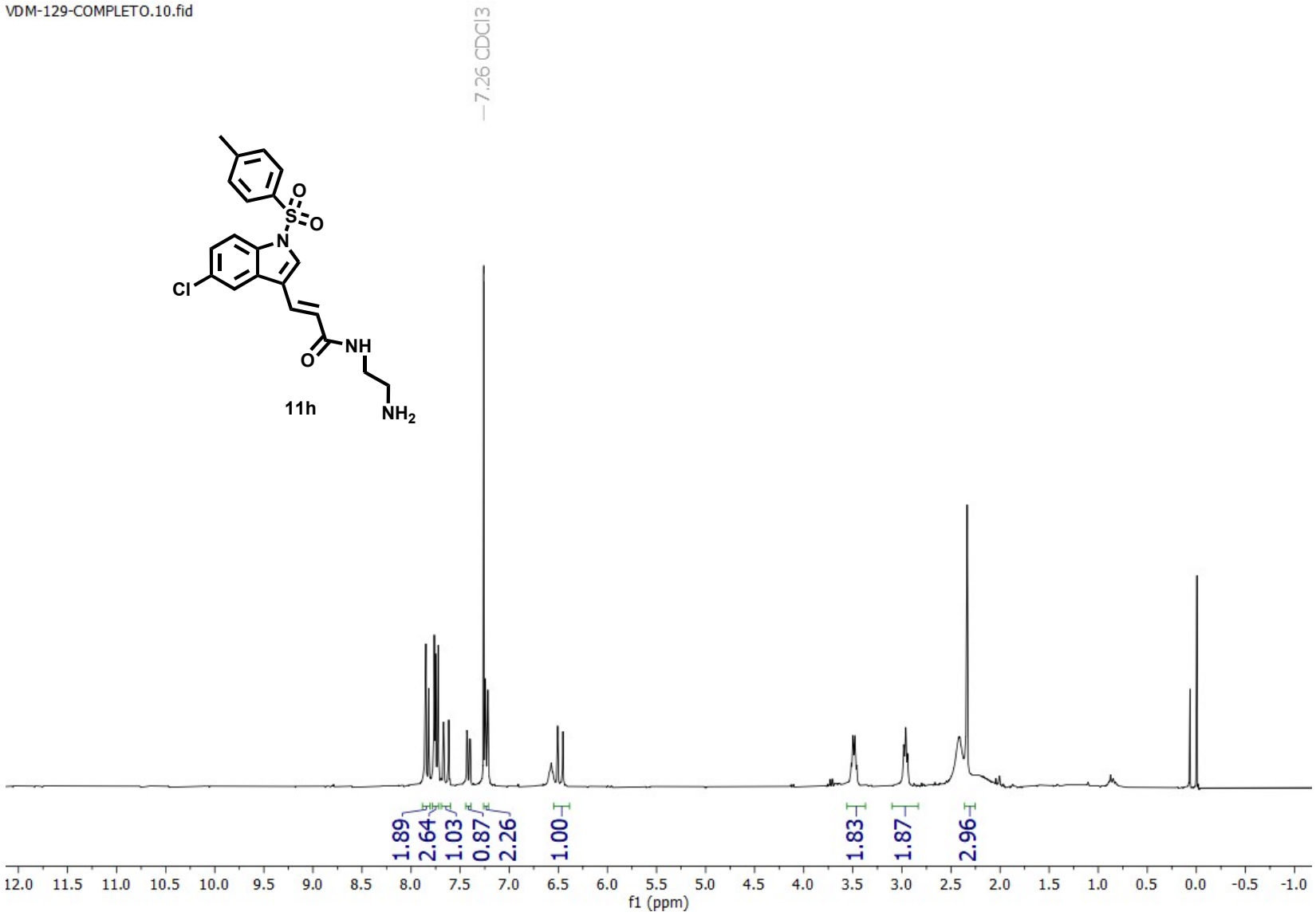


Figure 62. ^{1}H NMR spectrum of **11h** (300 MHz, $CDCl_3$).

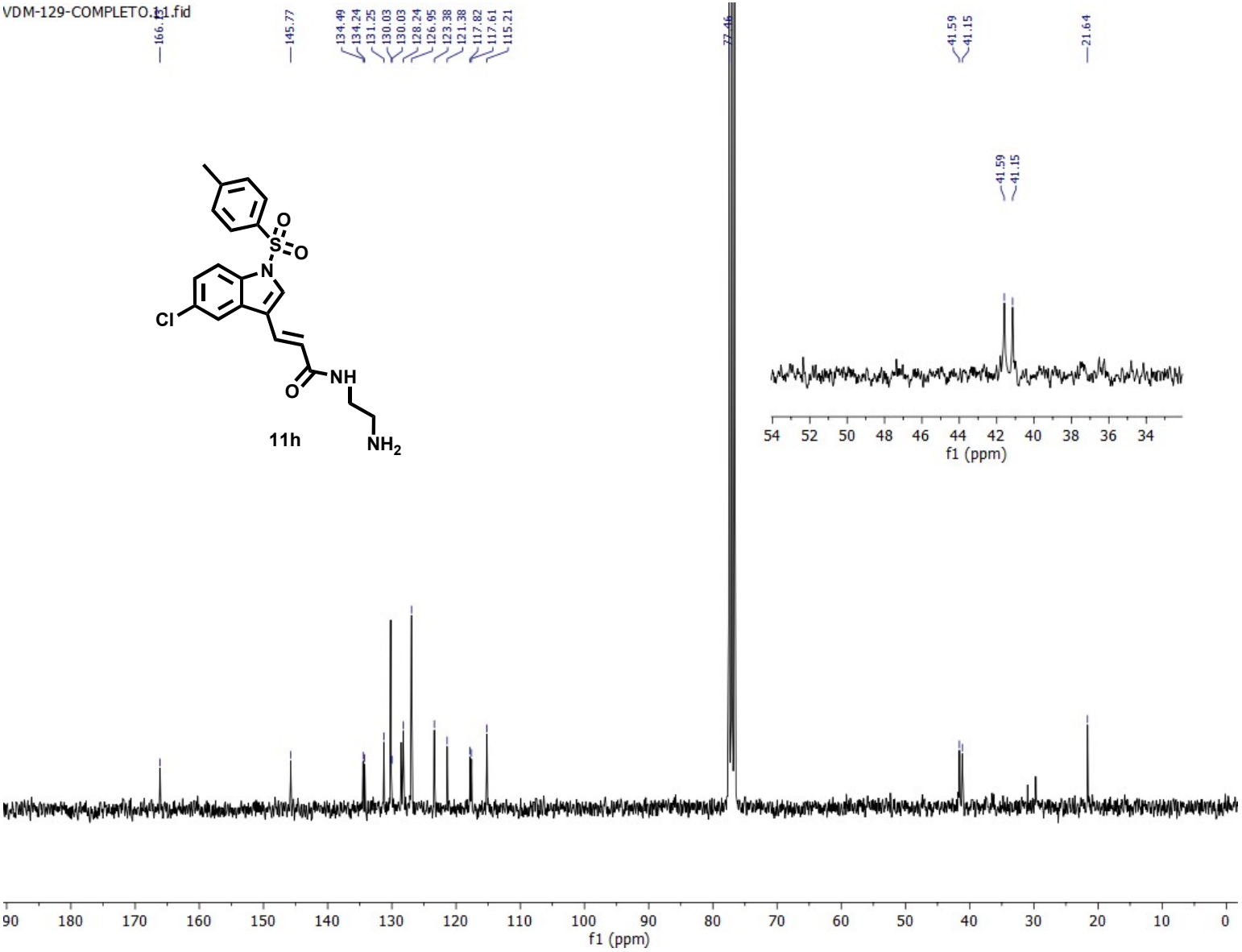
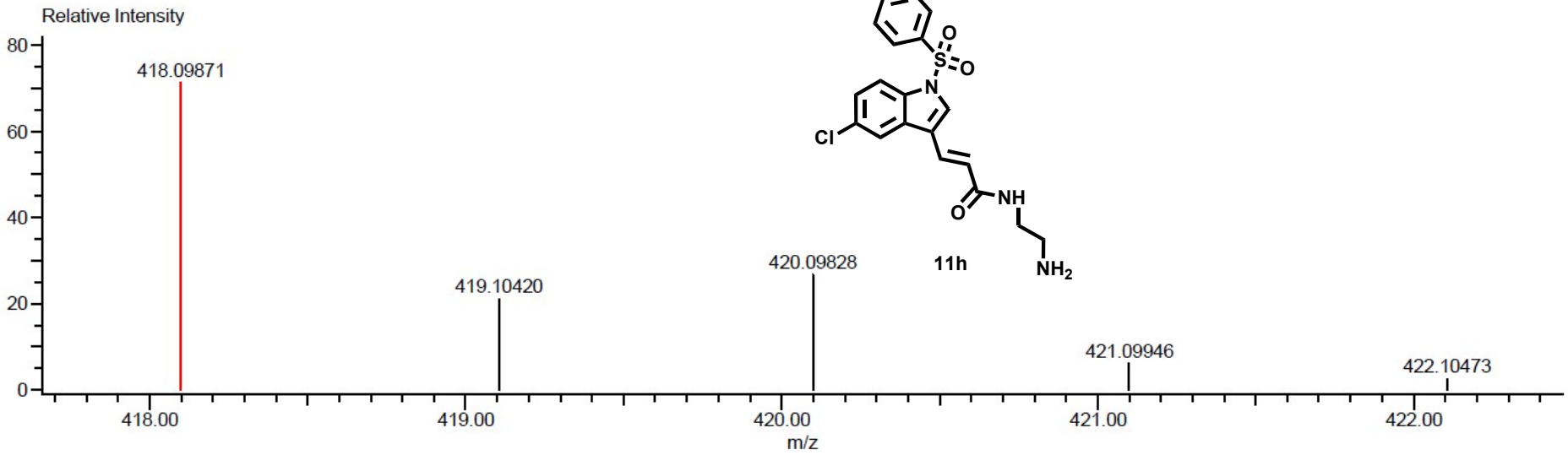


Figure 63. ^{13}C NMR spectrum of **11h** (75 MHz, $CDCl_3$).

Data:1711_VDM-129
Sample Name:DR. Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:6/20/2023 1:24:02 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:8/2/2023 1:44:36 PM
Created by:AccuTOF

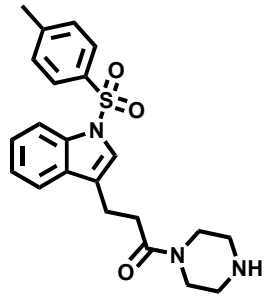
Charge number:1
Tolerance:2.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.0 .. 54.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{35}Cl:1 .. 1, ^{14}N:0 .. 3, ^{16}O:0 .. 3, ^{32}S:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
418.09871	30327.51	418.09921	-0.51	-1.21	$^{12}C_{20}{}^{1}H_{21}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{3}{}^{32}S_{1}$	12.5

Figure 64. ESI-HRMS spectrum of **11h.**

2.23 Compound 11a’



11a'

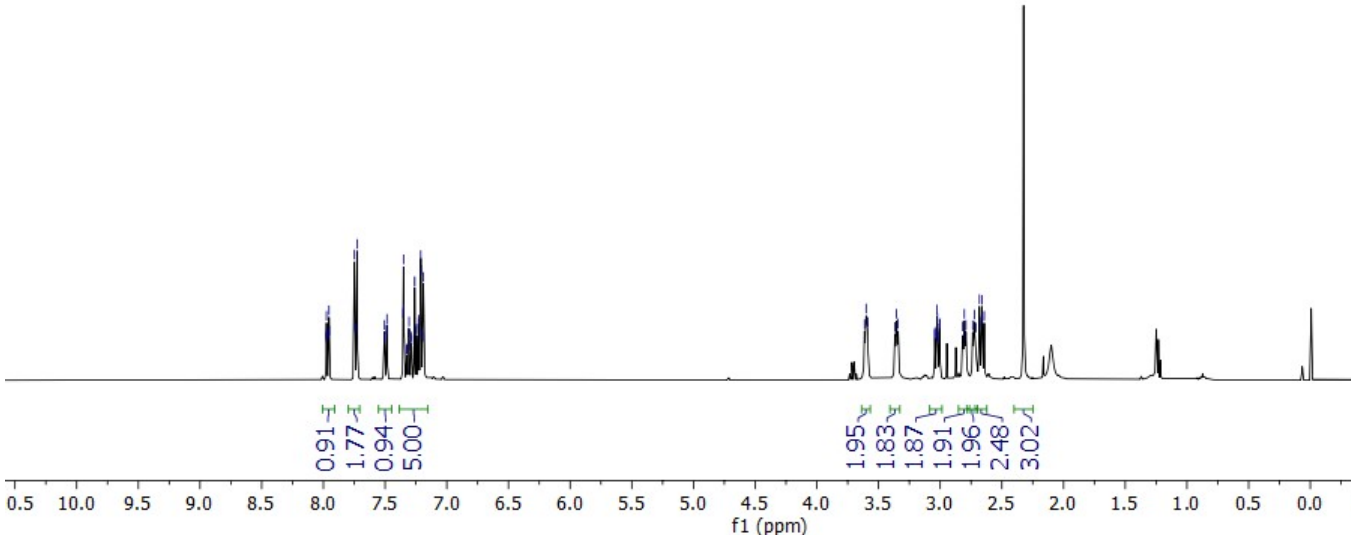


Figure 65. ^{1}H NMR spectrum of **11a'** (400 MHz, $CDCl_3$).

