Supporting Information

Direct Conversion of Carboxylic Acids to Free Thiols via Radical Relay Acridine Photocatalysis Enabled by N–O Bond Cleavage

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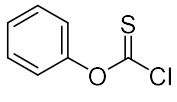
General Methods

Precoated silica gel plates F-254 were used for thin-layer analytical chromatography visualizing with UV and/or acidic aq. $KMnO_4$ solution. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and time-of-flight (TOF) mass analyzer. The measurements were done in a positive ion mode (interface capillary voltage – 4500 V) or in a negative ion mode (3200 V); mass range from m/z 50 to m/z 3000. For irradiation, a strip of light emitting diodes smd 3528, 50 cm (3528-120LED-1M, 12 V, IP 33; 60W 400 nm) was used. Reactions were performed in a glass tube (outer diameter 12 mm, inner diameter 9 mm). The reaction tube was placed in a glass jacket cooled with water (water temperature *ca*. 20 °C), and the system was wrapped by a strip of LEDs. The distance between the reaction vessel and diodes was about 1 cm.

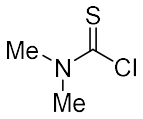
Starting materials

All reactions were performed under air atmosphere unless otherwise noted. Acetonitrile, ethylacetate, 1,2-dichloroethane, toluene and dichloromethane were distilled from CaH_2. All commercial reagents were used without further purification unless otherwise stated.

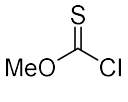
Following compounds were prepared according to literature procedures:



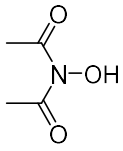
SI–1 [1]



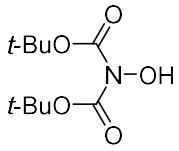
SI–2 [2]



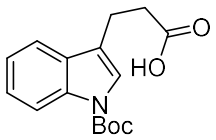
SI–3 [3]



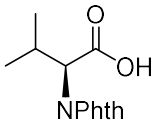
SI–4 [4]



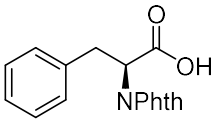
SI–5 [5]



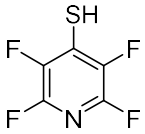
1j [6]



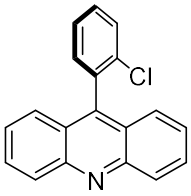
1z [7]



1aa [7]



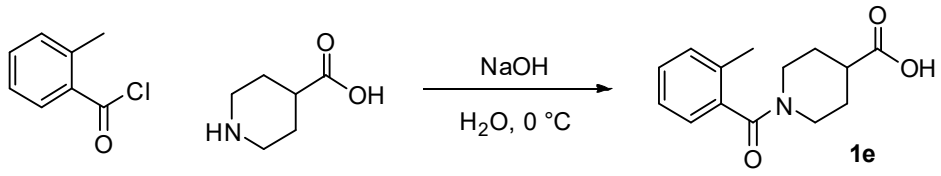
SI–6 [8]



A–1 [8]

CAUTION: due to the toxicity and volatility of thiophosgene (b.p. 72 °C), it should only be handled with adequate ventilation (preparation of compounds **SI–1**, **SI–2**, **SI–3**).

1-(2-Methylbenzoyl)piperidine-4-carboxylic acid (1e).



2-Methylbenzoyl chloride (1 equiv, 20 mmol, 3.08 g, 2.85 mL) and a solution of NaOH (1 equiv, 20 mmol, 0.8 g) in water (10 mL) were added dropwise simultaneously from two different dropping funnels into a three-necked 100 mL flask containing a solution of piperidine-4-carboxylic acid (1 equiv, 20 mmol, 2.58 g) and NaOH (1 equiv, 20 mmol, 0.8 g) in water (20 mL) at 0 °C (ice bath). The cooling bath was removed, and mixture was stirred for 1 hour at room temperature. The mixture was cooled to 0 °C, acidified with 2M aq. HCl to pH = 4 and extracted with EtOAc (4×30 mL). The combined organic layers were washed with water (10 mL), brine (10 mL), filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was recrystallised from ethyl acetate.

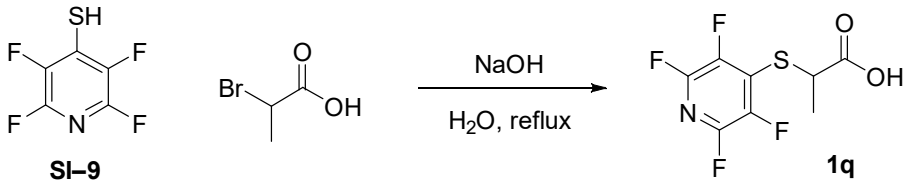
Yield 4.11 g, 83%. Colorless solid. Mp 164-166 °C.

^{1}H NMR (300 MHz, DMSO-d_6), δ: 7.43 – 7.02 (m, 4H), 4.53 – 4.30 (m, 1H), 3.41 – 3.17 (m, 2H), 3.13 – 2.82 (m, 2H), 2.20 (s, 3H), 2.02 – 1.86 (m, 1H), 1.82 – 1.65 (m, 1H), 1.61 – 1.32 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6), δ: 176.0, 168.9, 137.1, 133.9, 130.6, 128.9, 126.3, 125.9, 45.9, 40.5, 28.9, 28.2, 19.0.

HRMS (ESI): calcd for $C_{14}H_{18}NO_3$ (M+H) 248.1281, found 248.1277, for $C_{14}H_{17}NO_3Na$ (M+Na) 270.1101, found 270.1097, for $C_{14}H_{17}NO_3K$ (M+K) 286.0840, found 286.0837.

2-(2,3,5,6-Tetrafluoropyridin-4-ylsulfanyl)propionic acid (1q).



2-Bromopropionic acid (1.1 equiv, 22 mmol, 3.34 g) was added into a 50 mL flask containing a solution of 2,3,5,6-tetrafluoro-pyridine-4-thiol **SI-6** (1 equiv, 20 mmol, 3.64 g) and NaOH (2.1 equiv, 42 mmol, 1.68 g) in water (25 mL) at room temperature, and the mixture was stirred for 5 hours at 90 °C (water bath). The mixture was cooled to 0 °C, acidified with 2M aq. HCl to pH = 4. The precipitate was filtered off, washed with water and air dried, and then recrystallized from ethanol.

Yield 4.69 g, 92%. Colorless solid. Mp 77-79 °C.

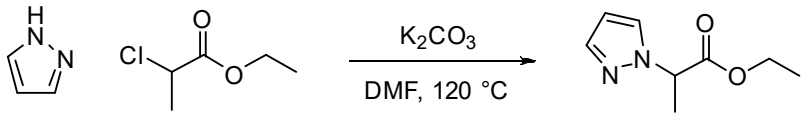
^{1}H NMR (300 MHz, DMSO-d_6), δ: 4.27 (q, J = 7.2 Hz, 1H), 1.46 (d, J = 7.2 Hz, 3H).

^{19}F NMR (282 MHz, DMSO-d_6), δ: -92.9 – -93.6 (m, 2F), -136.8 – -137.3 (m, 2F).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6), δ: 172.2, 143.2 (dm, J = 242.8 Hz), 141.6 (dd, J = 253.9 Hz, J = 19 Hz), 129.2 (m), 44.7, (t, J = 3.3 Hz), 18.1.

HRMS (ESI): calcd for $C_8H_5F_4NO_2SNa$ (M+Na) 277.9869, found 277.9860.

Ethyl 2-(1*H*-pyrazol-1-yl)propanoate (SI–7).



SI–7

Ethyl 2-chloropropionionate (1.1 equiv, 55 mmol, 7.5 g, 7 mL) was added into a 100 mL flask containing a solution of pyrazole (1 equiv, 50 mmol, 3.4 g) in DMF (35 mL) at room temperature. Then, solid K_2CO_3 (1.1 equiv, 55 mmol, 7.6 g) was added and the mixture was stirred for 5 hours at 120-130 °C (oil bath). The mixture was cooled to room temperature, concentrated under reduced pressure, diluted with water (20 mL) and extracted with EtOAc (4×25 mL). The combined organic layers were washed with brine (2×25 mL), filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (EtOAc/CH_2Cl_2 1/5).

Yield 6.13 g, 73%. Colorless oil.

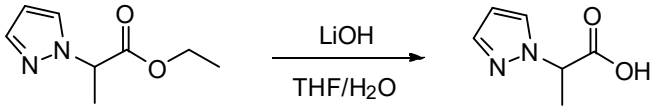
Chromatography: EtOAc/CH_2Cl_2 1/5. R_f 0.75.

^{1}H NMR (300 MHz, DMSO-d_6), δ: 7.81 (d, J = 1.9 Hz, 1H), 7.48 (d, J = 1.4 Hz, 1H), 6.32 – 6.24 (m, 1H), 5.25 (q, J = 7.2 Hz, 1H), 4.11 (q, J = 7.1 Hz, 2H), 1.67 (d, J = 7.2 Hz, 3H), 1.15 (t, J = 7 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6), δ: 170.7, 139.3, 129.9, 105.7, 61.5, 59.0, 17.4, 14.3.

HRMS (ESI): calcd for $C_8H_{12}N_2O_2Na$ (M+Na) 191.0791, found 191.0789, $C_8H_{12}N_2O_2K$ (M+K) 207.0530, found 207.0528.

2-Pyrazol-1-yl-propionic acid (1t).



SI–7 **1t**

A solution of lithium hydroxide (2.5 equiv, 25 mmol, 600 mg) in water (10 mL) was added into a 50 mL flask containing a solution of ethyl 2-pyrazol-1-yl-propionionate **SI-7** (1 equiv, 10 mmol, 1.68 g) in THF (15 mL) at room temperature. The mixture was stirred at room temperature for 4

hours, acidified with 1M aq. HCl to pH = 4 and extracted with EtOAc (5×25 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was recrystallized from ethyl acetate.

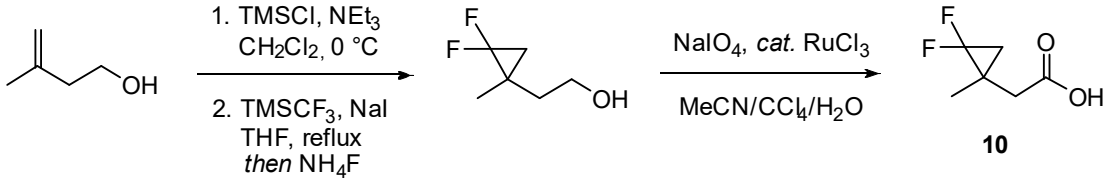
Yield 1.30 g, 93%. Colorless solid. Mp 89-91 °C.

^{1}H NMR (300 MHz, DMSO-d_6), δ: 7.78 (s, 1H), 7.45 (s, 1H), 6.26 (s, 1H), 5.13 (q, J = 6.5 Hz, 1H), 1.66 (d, J = 6.5 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6), δ: 172.4, 139.1, 129.9, 105.6, 59.1, 17.6.

HRMS (ESI): calcd for $C_6H_8N_2O_2Na$ (M+Na) 163.0478, found 163.0473.

2-(2,2-Difluoro-1-methylcyclopropyl)acetic acid (10).



Under argon atmosphere, trimethylsilyl chloride (1.1 equiv, 22 mmol, 2.4 g) was added dropwise into a 50 mL flask containing a solution of 3-methylbut-3-en-1-ol (1 equiv, 20 mmol, 1.72 g) and triethylamine (1.1 equiv, 22 mmol, 3.07 mL) in dichloromethane (20 mL) at 0 °C (ice bath), the cooling bath was removed, and the mixture was stirred for 15 min at room temperature. The solvent was removed from the reaction mixture under reduced pressure, the residue was diluted with water (50 mL), slightly acidified with 1M aq. HCl to pH = 6 and extracted with hexane (3×20 mL). The combined organic layers were filtered through Na_2SO_4 and concentrated under reduced pressure. The resulting alkene was introduced into the next reaction without further purification.

Under argon atmosphere, a 100 mL flask equipped with magnetic stirring bar and condenser was charged with trimethyl((3-methylbut-3-en-1-yl)oxy)silane (1 equiv, 19 mmol, 3.0 g), sodium iodide (0.45 equiv, 8.55 mmol, 1.28 g) and THF (25 mL). The flask was heated to reflux, and $TMSCF_3$ (3.0 equiv, 57 mmol, 8.42 mL) was added dropwise over 30 min, while maintaining the reflux. The mixture was refluxed for another 6 hours, and then cooled to room temperature. The mixture was diluted with water (40 mL), extracted with dichloromethane (3×40 mL) and concentrated under reduced pressure. The residue was diluted with methanol (50 mL), and ammonium fluoride (2.5 equiv, 47.5 mmol, 1.76 g) was added. The mixture was stirred overnight at room temperature, then diluted with water (80 mL) and extracted with dichloromethane (3×50 mL). The combined organic layers were filtered through Na_2SO_4 and

concentrated under reduced pressure. The resulting alcohol was introduced into the next reaction without further purification.

A 100 mL flask equipped with magnetic stirring bar and condenser was charged with 2-(2,2-difluoro-1-methylcyclopropyl)ethan-1-ol (1 equiv, 14.4 mmol, 1.96 g), sodium periodate (2.5 equiv, 36 mmol, 7.7 g), ruthenium (III) chloride (1 mol.%, 32 mg), acetonitrile (7 mL), carbon tetrachloride (7 mL) and water (14 mL). The mixture was stirred overnight at room temperature, then diluted with water (100 mL) and extracted with dichloromethane (3×50 mL). The combined organic layers were treated with 0.5M aqueous sodium hydroxide (200 mL) in a speratory funnel, and the mixture was stirred vigorously. The aqueous layer was separated and extracted with dichloromethane (2×50 mL). The aqueous layer was acidified with 1M aq. HCl to pH = 3 and extracted with dichloromethane (3×50 mL). The combined organic layers were filtered through Na_2SO_4 and concentrated under reduced pressure.

Yield 1.51 g, 50% (3 steps). Colorless solid. Mp 49-52 °C.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 12.0 – 10.0 (br s, 1H), 2.57 (dt, *J* = 16.9, 1.8 Hz, 1H), 2.49 (d, *J* = 16.9 Hz, 1H), 1.31 (dd, *J* = 2.8, 1.7 Hz, 3H), 1.30 – 1.11 (m, 2H).

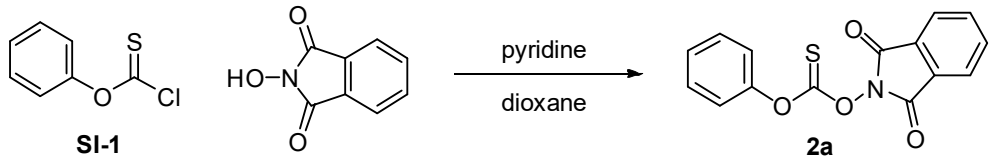
^{19}F NMR (282 MHz, $CDCl_3$), δ: -137.82 (dd, *J* = 154.6, 12.9 Hz, 1F), -140.27 (dd, *J* = 154.6, 12.4 Hz, 1F).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 177.7, 115.2 (dd, *J* = 289.0, 287.3 Hz), 37.5 (dd, *J* = 6.5, 1.3 Hz), 22.9 (dd, *J* = 11.3, 9.5 Hz), 22.31 (t, *J* = 10.2 Hz), 16.83 (dd, *J* = 6.3, 1.4 Hz).

HRMS (ESI): calcd for $C_6H_8F_2O_2Na$ (M+Na) 133.0385, found 173.0378.

Synthesis of thionocarbonates 2

Phthalimido phenyl thionocarbonate (2a). [9]



SI-1 **2a**

Carbonothiolate chloride **SI-1** (1.1 equiv, 55 mmol, 9.5 g) was added dropwise into a 200 mL flask containing a solution of *N*-hydroxyphthalimide (1 equiv, 50 mmol, 8.2 g) and pyridine (1.25 equiv, 62.5 mmol, 5.5 mL) in dry dioxane (70 mL) at 0 °C (ice bath). The mixture was stirred for 2 hours at room temperature, then poured into ice water. The precipitate was filtered off and recrystallized from ethanol.

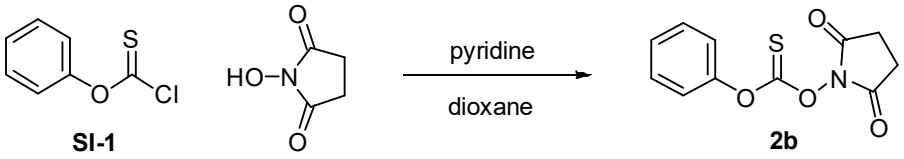
Yield 14.1 g (94%). Colorless crystalls. Mp 108-110 °C.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.97 – 7.94 (m, 2H), 7.86 – 7.83 (m, 2H), 7.51 – 7.46 (m, 2H), 7.39 – 7.34 (m, 1H), 7.30 – 7.27 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 191.7. 160.9, 154.0, 135.0, 129.9, 128.7, 127.4, 124.2, 121.1.

HRMS (ESI): calcd for $C_{15}H_{10}NO_4S$ (M+H) 300.0325; found 300.0315, calcd for $C_{15}H_{13}N_2O_4S$ ($M+NH_4$) 317.0580; found 317.0591, calcd for $C_{15}H_9NO_4SNa$ (M+Na) 322.0144; found 322.0139, calcd for $C_{15}H_9NO_4SK$ (M+K) 337.9883; found 337.9879.

Succinimido phenyl thionocarbonate (2b).



SI-1 **2b**

O-Phenyl chlorothiocarbonate **SI-1** (1 equiv, 10 mmol, 1.72 g) was added into a 100 mL flask containing a solution of *N*-hydroxysuccinimide (1 equiv, 10 mmol, 1.15 g) and pyridine (1.6 equiv, 16 mmol, 1.29 g, 1.32 mL) in dioxane (25 mL) at room temperature, and the mixture was stirred for 1 hour at room temperature and 1 hour at 50-60 °C. The mixture was cooled to room temperature and diluted with water (125 mL). The precipitate was filtered off and recrystallized from ethanol.

Yield 2.32 g, 92%. Colorless solid. Mp 141-143 °C.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.50 – 7.45 (m, 2H), 7.38 – 7.34 (m, 1H), 7.26 – 7.23 (m, 2H), 2.9 (s, 4H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 190.7. 168.1, 153.9, 129.9, 127.4, 121.1, 25.6.

HRMS (ESI): calcd for $C_{11}H_{10}NO_4S$ (M+H) 252.0325; found 252.0331, calcd for $C_{11}H_{13}N_2O_4S$ (M+NH_4) 269.0591; found 269.0599, calcd for $C_{11}H_9NO_4SNa$ (M+Na) 274.0144; found 274.0151, calcd for $C_{11}H_9NO_4SK$ (M+K) 289.9884; found 289.9895.

***N*-Acetylacetamido phenyl thionocarbonate (2c).**

SI-1 **SI-4** **2c**

O-Phenyl chlorothiocarbonate **SI-1** (1 equiv, 5 mmol, 870 mg) was added into a 25 mL flask containing a solution of *N,N*-diacetylhydroxylamine **SI–4** (1 equiv, 5 mmol, 580 mg) and triethylamine (1 equiv, 5 mmol, 550 mg, 0.7 mL) in acetonitrile (10 mL) at 0 °C. The mixture was stirred for 1 hour at 0 °C, warmed to room temperature, diluted with water (50 mL) and and extracted with ethyl acetate (4×25 mL). The combined organic layers were washed with water (20 mL), brine (20 mL), filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

Yield 749 mg, 59%. Colorless oil.

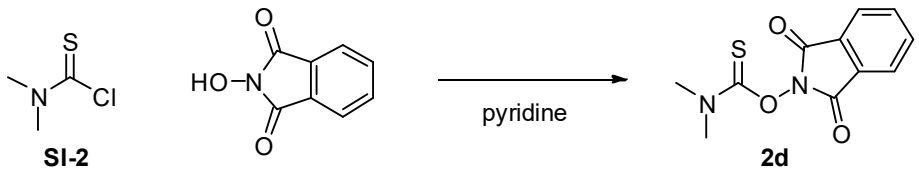
Chromatography: CH_2Cl_2. R_f 0.45.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.50 – 7.45 (m, 2H), 7.38 – 7.33 (m, 1H), 7.15 – 7.12 (m, 2H), 2.72 (s, 3H), 2.34 (s, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 166.9, 165.4, 160.2, 152.7, 129.8, 127.1, 122.0, 26.4, 18.1.

HRMS (ESI): calcd for $C_{11}H_{12}NO_4S$ (M+H) 254.0482; found 254.0483, calcd for $C_{11}H_{15}N_2O_4S$ (M+NH_4) 271.0747; found 271.0751, calcd for $C_{11}H_{11}NO_4SNa$ (M+Na) 276.0301; found 276.0307, calcd for $C_{11}H_{11}NO_4SK$ (M+K) 292.0040; found 292.0041.

***N*,*N*-Dimethyl *O*-phthalimidyl thionocarbamate (2d).** [10]



SI-2 **2d**

Thiocarbamoyl chloride **SI-2** (1.025 equiv, 51.25 mmol, 6.33 g) was added dropwise into a 200 mL flask containing a solution of *N*-hydroxyphthalimide (1 equiv, 50 mmol, 8.2 g) in pyridine (40 mL) at 0 °C (ice bath). The cooling bath was removed, and mixture was stirred overnight at room temperature, then poured into ice water. The precipitate was filtered off and recrystallized from ethanol.

