Supplementary information

Synthesis of benzosultams *via* Ag(I)-catalyzed alkylative cyclization of vinyl sulfonamides

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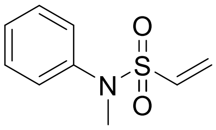
Table of Contents

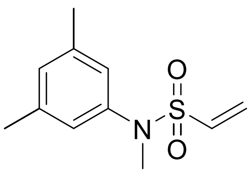
1. General information

All the reactions were performed in oven-dried glass apparatus, the air and moisture sensitive reactions were carried out under inert atmosphere (nitrogen) using freshly distilled anhydrous solvents. Commercially available reagents were used as such without further purification. All reactions were monitored by thin-layer chromatography carried out on silica plates using UV-light and anisaldehyde for visualization. Column chromatography was performed on silica gel (100-200 mesh) using hexanes and ethyl acetate as eluent. NMR spectra were recorded on 400, 500, and 600 MHz spectrometers. δ 7.26 and δ 77 ppm are corresponding to $CDCl_3$ in ^{1}H NMR and ^{13}C NMR respectively, δ 1.56 ppm is related to moisture present in $CDCl_3$. Chemical shifts were reported in δ (ppm) relative to TMS as an internal standard and *J* values are given in Hz (hertz). Multiplicity is indicated as, s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. High resolution mass spectra (HRMS) [ESI+] were obtained using either a TOF or a double focusing spectrometer. Melting point of all solid compounds was determined using a melting point apparatus.

2. List of starting materials



1a



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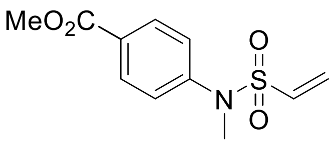

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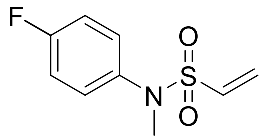

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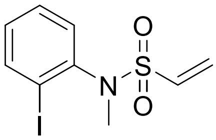

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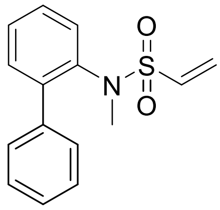

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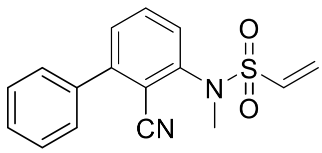

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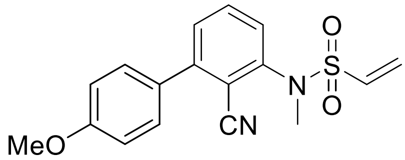

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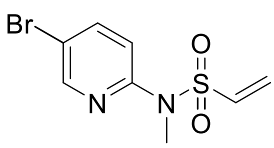

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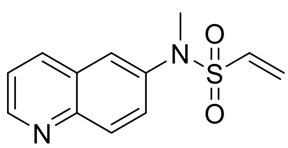

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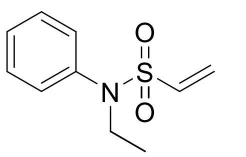
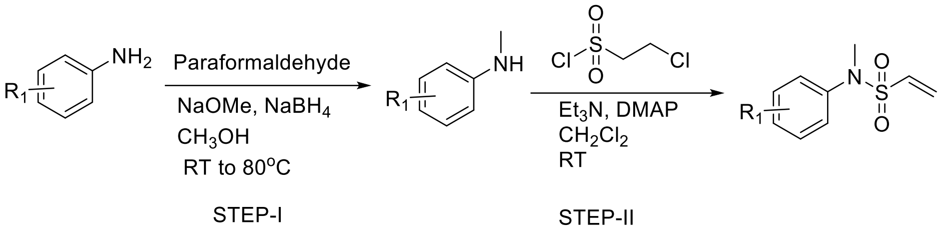


1k

3. Synthesis of starting materials

3.1. General procedure

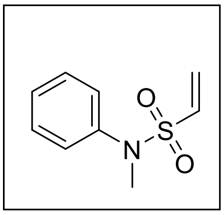


Step-I: To a solution of aniline (1 equiv.) in dry MeOH was added NaOMe (4 equiv.), followed by paraformaldehyde (4 equiv.) and stirred for 14 h. Then added $NaBH_4$ (4 equiv.) and heated the reaction mixture at 80 ˚C for one hour. The reaction mixture was then concentrated under reduced vacuum. Water (15 mL) was added to the reaction mixture, and the aqueous layer was extracted with ethyl acetate (2 x 25 mL). The combined organic layer was dried over anhydrous Na_2SO_4, concentrated in vacuo, and purified by column chromatography using hexane and ethyl acetate.

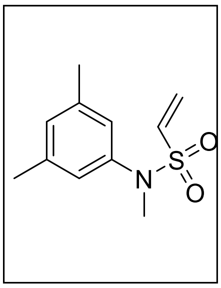
Step-II: DMAP (0.05 equiv.) was added to a stirring solution of *N*-Methyl aniline (1.0 equiv.) and Triethylamine (3.0 equiv.) in DCM, followed by addition of 2-Chloroethylsulfonyl chloride (1.5 equiv.) at 0 ˚C dropwise, and then the resulting mixture was stirred for 2-3 h under nitrogen atmosphere. After the reaction was completed (monitored by TLC), The reaction mixture was concentrated under reduced pressure and purified by column chromatography.

3.2. Characterization data

***N*-methyl-*N*-phenylethenesulfonamide (1a):** Compound **1a** was prepared according to the general procedure and spectral data matched with the literature reports[1].

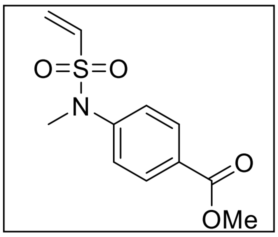


***N*-(3,5-dimethylphenyl)-*N*-methylethenesulfonamide (1b):** yellow oil (383 mg, 93% yield in step II); R_f = 0.4 (Hexane: Ethyl Acetate = 8:2).



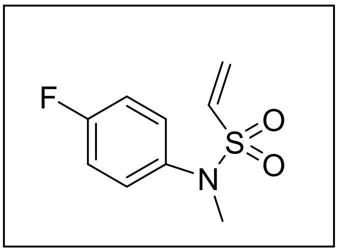
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 3H), 6.47 (dd, *J* = 16.6, 9.9 Hz, 1H), 6.21 (d, *J* = 16.6 Hz, 1H), 6.01 (d, *J* = 9.9 Hz, 1H), 3.20 (s, 3H), 2.31 (s, 6H); $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 141.1, 138.9, 132.5, 129.3, 128.1, 124.4, 38.3, 21.3; HRMS (ESI): *m/z* calcd for $C_{11}H_{15}NO_2S$ $[M+H]^+$: 225.0823, found: 225.0793.

Methyl 4-(*N*-methylvinylsulfonamido)benzoate (1c): yellow solid (395 mg, 73% yield in step II), m.p: 64-66 °C; R_f = 0.5 (Hexane: Ethyl Acetate = 8:2).



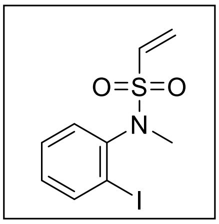
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.7 Hz, 2H), 7.40 (d, *J* = 8.7 Hz, 2H), 6.43 (dd, *J* = 16.6, 9.9 Hz, 1H), 6.21 (d, *J* = 16.6 Hz, 1H), 6.04 (d, *J* = 9.9 Hz, 1H), 3.92 (s, 3H), 3.28 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 166.3, 145.3, 132.2, 130.5, 129.0, 128.5, 125.3, 52.3, 37.6; HRMS (ESI): *m/z* calcd for $C_{11}H_{14}NO_4S$ $[M+H]^+$: 256.0644, found: 256.0635.

***N*-(4-fluorophenyl)-*N*-methylethenesulfonamide (1d):** Dark yellow oil (344 mg, 66% yield in step II); R_f = 0.4 (Hexane: Ethyl Acetate = 8:2).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.10 – 7.00 (m, 2H), 6.45 (dd, *J* = 16.6, 9.9 Hz, 1H), 6.19 (d, *J* = 16.6 Hz, 1H), 6.03 (d, *J* = 9.9 Hz, 1H), 3.22 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 161.6 (d, *J* = 247.6 Hz), 137.1 (d, *J* = 2.7 Hz), 132.1, 128.8, 128.6 (d, *J* = 8.6 Hz), 116.1 (d, *J* = 22.7 Hz), 38.3; ^{19}F NMR (376 MHz, CDCl3) δ -113.7; HRMS (ESI): *m/z* calcd for $C_9H_{11}NO_2SF$ $[M+H]^+$: 216.0495, found: 216.0494.

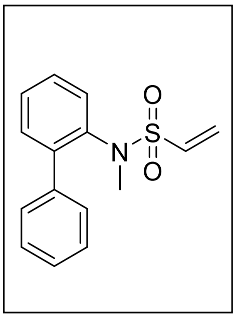
***N*-(2-iodophenyl)-*N*-methylethenesulfonamide (1e):** Black Solid (301 mg, 93% yield in step II); m.p: 60-62 °C; R_f = 0.6 (Hexane: Ethyl Acetate = 8:2).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.90 (m, 1H), 7.38 (dd, *J* = 5.3, 2.1 Hz, 2H), 7.08 – 7.03 (m, 1H), 6.71 (dd, *J* = 16.5, 9.9 Hz, 1H), 6.27 (d, *J* = 16.5 Hz, 1H), 6.05 (d, *J* = 9.9 Hz, 1H), 3.16 (s, 3H); $^{13}C\{^{1}H\}$NMR (75 MHz, $CDCl_3$) δ 143.2, 140.3, 134.9, 130.2, 129.9, 129.5, 128.1, 101.3, 38.2;

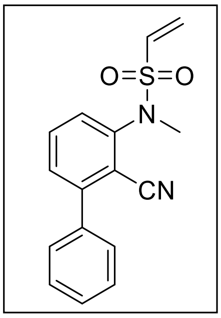
HRMS (ESI): *m/z* calcd for $C_9H_{11}NO_2SI$ $[M+H]^+$:323.9555 found: 323.9531.

***N*-([1,1'-biphenyl]-2-yl)-*N*-methylethenesulfonamide (1f):** Brown oil (407 mg, 91% yield in step II), R_f = 0.5(Hexane: Ethyl Acetate = 8:2).



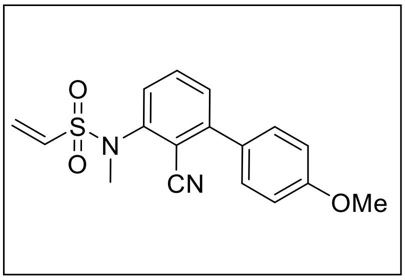
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 4.5 Hz, 4H), 7.41 – 7.36 (m, 5H), 6.19 – 6.06 (m, 2H), 5.87 (dd, *J* = 8.6, 1.1 Hz, 1H), 2.97 (s, 3H); ^{13}C{^{1}H}NMR (101 MHz, $CDCl_3$) δ 142.1, 139.3, 139.0, 134.6, 131.4, 129.2, 128.5, 128.4, 128.2, 127.5, 127.4, 38.6.; HRMS (ESI): *m/z* calcd for $C_{15}H_{15}NO_2NaS$ $[M+Na]^+$: 296.0721, found: 296.0667.

***N*-(2-cyano-[1,1'-biphenyl]-3-yl)-*N*-methylethenesulfonamide (1g):** yellow solid (269 mg, 75% yield in step II), m.p: 106-108°C; R_f = 0.5(Hexane: Ethyl Acetate = 8:2).



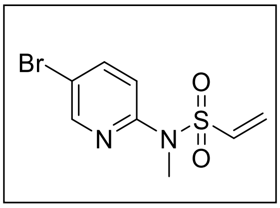
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (t, *J* = 7.9 Hz, 1H), 7.56 – 7.45 (m, 7H), 6.76 (dd, *J* = 16.5, 9.8 Hz, 1H), 6.34 (d, *J* = 16.5 Hz, 1H), 6.11 (d, *J* = 9.8 Hz, 1H), 3.34 (s, 3H); ^{13}C{^{1}H}NMR (101 MHz, $CDCl_3$) δ 147.6, 144.6, 137.5, 136.2, 134.5, 133.3, 129.8, 129.1, 129.0, 128.9, 128.8, 116.3, 112.5, 38.3; HRMS (ESI): *m/z* calcd for $C_{16}H_{15}N_2O_2S$ $[M+H]^+$: 299.0854, found: 299.0852.

***N*-(2-cyano-4'-methoxy-[1,1'-biphenyl]-3-yl)-*N*-methylethenesulfonamide (1h):** yellow solid (273 mg, 79% yield in step II), m.p: 110-112 °C; R_f = 0.4 (Hexane: Ethyl Acetate = 8:2).



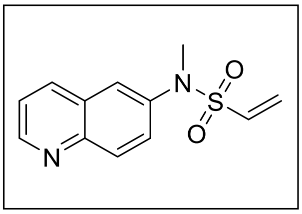
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (t, *J* = 7.9 Hz, 1H), 7.52 – 7.44 (m, 4H), 7.04 – 6.99 (m, 2H), 6.76 (dd, *J* = 16.5, 9.8 Hz, 1H), 6.34 (d, *J* = 16.5 Hz, 1H), 6.11 (d, *J* = 9.8 Hz, 1H), 3.87 (s, 3H), 3.34 (s, 3H); ^{13}C{^{1}H}NMR (101 MHz, $CDCl_3$) δ 160.4, 147.4, 144.6, 134.5, 133.3, 130.2, 129.8, 129.6, 129.0, 128.4, 116.6, 114.3, 112.2, 55.4, 38.3; HRMS (ESI): *m/z* calcd for $C_{17}H_{17}N_2O_3S$ $[M+H]^+$: 329.096, found: 329.0945.

***N*-(5-bromopyridin-2-yl)-*N*-methylethenesulfonamide (1i):** yellow oil (394 mg, 83% yield in step II), R_f = 0.6 (Hexane: Ethyl Acetate = 7:3).



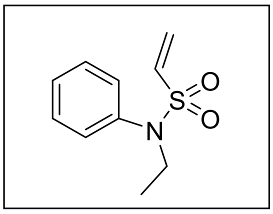
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 2.5, 0.5 Hz, 1H), 7.79 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.43 (dd, *J* = 8.7, 0.7 Hz, 1H), 6.49 (dd, *J* = 16.6, 9.9 Hz, 1H), 6.27 (d, *J* = 16.6 Hz, 1H), 6.04 (d, *J* = 9.9 Hz, 1H), 3.31 (s, 3H); $^{13}C\{^{1}H\}$NMR (126 MHz, $CDCl_3$) δ 152.3, 149.1, 140.4, 133.0, 128.8, 121.3, 117.5, 35.6; HRMS (ESI): *m/z* calcd for $C_8H_{10}N_2O_2SBr$ $[M+H]^+$: 276.9646, found: 276.9630.

***N*-methyl-*N*-(quinolin-6-yl)ethenesulfonamide (1j):** yellow oil (221 mg, 70% yield in step II); R_f = 0.5 (Hexane: Ethyl Acetate = 7:3).



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.19 – 8.07 (m, 2H), 7.78 (d, *J* = 2.4 Hz, 1H), 7.70 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 6.49 (dd, *J* = 16.6, 9.9 Hz, 1H), 6.23 (d, *J* = 16.6 Hz, 1H), 6.05 (d, *J* = 9.9 Hz, 1H), 3.36 (s, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 150.9, 146.9, 139.2, 136.1, 132.2, 130.6, 129.0, 128.2, 128.0, 124.7, 121.8, 38.1.; HRMS (ESI): *m/z* calcd for $C_{12}H_{13}N_2O_2S$ $[M+H]^+$: 249.0698, found: 249.0691.

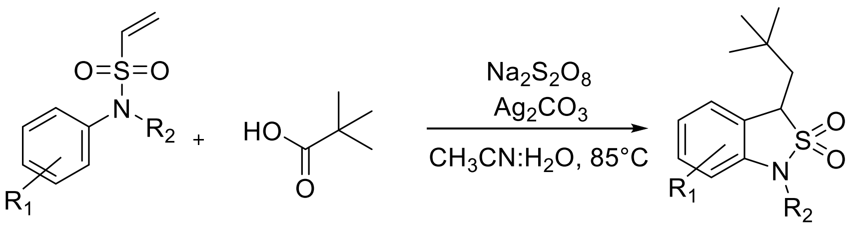
***N*-ethyl-*N*-phenylethenesulfonamide (1k)**:(Commercial available N-ethyl aniline is subjected to step-II) pale yellow oil (311 mg, 79% yield in step II); R_f = 0.5 (Hexane: Ethyl Acetate = 8:2).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.27 (m, 5H), 6.54 (dd, *J* = 16.6, 9.9 Hz, 1H), 6.15 (d, *J* = 16.6 Hz, 1H), 5.94 (d, *J* = 9.9 Hz, 1H), 3.65 (q, *J* = 7.1 Hz, 2H), 1.13 (t, *J* = 7.1 Hz, 3H); $^{13}C\{^{1}H\}$NMR (101 MHz, $CDCl_3$) δ 138.7, 134.1, 129.3, 129.0, 128.1, 127.3, 45.9, 14.4; HRMS (ESI): *m/z* calcd for $C_{10}H_{14}NO_2S[M+H]^+$: 212.0745, found: 212.0766.

4. Synthesis of benzo-fused-γ-sultams:

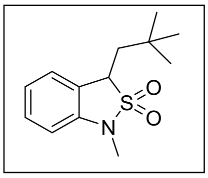
4.1. General procedure



N-phenyl Sulfonamide (0.253 mmol, 1 equiv.), Sodium per sulphate (1.27 mmol, 5 equiv.), and Silver carbonate (0.025 mmol, 0.1 equiv.) and pivalic acid (0.761 mmol, 3 equiv.) were taken in a reaction vial, and 3-mL of CH_3CN:H_2O (1:1) was added. The reaction mixture was stirred at 85°C (oil bath temperature) for 2h. After completion of the reaction (monitored by TLC), the reaction was quenched with cold water (5 mL) and extracted with ethyl acetate (10 mL X 3). The combined organic extracts were dried over Na_2SO_4, and the solvent was removed under reduced pressure. The crude reaction mixture was then purified by column chromatography on silica gel (100-200) using ethyl acetate and hexane as an eluent to afford the desired product.

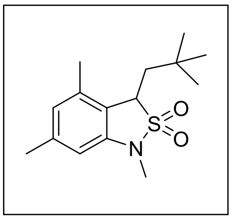
4.2. Characterization data

1-methyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3a): Brown oil (57 mg, 88% yield); R_f = 0.7 (Hexane: Ethyl acetate = 8:2).



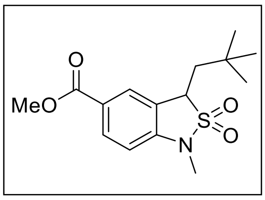
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.8 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.01 (td, *J* = 7.6, 0.9 Hz, 1H), 6.68 (d, *J* = 7.9 Hz, 1H), 4.30 – 4.14 (m, 1H), 3.13 (s, 3H), 2.38 (dd, *J* = 15.6, 7.6 Hz, 1H), 1.83 (dd, *J* = 15.6, 2.5 Hz, 1H), 1.12 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 141.0, 129.2, 124.3, 124.2, 121.8, 108.8, 57.9, 42.4, 30.5, 29.4, 26.8; HRMS (ESI): *m/z* calcd for $C_{17}H_{19}NO_2NaS$ $[M+Na]^+$: 276.1034, found: 276.1022.

1,4,6-trimethyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3b): White solid (56 mg, 91% yield); m.p: 102-104 °C; R_f = 0.6 (Hexane: Ethyl acetate = 8:2).



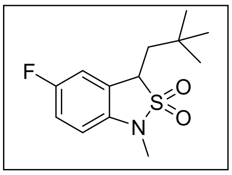
^{1}H NMR (300 MHz, $CDCl_3$) δ 6.64 (s, 1H), 6.35 (s, 1H), 4.16 (d, *J* = 9.1 Hz, 1H), 3.08 (s, 3H), 2.31 (s, 3H), 2.27 (s, 3H), 2.23 (d, *J* = 9.2 Hz, 1H), 1.53 (dd, *J* = 15.7, 0.6 Hz, 1H), 1.11 (s, 9H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 140.4, 139.2, 134.1, 124.8, 120.5, 107.5, 57.9, 43.4, 31.2, 29.6, 26.8, 21.6, 19.2; HRMS (ESI): *m/z* calcd for $C_{15}H_{24}NO_2S$ $[M+H]^+$: 282.1528, found: 282.1553.

Methyl 1-methyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole-5-carboxylate 2,2-dioxide (3c): white solid (42 mg, 69 % yield); m.p: 78-80 °C; R_f = 0.6 (Hexane: Ethyl Acetate = 8:2).



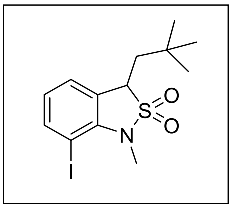
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 – 8.01 (m, 1H), 7.85 (s, 1H), 6.70 (d, *J* = 8.4 Hz, 1H), 4.25 (d, *J* = 8.1 Hz, 1H), 3.91 (s, 3H), 3.19 (s, 3H), 2.38 (dd, *J* = 15.6, 8.2 Hz, 1H), 1.91 (dd, *J* = 15.6, 2.1 Hz, 1H), 1.14 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.3, 144.5, 131.6, 125.8, 123.8, 123.6, 108.0, 57.8, 52.2, 42.5, 30.5, 29.4, 26.7; HRMS (ESI): *m/z* calcd for $C_{15}H_{14}NO_4S$ $[M+H]^+$: 312.1270, found: 312.1292.

5-fluoro-1-methyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3d): yellow Solid (50 mg, 79% yield; m.p: 85-87 °C; R_f = 0.8 (Hexane: Ethyl Acetate = 8:2).



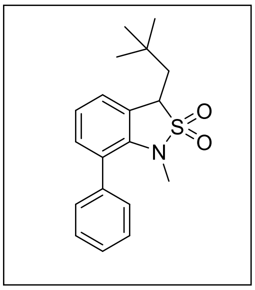
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 – 6.98 (m, 1H), 6.97 – 6.93 (m, 1H), 6.63 (dd, J = 8.7, 4.3 Hz, 1H), 4.22 – 4.16 (m, 1H), 3.12 (s, 3H), 2.38 (dd, *J* = 15.6, 7.5 Hz, 1H), 1.77 (dd, J = 15.6, 2.6 Hz, 1H), 1.12 (s, 9H); ^{13}C{^{1}H}NMR (126 MHz, $CDCl_3$) 158.1 (d, *J* = 241.2 Hz),137.2, 125.8 (d, *J* = 8.2 Hz), 115.7 (d, *J* = 23.1 Hz), 112.2 (d, *J* = 25.4 Hz), 109.9 (d, *J* = 8.0 Hz), 58.1, 42.3, 30.5, 29.4, 27.2; ^{19}F NMR (377 MHz, $CDCl_3$) δ -120.3; HRMS (ESI): *m/z* calcd for $C_{13}H_{19}NO_2FS$ $[M+H]^+$: 272.1121, found: 272.1113.

7-iodo-1-methyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3e): Yellow solid (44 mg, 74% yield); m.p: 83-85 °C; R_f = 0.8 (Hexane: Ethyl Acetate = 8:2).



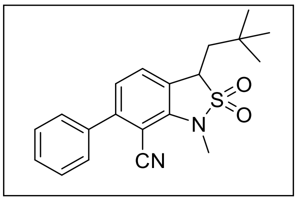
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 6.90 (t, *J* = 7.8 Hz, 1H), 4.20 (dd, *J* = 7.5, 2.4 Hz, 1H), 3.37 (s, 3H), 2.30 (dd, *J* = 15.3, 7.6 Hz, 1H), 1.70 (dd, *J* = 15.3, 2.6 Hz, 1H), 1.11 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 140.4, 132.3, 126.6, 124.7, 83.7, 59.3, 44.1, 37.5, 30.7, 29.4; HRMS (ESI): *m/z* calcd for $C_{13}H_{19}NO_2SI$ $[M+H]^+$: 380.0181 found: 380.0187.

1-methyl-3-neopentyl-7-phenyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3f): yellow solid (42 mg, 68% yield); m.p: 84- 85 °C; R_f = 0.6 (Hexane: Ethyl Acetate = 8:2).



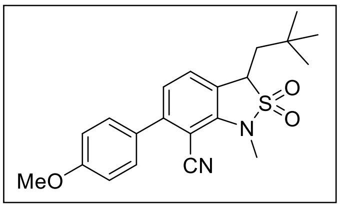
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 – 7.41 (m, 2H), 7.40 – 7.29 (m, 3H), 7.22 – 7.16 (m, 1H), 7.14 – 7.09 (m, 2H), 4.13 (dd, *J* = 7.7, 2.2 Hz, 1H), 2.62 (s, 3H), 2.29 (dd, *J* = 15.4, 7.7 Hz, 1H), 1.71 (dd, *J* = 15.4, 2.3 Hz, 1H), 1.06 (s, 9H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 139.6, 138.0, 131.3, 129.6, 129.5, 128.7, 128.6, 127.9, 124.1, 123.6, 58.3, 44.4, 35.0, 30.7, 29.4; HRMS (ESI): *m/z* calcd for $C_{19}H_{23}NO_2NaS$ $[M+Na]^+$: 352.1347, found: 352.1339.

1-methyl-3-neopentyl-6-phenyl-1,3-dihydrobenzo[*c*]isothiazole-7-carbonitrile 2,2-dioxide (3g): yellow solid (43 mg, 72% yield); m.p: 136-138 °C; R_f = 0.6 (Hexane: Ethyl Acetate = 8:2).



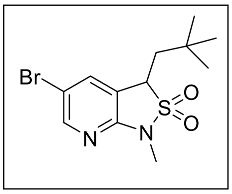
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (s, 5H), 7.38 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 4.19 (d, *J* = 7.2 Hz, 1H), 3.61 (s, 3H), 2.41 (dd, *J* = 15.5, 7.9 Hz, 1H), 1.80 (dd, *J* = 15.5, 2.2 Hz, 1H), 1.14 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.7, 143.6, 137.8, 129.1, 128.9, 128.7, 128.3, 125.2, 123.2, 116.2, 94.7, 56.7, 43.2, 30.7, 30.0, 29.4; HRMS (ESI): *m/z* calcd for $C_{20}H_{23}N_2O_2S$ $[M+H]^+$: 355.148, found: 355.1466.

6-(4-methoxyphenyl)-1-methyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole-7-carbonitrile 2,2-dioxide (3h): yellow solid (44mg, 75% yield); m.p: 188-190 °C; R_f = 0.5 (Hexane: Ethyl Acetate = 8:2).



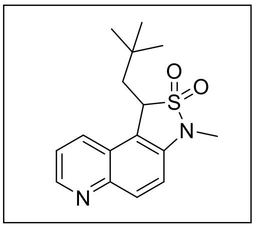
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.8 Hz, 2H), 7.37 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 7.03 (d, *J* = 8.8 Hz, 2H), 4.20 (d, *J* = 7.0 Hz, 1H), 3.89 (s, 3H), 3.63 (s, 3H), 2.42 (dd, *J* = 15.5, 7.9 Hz, 1H), 1.81 (dd, *J* = 15.5, 2.2 Hz, 1H), 1.16 (s, 9H); ^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$) δ 148.5, 144.6, 138.7, 130.0, 129.8, 129.6, 129.3, 126.4, 124.1, 117.1, 95.5, 55.9, 44.9, 43.0, 37.6, 33.2, 30.9; HRMS (ESI): *m/z* calcd for $C_{21}H_{25}N_2O_3S$ $[M+H]^+$: 385.1586, found: 385.1579.

5-bromo-1-methyl-3-neopentyl-1,3-dihydroisothiazolo[3,4-*b*]pyridine 2,2-dioxide (3i): pale-yellow solid (43 mg, 71% yield); m.p: 113-115 °C; R_f = 0.7 (Hexane: Ethyl Acetate = 8:2).



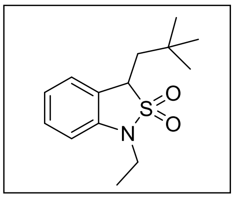
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.52 – 7.48 (m, 1H), 4.27 (d, *J* = 7.9 Hz, 1H), 3.24 (s, 3H), 2.41 (dd, *J* = 15.6, 7.9 Hz, 1H), 1.76 (dd, *J* = 15.6, 2.4 Hz, 1H), 1.12 (s, 9H); ^{13}C{^{1}H}NMR (126 MHz, $CDCl_3$) ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.1, 148.7, 134.6, 120.8, 112.1, 58.2, 42.4, 30.5, 29.3, 25.4; HRMS (ESI): *m/z* calcd for $C_{12}H_{18}N_2O_2SBr$ $[M+H]^+$: 333.0272, found: 333.0265.

3-methyl-1-neopentyl-1,3-dihydroisothiazolo[4,3-f]quinoline 2,2-dioxide (3j): yellow solid (38 mg, 63% yield); m.p: 170-172 °C; R_f = 0.2 (Hexane: Ethyl Acetate = 7:3).



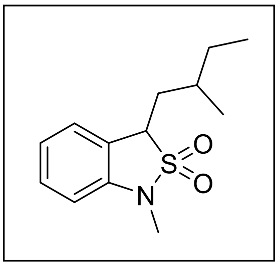
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.84 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.45 (dd, *J* = 8.6, 4.2 Hz, 1H), 7.24 (d, *J* = 4.5 Hz, 1H), 4.62 (d, *J* = 9.2 Hz, 1H), 3.27 (s, 3H), 2.36 (dd, *J* = 15.8, 9.3 Hz, 1H), 1.71 (d, *J* = 15.7 Hz, 1H), 1.22 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 148.4, 144.8, 138.5, 132.1, 129.9, 124.5, 122.3, 116.2, 113.8, 58.1, 44.0, 31.4, 29.7, 27.7; HRMS (ESI): *m/z* calcd for $C_{16}H_{21}N_2O_2S$ $[M+H]^+$: 305.1323, found: 305.0319.

1-ethyl-3-neopentyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3k): yellow solid (56 mg, 85% yield); m.p: 80-82 °C; R_f = 0.7 (Hexane: Ethyl Acetate = 8:2).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 6.99 (td, *J* = 7.6, 0.8 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 4.18 (d, *J* = 7.6 Hz, 1H), 3.70 (qd, *J* = 7.3, 3.6 Hz, 2H), 2.38 (dd, *J* = 15.5, 7.7 Hz, 1H), 1.80 (dd, *J* = 15.5, 2.3 Hz, 1H), 1.39 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 9H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 139.8, 129.1, 124.5, 124.3, 121.4, 108.8, 58.3, 42.8, 36.6, 30.5, 29.4, 13.4; HRMS (ESI): *m/z* calcd for $C_{14}H_{21}NO_2NaS$ $[M+H]^+$: 290.1191, found: 290.1175.

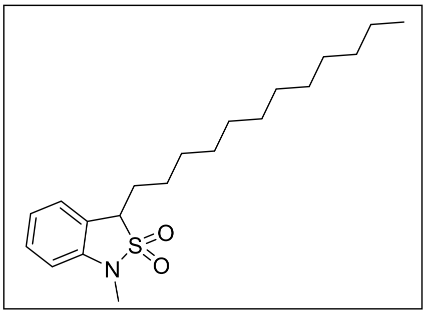
1-methyl-3-(2-methylbutyl)-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3l): yellow oil (55 mg, 86% yield); R_f = 0.7 (Hexane: Ethyl Acetate = 8:2). (Mixture of diastereomers)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 8.3 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.71 (dd, *J* = 7.9, 4.3 Hz, 1H), 4.31 (dd, *J* = 10.0, 4.9 Hz, 1H), 3.12 (s, 3H), 2.23 – 2.14 (m, 1H), 1.89 – 1.80 (m, 1H), 1.77 – 1.69 (m, 1H), 1.56 – 1.45 (m, 1H), 1.36 – 1.24 (m, 1H), 1.07 (d, *J* = 2.8 Hz, 3H), 0.99 – 0.90 (m, 3H); $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 141.0, 129.3, 124.7, 123.4, 121.8, 109.1, 58.6, 36.2, 31.8, 29.8, 26.5, 19.1, 11.1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 8.3 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.71 (dd, *J* = 7.9, 4.3 Hz, 1H), 4.26 (t, *J* = 7.1 Hz, 1H), 3.12 (s, 3H), 2.05 – 1.97 (m, 1H), 1.89 – 1.80 (m, 1H), 1.56 – 1.45 (m, 1H), 1.36 – 1.24 (m, 2H), 1.06 (d, *J* = 2.6 Hz, 3H), 0.99 – 0.90 (m, 3H); $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 140.9, 129.2, 124.3, 123.4, 121.8, 109.0, 58.6, 35.9, 31.5, 28.8, 26.4, 18.7, 11.0; HRMS (ESI): m/z calcd for $C_{13}H_{19}NO_2NaS$ [M+Na]+: 276.1034, found: 276.1022.

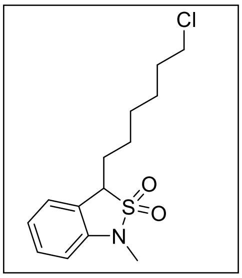
3-dodecyl-1-methyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3m): yellow liquid (67 mg, 75% yield); R_f = 0.6 (Hexane: Ethyl Acetate = 8:2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.00 (dd, *J* =



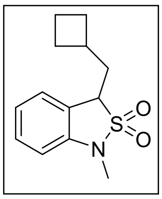
11.0, 4.2 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 4.17 (dd, *J* = 8.4, 6.0 Hz, 1H), 3.12 (s, 3H), 2.17 – 2.06 (m, 1H), 2.02 – 1.92 (m, 1H), 1.73 – 1.60 (m, 3H), 1.45 – 1.37 (m, 3H), 1.35 – 1.21 (m, 14H), 0.88 (t, *J* = 6.8 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 140.9, 129.3, 124.6, 123.1, 121.8, 109.0, 60.7, 31.8, 29.7, 29.4, 29.3, 29.2, 29.2, 26.6, 26.5, 22.7, 14.1.; HRMS (ESI): m/z calcd for $C_{20}H_{34}NO_2S$ [M+H]+: 352.2310, found: 352.2304.

3-(6-chlorohexyl)-1-methyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3n): yellow oil(56 mg, 74% yield); R_f = 0.8 (Hexane: Ethyl Acetate = 8:2).



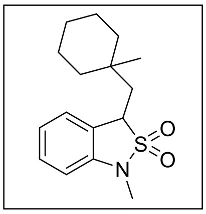
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (t, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.1 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 4.17 (dd, *J* = 8.7, 5.6 Hz, 1H), 3.54 (t, *J* = 6.7 Hz, 2H), 3.12 (s, 3H), 2.17 – 2.07 (m, 1H), 2.05 – 1.96 (m, 1H), 1.83 – 1.76 (m, 2H), 1.73 – 1.65 (m, 2H), 1.54 – 1.43 (m, 4H); $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 140.9, 129.4, 124., 122.9, 121.8, 109.1, 60.7, 45.0, 32.4, 29.2, 28.7, 26.6, 26.5, 26.4; HRMS (ESI): *m/z* calcd for $C_{14}H_{20}ClNO_2NaS$ $[M+Na]^+$: 324.0801, found: 324.0792.

3-(cyclobutylmethyl)-1-methyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3o): yellow oil (46 mg, 73% yield); R_f = 0.7 (Hexane: Ethyl Acetate = 8:2).



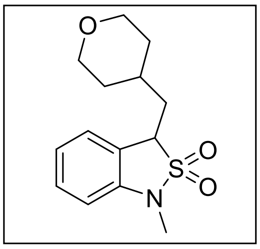
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 7.9 Hz, 1H), 4.13 – 4.04 (m, 1H), 3.11 (s, 3H), 2.70 (m, 1H), 2.30 – 2.11 (m, 3H), 2.08 – 1.81 (m, 3H), 1.74 (dd, *J* = 18.2, 9.1 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 141.0, 129.3, 124.6, 123.0, 121.7, 109.1, 58.9, 36.0, 32.9, 28.3, 28.1, 26.4, 18.2; HRMS (ESI): *m/z* calcd for $C_{13}H_{17}NO_2NaS$ $[M+Na]^+$: 274.0878, found: 274.0865.

1-methyl-3-((1-methylcyclohexyl)methyl)-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3p): yellow oil(62 mg, 83% yield); R_f = 0.7 (Hexane: Ethyl Acetate = 8:2).



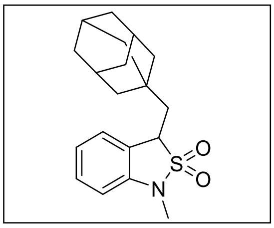
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.8 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 7.9 Hz, 1H), 4.24 (dd, *J* = 6.3, 1.0 Hz, 1H), 3.13 (s, 3H), 2.41 (dd, *J* = 15.7, 7.4 Hz, 1H), 1.84 (dd, *J* = 15.7, 2.5 Hz, 1H), 1.61 – 1.49 (m, 6H), 1.48 – 1.40 (m, 4H), 1.10 (s, 3H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 141.0, 129.2, 124.4, 124.3, 121.8, 108.8, 57.1, 41.4, 37.8, 37.4, 32.8, 26.8, 26.2, 24.4, 22.0, 21.9; HRMS (ESI): *m/z* calcd for $C_{16}H_{23}NO_2NaS$ $[M+Na]^+$: 316.1347, found: 316.1379.

1-methyl-3-((tetrahydro-2H-pyran-4-yl)methyl)-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3q): White Solid (59 mg, 82% yield); m.p: 112-114 °C; R_f = 0.6 (Hexane: Ethyl Acetate = 8:2).