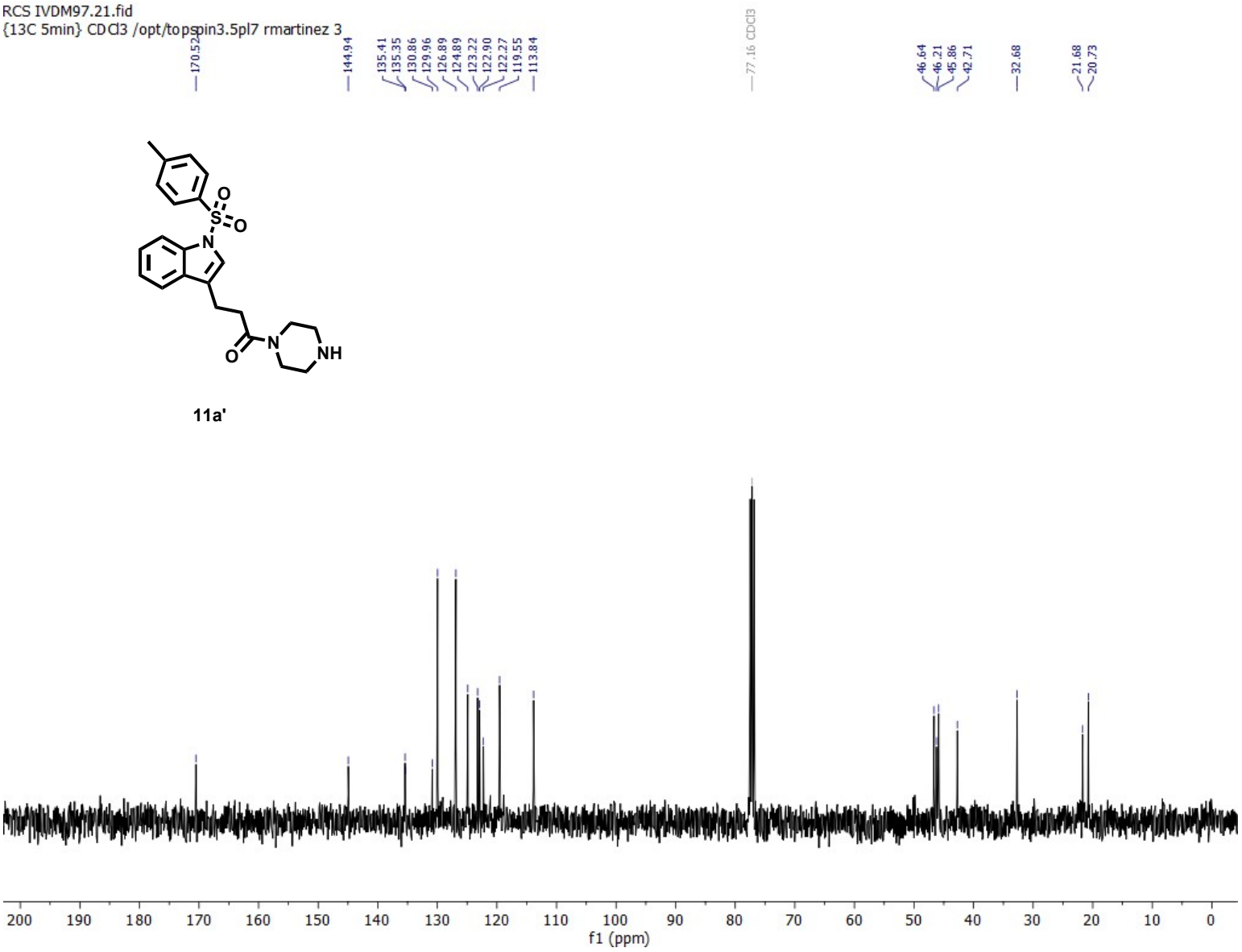
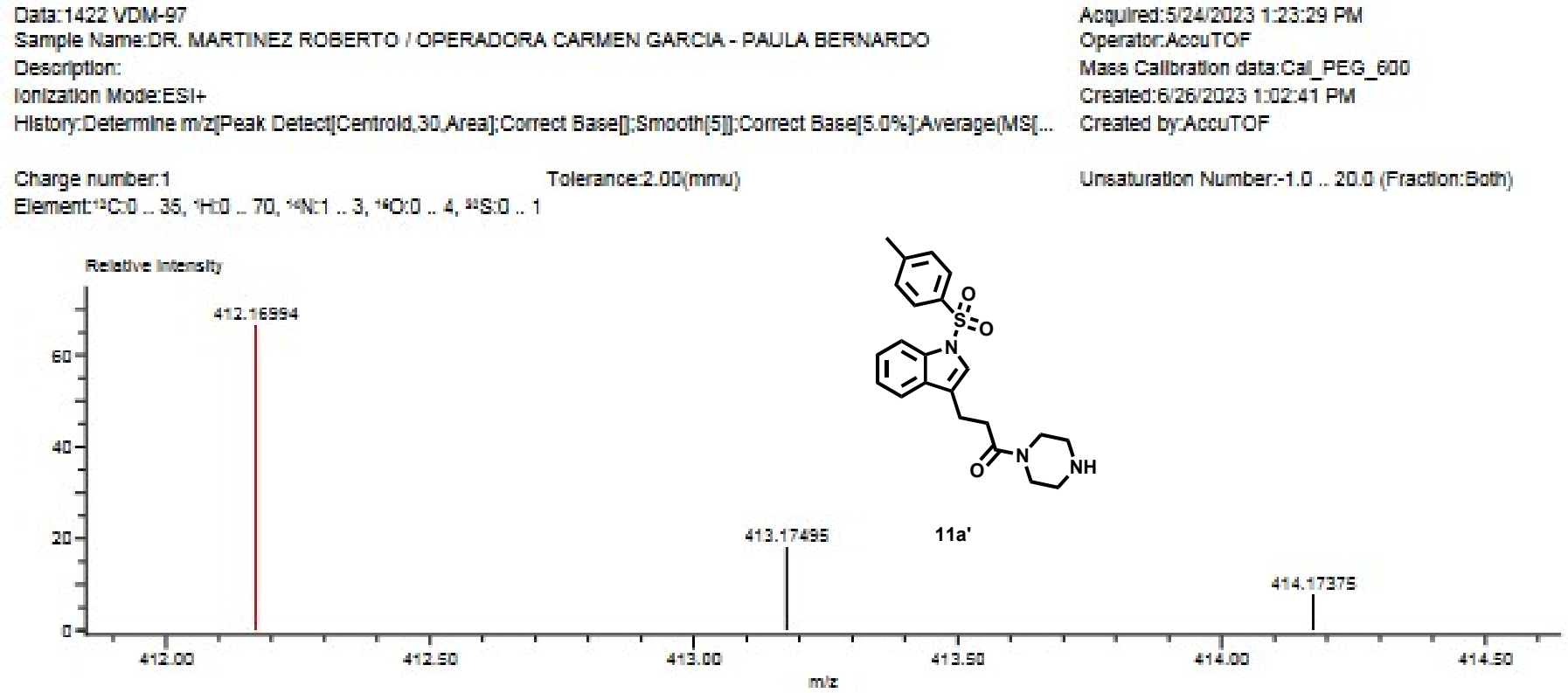


Figure 66. ^{13}C NMR spectrum of **11a'** (101 MHz, $CDCl_3$).



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
412.16994	259170.28	412.16949	0.45	1.09	$^{12}C_{22}{}^{1}H_{26}{}^{14}N_{2}{}^{16}O_{2}{}^{32}S_{1}$	12.5

Figure 67. ESI-HRMS spectrum of **11a'.**

2.24 Compound 12a

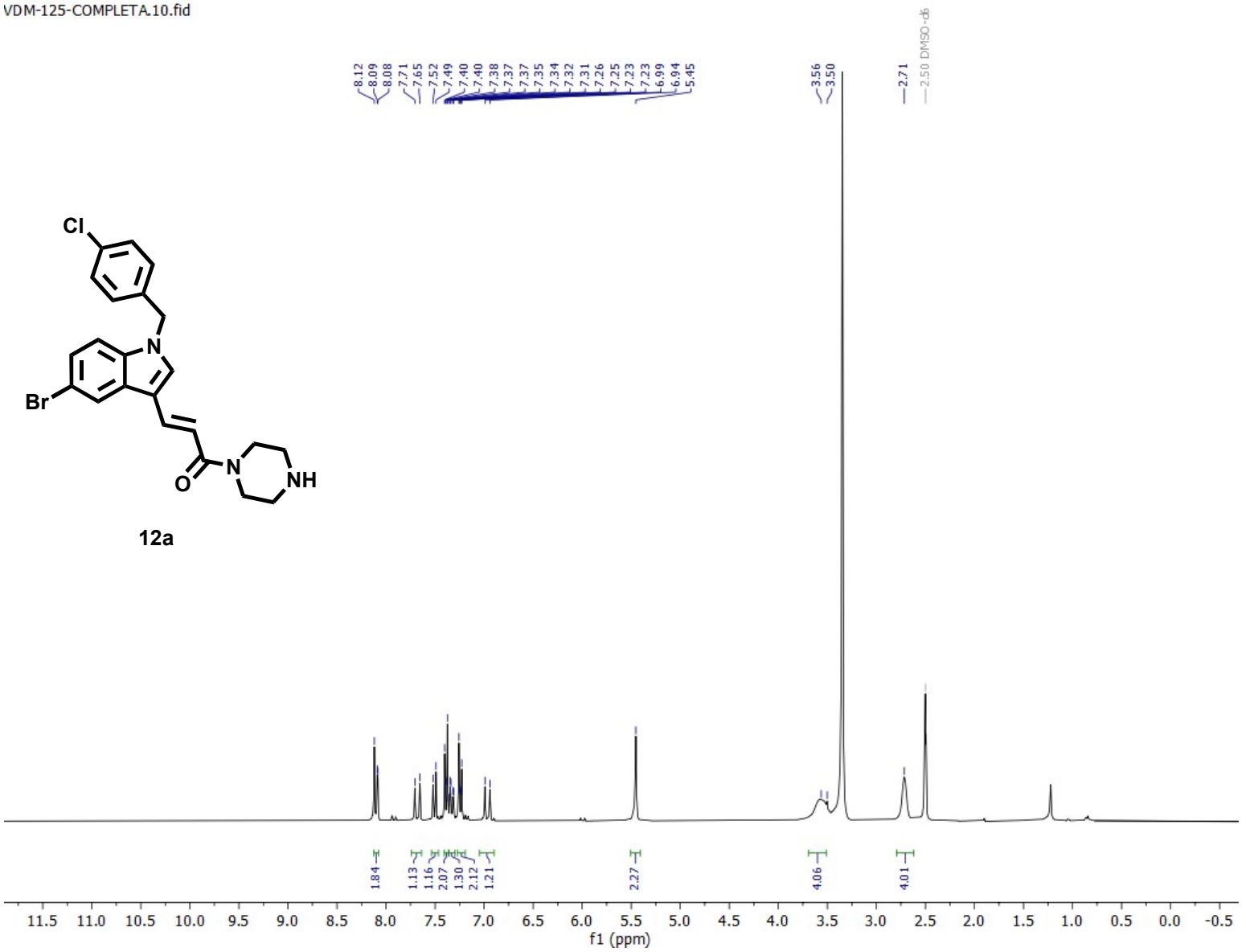


Figure 68. ^{1}H NMR spectrum of **12a** (300 MHz, DMSO-d_6).

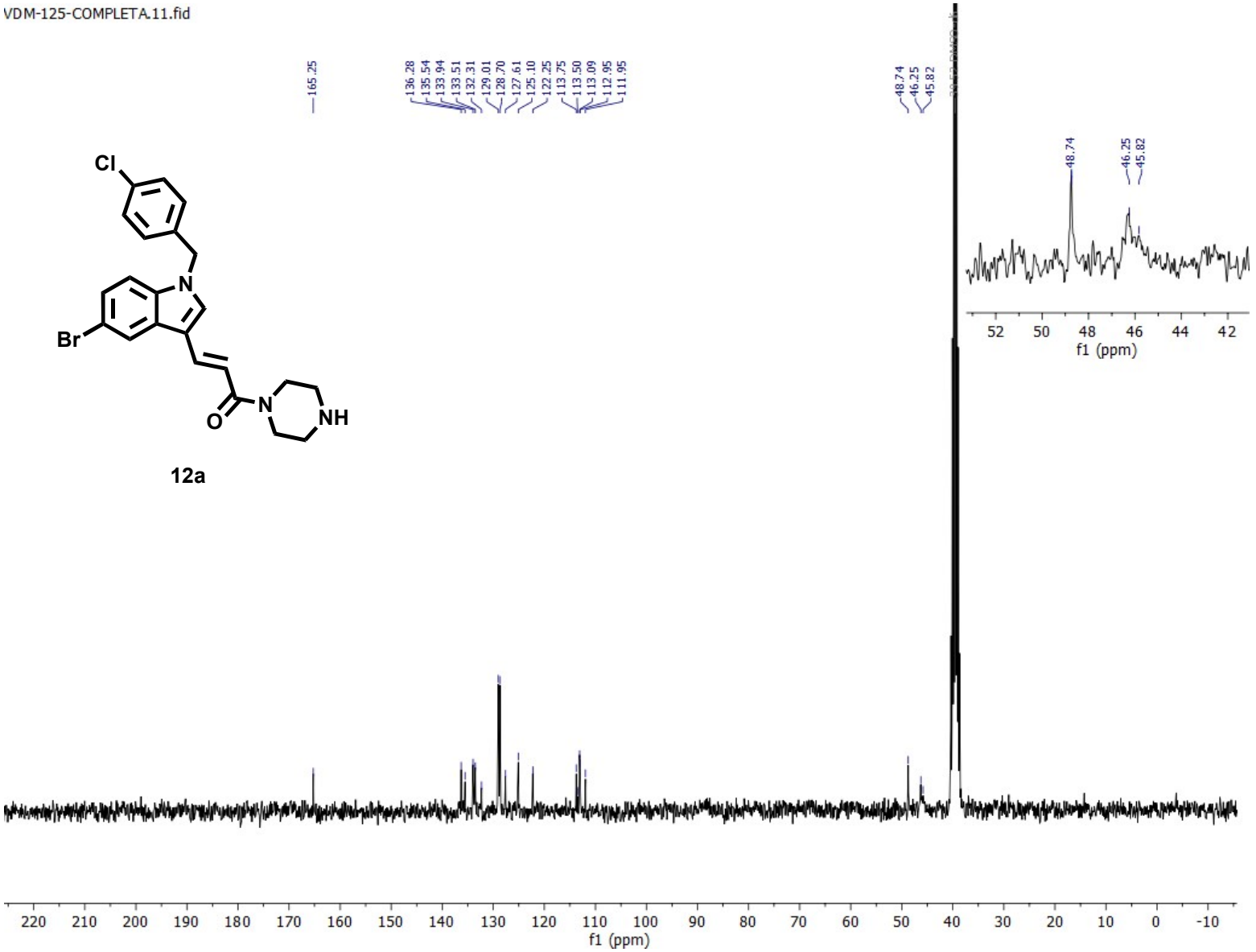


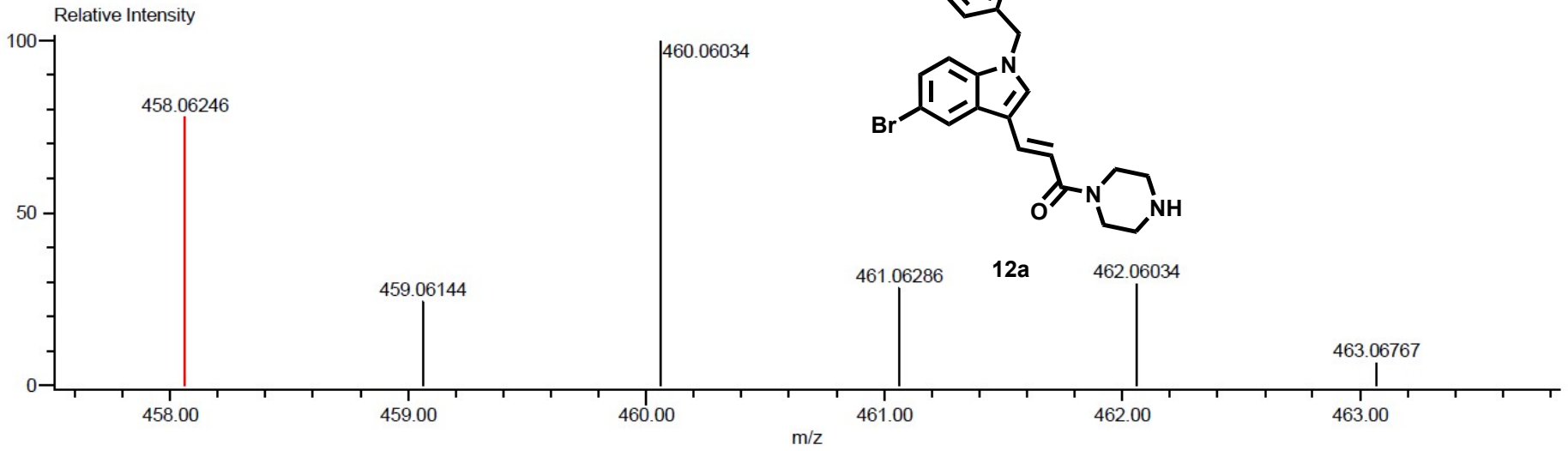
Figure 69. ^{13}C NMR spectrum of **12a** (75 MHz, DMSO-d_6).

Data:1420 VDM-125
Sample Name:DR. MARTINEZ ROBERTO / OPERADORA CARMEN GARCIA - PAULA BERNARDO
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:5/24/2023 1:14:55 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:6/26/2023 1:21:08 PM
Created by:AccuTOF

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 35, ^{1}H:0 .. 70, ^{79}Br:1 .. 1, ^{35}Cl:1 .. 1, ^{14}N:1 .. 3, ^{16}O:0 .. 3

Unsaturation Number:-1.0 .. 50.0 (Fraction:Both)



12a

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
458.06246	26215.80	458.06348	-1.02	-2.22	$^{12}C_{22}{}^{1}H_{22}{}^{79}Br_{1}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{1}$	12.5

Figure 70. ESI-HRMS spectrum of **12a.**

2.25 Compound 12b

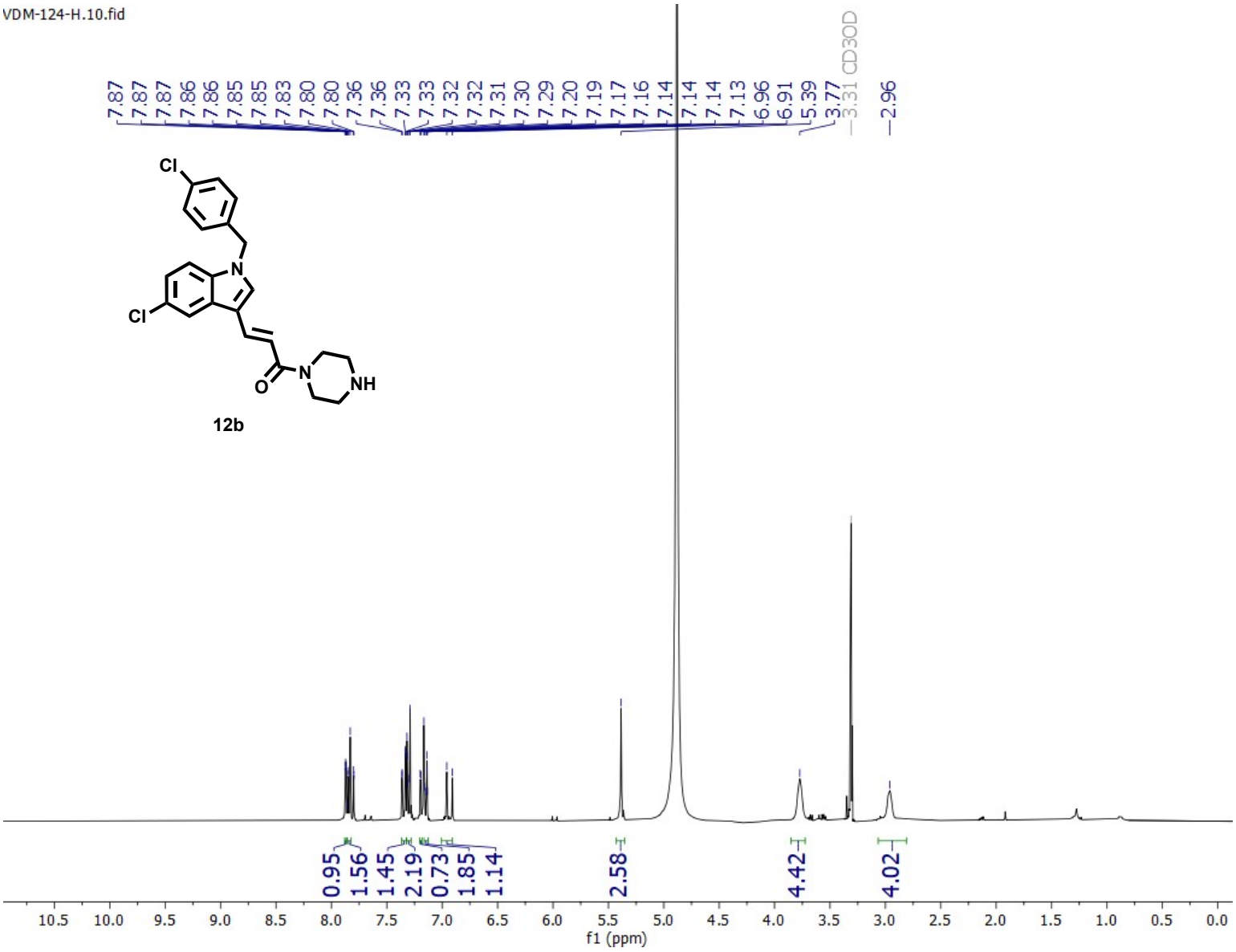


Figure 71. ^{1}H NMR spectrum of **12b** (300 MHz, CD_3OD-d_4).