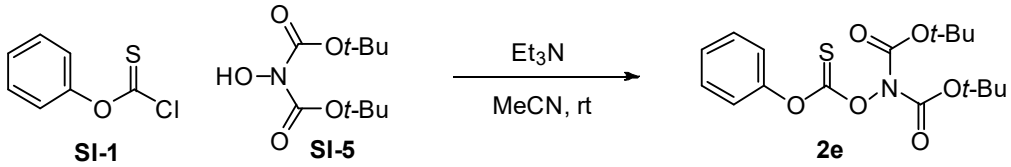
Yield 11.0 g (88%). Colorless crystalls. Mp 181-183 °C.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.89 – 7.86 (m, 2H), 7.79 – 7.76 (m, 2H), 3.41 (s, 3H), 3.88 (s, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 185.3. 162.0, 134.8, 128.7, 124.0, 45.1, 39.0.

HRMS (ESI): calcd for $C_{11}H_{11}N_2O_3S$ (M+H) 251.0485; found 251.0489, calcd for $C_{11}H_{14}N_3O_4S$ ($M+NH_4$) 268.07580; found 268.0748, calcd for $C_{11}H_{10}N_2O_3SNa$ (M+Na) 273.0304; found 273.0306, calcd for $C_{11}H_{10}N_2O_3SK$ (M+K) 289.0044; found 289.0045.

Di-*tert*-butyl [(phenoxycarbonothioyl)oxy]imidodicarbonate (2e).



O-Phenyl chlorothiocarbonate **SI-1** (1 equiv, 10 mmol, 1.72 g) was added into a 50 mL flask containing a solution of *N,N*-di(*tert*-buthoxycarbonyl)hydroxylamine **SI–5** (1 equiv, 10 mmol, 2.33 g) and triethylamine (1 equiv, 10 mmol, 1.01 g, 1.39 mL) in acetonitrile (28 mL) at 0 °C. The mixture was stirred for 1 hour at 0 °C, warmed to room temperature, diluted with water (160 mL) and and extracted with dichloromethane (4×50 mL). The combined organic layers were washed with brine (2×25 mL), filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

Yield 2.38 g, 64%. Colorless oil.

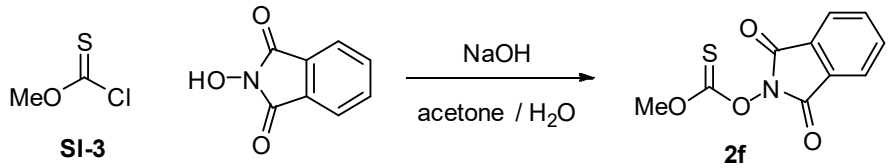
Chromatography: CH_2Cl_2. R_f 0.55.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.41 (m, 2H), 7.33 – 7.31 (m, 1H), 7.16 – 7.12 (m, 2H), 1.59 (s, 9H), 1.58 (s, 9H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 185.3. 153.2, 147.4, 129.5, 126.6, 122.1, 86.7. 86.1, 27.9, 27.6.

HRMS (ESI): calcd for $C_{17}H_{24}NO_6S$ (M+H) 370.1319; found 370.1317, calcd for $C_{17}H_{27}N_2O_6S$ ($M+NH_4$) 387.1584; found 387.1576, calcd for $C_{17}H_{23}NO_6SNa$ (M+Na) 392.1138; found 392.1132, calcd for $C_{17}H_{23}NO_6SK$ (M+K) 408.0878; found 408.0872.

Phthalimido methyl thionocarbonate (2f).



SI-3 2f

A solution of *O*-methyl chlorothiocarbonate **SI-3** (1 equiv, 10 mmol, 1.1 g) in 5 mL of acetone was added into a 50 mL flask containing a solution of *N*-hydroxyphthalimide (1 equiv, 10 mmol, 1.64 g) and NaOH (1.1 equiv, 11 mmol, 440 mg) in water (20 mL) at room temperature, and the mixture was stirred for 30 min at room temperature. The mixture was diluted with water (20 mL), the precipitate was filtered off and recrystallized from ethanol.

Yield 1.96 g, 83%. Colorless solid. Mp 136-138 °C.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.95 – 7.93 (m, 2H), 7.85 – 7.83 (m, 2H), 4.27 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ: 193.4. 161.0, 134.9, 128.7, 124.2, 62.6.

HRMS (ESI): calcd for $C_{10}H_8NO_4S$ (M+H) 238.0169; found 238.0176, calcd for $C_{10}H_{11}N_2O_4S$ ($M+NH_4$) 255.0434; found 255.0428, calcd for $C_{10}H_7NO_4SNa$ (M+Na) 259.9988; found 259.9989.

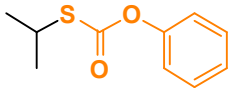
Synthesis of thiocarbonates 3 (General procedure I)

A tube containing a stirring bar was charged with carboxylic acid **1** (1.0 equiv, 0.5 mmol), thionocarbonate **2a** (1.5 equiv, 0.75 mmol, 224 mg), 9-(2-chlorophenyl)acridine **A-1** (2.5 mol%, 3.6 mg) and solvent (2 mL; for **3a-3ad, 3af**, dichloromethane; for **3ae**, acetonitrile; for **3ag**, DMSO). The tube was closed with a puncturable screw cap, and a needle was introduced as a pressure compensator. The mixture was irradiated by 60W 400 nm LEDs for 4 hours at 20 °C; during irradiation a solution of 9-(2-chlorophenyl)acridine **A-1** (5 mol%, 7.2 mg) in the same solvent (0.5 mL) was added using a syringe pump (150 μL/h).

For compounds **3a-3af**, the precipitate of phthalimide byproduct was filtered off, washed with dichloromethane (2×3 mL), the combined filtrate was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

For compound **3ag**, the reaction mixture was diluted with water (10 mL), extracted with dichloromethane (3×5 mL), filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

***S*-Isopropyl *O*-phenyl thiocarbonate (3a).**



Yield 83 mg (85%). Colorless oil.

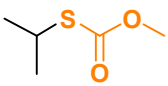
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.36 (m, 2H), 7.31 – 7.23 (m, 1H), 7.22 – 7.16 (m, 2H), 3.64 (hept, J = 6.8 Hz, 1H), 1.45 (d, J = 6.8 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 169.8, 151.2, 129.5, 126.1, 121.5, 37.2, 23.1.

HRMS (ESI): calcd for $C_{10}H_{13}O_2S$ (M+H) 197.0631, found 197.0626, calcd for $C_{10}H_{16}NO_2S$ ($M+NH_4$) 214.0896, found 214.0890, calcd for $C_{10}H_{12}O_2SNa$ (M+Na) 219.0450, found 219.0442, calcd for $C_{10}H_{12}O_2SK$ (M+K) 235.0190, found 235.0178.

***S*-Isopropyl *O*-methyl thiocarbonate (3a-Me).**



Yield 30 mg (44%). Colorless oil.

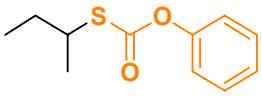
Chromatography: CH_2Cl_2. R_f 0.8.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 4.17 (s, 3H), 3.82 (hept, J = 6.8 Hz, 1H), 1.41 (d, J = 6.8 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 167.3, 56.1, 36.7, 23.1.

HRMS (ESI): calcd for $C_5H_{10}O_2SNa$ (M+Na) 157.0294, found 157.0300.

_S_-(sec-Butyl) _O_-phenyl thiocarbonate (3b).



Yield 71 mg (68%). Colorless oil.

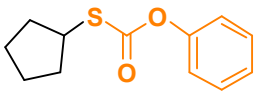
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.46 – 7.36 (m, 2H), 7.31 – 7.22 (m, 1H), 7.21 – 7.15 (m, 2H), 3.47 (tq, J = 8.8, 7.0 Hz, 1H), 1.85 – 1.62 (m, 2H), 1.44 (d, J = 7.0 Hz, 3H), 1.06 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 170.1, 151.2, 129.5, 126.0, 121.4, 43.7, 29.5, 20.8, 11.4.

HRMS (ESI): calcd for $C_{11}H_{15}O_2S$ (M+H) 211.0787, found 211.0781, calcd for $C_{11}H_{14}O_2SNa$ (M+Na) 233.0607, found 233.0600.

_S_-Cyclopentyl _O_-phenyl thiocarbonate (3c).



Yield 63 mg (57%). Colorless oil.

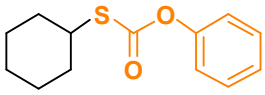
Chromatography: CH_2Cl_2. R_f 0.7.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.44 – 7.34 (m, 2H), 7.29 – 7.21 (m, 1H), 7.20 – 7.14 (m, 2H), 3.78 – 3.65 (m, 1H), 2.28 – 2.13 (m, 2H), 1.89 – 1.61 (m, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 169.8, 151.3, 129.3, 125.9, 121.4, 44.4, 33.3, 24.8.

HRMS (ESI): calcd for $C_{12}H_{15}O_2S$ (M+H) 223.0787, found 223.0791, calcd for $C_{12}H_{18}NO_2S$ ($M+NH_4$) 240.1053, found 240.1056, calcd for $C_{12}H_{14}O_2SNa$ (M+Na) 245.0807, found 245.0807, calcd for $C_{12}H_{14}O_2SK$ (M+K) 261.0346, found 261.0350.

_S_-Cyclohexyl _O_-phenyl thiocarbonate (3d).



Yield 93 mg (79%). Colorless oil.

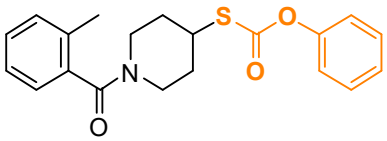
Chromatography: CH_2Cl_2. R_f 0.7.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.33 (m, 2H), 7.31 – 7.22 (m, 1H), 7.22 – 7.14 (m, 2H), 3.53 – 3.38 (m, 1H), 2.17 – 2.02 (m, 2H), 1.86 – 1.72 (m, 2H), 1.71 – 1.35 (m, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 169.9, 151.2, 129.4, 126.0, 121.4, 45.0, 33.1, 25.9, 25.2.

HRMS (ESI): calcd for $C_{13}H_{17}O_2S$ (M+H) 237.0944, found 237.0947, calcd for $C_{13}H_{20}NO_2S$ ($M+NH_4$) 254.1209, found 254.1212, calcd for $C_{13}H_{16}O_2SNa$ (M+Na) 259.0763, found 259.0762, calcd for $C_{13}H_{16}O_2SK$ (M+K) 275.0503, found 275.0483.

_S_-(1-(2-Methylbenzoyl)piperidin-4-yl) _O_-phenyl thiocarbonate (3e).



Yield 114 mg (64%). Colorless oil.

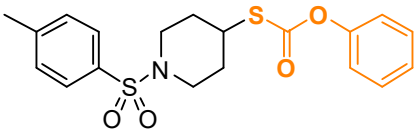
Chromatography: CH_2Cl_2. R_f 0.35.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.45 – 7.35 (m, 2H), 7.32 – 7.1 (m, 7H), 7.65 – 7.41 (m, 1H), 3.74 – 3.42 (m, 2H), 3.40 – 3.33 (m, 2H), 2.43 – 2.12 (m, 4H), 2.10 – 1.91 (m, 1H), 1.90 – 1.53 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 170.0, 169.0, 151.0, 136.0, 132.7, 130.5, 129.6, 126.3, 126.0, 125.7, 123.6, 121.3, 42.4, 31.8, 29.7, 19.0.

HRMS (ESI): calcd for $C_{20}H_{22}NO_3S$ (M+H) 356.1315, found 356.1317, calcd for $C_{20}H_{21}NO_3SNa$ (M+Na) 378.1134, found 378.1134, calcd for $C_{20}H_{21}NO_3SK$ (M+K) 394.0874, found 394.0865.

***O*-Phenyl *S*-(1-tosylpiperidin-4-yl) thiocarbonate (3f).**



Yield 125 mg (64%). Colorless crystalls. Mp 185-188 °C (1,2-dichloroethane/hexane).

Chromatography: CH_2Cl_2. R_f 0.3.

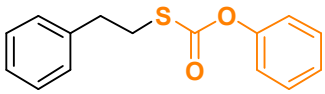
^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.71 – 7.62 (m, 2H), 7.42 – 7.31 (m, 4H), 7.30 – 7.22 (m, 1H), 7.17 – 7.10 (m, 2H), 3.64 – 3.52 (m, 2H), 3.42 – 3.31 (m, 1H), 2.75 – 2.61 (m, 2H), 2.45 (s, 3H), 2.22 – 2.09 (m, 2H), 1.93 – 1.76 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.9, 151.0, 143.8, 133.1, 129.8, 129.5, 127.7, 126.3, 121.3, 45.6, 41.4, 31.3, 21.5.

HRMS (ESI): calcd for $C_{19}H_{22}NO_4S_2$ (M+H) 392.0985, found 392.0988, calcd for $C_{19}H_{25}N_2O_4S_2$ ($M+NH_4$) 409.1250, found 409.1253, calcd for $C_{19}H_{21}NO_4S_2Na$ (M+Na) 414.0804, found 414.0809, calcd for $C_{19}H_{21}NO_4S_2K$ (M+K) 430.0544, found 430.0546.

The single crystal suitable for X-ray diffraction analysis was prepared by slow diffusion of hexane into 1,2-dichloroethane solution at 0 °C.

***S*-Phenethyl *O*-phenyl thiocarbonate (3g).**



Yield 72 mg (56%). Colorless oil.

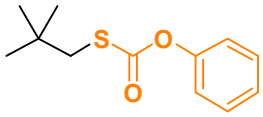
Chromatography: CH_2Cl_2. R_f 0.65.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.38 (m, 2H), 7.37 – 7.32 (m, 1H), 7.31 – 7.15 (m, 7H), 3.22 (t, J = 8.4 Hz, 2H), 3.04 (t, J = 8.4 Hz, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 170.1, 151.2, 139.6, 129.5, 128.9, 128.6, 126.7, 126.1, 121.3, 36.0, 32.7.

HRMS (ESI): calcd for $C_{15}H_{14}O_2SNa$ (M+Na) 281.0607, found 281.0812.

***S*-Neopentyl *O*-phenyl thiocarbonate (3h).**



Yield 93 mg (83%). Colorless oil.

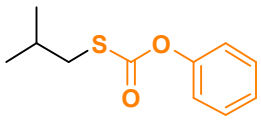
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.44 – 7.34 (m, 2H), 7.31 – 7.23 (m, 1H), 7.20 – 7.12 (m, 2H), 2.95 (s, 2H), 1.04 (s, 9H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 170.8, 151.4, 129.5, 126.1, 121.3, 45.0, 31.9, 28.5.

HRMS (ESI): calcd for $C_{12}H_{17}O_2S$ (M+H) 225.0944, found 225.0934, calcd for $C_{12}H_{20}NO_2S$ ($M+NH_4$) 242.1209, found 242.1202, calcd for $C_{12}H_{16}O_2SNa$ (M+Na) 247.0763, found 247.0757, calcd for $C_{12}H_{16}O_2SK$ (M+K) 263.0503, found 263.0499.

***S*-Isobutyl *O*-phenyl thiocarbonate (3i).**



Yield 54 mg (51%). Colorless oil.

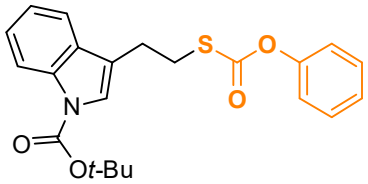
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.46 – 7.36 (m, 2H), 7.31 – 7.25 (m, 1H), 7.21 – 7.15 (m, 2H), 2.90 (d, J = 6.7 Hz, 2H), 1.98 (m, 1H), 1.06 (d, J = 6.7 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, C $CDCl_3$), δ: 170.6, 151.3, 129.5, 126.1, 121.3, 39.8, 28.8, 21.7.

HRMS (ESI): calcd for $C_{11}H_{15}O_2S$ (M+H) 211.0787, found 211.0786, calcd for $C_{11}H_{18}NO_2S$ ($M+NH_4$) 228.1053, found 228.1045, calcd for $C_{11}H_{14}O_2SNa$ (M+Na) 233.0607, found 233.0598, calcd for $C_{11}H_{14}O_2SK$ (M+K) 249.0346, found 249.0339.

***tert*-Butyl 3-(2-((phenoxycarbonyl)thio)ethyl)-1*H*-indole-1-carboxylate (3j).**



Yield 81 mg (41%). Colorless oil.

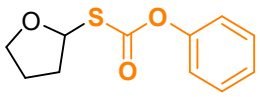
Chromatography: CH_2Cl_2. R_f 0.3.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 8.55 (d, *J* = 8.2 Hz, 1H), 7.62 (s, 1H), 7.51 – 7.46 (m, 2H), 7.44 – 7.37 (m, 2H), 7.32 – 7.26 (m, 2H), 7.22 – 7.16 (m, 2H), 3.34 –3.24 (m, 2H), 3.22 – 3.12 (m, 2H), 1.54 (s, 9H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.6, 151.1, 148.6, 136.7, 135.1, 131.6, 129.4, 128.3, 126.2, 123.7, 123.0, 121.2, 120.9, 116.1, 61.4, 31.8, 29.7, 26.9.

HRMS (ESI): calcd for $C_{22}H_{24}NO_4S$ (M+H) 398.1421, found 398.1428.

***O*-Phenyl *S*-(tetrahydrofuran-2-yl) thiocarbonate (3k).**



Yield 57 mg (51%). Colorless oil.

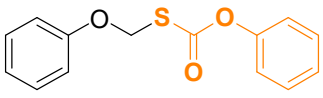
Chromatography: CH_2Cl_2. R_f 0.65.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.44 – 7.35 (m, 2H), 7.30 – 7.23 (m, 1H), 7.22 – 7.15 (m, 2H), 6.04 (dd, *J* = 7.0, 3.1 Hz, 1H), 4.02 (t, *J* = 7.0 Hz, 2H), 2.53 – 2.36 (m, 1H), 2.21 – 1.92 (m, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 170.0, 151.1, 129.5, 126.2, 121.4, 85.8, 68.4, 32.5, 24.5.

HRMS (ESI): calcd for $C_{11}H_{13}O_3S$ (M+H) 225.0580, found 225.0574, calcd for $C_{11}H_{16}NO_3S$ (M+NH_4) 242.0845, found 242.0839, calcd for $C_{11}H_{12}O_3SNa$ (M+Na) 247.0399, found 247.0391, calcd for $C_{11}H_{12}O_3SK$ (M+K) 263.0139, found 263.0132.

***S*-(Phenoxymethyl) *O*-phenyl thiocarbonate (3l).**



Yield 113 mg (87%). Colorless oil.

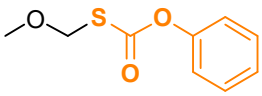
Chromatography: CH_2Cl_2. R_f 0.6.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.44 – 7.23 (m, 5H), 7.21 – 7.15 (m, 2H), 7.11 – 7.04 (m, 1H), 7.03 – 7.97 (m, 2H), 5.66 (s, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.1, 156.5, 151.2, 129.7, 129.6, 126.4, 122.6, 121.2, 116.0, 69.4.

HRMS (ESI): calcd for $C_{14}H_{16}NO_3S$ (M+NH_4) 278.0845, found 278.0839, calcd for $C_{14}H_{12}O_3SNa$ (M+Na) 283.0399, found 283.0393, calcd for $C_{14}H_{12}O_3SK$ (M+K) 299.0139, found 299.0134.

_S_-(Methoxymethyl) _O_-phenyl thiocarbonate (3m).



Yield 87 mg (88%). Colorless oil.

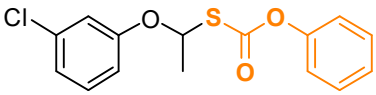
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.42 – 7.36 (m, 2H), 7.31 – 7.26 (m, 1H), 7.23 – 7.16 (m, 2H), 5.16 (s, 2H), 3.45 (s, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 166.4, 151.2, 129.6, 126.3, 121.2, 75.0, 57.2.

HRMS (ESI): calcd for $C_9H_{11}O_3S$ (M+H) 199.0423, found 199.0422, calcd for $C_9H_{14}NO_3S$ (M+NH_4) 216.0689, found 216.0702, calcd for $C_9H_{10}O_3SNa$ (M+Na) 221.0243, found 221.0237, calcd for $C_9H_{10}O_3SK$ (M+K) 236.9982, found 236.9978.

_S_-(1-(3-Chlorophenoxy)ethyl) _O_-phenyl thiocarbonate (3n).



Yield 109 mg (71%). Colorless oil.

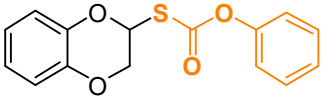
Chromatography: CH_2Cl_2. R_f 0.55.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.46 – 7.37 (m, 2H), 7.32 – 7.23 (m, 2H), 7.19 – 7.14 (m, 2H), 7.12 – 7.04 (m, 2H), 6.99 (dm, J = 8.3 Hz, 1H), 6.08 (q, J = 6.3 Hz, 1H), 1.92 (d, J = 6.3 Hz, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 168.5, 156.9, 151.0, 135.0, 130.4, 129.6, 126.4, 123.0, 121.2, 117.8, 115.3, 81.4, 23.3.