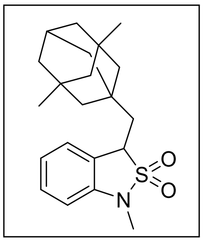
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (t, *J* = 7.8 Hz, 1H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.9 Hz, 1H), 4.32 (dd, *J* = 9.6, 5.2 Hz, 1H), 4.05 – 3.97 (m, 2H), 3.46 (td, *J* = 11.9, 2.2 Hz, 2H), 3.13 (s, 3H), 2.19 – 2.08 (m, 1H), 2.07 – 1.95 (m, 1H), 1.92 – 1.82 (m, 2H), 1.76 (ddd, *J* = 13.2, 3.6, 2.0 Hz, 1H), 1.50 – 1.32 (m, 2H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 141.0, 129.4, 124.3, 122.9, 121.9, 109.1, 67.7, 57.4, 36.11, 33.3, 32.3, 32.2, 26.5; HRMS (ESI): m/z calcd for $C_{14}H_{19}NO_3NaS$ [M+Na]+: 304.0983, found: 304.0979.

3-(adamantan-1-ylmethyl)-1-methyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3r): yellow solid (68 mg, 81% yield); m.p: 130-132 °C; R_f = 0.3 (hexanes: Ethyl Acetate = 8:2).



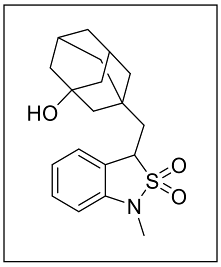
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 7.9 Hz, 1H), 4.28 (d, *J* = 7.2 Hz, 1H), 3.13 (s, 3H), 2.26 (dd, *J* = 15.7, 7.4 Hz, 1H), 2.11 – 2.04 (m, 3H), 1.83 – 1.76 (m, 2H), 1.75 – 1.64 (m, 11H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 141.0, 129.1, 124.5, 124.4, 121.8, 108.7, 56.1, 43.1, 42.1, 38.3, 36.8, 36.6, 32.1, 28.5, 28.0, 26.8; HRMS (ESI): *m/z* calcd for $C_{19}H_{26}NO_2S$ $[M+H]^+$: 332.1684, found: 332.1697.

3-((3,5-dimethyladamantan-1-yl)methyl)-1-methyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3s): White solid (82 mg, 90% yield); m.p: 93-95 °C; R_f = 0.4 (Hexane: Ethyl Acetate = 8:2).



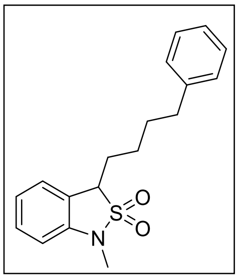
[1]H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 7.9 Hz, 1H), 4.27 (d, *J* = 6.4 Hz, 1H), 3.13 (s, 3H), 2.29 (dd, *J* = 15.7, 7.5 Hz, 1H), 2.14 (m, 1H), 1.70 (dd, *J* = 15.7, 2.5 Hz, 1H), 1.51 (s, 2H), 1.36 (s, 4H), 1.34 – 1.29 (m, 2H), 1.25 (dd, *J* = 12.2, 4.0 Hz, 2H), 1.16 (q, *J* = 12.4 Hz, 2H), 0.86 (s, 6H); $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 141.0, 129.1, 124.5, 124.4, 121.8, 108.7, 56.2, 51.0, 48.6, 48.3, 43.0, 42.5, 40.7, 33.9, 31.3, 30.6, 29.6, 26.8; HRMS (ESI): *m/z* calcd for $C_{21}H_{30}NO_2S$ $[M+H]^+$: 360.1997, found: 360.2009.

3-((3-hydroxyadamantan-1-yl)methyl)-1-methyl-1,3-dihydrobenzo[*c*]isothiazole 2,2-dioxide (3t): White solid (75 mg, 85% yield); m.p: 138-140 °C; R_f = 0.3 (Hexane: Ethyl Acetate = 8:2).



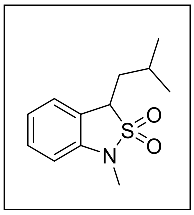
[1]H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.6, Hz, 1H), 6.68 (d, *J* = 7.9 Hz, 1H), 4.26 (d, *J* = 7.6 Hz, 1H), 3.13 (s, 3H), 2.38 – 2.27 (m, 3H), 1.77 (dd, *J* = 15.7, 2.4 Hz, 1H), 1.73 – 1.66 (m, 4H), 1.65 – 1.58 (m, 8H); $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 141.0, 129.3, 124.3, 124.0, 121.9, 108.8, 68.8, 56.3, 49.8, 44.5, 44.5, 42.2, 41.0, 40.5, 35.8, 35.2, 30.6, 30.5, 26.8; HRMS (ESI): *m/z* calcd for $C_{19}H_{25}NO_3NaS$ $[M+Na]^+$: 370.1453, found: 370.1432.

1-methyl-3-(4-phenylbutyl)-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide (3u): Yellow oil (57 mg, 72% yield); R_f = 0.8 (Hexane: Ethyl Acetate = 8:2).



[1]H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.26 (m, 3H), 7.21 – 7.17 (m, 3H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.01 – 6.97 (m, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 4.15 (dd, *J* = 8.6, 5.8 Hz, 1H), 3.12 (s, 3H), 2.66 (t, *J* = 7.2 Hz, 2H), 2.19 – 2.11 (m, 1H), 2.04 – 1.96 (m, 1H), 1.77 – 1.70 (m, 4H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 142.1, 140.9, 129.4, 128.4, 128.4, 125.9, 124.6, 122.9, 121.8, 109.1, 60.6, 35.6, 31.2, 29.3, 26.5, 26.2; HRMS (ESI): *m/z* calcd for $C_{18}H_{21}NO_2NaS$ $[M+Na]^+$: 338.1191, found: 338.1155.

3-isobutyl-1-methyl-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide (3v): Yellow oil (47 mg, 78% yield); R_f = 0.8 (Hexane: Ethyl Acetate = 8:2).



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 4.35 – 4.14 (m, 1H), 3.12 (s, 3H), 2.14 – 2.02 (m, 2H), 1.83 – 1.69 (m, 1H), 1.08 (d, *J* = 6.2 Hz, 6H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 140.9, 129.3, 124.5, 123.3, 121.8, 109.1, 58.7, 38.0, 26.5, 25.5, 22.8, 22.0; HRMS (ESI): *m/z* calcd for $C_{12}H_{17}NO_2NaS$ $[M+Na]^+$: 262.0878, found: 262.0848.

5. Crystal structure details

X-ray data for the compound was collected on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-III detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs.[2] The structure was solved using intrinsic phasing method and further refined with the SHELXL program and expanded using Fourier techniques.[3] Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and Uiso(H) = 1.5Ueq(C) for methyl H or 1.2Ueq(C) for other H atoms]. The carbon atoms C15, C16, C17, C18, and C19 are disordered over two positions, the major and minor occupancy factors were refined to 0.595 (5) and 0.405 (5) respectively.

Compound 3f:

Crystal of compound **3f** was developed in DCM, and X-ray data was collected at low temperature.

Crystal Data for $C_{19}H_{23}NO_2S$ (M =329.44 g/mol): monoclinic, space group P21/c (no.14), a =13.6647(4) Å, b =17.8621(5) Å, c = 7.4013(2) Å, β = 97.8140(10)°, V = 1789.74(9) Å 3 , Z = 4, T = 100.15 K, μ(MoKα) = 0.190 mm -1 , Dcalc = 1.223 g/cm^3, 14932 reflections measured (4.56° ≤ 2θ ≤ 52.666°), 3606 unique (Rint = 0.0644, Rsigma = 0.0719) which were used in all calculations. The final R1 was 0.0771 (I & gt; 2σ(I)) and wR 2 was 0.1943.

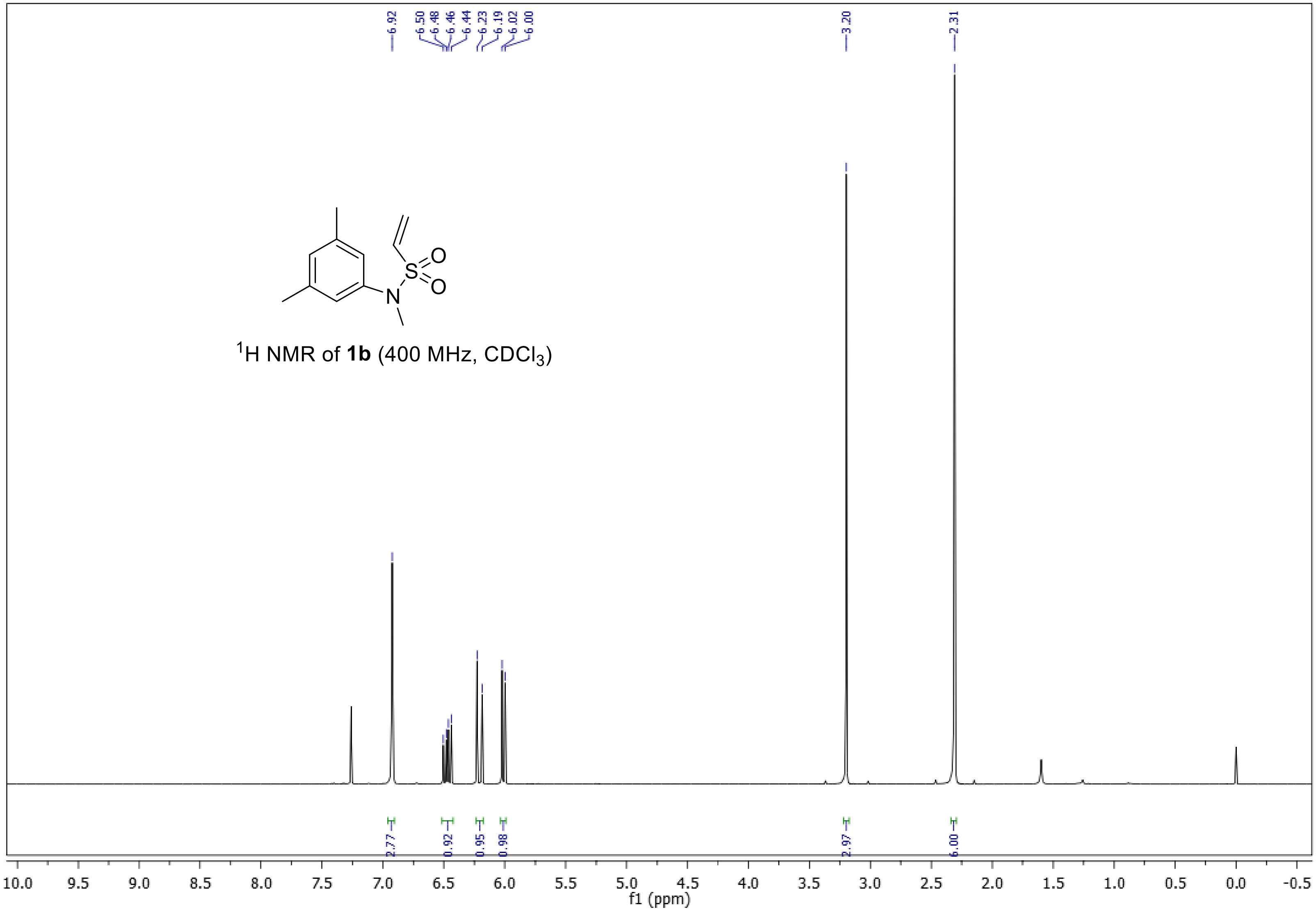
Compound 3g:

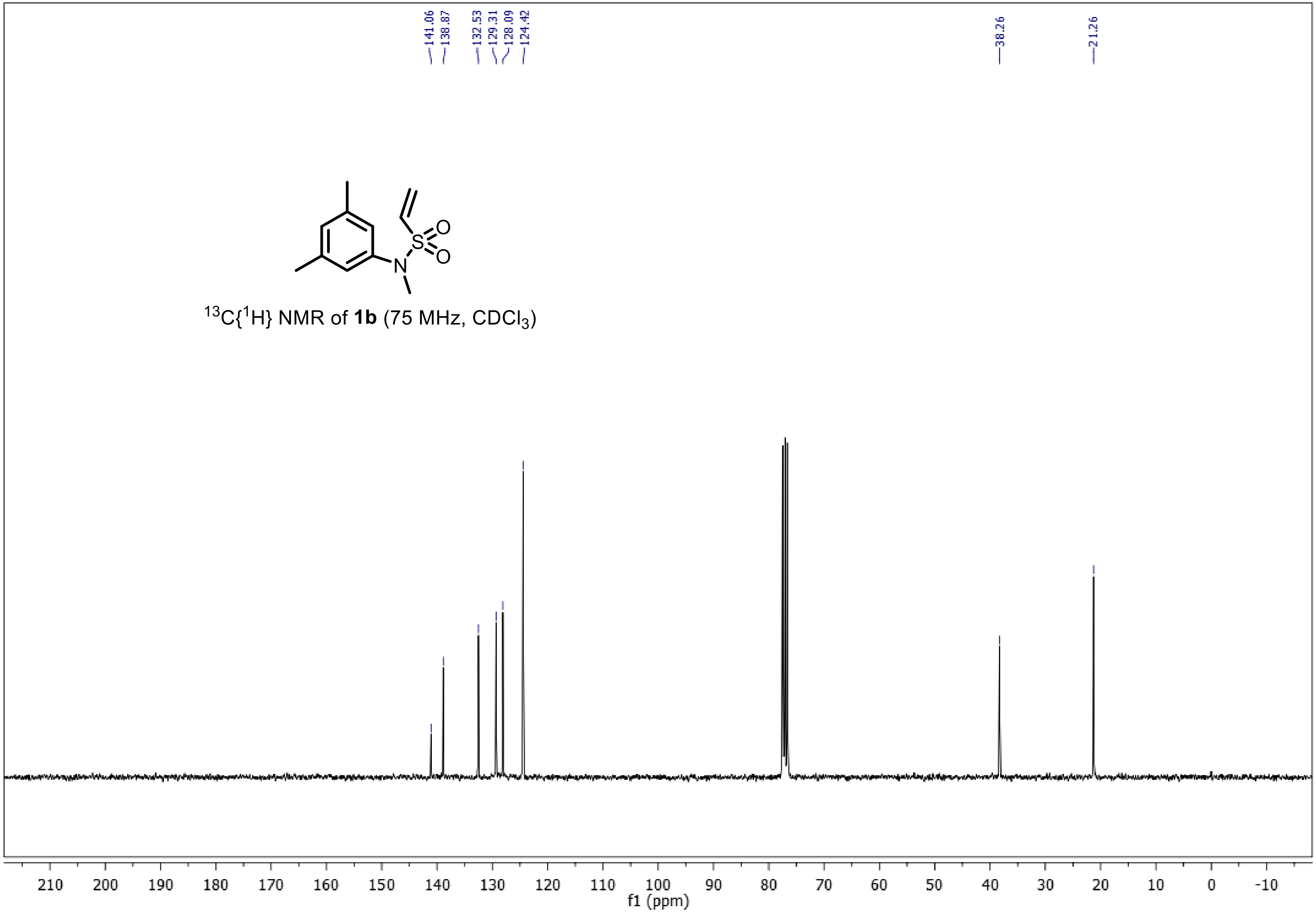
Crystal of compound **3g** was developed in Chloroform, and X-ray data was collected at room temperature.

Crystal Data for $C_{20}H_{22}N_2O_2S$ (M =354.45 g/mol): orthorhombic, space group Pbca (no. 61), a = 14.3600(4) Å, b = 9.5280(3) Å, c = 28.4766(8) Å, V = 3896.2(2) Å 3, Z = 8, T =

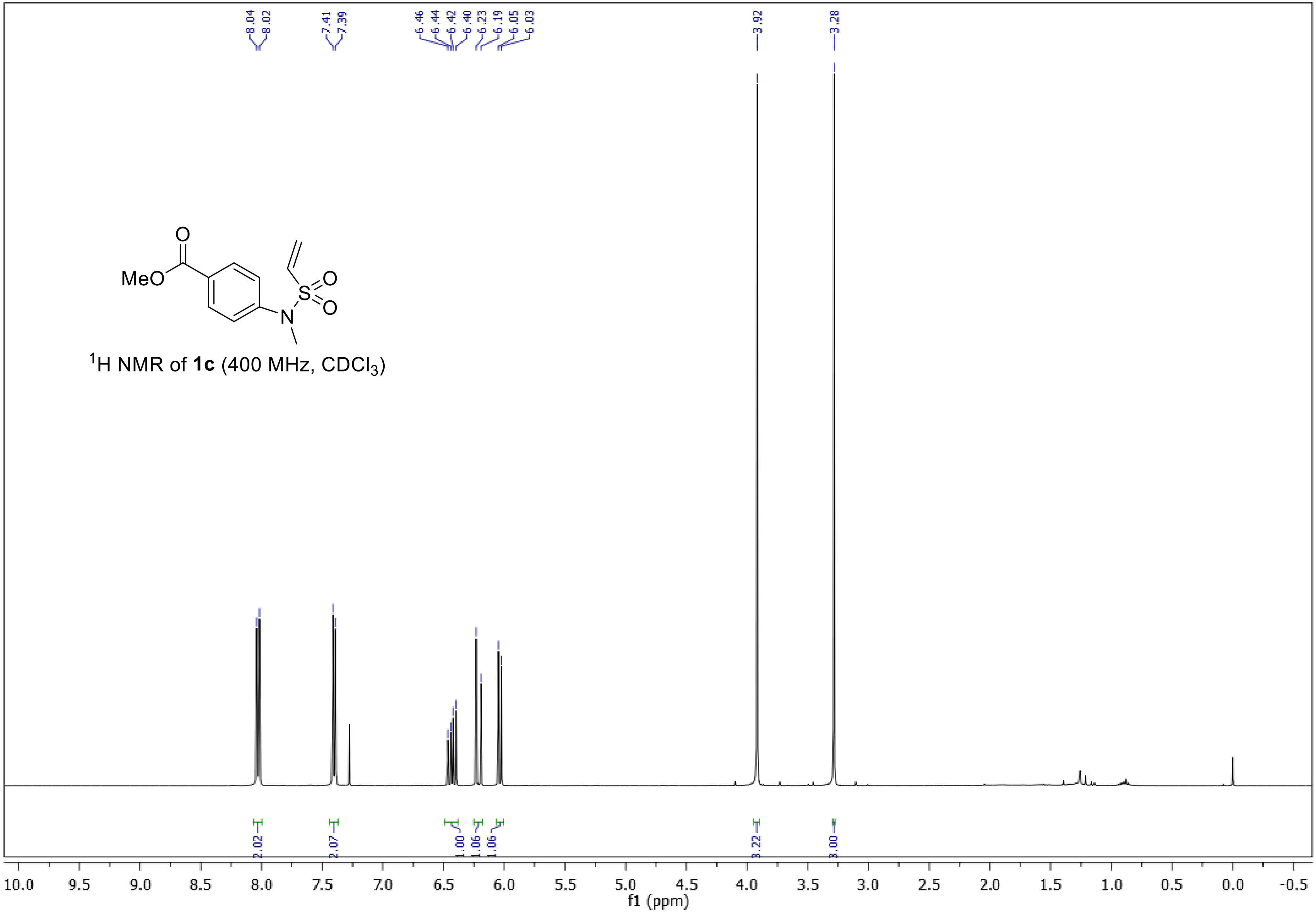
294.15 K, μ(MoKα) = 0.181 mm^{-1} , Dcalc = 1.209 g/cm^3, 28438 reflections measured (5.326° ≤ 2Θ ≤ 56.676°), 4854 unique (Rint = 0.0532, Rsigma = 0.0479) which were used in all calculations. The final R1 was 0.0689 (I & gt; 2σ(I)) and wR2 was 0.2536.

5. Copies of NMR spectra

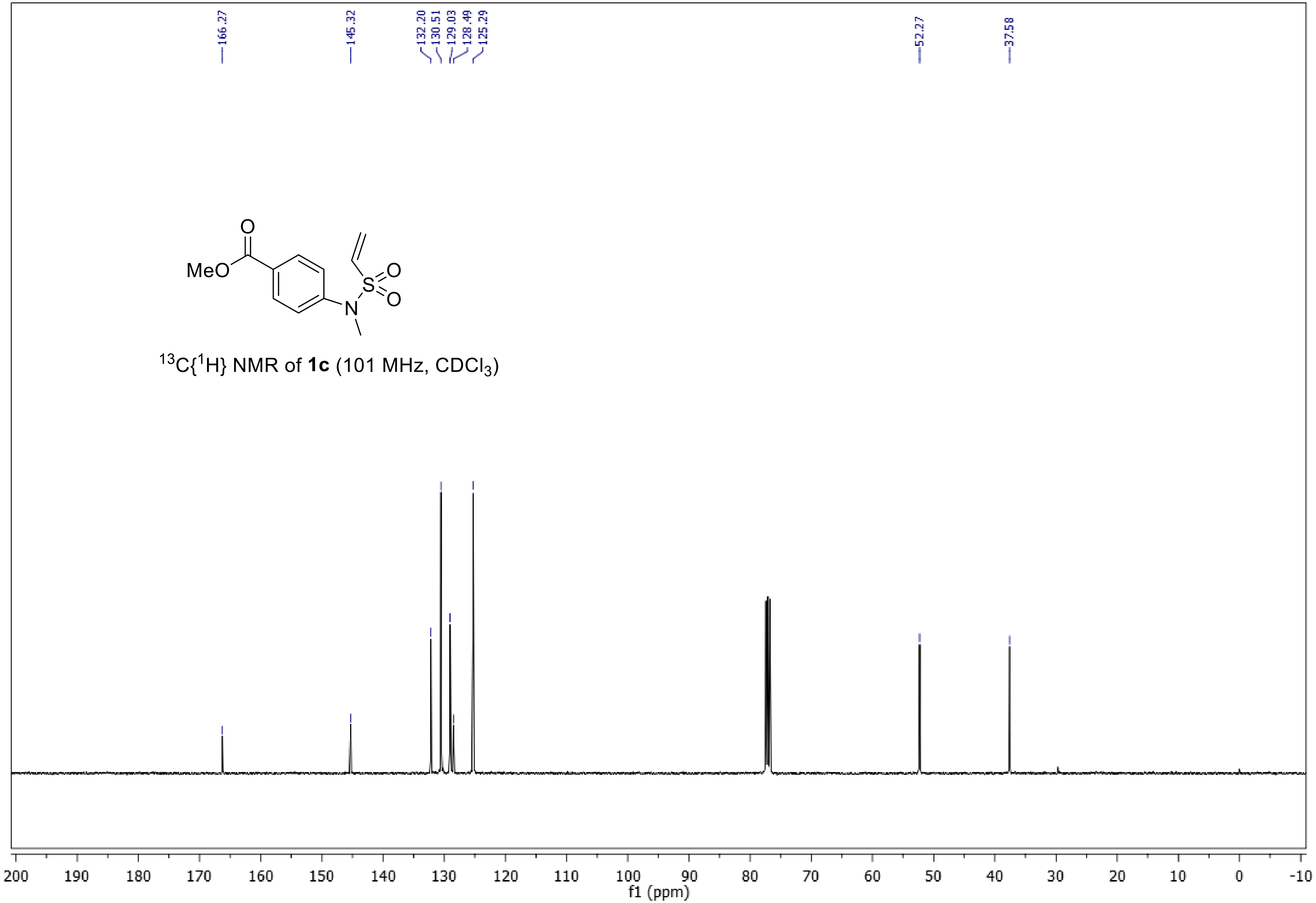




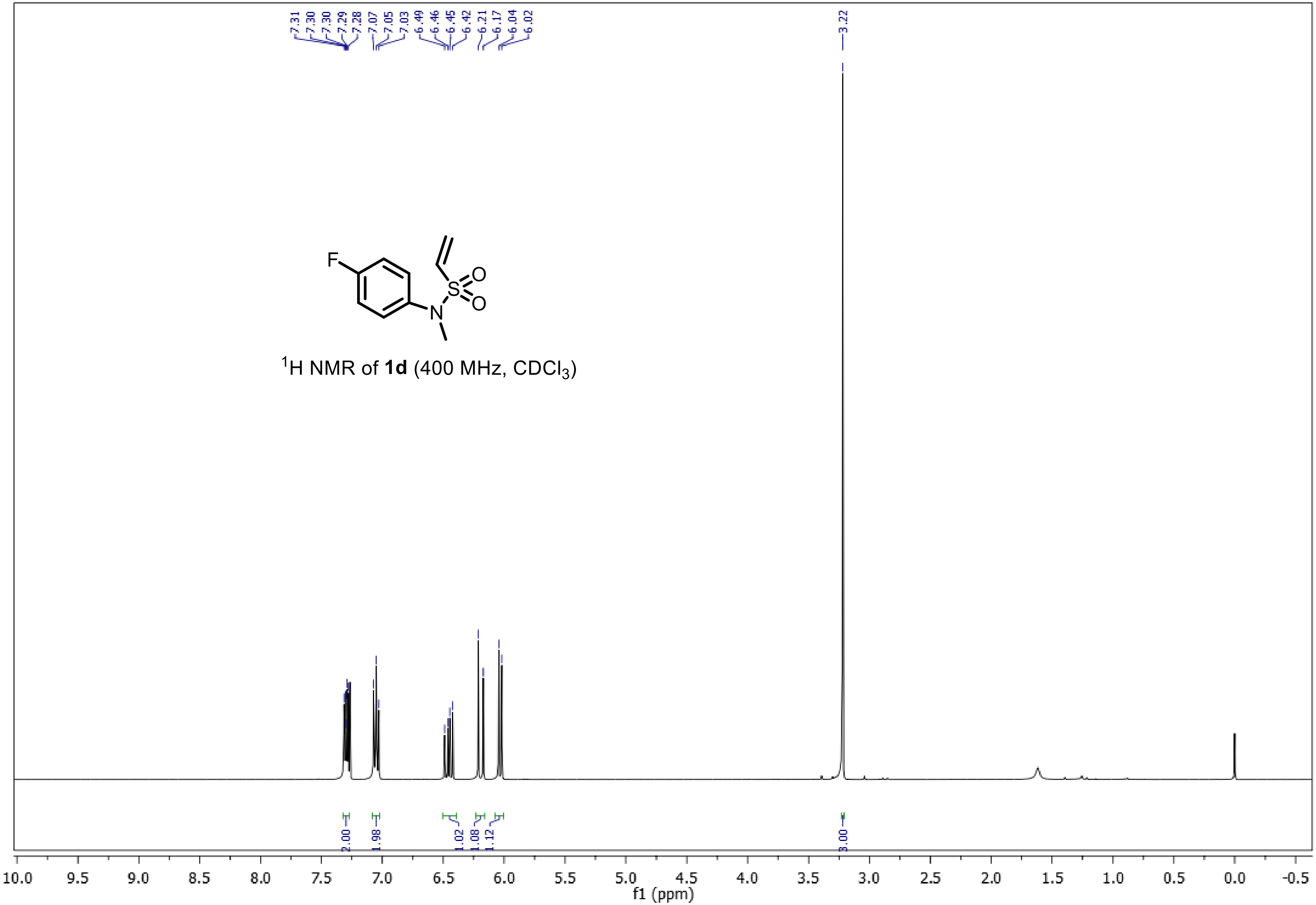
$^{13}C\{^{1}H\}$ NMR of **1b** (75 MHz, $CDCl_3$)

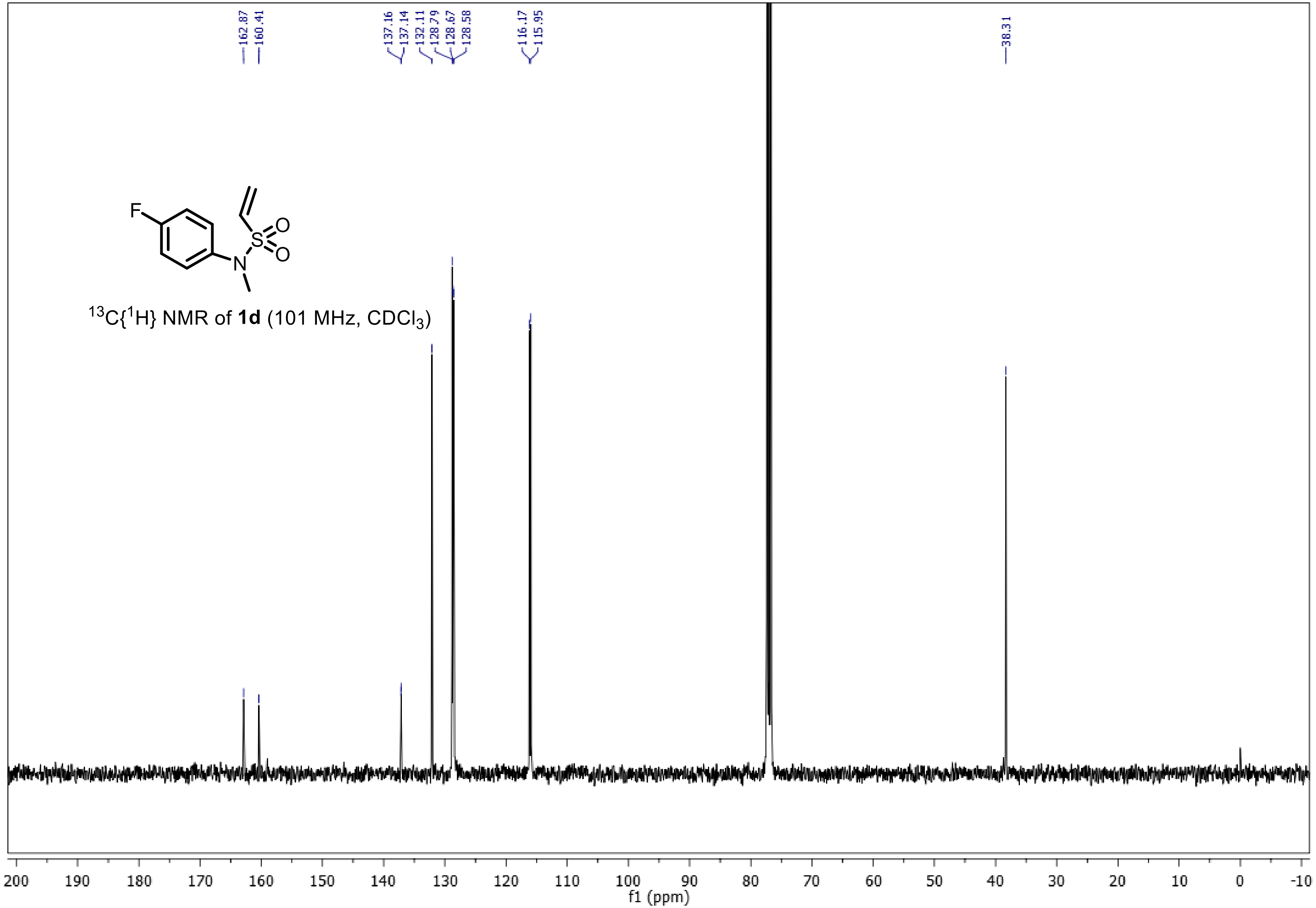


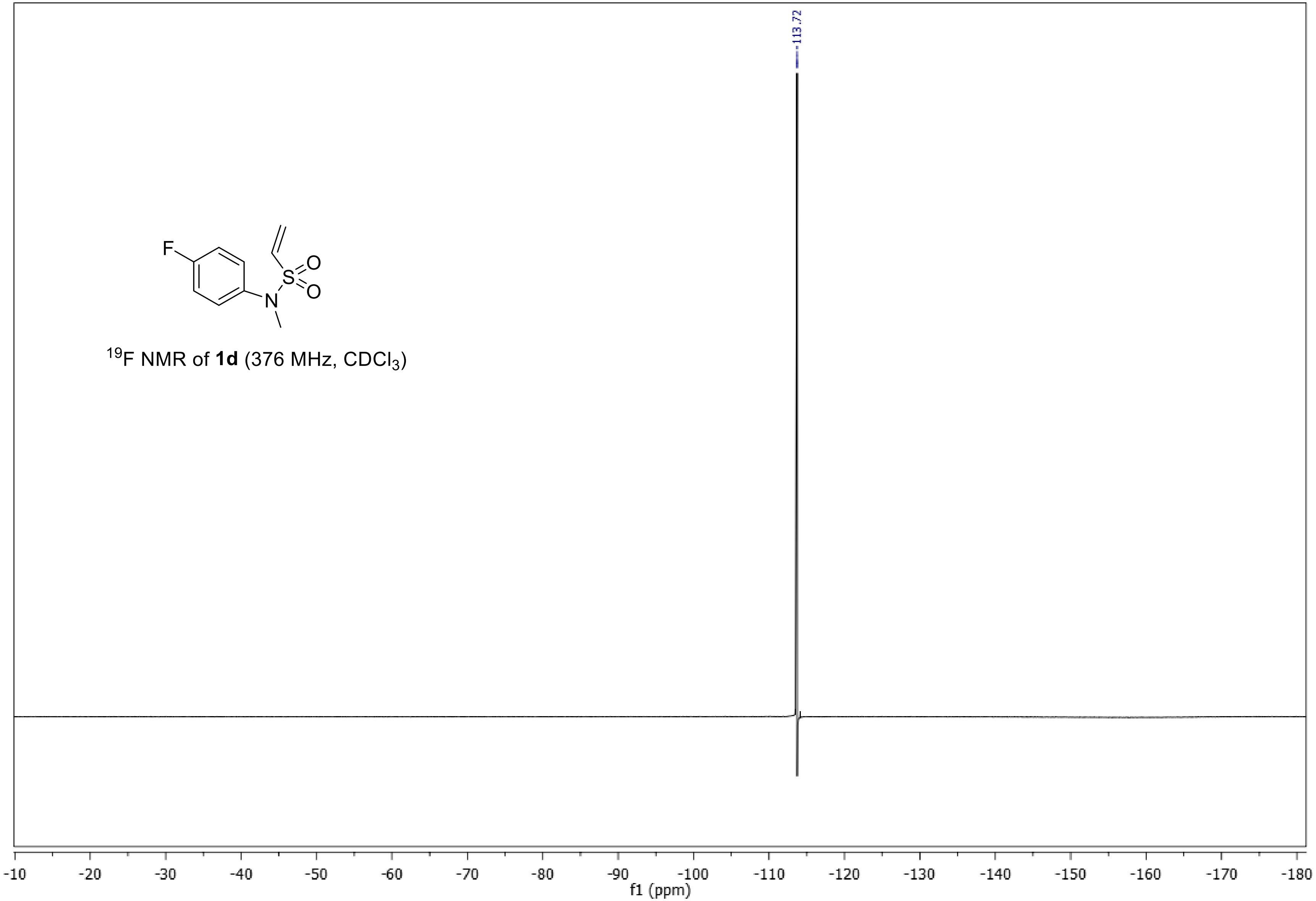
[1]H NMR of **1c** (400 MHz, $CDCl_3$)



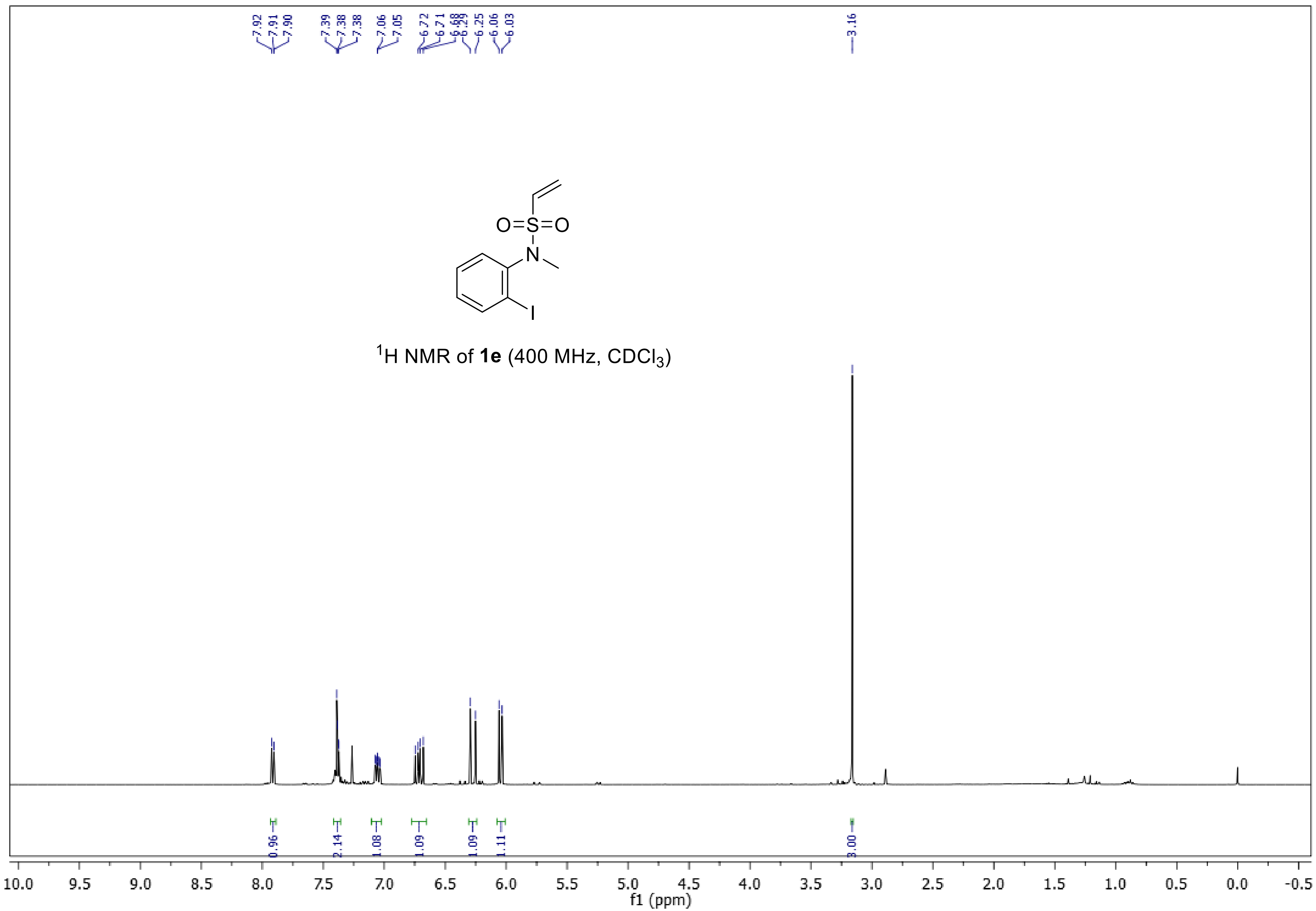
$^{13}C\{^{1}H\}$ NMR of **1c** (101 MHz, $CDCl_3$)