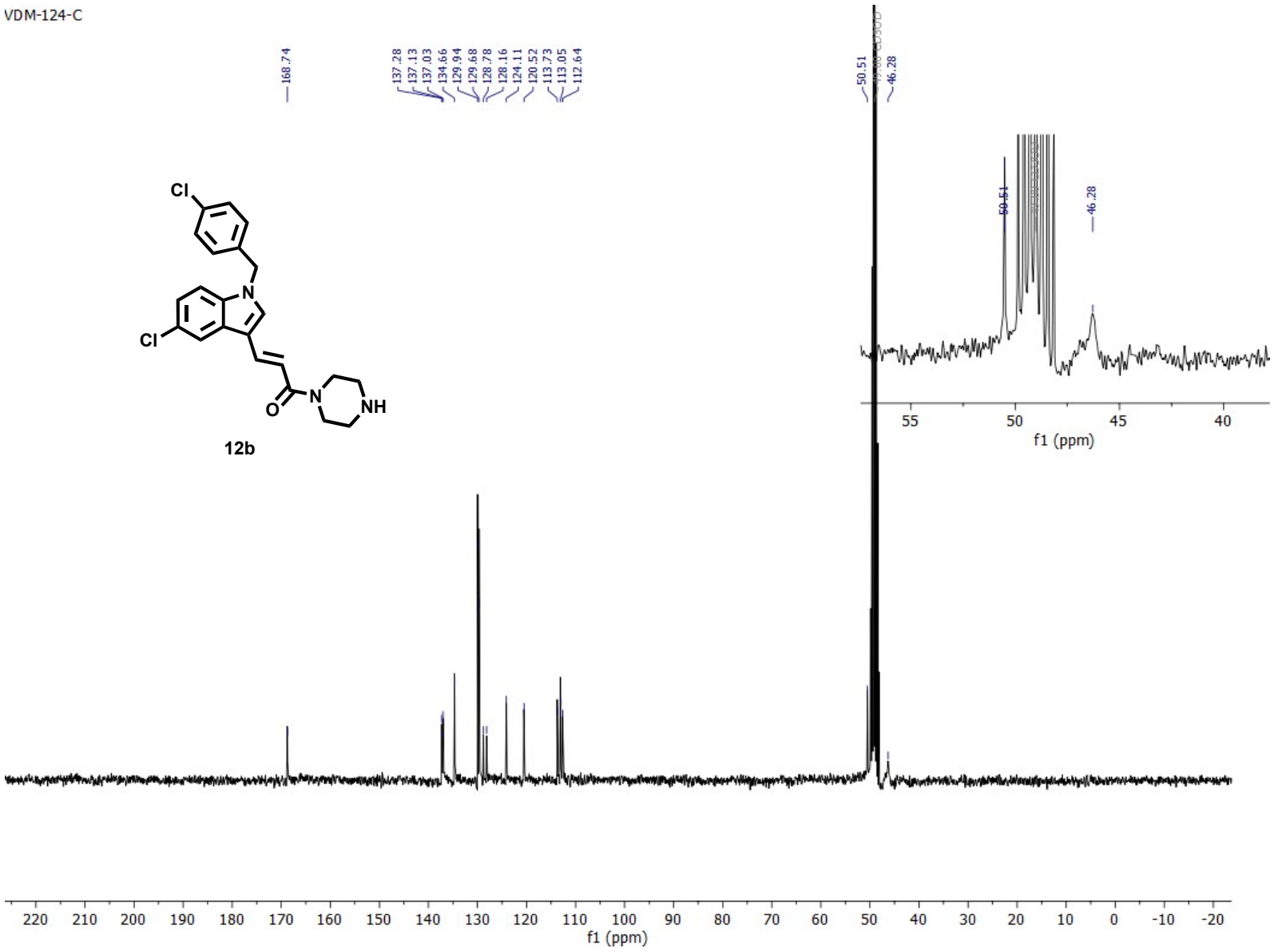
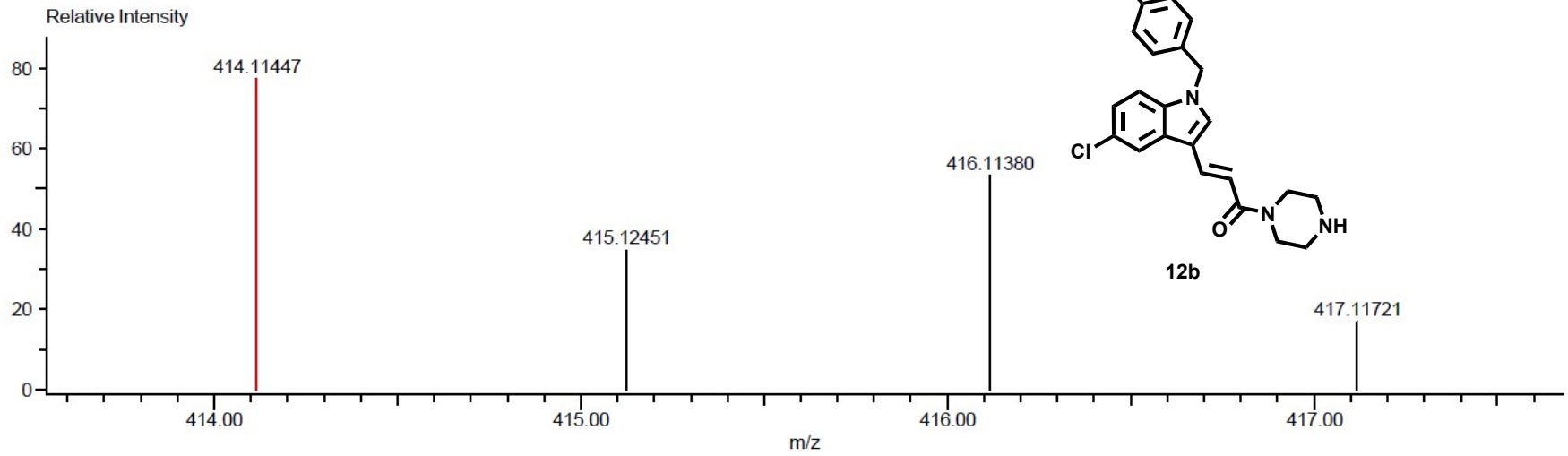


Figure 72 ^{13}C NMR spectrum of **12b** (75 MHz, MeOD-d_4).

Data:1419 VDM-124
Sample Name:DR. MARTINEZ ROBERTO / OPERADORA CARMEN GARCIA - PAULA BERNARDO
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:5/24/2023 1:09:51 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:6/26/2023 12:55:53 PM
Created by:AccuTOF

Charge number:1
Tolerance:2.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.0 .. 60.0 (Fraction:Both)
Element:^{12}C:0 .. 35, ^{1}H:0 .. 70, ^{35}Cl:2 .. 2, ^{14}N:1 .. 4, ^{16}O:0 .. 3



12b

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
414.11447	21806.25	414.11399	0.48	1.17	$^{12}C_{22}{}^{1}H_{22}{}^{35}Cl_2{}^{14}N_3{}^{16}O_1$	12.5

Figure 73. ESI-HRMS spectrum of **12b.**

2.26 Compound 12c

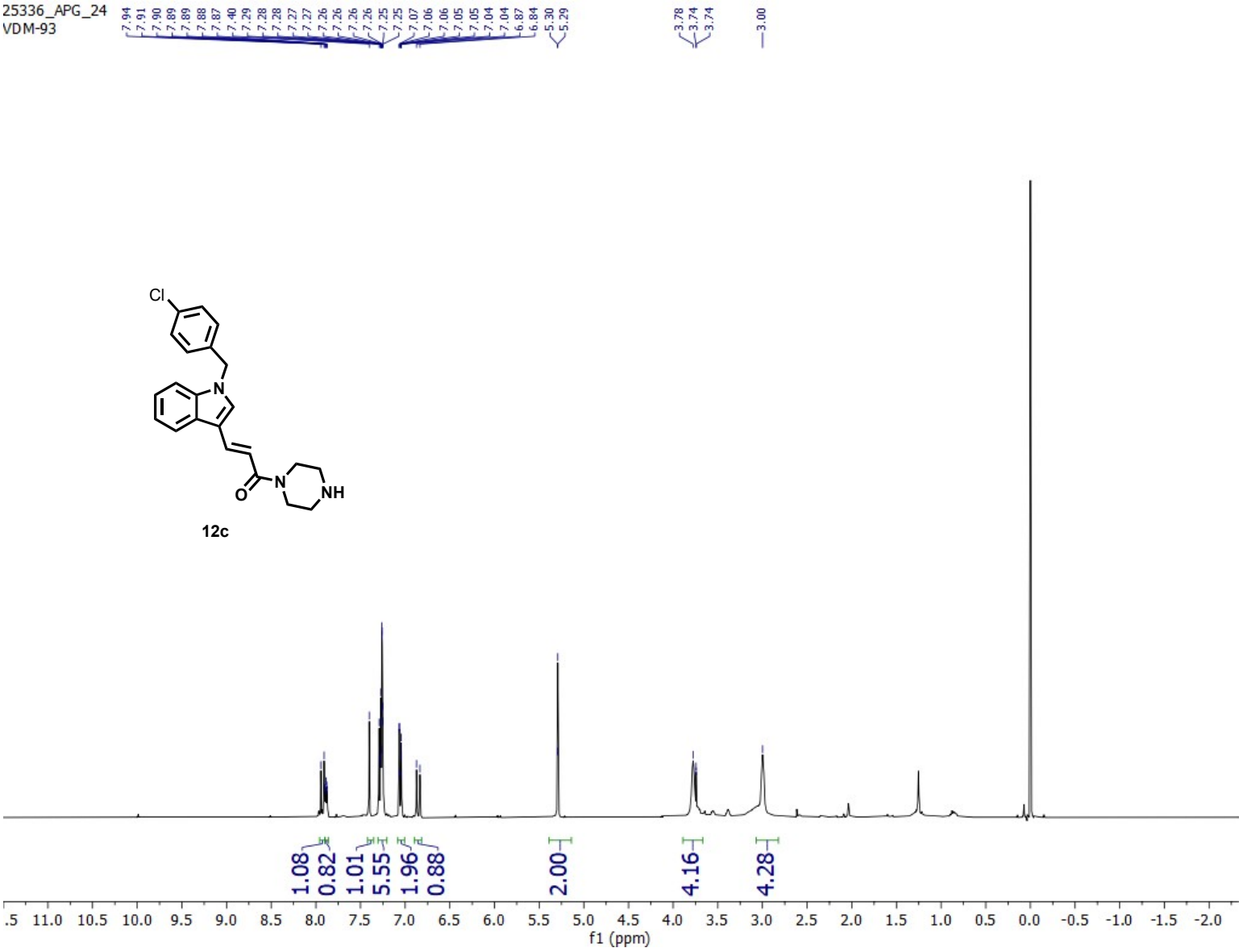


Figure 74. ^{1}H NMR spectrum of **12c** (400 MHz, $CDCl_3$)