HRMS (ESI): calcd for $C_{15}H_{17}{}^{35}ClNO_3S$ (M+NH_4) 326.0612, found 326.0602, calcd for $C_{15}H_{17}{}^{37}ClNO_3S$ (M+NH_4) 328.0588, found 328.0574, calcd for $C_{15}H_{13}{}^{35}ClO_3SNa$ (M+Na) 331.0166, found 331.0157, calcd for $C_{15}H_{13}{}^{37}ClO_3SNa$ (M+Na) 333.0142, found 333.0132.

_S_-(2,3-Dihydrobenzo[b][1,4]dioxin-2-yl) _O_-phenyl thiocarbonate (3o).



Yield 98 mg (68%). Colorless oil.

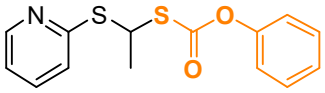
Chromatography: CH_2Cl_2. R_f 0.55.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.48 – 7.37 (m, 2H), 7.34 – 7.26 (m, 1H), 7.24 – 7.17 (m, 2H), 7.03 – 6.91 (m, 4H), 6.29 (t, *J* = 2.3 Hz, 1H), 4.51 (dd, *J* = 11.7, 2.3 Hz, 1H), 4.46 (dd, *J* = 11.7, 2.3, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 167.7, 151.0, 142.8, 140.8, 129.6, 126.5, 122.8, 122.5, 121.2, 118.3, 117.5, 79.0, 67.2.

HRMS (ESI): calcd for $C_{15}H_{16}NO_4S$ (M+NH_4) 306.0795, found 306.0794, calcd for $C_{15}H_{12}O_4SNa$ (M+Na) 311.0349, found 311.0351, calcd for $C_{15}H_{12}O_4SK$ (M+K) 327.0088, found 327.0090.

_O_-Phenyl _S_-(1-(pyridin-2-ylthio)ethyl) thiocarbonate (3p).



Yield 77 mg (53%). Colorless oil.

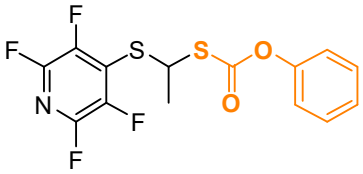
Chromatography: CH_2Cl_2. R_f 0.5.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 8.52 (dm, *J* = 4.39 Hz, 1H), 7.55 (dt, *J* = 8.2 Hz, *J* = 1.9 Hz, 1H), 7.45 – 7.35 (m, 2H), 7.31 – 7.14 (m, 4H), 7.07 (ddd, J = 7.3 Hz, *J* = 5 Hz, *J* = 1 Hz, 1H), 5.59 (q, *J* = 7 Hz, 1H), 1.96 (d, *J* = 7 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 169.2, 156.6, 151.1, 149.8, 130.4, 129.5, 126.2, 122.8, 121.3, 120.4, 44.8, 23.2.

HRMS (ESI): calcd for $C_{14}H_{14}NO_2S_2$ (M+H) 292.0460, found 292.0465.

_S_-(1-((Perfluoropyridin-4-yl)thio)ethyl) _O_-phenyl thiocarbonate (3q).



Yield 107 mg (59%). Colorless oil.

Chromatography: CH_2Cl_2. R_f 0.6.

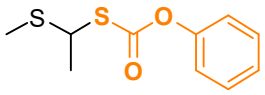
^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.42 – 7.31 (m, 2H), 7.26 – 7.17 (m, 1H), 7.16 – 7.09 (m, 2H), 5.29 (q, *J* = 7.2 Hz, 1H), 1.88 (d, *J* = 7.2 Hz, 3H).

^{19}F NMR (282 MHz, $CDCl_3$), δ: -90.8 – -91.5 (m, 2F), -136.2 – -136.9 (m, 2F).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 167.6, 150.8, 142.9 (dm, *J* = 289 Hz), 141.6 (dd, *J* = 232 Hz, *J* = 19 Hz), 129.7, 129.2 (m), 126.6, 121.0, 48.0, 22.9.

HRMS (ESI): calcd for $C_{14}H_{10}F_4NO_2S_2$ (M+H) 364.0084, found 364.0089.

***S*-(1-(Methylthio)ethyl) *O*-phenyl thiocarbonate (3r).**



Yield 83 mg (73%). Colorless oil.

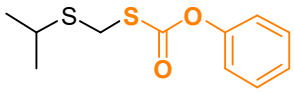
Chromatography: CH_2Cl_2. R_f 0.8.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.35 (m, 2H), 7.32 – 7.25 (m, 1H), 7.22 – 7.15 (m, 2H),4.53 (q, *J* = 7.1 Hz, 1H), 2.29 (s, 3H), 1.78 (d, *J* = 7.1 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 171.9, 150.9, 129.5, 126.2, 121.3, 48.8, 23.1, 15.1.

HRMS (ESI): calcd for $C_{10}H_{16}NO_2S_2$ (M+NH_4) 246.0617, found 246.0617, calcd for $C_{10}H_{12}O_2S_2Na$ (M+Na) 251.0171, found 251.0176.

***S*-((Isopropylthio)methyl) *O*-phenyl thiocarbonate (3s).**



Yield 97 mg (81%). Colorless oil.

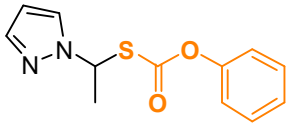
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.46 – 7.36 (m, 2H), 7.32 – 7.24 (m, 1H), 7.23 – 7.16 (m, 2H), 4.17 (s, 2H), 3.17 (hept, *J* = 6.7 Hz, 1H), 1.36 (d, *J* = 6.7 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 169.5, 151.2, 129.6, 126.3, 121.3, 35.5, 33.4, 23.0.

HRMS (ESI): calcd for $C_{11}H_{15}O_2S_2$ (M+H) 243.0507, found 243.0512, calcd for $C_{11}H_{14}O_2S_2Na$ (M+Na) 265.0327, found 265.0329, calcd for $C_{11}H_{12}O_2S_2K$ (M+K) 281.0067, found 281.0075.

***S*-(1-(1*H*-Pyrazol-1-yl)ethyl) *O*-phenyl thiocarbonate (3t).**



Yield 72 mg (58%). Colorless oil.

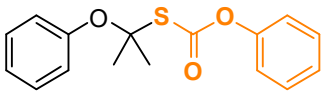
Chromatography: CH_2Cl_2. R_f 0.45.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.68 (d, *J* = 1.9 Hz, 1H), 7.45 – 7.34 (m, 2H), 7.33 – 7.24 (m, 1H), 7.19 – 7.11 (m, 2H), 6.98 – 6.90 (m, 1H), 6.29 (dd, *J* = 2.1 Hz, *J* = 1.9 Hz, 1H), 6.14 (q, *J* = 7.3 Hz, 1H), 2.07 (d, *J* = 7.2 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.7, 150.9, 140.9, 129.6, 126.5, 121.2, 120.4, 115.5, 61.7, 21.3.

HRMS (ESI): calcd for $C_{12}H_{13}N_2O_2S$ (M+H) 249.0692, found 249.0695, calcd for $C_{12}H_{12}N_2O_2SNa$ (M+Na) 271.0512, found 271.0513, calcd for $C_{12}H_{12}N_2O_2SK$ (M+K) 287.0251, found 287.0249.

***S*-(2-Phenoxypropan-2-yl) *O*-phenyl thiocarbonate (3u).**



Yield 114 mg (79%). Colorless oil.

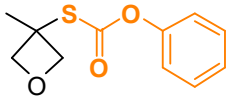
Chromatography: CH_2Cl_2. R_f 0.6.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.31 – 7.20 (m, 3H), 7.19 – 7.13 (m, 2H), 7.23 – 7.14 (m, 5H), 1.95 (s, 6H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 167.6, 154.0, 150.9, 129.5, 129.1, 126.2, 124.7, 123.6, 121.4, 92.3, 29.1.

HRMS (ESI): calcd for $C_{16}H_{20}NO_3S$ (M+NH_4) 306.1158, found 306.1157, calcd for $C_{16}H_{16}O_3SNa$ (M+Na) 311.0712, found 311.0715, calcd for $C_{16}H_{16}O_3SK$ (M+K) 327.0452, found 327.0454.

***S*-(3-Methyloxetan-3-yl) *O*-phenyl thiocarbonate (3v).**



Yield 71 mg (63%). Colorless oil.

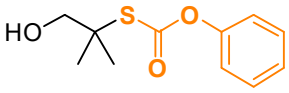
Chromatography: CH_2Cl_2. R_f 0.65.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.46 – 7.36 (m, 2H), 7.32 – 7.23 (m, 1H), 7.22 – 7.15 (m, 2H), 4.87 (d, *J* = 6.7 Hz, 2H), 4.68 (d, *J* = 6.7 Hz, 2H), 1.92 (s, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 168.1, 150.9, 129.6, 126.4, 121.3, 83.0, 47.5, 26.1.

HRMS (ESI): calcd for $C_{11}H_{13}O_3S$ (M+H) 225.0580, found 225.0584, calcd for $C_{11}H_{16}NO_3S$ (M+NH_4) 242.0845, found 242.0852, calcd for $C_{11}H_{12}O_3SNa$ (M+Na) 247.0399, found 247.0403.

***S*-(1-Hydroxy-2-methylpropan-2-yl) *O*-phenyl thiocarbonate (3w).**



Yield 98 mg (87%). Colorless oil.

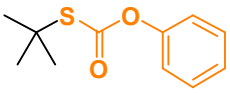
Chromatography: CH_2Cl_2. R_f 0.45.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.46 – 7.35 (m, 2H), 7.31 – 7.22 (m, 1H), 7.20 – 7.13 (m, 2H), 3.82 (s, 2H), 2.32 – 2.07 (br s, 1H), 1.51 (s, 6H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 169.1, 150.8, 129.5, 126.2, 121.4, 69.4, 53.0, 24.7.

HRMS (ESI): calcd for $C_{11}H_{15}O_3S$ (M+H) 227.0736, found 227.0744, calcd for $C_{11}H_{14}O_3SNa$ (M+Na) 249.0556, found 249.0558.

***S*-(tert-Butyl) *O*-phenyl thiocarbonate (3x).**



Yield 84 mg (80%). Colorless oil.

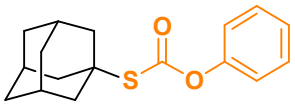
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.42 – 7.31 (m, 2H), 7.25 – 7.17 (m, 1H), 7.19 – 7.09 (m, 2H), 1.52 (s, 9H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 169.0, 150.9, 129.4, 126.0, 121.5, 47.8, 29.9.

HRMS (ESI): calcd for $C_{11}H_{14}O_2S$ (M+H) 211.0787, found 211.0797.

***S*-(Adamantan-1-yl) *O*-phenyl thiocarbonate (3y).**



Yield 114 mg (79%). Colorless oil.

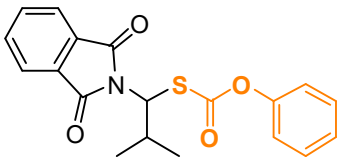
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.45 – 7.34 (m, 2H), 7.28 – 7.22 (m, 1H), 7.21 – 7.14 (m, 2H), 2.26 – 2.17 (m, 4H), 2.15 – 2.08 (m, 2H), 1.96 – 1.71 (m, 9H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 168.4, 150.9, 129.4, 125.9, 121.5, 50.5, 41.9, 36.2, 29.8.

HRMS (ESI): calcd for $C_{17}H_{21}O_2S$ (M+H) 289.1257, found 289.1258, calcd for $C_{17}H_{24}NO_2S$ ($M+NH_4$) 306.1527, found 306.1526, calcd for $C_{17}H_{20}O_2SNa$ (M+Na) 311.1076, found 311.1078, calcd for $C_{17}H_{20}O_2SK$ (M+K) 327.0816, found 327.0815.

***S*-(1-(Phthalimidyl)-2-methylpropyl) *O*-phenyl thiocarbonate (3z).**



Yield 85 mg (48%). Colorless oil.

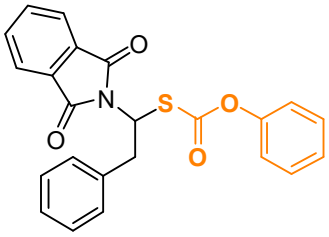
Chromatography: CH_2Cl_2. R_f 0.25.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.93 – 7.85 (m, 2H), 7.81 – 7.72 (m, 2H), 7.43 – 7.31 (m, 2H), 7.26 – 7.19 (m, 1H), 7.17 – 7.11 (m, 2H), 5.71 (d, J = 7.7 Hz, 1H), 2.77 – 2.61 (m, 1H), 1.26 (d, J = 6.6 Hz, 3H), 0.99 (d, J = 6.6 Hz, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 168.7, 167.0, 151.0, 134.3, 131.6, 129.4, 126.2, 123.7, 121.2, 61.4, 31.8, 20.4, 19.6.

HRMS (ESI): calcd for $C_{19}H_{18}NO_4S$ (M+H) 356.0951, found 356.0940, calcd for $C_{19}H_{21}N_2O_4S$ (M+NH_4) 373.1217, found 373.1211, calcd for $C_{19}H_{17}NO_4SNa$ (M+Na) 378.0770, found 378.0756, calcd for $C_{19}H_{17}NO_4SK$ (M+K) 394.0510, found 394.0494.

***S*-(1-(Phthalimidyl)-2-phenylethyl) *O*-phenyl thiocarbonate (3aa).**



Yield 111 mg (55%). Colorless oil.

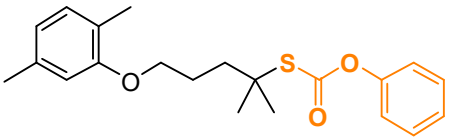
Chromatography: CH_2Cl_2. R_f 0.3.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 8.08 – 8.01 (m, 2H), 7.91 – 7.81 (m, 4H), 7.78 – 7.71 (m, 2H), 7.46 – 7.12 (m, 6H), 6.29 (dd, *J* = 11.9 Hz, *J* = 10.9 Hz, 1H), 3.71 (dd, *J* = 14.0, 10.9, 1H), 3.53 (dd, *J* = 14.0, 11.9, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.3, 166.7, 151.0, 135.9, 134.3, 132.0, 129.7, 129.5, 128.6, 127.3, 126.4, 123.6, 120.9, 55.3, 39.7.

HRMS (ESI): calcd for $C_{23}H_{18}NO_4S$ (M+H) 404.0951, found 404.0968, calcd for $C_{23}H_{21}N_2O_4S$ (M+NH_4) 421.1217, found 421.1231, calcd for $C_{23}H_{17}NO_4SNa$ (M+Na) 426.0770, found 426.0780, calcd for $C_{23}H_{17}NO_4SK$ (M+K) 442.0510, found 442.0523.

***S*-(5-(2,5-Dimethylphenoxy)-2-methylpentan-2-yl) *O*-phenyl thiocarbonate (3ab).**



Yield 127 mg (71%). Colorless oil.

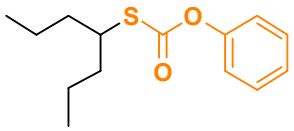
Chromatography: CH_2Cl_2. R_f 0.65.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.37 (m, 2H), 7.31 – 7.22 (m, 1H), 7.22 – 7.16 (m, 2H), 7.03 (d, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 7.5 Hz), 1H), 6.64 (s, 1H), 4.02 (t, *J* = 5.2 Hz, 2H), 2.37 (s, 3H), 2.24 (s, 3H), 2.13 – 1.95 (m, 4H), 1.62 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.5, 156.9, 151.0, 136.3, 130.4, 129.4, 125.9, 123.5, 121.6, 120.8, 111.0, 67.6, 51.1, 37.9, 28.0, 25.3, 21.5, 15.9.

HRMS (ESI): calcd for $C_{21}H_{27}O_3S$ (M+H) 359.1675, found 359.1666, calcd for $C_{21}H_{30}NO_3S$ (M+NH_4) 376.1941, found 376.1934, calcd for $C_{21}H_{26}O_3SNa$ (M+Na) 381.1495, found 381.1484, calcd for $C_{21}H_{26}O_3SK$ (M+K) 397.1234, found 397.1228.

***S*-(Heptan-4-yl) *O*-phenyl thiocarbonate (3ac).**



Yield 87 mg (69%). Colorless oil.

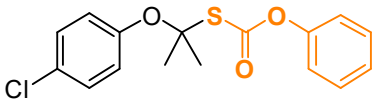
Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.45 – 7.34 (m, 2H), 7.30 – 7.22 (m, 1H), 7.21 – 7.14 (m, 2H), 3.53 – 2.42 (m, 1H), 1.77 – 1.62 (m, 4H), 1.59 – 1.42 (m, 4H), 0.97 (t, *J* = 8.7 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 170.4, 151.3, 129.4, 126.0, 121.4, 47.2, 37.0, 20.0, 13.9.

HRMS (ESI): calcd for $C_{14}H_{21}O_2S$ (M+H) 253.1257, found 253.1264, calcd for $C_{14}H_{24}NO_2S$ ($M+NH_4$) 270.1522, found 270.1529, calcd for $C_{14}H_{20}O_2SNa$ (M+Na) 275.1076, found 2751064, calcd for $C_{14}H_{20}O_2SK$ (M+K) 291.0816, found 291.0821.

***S*-(2-(4-Chlorophenoxy)propan-2-yl) *O*-phenyl thiocarbonate (3ad).**



Yield 92 mg (57%). Colorless oil.

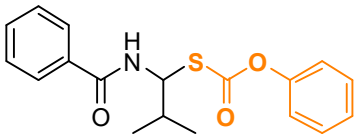
Chromatography: CH_2Cl_2. R_f 0.45.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.44 – 7.37 (m, 2H), 7.33 – 7.24 (m, 3H), 7.20 – 7.11 (m, 4H), 1.93 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 167.3, 152.5, 150.8, 129.5, 129.2, 126.2, 124.8, 121.4, 117.2, 92.3, 29.0.

HRMS (ESI): calcd for $C_{16}H_{19}{}^{35}ClNO_3S$ ($M+NH_4$) 340.0769, found 340.0777, calcd for $C_{16}H_{19}{}^{37}ClNO_3S$ ($M+NH_4$) 342.0740, found 342.0748, calcd for $C_{16}H_{15}{}^{35}ClO_3SNa$ (M+Na) 345.0323, found 345.0330, calcd for $C_{16}H_{15}{}^{37}ClO_3SNa$ (M+Na) 347.0294, found 347.0302.

***S*-(1-Benzamido-2-methylpropyl) *O*-phenyl thiocarbonate (3ae).**



Yield 61 mg (37%). Colorless crystalls.

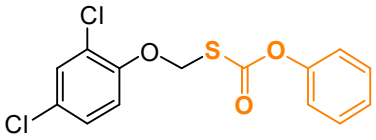
Chromatography: CH_2Cl_2. R_f 0.2.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.82 – 7.72 (m, 2H), 7.59 – 7.37 (m, 3H), 7.35 – 7.22 (m, 2H), 7.14 – 7.05 (m, 2H), 7.02 – 6.93 (m, 1H), 6.53 – 6.41 (br d, *J* = 9.3 Hz, 1H), 6.03 (dd, *J* = 9.3, 5.9 Hz, 1H),2.20 (dq, *J* = 13.3, 6.3 Hz, 1H), 1.13 (t, *J* = 6.3 Hz, 6H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ: 167.6, 167.0, 156.7, 133.9, 131.9, 129.7, 128.7, 127.0, 121.6, 115.8, 82.3, 33.9, 17.6, 17.2.

HRMS (ESI): calcd for $C_{18}H_{20}NO_3S$ (M+H) 330.1158, found 330.1159, calcd for $C_{18}H_{23}N_2O_3S$ ($M+NH_4$) 347.1413, found 347.1422, calcd for $C_{18}H_{19}NO_3SK$ (M+K) 368.0717, found 368.0706.

_S_-((2,4-Dichlorophenoxy)methyl) _O_-phenyl thiocarbonate (3af).



Yield 134 mg (82%). Colorless oil.

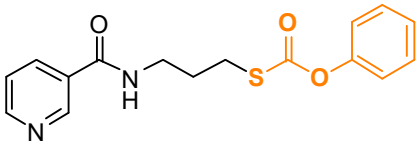
Chromatography: CH_2Cl_2. R_f 0.55.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.48 –7.41 (m, 2H), 7.39 (s, 1H), 7.34 – 7.20 (m, 4H), 7.04 (d, J = 8.7 Hz, 1H), 5.69 (s, 2H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ: 167.7, 151.1, 151.0, 130.5, 129.6, 127.8, 127.7, 126.5, 126.0, 121.1, 118.1, 71.3.

HRMS (ESI): calcd for $C_{14}H_{14}{}^{35}Cl^{35}ClNO_3S$ ($M+NH_4$) 346.0066, found 346.0054, calcd for $C_{14}H_{14}{}^{35}Cl^{37}ClNO_3S$ ($M+NH_4$) 348.0037, found 348.0028, calcd for $C_{14}H_{14}{}^{37}Cl^{37}ClNO_3S$ ($M+NH_4$) 350.0007, found 350.0008, calcd for $C_{14}H_{10}{}^{35}Cl^{35}ClO_3SNa$ (M+Na) 390.9620, found 390.9618. calcd for $C_{14}H_{10}{}^{35}Cl^{37}ClO_3SNa$ (M+Na) 352.9591, found 352.9581.

_S_-(3-(Nicotinamido)propyl) _O_-phenyl thiocarbonate (3ag).