7.31
7.30
7.30
7.29
7.28
7.07
7.05
7.03
6.49
6.46
6.45
6.42
6.21
6.17
6.04
6.02
3.22
F
S
O
O
N
^{1}H NMR of **1d** (400 MHz, $CDCl_3$)
2.00
1.98
1.02
1.08
1.12
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

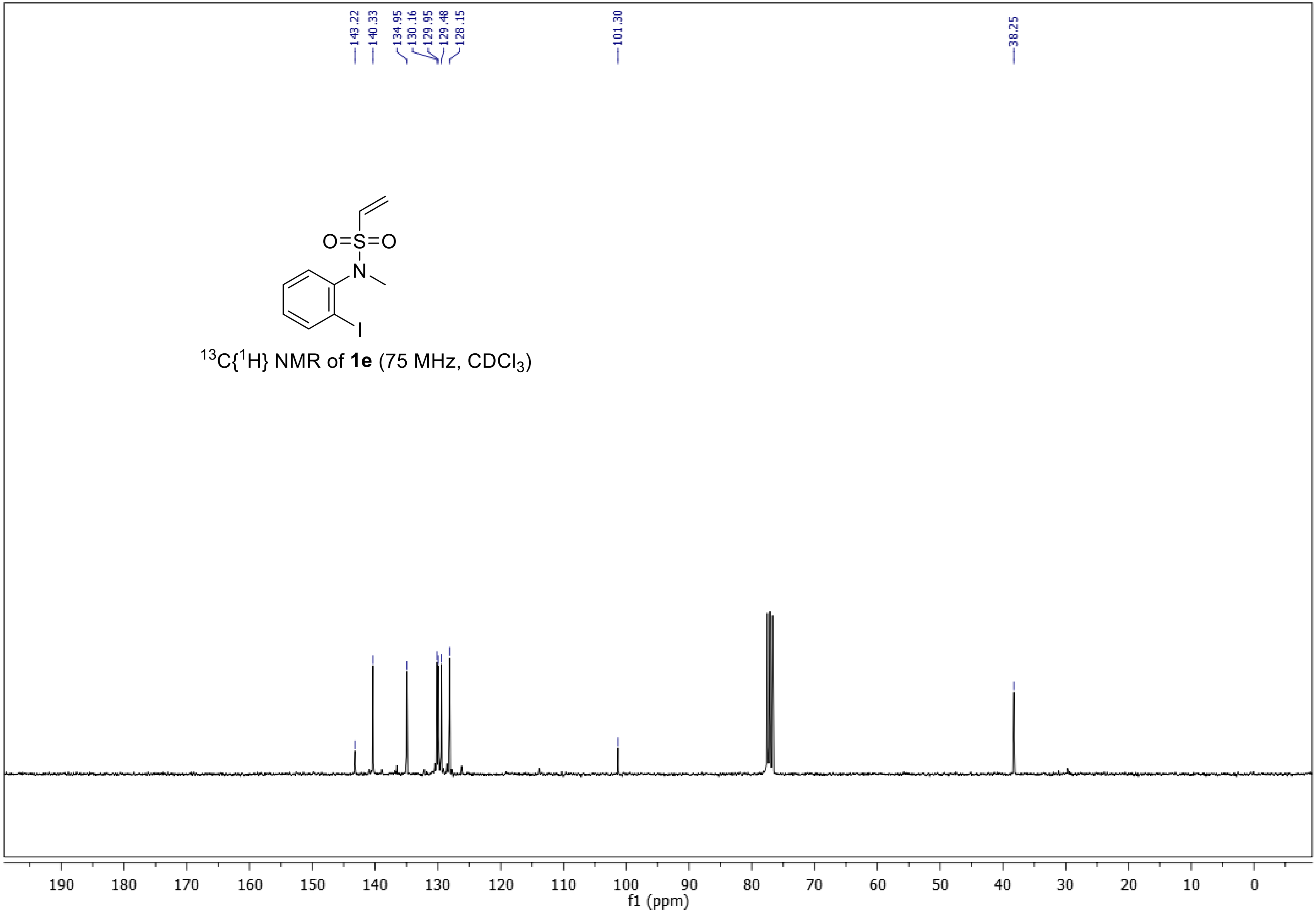

162.87
160.41
137.16
137.14
132.11
128.79
128.67
128.58
116.17
115.95
38.31
F
S
O
O
N
$^{13}C\{^1H\}$ NMR of **1d** (101 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



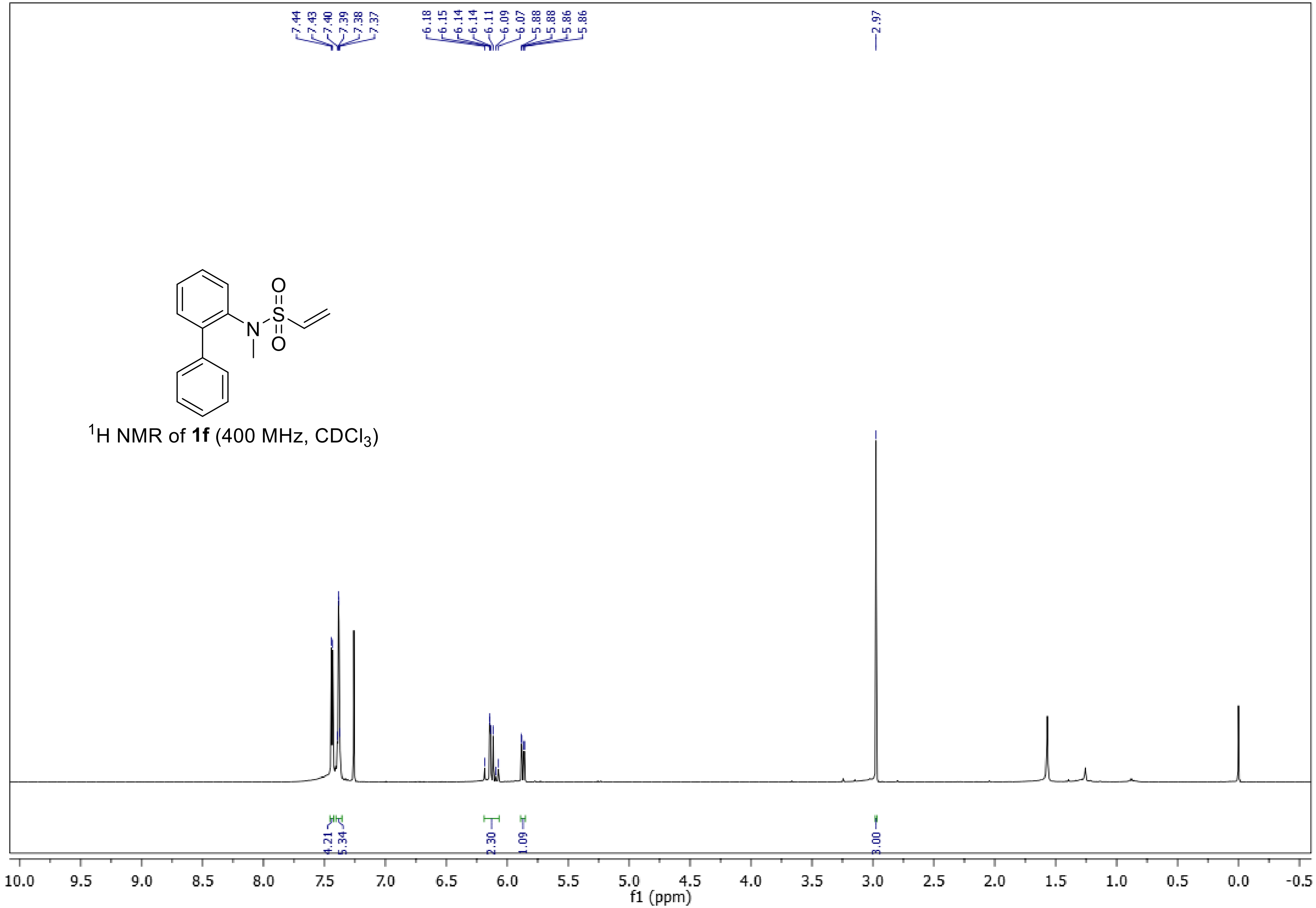
^{19}F NMR of **1d** (376 MHz, $CDCl_3$)



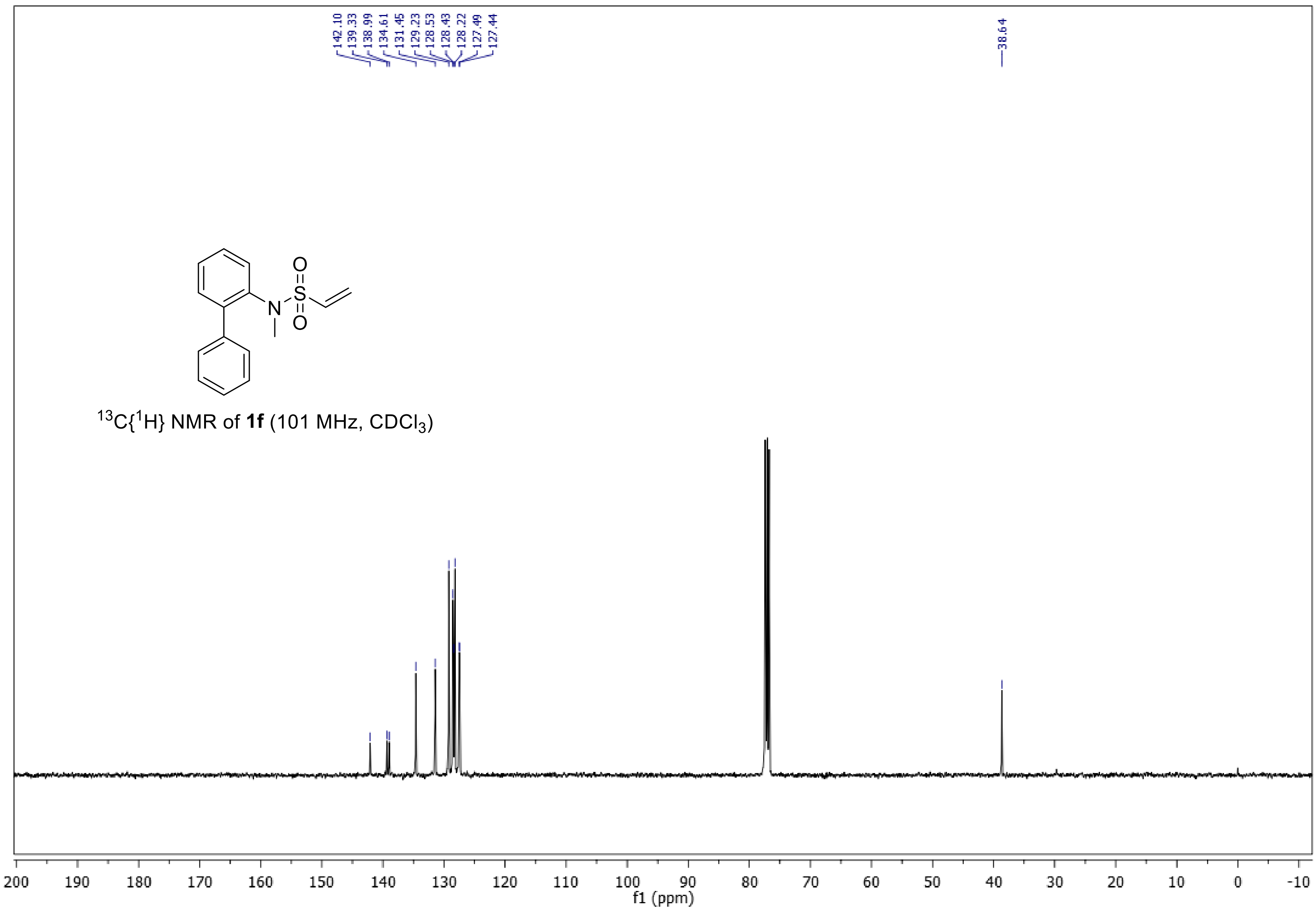
^{1}H NMR of **1e** (400 MHz, $CDCl_3$)



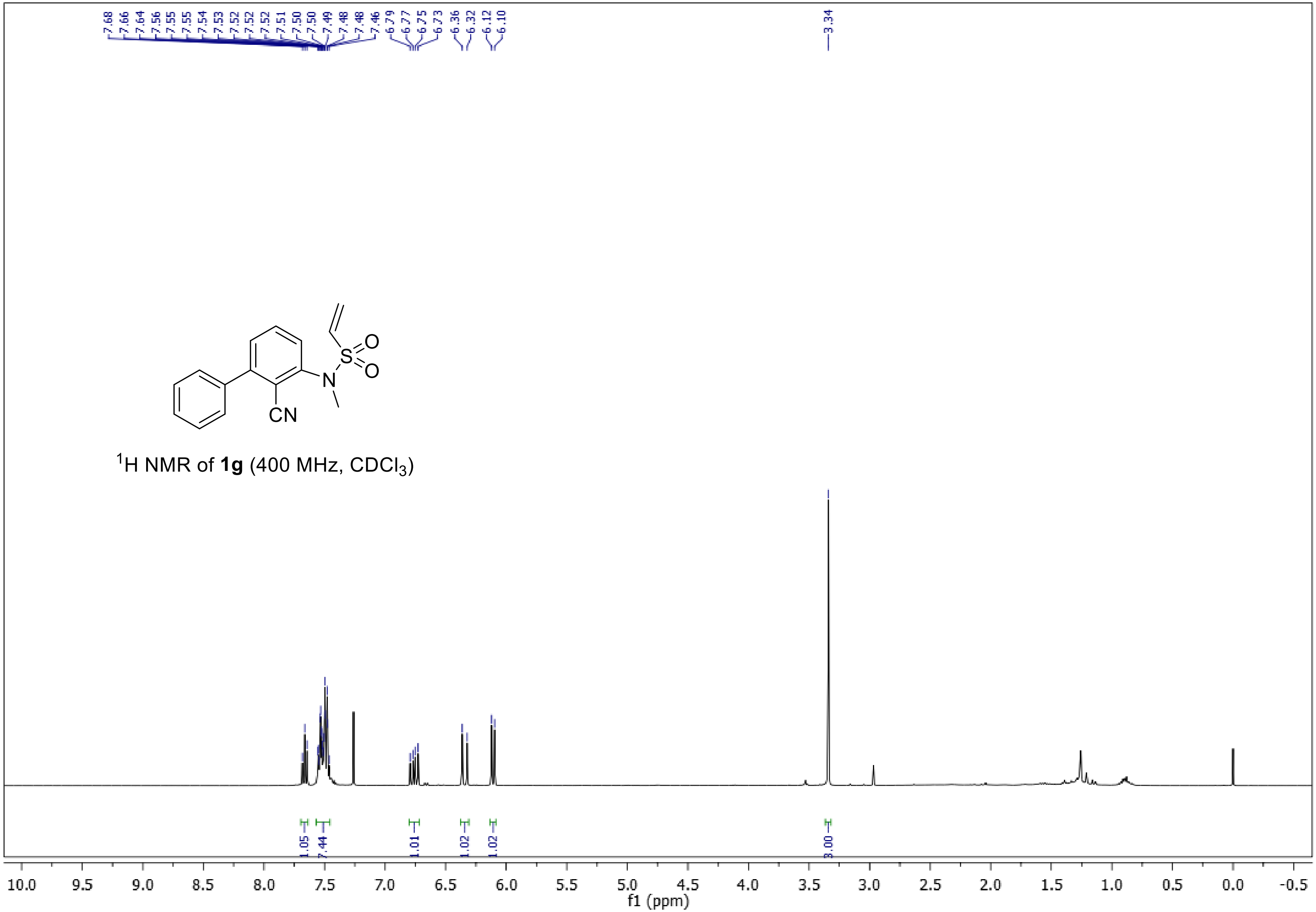
$^{13}C\{^1H\}$ NMR of **1e** (75 MHz, $CDCl_3$)



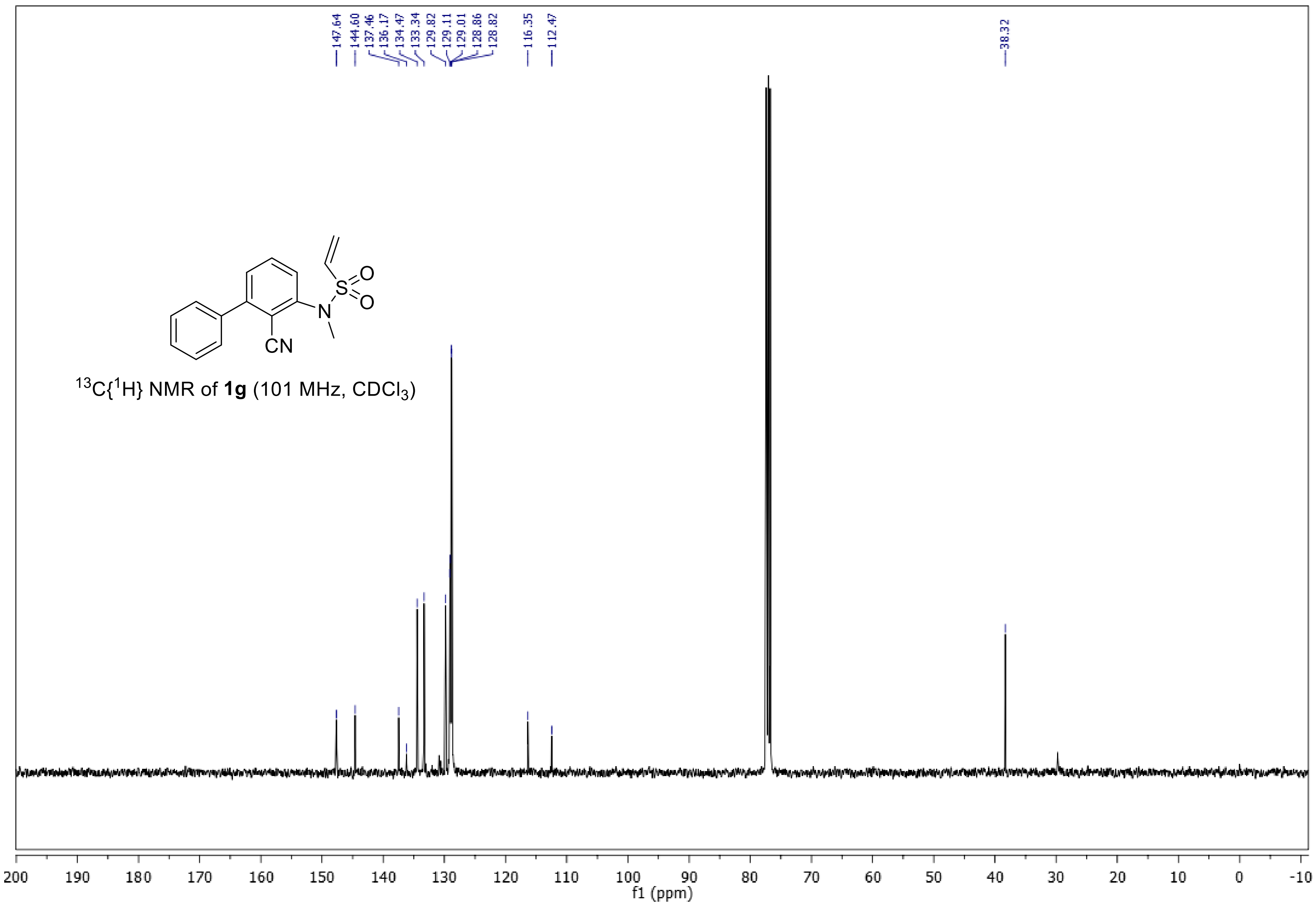
^{1}H NMR of **1f** (400 MHz, $CDCl_3$)



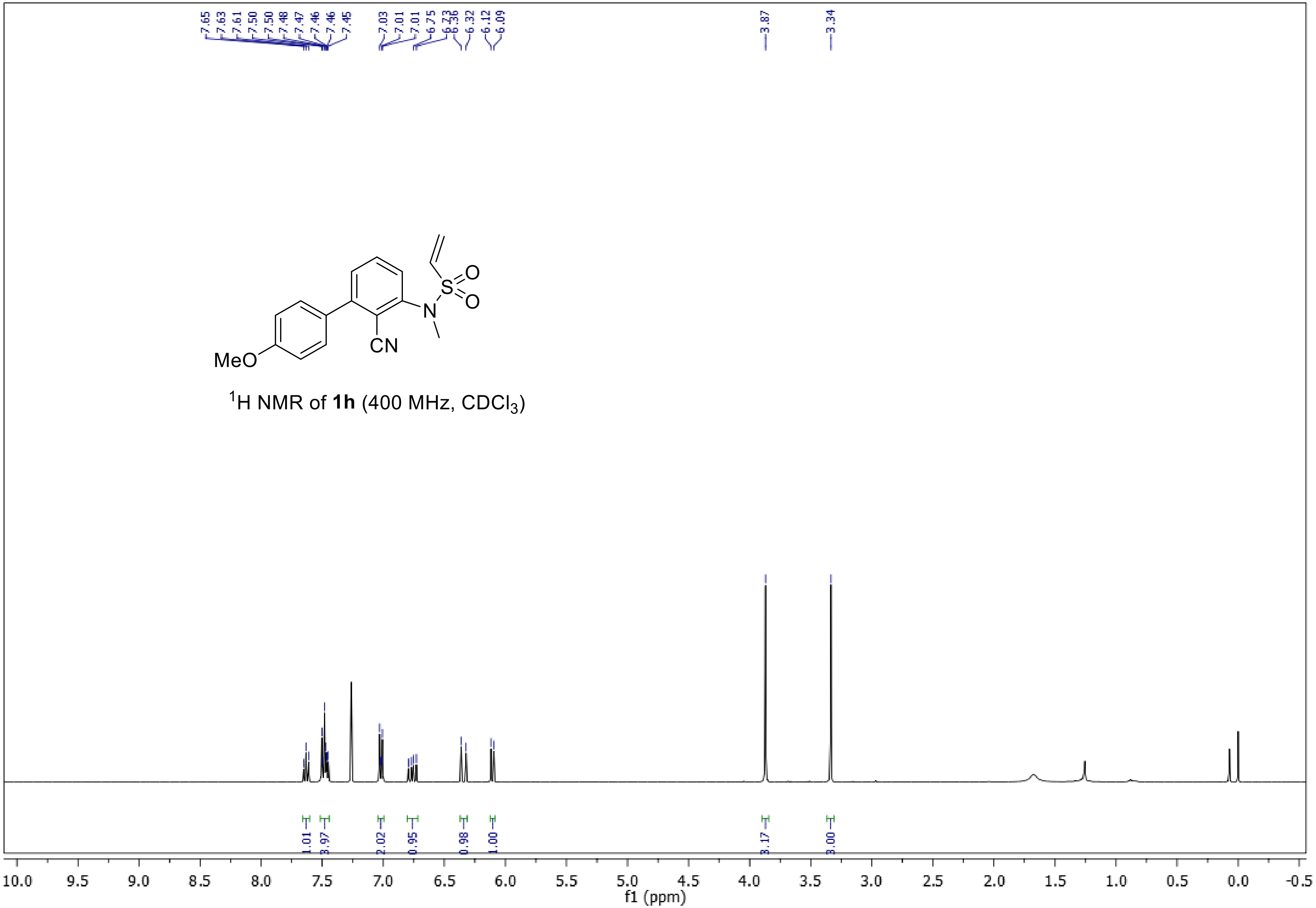
$^{13}C\{^{1}H\}$ NMR of **1f** (101 MHz, $CDCl_3$)



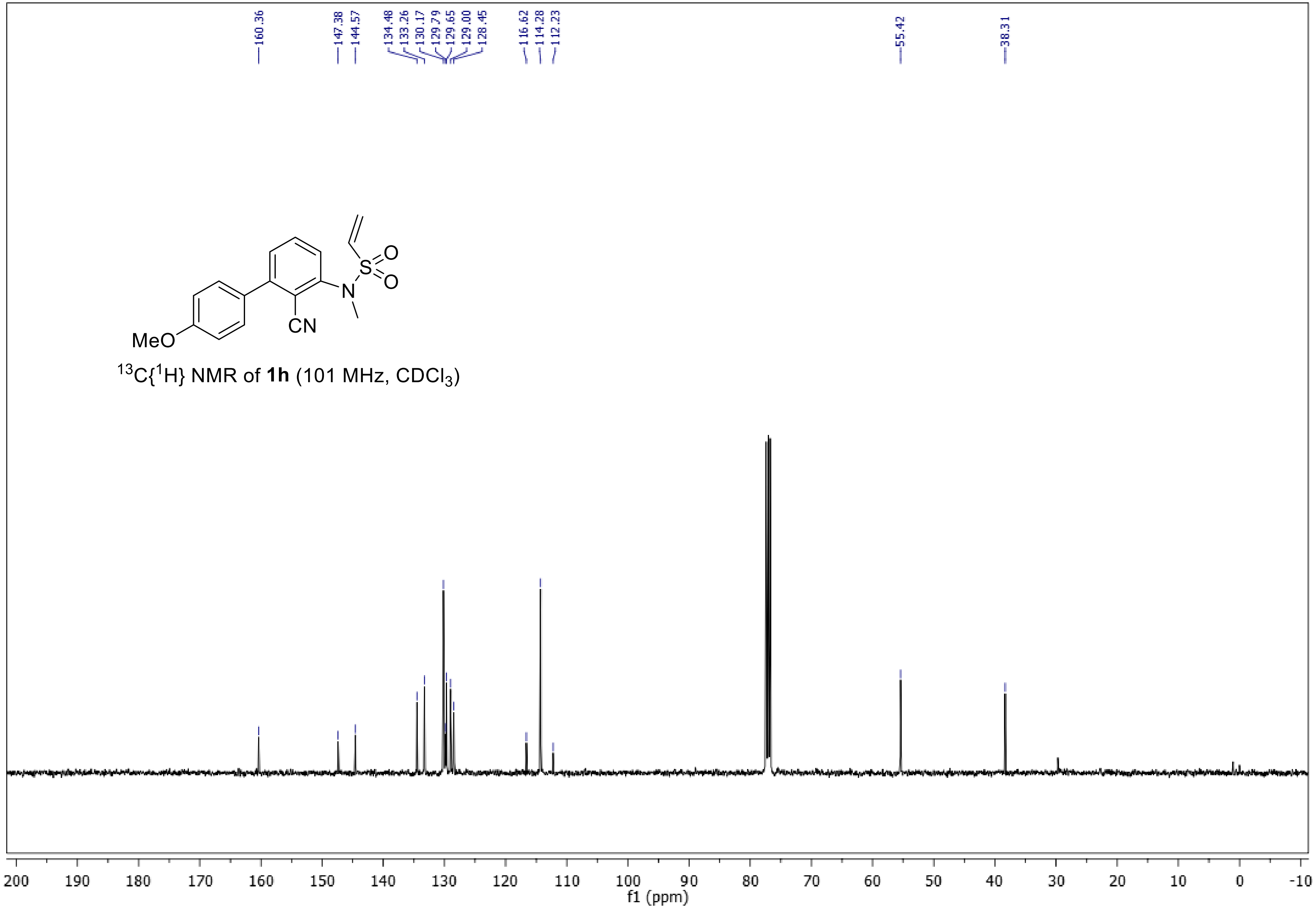
[1]H NMR of **1g** (400 MHz, $CDCl_3$)



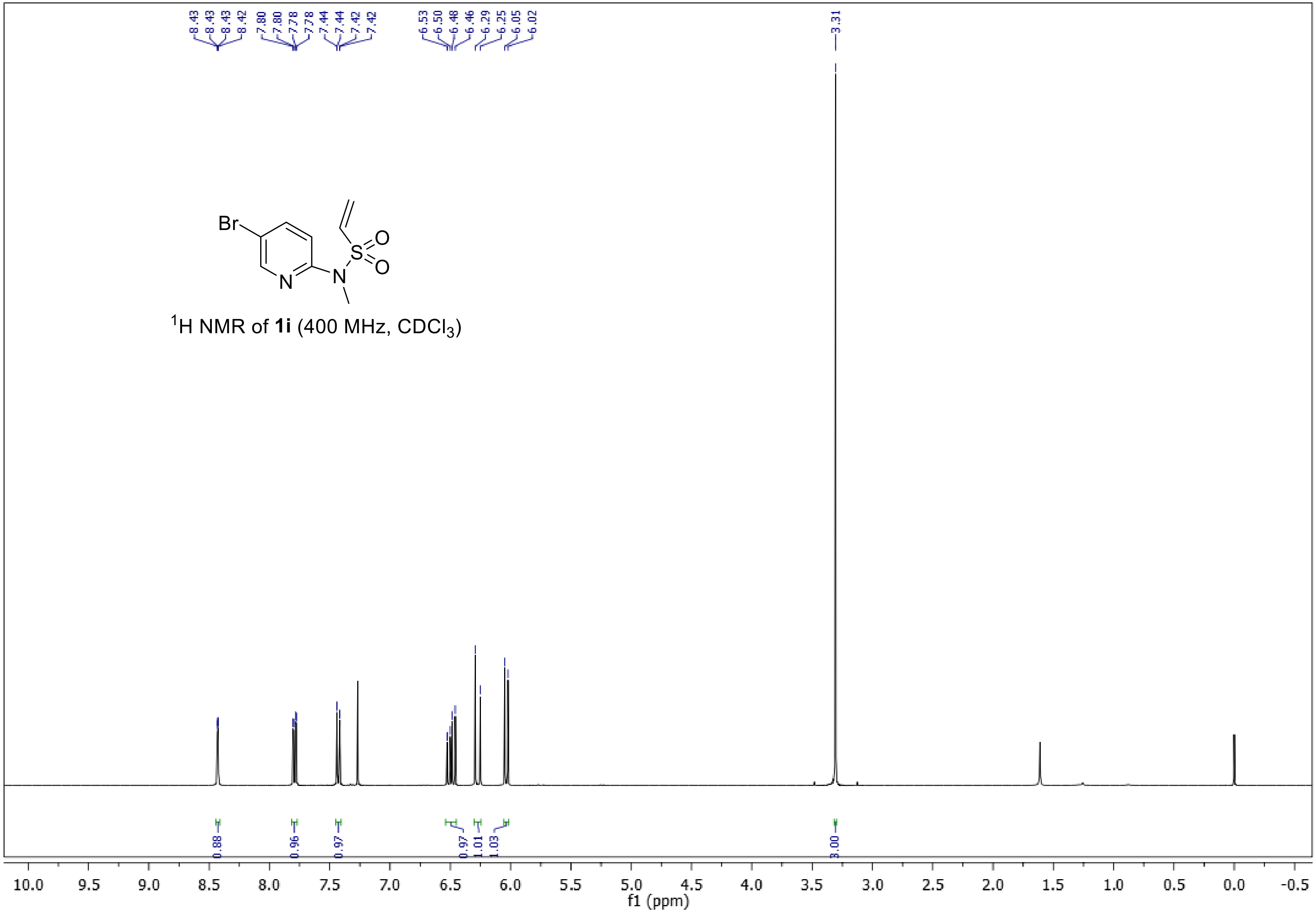
$^{13}C\{^{1}H\}$ NMR of **1g** (101 MHz, $CDCl_3$)



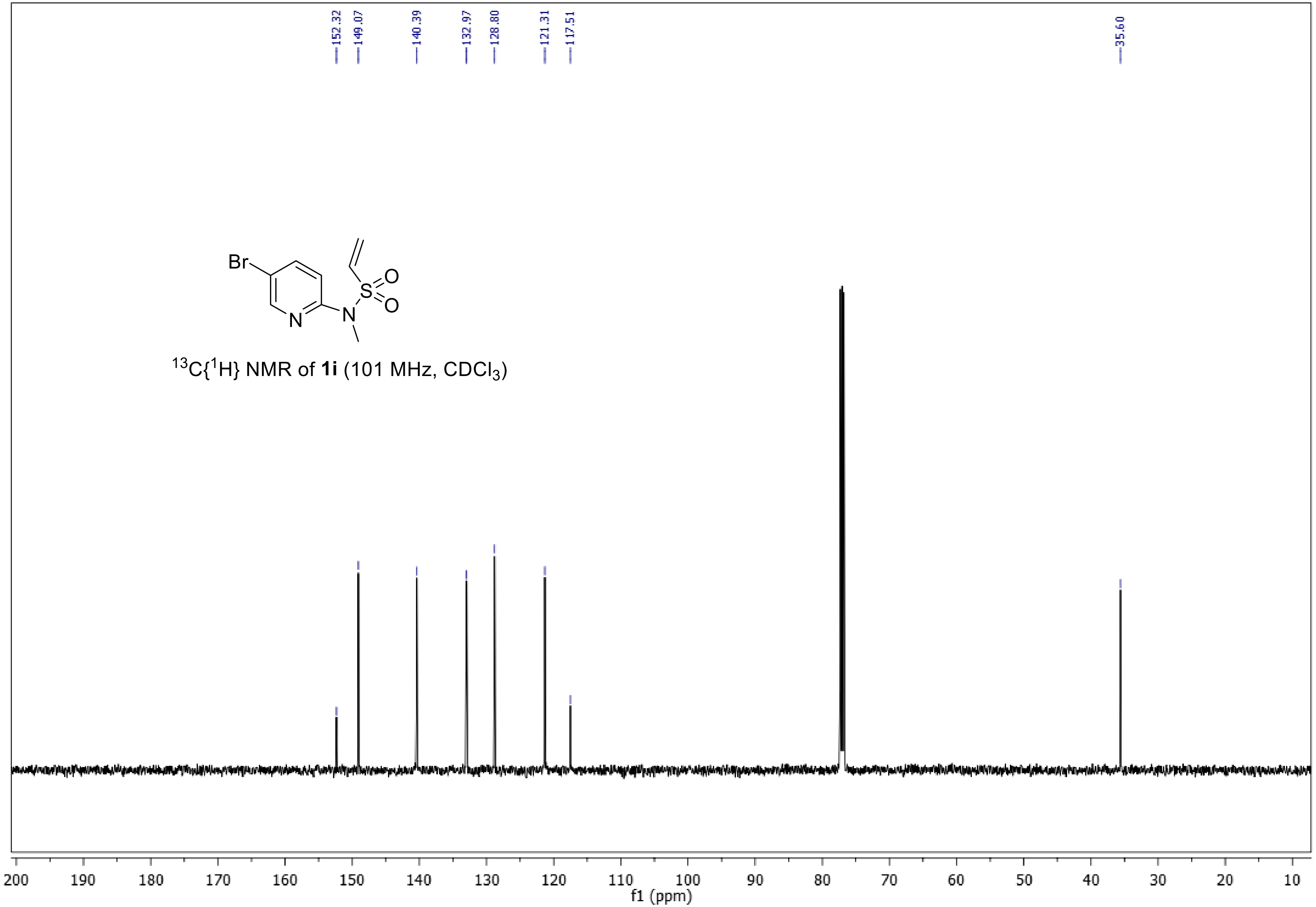
^{1}H NMR of **1h** (400 MHz, $CDCl_3$)