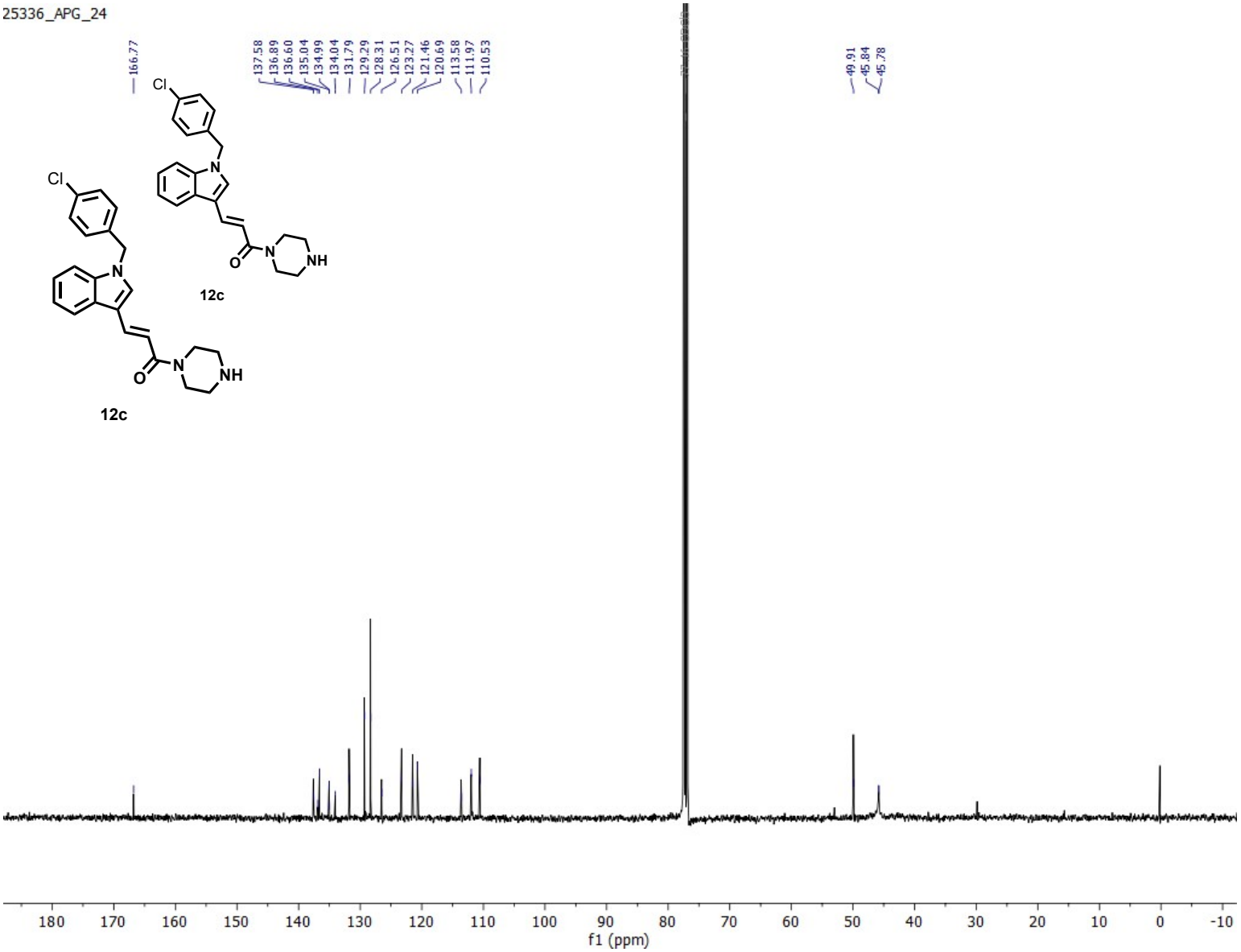
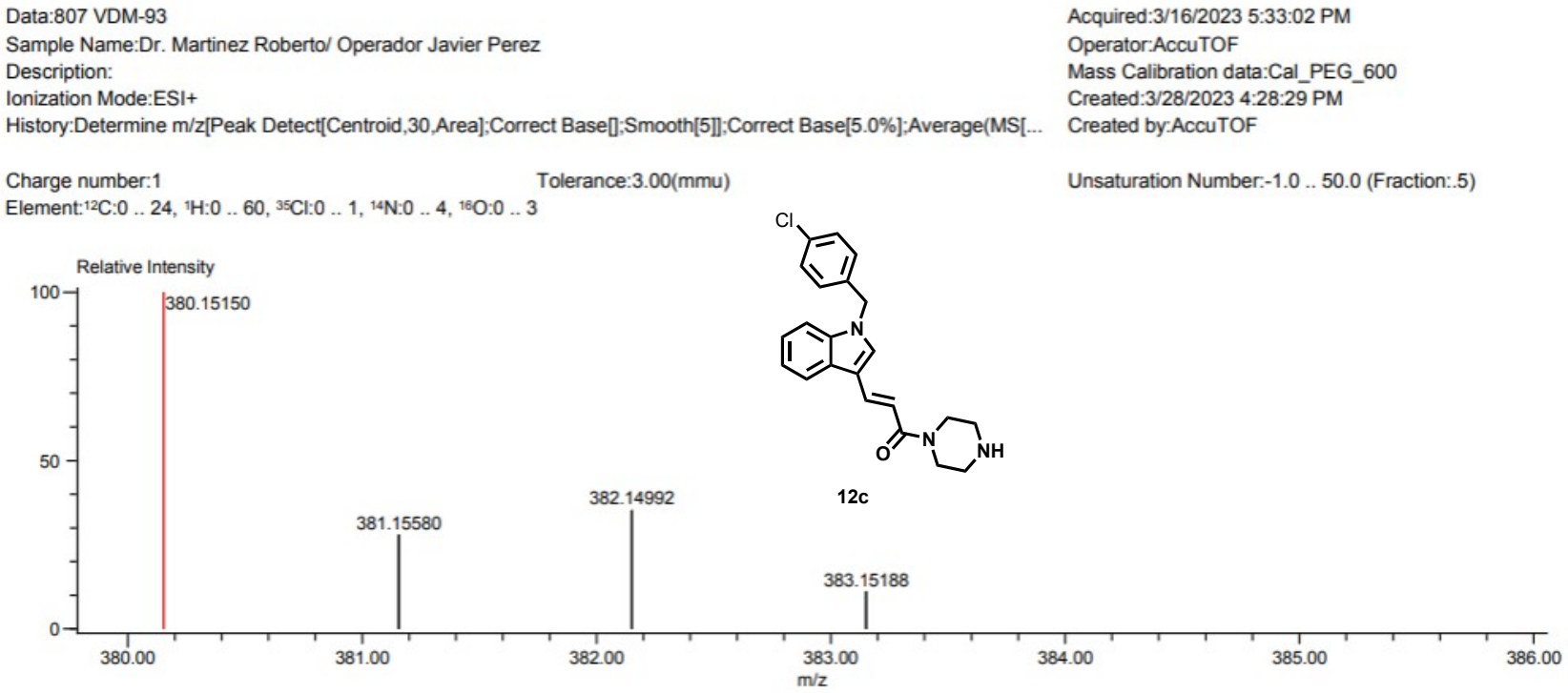


Figure 75. ^{13}C NMR spectrum of **12c** (101 MHz, $CDCl_3$).



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
380.15150	246657.64	380.15296	-1.47	-3.86	$^{12}C_{22}{}^{1}H_{23}{}^{35}Cl_1{}^{14}N_3{}^{16}O_1$	12.5

Figure 76. ESI-HRMS spectrum of **12c.**

2.27Compound 12d

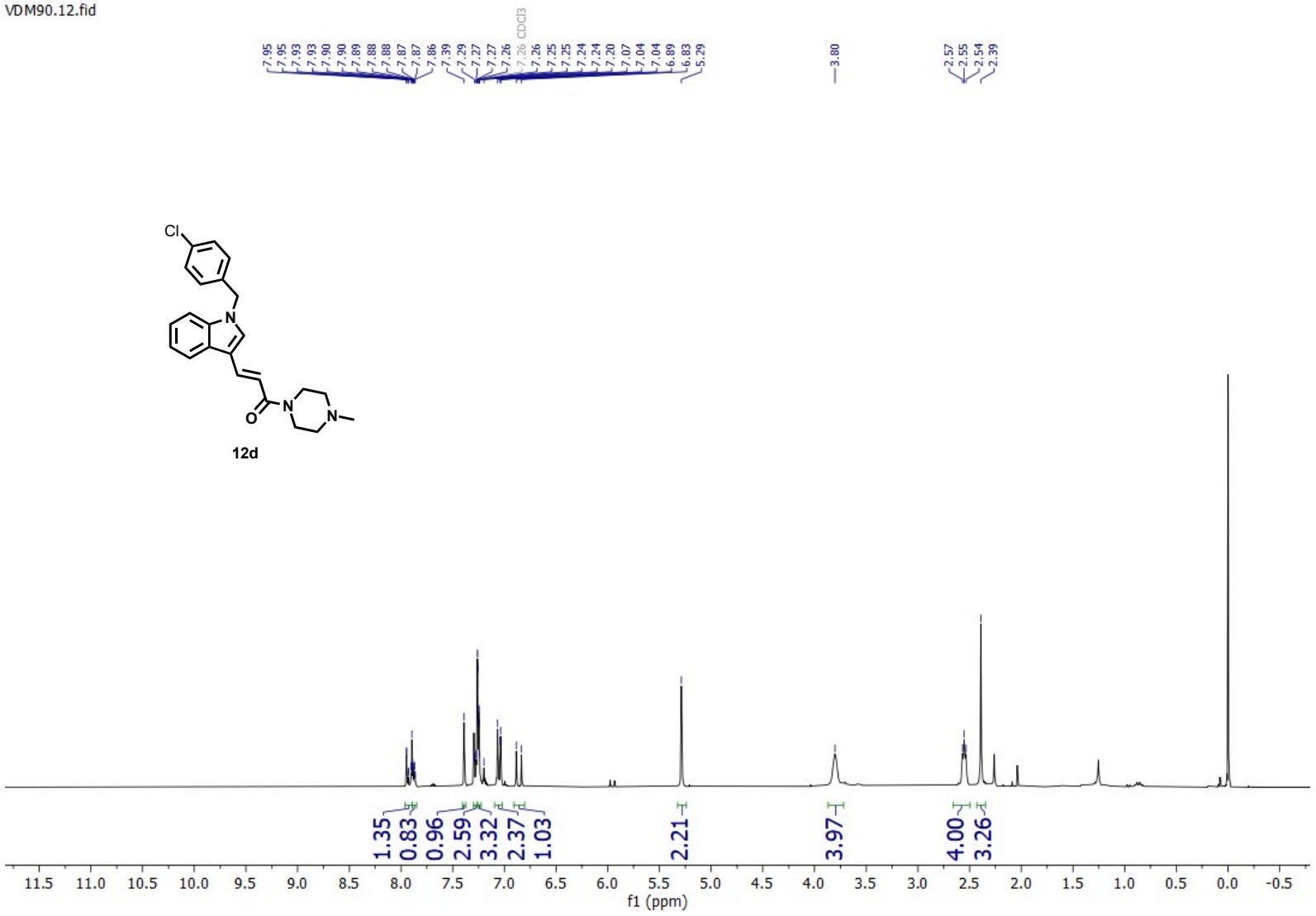


Figure 77. ^{1}H NMR spectrum of **12d** (300 MHz, $CDCl_3$)

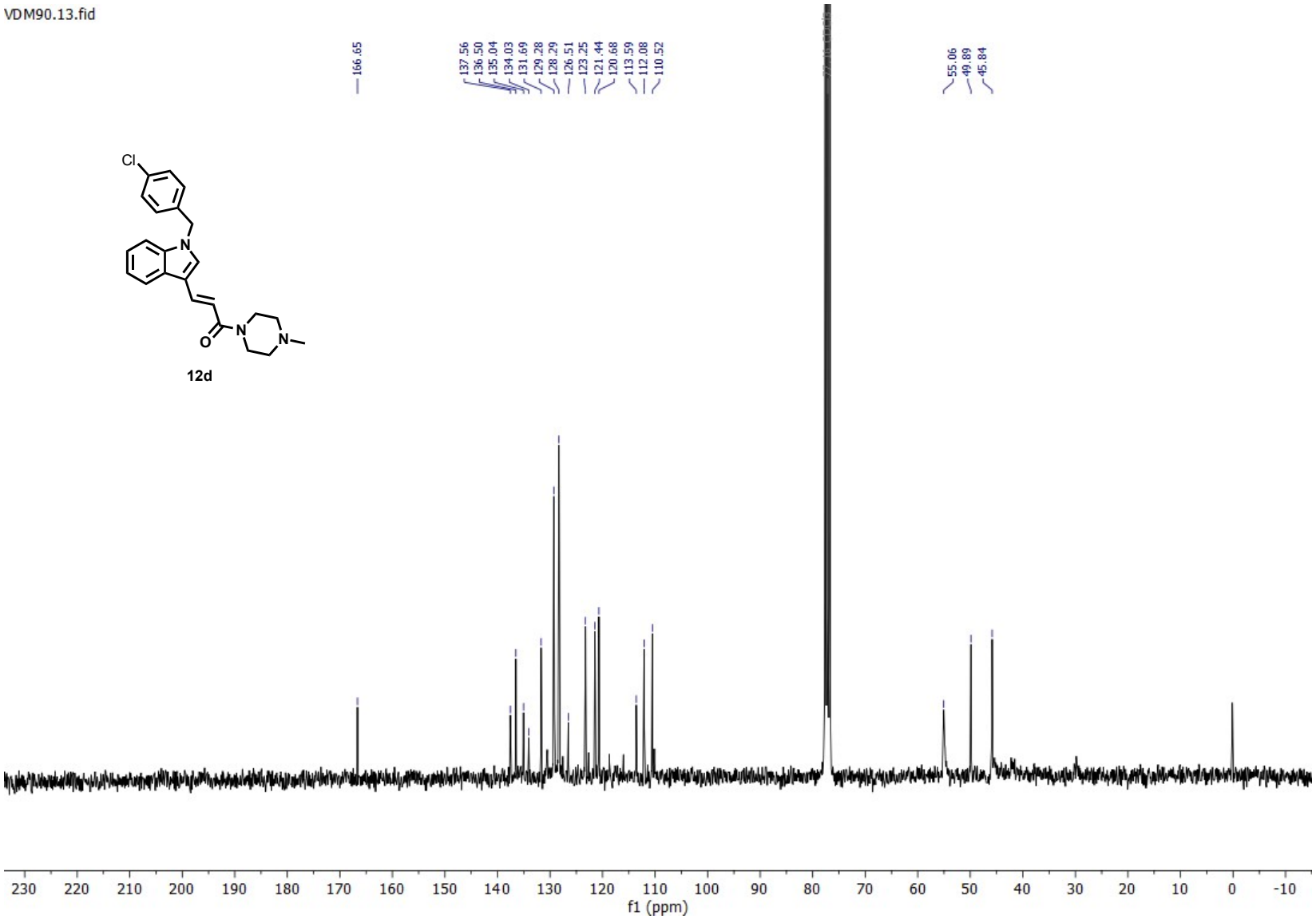


Figure 78. ^{13}C NMR spectrum of **12d** (75 MHz, $CDCl_3$)

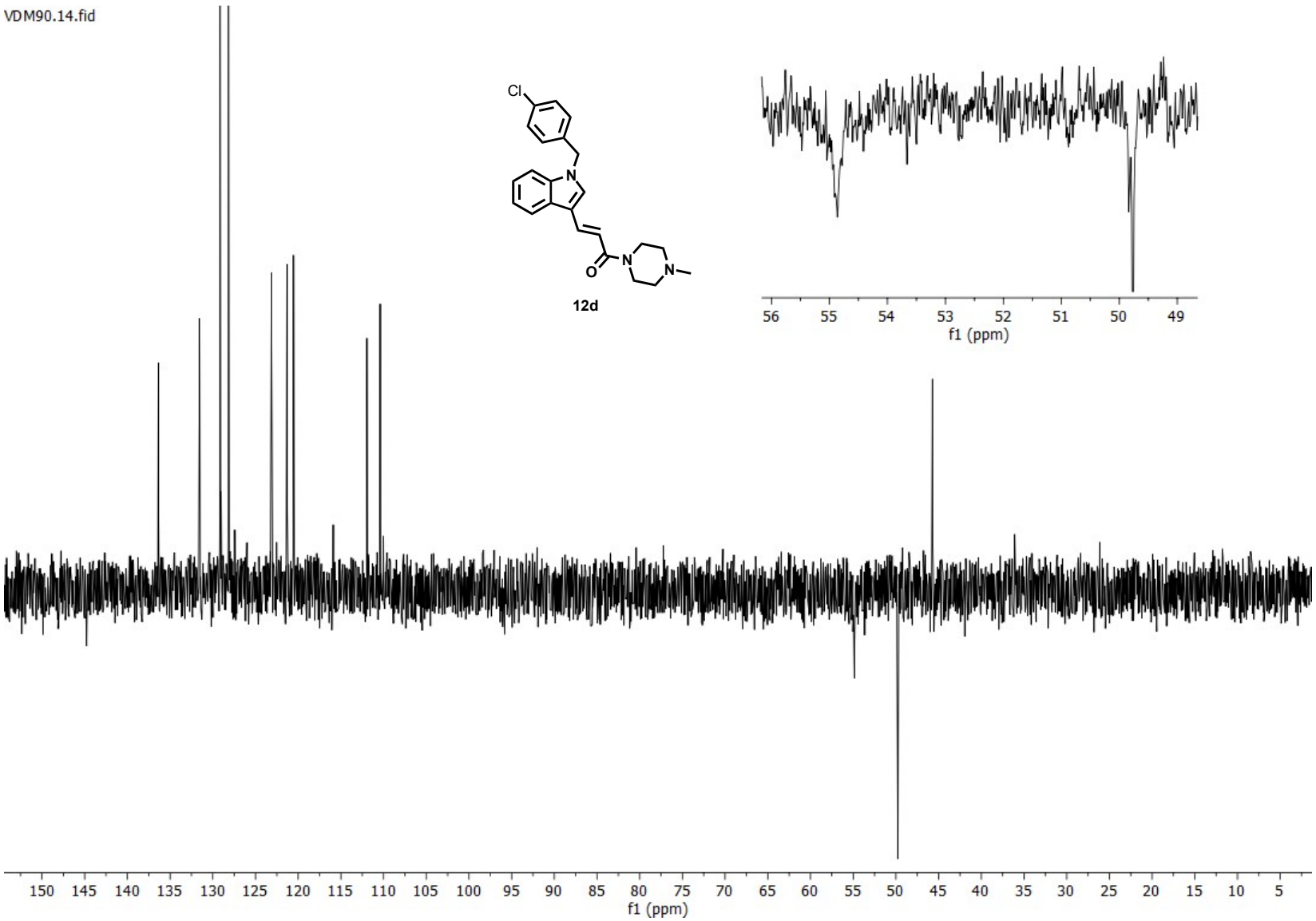
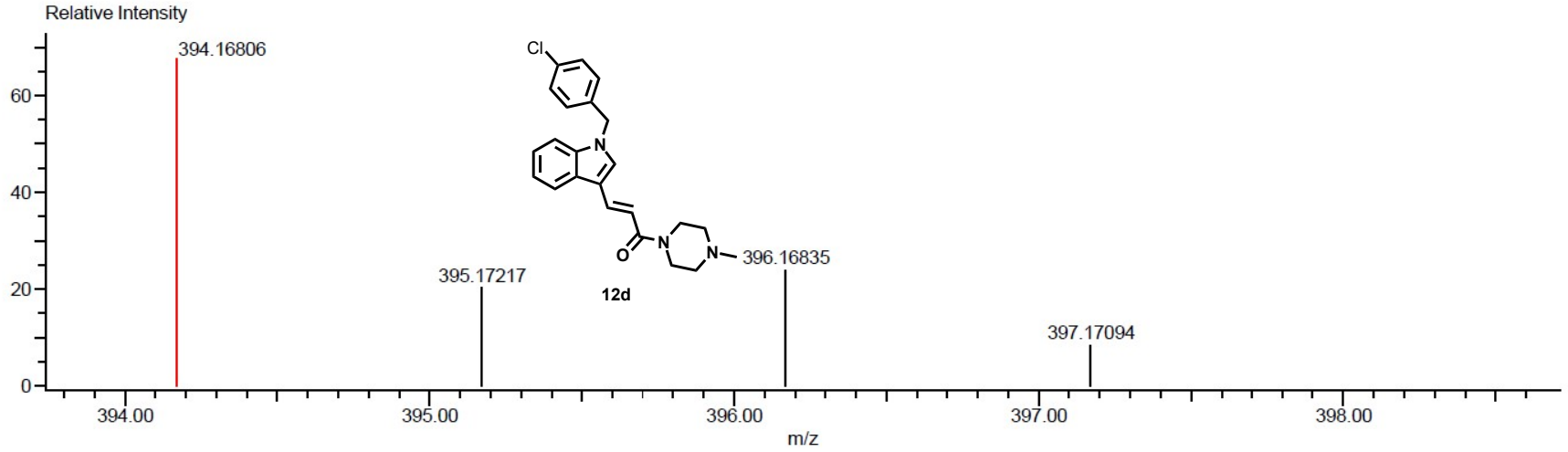


Figure 79. ^{13}C NMR, DEPT-135, spectrum of **12d** (75 MHz, $CDCl_3$).