Yield 55 mg (35%). Colorless oil.

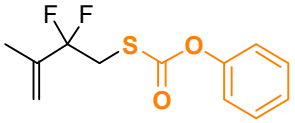
Chromatography: CH_2Cl_2/EtOAc 5/1. R_f 0.35.

^{1}H NMR (300 MHz, DMSO-d_6), δ: 9.40 (s, 1H), 9.07 (s, 1H), 8.67 (d, J = 3.9 Hz, 1H), 8.25 (d, J = 7.9 Hz), 7.51 – 7.39 (m, 1H), 7.19 – 7.04 (m, 2H), 6.89 – 6.77 (m, 2H), 6.75 – 6.65 (m, 1H), 3.38 – 3.25 (m, 2H), 2.61 – 2.51 (m, 2H), 2.18 (t, J = 6.7 Hz, 2H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, DMSO-d_6), δ: 170.8, 165.1, 158.5, 152.0, 149.0, 135.3, 130.6, 129.7, 123.8, 120.9, 118.9, 40.5, 29.7, 25.8.

HRMS (ESI): calcd for $C_{16}H_{17}N_2O_3S$ (M+H) 317.0954, found 317.0949, for $C_{16}H_{16}N_2O_3SNa$ (M+Na) 339.0774, found 339.0776.

***S*-(2,2-Difluoro-3-methylbut-3-en-1-yl) *O*-phenyl thiocarbonate (11).**



Yield 37 mg (29%). Colorless oil.

Chromatography: CH_2Cl_2. R_f 0.75.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.47 – 7.37 (m, 2H), 7.36 – 7.25 (m, 1H), 7.22 – 7.15 (m, 2H), 5.44 (s, 1H), 5.26 (s, 1H), 3.56 (t, J = 13.4 Hz, 2H), 1.91 (s, 3H).

^{19}F NMR (282 MHz, $CDCl_3$), δ: -100.2 (t, J = 13.4 Hz).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 168.9, 151.2, 138.6 (t, J = 24.2 Hz), 129.6, 126.4, 121.1, 119.9 (t, J = 247.3 Hz), 116.9 (t, J = 8.0 Hz), 36.1 (t, J = 31.4 Hz), 17.3 (t, J = 3.0 Hz).

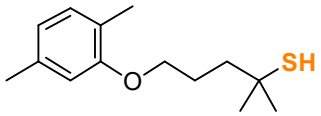
HRMS (ESI): calcd for $C_{12}H_{12}F_2O_3SNa$ (M+Na) 281.0418, found 281.0412.

Synthesis of thiols 4 (General procedure II)

A 50 mL flask containing a stirring bar was charged with carboxylic acid **1** (1.0 equiv, 2 mmol), thionocarbonate **2a** (1.5 equiv, 3 mmol, 898 mg), 9-(2-chlorophenyl)acridine **A-1** (2.5 mol%, 14.4 mg) and dichloromethane (8 mL). The flask was closed with a rubber septum, and a needle was introduced as a pressure compensator. The mixture was irradiated by 60W 400 nm LEDs for 4 hours at 20 °C; during irradiation a solution of 9-(2-chlorophenyl)acridine **A-1** (5 mol%, 28.8 mg) in dichloromethane (1 mL) was added using a syringe pump (250 μL/h). Then, K_2CO_3 (5 equiv, 5 mmol, 690 mg), methanol (10 mL) and water (2 mL) were added, dichloromethane was evaporated under vacuum at room temperature (until vacuum reached *ca*. 25 Torr), the flask was filled with argon, and the mixture was stirred at room temperature for 4 hours. The mixture was diluted with water (20 mL) and extracted with hexanes (4×20 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

NOTE: After completion of the treatment with potassium carbonate, extraction and chromatography should be carried out within two hours to avoid oxidation of thiols.

5-(2,5-Dimethyl-phenoxy)-2-methyl-pentane-2-thiol (4a). [11]



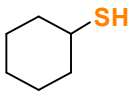
Yield 336 mg (71%). Colorless oil.

Chromatography: hexanes/EtOAc, 20/1. R_f 0.30.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.05 (d, J = 7.4 Hz, 1H), 6.71 (d, J = 7.4 Hz, 1H), 6.67 (s, 1H), 4.00 (t, J = 6.3, 2H), 2.36 (s, 3H), 2.23 (s, 3H), 2.04 – 1.93 (m, 2H), 1.84 – 1.75 (m, 2H), 1.46 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 157.0, 136.5, 130.3, 123.6, 120.8, 112.0, 68.0, 44.5, 43.1, 32.8, 25.7, 21.4, 15.8.

Cyclohexanethiol (4b). [12]



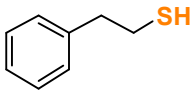
Yield 172 mg (74%). Colorless oil.

Chromatography: hexanes/EtOAc, 20/1. R_f 0.45.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 2.85 – 2.65 (m, 1H), 2.05 – 1.85 (m, 2H), 1.79 – 1.64 (m, 2H), 1.62 – 1.51 (m, 1H), 1.46 (d, *J* = 6.5 Hz, 1H), 1.40 – 1.04 (m 5H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ:38.4, 37.9, 26.3, 25.3.

2-Phenyl-ethanethiol (4c). [13]



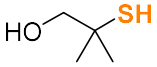
Yield 158 mg (58%). Colorless oil.

Chromatography: hexanes/EtOAc, 20/1. R_f 0.40.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.42 – 7.21 (m, 5H), 3.04 – 2.93 (m, 2H), 2.89 – 2.77 (m, 2H), 1.43 (t, *J* = 7.8 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 139.9, 128.8, 128.6, 126.6, 40.3, 26.1.

2-Mercapto-2-methyl-propan-1-ol (4d). [14]



Yield 176 mg (83%). Colorless oil.

Chromatography: hexanes/EtOAc, 10/1. R_f 0.6.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 3.65 (s, 2H), 2.18 – 1.97 (br s, 1H), 1.93 – 1.86 (br s, 1H), 1.35 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 73.0, 49.5, 28.2.

2-Methyl-propane-2-thiol (4e).

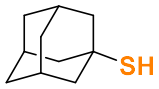
Yield 116 mg (64%). Colorless oil.

Chromatography: pentane. R_f 0.30.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 1.84 (s, 1H), 1.45 (s, 9H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 41.2, 35.0.

Adamantane-1-thiol (4f). [13]



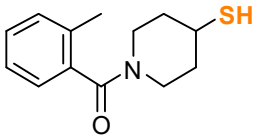
Yield 288 mg (85%). Colorless solid. Mp 100-103 °C.

Chromatography: hexanes/EtOAc, 20/1. R_f 0.55.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 2.17 – 2.06 (m, 3H), 1.95 – 1.76 (br s, 1H), 1.74 – 1.67 (m, 6H), 1.63 – 1.55 (m, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 45.3, 42.2, 36.1, 30.7.

(4-Mercapto-piperidin-1-yl)-o-tolyl-methanone (4g).



Yield 136 mg (29%). Colorless oil.

Chromatography: CH_2Cl_2/EtOAc, 4/1. R_f 0.35.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 8.21 (dd, *J* = 7.9 Hz, *J* = 1.1 Hz, 1H), 7.56 – 7.47 (m, 1H), 7.39 – 7.26 (m, 2H), 4.02 – 3.85 (m, 4H), 2.63 – 2.52 (m, 7H), 2.39 – 2.30 (m, 1H), 1.37 – 1.22 (br s, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 167.5, 141.4, 134.2, 133.9, 132.4, 131.9, 126.4, 42.6, 40.9, 30.2, 22.0.

HRMS (ESI): calcd for $C_{12}H_{18}NOS$ (M+H) 236.1104, found 236.1109.

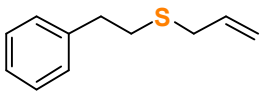
Synthesis of sulfides 5 (General procedure III)

A 50 mL flask containing a stirring bar was charged with 3-phenylpropionic acid (1.0 equiv, 2 mmol, 300 mg), thionocarbonate **2a** (1.5 equiv, 3 mmol, 898 mg), 9-(2-chlorophenyl)acridine **A-1** (2.5 mol%, 14.4 mg) and dichloromethane (8 mL). The flask was closed with a rubber septum, and a needle was introduced as a pressure compensator. The mixture was irradiated by 60W 400 nm LEDs for 4 hours at 20 °C; during irradiation a solution of 9-(2-chlorophenyl)acridine **A-1** (5 mol%, 28.8 mg) in dichloromethane (1 mL) was added using a syringe pump (250 μL/h). Then, halide (5 equiv, 5 mmol), K_2CO_3 (5 equiv, 5 mmol, 690 mg), solvent (10 mL; for **5a**, **5b**, **5f**, methanol; for **5d**, **5e**, **5g**, acetonitrile; for **5c**, ethanol) and water (2 mL) were added, dichloromethane was evaporated under reduced pressure at room temperature (until vacuum reached *ca*. 25 Torr), the flask was filled with argon, and the mixture was stirred under argon atmosphere while heating at 60-70 °C (oil bath temperature) for 4 hours.

For compounds **5a**, **5b**, **5d-g**, the mixture was cooled to room temperature, diluted with dichloromethane (40 mL) and washed with water (3×5 mL) and brine (5 mL). The organic layer was filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

For compound **5c**, the mixture was cooled to room temperature, concentrated under reduced pressure, diluted with water (10 mL) and extracted with EtOAc (3×10 mL). The aqueous layer was acidified with 1M aqueous HCl to pH = 2 and extracted with EtOAc (4×15 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

(2-Allylsulfanyl-ethyl)-benzene (5a). [15]



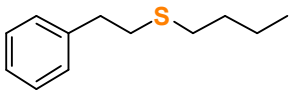
Yield 230 mg (64%). Colorless oil.

Chromatography: hexanes/EtOAc, 10/1. R_f 0.70.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.38 – 7.23 (m, 5H), 5.94 – 5.78 (m, 1H), 5.20 – 5.12 (m, 2H), 3.19 (dt, *J* = 7.1 Hz, *J* = 0.9 Hz, 2H), 2.96 – 2.88 (m, 2H), 2.81 – 2.73 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 140.7, 134.5, 128.6, 128.5, 126.4, 117.0, 36.1, 34.9, 32.1.

(2-Butylsulfanyl-ethyl)-benzene (5b). [16]



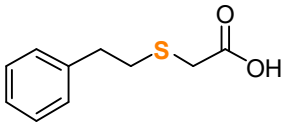
Yield 237 mg (61%). Colorless oil.

Chromatography: hexanes/EtOAc, 10/1. R_f 0.70.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.41 – 7.32 (m, 2H), 7.31 – 7.23 (m, 3H), 3.00 – 2.91 (m, 2H), 2.88 – 2.74 (m, 2H), 2.60 (t, *J* = 7.4 Hz, 2H), 1.71 – 1.59 (m, 2H), 1.55 – 1.41 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 140.9, 128.6, 128.5, 126.3, 36.5, 33.7, 32.1, 31.8, 22.1, 13.8.

Phenethylsulfanyl-acetic acid (5c). [17]



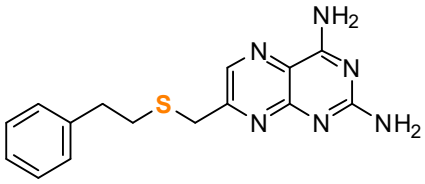
Yield 227 mg (58%). White solid. Mp 55-57 °C (ethanol/water 1:1).

Chromatography: EtOAc. R_f 0.4.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 11.25 – 10.85 (br s, 1H), 7.41 – 7.20 (m, 5H), 3.35 – 3.22 (br s, 2H), 3.04 – 2.91 (br s, 4H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 177.0, 139.9, 128.7, 128.6, 126.6, 35.6, 34.2, 33.6.

7-Phenethylsulfanylmethyl-pteridine-2,4-diamine (5d).



Yield 181 mg (29%). Colorless solid. Mp 194-197 °C (ethanol, dec.).

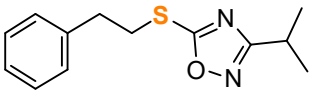
Chromatography: CH_2Cl_2/MeOH, 5/1. R_f 0.30.

^{1}H NMR (300 MHz, DMSO-d_6), δ: 8.75 (s, 1H), 7.7 – 7.45 (br, 2H), 7.31 – 7.14 (m, 5H), 6.7 – 6.55 (br s, 2H), 3.94 (s, 2H), 2.86 – 2.67 (m, 4H).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6), δ: 163.8, 163.3, 155.4, 151.4, 147.0, 140.8, 129.0, 128.7, 126.6, 121.2, 35.7, 34.5, 32.6.

HRMS (ESI): calcd for $C_{15}H_{17}N_6S$ (M+H) 313.1230, found 313.1227; calcd for $C_{15}H_{16}N_6SNa$ (M+Na) 335.1049, found 335.1043.

3-Isopropyl-5-phenethylsulfanyl-[1,2,4]oxadiazole (5e).



Yield 378 mg (76%). Colorless oil.

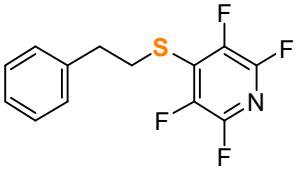
Chromatography: CH_2Cl_2. R_f 0.60.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.40 – 7.20 (m, 5H), 3.58 – 3.44 (m, 2H), 3.17 – 3.08 (m, 2H), 3.04 – 2.96 (m, 1H), 1.38 (d, J = 7 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 177.2, 175.3, 139.1, 128.7, 128.6, 126.9, 35.8, 34.0, 26.8, 20.4.

HRMS (ESI): calcd for $C_{13}H_{17}N_2OS$ (M+H) 249.1056, found 249.1051.

2,3,5,6-Tetrafluoro-4-phenethylsulfanyl-pyridine (5f). [18]



Yield 384 mg (67%). Colorless oil.

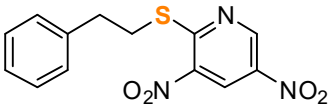
Chromatography: hexanes/EtOAc, 10/1. R_f 0.65.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.36 – 7.17 (m, 5H), 3.39 (t, J = 7.9 Hz, 2H), 2.98 (t, J = 7.9 Hz, 2H).

^{19}F NMR (282 MHz, $CDCl_3$), δ: -95.3 – -95.6 (m, 2F), -138.4 – -138.6 (m, 2F).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 142.5 (dm, J = 254.3 Hz), 140.8 (dm, J = 246.5 Hz), 138.9, 131.4 – 130.7 (m), 128.6, 128.5, 126.7, 36.6, 34.3 (t, J = 4.6 Hz).

3,5-Dinitro-2-phenethylsulfanyl-pyridine (5g).



Yield 363 mg (59%). Light yellow solid. Mp 122-124 °C (ethanol).

Chromatography: CH_2Cl_2. R_f 0.35.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 9.41 (d, J = 2.4 Hz, 1H), 9.20 (d, J = 2.4 Hz, 1H), 7.40 – 7.20 (m, 5H), 3.65 – 3.56 (m, 2H), 3.13 – 3.03 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 165.1, 147.2, 140.7, 139.7, 139.5, 128.8, 128.7, 128.6, 126.9, 34.7, 32.9.

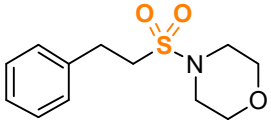
^{14}N NMR (21.69 MHz, $CDCl_3$), δ: -18.9.

HRMS (ESI): calcd for $C_{13}H_{12}N_3O_4S$ (M+H) 306.0543, found 306.0548.

Synthesis of sulfonamides 6 (General procedure IV)

A 50 mL flask containing a stirring bar was charged with 3-phenylpropionic acid (1.0 equiv, 2 mmol, 300 mg), thionocarbonate **2a** (1.5 equiv, 3 mmol, 898 mg), 9-(2-chlorophenyl)acridine **A-1** (2.5 mol%, 14.4 mg) and dichloromethane (8 mL). The flask was closed with a rubber septum, and a needle was introduced as a pressure compensator. The mixture was irradiated by 60W 400 nm LEDs for 4 hours at 20 °C; during irradiation a solution of 9-(2-chlorophenyl)acridine **A-1** (5 mol%, 28.8 mg) in dichloromethane (1 mL) was added using a syringe pump (250 μL/h). Then, acetic acid (10 mL) and water (5 equiv, 5 mmol, 90 μL) were added, dichloromethane was evaporated under reduced pressure at room temperature (until vacuum reached *ca*. 25 Torr), and a slow stream of chlorine was bubbled at room temperature until the mixture was saturated. The mixture was stirred at room temperature for 15 minutes, concentrated under reduced pressure, diluted with acetonitrile (10 mL) followed by addition of amine (5 equiv, 5 mmol) at 0 °C (ice bath). The mixture was stirred at room temperature for 15 min, diluted with water (10 mL) and extracted with EtOAc (3×20 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

4-(2-Phenyl-ethanesulfonyl)-morpholine (6a). [19]



Yield 352 mg (69%). Colorless oil.

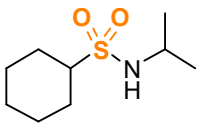
Chromatography: CH_2Cl_2. R_f 0.5.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.41 – 7.19 (m, 5H), 3.79 – 3.71 (m, 4H), 3.34 – 3.23 (m, 4H), 3.231 – 3.11 (m, 4H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ: 137.9, 128.9, 128.4, 127.0, 66.6, 50.4, 45.8, 29.2.

HRMS (ESI): calcd for $C_{12}H_{18}NO_3S$ (M+H) 256.1002, found 256.1009.

Cyclohexanesulfonic acid isopropylamide (6b). [20]



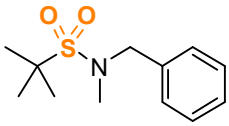
Yield 291 mg (71%). Colorless solid. Mp 65-67 °C (hexane).

Chromatography: CH_2Cl_2. R_f 0.35.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 5.72 – 5.31 (br s, 1H), 4.02 (hept, *J* = 7.0 Hz, 1H), 3.53 (tt, *J* = 11.8, 3.5 Hz, 1H), 2.47 – 2.34 (m, 2H), 2.05 – 1.92 (m, 2H), 1.81 – 1.62 (m, 3H), 1.47 – 1.20 (m, 3H), 1.14 (d, *J* = 7.0 Hz, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 74.9, 49.9, 27.2, 25.0, 24.7, 24.0.

2-Methyl-propane-2-sulfonic acid benzyl-methyl-amide (6c).



Yield 390 mg (81%). Colorless oil.

Chromatography: CH_2Cl_2. R_f 0.55.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.38 – 7.17 (m, 5H), 4.65 (s, 2H), 2.99 (s, 3H), 1.34 (s, 9H).

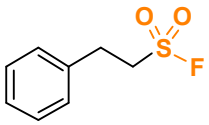
^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 137.6, 129.6, 127.3, 127.2, 53.2, 38.9, 36.1, 28.4.

HRMS (ESI): calcd for $C_{12}H_{20}NO_2S$ (M+H) 242.1209, found 242.1215; calcd for $C_{12}H_{19}NO_2SNa$ (M+Na) 264.1029, found 264.1038.

Synthesis of sulfonyl fluorides 7 (General procedure V)

Selectfluor (7.5 equiv, 664 mg, 1.875 mmol) was added to a stirred solution of thiocarbonate **3** (1 equiv, 0.25 mmol) in acetonitrile (2.5 mL) and water (0.25 mL) at room temperature, and the mixture was heated at reflux (*ca.* 85 °C) for 2 hours. At this point, TLC control indicated consumption of the starting thiocompound. For the work-up, water (2.5 mL) was added, and the mixture was extracted with dichloromethane (3×10 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

2-Phenyl-ethanesulfonyl fluoride (7a). [21]



Yield 36 mg (77%) from **3g**, 42 mg (89%) from **4c**. Colorless oil.

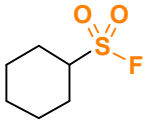
Chromatography: CH_2Cl_2. R_f 0.9.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 7.34 – 7.09 (m, 5H), 3.59 – 3.48 (m, 2H), 3.23 – 3.10 (m, 2H).

^{19}F NMR (282 MHz, $CDCl_3$), δ: 52.5.

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 136.0, 129.1, 128.4, 127.6, 52.1 (d, J = 15.4 Hz), 29.6.

Cyclohexanesulfonyl fluoride (7b). [22]



Yield 32 mg (77%). Colorless oil.

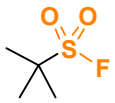
Chromatography: CH_2Cl_2. R_f 0.9.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 3.39 – 3.26 (m, 1H), 2.41 – 2.24 (m, 2H), 2.06 – 1.90 (m, 2H), 1.84 – 1.64 (m, 3H), 1.44 – 1.26 (m, 3H).

^{19}F NMR (282 MHz, $CDCl_3$), δ: 40.7.

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ: 61.0 (d, J = 12.8 Hz), 26.5, 24.7, 24.6.

2-Methyl-propane-2-sulfonyl fluoride (7c).



Yield 11 mg (31%). Colorless oil.

Chromatography: CH_2Cl_2. R_f 0.9.

^{1}H NMR (300 MHz, $CDCl_3$), δ: 1.36 (s, 9H).

^{19}F NMR (282 MHz, $CDCl_3$), δ: 47.9.

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ: 68.3 (d, J = 10.5 Hz), 28.8.

HRMS (ESI): calcd for $C_4H_{10}FO_2S$ (M+H) 141.0380, found 141.0386.