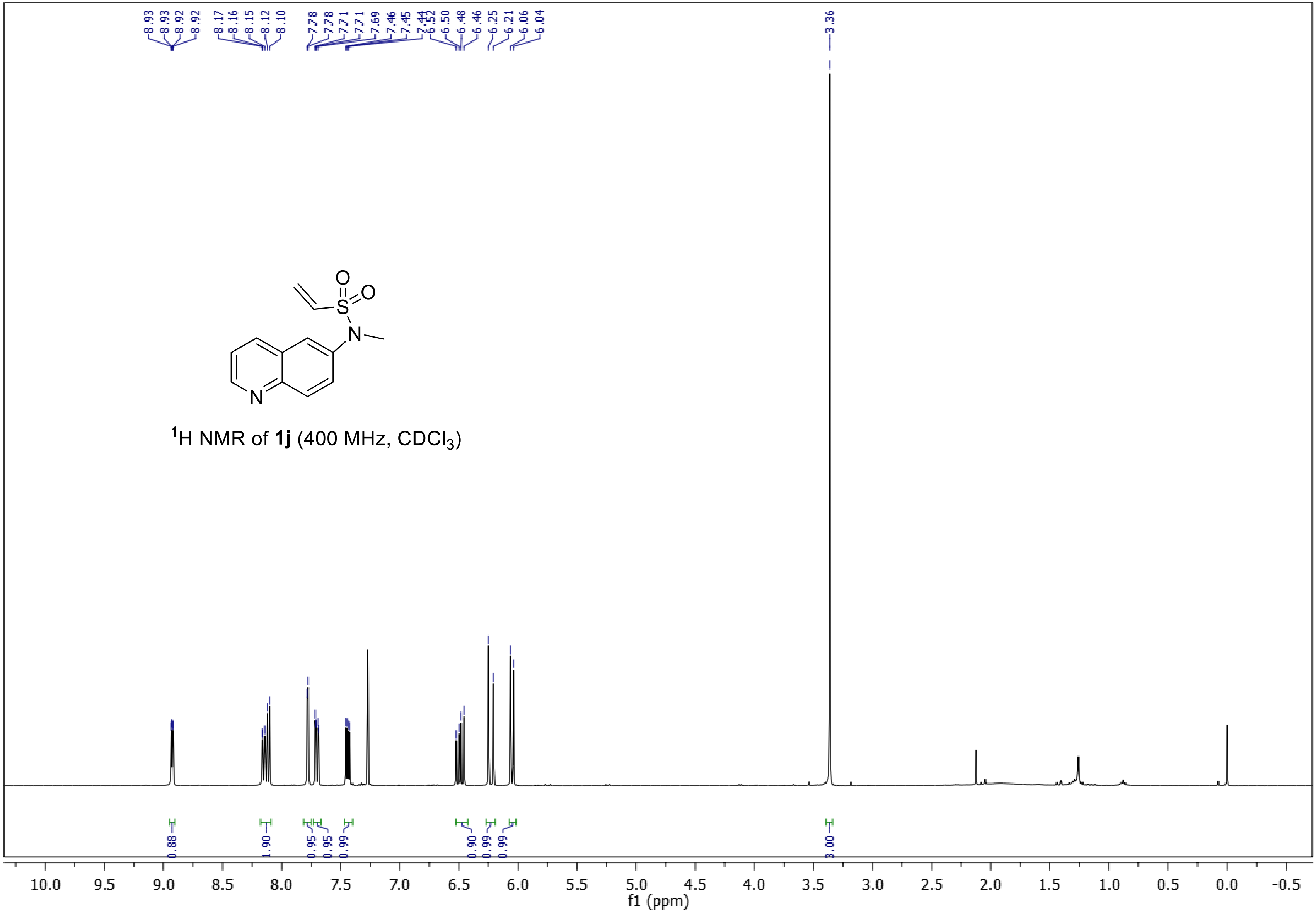
$^{13}C\{^{1}H\}$ NMR of **1h** (101 MHz, $CDCl_3$)



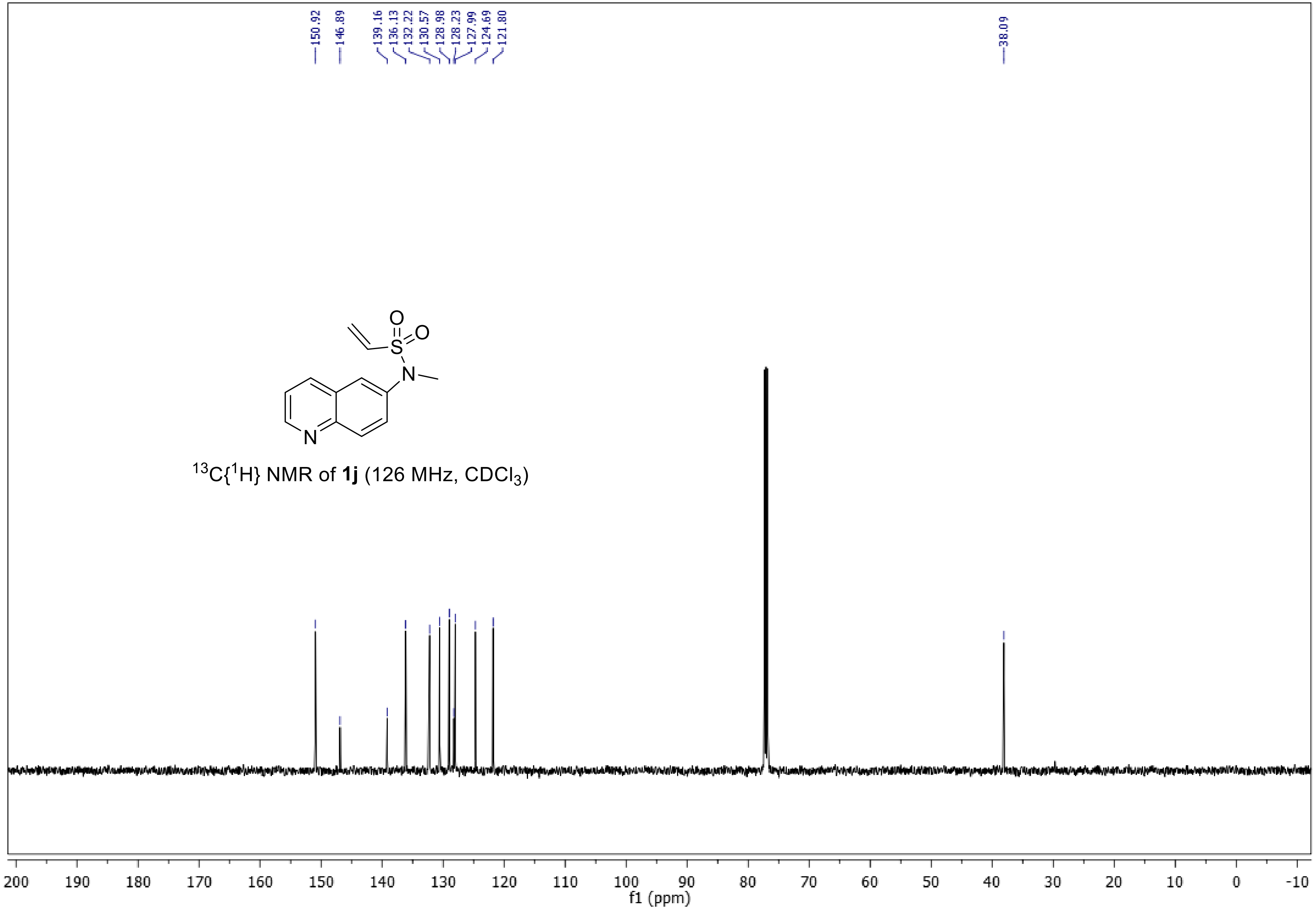
^1H NMR of **1i** (400 MHz, $CDCl_3$)



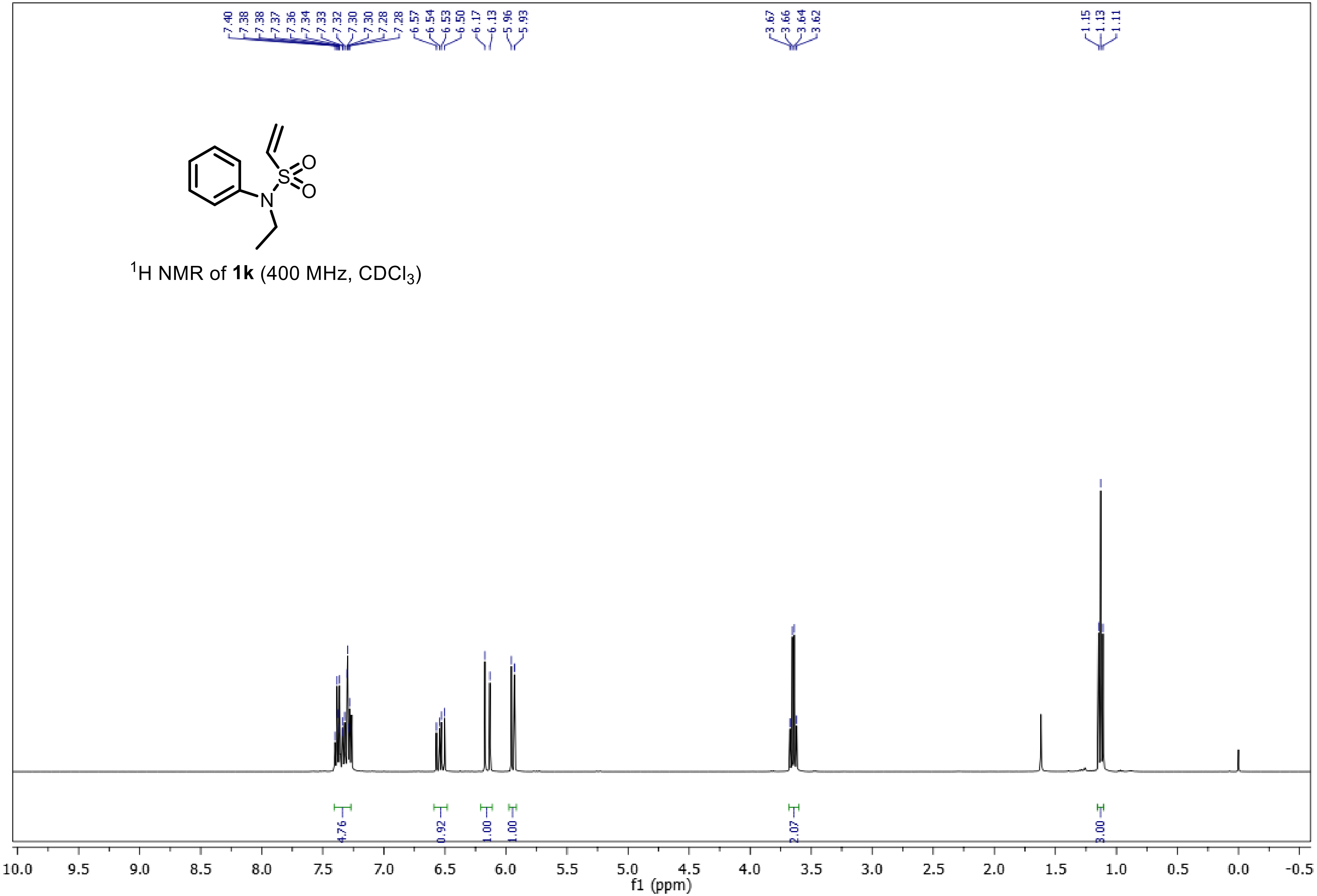
$^{13}C\{^{1}H\}$ NMR of **1i** (101 MHz, $CDCl_3$)



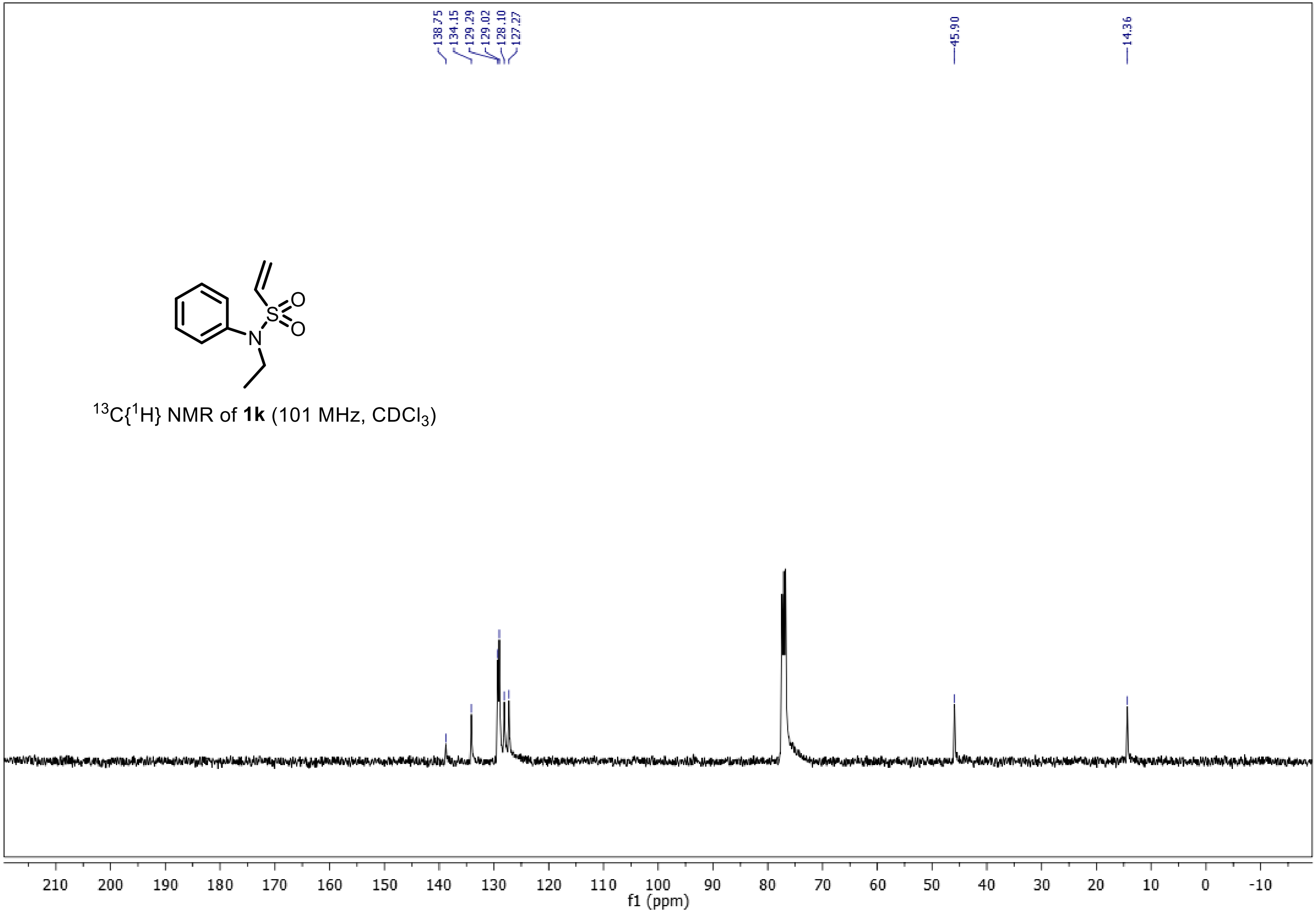
[1]H NMR of **1j** (400 MHz, $CDCl_3$)



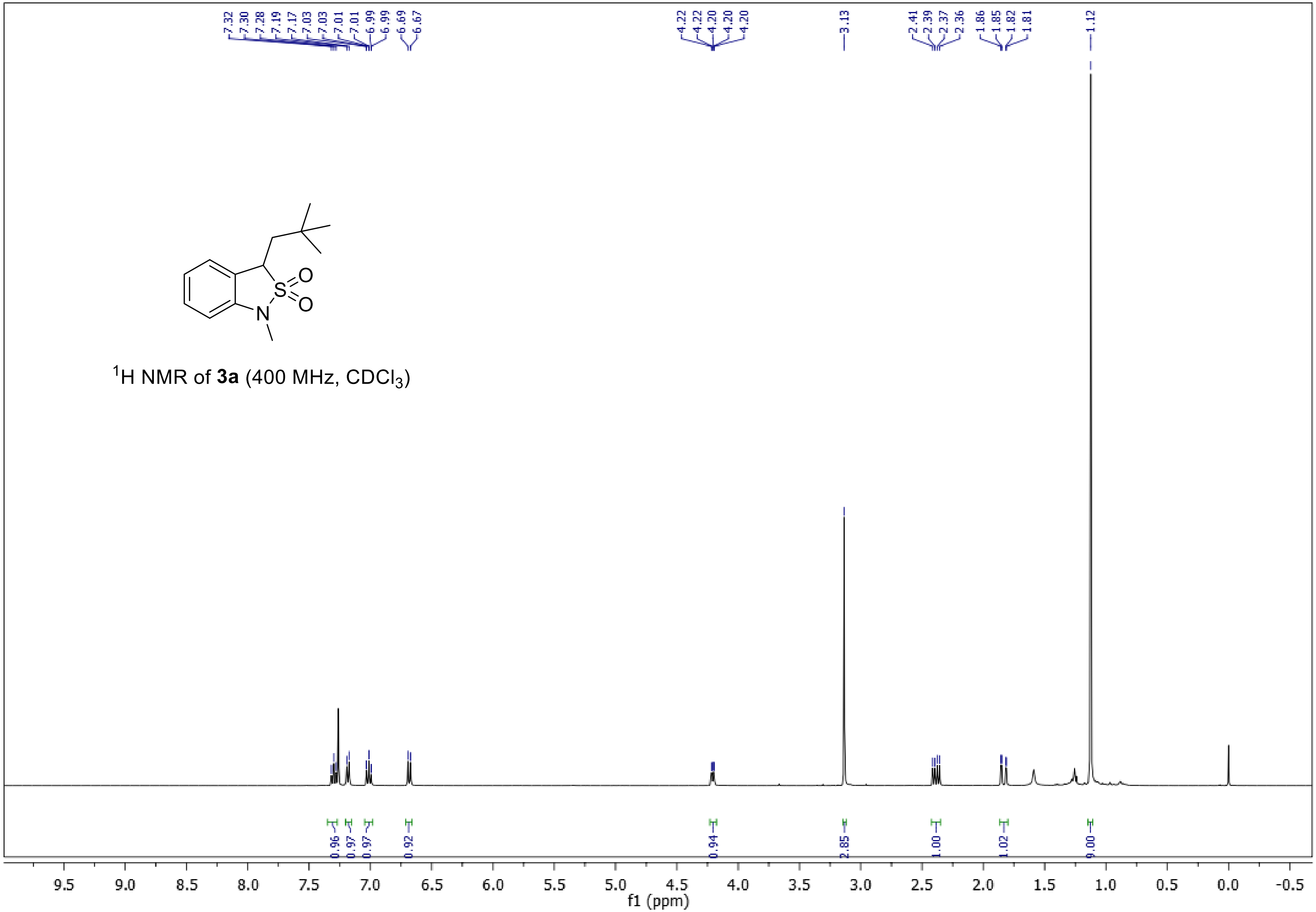
$^{13}C\{^{1}H\}$ NMR of **1j** (126 MHz, $CDCl_3$)



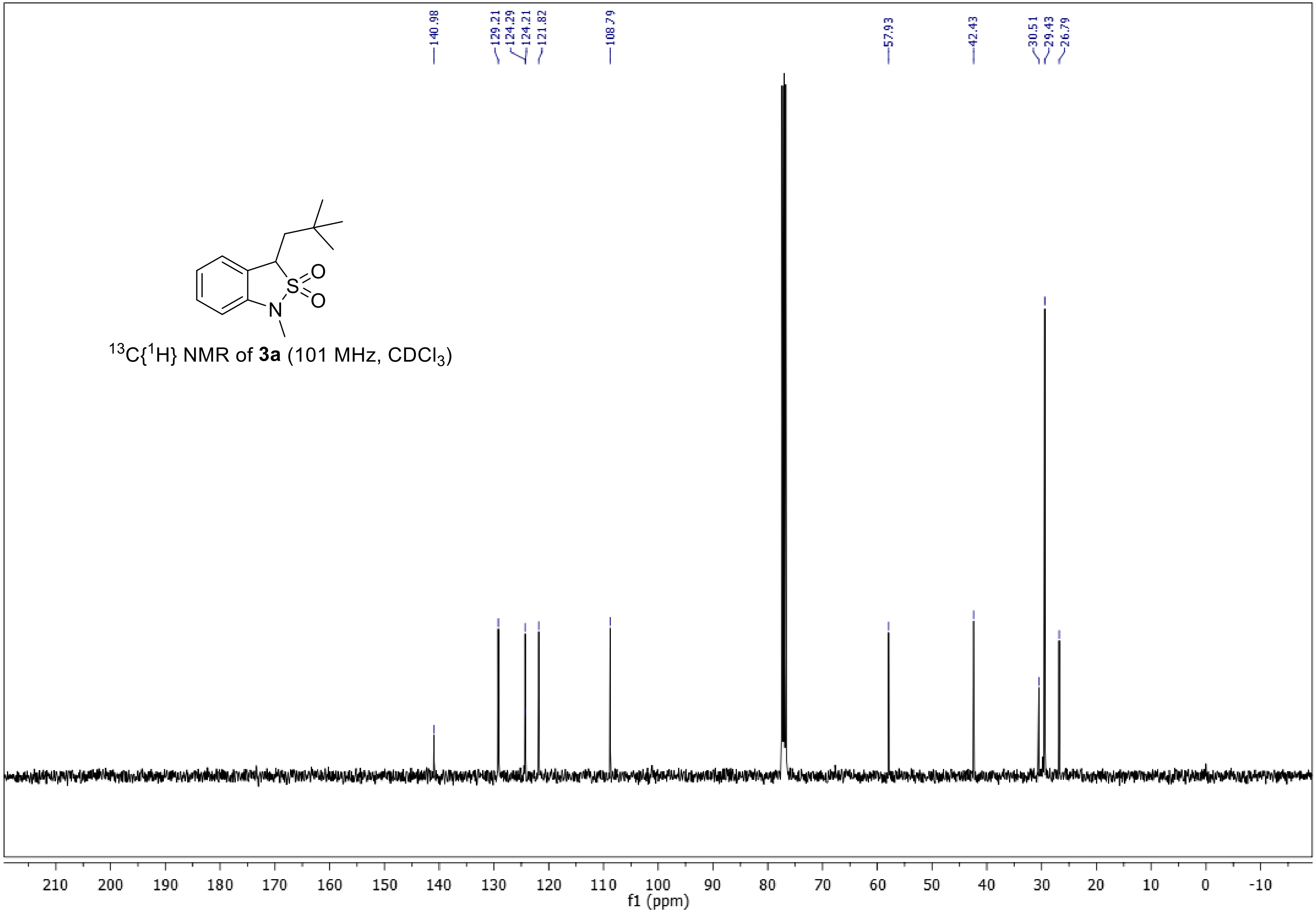
[1]H NMR of **1k** (400 MHz, $CDCl_3$)



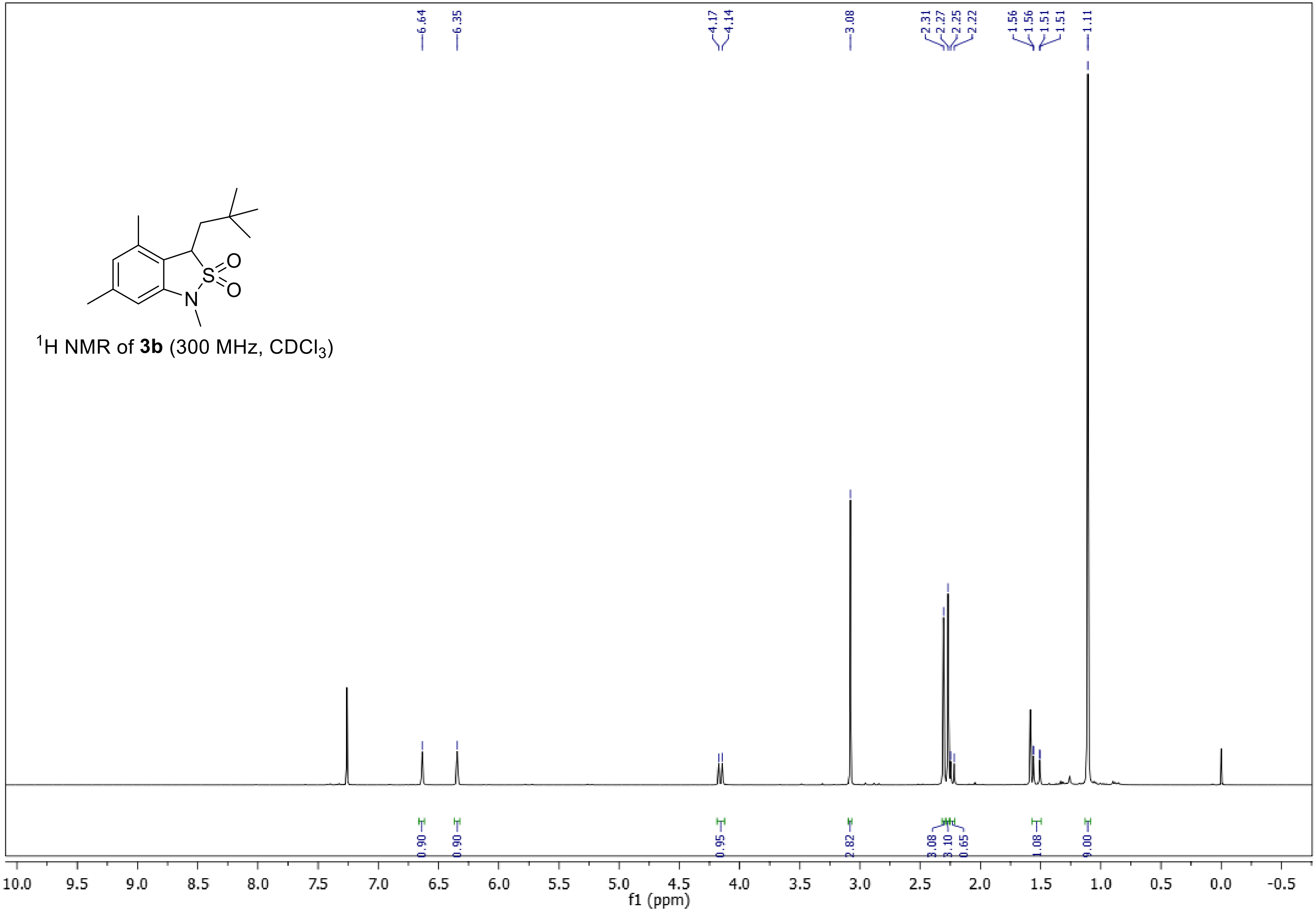
$^{13}C\{^1H\}$ NMR of **1k** (101 MHz, $CDCl_3$)



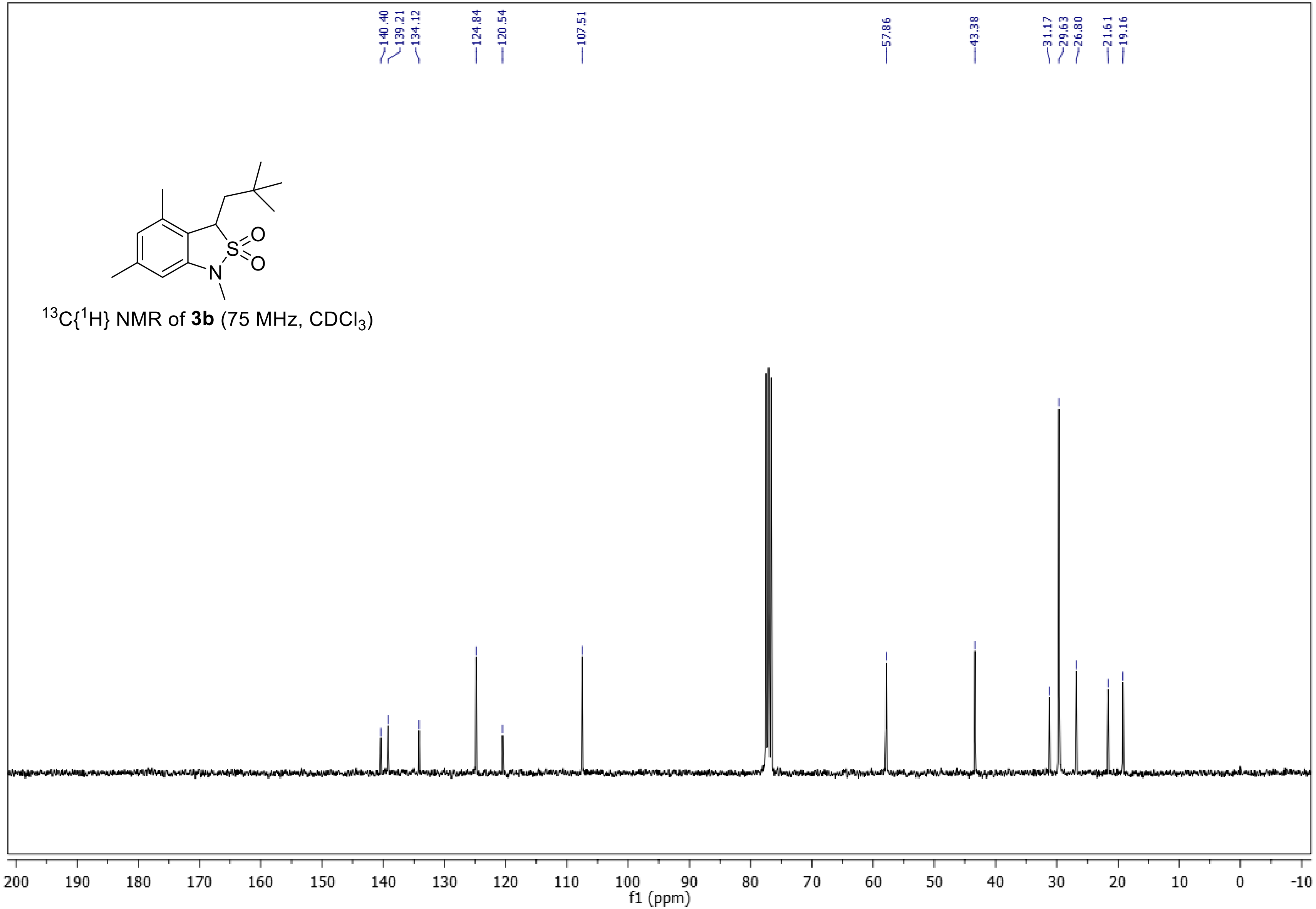
^{1}H NMR of **3a** (400 MHz, $CDCl_3$)



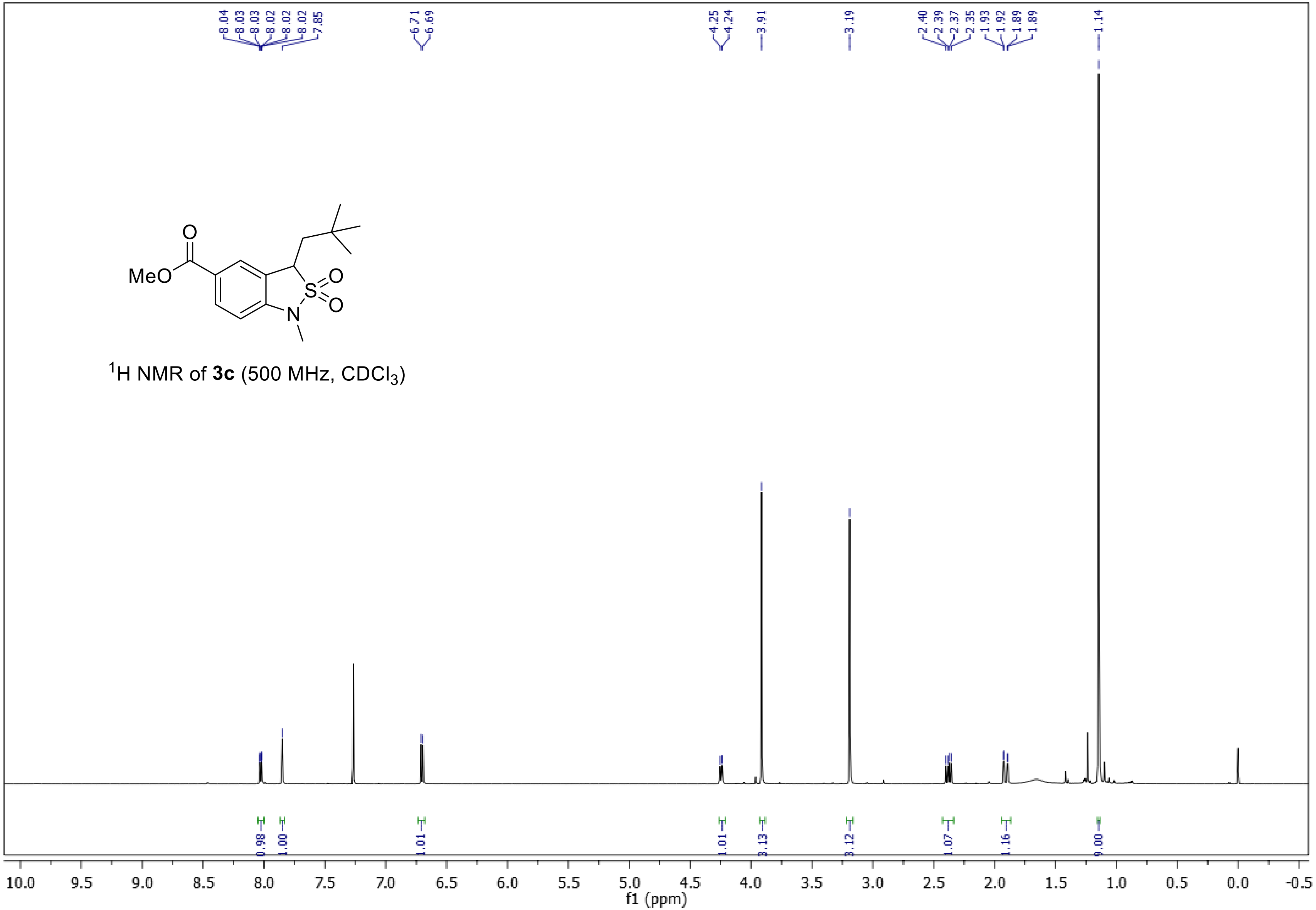
$^{13}C\{^1H\}$ NMR of **3a** (101 MHz, $CDCl_3$)



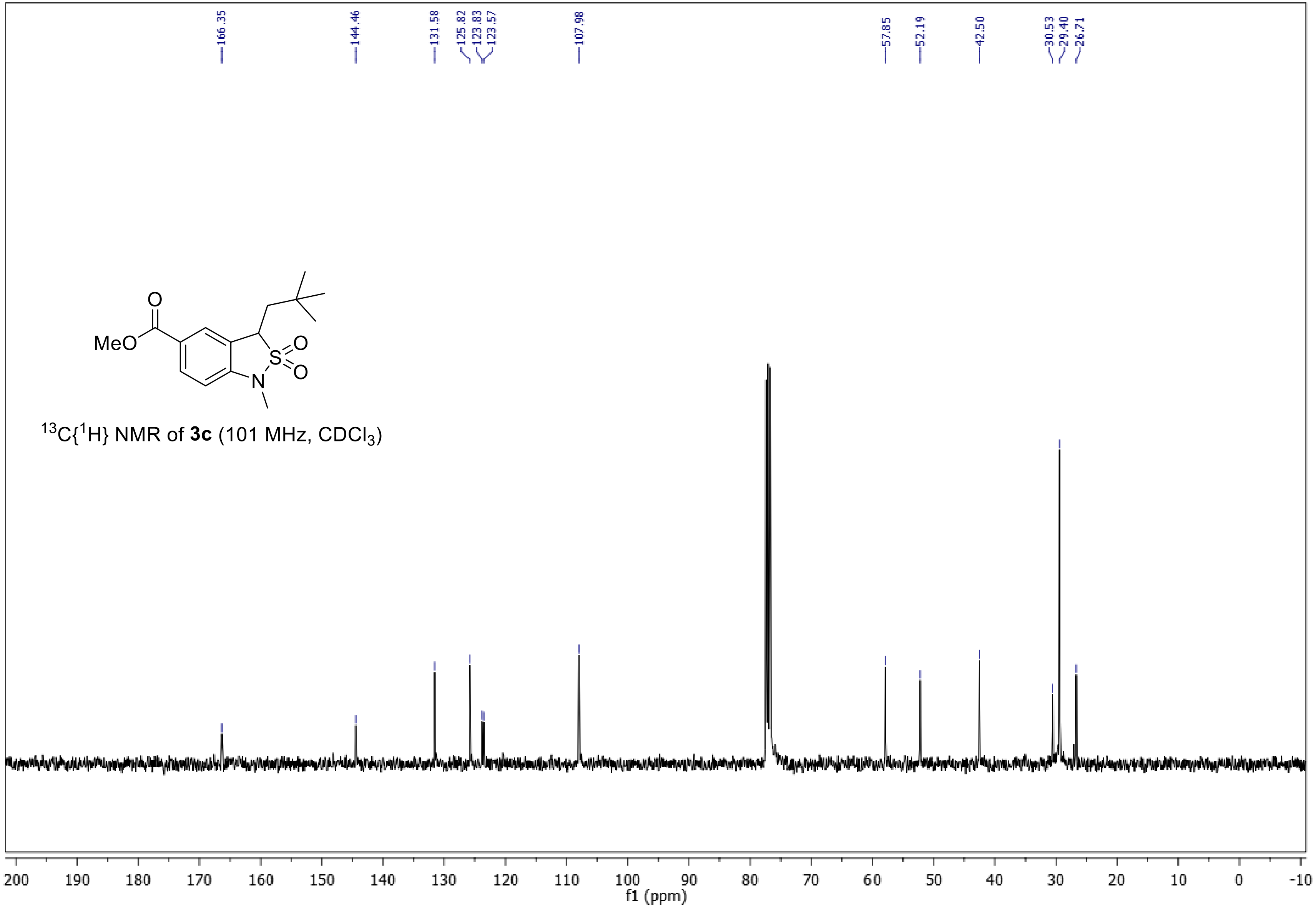
6.64
6.35
4.17
4.14
3.08
2.31
2.27
2.25
2.22
1.56
1.56
1.51
1.51
1.11
0.90
0.90
0.95
2.82
3.08
3.10
0.65
1.08
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