Data:805 VDM-90
Sample Name:Dr. Martinez Roberto/ Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:3/16/2023 5:27:05 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:3/28/2023 4:22:51 PM
Created by:AccuTOF

Charge number:1
Tolerance:4.00(mmu)
Unsaturation Number:-1.0 .. 50.0 (Fraction:.5)
Element:^{12}C:0 .. 24, ^{1}H:0 .. 60, ^{35}Cl:0 .. 1, ^{14}N:0 .. 4, ^{16}O:0 .. 3



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
394.16806	54609.41	394.16861	-0.55	-1.40	$^{12}C_{23}{}^{1}H_{25}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{1}$	12.5

Figure 80. ESI-HRMS spectrum of **12d.**

2.28 Compound 12e

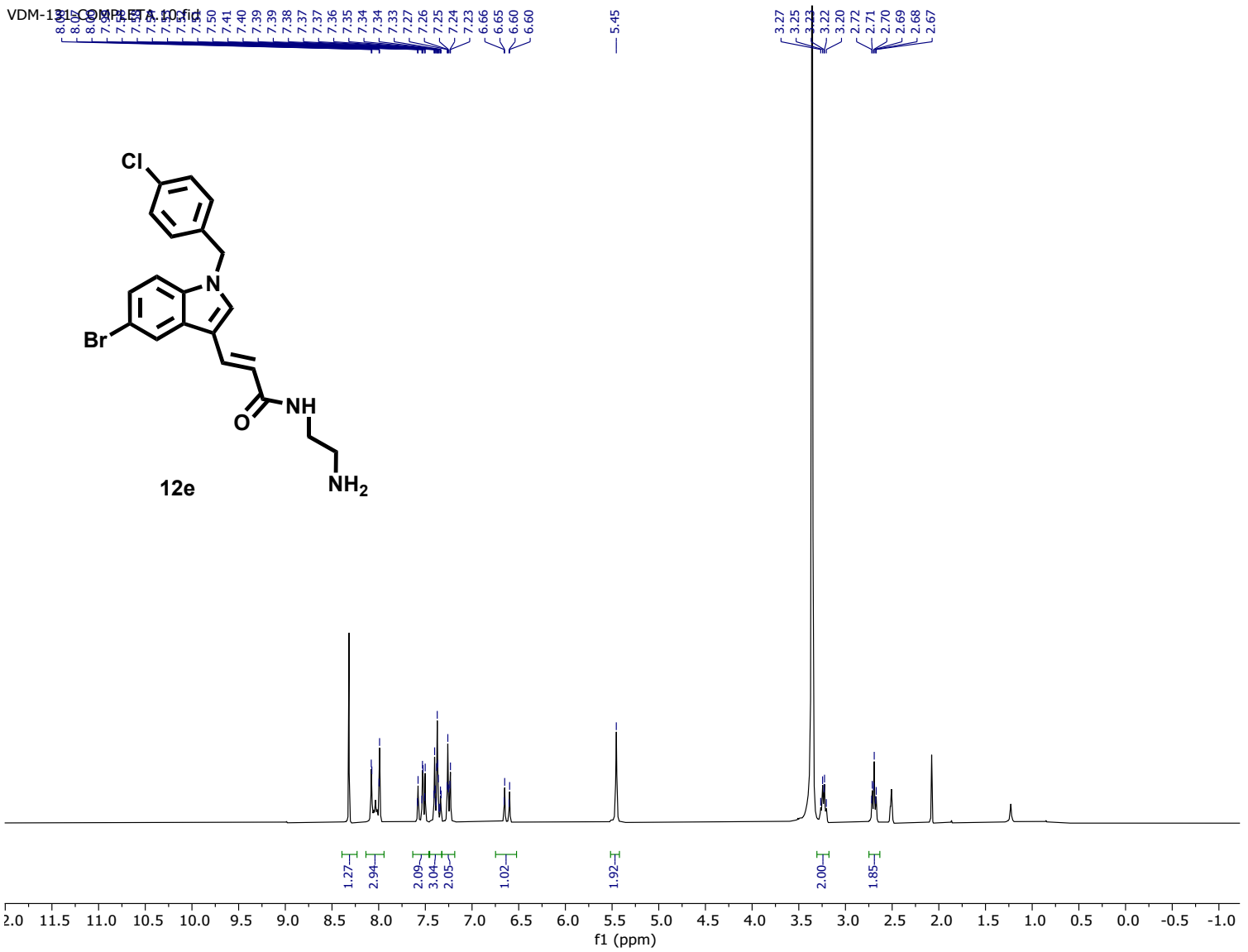


Figure 81. ^{1}H NMR spectrum of **12e** (300 MHz, DMSO-d_6).

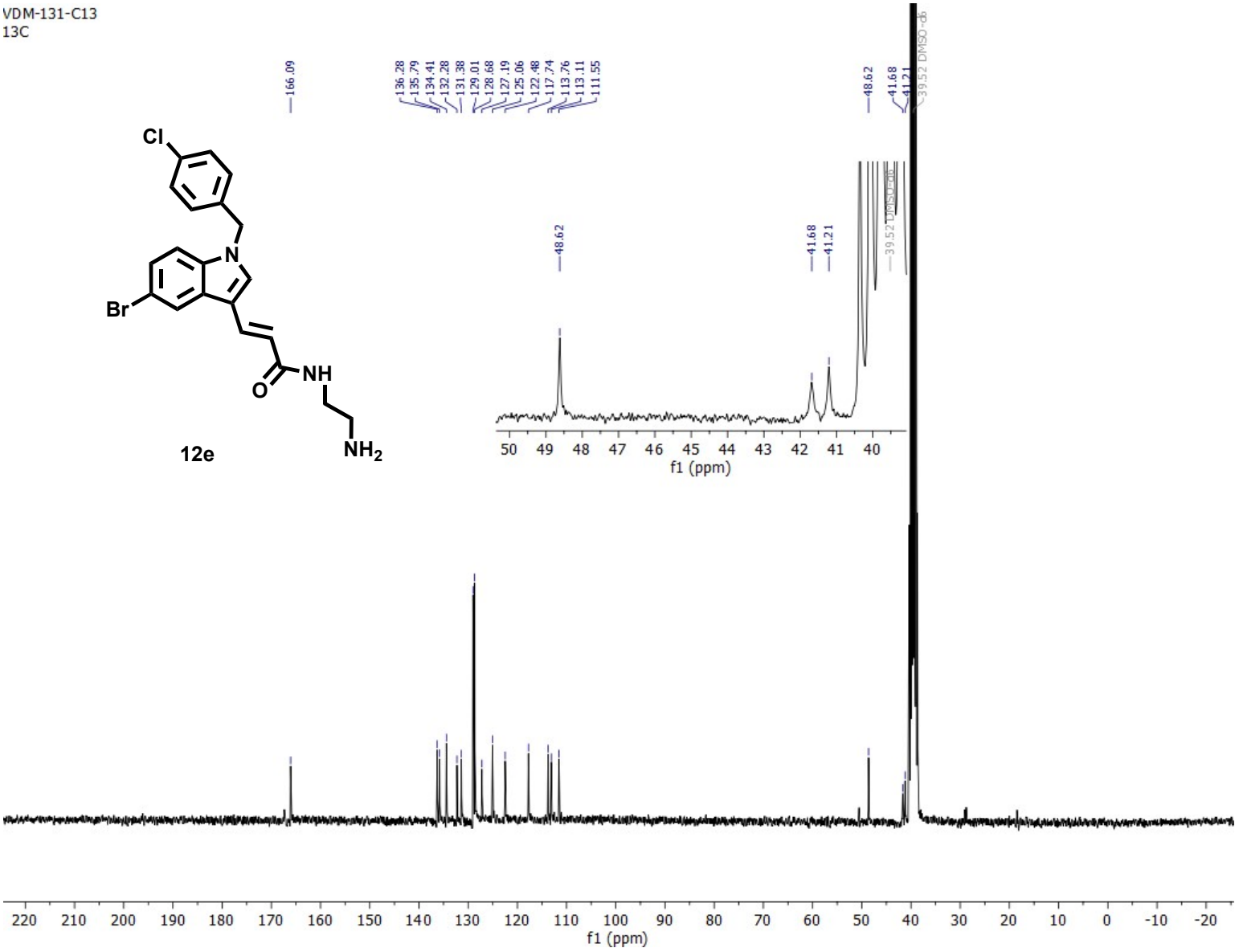
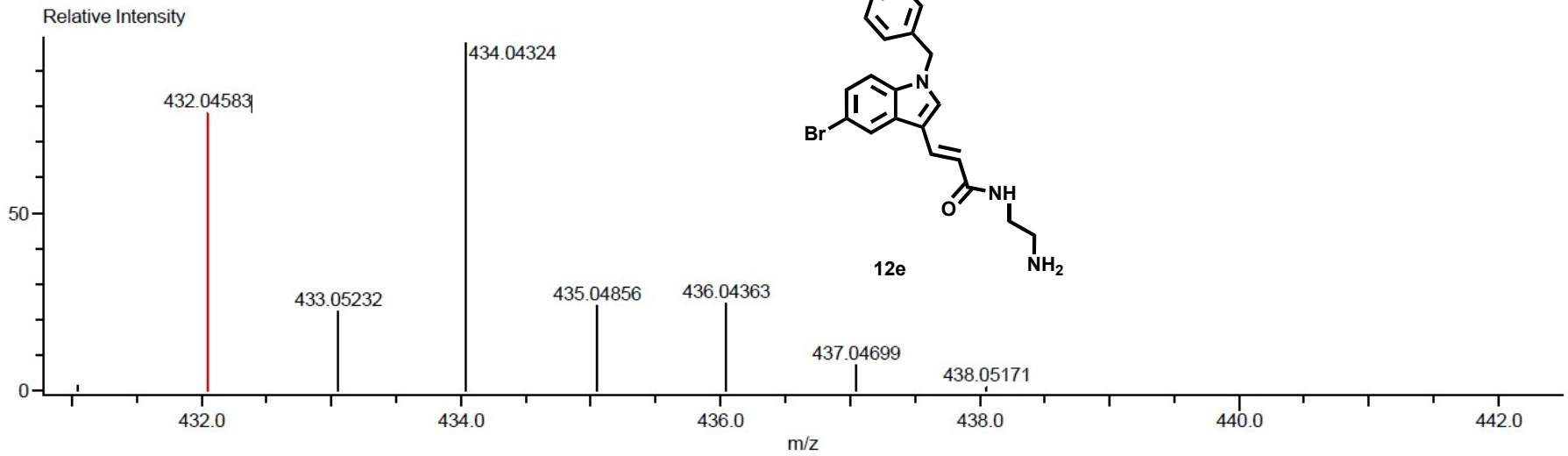


Figure 82. ^{13}C NMR spectrum of **12e** (75 MHz, DMSO-d_6).

Data:1709_VDM-131
Sample Name:DR. Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:6/20/2023 1:19:46 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:8/2/2023 1:55:37 PM
Created by:AccuTOF

Charge number:1
Tolerance:4.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.0 .. 54.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{79}Br:0 .. 2, ^{35}Cl:1 .. 1, ^{14}N:3 .. 3, ^{16}O:1 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
432.04583	60643.74	432.04783	-1.99	-4.61	$^{12}C_{20}{}^{1}H_{20}{}^{79}Br_{1}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{1}$	11.5

Figure 83. ESI-HRMS spectrum of **12e.**

2.29 Compound 12f

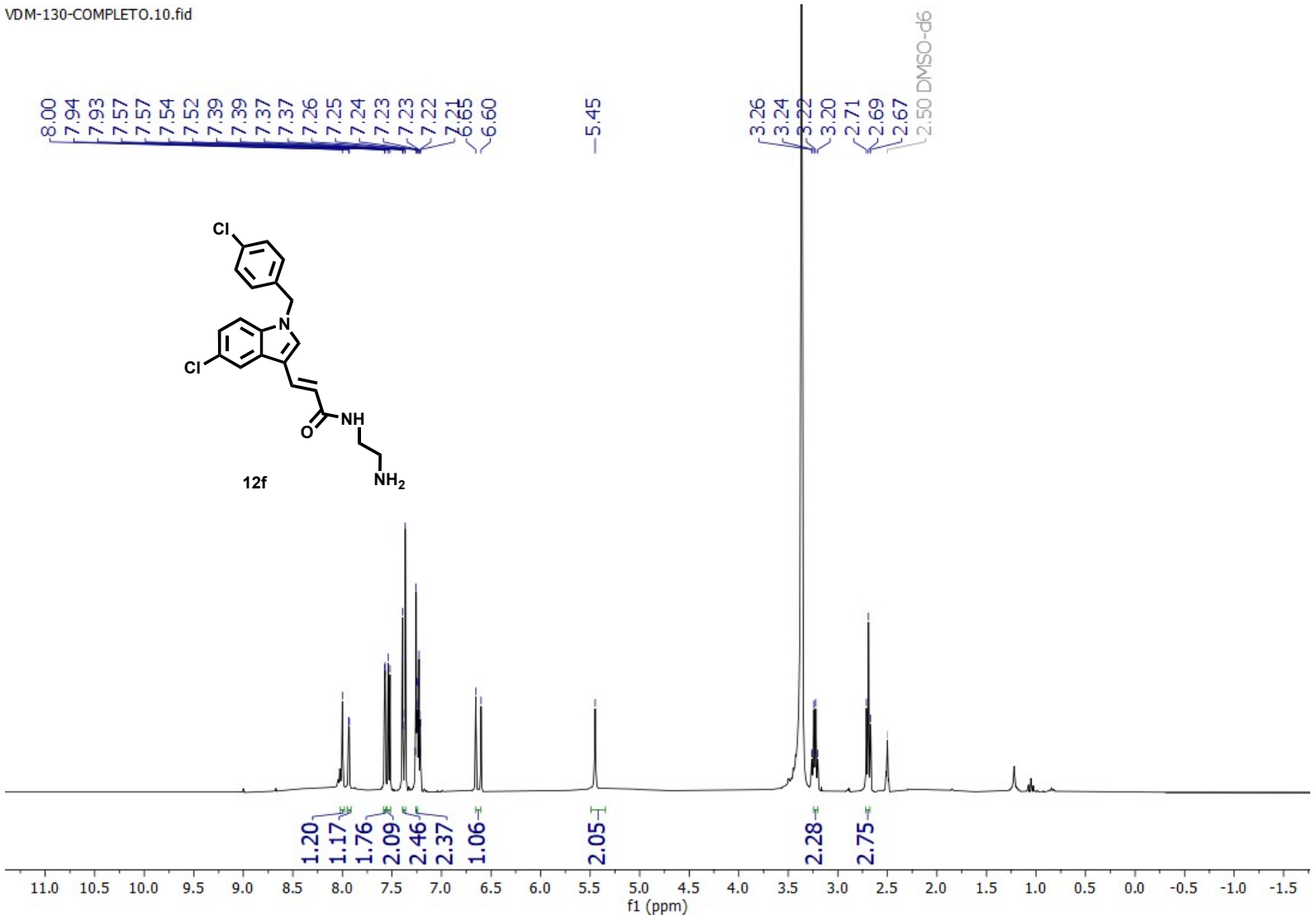


Figure 84. ^{1}H NMR spectrum of **12f** (300 MHz, DMSO-d_6).