X-ray crystallographic data

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program. [23] The structure was solved by direct methods using SHELXT [24] and refined on F^2 using SHELXL-2018 [25] in the OLEX2 program. [26] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters. A rotating group model was applied for methyl groups.

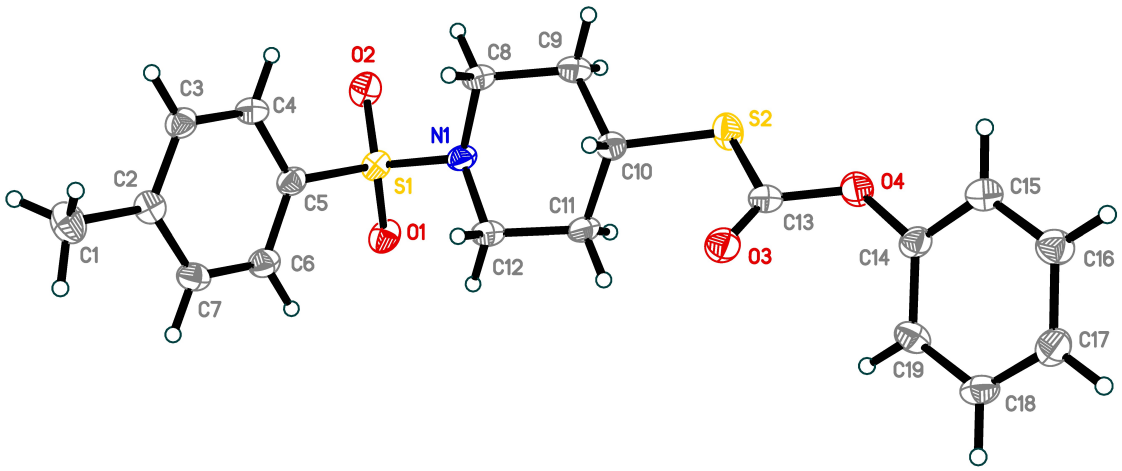


Figure S1. X-ray structure of compound **3f**. Anisotropic displacement parameters are drawn at the 50% probability.

Table S1. Crystal data and structure refinement for compound **3f**.

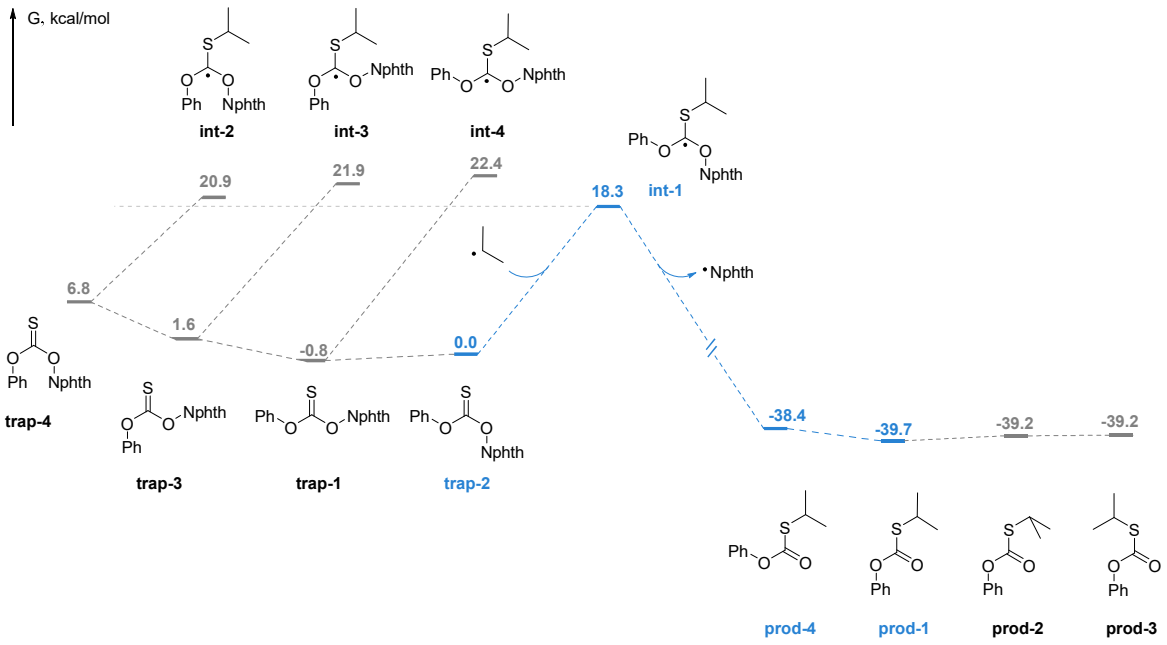
CCDC number	2271075
Empirical formula	$C_{19}H_{21}NO_4S_2$
Formula weight	391.49
Temperature	99.9(3) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 6.29180(10) Å α= 90° b = 7.95790(10) Å ω= 90° c = 37.0360(5) Å γ= 90°
Volume	1854.37(5) $Å^3$
Z	4
Density (calculated)	1.402 Mg/m^3
Absorption coefficient	2.815 mm^{-1}
F(000)	824
Crystal size	0.5 × 0.3 × 0.3 mm^3
Theta range for data collection	2.386 to 77.798°
Index ranges	$-6 \le h \le 7$ $-10 \le k \le 10$ $-46 \le l \le 46$
Reflections collected	13457
Independent reflections	3782 [R(int) = 0.0488]
Completeness to theta = 67.684°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max and min transmission	1.00000 and 0.53768
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3782 / 0 / 237
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1209
R indices (all data)	R1 = 0.0481, wR2 = 0.1219
Absolute structure parameter	0.18(3)
Largest diff. peak and hole	0.517 and -0.437 $e \cdot Å^{-3}$

Crystal structure determination was performed in the Department of Structural Studies of Zelinsky Institute of Organic Chemistry, Moscow.

DFT calculations

All calculations were carried out using the Gaussian09 package [27]. Geometries of stationary points were optimized using the (u)ωB97XD functional with the def2-TZVP basis set. Stationary points were verified by vibrational analysis (no imaginary frequencies for intermediates and single imaginary frequency for the transition states). Solvation effects were evaluated using the PCM model (dichloromethane as solvent). Structures are given in the xyz format (visualized with CYLview26 [28]) with energies in Hartrees.

The simplified reaction pathway given in the main text (Scheme S1, blue) was chosen according to the conformational analysis – the addition of isopropyl radical was considered through conformer **trap-2** of reagent **2a** in accordance with the Curtin–Hammett principle.



Scheme S1. Gibbs free energy profile for the addition-elimination step considering various conformers.

Activation barrier $\Delta G^{\neq}$ of a single electron transfer between phthalimide radical (•Nphth) and acridinyl radical (•Acr-H) was estimated according to the Marcus-Hush theory [29,30].

$A + D \rightarrow A^{-\cdot} + D^{+\cdot}$ (ΔG),

where A = •Nphth, D = •Acr-H

$\Delta G^{\neq} = (\lambda + \Delta G)^2 / 4\lambda$

The reorganization energy λ was calculated as the sum of two contributions – inner-sphere (λ_i) and outer-sphere (λ_o). The first contribution was estimated via the improved Nelsen's four-point method [31,32]:

$\lambda = \lambda_i + \lambda_o$

$\lambda_i^2 = \lambda_{for} \cdot \lambda_{back} = (E_{ncg} - E_n)\,(E_{cng} - E_c)$

where E_{ncg} – electronic energy of **n**eutral species at the **c**harged species' **g**eometry,

E_{cng} – electronic energy of **c**harged species at the **n**eutral species' **g**eometry,

E_n – electronic energy of ground state of **n**eutral species,

E_c – electronic energy of ground state of **c**harged species.

$\lambda_i^2 = 21.60 \cdot 12.44 = 268.77$

$\lambda_i = 16.39$ kcal/mol

The outer-sphere (solvent) contribution was estimated using the Born model for the solvation of a charged species [29,33]:

$\lambda_o = 332.2$ kcal·Å/mol $(1/\varepsilon_s - 1/\varepsilon_{op})\,(1/2r_1 + 1/2r_2 - 1/(r_1+r_2))$

For dichloromethane static dielectric constant $\varepsilon_s = 4.90$, optical dielectric constant (which is square of refractive index) $\varepsilon_{op} = 1.4244^2 = 2.03$. The radii of phthalimide ($r_1 = 3.08$ Å) and acridinyl ($r_2 = 3.82$ Å) species are estimated as the radii of spheres with the same volume of the molecule using the VEGA ZZ program [34].

$\lambda_o = 332.2\,(1/2.03 - 1/4.90)\,(1/3.08 + 1/7.65 - 1/6.90) = 14.23$ kcal/mol

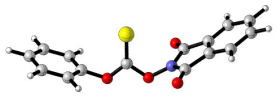
$\lambda = 14.23 + 16.39 = 30.62$ kcal/mol

Having the $\Delta G = -38.81$ kcal/mol, we obtain:

$\Delta G^{\neq} = (\lambda + \Delta G)^2 / 4\lambda = (30.62 - 38.81)^2 / (4 \cdot 30.62) = 0.55$ kcal/mol

Energies and Cartesian coordinates

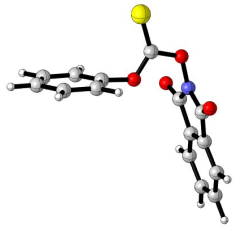
Thionocarbonate **2a** (**trap-1**)



SCF Energy = -1330.86349727
Zero-point correction = 0.214250
Thermal correction to Energy = 0.230865
Thermal correction to Enthalpy = 0.231810
Thermal correction to Gibbs Free Energy = 0.166444
Sum of electronic and zero-point Energies = -1330.649247
Sum of electronic and thermal Energies = -1330.632632
Sum of electronic and thermal Enthalpies = -1330.631688
Sum of electronic and thermal Free Energies = -1330.697053

S	-0.846479000	-0.000077000	1.248460000
C	-1.058102000	0.000083000	-0.359354000
O	-2.168121000	0.000154000	-1.057324000
C	-3.405119000	0.000052000	-0.400669000
C	-4.006814000	1.210742000	-0.126297000
C	-4.006762000	-1.210734000	-0.126622000
C	-5.262981000	1.202526000	0.461412000
C	-5.262929000	-1.202734000	0.461091000
C	-5.889472000	-0.000158000	0.755533000
H	-3.499901000	2.135885000	-0.365400000
H	-3.499807000	-2.135791000	-0.365970000
H	-5.752329000	2.141119000	0.685627000
H	-5.752231000	-2.141410000	0.685057000
H	-6.869850000	-0.000240000	1.213440000
O	-0.075227000	0.000203000	-1.309836000
N	1.188304000	0.000129000	-0.828908000
C	1.882667000	-1.179747000	-0.538920000
C	1.882695000	1.179891000	-0.538622000
C	3.197908000	0.694834000	-0.044617000
C	5.412479000	0.694817000	0.786506000
C	5.412480000	-0.695100000	0.786285000
C	4.296479000	1.414987000	0.367760000
H	6.295044000	-1.225546000	1.118318000
H	4.290604000	2.496642000	0.366260000
C	4.296478000	-1.415138000	0.367315000
H	4.290598000	-2.496793000	0.365483000
C	3.197904000	-0.694855000	-0.044830000
H	6.295044000	1.225158000	1.118706000
O	1.453379000	2.288554000	-0.680476000
O	1.453334000	-2.288349000	-0.681160000

Thionocarbonate **2a** (**trap-2**)

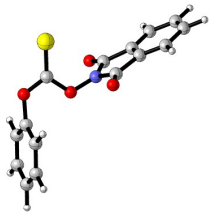


SCF Energy = -1330.86137846

Zero-point correction = 0.213976
Thermal correction to Energy = 0.230657
Thermal correction to Enthalpy = 0.231601
Thermal correction to Gibbs Free Energy = 0.165560
Sum of electronic and zero-point Energies = -1330.647403
Sum of electronic and thermal Energies = -1330.630722
Sum of electronic and thermal Enthalpies = -1330.629777
Sum of electronic and thermal Free Energies = -1330.695819

S	2.555049000	-2.422477000	0.001473000
C	1.230512000	-1.487727000	0.000490000
O	1.124343000	-0.182147000	-0.000332000
C	2.273025000	0.620969000	-0.000409000
C	2.790686000	1.028370000	-1.211865000
C	2.788874000	1.031037000	1.210917000
C	3.885484000	1.879545000	-1.203568000
C	3.883690000	1.882197000	1.202358000
C	4.431029000	2.305217000	-0.000662000
H	2.346381000	0.683496000	-2.135821000
H	2.343177000	0.688233000	2.134973000
H	4.310092000	2.211877000	-2.141599000
H	4.306899000	2.216638000	2.140274000
H	5.283506000	2.971723000	-0.000755000
O	0.004444000	-2.081805000	0.000411000
N	-1.071714000	-1.243599000	0.000194000
C	-1.628490000	-0.735348000	-1.178627000
C	-1.628194000	-0.734528000	1.178792000
C	-2.732059000	0.135303000	0.694921000
C	-4.572574000	1.620249000	0.694618000
C	-4.572830000	1.619670000	-0.695312000
C	-3.644882000	0.872258000	1.415282000
H	-5.305319000	2.212955000	-1.226376000
H	-3.638679000	0.870717000	2.496905000
C	-3.645400000	0.871089000	-1.415700000
H	-3.639578000	0.868681000	-2.497324000
C	-2.732297000	0.134741000	-0.695070000
H	-5.304874000	2.213966000	1.225462000
O	-1.241481000	-0.975336000	2.286204000
O	-1.242286000	-0.977177000	-2.285990000

Thionocarbonate **2a** (**trap-3**)



SCF Energy = -1330.85980209
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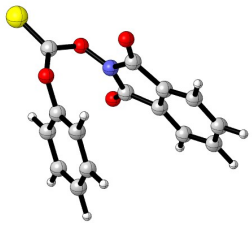
Thermal correction to Energy = 0.230883
Thermal correction to Enthalpy = 0.231827
Thermal correction to Gibbs Free Energy = 0.166594
Sum of electronic and zero-point Energies = -1330.645538
Sum of electronic and thermal Energies = -1330.628919
Sum of electronic and thermal Enthalpies = -1330.627975
Sum of electronic and thermal Free Energies = -1330.693208

S	0.096971000	2.219944000	-1.509885000
C	1.068149000	1.176221000	-0.735429000
O	2.376235000	1.237060000	-0.766306000
C	3.188101000	0.256555000	-0.164203000
C	3.426679000	-0.922658000	-0.841110000
C	3.784358000	0.555885000	1.042678000

C	4.291540000	-1.844409000	-0.272169000
C	4.650246000	-0.375627000	1.597692000
C	4.902261000	-1.573193000	0.944520000
H	2.943012000	-1.113201000	-1.789855000
H	3.574842000	1.496930000	1.532927000
H	4.488427000	-2.776997000	-0.784246000
H	5.127918000	-0.160926000	2.544527000
H	5.579383000	-2.295203000	1.381594000
O	0.673200000	0.126326000	0.042734000
N	-0.662172000	-0.064239000	0.127616000
C	-1.361683000	-0.868075000	-0.779913000
C	-1.453982000	0.559254000	1.098840000
C	-2.822004000	0.061854000	0.798379000
C	-5.159399000	-0.275021000	0.937320000
C	-5.104464000	-1.116606000	-0.167397000
C	-4.010184000	0.330045000	1.439921000
H	-6.014781000	-1.571077000	-0.535185000
H	-4.047568000	0.987500000	2.297994000
C	-3.897875000	-1.382694000	-0.809766000
H	-3.849138000	-2.036478000	-1.670089000
C	-2.767424000	-0.779277000	-0.306956000
H	-6.112190000	-0.087394000	1.414228000
O	-1.053271000	1.305317000	1.944762000
O	-0.872683000	-1.459467000	-1.698877000

Thionocarbonate **2a** (**trap-4**)



SCF Energy = -1330.85241438
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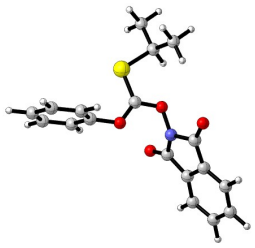
Thermal correction to Energy = 0.230398
Thermal correction to Enthalpy = 0.231342
Thermal correction to Gibbs Free Energy = 0.167533
Sum of electronic and zero-point Energies = -1330.638558
Sum of electronic and thermal Energies = -1330.622017
Sum of electronic and thermal Enthalpies = -1330.621072
Sum of electronic and thermal Free Energies = -1330.684882

S	-0.846479000	-0.000077000	1.248460000
C	-1.058102000	0.000083000	-0.359354000
O	-2.168121000	0.000154000	-1.057324000
C	-3.405119000	0.000052000	-0.400669000
C	-4.006814000	1.210742000	-0.126297000
C	-4.006762000	-1.210734000	-0.126622000
C	-5.262981000	1.202526000	0.461412000
C	-5.262929000	-1.202734000	0.461091000
C	-5.889472000	-0.000158000	0.755533000
H	-3.499901000	2.135885000	-0.365400000
H	-3.499807000	-2.135791000	-0.365970000
H	-5.752329000	2.141119000	0.685627000
H	-5.752231000	-2.141410000	0.685057000
H	-6.869850000	-0.000240000	1.213440000
O	-0.075227000	0.000203000	-1.309836000
N	1.188304000	0.000129000	-0.828908000
C	1.882667000	-1.179747000	-0.538920000
C	1.882695000	1.179891000	-0.538622000
C	3.197908000	0.694834000	-0.044617000
C	5.412479000	0.694817000	0.786506000
C	5.412480000	-0.695100000	0.786285000

C	4.296479000	1.414987000	0.367760000
H	6.295044000	-1.225546000	1.118318000
H	4.290604000	2.496642000	0.366260000
C	4.296478000	-1.415138000	0.367315000
H	4.290598000	-2.496793000	0.365483000
C	3.197904000	-0.694855000	-0.044830000
H	6.295044000	1.225158000	1.118706000
O	1.453379000	2.288554000	-0.680476000
O	1.453334000	-2.288349000	-0.681160000

Radical addition product (**int-1**)

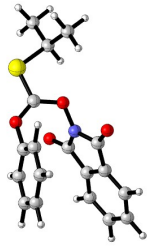


SCF Energy = -1449.34099197
Zero-point correction = 0.308018
Thermal correction to Energy = 0.329524
Thermal correction to Enthalpy = 0.330468
Thermal correction to Gibbs Free Energy = 0.254592
Sum of electronic and zero-point Energies = -1449.032974
Sum of electronic and thermal Energies = -1449.011468
Sum of electronic and thermal Enthalpies = -1449.010524
Sum of electronic and thermal Free Energies = -1449.086400

S	-2.442580000	1.265843000	-0.270964000
C	-0.985323000	0.429986000	-0.029059000
O	-0.933514000	-0.822929000	0.220835000
C	-2.126532000	-1.589108000	0.272198000
C	-2.578405000	-2.161677000	-0.896911000
C	-2.729990000	-1.767082000	1.498006000
C	-3.721219000	-2.944319000	-0.829101000
C	-3.870412000	-2.554782000	1.543669000
C	-4.364576000	-3.137327000	0.385308000
H	-2.051268000	-1.999809000	-1.827290000
H	-2.319421000	-1.305063000	2.385276000
H	-4.104510000	-3.405593000	-1.729123000
H	-4.369011000	-2.713224000	2.490265000
H	-5.254823000	-3.750511000	0.429891000
O	0.129799000	1.087059000	-0.095523000
N	1.284652000	0.336990000	0.045563000
C	1.843047000	-0.293526000	-1.100653000
C	2.208388000	0.688638000	1.063399000
C	3.404195000	0.048305000	0.605458000
C	5.664142000	-0.726780000	0.570609000
C	5.448560000	-1.305786000	-0.707455000
C	4.658160000	-0.060096000	1.223680000
H	6.264463000	-1.824206000	-1.195330000
H	4.822842000	0.381496000	2.198932000
C	4.228644000	-1.216970000	-1.328531000
H	4.066112000	-1.661422000	-2.302825000
C	3.186452000	-0.535622000	-0.680377000
H	6.638734000	-0.817519000	1.033381000
O	1.912069000	1.363938000	2.048068000
O	1.188733000	-0.522638000	-2.119126000
C	-1.882319000	3.007974000	-0.524382000
H	-1.052026000	2.952104000	-1.225828000
C	-1.455921000	3.651056000	0.783678000
C	-3.064425000	3.712733000	-1.177686000
H	-3.338106000	3.252083000	-2.126339000
H	-3.936460000	3.722057000	-0.521113000

H	-2.779667000	4.747510000	-1.369060000
H	-2.279972000	3.664721000	1.497967000
H	-1.166016000	4.683088000	0.578900000
H	-0.603642000	3.144728000	1.233636000

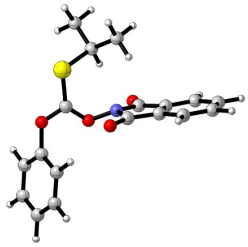
Radical addition product (**int-2**)



SCF Energy = -1449.33868209
Zero-point correction = 0.308246
Thermal correction to Energy = 0.329532
Thermal correction to Enthalpy = 0.330477
Thermal correction to Gibbs Free Energy = 0.256437
Sum of electronic and zero-point Energies = -1449.030436
Sum of electronic and thermal Energies = -1449.009150
Sum of electronic and thermal Enthalpies = -1449.008205
Sum of electronic and thermal Free Energies = -1449.082245