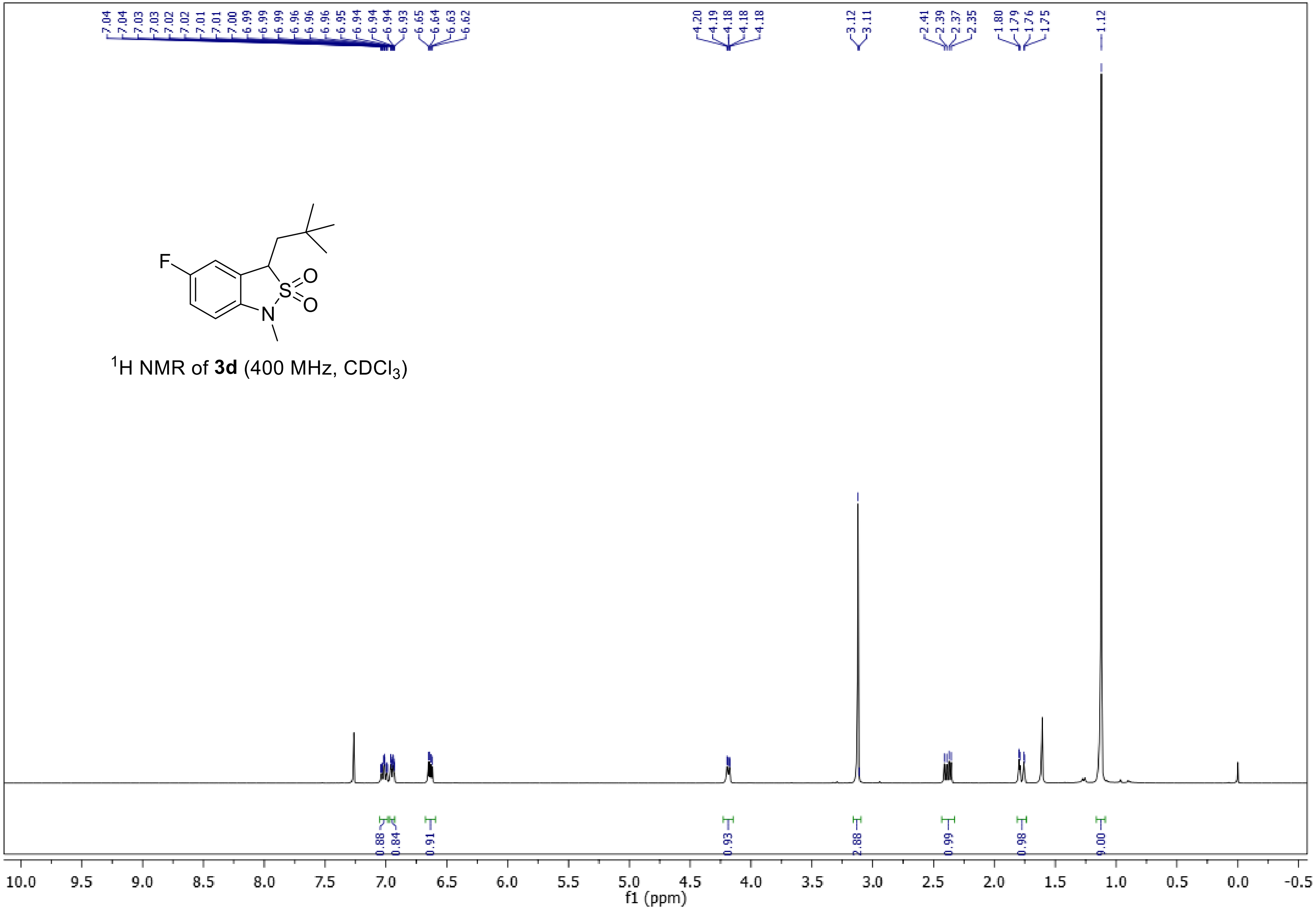


$^{13}C\{^{1}H\}$ NMR of **3b** (75 MHz, $CDCl_3$)

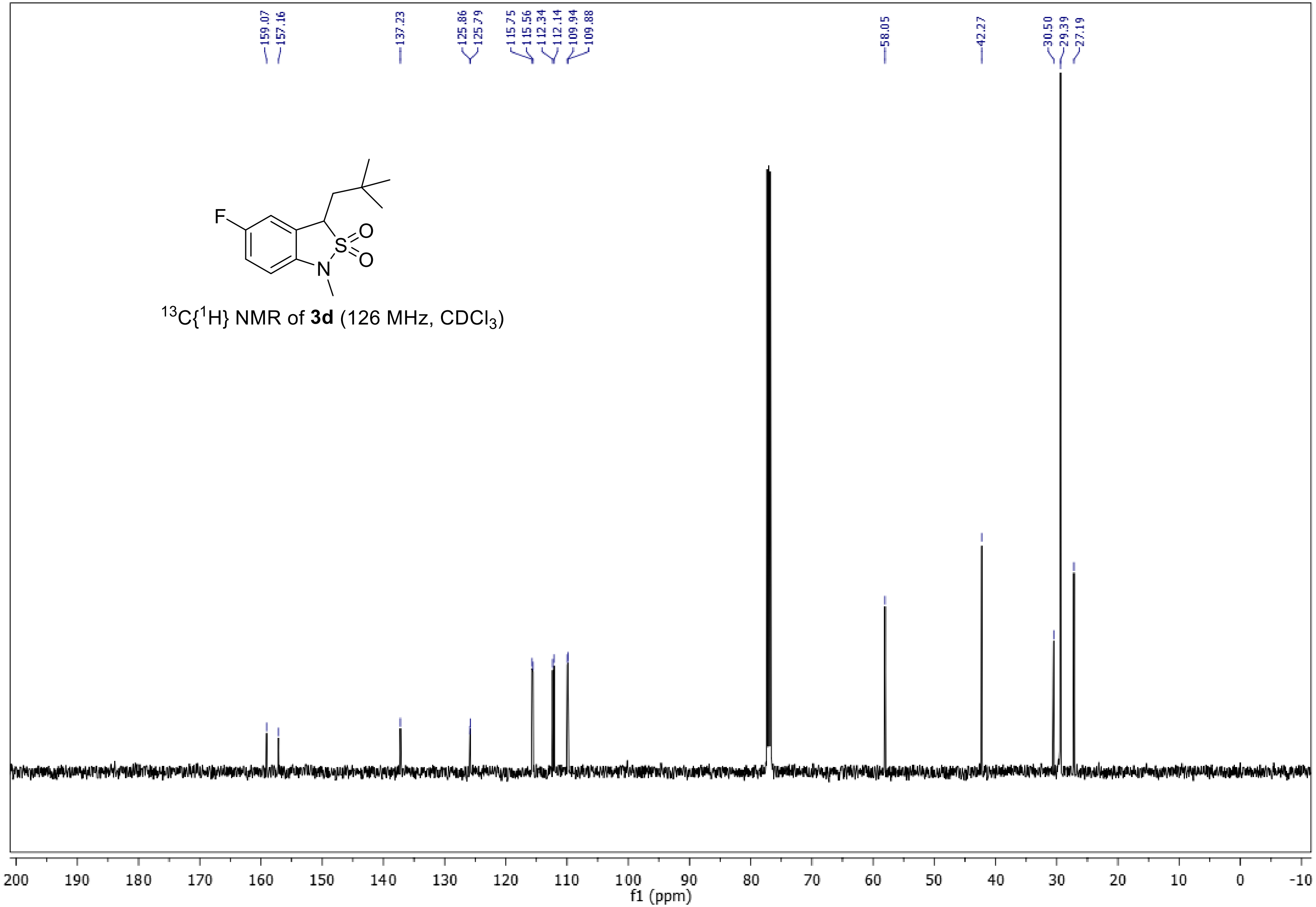


[1]H NMR of **3c** (500 MHz, $CDCl_3$)

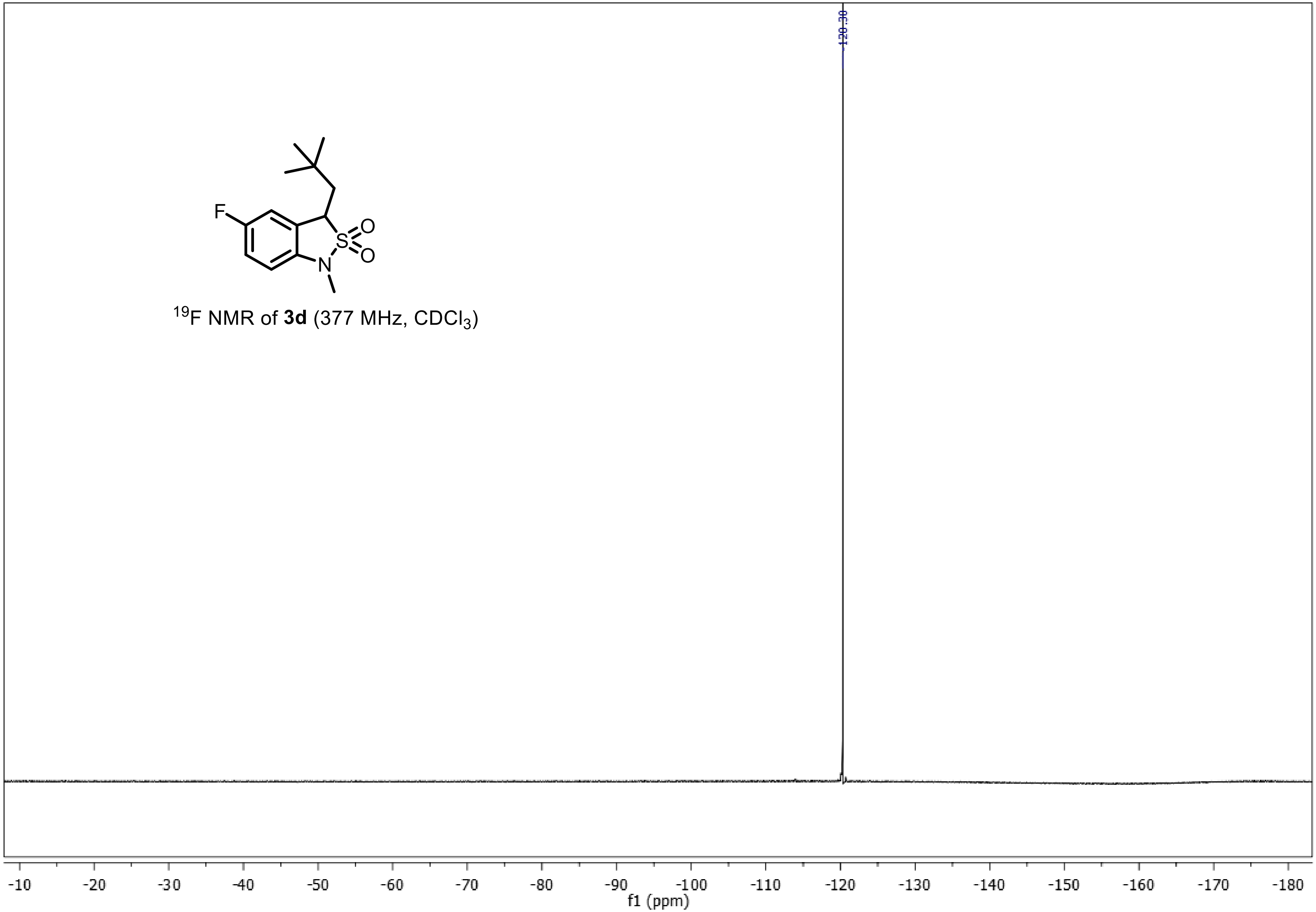

166.35
144.46
131.58
125.82
123.83
123.57
107.98
57.85
52.19
42.50
30.53
29.40
26.71
MeO
O
S
O
O
N
$^{13}C\{^{1}H\}$ NMR of **3c** (101 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

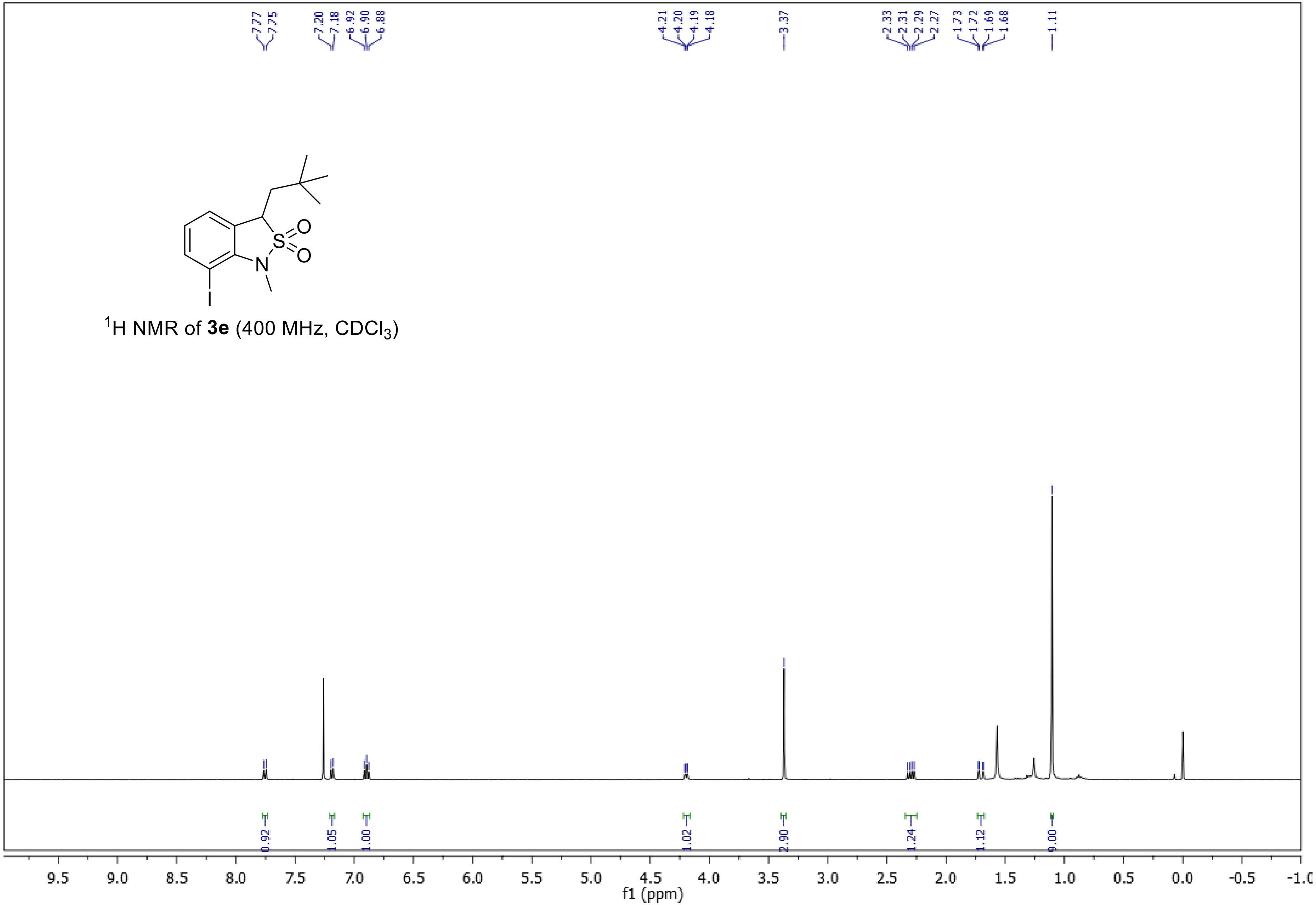


^{1}H NMR of **3d** (400 MHz, $CDCl_3$)

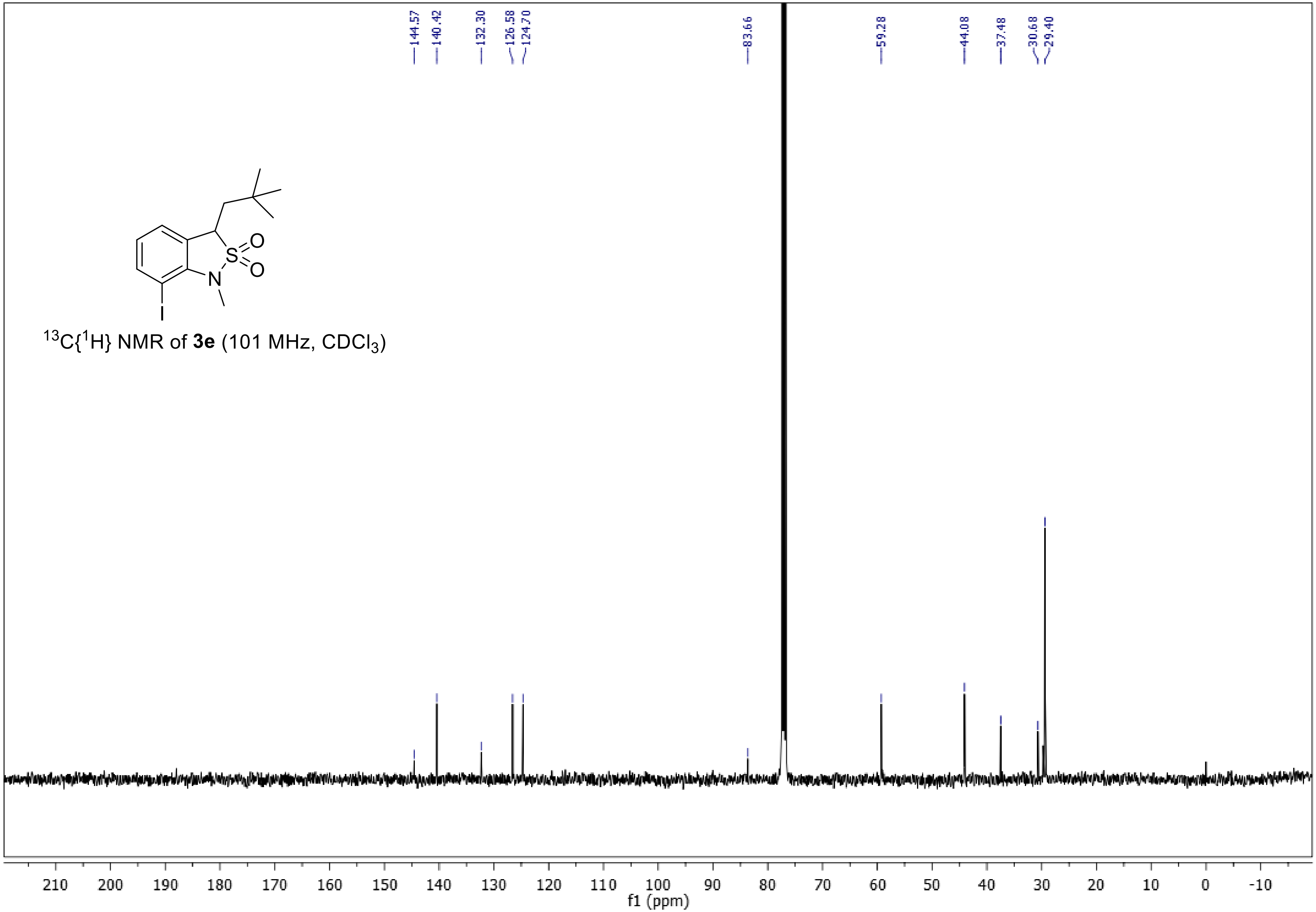


$^{13}C\{^{1}H\}$ NMR of **3d** (126 MHz, $CDCl_3$)

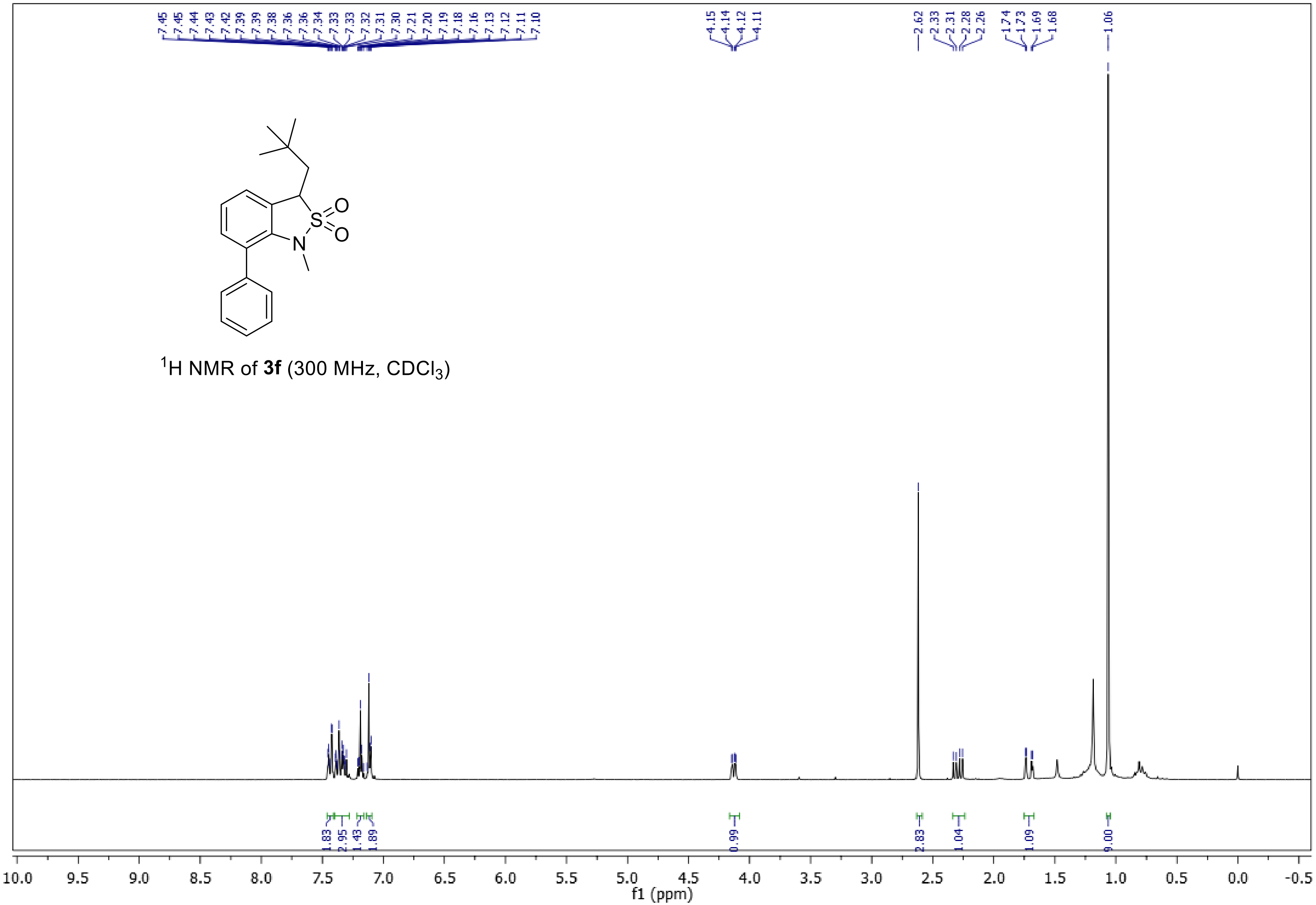

-120.30
F
S
O
O
N
19F NMR of 3d (377 MHz, CDCl3)
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)



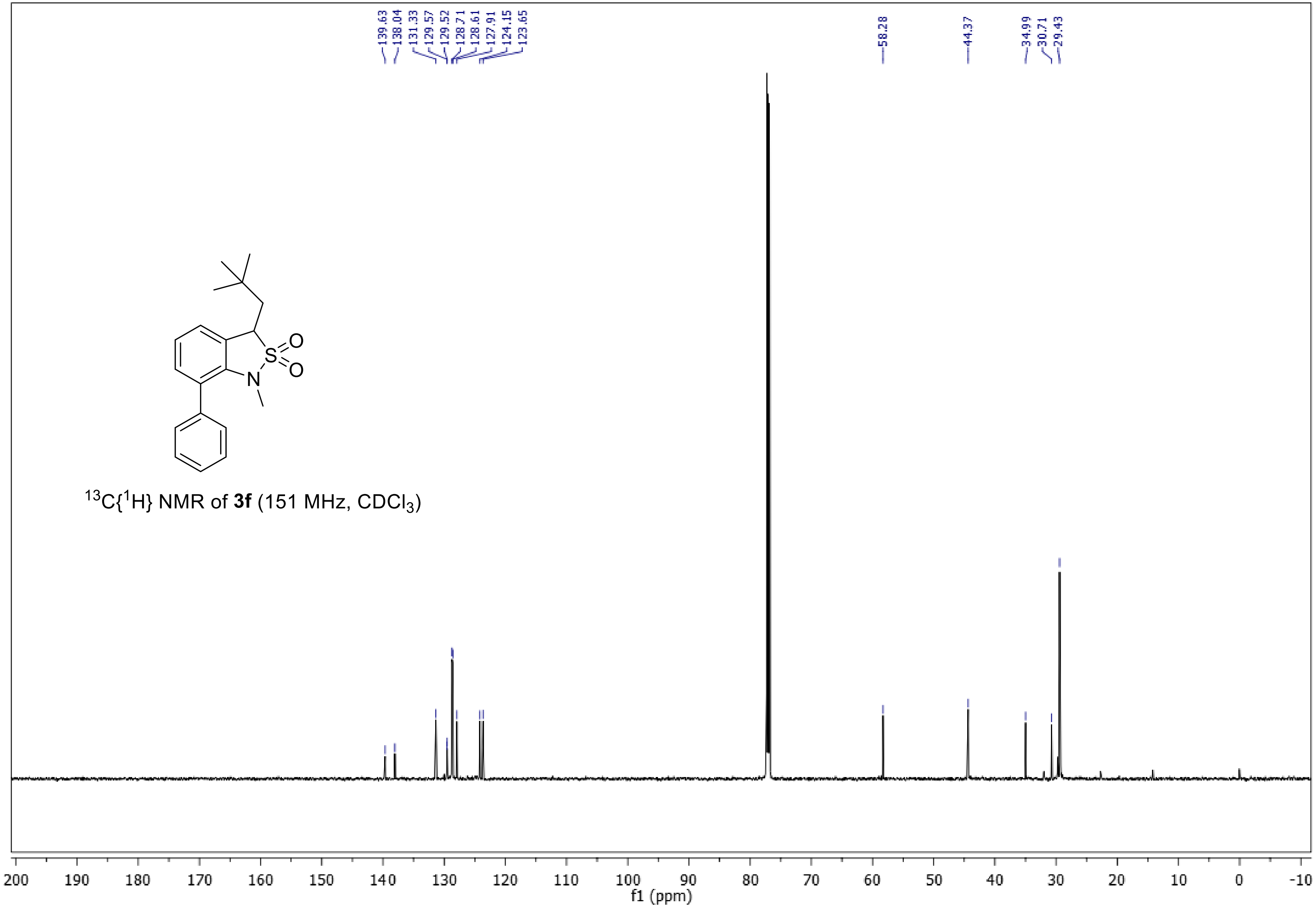
7.77
7.75
7.20
7.18
6.92
6.90
6.88
4.21
4.20
4.19
4.18
3.37
2.33
2.31
2.29
2.27
1.73
1.72
1.69
1.68
1.11
S
O
O
N
I
^{1}H NMR of **3e** (400 MHz, $CDCl_3$)
0.92
1.05
1.00
1.02
2.90
1.24
1.12
9.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)



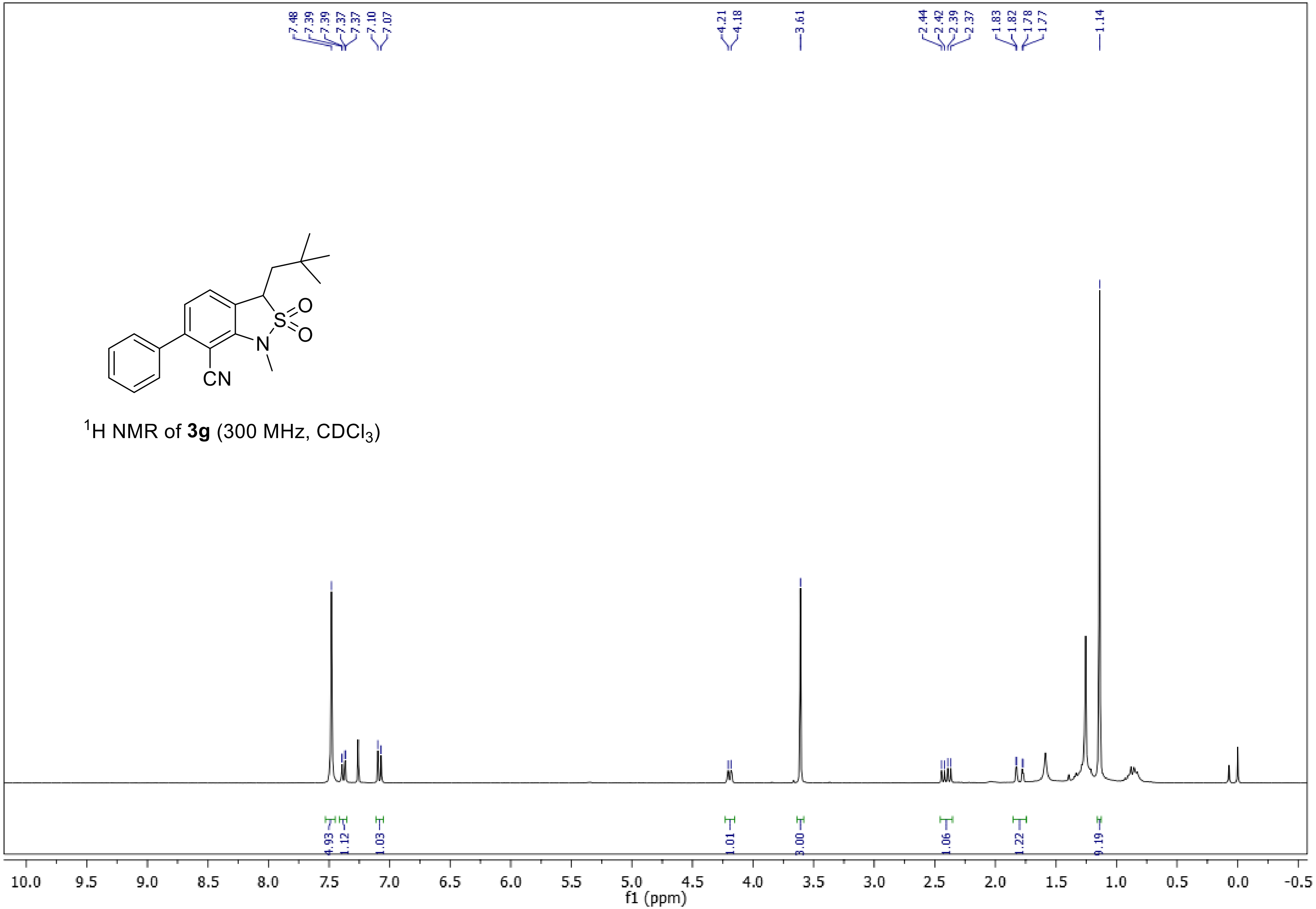
$^{13}C\{^{1}H\}$ NMR of **3e** (101 MHz, $CDCl_3$)



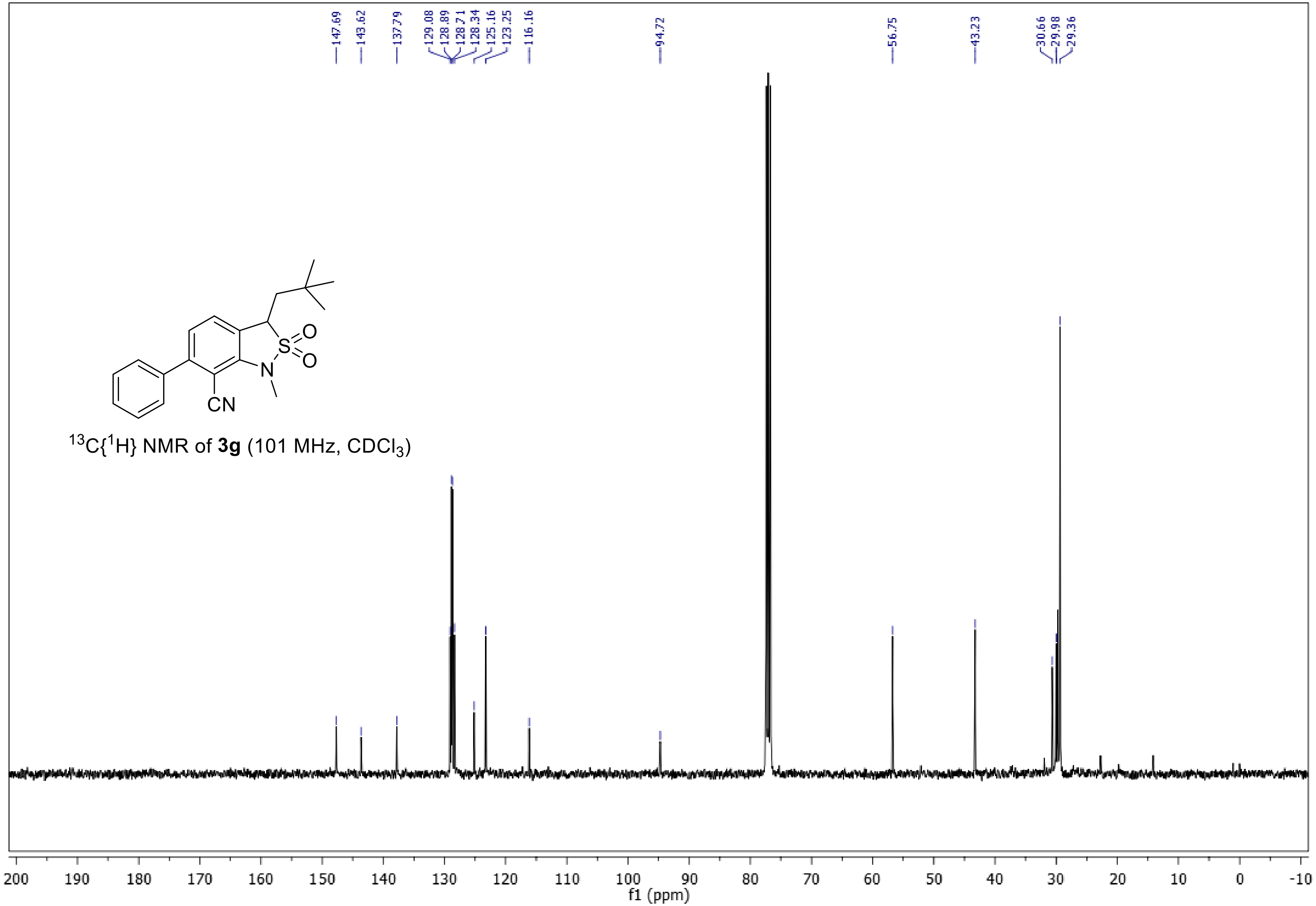
^{1}H NMR of **3f** (300 MHz, $CDCl_3$)



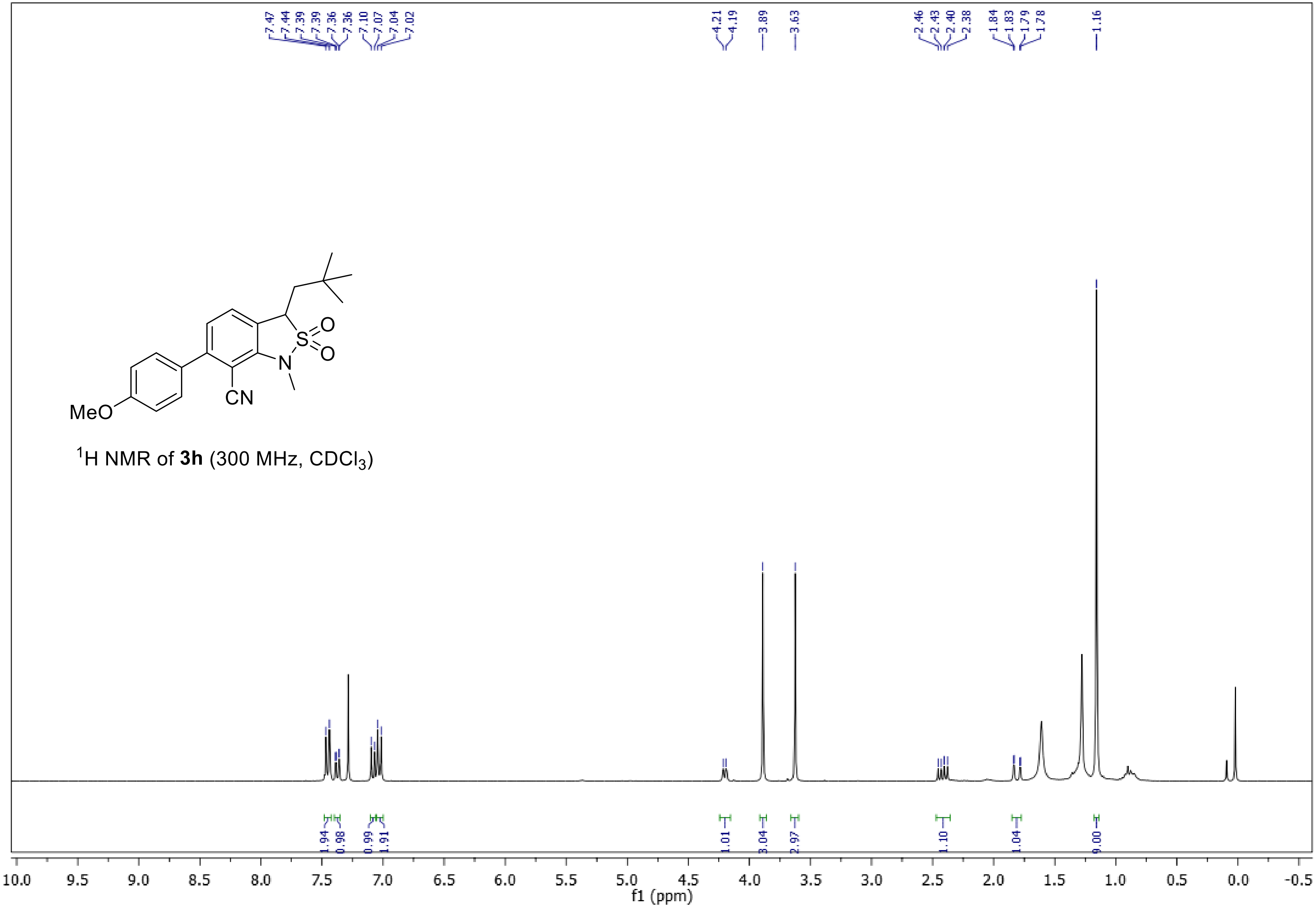
$^{13}C\{^{1}H\}$ NMR of **3f** (151 MHz, $CDCl_3$)