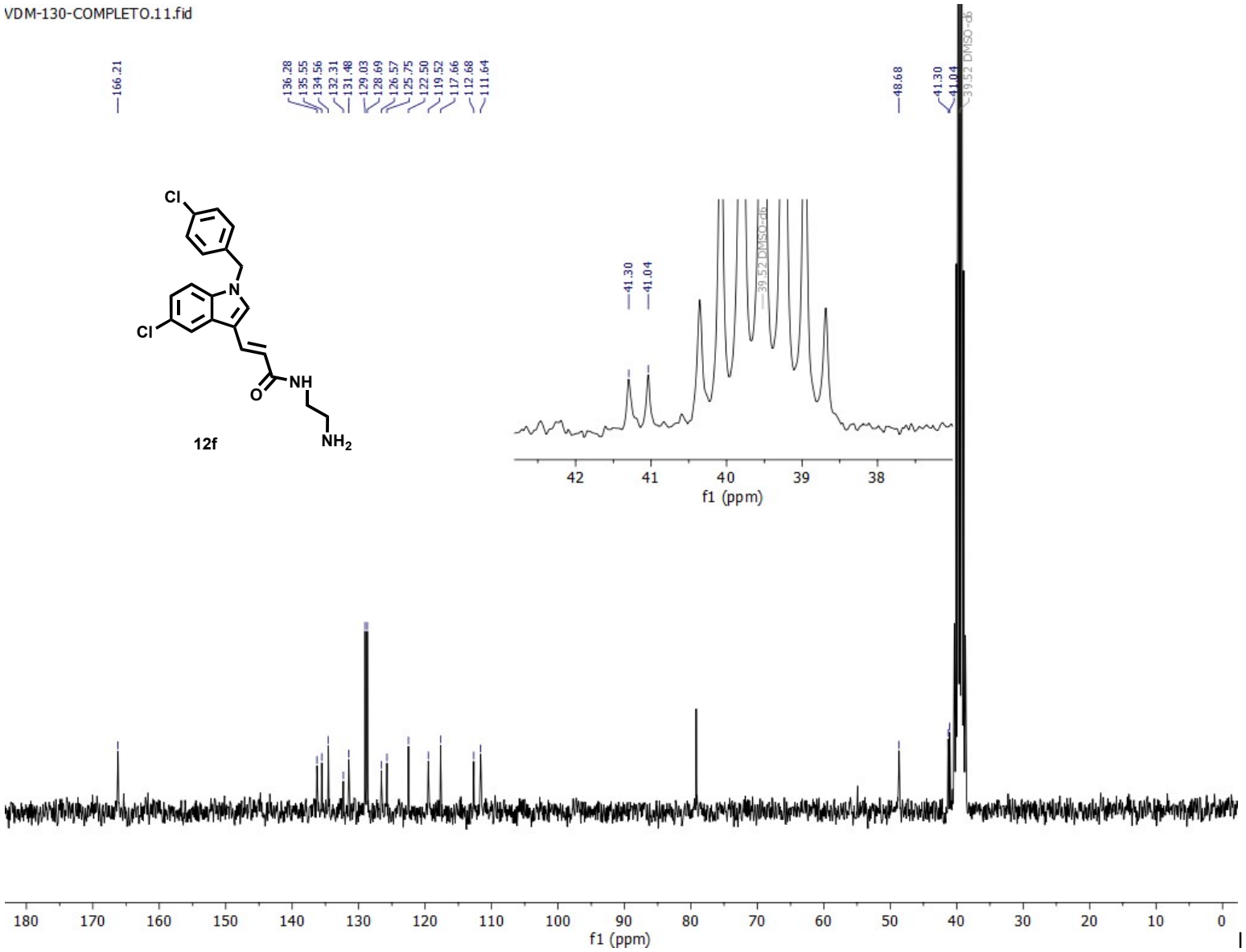
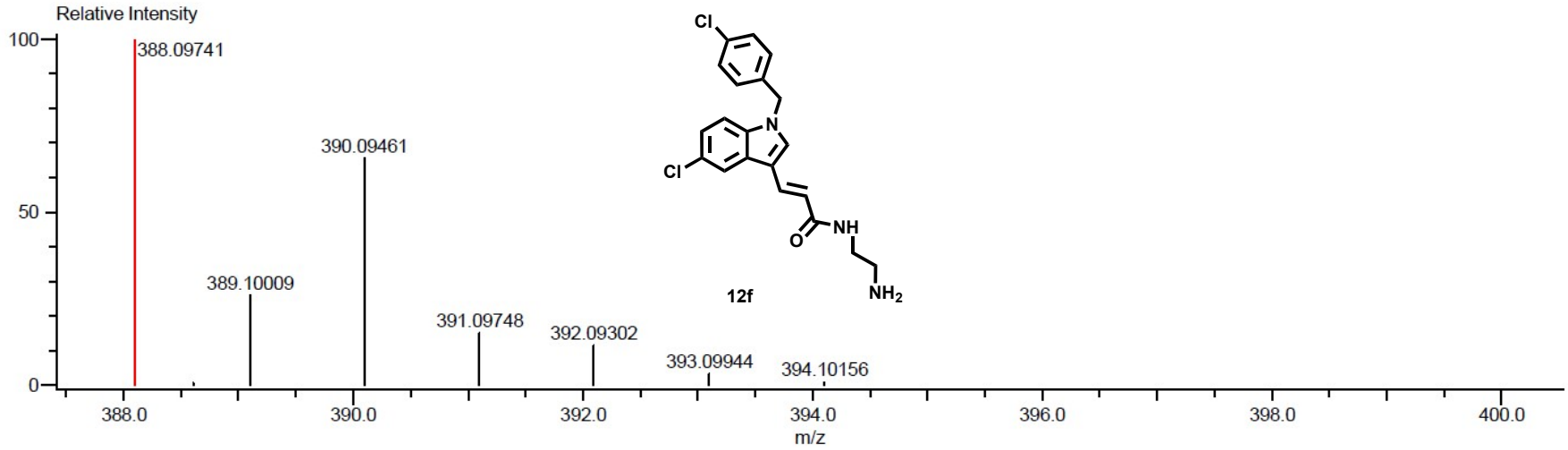


Figure 85. ^{13}C NMR spectrum of **12f** (75 MHz, DMSO-d_6).

Data:1712_VDM-130
Sample Name:DR. Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:6/20/2023 1:26:03 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:8/2/2023 1:51:52 PM
Created by:AccuTOF

Charge number:1
Tolerance:20.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.0 .. 54.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{35}Cl:1 .. 2, ^{14}N:0 .. 3, ^{16}O:0 .. 3



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
388.09741	663844.19	388.09834	-0.93	-2.39	$^{12}C_{20}{}^{1}H_{20}{}^{35}Cl_2{}^{14}N_3{}^{16}O_1$	11.5

Figure 86. ESI-HRMS spectrum of **12f.**

2.30 Compound 12g

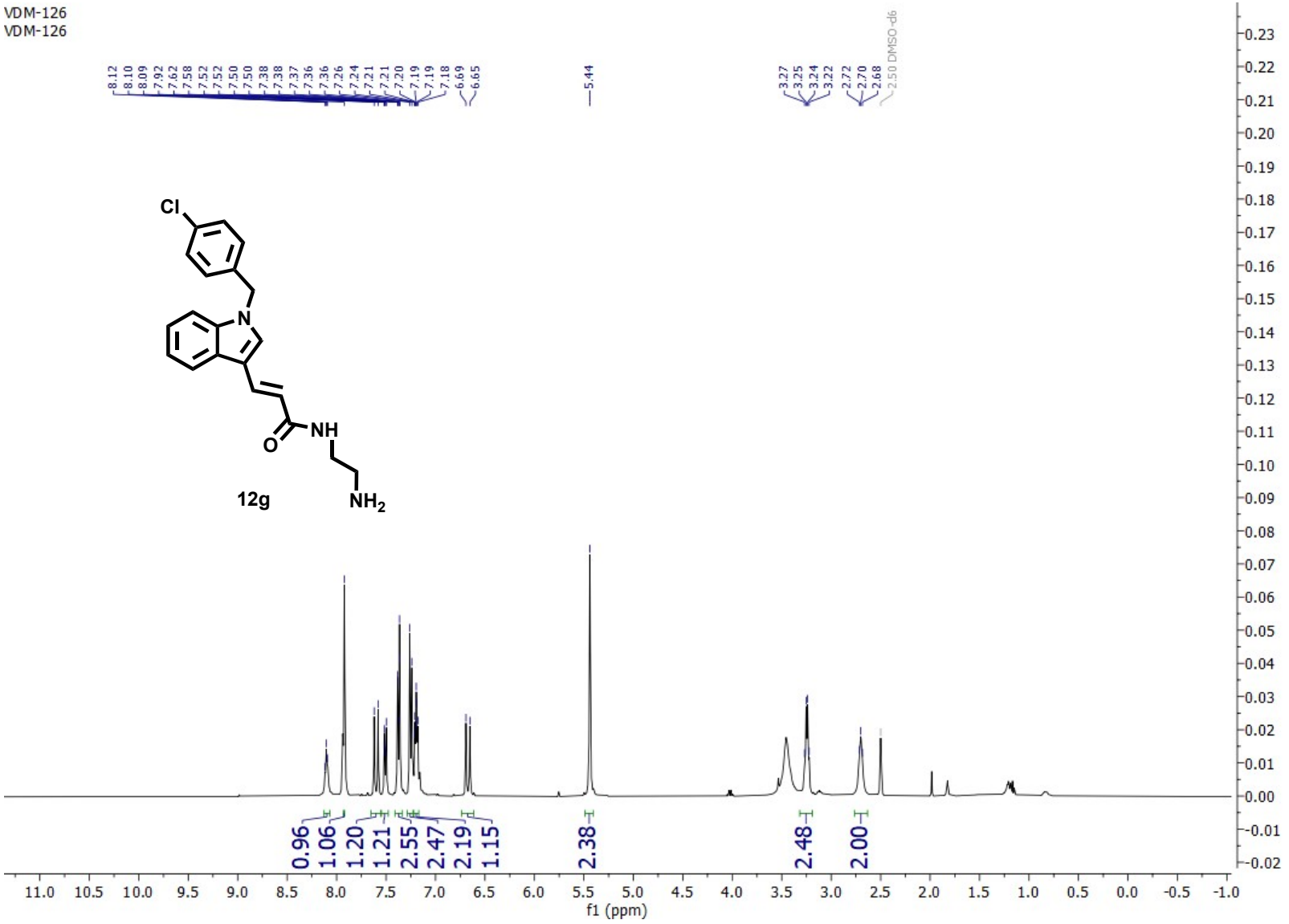


Figure 87. ^{1}H NMR spectrum of **12g** (300 MHz, DMSO-d_6).

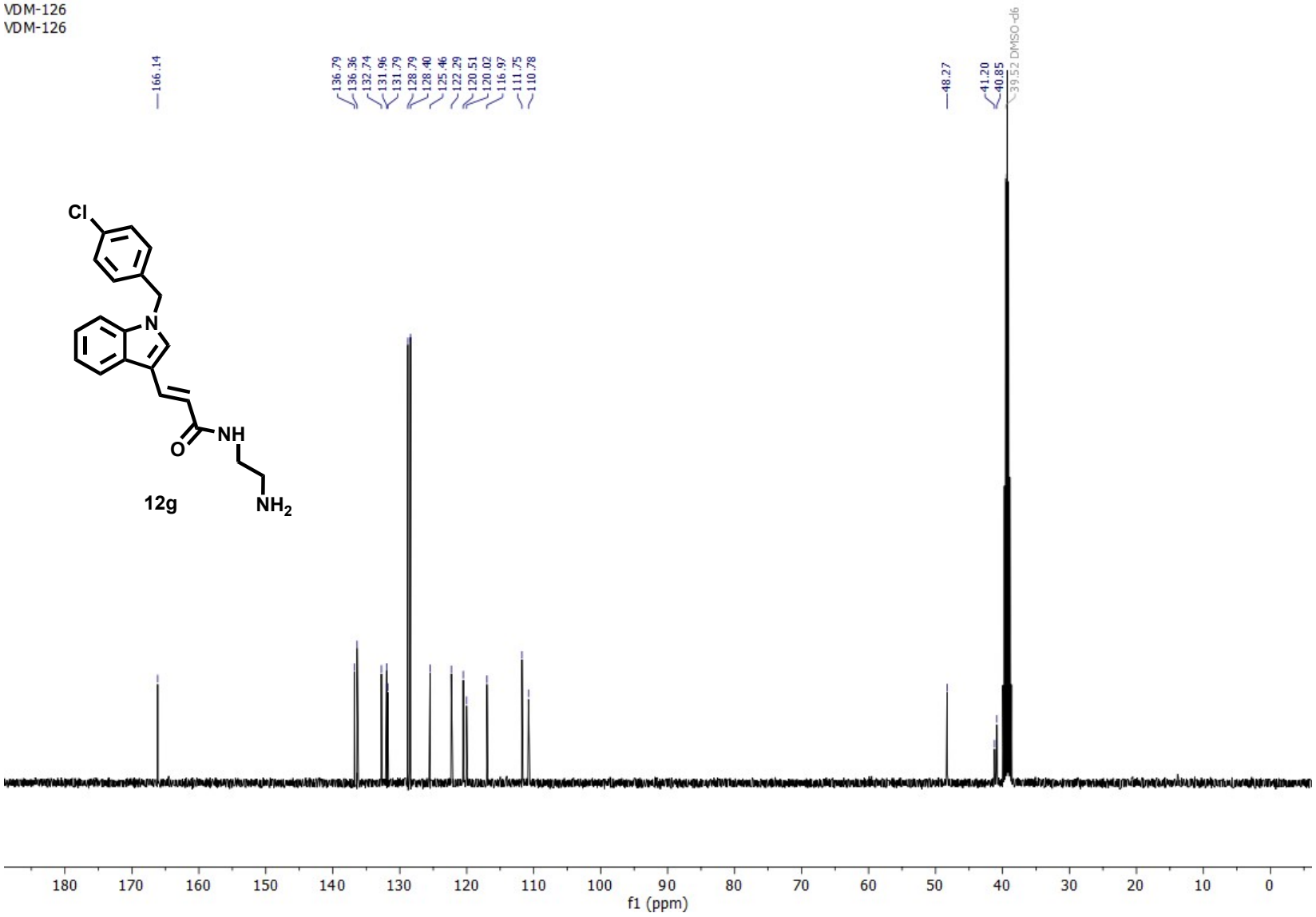
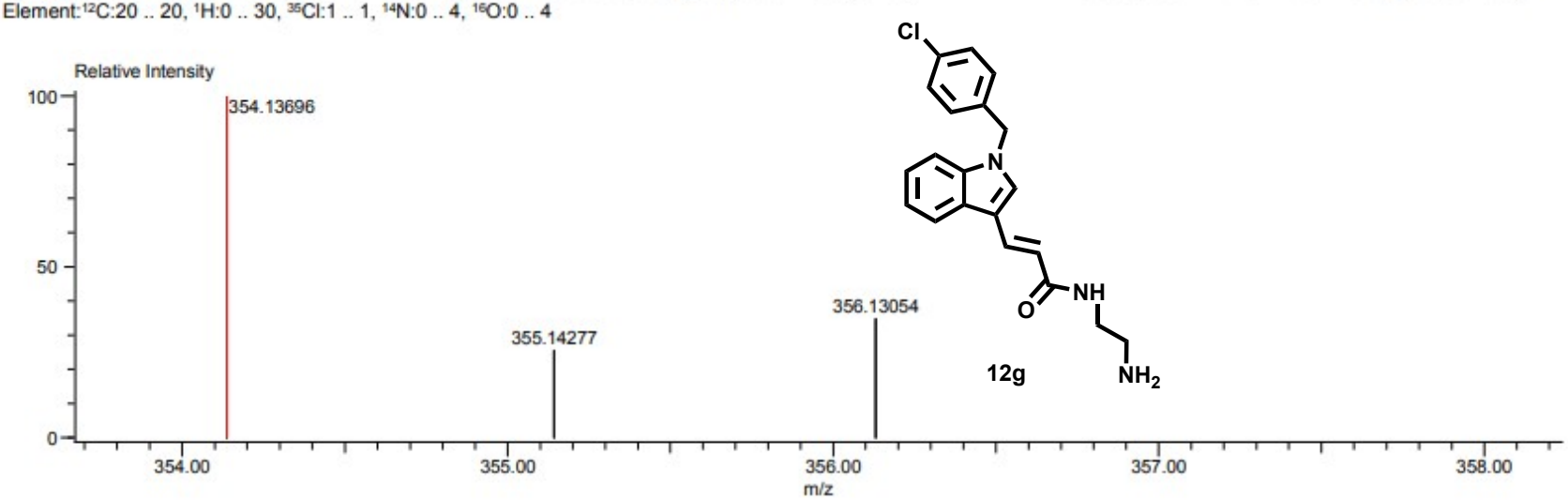


Figure 88. ^{13}C NMR spectrum of **12g** (75MHz, DMSO-d_6).