S	-3.468108000	-0.610378000	-0.564896000
C	-1.796697000	-0.577443000	-0.287934000
O	-1.128129000	-1.509884000	-0.854948000
C	0.177971000	-1.942147000	-0.488372000
C	0.368104000	-2.536591000	0.738862000
C	1.161980000	-1.824488000	-1.444893000
C	1.637618000	-3.014452000	1.029887000
C	2.422771000	-2.306273000	-1.132280000
C	2.660356000	-2.896807000	0.101163000
H	-0.439671000	-2.615978000	1.453248000
H	0.948369000	-1.346860000	-2.390582000
H	1.820885000	-3.477427000	1.989927000
H	3.220249000	-2.214616000	-1.857182000
H	3.647971000	-3.269649000	0.337758000
O	-1.315679000	0.353346000	0.487876000
N	0.020877000	0.647983000	0.334182000
C	0.494220000	1.190433000	-0.883291000
C	0.918927000	0.644712000	1.422175000
C	2.108166000	1.159149000	0.803115000
C	4.383764000	1.830962000	0.537157000
C	4.134639000	2.142185000	-0.823027000
C	3.385426000	1.343820000	1.345337000
H	4.944893000	2.519603000	-1.434265000
H	3.575862000	1.101550000	2.383605000
C	2.889127000	1.973117000	-1.374258000
H	2.702833000	2.208618000	-2.414776000
C	1.854067000	1.482231000	-0.564259000
H	5.377602000	1.978884000	0.940291000
O	0.632110000	0.261311000	2.553763000
O	-0.217947000	1.260600000	-1.890806000
C	-4.057949000	0.979505000	0.157451000
H	-3.303515000	1.717191000	-0.111075000
C	-4.214675000	0.879911000	1.665333000
C	-5.366160000	1.294230000	-0.556982000
H	-5.223705000	1.406757000	-1.631080000
H	-6.116796000	0.522640000	-0.376292000
H	-5.752895000	2.234088000	-0.161957000
H	-4.945577000	0.115393000	1.931839000
H	-4.574084000	1.839433000	2.041245000
H	-3.271605000	0.655234000	2.160190000

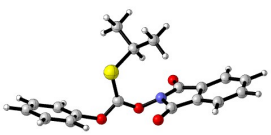
Radical addition product (**int-3**)



SCF Energy = -1449.33665754
Zero-point correction = 0.307873
Thermal correction to Energy = 0.329213
Thermal correction to Enthalpy = 0.330157
Thermal correction to Gibbs Free Energy = 0.255922
Sum of electronic and zero-point Energies = -1449.028784
Sum of electronic and thermal Energies = -1449.007444
Sum of electronic and thermal Enthalpies = -1449.006500
Sum of electronic and thermal Free Energies = -1449.080735

S	2.555049000	-2.422477000	0.001473000
C	1.230512000	-1.487727000	0.000490000
O	1.124343000	-0.182147000	-0.000332000
C	2.273025000	0.620969000	-0.000409000
C	2.790686000	1.028370000	-1.211865000
C	2.788874000	1.031037000	1.210917000
C	3.885484000	1.879545000	-1.203568000
C	3.883690000	1.882197000	1.202358000
C	4.431029000	2.305217000	-0.000662000
H	2.346381000	0.683496000	-2.135821000
H	2.343177000	0.688233000	2.134973000
H	4.310092000	2.211877000	-2.141599000
H	4.306899000	2.216638000	2.140274000
H	5.283506000	2.971723000	-0.000755000
O	0.004444000	-2.081805000	0.000411000
N	-1.071714000	-1.243599000	0.000194000
C	-1.628490000	-0.735348000	-1.178627000
C	-1.628194000	-0.734528000	1.178792000
C	-2.732059000	0.135303000	0.694921000
C	-4.572574000	1.620249000	0.694618000
C	-4.572830000	1.619670000	-0.695312000
C	-3.644882000	0.872258000	1.415282000
H	-5.305319000	2.212955000	-1.226376000
H	-3.638679000	0.870717000	2.496905000
C	-3.645400000	0.871089000	-1.415700000
H	-3.639578000	0.868681000	-2.497324000
C	-2.732297000	0.134741000	-0.695070000
H	-5.304874000	2.213966000	1.225462000
O	-1.241481000	-0.975336000	2.286204000
O	-1.242286000	-0.977177000	-2.285990000

Radical addition product (**int-4**)

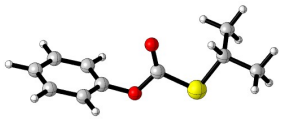


SCF Energy = -1449.33548132
Zero-point correction = 0.307983
Thermal correction to Energy = 0.329316
Thermal correction to Enthalpy = 0.330260

Thermal correction to Gibbs Free Energy = 0.255642
Sum of electronic and zero-point Energies = -1449.027498
Sum of electronic and thermal Energies = -1449.006166
Sum of electronic and thermal Enthalpies = -1449.005221
Sum of electronic and thermal Free Energies = -1449.079840

S	1.285049000	0.832707000	-0.751875000
C	1.089208000	-0.142738000	0.623448000
O	2.072047000	-0.821321000	1.100941000
C	3.368097000	-0.723477000	0.538851000
C	4.247580000	0.188631000	1.081333000
C	3.699072000	-1.591721000	-0.478524000
C	5.526815000	0.244654000	0.550606000
C	4.984711000	-1.520566000	-0.994726000
C	5.892958000	-0.604394000	-0.484819000
H	3.937254000	0.838552000	1.888131000
H	2.972310000	-2.299881000	-0.853261000
H	6.238322000	0.954548000	0.950376000
H	5.273762000	-2.188625000	-1.794734000
H	6.893092000	-0.553594000	-0.894128000
O	0.035944000	-0.291815000	1.380707000
N	-1.176633000	-0.217883000	0.726471000
C	-1.580139000	-1.327519000	-0.068499000
C	-2.229483000	0.568163000	1.255788000
C	-3.371618000	0.015624000	0.594117000
C	-5.634829000	-0.270779000	-0.113607000
C	-5.251844000	-1.392320000	-0.894197000
C	-4.711231000	0.429839000	0.620383000
H	-6.006929000	-1.922963000	-1.460358000
H	-5.004392000	1.286524000	1.214756000
C	-3.946313000	-1.810227000	-0.941538000
H	-3.655227000	-2.664806000	-1.539783000
C	-2.985296000	-1.111131000	-0.194330000
H	-6.674289000	0.031834000	-0.100397000
O	-2.050009000	1.503663000	2.036442000
O	-0.773914000	-2.157394000	-0.491972000
C	-0.058951000	2.113233000	-0.711100000
H	-0.490496000	2.086703000	0.286404000
C	-1.098949000	1.834878000	-1.781539000
C	0.655815000	3.443153000	-0.917798000
H	1.373021000	3.645642000	-0.123653000
H	1.171083000	3.479414000	-1.879246000
H	-0.098046000	4.231543000	-0.911926000
H	-0.654664000	1.879368000	-2.777026000
H	-1.868060000	2.606301000	-1.719346000
H	-1.577257000	0.866425000	-1.653145000

Thiocarbonate **3a** (**prod-1**)

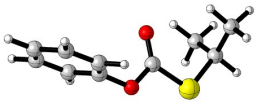


SCF Energy = -936.987832805
Zero-point correction = 0.202023
Thermal correction to Energy = 0.214912
Thermal correction to Enthalpy = 0.215856
Thermal correction to Gibbs Free Energy = 0.160918
Sum of electronic and zero-point Energies = -936.785810
Sum of electronic and thermal Energies = -936.772921
Sum of electronic and thermal Enthalpies = -936.771977
Sum of electronic and thermal Free Energies = -936.826915

S	2.023633000	-0.589212000	-0.740011000

C	0.511805000	-0.073156000	-0.001543000
O	-0.499888000	-0.459026000	-0.803467000
C	-1.802273000	-0.206883000	-0.369030000
C	-2.381285000	1.020428000	-0.629243000
C	-2.496934000	-1.224239000	0.256385000
C	-3.697288000	1.232374000	-0.246675000
C	-3.813222000	-1.001415000	0.632739000
C	-4.413471000	0.224435000	0.383979000
H	-1.807917000	1.793464000	-1.123619000
H	-2.011238000	-2.173512000	0.439559000
H	-4.163099000	2.189334000	-0.442800000
H	-4.369021000	-1.790580000	1.122321000
H	-5.441102000	0.394040000	0.677776000
O	0.380206000	0.506564000	1.037700000
C	3.226602000	0.085458000	0.460163000
H	2.792648000	-0.102117000	1.441646000
C	3.435931000	1.578772000	0.263749000
C	4.518588000	-0.707328000	0.308797000
H	4.361142000	-1.771124000	0.486923000
H	4.948236000	-0.581035000	-0.687422000
H	5.247345000	-0.342052000	1.034043000
H	3.850610000	1.784050000	-0.724976000
H	4.139752000	1.948856000	1.012649000
H	2.501259000	2.127081000	0.374282000

Thiocarbonate **3a** (**prod-2**)

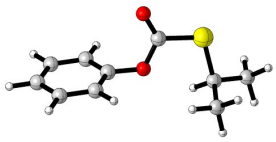


SCF Energy = -936.986112546
Zero-point correction = 0.201514
Thermal correction to Energy = 0.214630
Thermal correction to Enthalpy = 0.215575
Thermal correction to Gibbs Free Energy = 0.159972
Sum of electronic and zero-point Energies = -936.784598
Sum of electronic and thermal Energies = -936.771482
Sum of electronic and thermal Enthalpies = -936.770538
Sum of electronic and thermal Free Energies = -936.826140

S	2.063632000	-0.197979000	-1.162051000
C	0.611952000	-0.038642000	-0.179469000
O	-0.448771000	-0.185190000	-1.001577000
C	-1.720893000	-0.078081000	-0.438800000
C	-2.300962000	1.169891000	-0.314362000
C	-2.389403000	-1.232414000	-0.079493000
C	-3.588777000	1.261350000	0.191576000
C	-3.678078000	-1.128958000	0.423798000
C	-4.277656000	0.114573000	0.561387000
H	-1.748816000	2.052435000	-0.609451000
H	-1.904923000	-2.192887000	-0.194941000
H	-4.054154000	2.232781000	0.296335000
H	-4.212903000	-2.025644000	0.709019000
H	-5.282138000	0.191081000	0.956808000
O	0.536892000	0.161703000	0.998276000
C	3.424934000	0.006508000	0.042341000
H	4.277182000	-0.098972000	-0.634632000
C	3.482647000	-1.114294000	1.070762000
C	3.469721000	1.396940000	0.660901000
H	3.458958000	2.171524000	-0.105634000
H	2.626852000	1.553473000	1.332524000
H	4.390907000	1.499981000	1.238187000
H	2.637649000	-1.061317000	1.755891000

H	4.401171000	-1.015729000	1.653114000
H	3.486240000	-2.092412000	0.590153000

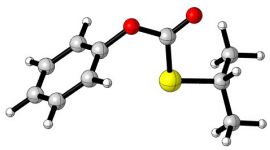
Thiocarbonate **3a** (**prod-3**)



SCF Energy = -936.985621741
Zero-point correction = 0.201498
Thermal correction to Energy = 0.214563
Thermal correction to Enthalpy = 0.215508
Thermal correction to Gibbs Free Energy = 0.159507
Sum of electronic and zero-point Energies = -936.784124
Sum of electronic and thermal Energies = -936.771058
Sum of electronic and thermal Enthalpies = -936.770114
Sum of electronic and thermal Free Energies = -936.826114

S	2.271696000	-0.953395000	-0.415308000
C	0.516896000	-0.962755000	-0.514768000
O	-0.064235000	0.057745000	0.138212000
C	-1.458445000	0.122739000	0.139507000
C	-2.174215000	-0.634706000	1.047070000
C	-2.075839000	1.005250000	-0.724886000
C	-3.553924000	-0.502993000	1.083789000
C	-3.456708000	1.130889000	-0.676429000
C	-4.195892000	0.377936000	0.224340000
H	-1.655772000	-1.313132000	1.711612000
H	-1.480074000	1.585012000	-1.417402000
H	-4.128189000	-1.091489000	1.787438000
H	-3.954140000	1.820109000	-1.346326000
H	-5.272634000	0.480252000	0.259873000
O	-0.072002000	-1.822949000	-1.107193000
C	2.703290000	0.578098000	0.495382000
H	2.000169000	0.647438000	1.323214000
C	2.597404000	1.810090000	-0.389644000
C	4.112655000	0.380922000	1.041125000
H	4.166839000	-0.471946000	1.717658000
H	4.833873000	0.232409000	0.234334000
H	4.409038000	1.275445000	1.591242000
H	3.299083000	1.747030000	-1.223461000
H	2.841920000	2.700165000	0.194649000
H	1.591310000	1.931838000	-0.788979000

Thiocarbonate **3a** (**prod-4**)

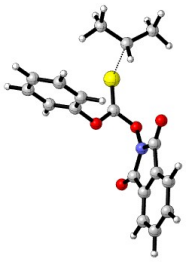


SCF Energy = -936.985508791
Zero-point correction = 0.201635
Thermal correction to Energy = 0.214567
Thermal correction to Enthalpy = 0.215511
Thermal correction to Gibbs Free Energy = 0.160712
Sum of electronic and zero-point Energies = -936.783873
Sum of electronic and thermal Energies = -936.770942

Sum of electronic and thermal Enthalpies = -936.769998
Sum of electronic and thermal Free Energies = -936.824797

S	-1.020642000	-0.463198000	-0.074209000
C	-0.707256000	1.263776000	-0.294468000
O	0.592200000	1.621206000	-0.267324000
C	1.600606000	0.678943000	-0.088683000
C	2.150585000	0.063668000	-1.198825000
C	2.074884000	0.438410000	1.188242000
C	3.191522000	-0.834209000	-1.018701000
C	3.117360000	-0.460369000	1.355344000
C	3.674128000	-1.097840000	0.255533000
H	1.760094000	0.283744000	-2.183610000
H	1.626614000	0.945348000	2.032467000
H	3.628194000	-1.324919000	-1.878666000
H	3.497016000	-0.659137000	2.349055000
H	4.486646000	-1.799679000	0.391181000
O	-1.544487000	2.102074000	-0.465493000
C	-2.848622000	-0.468014000	-0.136177000
H	-3.117603000	0.207504000	-0.947061000
C	-3.456023000	0.019829000	1.169414000
C	-3.277286000	-1.888750000	-0.481506000
H	-2.862618000	-2.214109000	-1.435734000
H	-2.966784000	-2.595765000	0.290788000
H	-4.365614000	-1.925981000	-0.549660000
H	-3.174282000	-0.635409000	1.995823000
H	-4.545166000	0.015141000	1.085430000
H	-3.137315000	1.035513000	1.398842000

Transition state of C–S bond formation (**TS-1**)

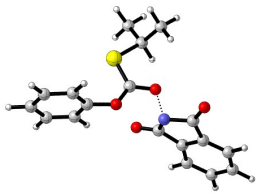


SCF Energy = -1449.33996447
Zero-point correction = 0.305315
Thermal correction to Energy = 0.327241
Thermal correction to Enthalpy = 0.328186
Thermal correction to Gibbs Free Energy = 0.250065
Sum of electronic and zero-point Energies = -1449.034649
Sum of electronic and thermal Energies = -1449.012723
Sum of electronic and thermal Enthalpies = -1449.011779
Sum of electronic and thermal Free Energies = -1449.089899

S	-2.273050000	-1.308572000	1.300803000
C	-0.809627000	-0.628885000	1.172512000
O	-0.480522000	0.618969000	0.836551000
C	-3.182245000	-1.808783000	-0.973135000
H	-2.317232000	-1.398763000	-1.483673000
O	0.323485000	-1.393854000	1.368135000
N	1.454783000	-0.922628000	0.774717000
C	2.446537000	-0.228774000	1.473353000
C	1.669981000	-1.016591000	-0.600429000
C	2.999276000	-0.382701000	-0.797703000
C	3.460096000	0.081548000	0.428053000
O	0.901266000	-1.494022000	-1.388353000
O	2.425637000	0.027379000	2.643284000
C	-1.456648000	1.456226000	0.301911000
C	-2.227158000	2.229274000	1.147157000

C	-1.574301000	1.525790000	-1.072614000
C	-3.156640000	3.095121000	0.591069000
C	-2.506336000	2.397175000	-1.616130000
C	-3.298236000	3.178879000	-0.787309000
H	-2.101281000	2.145348000	2.218093000
H	-0.946693000	0.904465000	-1.698187000
H	-3.771685000	3.706137000	1.238610000
H	-2.613639000	2.463215000	-2.690920000
H	-4.024799000	3.857126000	-1.215203000
C	3.733162000	-0.225063000	-1.951560000
H	3.367650000	-0.589109000	-2.902308000
C	4.963034000	0.419363000	-1.842725000
H	5.569098000	0.562610000	-2.727469000
C	5.424732000	0.883820000	-0.616976000
H	6.383983000	1.381486000	-0.564743000
C	4.673828000	0.720484000	0.544996000
H	5.028477000	1.082665000	1.500585000
C	-3.312357000	-3.293513000	-0.988464000
H	-3.717195000	-3.632731000	-1.951986000
H	-2.350688000	-3.785686000	-0.842984000
H	-4.003031000	-3.640284000	-0.215435000
C	-4.418087000	-0.976268000	-0.999572000
H	-4.919229000	-1.067106000	-1.972938000
H	-5.134163000	-1.303589000	-0.241287000
H	-4.197251000	0.079382000	-0.837557000

Transition state of N–O bond cleavage (**TS-2**)

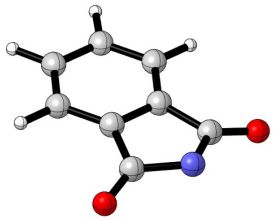


SCF Energy = -1449.33070852
Zero-point correction = 0.304736
Thermal correction to Energy = 0.326166
Thermal correction to Enthalpy = 0.327111
Thermal correction to Gibbs Free Energy = 0.251265
Sum of electronic and zero-point Energies = -1449.025972
Sum of electronic and thermal Energies = -1449.004542
Sum of electronic and thermal Enthalpies = -1449.003598
Sum of electronic and thermal Free Energies = -1449.079444

S	-2.105388000	1.517017000	-0.284028000
C	-0.990695000	0.470430000	0.488100000
O	-1.346238000	-0.699846000	0.908048000
C	-2.573720000	-1.260960000	0.502760000
C	-2.628448000	-1.884869000	-0.727019000
C	-3.634409000	-1.220591000	1.382268000
C	-3.822981000	-2.483078000	-1.096126000
C	-4.820450000	-1.827928000	0.995469000
C	-4.915151000	-2.454147000	-0.238875000
H	-1.751727000	-1.890827000	-1.362199000
H	-3.531968000	-0.730489000	2.340862000
H	-3.897481000	-2.977393000	-2.055512000
H	-5.669358000	-1.812388000	1.665927000
H	-5.842896000	-2.927215000	-0.532491000
O	0.199439000	0.864778000	0.721140000
N	1.219695000	-0.278614000	0.729316000
C	1.529515000	-0.668099000	-0.605175000
C	2.396681000	0.164915000	1.423440000
C	3.494274000	-0.337066000	0.609926000
C	5.697298000	-0.870562000	-0.107169000

C	5.165693000	-1.370759000	-1.311324000
C	4.856445000	-0.349768000	0.861273000
H	5.844895000	-1.777001000	-2.051207000
H	5.246000000	0.028568000	1.798185000
C	3.814429000	-1.352143000	-1.578138000
H	3.422690000	-1.738639000	-2.509814000
C	2.954484000	-0.798040000	-0.615061000
H	6.765099000	-0.907439000	0.061608000
O	2.373951000	0.827271000	2.431815000
O	0.639199000	-0.888979000	-1.442557000
C	-1.041944000	2.943476000	-0.753865000
H	-0.120824000	2.501636000	-1.130845000
C	-0.762379000	3.856971000	0.427158000
C	-1.775835000	3.651632000	-1.885626000
H	-1.943667000	2.990618000	-2.735368000
H	-2.735742000	4.048997000	-1.550271000
H	-1.164841000	4.491137000	-2.218881000
H	-1.687780000	4.284009000	0.816320000
H	-0.123928000	4.675862000	0.090577000
H	-0.247772000	3.336324000	1.232682000

Phthalimide radical



SCF Energy = -512.420865198
Zero-point correction = 0.102858
Thermal correction to Energy = 0.110743
Thermal correction to Enthalpy = 0.111688
Thermal correction to Gibbs Free Energy = 0.068888
Sum of electronic and zero-point Energies = -512.318007
Sum of electronic and thermal Energies = -512.310122
Sum of electronic and thermal Enthalpies = -512.309178
Sum of electronic and thermal Free Energies = -512.351977

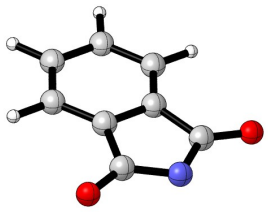
N	2.073722000	-0.000005000	0.266673000
C	1.267772000	-1.144971000	0.014126000
C	1.267767000	1.144998000	0.014283000
C	-0.144978000	0.695017000	0.010389000
C	-2.506914000	0.699145000	0.000966000
C	-2.506912000	-0.699148000	0.000994000
C	-1.322626000	1.419816000	0.009191000
H	-3.452613000	-1.224710000	-0.006719000
H	-1.317394000	2.501320000	0.011506000
C	-1.322620000	-1.419814000	0.009236000
H	-1.317382000	-2.501319000	0.011548000
C	-0.144976000	-0.695008000	0.010389000
H	-3.452618000	1.224702000	-0.006757000
O	1.719061000	2.246967000	-0.143421000
O	1.719048000	-2.246988000	-0.143295000