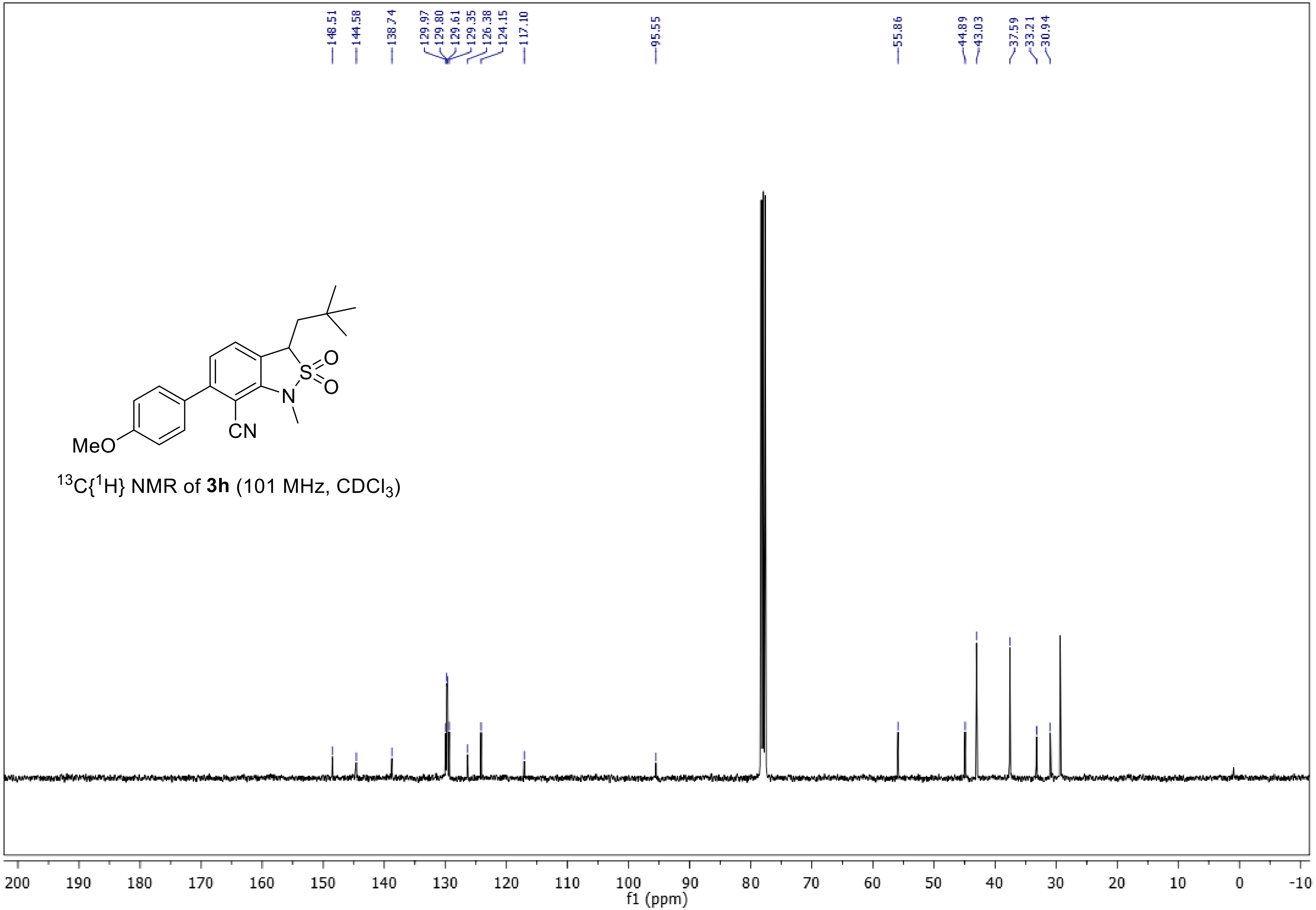
^{1}H NMR of **3g** (300 MHz, $CDCl_3$)



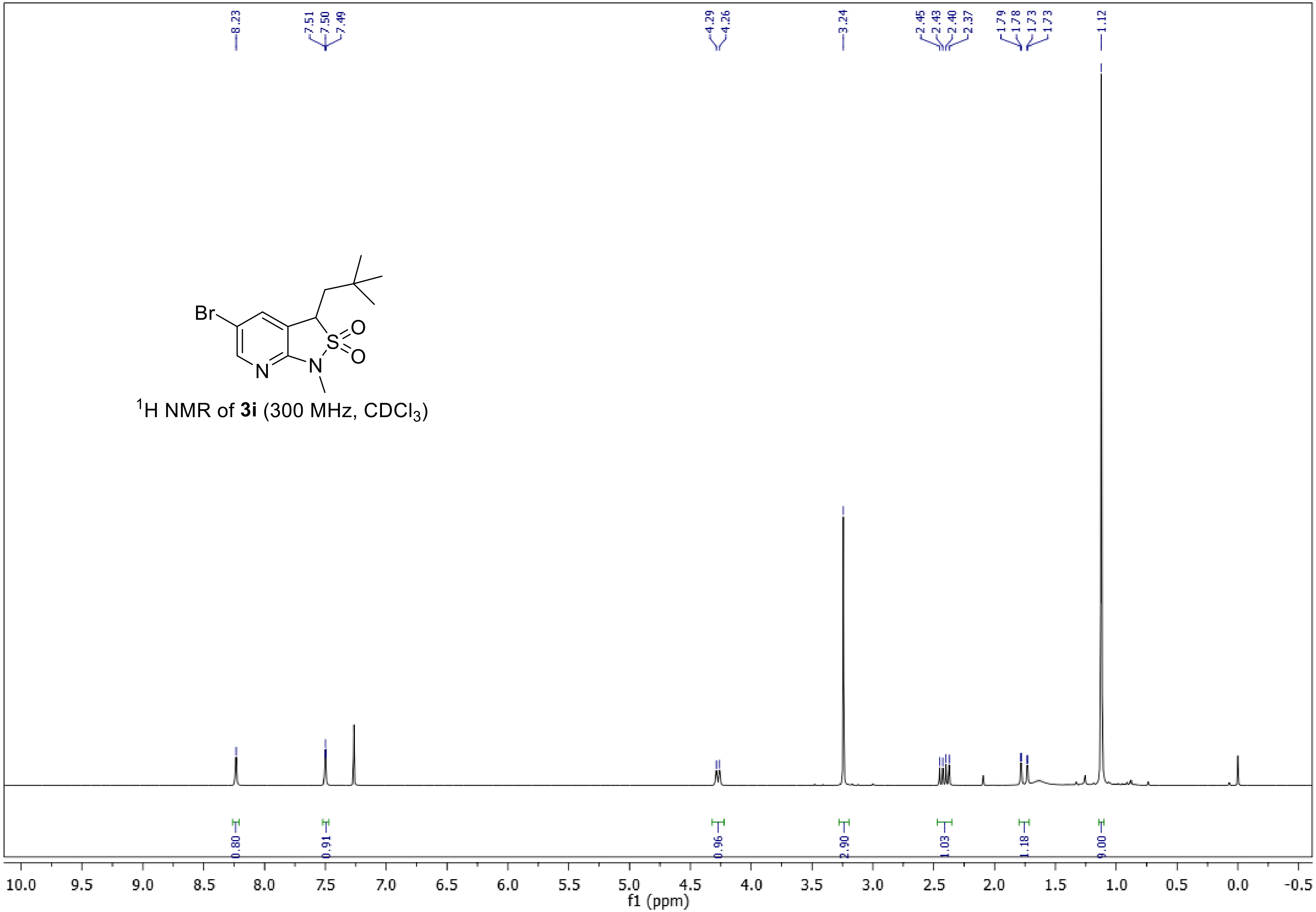
$^{13}C\{^1H\}$ NMR of **3g** (101 MHz, $CDCl_3$)



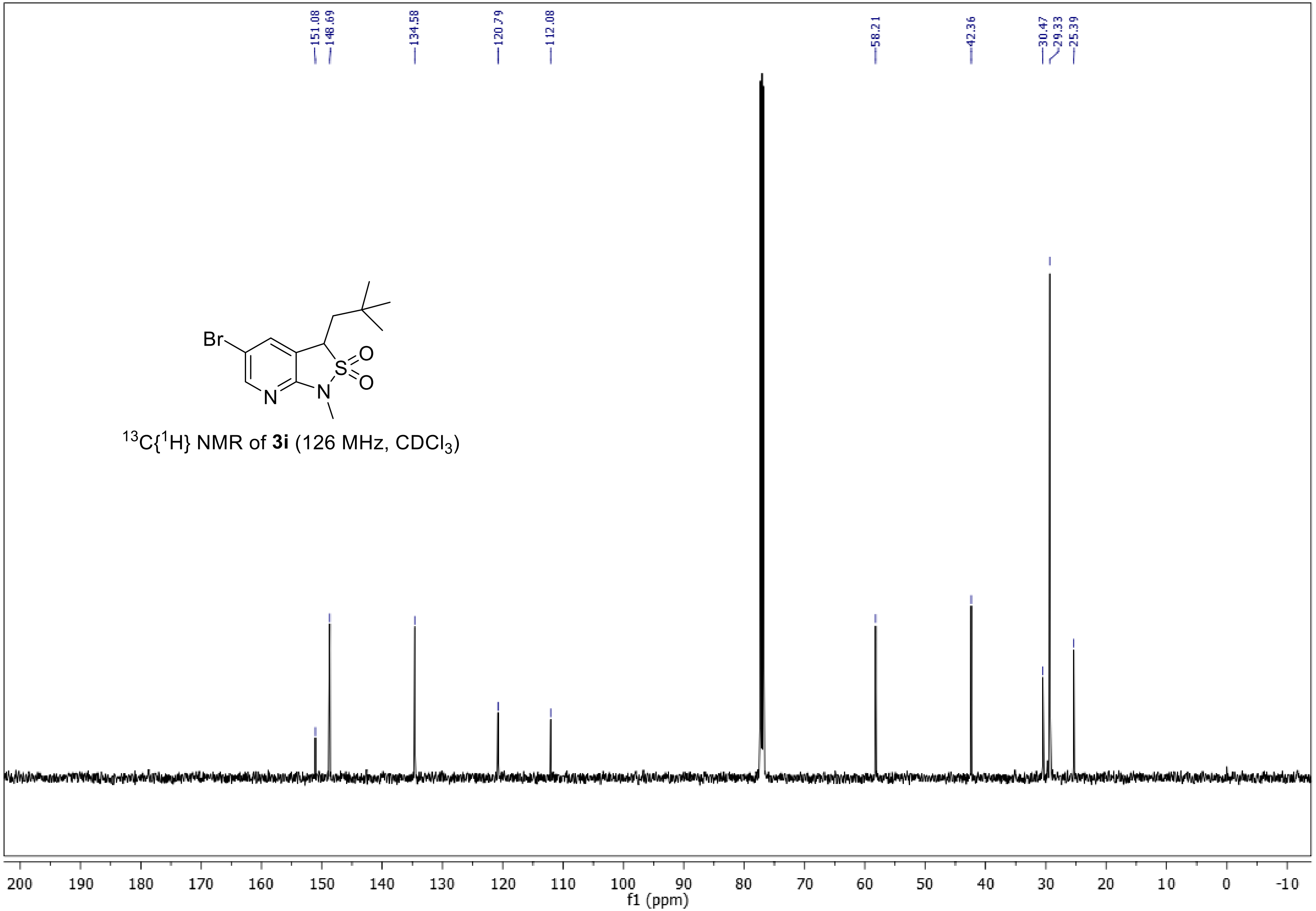
[1]H NMR of **3h** (300 MHz, $CDCl_3$)



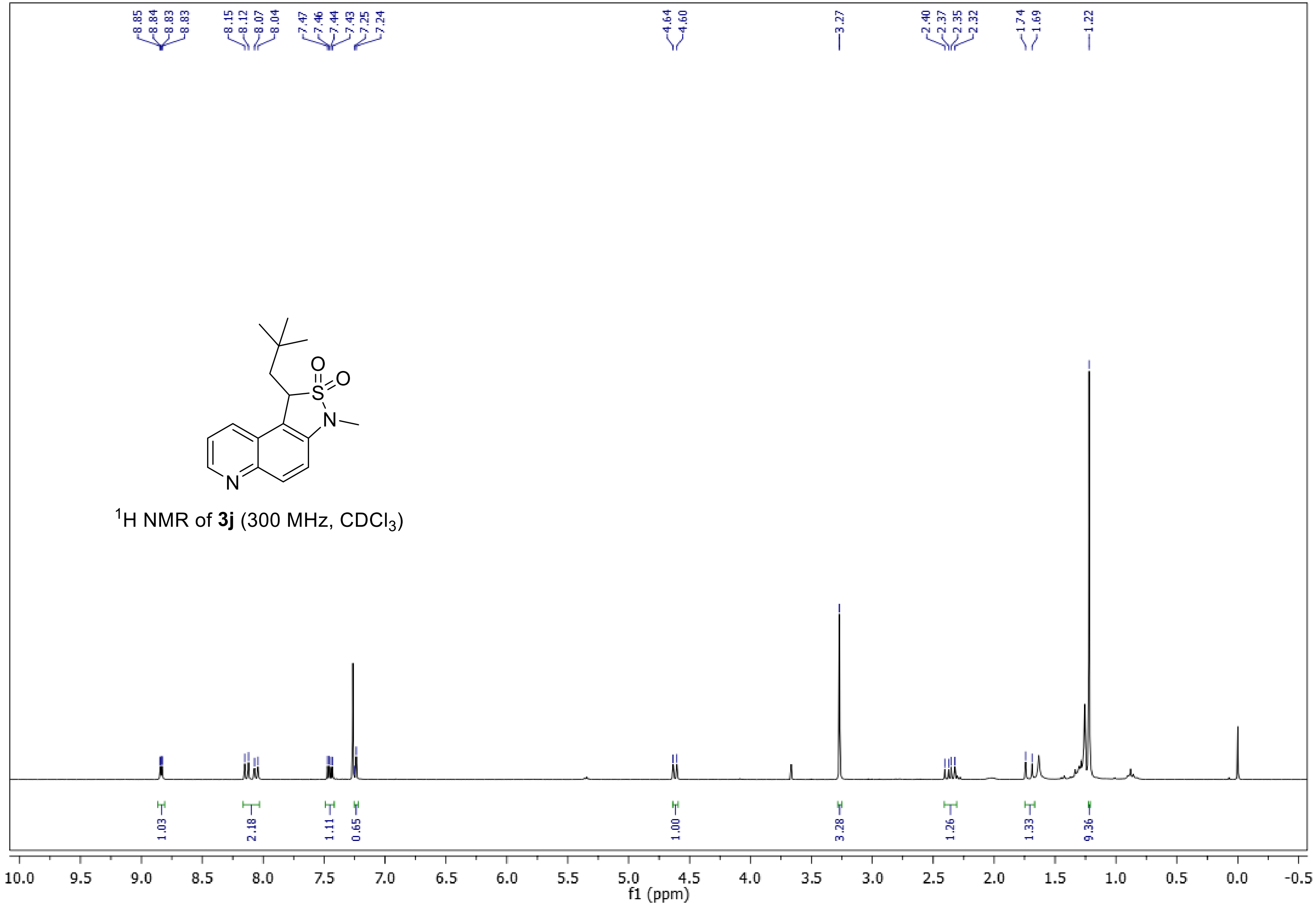
$^{13}C\{^{1}H\}$ NMR of **3h** (101 MHz, $CDCl_3$)



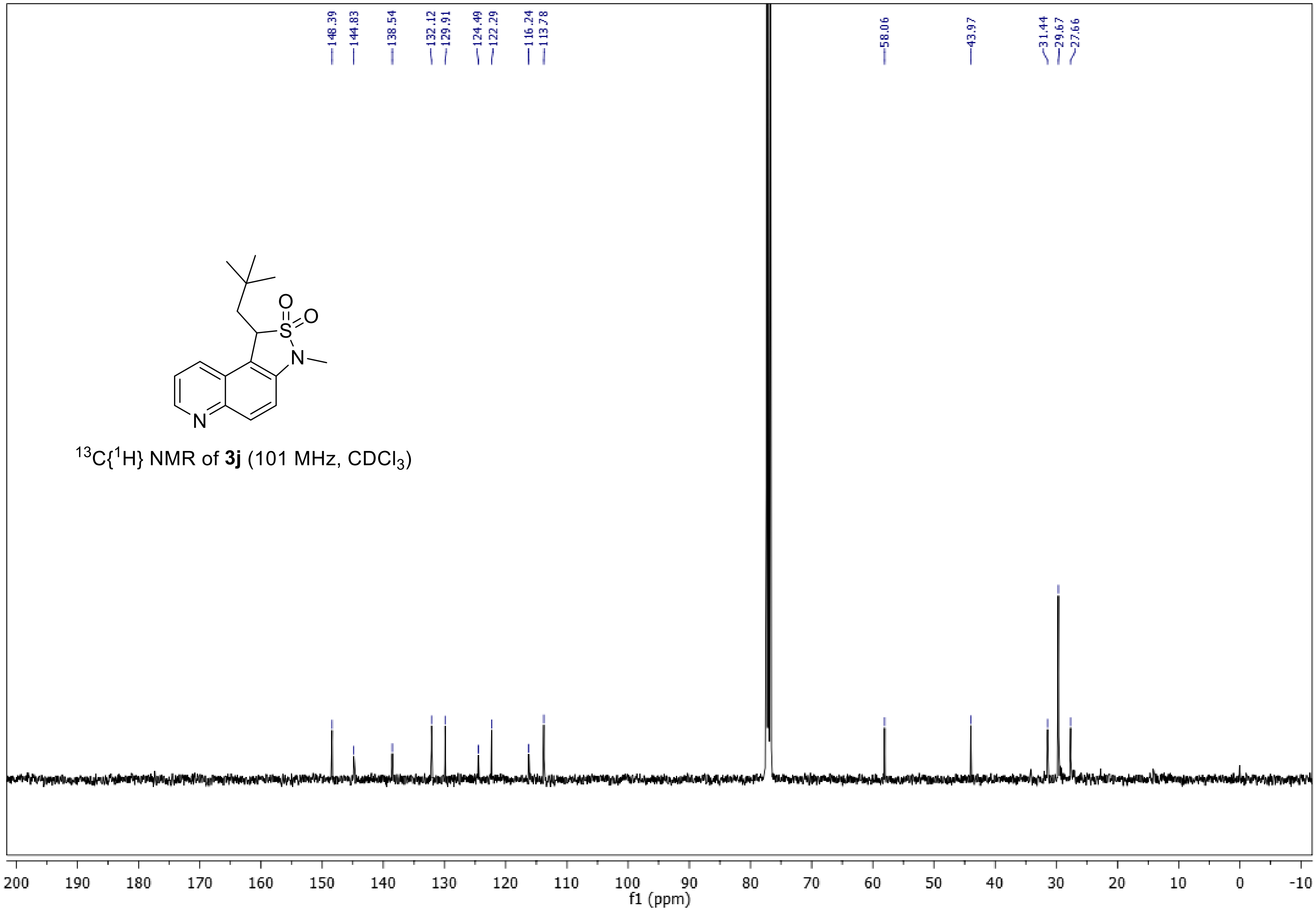
^{1}H NMR of **3i** (300 MHz, $CDCl_3$)



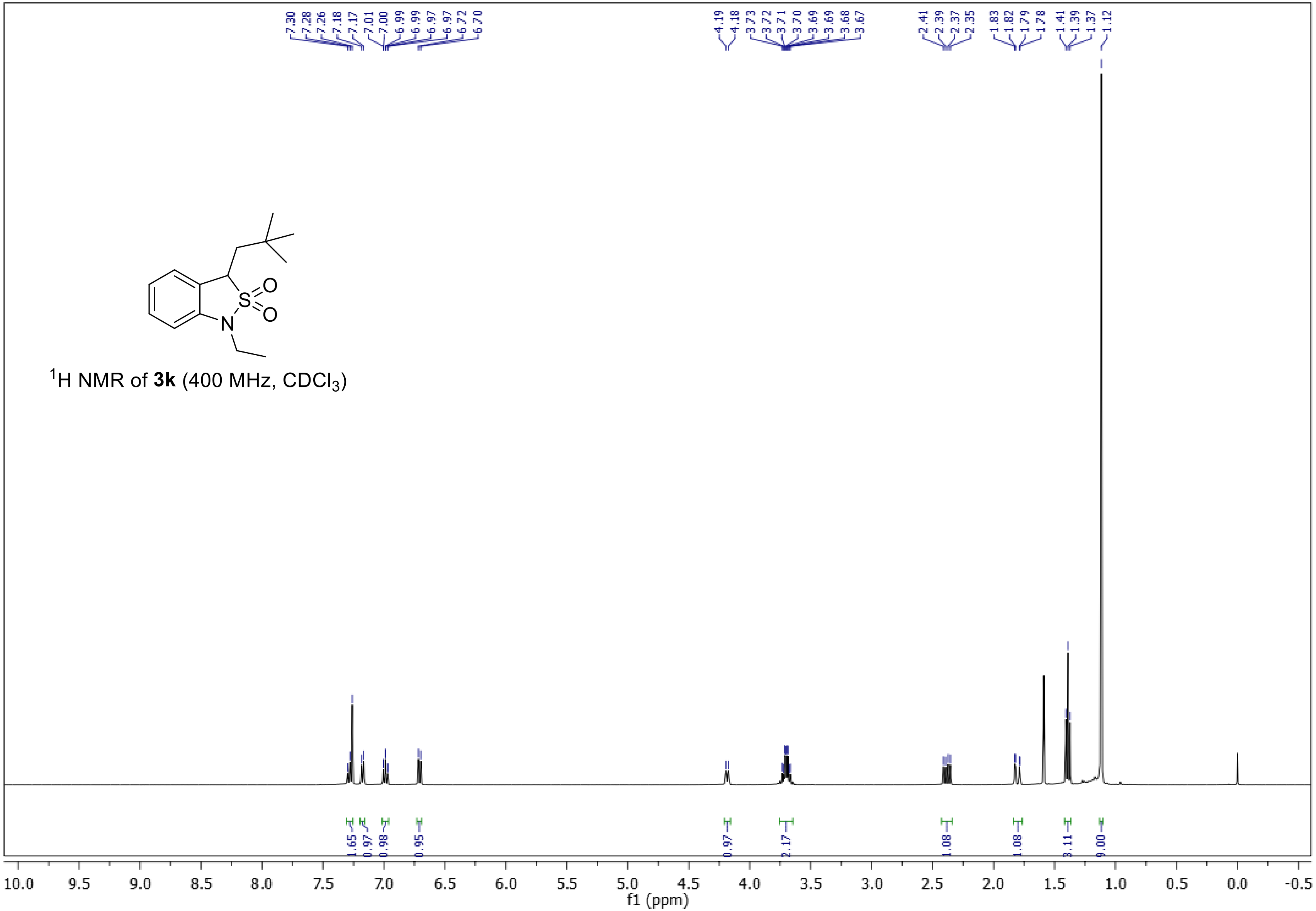
$^{13}C\{^{1}H\}$ NMR of **3i** (126 MHz, $CDCl_3$)



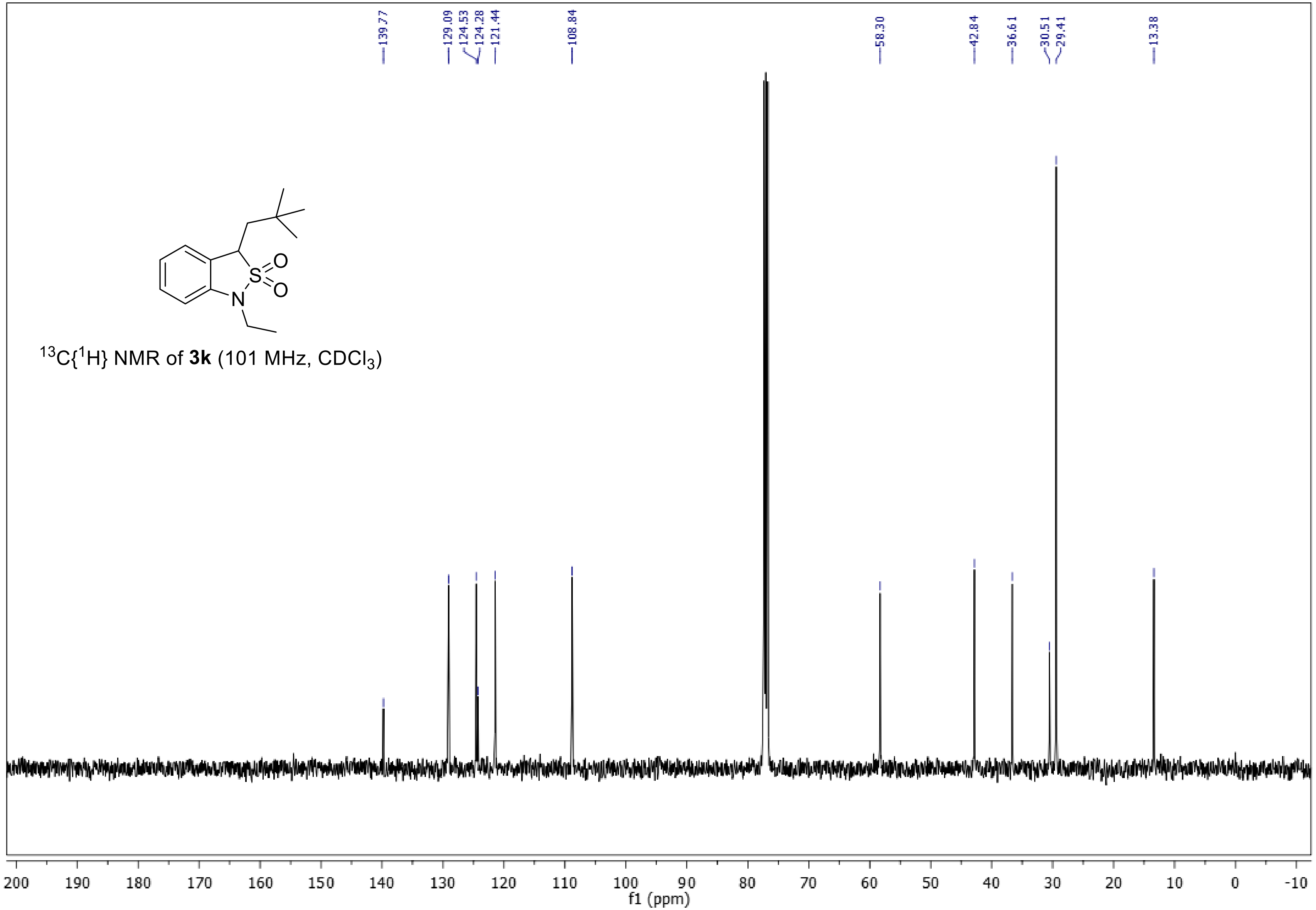
^{1}H NMR of **3j** (300 MHz, $CDCl_3$)



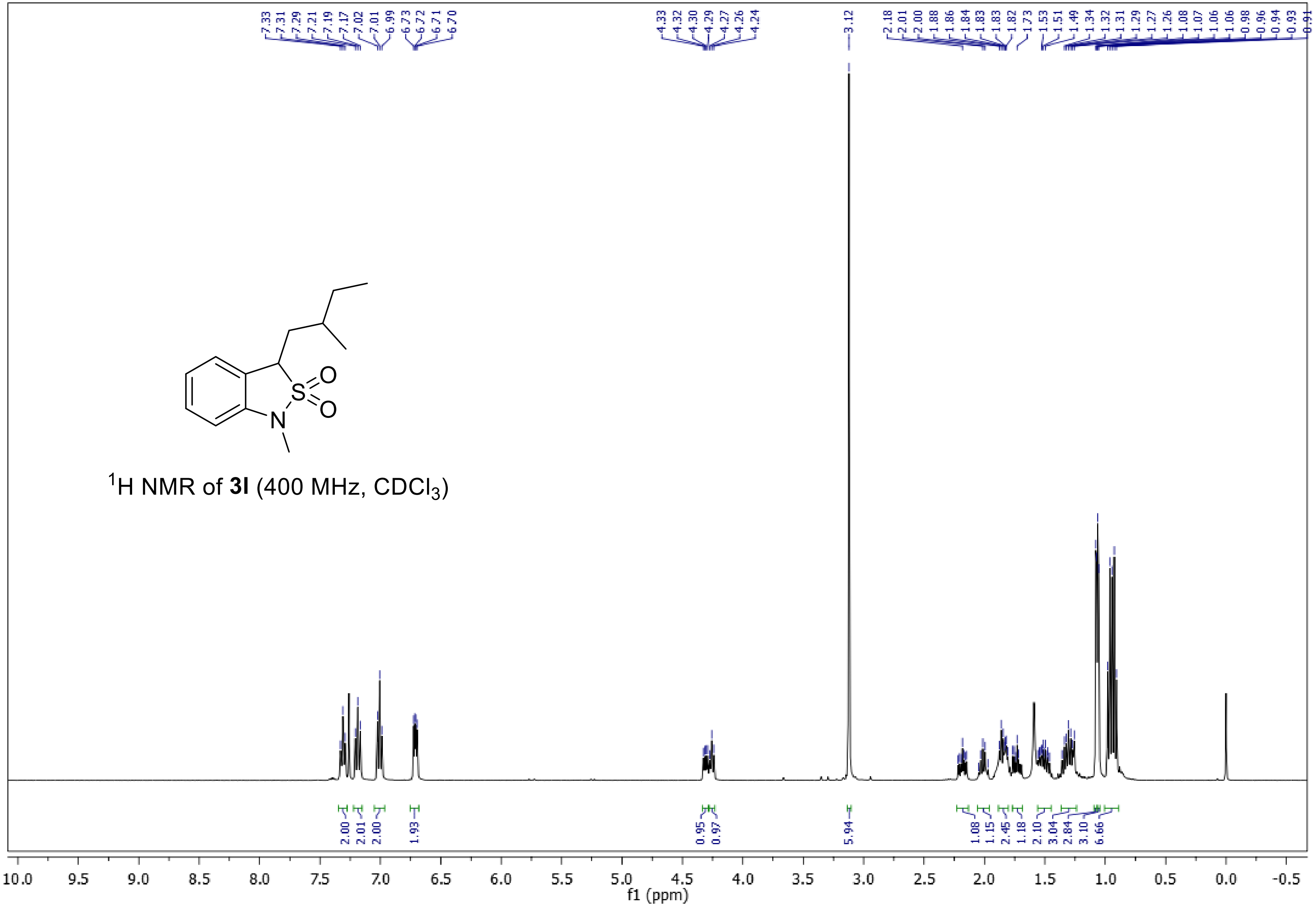
$^{13}C\{^{1}H\}$ NMR of **3j** (101 MHz, $CDCl_3$)



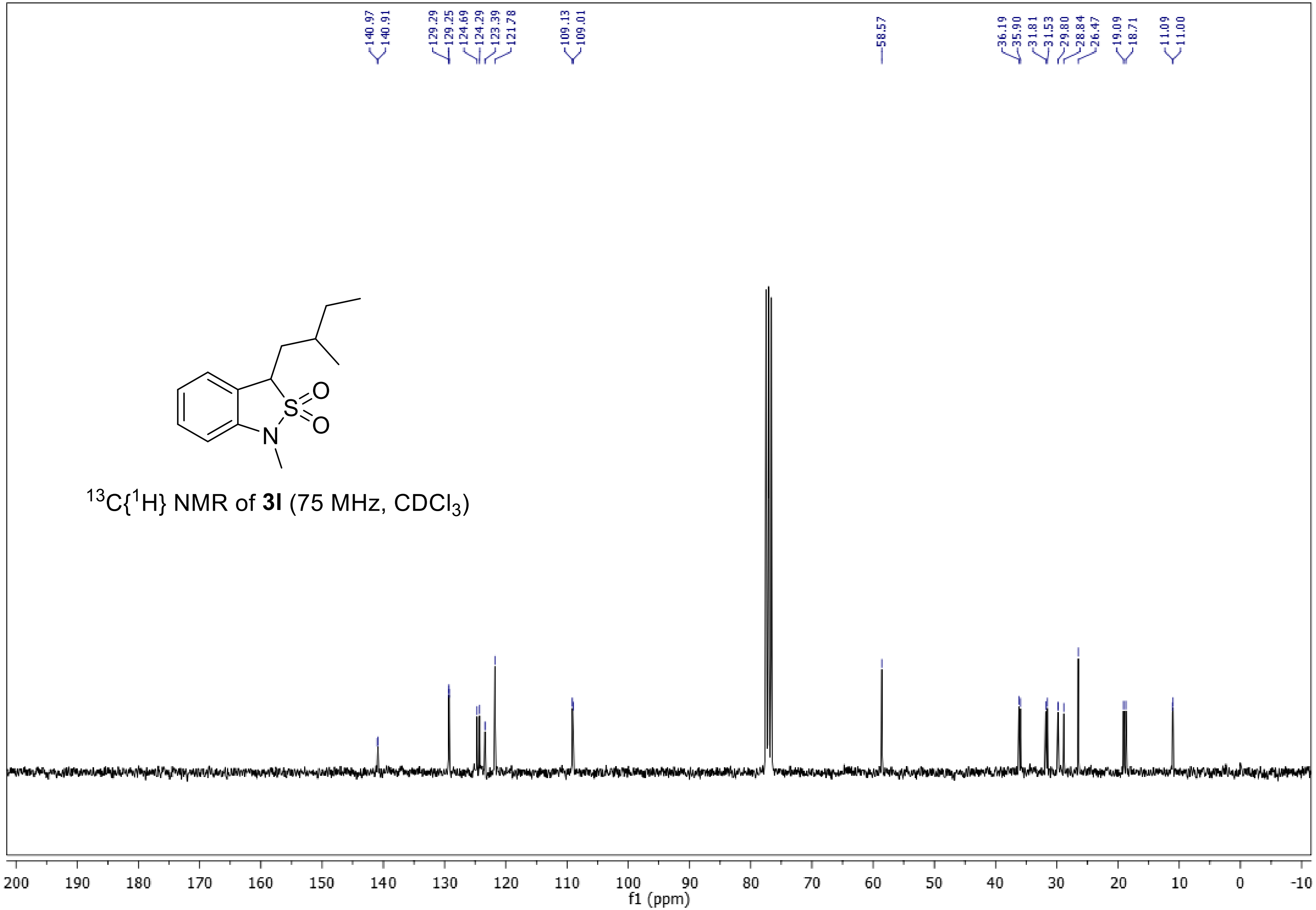
[1]H NMR of **3k** (400 MHz, $CDCl_3$)



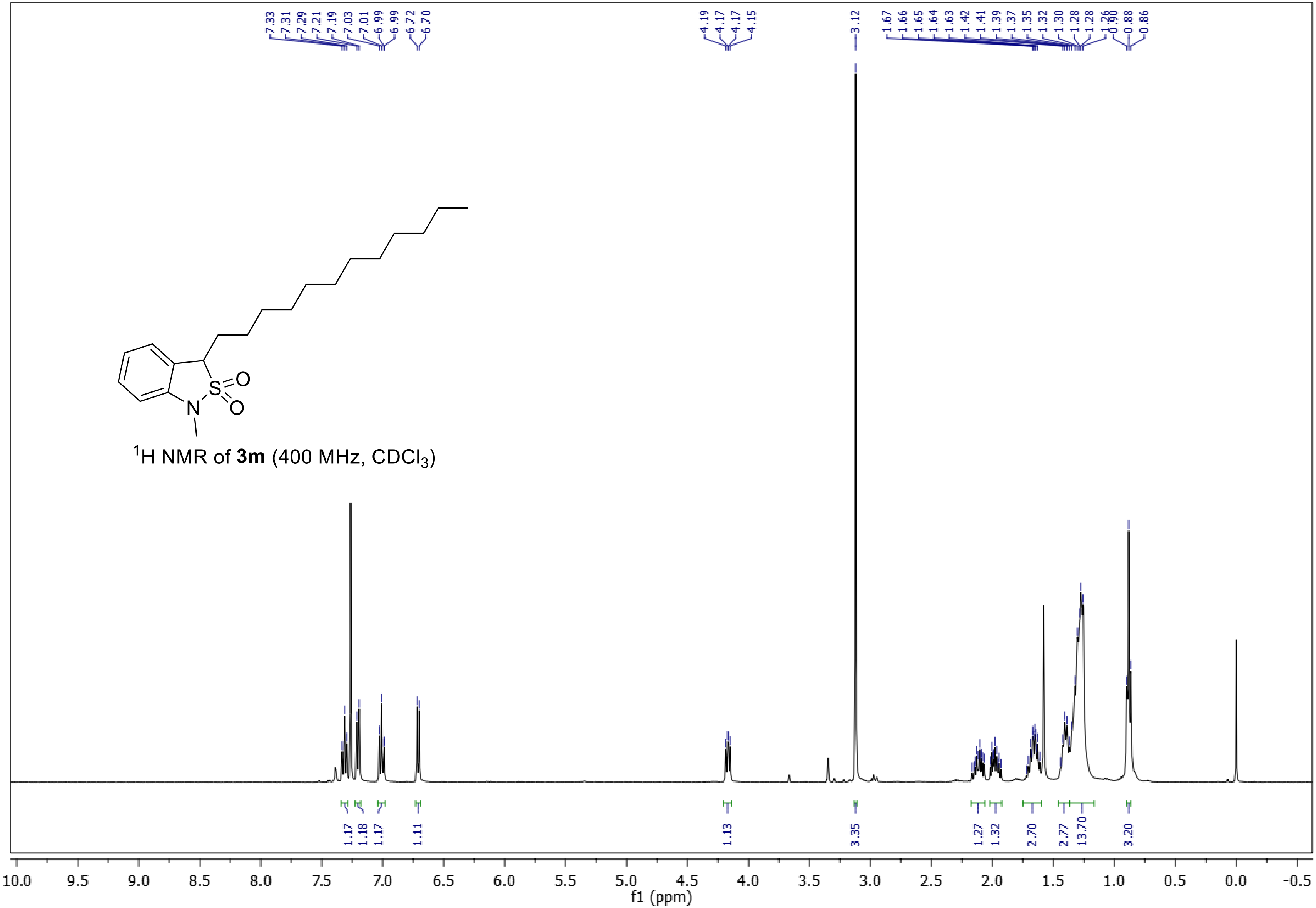
$^{13}C\{^{1}H\}$ NMR of **3k** (101 MHz, $CDCl_3$)