Data:1053_VDM-126
Sample Name:DR Martinez Roberto /Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:4/29/2024 11:12:27 AM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600_ok
Created:4/29/2024 12:24:14 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)
Element:^{12}C:20 .. 20, ^{1}H:0 .. 30, ^{35}Cl:1 .. 1, ^{14}N:0 .. 4, ^{16}O:0 .. 4



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
354.13696	9584.70	354.13731	-0.35	-1.00	$^{12}C_{20}{}^{1}H_{21}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{1}$	11.5

Figure 89. ESI-HRMS spectrum of **12g.**

2.31 Compound 12h

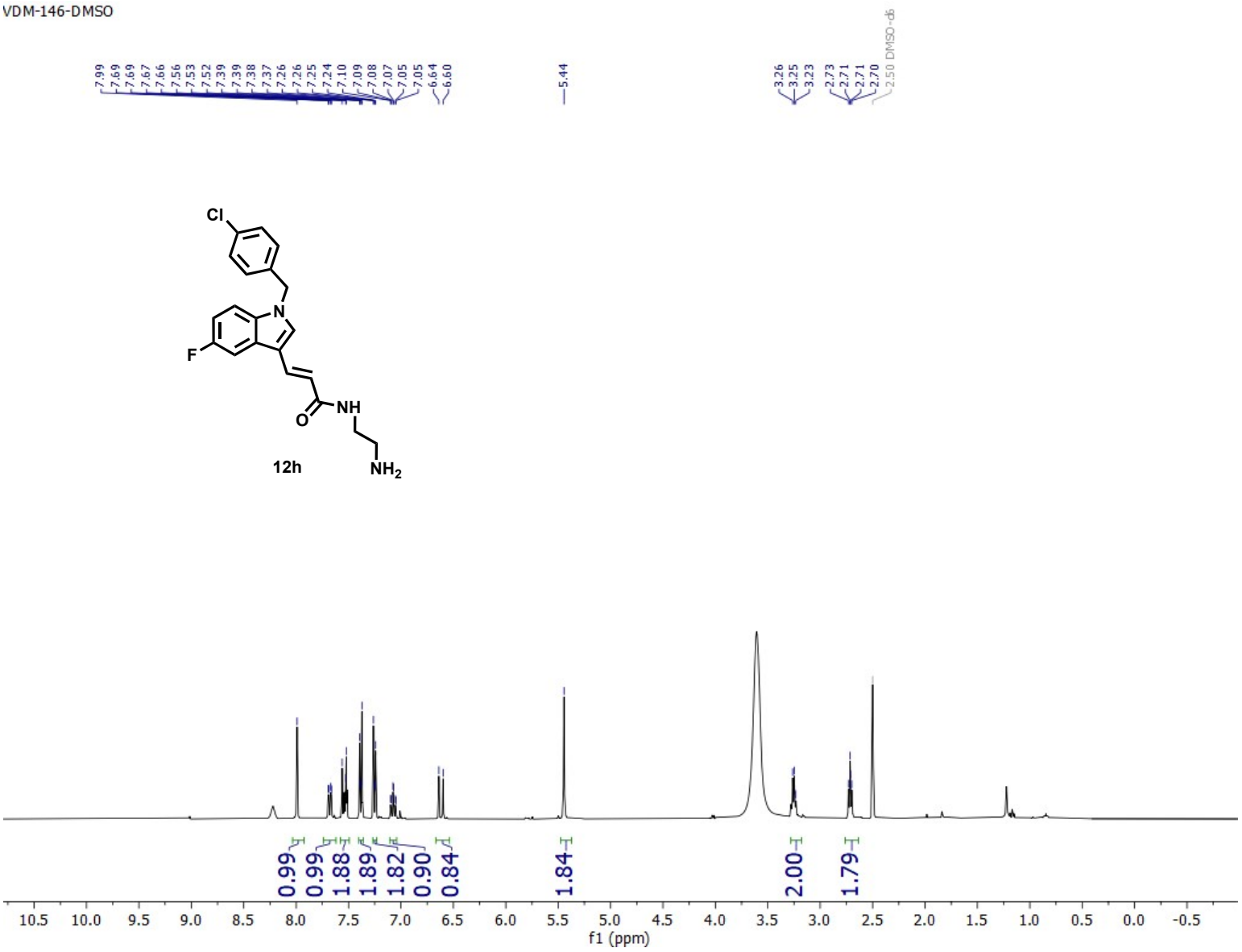


Figure 90. ^{1}H NMR spectrum of **12h** (400 MHz, DMSO-d_6).

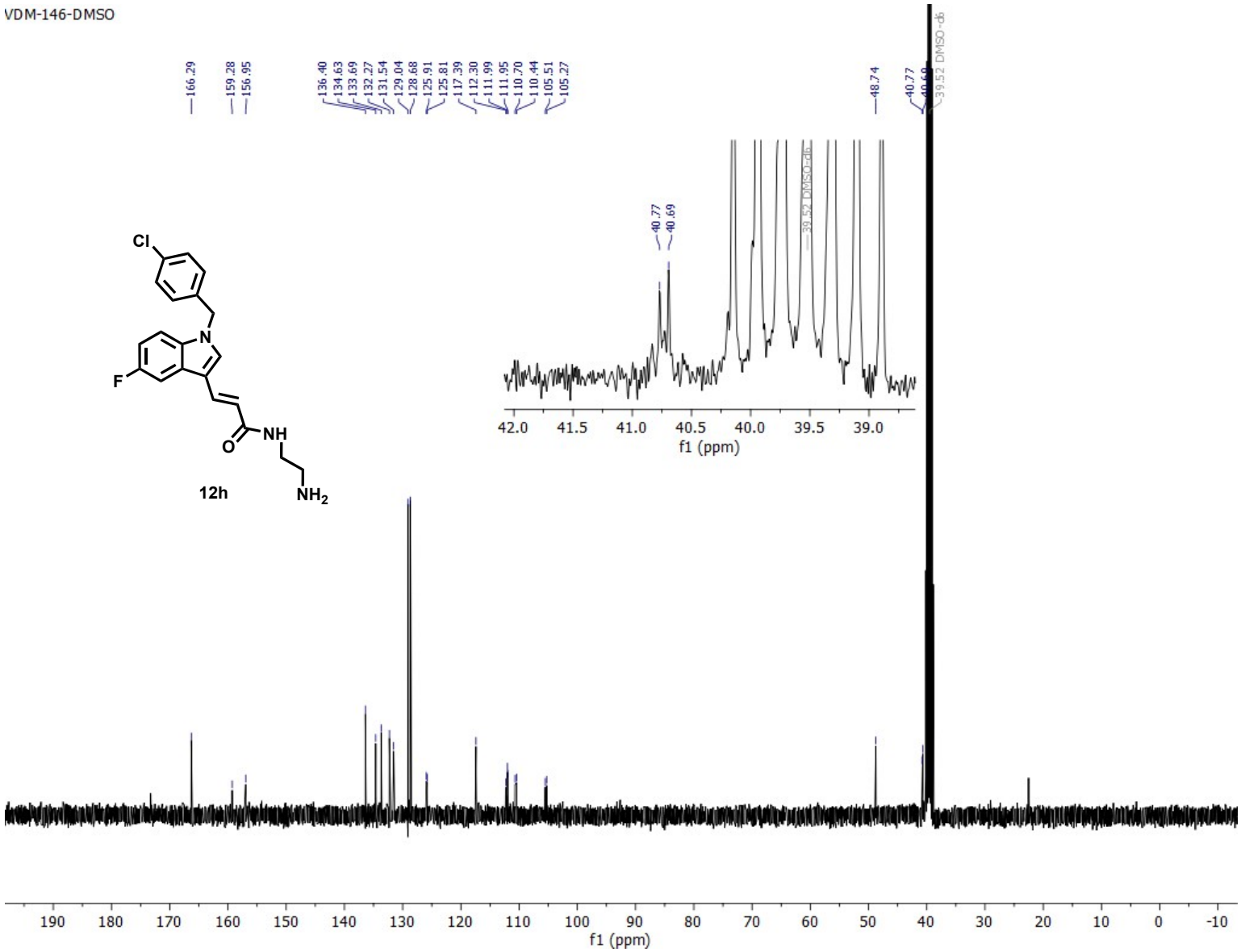
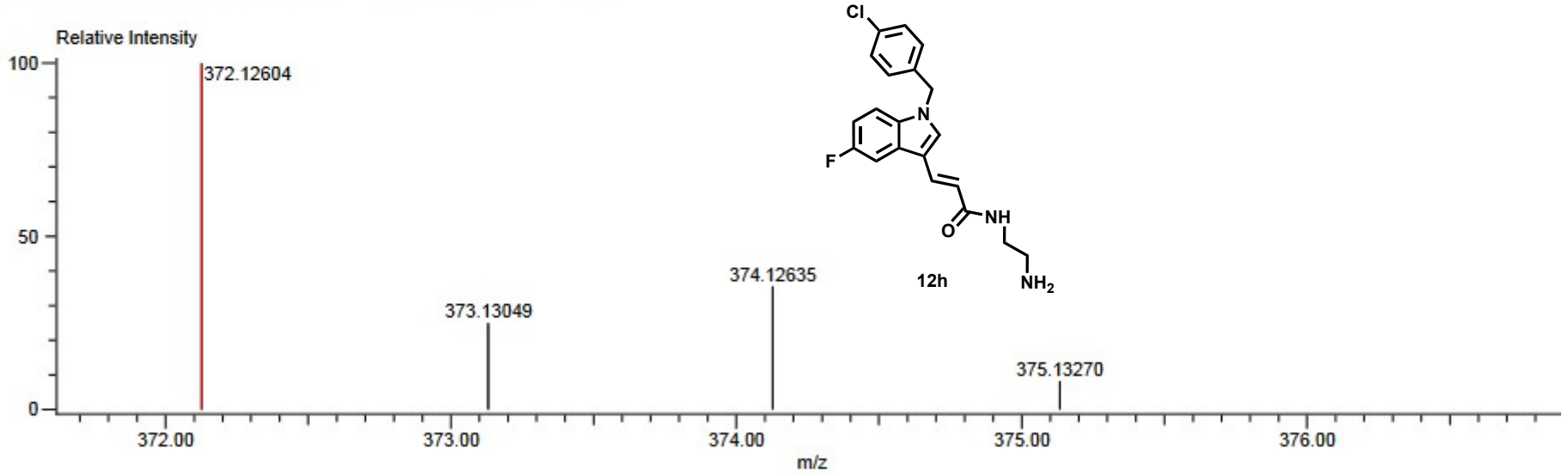


Figure 91. ^{13}C NMR spectrum of **12h** (101 MHz, DMSO-d_6).

Data:928_VDM-146
Sample Name:Dr Martinez Roberto /Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 1..1)

Acquired:4/18/2024 11:41:43 AM
Operator:AccuTOF
Mass Calibration data:CAL_PEG_600
Created:4/18/2024 11:47:36 AM
Created by:AccuTOF

Charge number:1
Tolerance:4.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.5 .. 100.0 (Fraction:Both)
Element:^{12}C:0 .. 20, ^{1}H:0 .. 50, ^{35}Cl:0 .. 1, ^{19}F:0 .. 1, ^{14}N:1 .. 3, ^{16}O:1 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
372.12604	45824.89	372.12789	-1.85	-4.97	$^{12}C_{20}{}^{1}H_{20}{}^{35}Cl_{1}{}^{19}F_{1}{}^{14}N_{3}{}^{16}O_{1}$	11.5

Figure 92. ESI-HRMS spectrum of **12h.**

2.32 Compound 12i

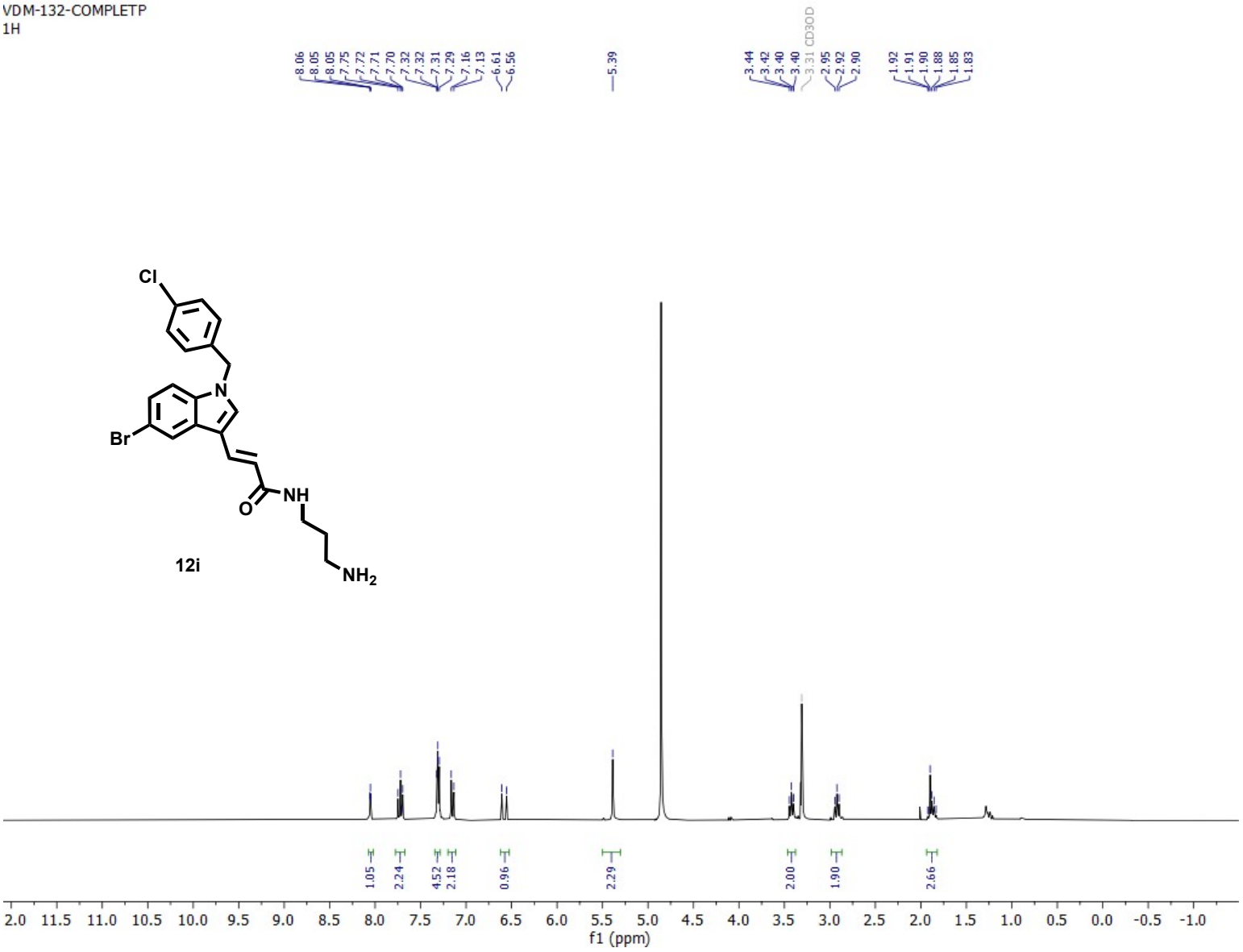


Figure 93. ^{1}H NMR spectrum of **12i** (300 MHz, MeOD-d_4).