Geometry of phthalimide radical – single point as anion

SCF Energy = -512.620446148
Zero-point correction = 0.103593
Thermal correction to Energy = 0.111307
Thermal correction to Enthalpy = 0.112251
Thermal correction to Gibbs Free Energy = 0.070500
Sum of electronic and zero-point Energies = -512.516853

Sum of electronic and thermal Energies = -512.509139
Sum of electronic and thermal Enthalpies = -512.508195
Sum of electronic and thermal Free Energies = -512.549946

Phthalimide anion



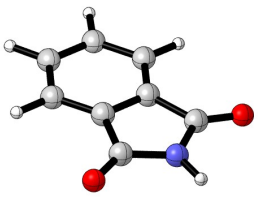
SCF Energy = -512.635818148
Zero-point correction = 0.104258
Thermal correction to Energy = 0.111679
Thermal correction to Enthalpy = 0.112624
Thermal correction to Gibbs Free Energy = 0.071709
Sum of electronic and zero-point Energies = -512.531560
Sum of electronic and thermal Energies = -512.524139
Sum of electronic and thermal Enthalpies = -512.523195
Sum of electronic and thermal Free Energies = -512.564109

N	-2.100425000	0.000000000	0.000050000
C	-1.308627000	-1.104917000	-0.000040000
C	-1.308628000	1.104917000	-0.000059000
C	0.145778000	0.690247000	-0.000057000
C	2.516523000	0.695352000	-0.000006000
C	2.516523000	-0.695352000	-0.000007000
C	1.319430000	1.411676000	-0.000048000
H	3.460726000	-1.226048000	0.000019000
H	1.314655000	2.494769000	-0.000035000
C	1.319431000	-1.411676000	-0.000049000
H	1.314655000	-2.494769000	-0.000032000
C	0.145778000	-0.690247000	-0.000056000
H	3.460725000	1.226049000	0.000020000
O	-1.682815000	2.272678000	0.000109000
O	-1.682814000	-2.272678000	0.000092000

Geometry of phthalimide anion – single point as radical

SCF Energy = -512.390909326
Zero-point correction = 0.100694
Thermal correction to Energy = 0.108069
Thermal correction to Enthalpy = 0.109013
Thermal correction to Gibbs Free Energy = 0.067590
Sum of electronic and zero-point Energies = -512.290215
Sum of electronic and thermal Energies = -512.282841
Sum of electronic and thermal Enthalpies = -512.281896
Sum of electronic and thermal Free Energies = -512.323319

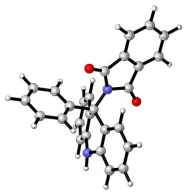
Phthalimide



SCF Energy = -513.126102463
Zero-point correction = 0.117364
Thermal correction to Energy = 0.125088
Thermal correction to Enthalpy = 0.126032
Thermal correction to Gibbs Free Energy = 0.084577
Sum of electronic and zero-point Energies = -513.008738
Sum of electronic and thermal Energies = -513.001014
Sum of electronic and thermal Enthalpies = -513.000070
Sum of electronic and thermal Free Energies = -513.041526

C	1.237520000	1.158744000	0.000113000
C	1.237527000	-1.158737000	0.000125000
C	-0.178857000	-0.693349000	0.000051000
C	-2.543819000	-0.695642000	-0.000054000
C	-2.543818000	0.695612000	-0.000052000
C	-1.352209000	-1.415203000	-0.000009000
H	-3.487406000	1.225296000	-0.000093000
H	-1.346374000	-2.497126000	-0.000011000
C	-1.352201000	1.415166000	-0.000006000
H	-1.346341000	2.497089000	-0.000009000
C	-0.178864000	0.693298000	0.000051000
H	-3.487405000	-1.225328000	-0.000094000
O	1.668481000	-2.282426000	-0.000057000
O	1.668352000	2.282487000	-0.000059000
N	2.001762000	0.000039000	-0.000003000
H	3.008856000	-0.000030000	-0.000157000

Acridine-phthalimide adduct (**Int-2**)

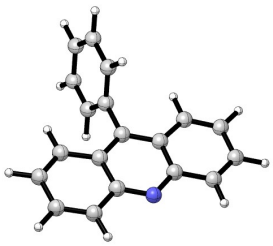


SCF Energy = -1299.74981651
Zero-point correction = 0.385884
Thermal correction to Energy = 0.408494
Thermal correction to Enthalpy = 0.409439
Thermal correction to Gibbs Free Energy = 0.333460
Sum of electronic and zero-point Energies = -1299.363933
Sum of electronic and thermal Energies = -1299.341322
Sum of electronic and thermal Enthalpies = -1299.340378
Sum of electronic and thermal Free Energies = -1299.416356

C	1.795865000	-1.147968000	-0.208639000
C	1.653230000	1.117228000	0.226930000
C	3.088614000	0.748040000	0.185405000
C	5.446641000	0.898494000	0.220759000
C	5.533087000	-0.467236000	-0.036118000
C	4.213268000	1.531650000	0.333468000
H	6.507532000	-0.929876000	-0.121983000
H	4.136764000	2.593385000	0.526053000
C	4.389081000	-1.244106000	-0.189733000
H	4.449401000	-2.304524000	-0.395247000
C	3.173906000	-0.604951000	-0.069453000
H	6.356103000	1.474333000	0.331556000
O	1.178336000	2.214433000	0.345064000
O	1.494237000	-2.264865000	-0.531378000
N	0.926697000	-0.079154000	0.070918000
C	-1.115896000	0.654425000	1.223527000
C	-2.362707000	1.267810000	1.108485000
N	-2.979433000	1.343433000	-0.132130000
C	-2.218304000	1.302223000	-1.289290000

C	-0.974639000	0.671197000	-1.268344000
C	-2.982173000	1.808278000	2.234845000
H	-3.950245000	2.283857000	2.131206000
C	-2.359626000	1.751859000	3.465967000
C	-0.496517000	0.631072000	2.465635000
H	0.480142000	0.173885000	2.564467000
C	-1.103981000	1.170651000	3.585421000
C	-0.218332000	0.646309000	-2.431666000
H	0.744199000	0.150745000	-2.434173000
C	-0.681372000	1.217339000	-3.604827000
C	-2.691255000	1.875720000	-2.468755000
H	-3.657458000	2.366148000	-2.471327000
C	-1.928414000	1.827780000	-3.619514000
H	-0.603281000	1.134730000	4.543661000
H	-2.848895000	2.177030000	4.332990000
H	-2.306201000	2.277050000	-4.529072000
H	-0.077797000	1.179184000	-4.501714000
C	-1.128634000	-1.498764000	0.015794000
C	-1.790951000	-2.028901000	-1.081671000
C	-1.039731000	-2.269253000	1.172399000
C	-2.339880000	-3.304163000	-1.030990000
C	-1.577655000	-3.541589000	1.223546000
C	-2.234667000	-4.066916000	0.118502000
H	-1.882028000	-1.455914000	-1.993690000
H	-0.538558000	-1.878255000	2.047180000
H	-2.851996000	-3.697403000	-1.900184000
H	-1.488535000	-4.123154000	2.132476000
H	-2.665328000	-5.059358000	0.159263000
H	-3.823067000	1.889994000	-0.174552000
C	-0.547653000	-0.062619000	-0.003002000

9-Phenylacridine

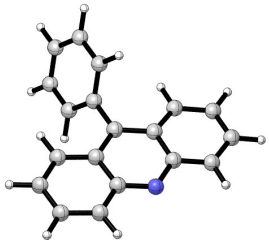


SCF Energy = -786.620241889
Zero-point correction = 0.265304
Thermal correction to Energy = 0.279419
Thermal correction to Enthalpy = 0.280363
Thermal correction to Gibbs Free Energy = 0.223416
Sum of electronic and zero-point Energies = -786.354938
Sum of electronic and thermal Energies = -786.340823
Sum of electronic and thermal Enthalpies = -786.339879
Sum of electronic and thermal Free Energies = -786.396826

C	0.000000000	0.000000000	-0.132122000
C	-0.007204000	1.203942000	0.580281000
C	-0.010006000	1.145817000	2.009030000
N	0.000000000	0.000000000	2.691085000
C	0.010006000	-1.145817000	2.009030000
C	0.007204000	-1.203942000	0.580281000
C	-0.020368000	2.367969000	2.745793000
H	-0.026453000	2.300661000	3.826153000
C	-0.020723000	3.564103000	2.105727000
C	0.000000000	2.483847000	-0.051870000
H	0.014016000	2.534319000	-1.132563000
C	-0.007111000	3.623515000	0.685480000
C	0.000000000	-2.483847000	-0.051870000
H	-0.014016000	-2.534319000	-1.132563000
C	0.007111000	-3.623515000	0.685480000

C	0.020368000	-2.367969000	2.745793000
H	0.026453000	-2.300661000	3.826153000
C	0.020723000	-3.564103000	2.105727000
H	-0.000067000	4.587616000	0.193730000
H	-0.028045000	4.485366000	2.674546000
H	0.028045000	-4.485366000	2.674546000
H	0.000067000	-4.587616000	0.193730000
C	0.000000000	0.000000000	-1.619242000
C	1.179158000	-0.224671000	-2.322332000
C	-1.179158000	0.224671000	-2.322332000
C	1.179183000	-0.222870000	-3.709187000
C	-1.179183000	0.222870000	-3.709187000
C	0.000000000	0.000000000	-4.405078000
H	2.099976000	-0.400503000	-1.779675000
H	-2.099976000	0.400503000	-1.779675000
H	2.103627000	-0.395777000	-4.245338000
H	-2.103627000	0.395777000	-4.245338000
H	0.000000000	0.000000000	-5.487694000

9-Phenylacridine (triplet)

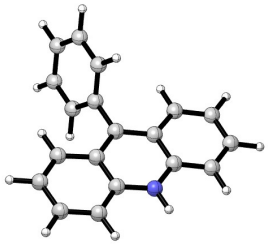


SCF Energy = -786.546464499
Zero-point correction = 0.261560
Thermal correction to Energy = 0.275929
Thermal correction to Enthalpy = 0.276873
Thermal correction to Gibbs Free Energy = 0.219023
Sum of electronic and zero-point Energies = -786.284905
Sum of electronic and thermal Energies = -786.270536
Sum of electronic and thermal Enthalpies = -786.269592
Sum of electronic and thermal Free Energies = -786.327442

C	0.000000000	0.000000000	-0.165139000
C	-0.023574000	1.236068000	0.576053000
C	-0.032439000	1.173638000	2.005981000
N	0.000000000	0.000000000	2.702801000
C	0.032439000	-1.173638000	2.005981000
C	0.023574000	-1.236068000	0.576053000
C	-0.055759000	2.352150000	2.743356000
H	-0.065664000	2.272824000	3.822952000
C	-0.057727000	3.604327000	2.114482000
C	0.000000000	2.486408000	-0.020525000
H	0.043518000	2.564598000	-1.098461000
C	-0.023607000	3.667887000	0.744421000
C	0.000000000	-2.486408000	-0.020525000
H	-0.043518000	-2.564598000	-1.098461000
C	0.023607000	-3.667887000	0.744421000
C	0.055759000	-2.352150000	2.743356000
H	0.065664000	-2.272824000	3.822952000
C	0.057727000	-3.604327000	2.114482000
H	-0.011940000	4.624857000	0.239104000
H	-0.077405000	4.507830000	2.709443000
H	0.077405000	-4.507830000	2.709443000
H	0.011940000	-4.624857000	0.239104000
C	0.000000000	0.000000000	-1.638909000
C	1.070057000	-0.542251000	-2.352754000
C	-1.070057000	0.542251000	-2.352754000
C	1.071517000	-0.539224000	-3.738623000
C	-1.071517000	0.539224000	-3.738623000

C	0.000000000	0.000000000	-4.435933000
H	1.910754000	-0.961343000	-1.813646000
H	-1.910754000	0.961343000	-1.813646000
H	1.914062000	-0.957932000	-4.274315000
H	-1.914062000	0.957932000	-4.274315000
H	0.000000000	0.000000000	-5.518562000

9-Phenylacridine–H radical



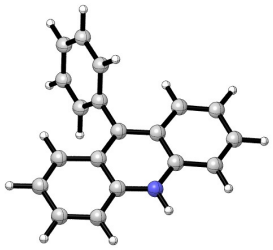
SCF Energy = -787.215901161
Zero-point correction = 0.275672
Thermal correction to Energy = 0.290259
Thermal correction to Enthalpy = 0.291203
Thermal correction to Gibbs Free Energy = 0.233053
Sum of electronic and zero-point Energies = -786.940229
Sum of electronic and thermal Energies = -786.925642
Sum of electronic and thermal Enthalpies = -786.924698
Sum of electronic and thermal Free Energies = -786.982848

C	0.000000000	0.000000000	-0.153137000
C	-0.011261000	1.233888000	0.562831000
C	-0.013944000	1.214650000	1.979935000
N	0.000000000	0.000000000	2.624236000
C	0.013944000	-1.214650000	1.979935000
C	0.011261000	-1.233888000	0.562831000
C	-0.024588000	2.398015000	2.711183000
H	-0.030021000	2.352393000	3.794062000
C	-0.024786000	3.619931000	2.061615000
C	0.000000000	2.496950000	-0.061811000
H	0.018298000	2.542297000	-1.142586000
C	-0.008761000	3.666524000	0.669854000
C	0.000000000	-2.496950000	-0.061811000
H	-0.018298000	-2.542297000	-1.142586000
C	0.008761000	-3.666524000	0.669854000
C	0.024588000	-2.398015000	2.711183000
H	0.030021000	-2.352393000	3.794062000
C	0.024786000	-3.619931000	2.061615000
H	-0.000176000	4.620658000	0.158955000
H	-0.032850000	4.535188000	2.639220000
H	0.032850000	-4.535188000	2.639220000
H	0.000176000	-4.620658000	0.158955000
C	0.000000000	0.000000000	-1.635622000
C	1.145655000	-0.349924000	-2.347726000
C	-1.145655000	0.349924000	-2.347726000
C	1.147060000	-0.350031000	-3.734545000
C	-1.147060000	0.350031000	-3.734545000
C	0.000000000	0.000000000	-4.432360000
H	2.043061000	-0.623714000	-1.805768000
H	-2.043061000	0.623714000	-1.805768000
H	2.047692000	-0.621893000	-4.270862000
H	-2.047692000	0.621893000	-4.270862000
H	0.000000000	0.000000000	-5.515112000
H	0.000000000	0.000000000	3.630106000

9-Phenylacridine–H radical geometry – single point as cation

SCF Energy = -787.066235309
Zero-point correction = 0.278386
Thermal correction to Energy = 0.291803
Thermal correction to Enthalpy = 0.292747
Thermal correction to Gibbs Free Energy = 0.237176
Sum of electronic and zero-point Energies = -786.787849
Sum of electronic and thermal Energies = -786.774433
Sum of electronic and thermal Enthalpies = -786.773489
Sum of electronic and thermal Free Energies = -786.829060

9-Phenylacridine–H cation



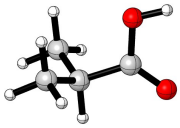
SCF Energy = -787.070695140
Zero-point correction = 0.279665
Thermal correction to Energy = 0.293859
Thermal correction to Enthalpy = 0.294803
Thermal correction to Gibbs Free Energy = 0.238128
Sum of electronic and zero-point Energies = -786.791031
Sum of electronic and thermal Energies = -786.776836
Sum of electronic and thermal Enthalpies = -786.775892
Sum of electronic and thermal Free Energies = -786.832567

C	0.000000000	0.000000000	-0.146742000
C	-0.014211000	1.216381000	0.557132000
C	-0.019144000	1.192299000	1.974983000
N	0.000000000	0.000000000	2.607016000
C	0.019144000	-1.192299000	1.974983000
C	0.014211000	-1.216381000	0.557132000
C	-0.035208000	2.387632000	2.718417000
H	-0.044207000	2.347048000	3.799793000
C	-0.035938000	3.579496000	2.058086000
C	0.000000000	2.486173000	-0.084981000
H	0.027313000	2.524575000	-1.164434000
C	-0.012542000	3.632524000	0.645172000
C	0.000000000	-2.486173000	-0.084981000
H	-0.027313000	-2.524575000	-1.164434000
C	0.012542000	-3.632524000	0.645172000
C	0.035208000	-2.387632000	2.718417000
H	0.044207000	-2.347048000	3.799793000
C	0.035938000	-3.579496000	2.058086000
H	0.000891000	4.592910000	0.149044000
H	-0.047382000	4.501730000	2.623671000
H	0.047382000	-4.501730000	2.623671000
H	-0.000891000	-4.592910000	0.149044000
C	0.000000000	0.000000000	-1.629014000
C	1.147001000	-0.366132000	-2.326410000
C	-1.147001000	0.366132000	-2.326410000
C	1.146300000	-0.358320000	-3.712095000
C	-1.146300000	0.358320000	-3.712095000
C	0.000000000	0.000000000	-4.406187000
H	2.040427000	-0.649899000	-1.784253000
H	-2.040427000	0.649899000	-1.784253000
H	2.043990000	-0.635230000	-4.249173000
H	-2.043990000	0.635230000	-4.249173000
H	0.000000000	0.000000000	-5.488454000
H	0.000000000	0.000000000	3.618054000

9-Phenylacridine–H cation geometry – single point as radical

SCF Energy = -787.211440093
Zero-point correction = 0.276414
Thermal correction to Energy = 0.290175
Thermal correction to Enthalpy = 0.291120
Thermal correction to Gibbs Free Energy = 0.235410
Sum of electronic and zero-point Energies = -786.935026
Sum of electronic and thermal Energies = -786.921265
Sum of electronic and thermal Enthalpies = -786.920320
Sum of electronic and thermal Free Energies = -786.976030

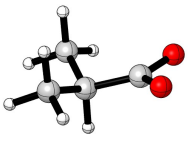
i-PrCO$_2$H



SCF Energy = -307.750080931
Zero-point correction = 0.119491
Thermal correction to Energy = 0.126528
Thermal correction to Enthalpy = 0.127472
Thermal correction to Gibbs Free Energy = 0.087842
Sum of electronic and zero-point Energies = -307.630590
Sum of electronic and thermal Energies = -307.623553
Sum of electronic and thermal Enthalpies = -307.622609
Sum of electronic and thermal Free Energies = -307.662239

H	2.017422000	0.000378000	1.327836000
O	1.061559000	0.000361000	1.189994000
O	1.730994000	-0.000271000	-0.934153000
C	0.832659000	-0.000019000	-0.129796000
C	-0.639215000	-0.000103000	-0.469515000
H	-0.680022000	-0.000336000	-1.559017000
C	-1.320106000	-1.265207000	0.056076000
H	-2.360420000	-1.280417000	-0.271209000
H	-0.833186000	-2.166608000	-0.318850000
H	-1.304733000	-1.291628000	1.146354000
C	-1.320161000	1.265189000	0.055544000
H	-0.833279000	2.166454000	-0.319755000
H	-2.360475000	1.280218000	-0.271753000
H	-1.304796000	1.292067000	1.145811000

i-PrCO$_2$ radical

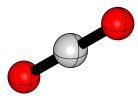


SCF Energy = -307.066295139
Zero-point correction = 0.105151
Thermal correction to Energy = 0.112152
Thermal correction to Enthalpy = 0.113097
Thermal correction to Gibbs Free Energy = 0.072631
Sum of electronic and zero-point Energies = -306.961144
Sum of electronic and thermal Energies = -306.954143
Sum of electronic and thermal Enthalpies = -306.953198
Sum of electronic and thermal Free Energies = -306.993664

O	1.527509000	-1.022160000	0.068563000

O	1.527516000	1.022154000	0.068545000
C	0.815946000	-0.000002000	-0.067309000
C	-0.647338000	0.000003000	-0.378869000
H	-0.682675000	0.000008000	-1.475000000
C	-1.316919000	-1.274580000	0.127678000
H	-2.354829000	-1.294472000	-0.204063000
H	-0.821870000	-2.167913000	-0.252697000
H	-1.306409000	-1.311197000	1.218235000
C	-1.316912000	1.274585000	0.127690000
H	-0.821867000	2.167918000	-0.252690000
H	-2.354826000	1.294478000	-0.204037000
H	-1.306386000	1.311198000	1.218247000

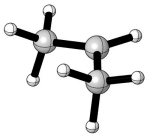
Carbon dioxide



SCF Energy = -188.607636072
Zero-point correction = 0.011812
Thermal correction to Energy = 0.014420
Thermal correction to Enthalpy = 0.015364
Thermal correction to Gibbs Free Energy = -0.008868
Sum of electronic and zero-point Energies = -188.595824
Sum of electronic and thermal Energies = -188.593216
Sum of electronic and thermal Enthalpies = -188.592272
Sum of electronic and thermal Free Energies = -188.616504

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.155616000
O	0.000000000	0.000000000	-1.155616000