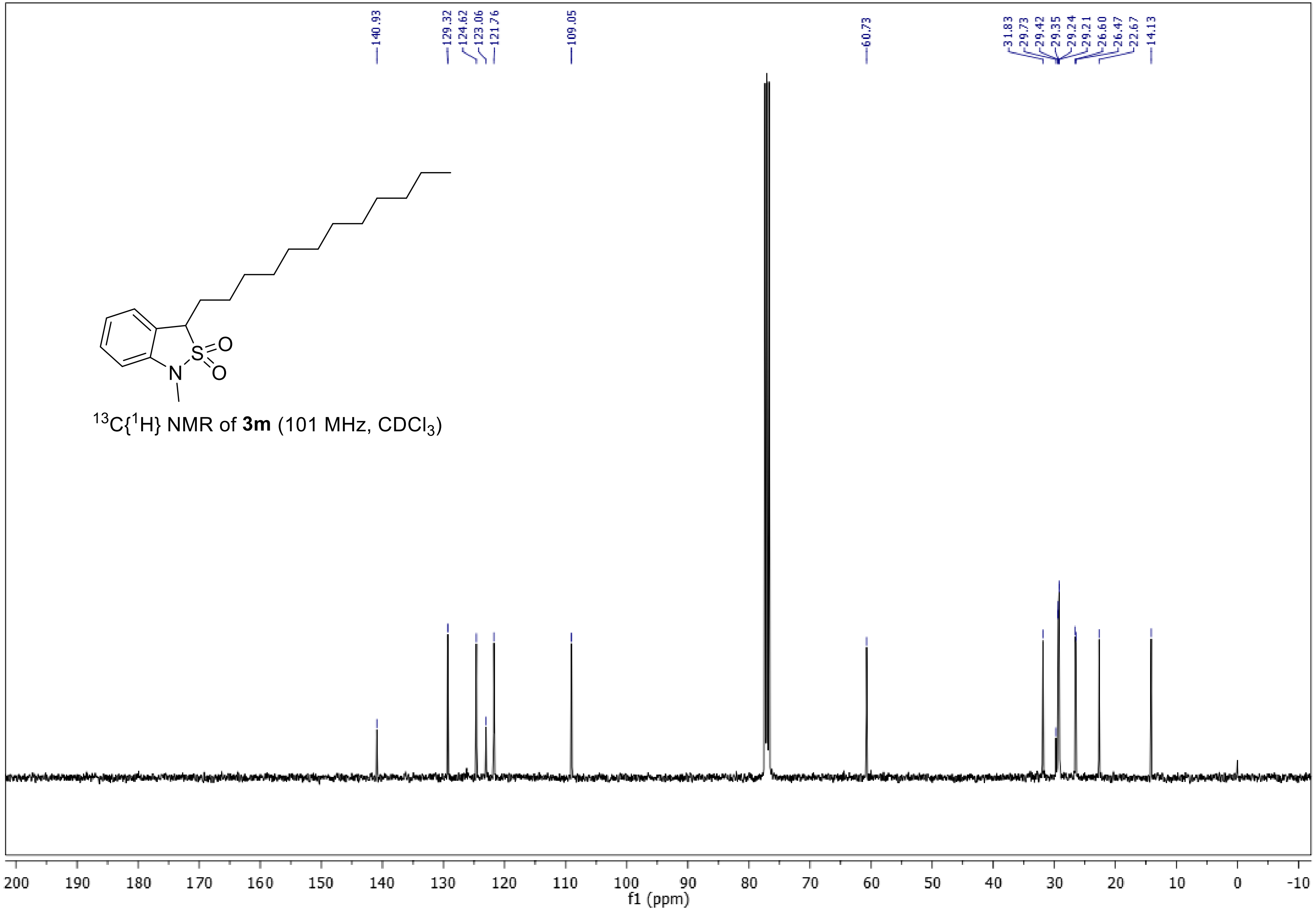
^{1}H NMR of **3l** (400 MHz, $CDCl_3$)



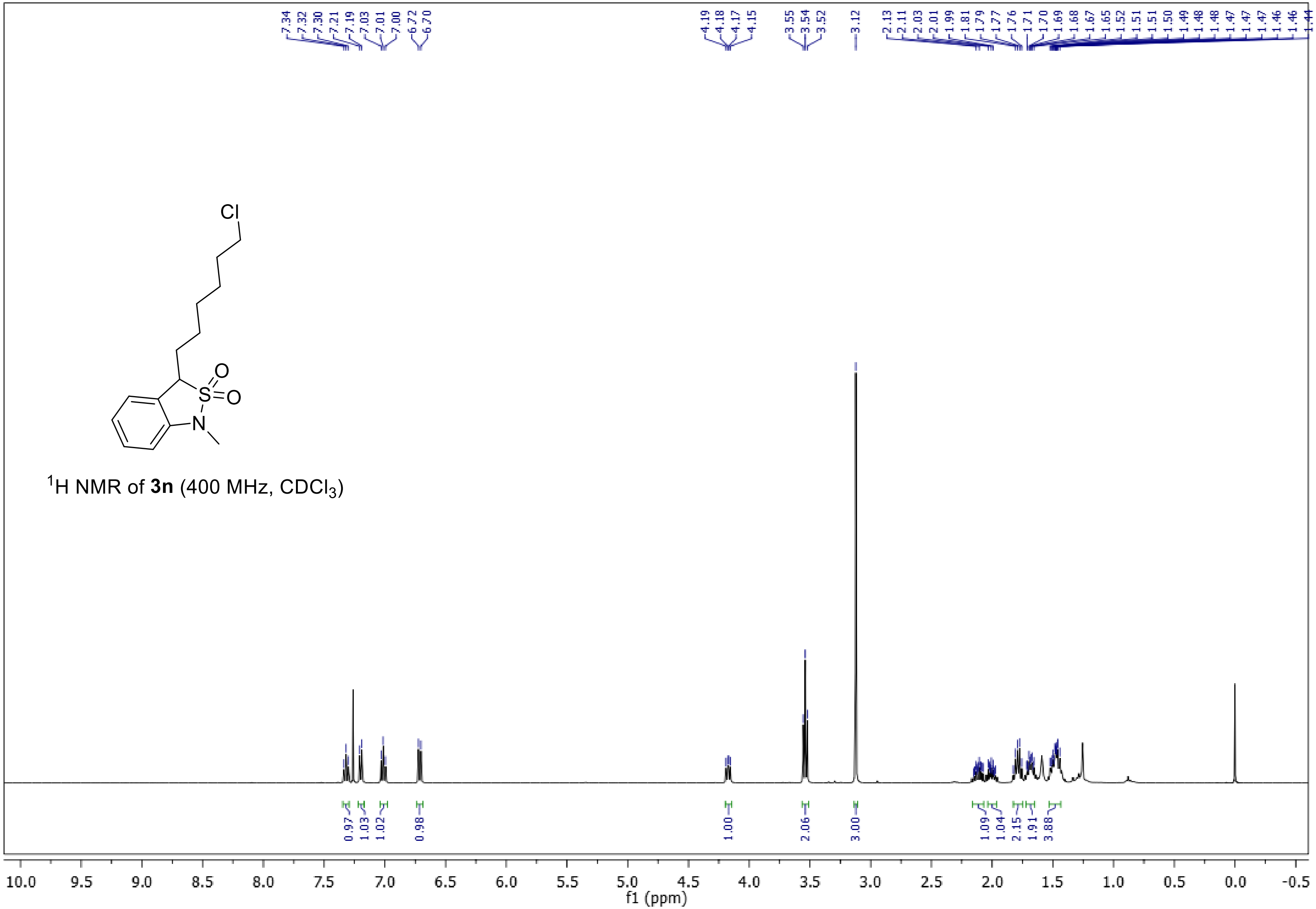
$^{13}C\{^{1}H\}$ NMR of **3l** (75 MHz, $CDCl_3$)



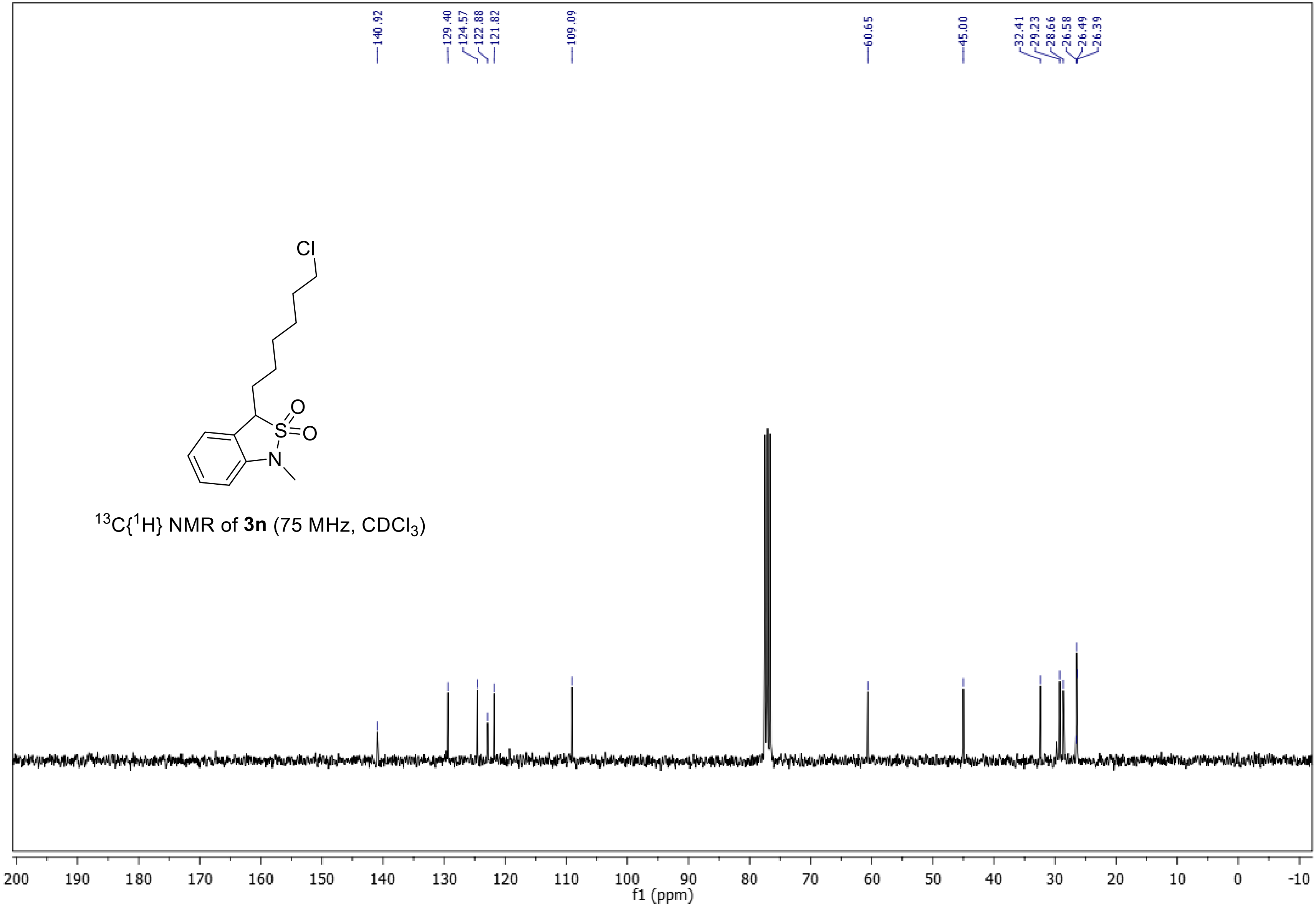
^{1}H NMR of **3m** (400 MHz, $CDCl_3$)



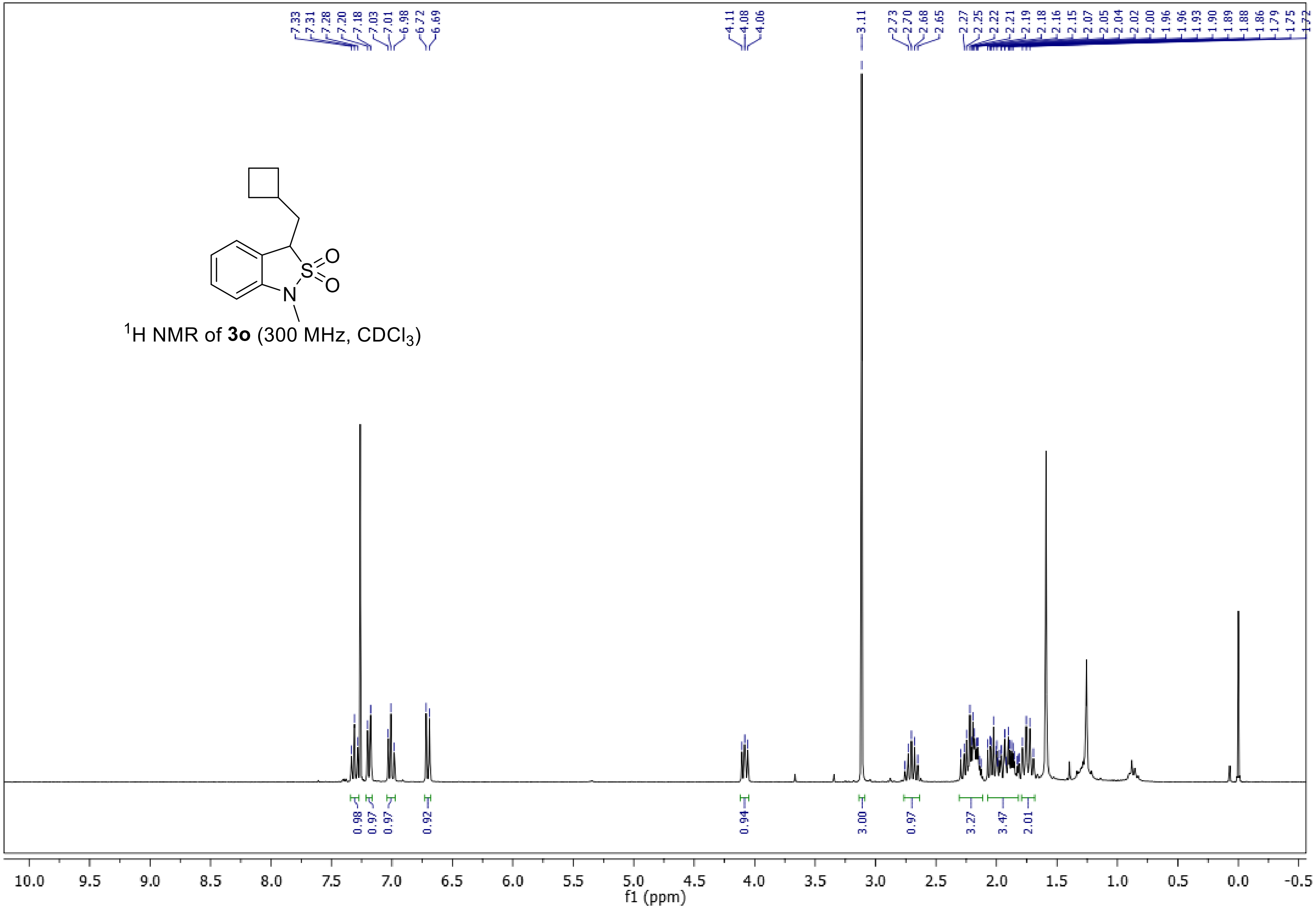
$^{13}C\{^1H\}$ NMR of **3m** (101 MHz, $CDCl_3$)

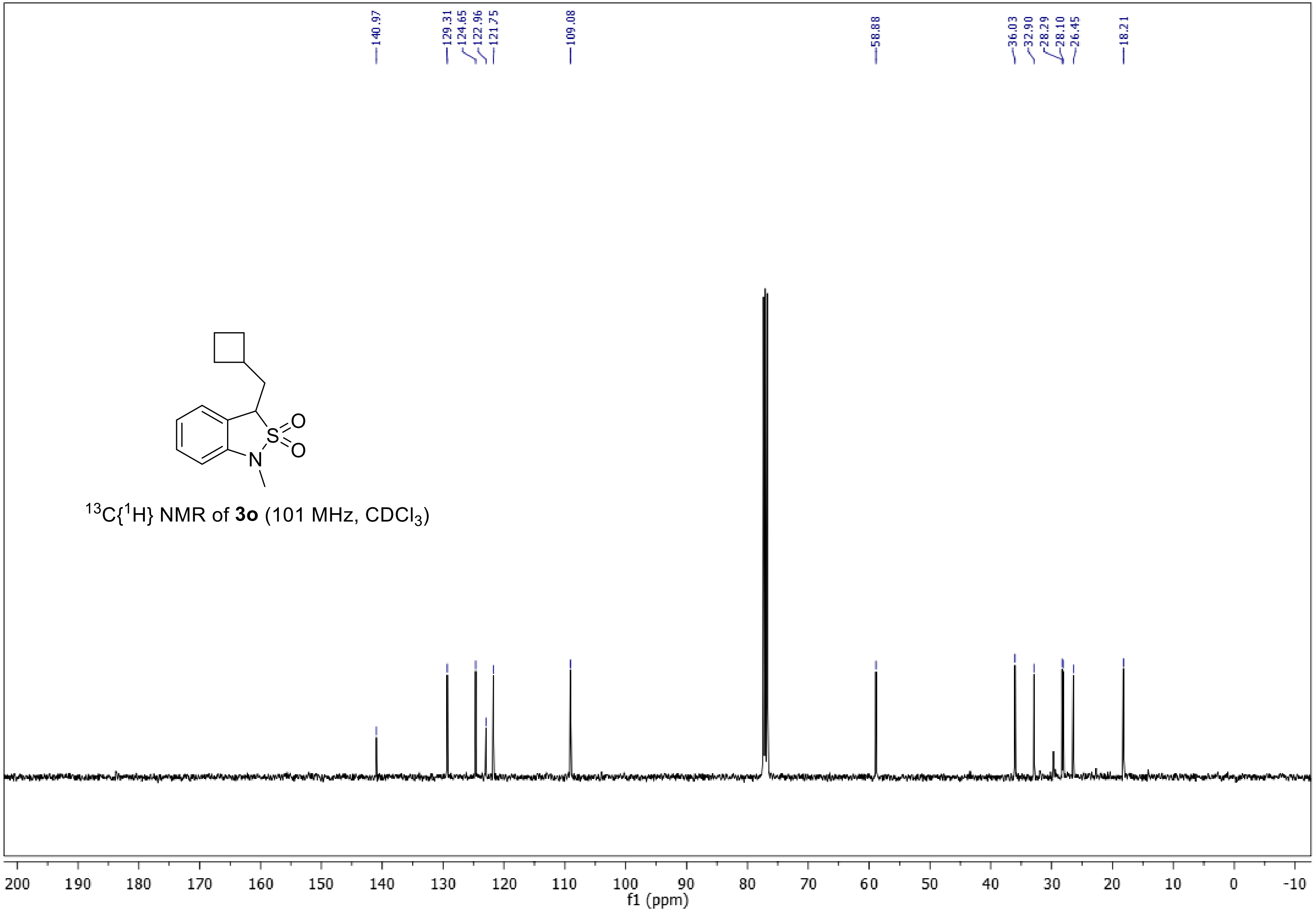


[1]H NMR of **3n** (400 MHz, $CDCl_3$)

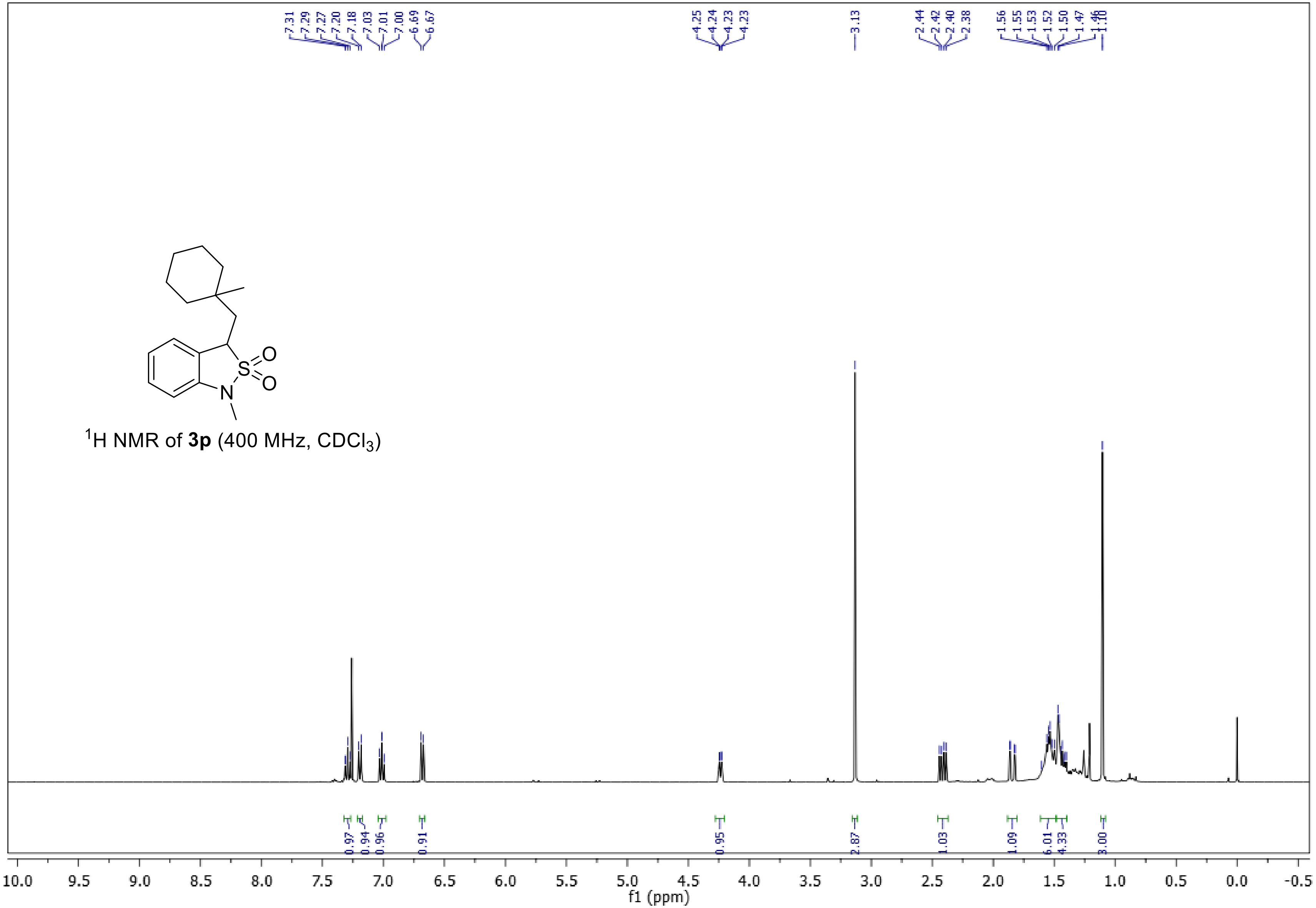


$^{13}C\{^{1}H\}$ NMR of **3n** (75 MHz, $CDCl_3$)

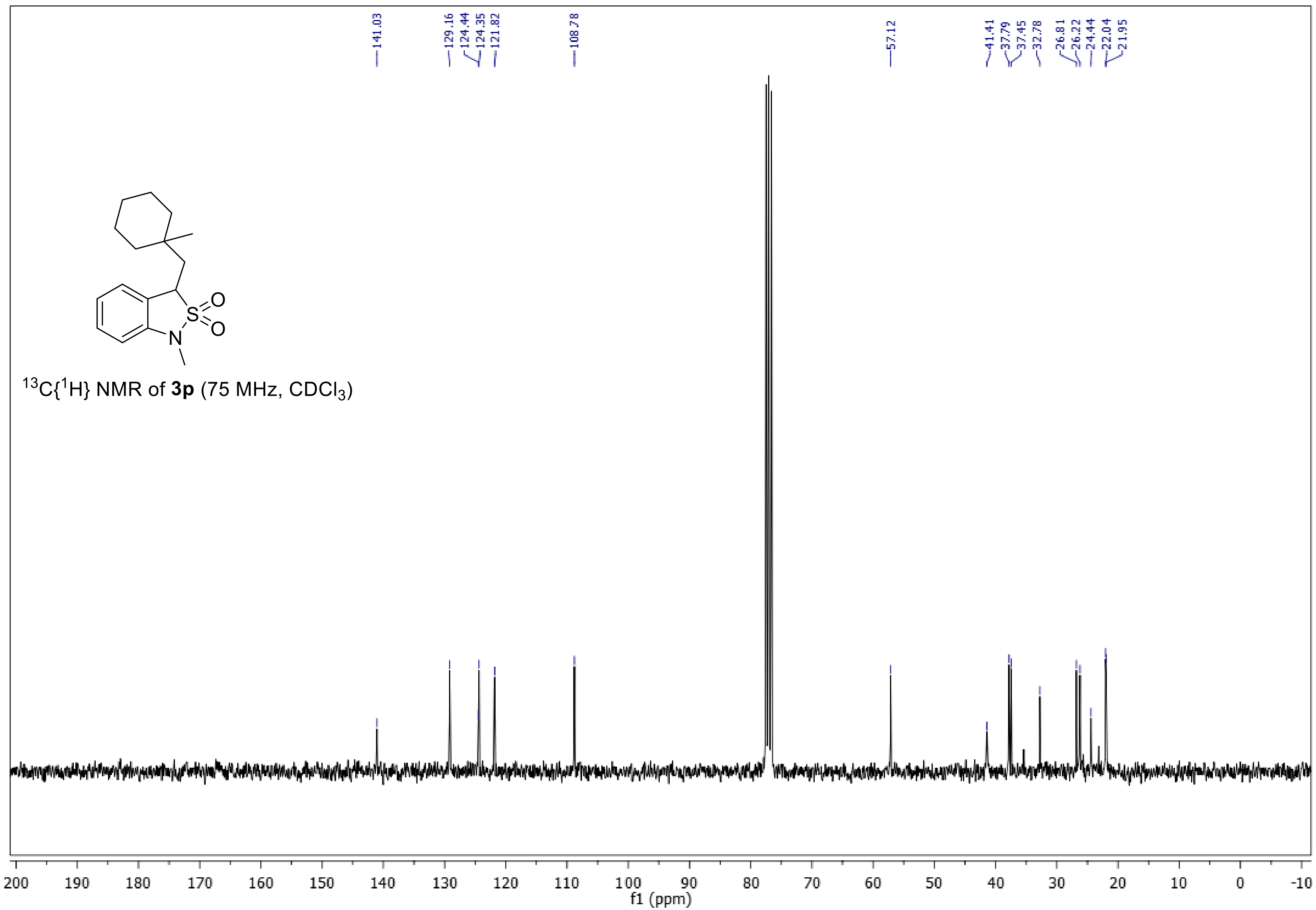

[1]H NMR of 3o (300 MHz, CDCl3)
f1 (ppm)



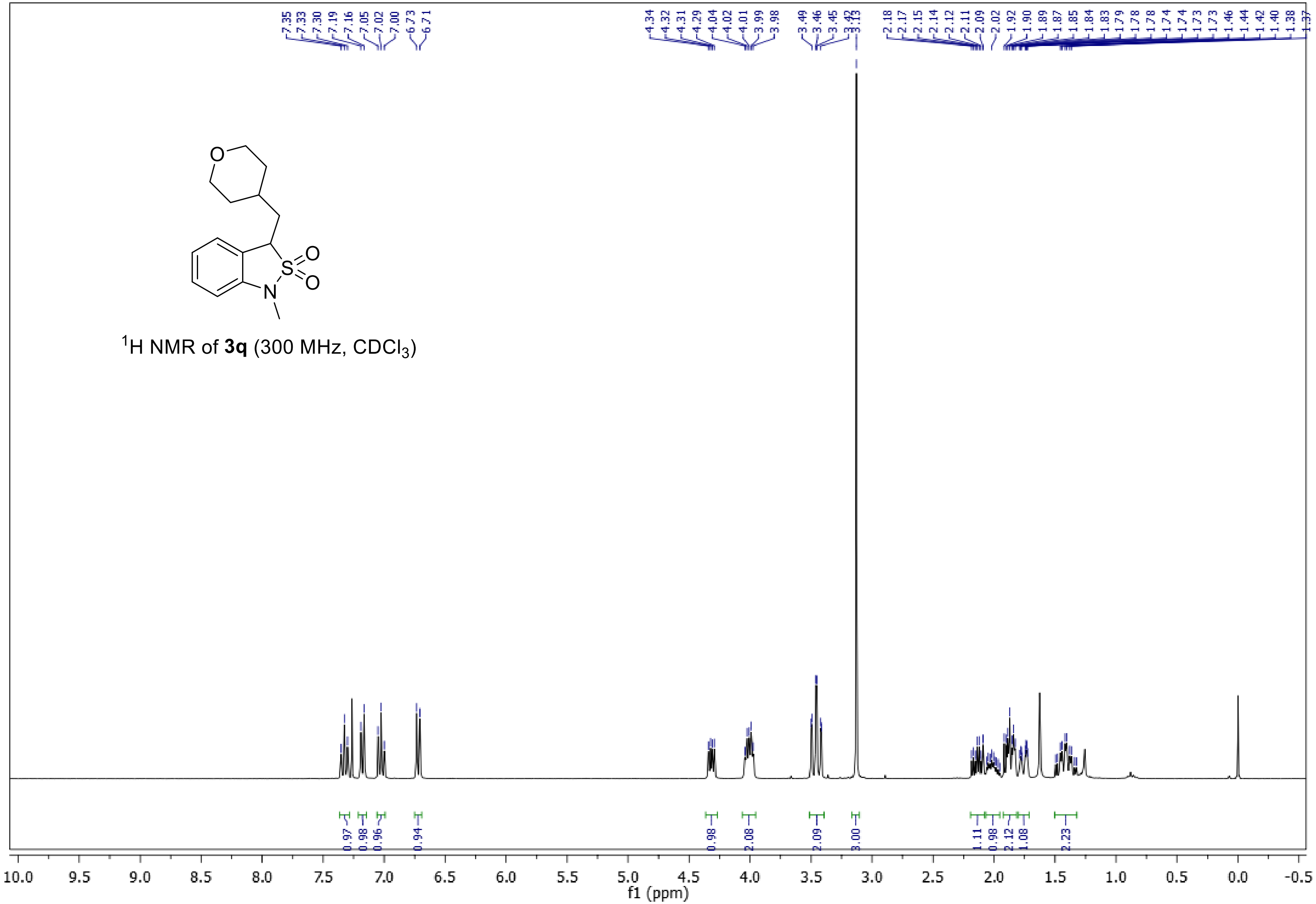
$^{13}C\{^{1}H\}$ NMR of **3o** (101 MHz, $CDCl_3$)



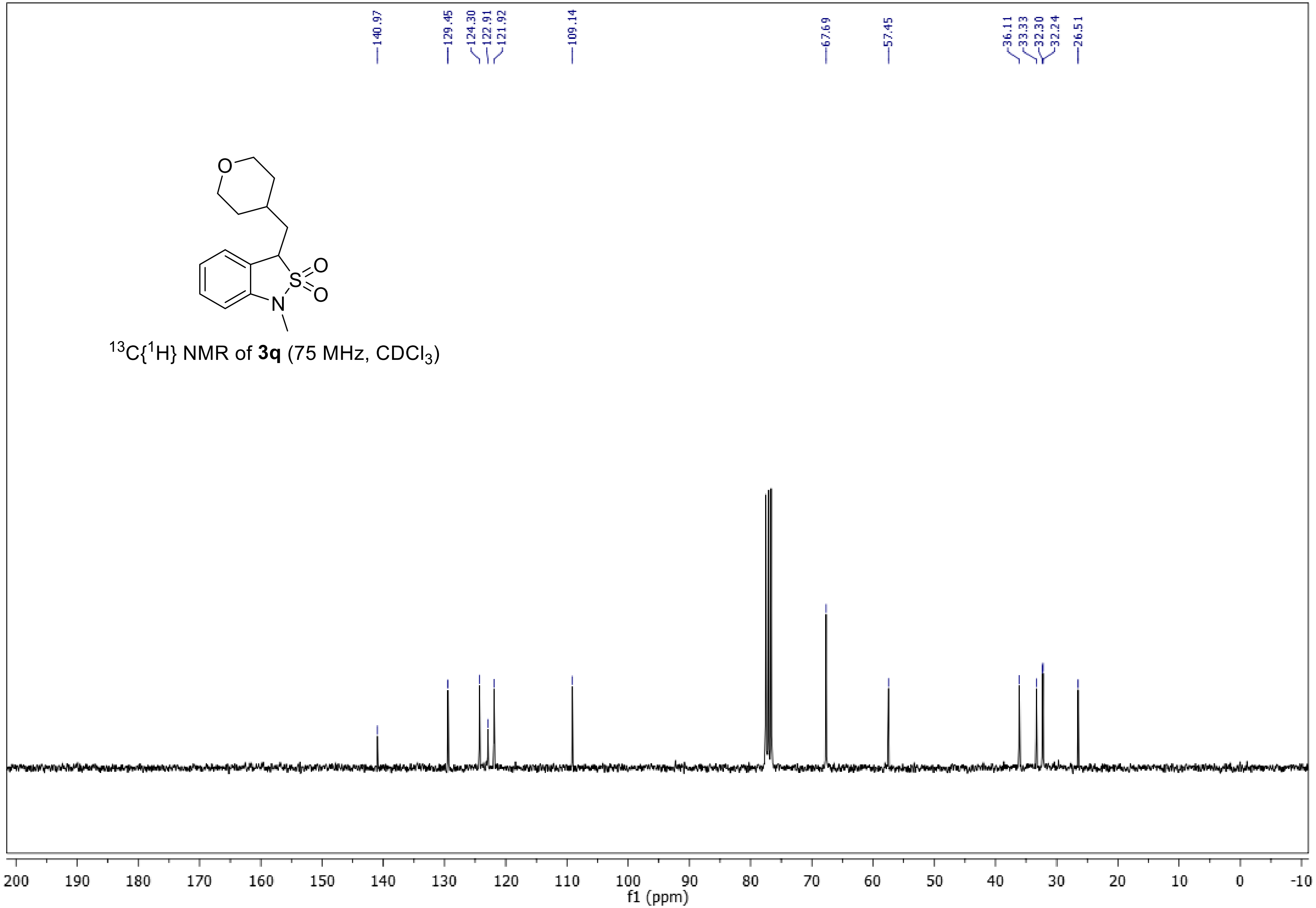
^{1}H NMR of **3p** (400 MHz, $CDCl_3$)