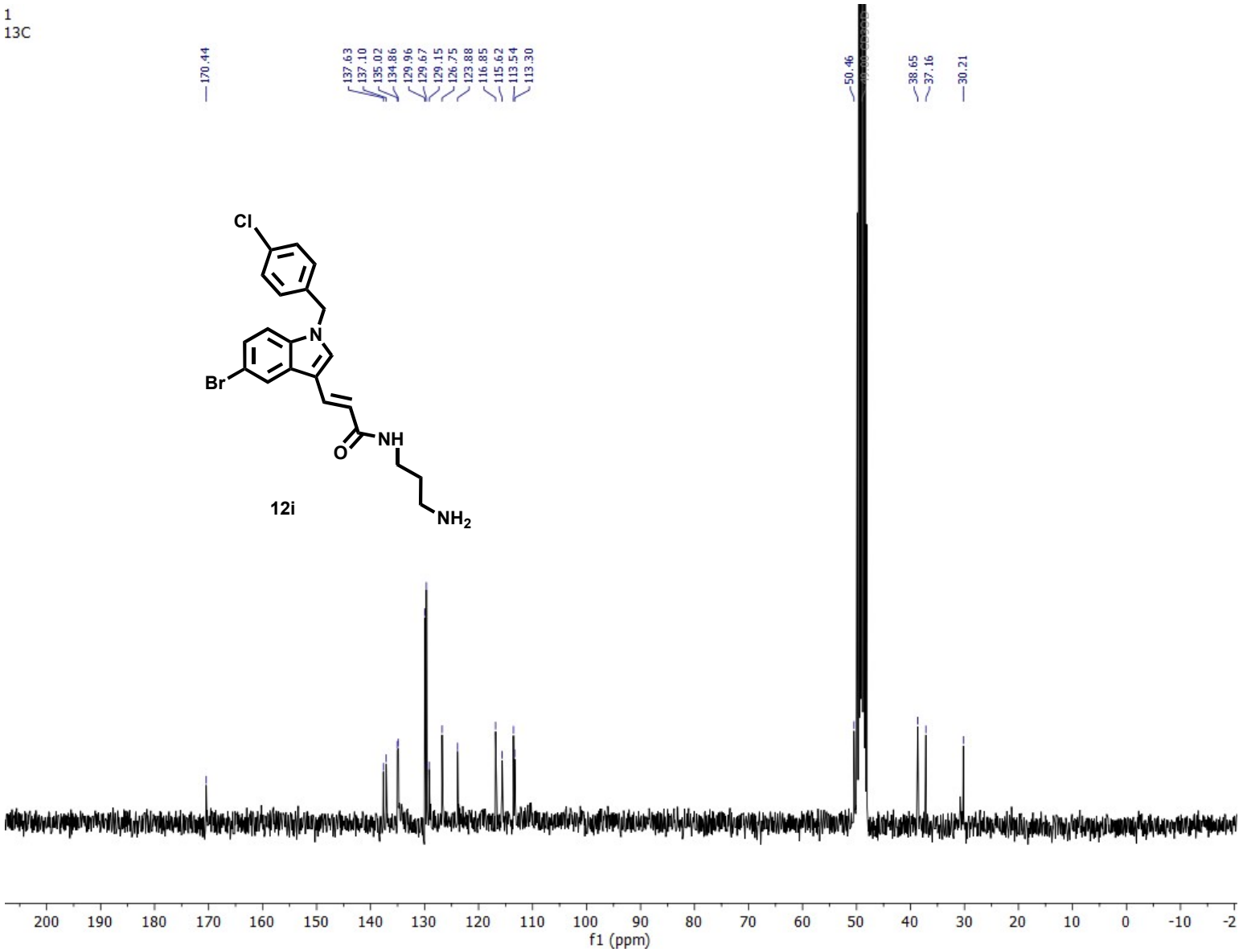


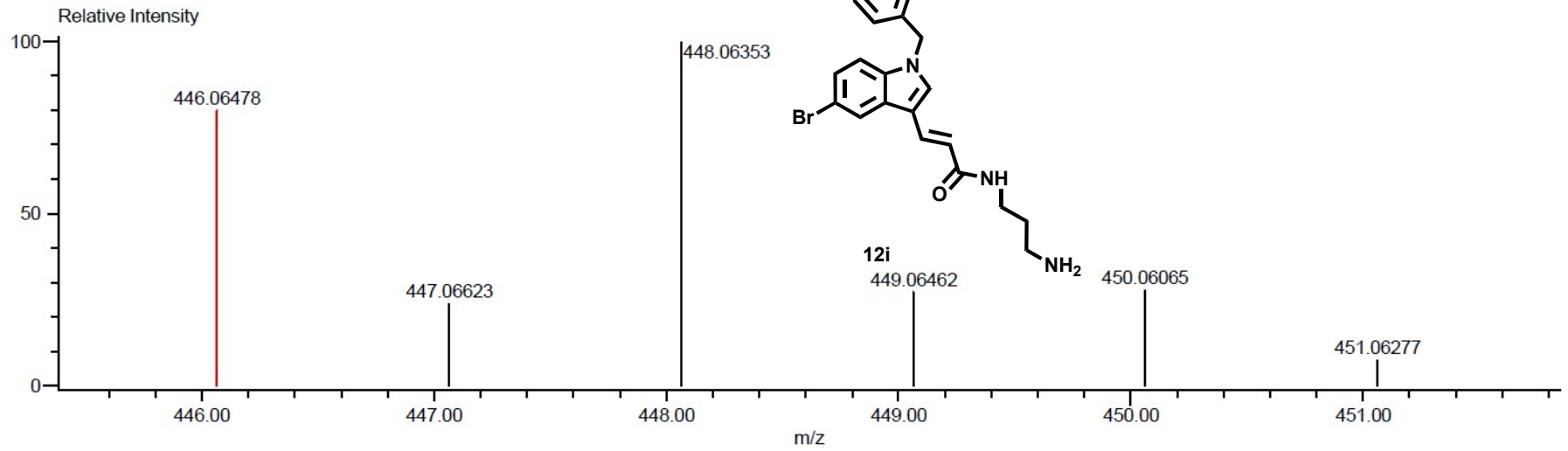
Figure 94. ^{13}C NMR spectrum of **12i** (75 MHz, MeOD-d_4).

Data:1974 VDM-132
Sample Name:Dr Martinez Roberto/ Operador Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:8/8/2023 6:23:36 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:8/21/2023 6:44:36 PM
Created by:AccuTOF

Charge number:1
Tolerance:5.00(mmu)
Element:^{12}C:0 .. 30, ^{1}H:0 .. 50, ^{79}Br:1 .. 1, ^{35}Cl:1 .. 1, ^{14}N:1 .. 4, ^{16}O:0 .. 2

Unsaturation Number:-1.0 .. 50.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
446.06478	2200124.35	446.06348	1.31	2.93	$^{12}C_{21}{}^{1}H_{22}{}^{79}Br_{1}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{1}$	11.5

Figure 95. ESI-HRMS spectrum of **12i.**

2.33 Compound 12j

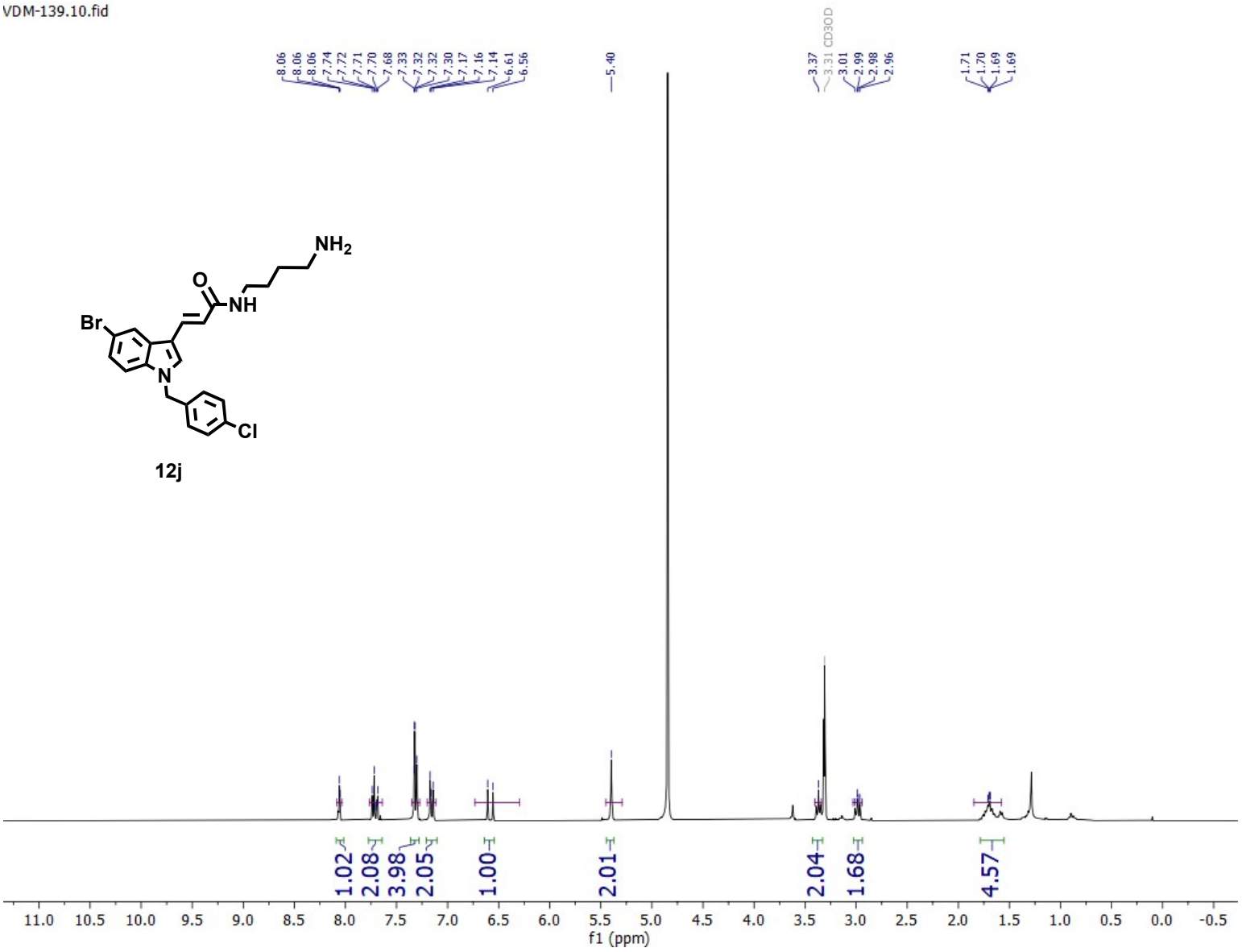


Figure 96. ^{1}H NMR spectrum of **12j** (300 MHz, MeOD-d_4).

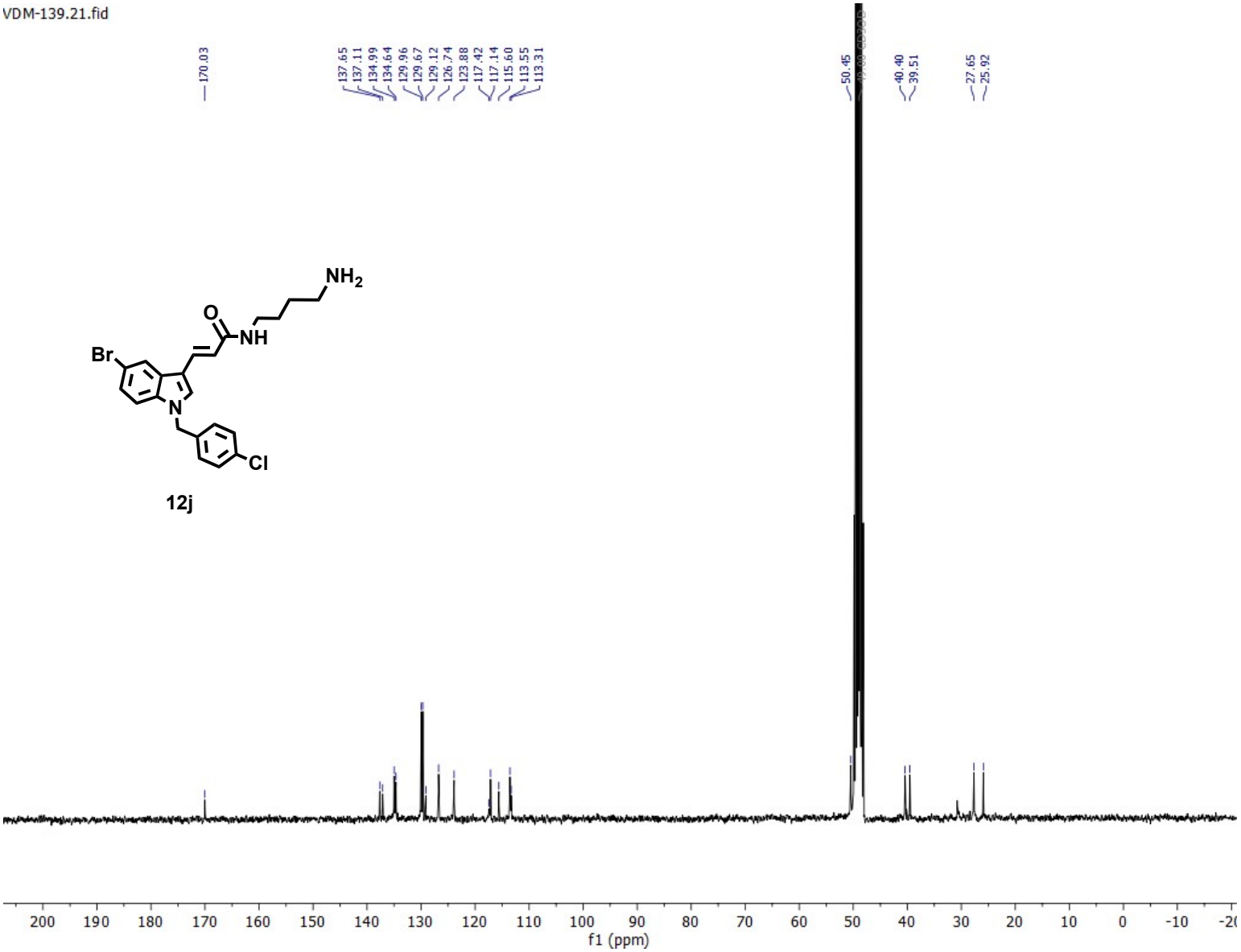
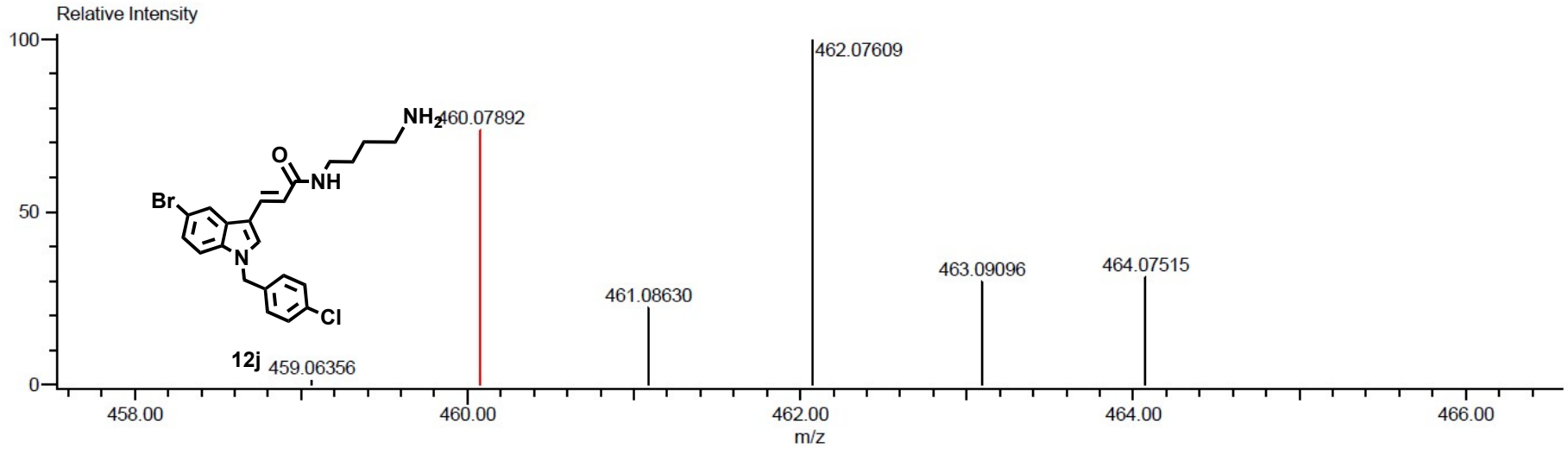


Figure 97. ^{13}C NMR spectrum of **12j** (75 MHz, MeOD-d_4).

Data:3027_VDM-139
Sample Name:Dr Martinez Roberto / Operador: Carmen Garcia
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[5]];Correct Base[5.0%];Average(MS[...

Acquired:11/14/2023 1:53:19 PM
Operator:AccuTOF
Mass Calibration data:Cal_PEG_600
Created:11/27/2023 9:45:22 AM
Created by:AccuTOF

Charge number:1
Tolerance:4.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:-1.0 .. 70.0 (Fraction:Both)
Element:^{12}C:0 .. 25, ^{1}H:0 .. 40, ^{79}Br:0 .. 1, ^{35}Cl:0 .. 1, ^{14}N:0 .. 3, ^{16}O:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
460.07892	6275.53	460.07913	-0.21	-0.46	$^{12}C_{22}{}^{1}H_{24}{}^{79}Br_{1}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{1}$	11.5

Figure 98. ESI-HRMS spectrum of **12j.**

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