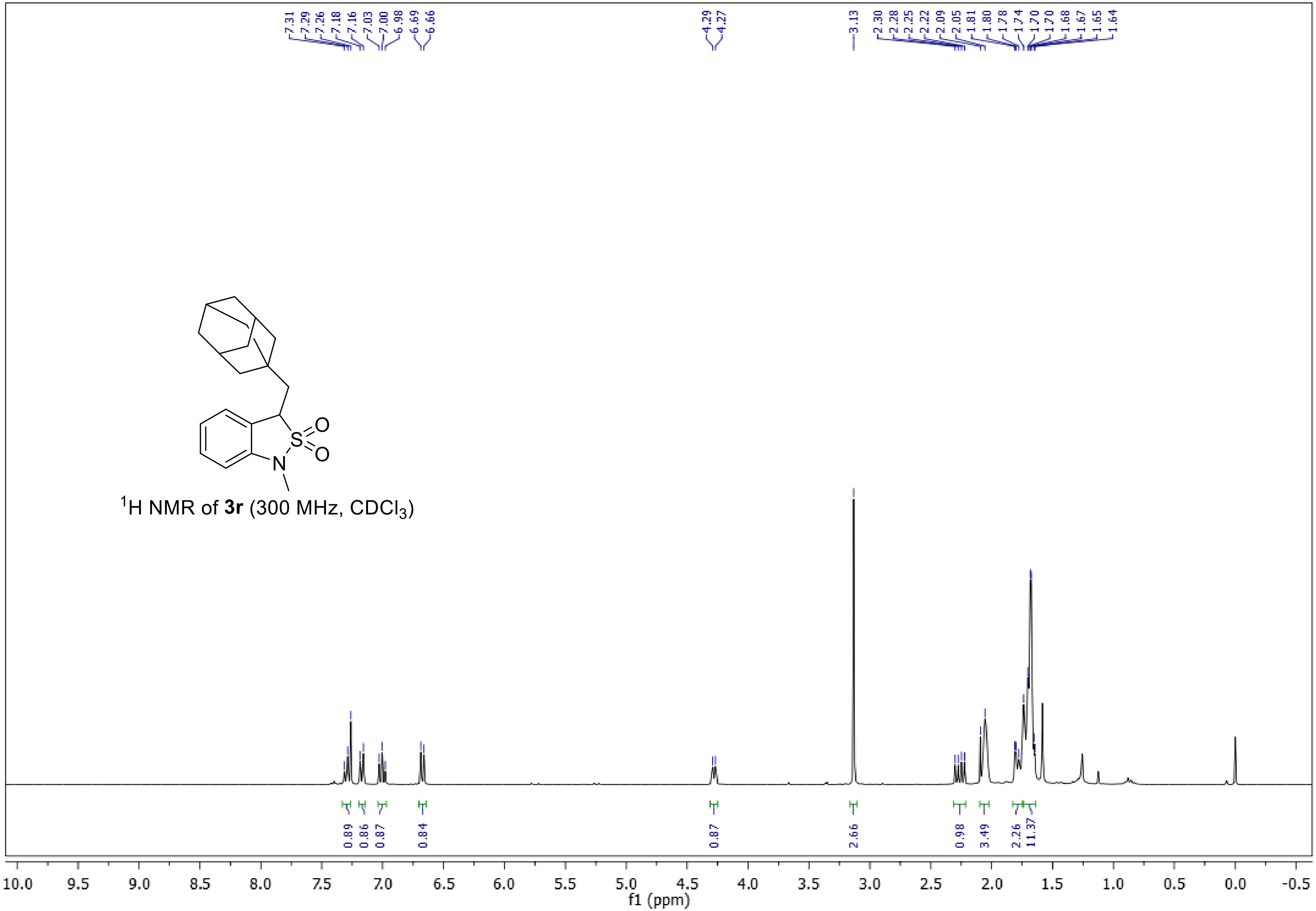
$^{13}C\{^{1}H\}$ NMR of **3p** (75 MHz, $CDCl_3$)



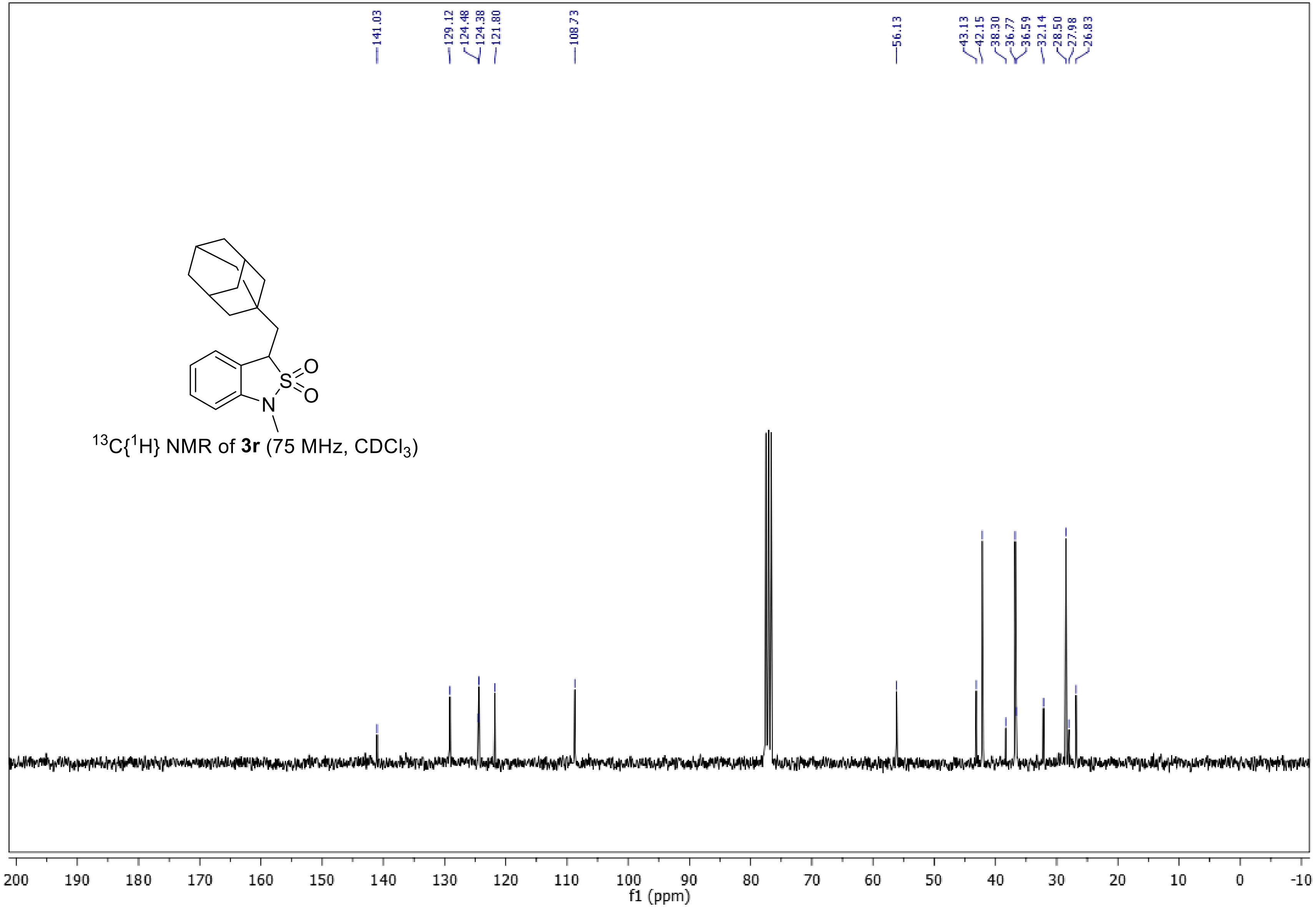
^{1}H NMR of **3q** (300 MHz, $CDCl_3$)



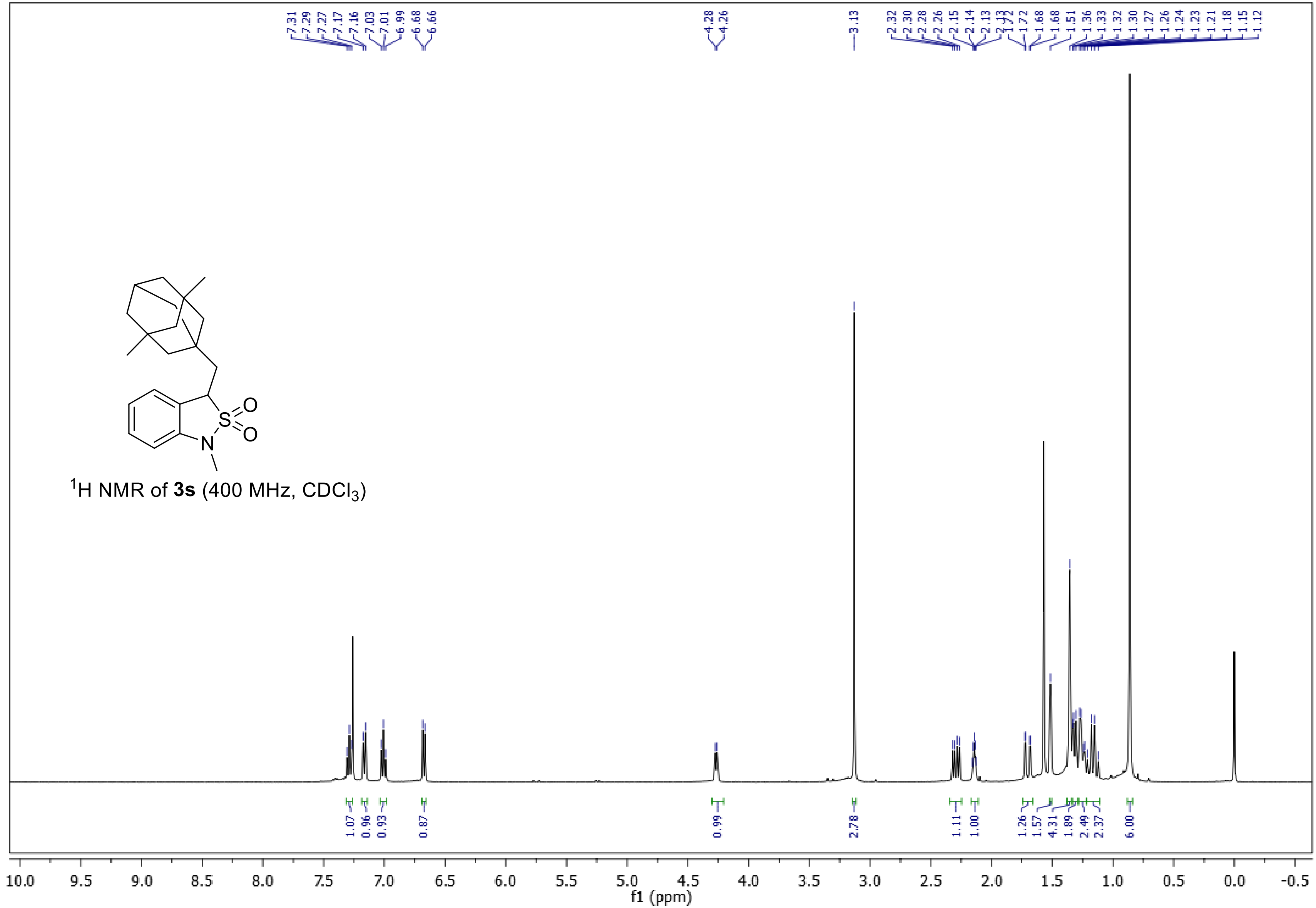
$^{13}C\{^1H\}$ NMR of **3q** (75 MHz, $CDCl_3$)



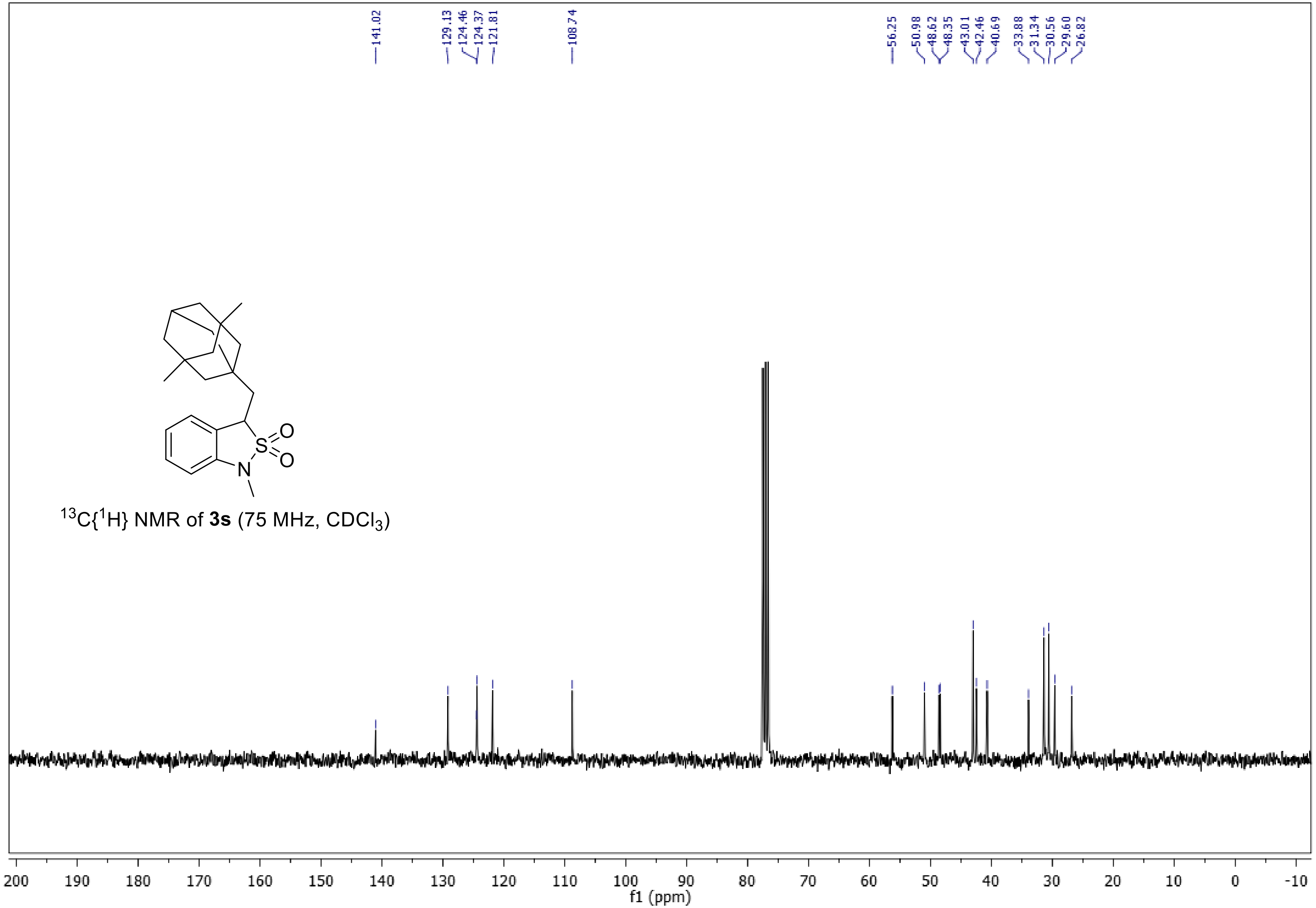
^{1}H NMR of **3r** (300 MHz, $CDCl_3$)



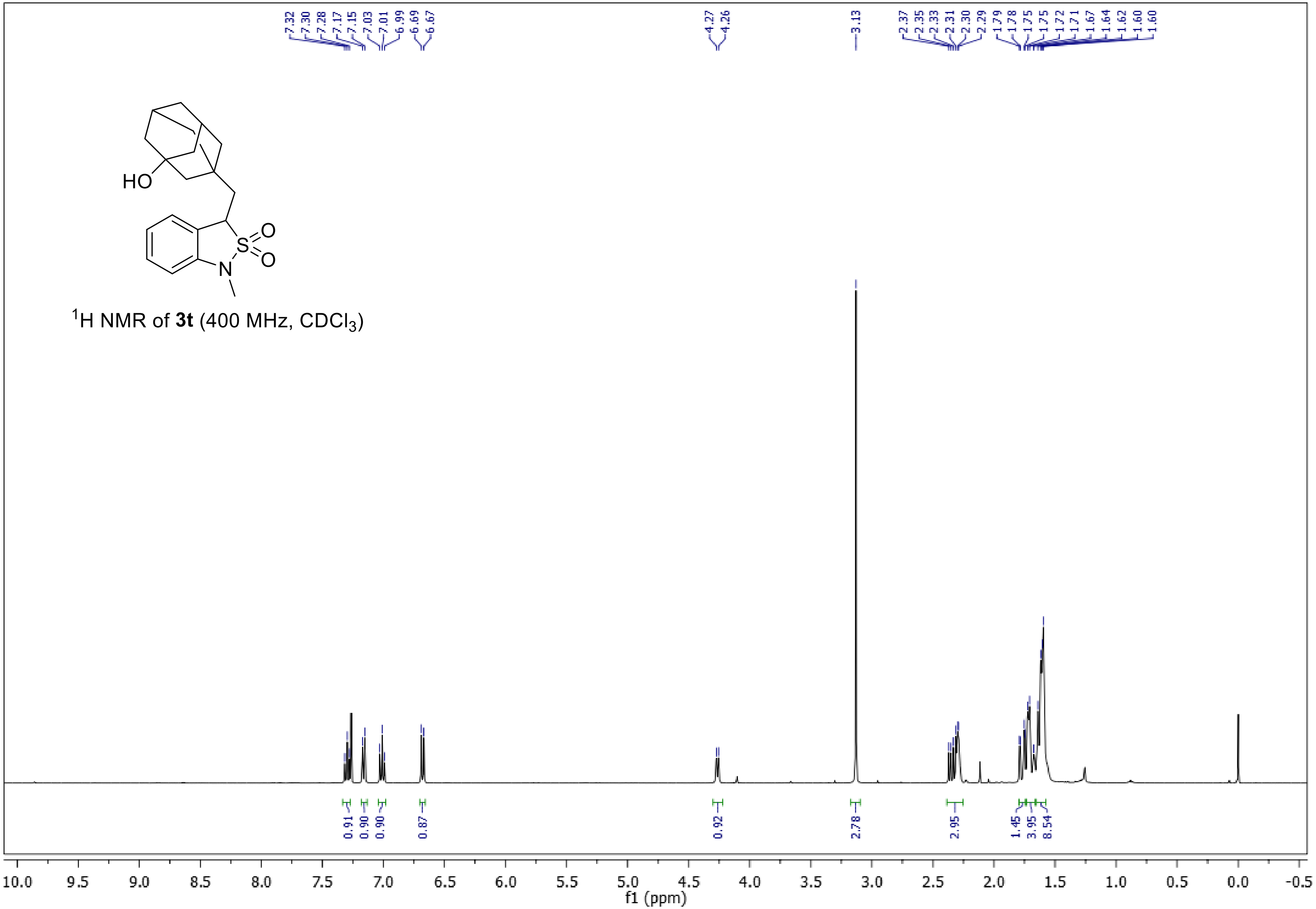
$^{13}C\{^{1}H\}$ NMR of **3r** (75 MHz, $CDCl_3$)



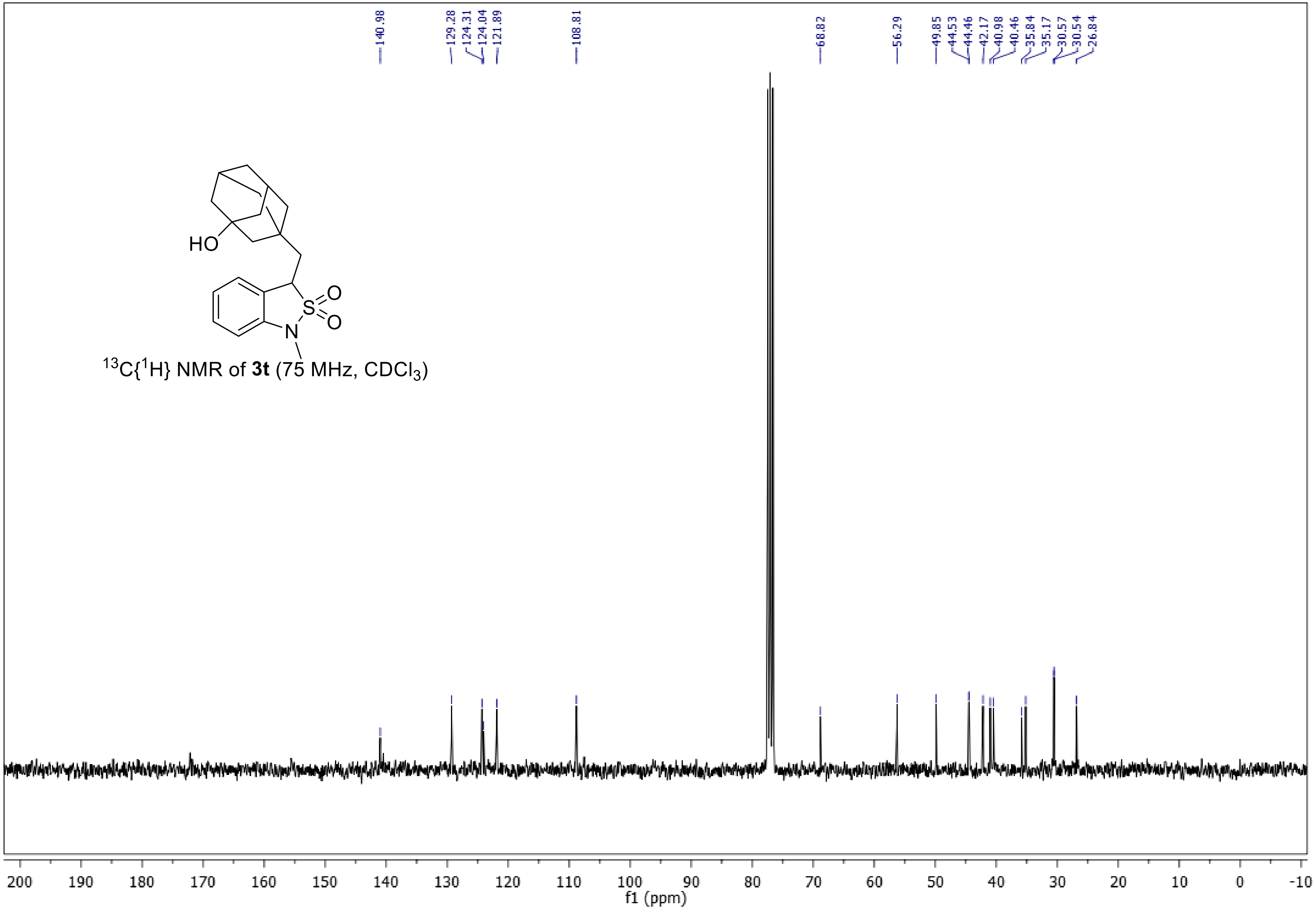
^{1}H NMR of **3s** (400 MHz, $CDCl_3$)



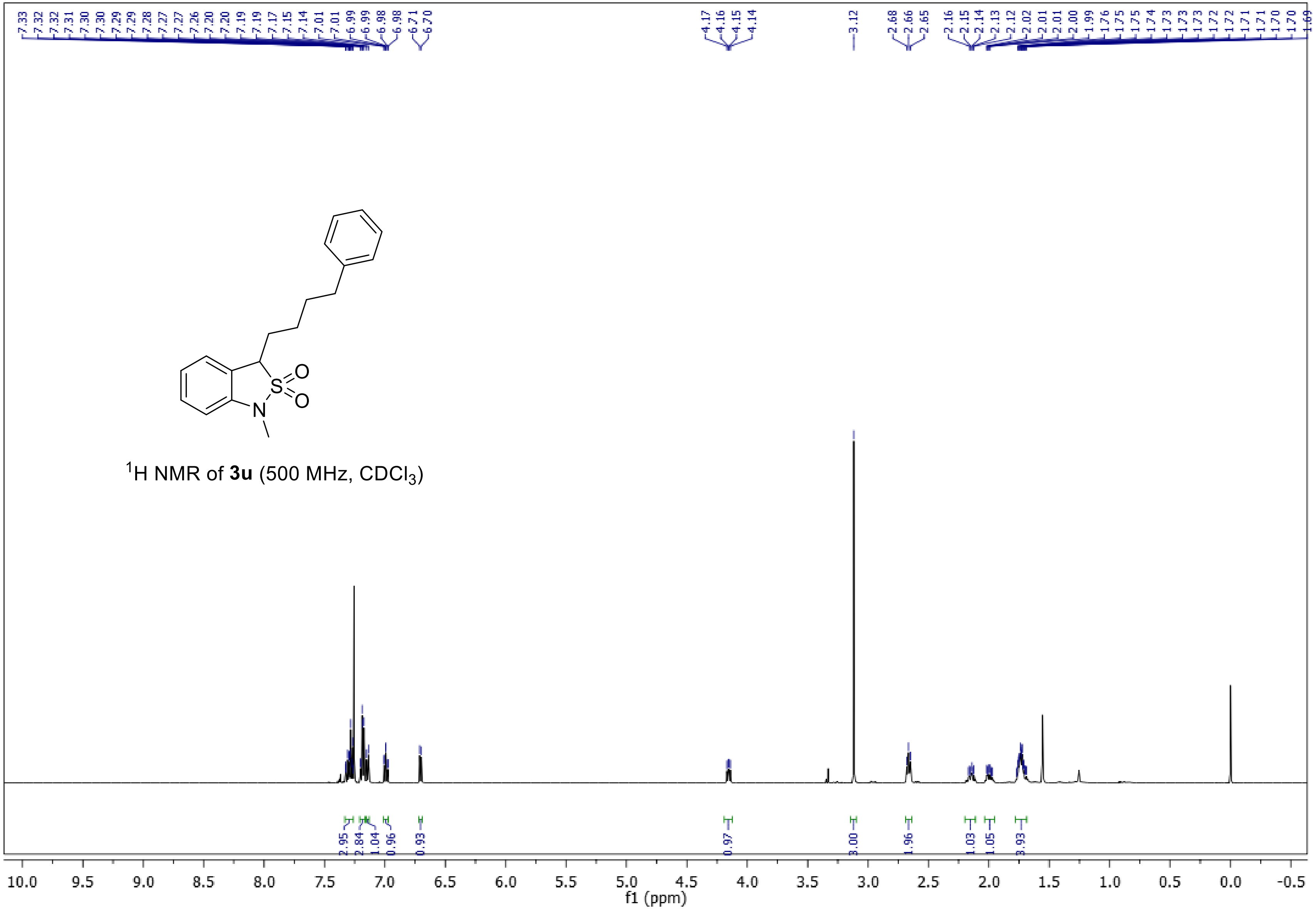
$^{13}C\{^{1}H\}$ NMR of **3s** (75 MHz, $CDCl_3$)



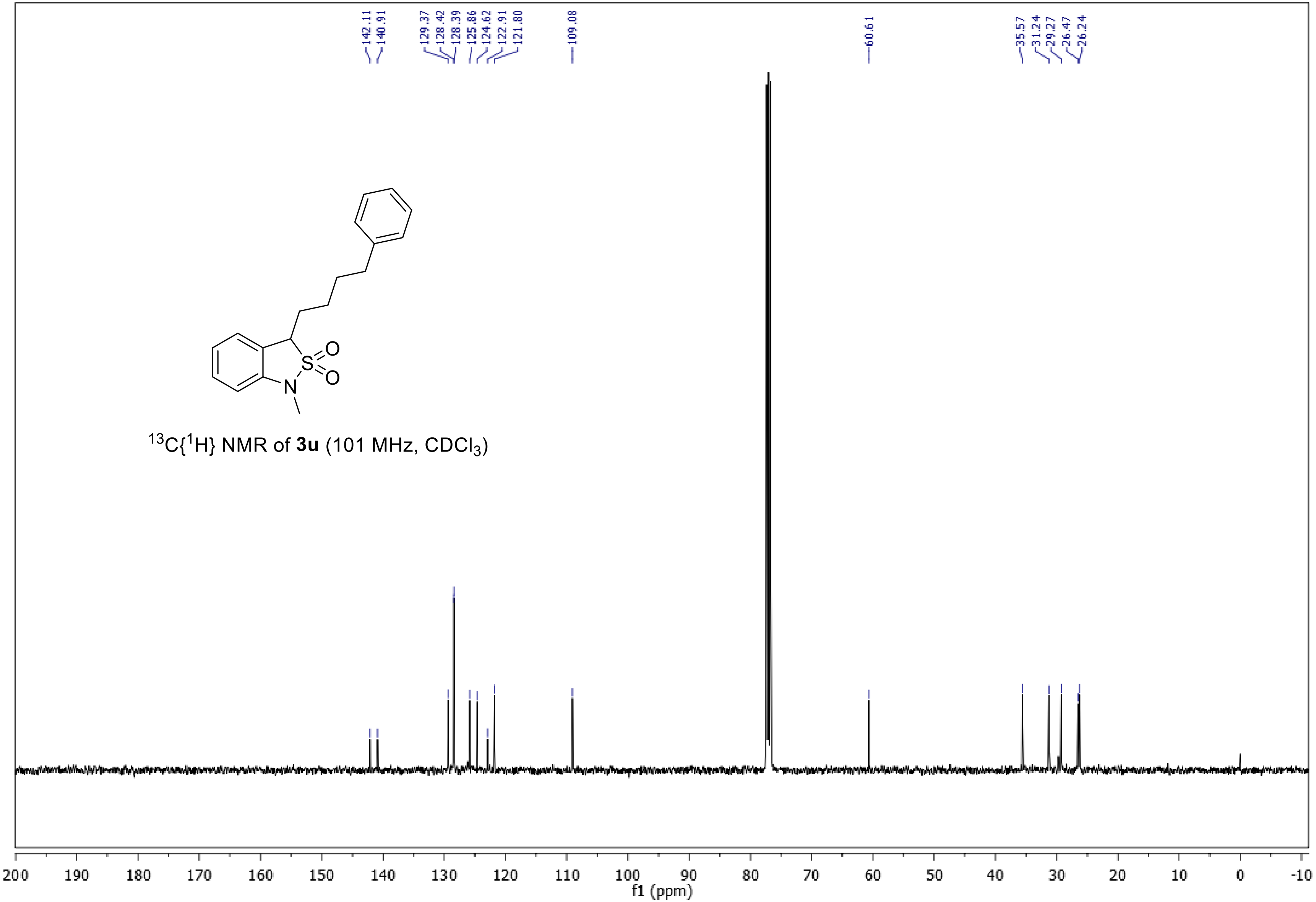
7.32
7.30
7.28
7.17
7.15
7.03
7.01
6.99
6.69
6.67
4.27
4.26
3.13
2.37
2.35
2.33
2.31
2.30
2.29
1.79
1.78
1.75
1.75
1.72
1.71
1.67
1.64
1.62
1.60
1.60
HO
S
O
O
N
^{1}H NMR of **3t** (400 MHz, $CDCl_3$)
0.91
0.90
0.90
0.87
0.92
2.78
2.95
1.45
3.95
8.54
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



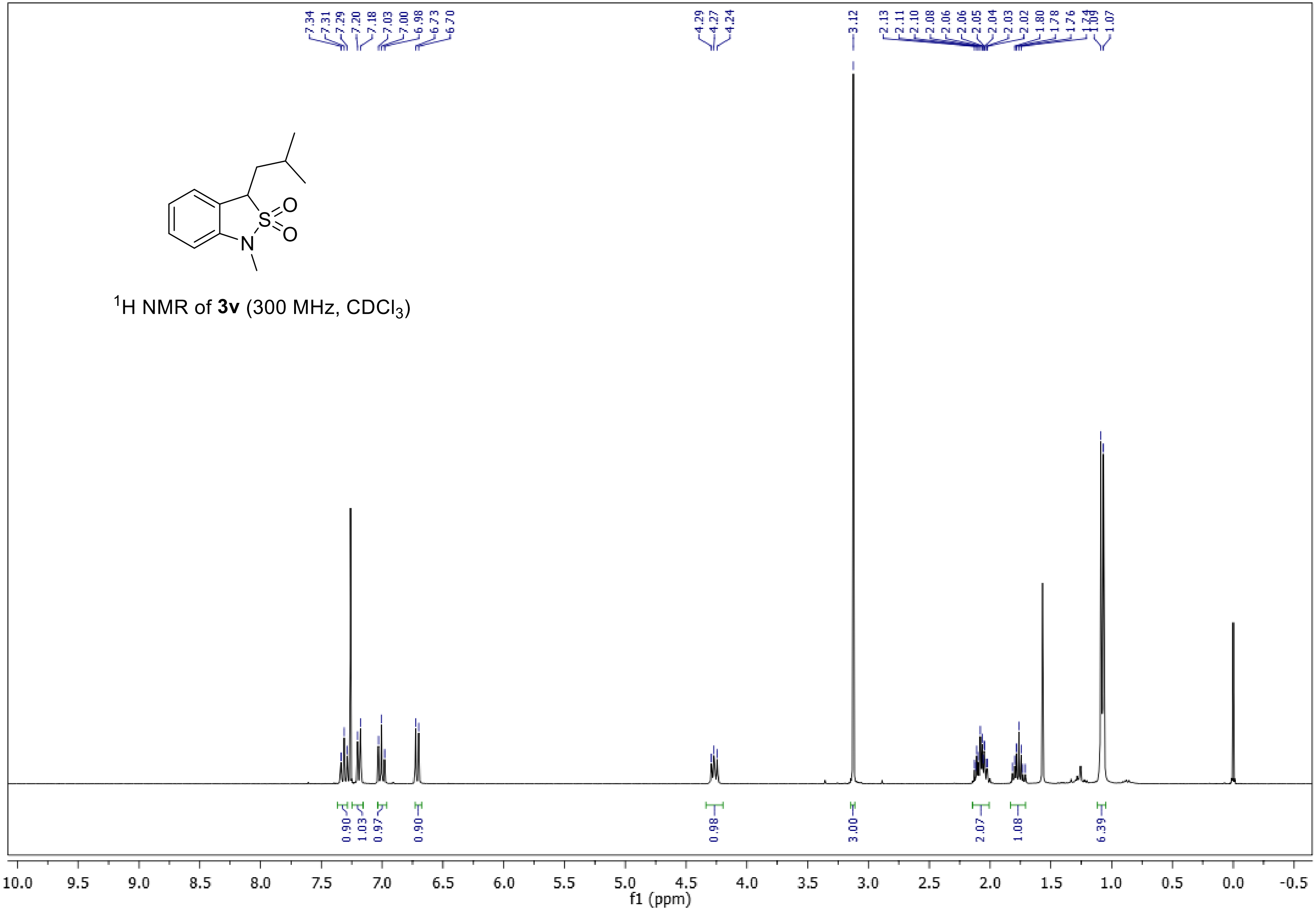
$^{13}C\{^{1}H\}$ NMR of **3t** (75 MHz, $CDCl_3$)



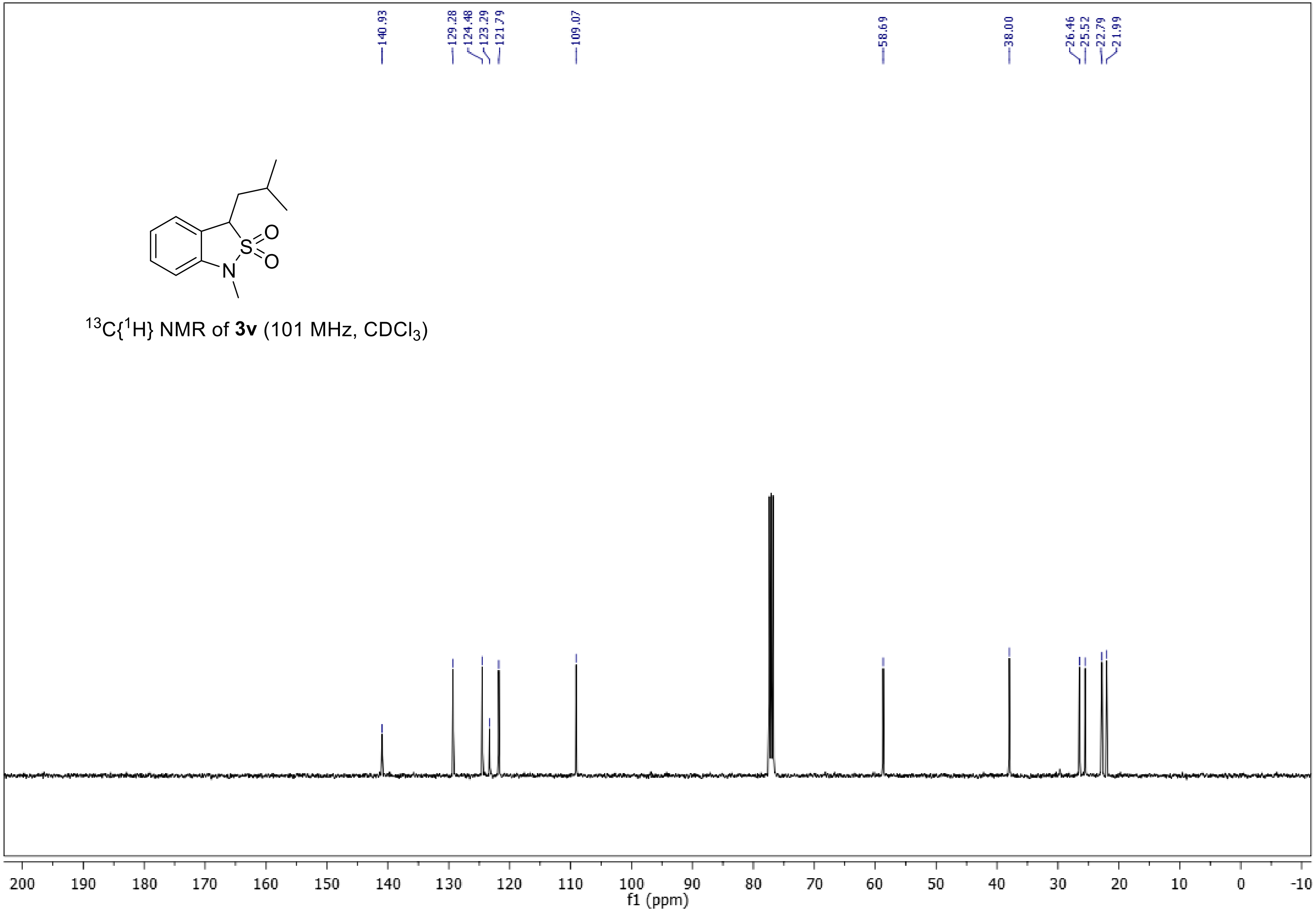
^{1}H NMR of **3u** (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR of **3u** (101 MHz, $CDCl_3$)



^{1}H NMR of **3v** (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR of **3v** (101 MHz, $CDCl_3$)

References:

1) D. Vytla, K. Kaliyaperumal, R. Velayuthaperumal, P. Shaw, R. Gautam, A. Mathur, A. Roy. *Synthesis*, 2022, **54**, 667– 682.
2) Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
3) Sheldrick G. M. (2015). ActaCrystallogr. C71: 3-8.