Isopropyl radical



SCF Energy = -118.481237272
Zero-point correction = 0.088364
Thermal correction to Energy = 0.093438
Thermal correction to Enthalpy = 0.094382
Thermal correction to Gibbs Free Energy = 0.061425
Sum of electronic and zero-point Energies = -118.392873
Sum of electronic and thermal Energies = -118.387799
Sum of electronic and thermal Enthalpies = -118.386855
Sum of electronic and thermal Free Energies = -118.419813

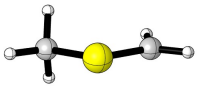
C	-0.000002000	0.537175000	-0.046179000
H	-0.000013000	1.610044000	0.103070000
C	1.288981000	-0.198386000	0.002917000
C	-1.288977000	-0.198392000	0.002915000
H	-2.140217000	0.451483000	-0.203008000
H	-1.304094000	-1.023372000	-0.717756000
H	-1.457144000	-0.654319000	0.990282000
H	1.304312000	-1.023007000	-0.718157000
H	1.456881000	-0.654818000	0.990100000
H	2.140259000	0.451610000	-0.202450000

Benzyl radical

SCF Energy = -270.913697526
Zero-point correction = 0.115343
Thermal correction to Energy = 0.120979
Thermal correction to Enthalpy = 0.121923
Thermal correction to Gibbs Free Energy = 0.085695
Sum of electronic and zero-point Energies = -270.798355
Sum of electronic and thermal Energies = -270.792718
Sum of electronic and thermal Enthalpies = -270.791774
Sum of electronic and thermal Free Energies = -270.828002

C	1.127298000	1.204755000	-0.000004000
C	-0.250806000	1.211368000	0.000027000
C	-0.988272000	0.000000000	0.000019000
C	-0.250806000	-1.211368000	0.000034000
C	1.127295000	-1.204756000	0.000004000
C	1.828319000	0.000000000	-0.000031000
H	1.668251000	2.142971000	0.000034000
H	-0.789252000	2.151788000	0.000101000
H	-0.789255000	-2.151787000	0.000113000
H	1.668250000	-2.142971000	0.000053000
H	2.910678000	-0.000003000	-0.000225000
C	-2.389519000	0.000002000	0.000039000
H	-2.944859000	-0.928563000	-0.000403000
H	-2.944869000	0.928559000	-0.000205000

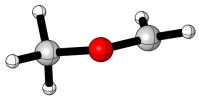
(Methylthio)methyl radical



SCF Energy = -477.371600848
Zero-point correction = 0.061540
Thermal correction to Energy = 0.066763
Thermal correction to Enthalpy = 0.067707
Thermal correction to Gibbs Free Energy = 0.033713
Sum of electronic and zero-point Energies = -477.310061
Sum of electronic and thermal Energies = -477.304838
Sum of electronic and thermal Enthalpies = -477.303894
Sum of electronic and thermal Free Energies = -477.337888

C	-1.343554000	0.566592000	0.018841000
H	-1.123223000	1.616278000	-0.106597000
H	-2.362431000	0.210416000	0.035243000
C	1.373730000	0.421641000	0.007585000
H	1.415326000	1.013716000	0.920303000
H	2.227189000	-0.252752000	-0.026309000
H	1.392728000	1.073782000	-0.864264000
S	-0.108165000	-0.599427000	-0.007308000

(Methoxy)methyl radical

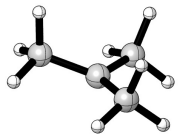


SCF Energy = -154.376737610
Zero-point correction = 0.066166

Thermal correction to Energy = 0.070616
Thermal correction to Enthalpy = 0.071560
Thermal correction to Gibbs Free Energy = 0.040205
Sum of electronic and zero-point Energies = -154.310572
Sum of electronic and thermal Energies = -154.306122
Sum of electronic and thermal Enthalpies = -154.305177
Sum of electronic and thermal Free Energies = -154.336533

C	1.197247000	0.224670000	-0.063176000
H	1.117551000	1.277192000	0.187588000
H	2.123212000	-0.318625000	0.057108000
O	0.092358000	-0.540967000	0.029530000
C	-1.133638000	0.167415000	-0.008630000
H	-1.245935000	0.690995000	-0.961503000
H	-1.929997000	-0.564905000	0.101025000
H	-1.185351000	0.890571000	0.810380000

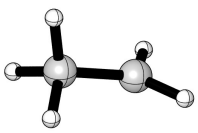
tert-Butyl radical



SCF Energy = -157.803344652
Zero-point correction = 0.117226
Thermal correction to Energy = 0.123406
Thermal correction to Enthalpy = 0.124350
Thermal correction to Gibbs Free Energy = 0.088193
Sum of electronic and zero-point Energies = -157.686119
Sum of electronic and thermal Energies = -157.679939
Sum of electronic and thermal Enthalpies = -157.678995
Sum of electronic and thermal Free Energies = -157.715152

C	0.001352000	0.000279000	-0.162409000
C	-0.662064000	-1.321465000	0.015886000
H	-1.651851000	-1.342825000	-0.446797000
H	-0.065355000	-2.133446000	-0.406417000
H	-0.807849000	-1.556756000	1.082482000
C	1.477330000	0.088390000	0.016084000
H	1.989292000	-0.767920000	-0.429668000
H	1.883988000	1.001946000	-0.424380000
H	1.753982000	0.101451000	1.082694000
C	-0.815367000	1.233179000	0.015844000
H	-0.320655000	2.111088000	-0.406321000
H	-1.800739000	1.135088000	-0.446505000
H	-0.988322000	1.449074000	1.082485000

Ethyl radical

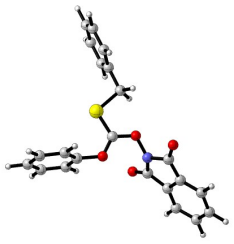


SCF Energy = -79.1595809251
Zero-point correction = 0.059380
Thermal correction to Energy = 0.063399
Thermal correction to Enthalpy = 0.064344
Thermal correction to Gibbs Free Energy = 0.035055

Sum of electronic and zero-point Energies = -79.100201
Sum of electronic and thermal Energies = -79.096181
Sum of electronic and thermal Enthalpies = -79.095237
Sum of electronic and thermal Free Energies = -79.124526

C	0.791091000	0.000000000	-0.020784000
H	1.344303000	-0.927310000	0.045266000
H	1.344311000	0.927306000	0.045263000
C	-0.690924000	0.000001000	-0.002006000
H	-1.102910000	0.886153000	-0.489512000
H	-1.102909000	-0.886081000	-0.489641000
H	-1.083792000	-0.000074000	1.025365000

Product of benzyl radical addition to **3a**

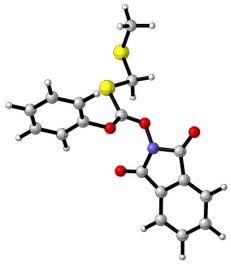


SCF Energy = -1601.75533474
Zero-point correction = 0.333358
Thermal correction to Energy = 0.356575
Thermal correction to Enthalpy = 0.357519
Thermal correction to Gibbs Free Energy = 0.275440
Sum of electronic and zero-point Energies = -1601.421977
Sum of electronic and thermal Energies = -1601.398760
Sum of electronic and thermal Enthalpies = -1601.397815
Sum of electronic and thermal Free Energies = -1601.479895

S	-1.883662000	0.180851000	-0.115991000
C	-0.198863000	0.350250000	-0.284371000
O	0.381997000	1.483358000	-0.392381000
C	-0.368267000	2.680566000	-0.264878000
C	-0.478868000	3.236179000	0.991408000
C	-0.887131000	3.251378000	-1.406375000
C	-1.171332000	4.431767000	1.105512000
C	-1.575250000	4.447801000	-1.269433000
C	-1.718213000	5.033076000	-0.019621000
H	-0.031077000	2.746804000	1.845822000
H	-0.754495000	2.776686000	-2.368919000
H	-1.278134000	4.894398000	2.077255000
H	-1.996660000	4.921796000	-2.145492000
H	-2.252973000	5.968423000	0.077960000
O	0.523937000	-0.722729000	-0.332554000
N	1.895237000	-0.521482000	-0.290230000
C	2.496545000	-0.274923000	0.977980000
C	2.718198000	-1.195337000	-1.231637000
C	3.992205000	-1.167277000	-0.577724000
C	6.331322000	-1.481873000	-0.207322000
C	6.199903000	-0.935313000	1.096309000
C	5.245429000	-1.595374000	-1.038823000
H	7.077395000	-0.859641000	1.726258000
H	5.346413000	-2.013816000	-2.032788000
C	4.985403000	-0.505839000	1.566640000
H	4.888083000	-0.088119000	2.561192000
C	3.859151000	-0.619051000	0.735149000
H	7.305220000	-1.812564000	-0.545687000
O	2.312035000	-1.625120000	-2.308996000
O	1.853156000	0.148874000	1.940422000
C	-2.062326000	-1.643253000	-0.006564000
H	-1.643944000	-2.071807000	-0.913639000
H	-1.495487000	-1.977875000	0.858781000
C	-3.530489000	-1.929605000	0.128694000

C	-4.324518000	-2.058059000	-1.006610000
C	-4.109243000	-2.056462000	1.386773000
C	-5.680917000	-2.313368000	-0.884950000
H	-3.877053000	-1.961877000	-1.988822000
C	-5.465826000	-2.314416000	1.507892000
H	-3.495947000	-1.958907000	2.274756000
C	-6.253153000	-2.441543000	0.372571000
H	-6.290310000	-2.416032000	-1.773471000
H	-5.908284000	-2.419116000	2.489996000
H	-7.312371000	-2.642607000	0.468615000

Product of (methylthio)methyl radical addition to **3a**

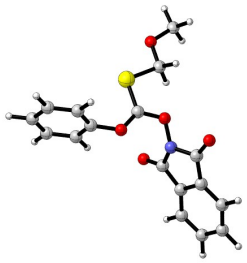


SCF Energy = -1808.21673439
Zero-point correction = 0.280662
Thermal correction to Energy = 0.302392
Thermal correction to Enthalpy = 0.303336
Thermal correction to Gibbs Free Energy = 0.226060
Sum of electronic and zero-point Energies = -1807.936073
Sum of electronic and thermal Energies = -1807.914343
Sum of electronic and thermal Enthalpies = -1807.913399
Sum of electronic and thermal Free Energies = -1807.990674

S	-2.340044000	0.644613000	-0.202934000
C	-0.768851000	0.093712000	0.160576000
O	-0.502564000	-1.119159000	0.458408000
C	-1.511584000	-2.112245000	0.358846000
C	-1.675352000	-2.734687000	-0.859750000
C	-2.221425000	-2.440341000	1.492771000
C	-2.630586000	-3.735524000	-0.945435000
C	-3.171232000	-3.445704000	1.384782000
C	-3.375880000	-4.087143000	0.171652000
H	-1.068720000	-2.441967000	-1.706301000
H	-2.035708000	-1.929029000	2.427328000
H	-2.786589000	-4.242464000	-1.887941000
H	-3.747502000	-3.727712000	2.255592000
H	-4.118426000	-4.870425000	0.097837000
O	0.196042000	0.957431000	0.154944000
N	1.472237000	0.421971000	0.232366000
C	2.036757000	-0.136398000	-0.950425000
C	2.402366000	0.969037000	1.153621000
C	3.649021000	0.527197000	0.602436000
C	5.999274000	0.161198000	0.381597000
C	5.783286000	-0.488481000	-0.861812000
C	4.949090000	0.662673000	1.109076000
H	6.634452000	-0.872817000	-1.409767000
H	5.114055000	1.157685000	2.058215000
C	4.519970000	-0.637167000	-1.374658000
H	4.358793000	-1.134037000	-2.323410000
C	3.430842000	-0.127295000	-0.648961000
H	7.009822000	0.260845000	0.757234000
O	2.081817000	1.621056000	2.144878000
O	1.341111000	-0.503726000	-1.900148000
C	-2.036399000	2.417368000	-0.570201000
H	-1.552796000	2.883066000	0.284581000
H	-1.396987000	2.476423000	-1.447348000
S	-3.598629000	3.194297000	-0.953685000
C	-4.270770000	3.435365000	0.702361000

H	-5.228429000	3.935432000	0.568906000
H	-4.437676000	2.484847000	1.206270000
H	-3.613588000	4.069597000	1.294616000

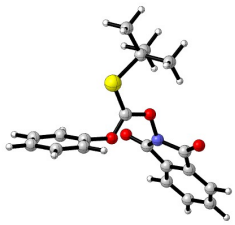
Product of (methoxy)methyl radical addition to **3a**



SCF Energy = -1485.22375357
Zero-point correction = 0.284006
Thermal correction to Energy = 0.305445
Thermal correction to Enthalpy = 0.306389
Thermal correction to Gibbs Free Energy = 0.229345
Sum of electronic and zero-point Energies = -1484.939747
Sum of electronic and thermal Energies = -1484.918309
Sum of electronic and thermal Enthalpies = -1484.917364
Sum of electronic and thermal Free Energies = -1484.994409

S	-2.424381000	1.136294000	0.055432000
C	-0.965776000	0.334278000	0.396293000
O	-0.899031000	-0.920489000	0.625531000
C	-2.020740000	-1.751016000	0.370909000
C	-2.125360000	-2.301224000	-0.888649000
C	-2.899370000	-2.008255000	1.400159000
C	-3.193624000	-3.150771000	-1.129762000
C	-3.961818000	-2.860669000	1.135734000
C	-4.108259000	-3.426744000	-0.122271000
H	-1.386593000	-2.065248000	-1.643320000
H	-2.757475000	-1.559293000	2.373775000
H	-3.307137000	-3.600305000	-2.106922000
H	-4.673000000	-3.083416000	1.919557000
H	-4.937599000	-4.093329000	-0.318178000
O	0.119086000	1.038438000	0.474480000
N	1.295709000	0.304564000	0.425341000
C	1.672191000	-0.234873000	-0.839678000
C	2.375454000	0.662105000	1.275701000
C	3.492190000	0.088998000	0.582493000
C	5.738074000	-0.570242000	0.105011000
C	5.319871000	-1.097774000	-1.144874000
C	4.839584000	0.013840000	0.962527000
H	6.055259000	-1.551101000	-1.797686000
H	5.159701000	0.417760000	1.915205000
C	4.006896000	-1.041043000	-1.535477000
H	3.690203000	-1.445789000	-2.488792000
C	3.071378000	-0.441979000	-0.675779000
H	6.783296000	-0.633275000	0.380130000
O	2.243880000	1.288638000	2.323680000
O	0.847021000	-0.421766000	-1.738696000
C	-1.796653000	2.834121000	-0.248394000
H	-1.366533000	3.225542000	0.677525000
H	-1.037033000	2.788508000	-1.033921000
O	-2.941964000	3.508340000	-0.637356000
C	-2.696329000	4.887401000	-0.866706000
H	-3.642536000	5.326812000	-1.170997000
H	-2.341825000	5.375067000	0.046199000
H	-1.956783000	5.023202000	-1.661411000

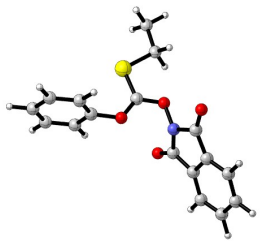
Product of *tert*-butyl radical addition to **3a**



SCF Energy = -1488.65754441
Zero-point correction = 0.335991
Thermal correction to Energy = 0.358773
Thermal correction to Enthalpy = 0.359717
Thermal correction to Gibbs Free Energy = 0.281373
Sum of electronic and zero-point Energies = -1488.321554
Sum of electronic and thermal Energies = -1488.298771
Sum of electronic and thermal Enthalpies = -1488.297827
Sum of electronic and thermal Free Energies = -1488.376171

S	-2.423723000	1.047729000	-0.129023000
C	-0.933376000	0.254921000	0.056174000
O	-0.843315000	-1.011791000	0.215379000
C	-2.007615000	-1.820769000	0.225936000
C	-2.429574000	-2.365097000	-0.967408000
C	-2.612238000	-2.068758000	1.438832000
C	-3.541513000	-3.193391000	-0.938017000
C	-3.721737000	-2.900375000	1.446304000
C	-4.185116000	-3.457393000	0.262747000
H	-1.902938000	-2.147518000	-1.886569000
H	-2.224694000	-1.625060000	2.345649000
H	-3.900417000	-3.635251000	-1.857678000
H	-4.220072000	-3.113484000	2.382262000
H	-5.049879000	-4.107439000	0.276946000
O	0.163978000	0.942299000	0.049659000
N	1.341194000	0.217884000	0.140039000
C	1.908132000	-0.320876000	-1.049644000
C	2.272065000	0.568518000	1.153038000
C	3.484698000	0.003735000	0.644685000
C	5.773568000	-0.672839000	0.536742000
C	5.558324000	-1.201753000	-0.763168000
C	4.753308000	-0.079697000	1.236546000
H	6.385283000	-1.664864000	-1.286710000
H	4.917386000	0.322877000	2.228664000
C	4.325042000	-1.134629000	-1.359975000
H	4.163152000	-1.541441000	-2.350673000
C	3.267651000	-0.527227000	-0.664089000
H	6.759201000	-0.744213000	0.979088000
O	1.968183000	1.189166000	2.170572000
O	1.247397000	-0.517011000	-2.070638000
C	-2.055126000	2.880319000	-0.273360000
C	-1.409412000	3.401602000	1.004077000
C	-3.472825000	3.438960000	-0.426143000
H	-3.964482000	3.056836000	-1.321711000
H	-4.092166000	3.217496000	0.444123000
H	-3.394864000	4.522723000	-0.519547000
H	-2.017806000	3.171129000	1.878560000
H	-1.332583000	4.487470000	0.918543000
H	-0.407513000	3.005563000	1.154744000
C	-1.229454000	3.173854000	-1.519047000
H	-0.215811000	2.788475000	-1.442011000
H	-1.699334000	2.763650000	-2.412571000
H	-1.170018000	4.258271000	-1.632159000

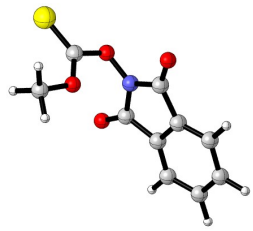
Product of ethyl radical addition to **3a**



SCF Energy = -1410.02193106
Zero-point correction = 0.279779
Thermal correction to Energy = 0.299963
Thermal correction to Enthalpy = 0.300907
Thermal correction to Gibbs Free Energy = 0.227414
Sum of electronic and zero-point Energies = -1409.742153
Sum of electronic and thermal Energies = -1409.721968
Sum of electronic and thermal Enthalpies = -1409.721024
Sum of electronic and thermal Free Energies = -1409.794517

S	-2.439069000	1.552315000	-0.171107000
C	-1.028252000	0.631816000	0.046194000
O	-1.037799000	-0.634152000	0.220302000
C	-2.267335000	-1.342617000	0.222161000
C	-2.724833000	-1.851814000	-0.973762000
C	-2.900002000	-1.534126000	1.431196000
C	-3.903087000	-2.583037000	-0.950912000
C	-4.075628000	-2.269374000	1.431556000
C	-4.575112000	-2.788721000	0.245708000
H	-2.175324000	-1.681850000	-1.889598000
H	-2.484020000	-1.122158000	2.340380000
H	-4.291481000	-2.995482000	-1.872214000
H	-4.596696000	-2.437392000	2.364288000
H	-5.492801000	-3.361684000	0.254729000
O	0.112142000	1.246366000	0.049115000
N	1.233511000	0.436640000	0.128247000
C	1.763873000	-0.115487000	-1.071608000
C	2.175887000	0.665115000	1.164919000
C	3.344188000	0.022251000	0.644176000
C	5.576300000	-0.821141000	0.525318000
C	5.333410000	-1.283117000	-0.794829000
C	4.597056000	-0.179152000	1.240778000
H	6.128172000	-1.786224000	-1.331272000
H	4.782255000	0.172719000	2.248330000
C	4.113813000	-1.101843000	-1.396034000
H	3.931080000	-1.456574000	-2.402969000
C	3.099091000	-0.441714000	-0.684730000
H	6.550458000	-0.980742000	0.969979000
O	1.912673000	1.263264000	2.206623000
O	1.095793000	-0.231727000	-2.100421000
C	-1.752395000	3.234730000	-0.352777000
H	-1.219181000	3.474435000	0.564071000
H	-1.055352000	3.218884000	-1.187151000
C	-2.908649000	4.188658000	-0.599692000
H	-3.614736000	4.191444000	0.230629000
H	-2.501611000	5.194144000	-0.702215000
H	-3.442640000	3.944405000	-1.517931000

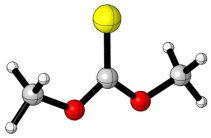
Thionocarbonate **2f**



SCF Energy = -1139.12847573
Zero-point correction = 0.161259
Thermal correction to Energy = 0.174972
Thermal correction to Enthalpy = 0.175916
Thermal correction to Gibbs Free Energy = 0.118347
Sum of electronic and zero-point Energies = -1138.967216
Sum of electronic and thermal Energies = -1138.953503
Sum of electronic and thermal Enthalpies = -1138.952559
Sum of electronic and thermal Free Energies = -1139.010129

S	4.011982000	-0.000329000	-0.440097000
C	2.425913000	-0.000336000	-0.075738000
O	1.842106000	0.000691000	1.082232000
O	1.523939000	-0.000964000	-1.101825000
N	0.208876000	-0.000622000	-0.742380000
C	-0.507920000	1.178079000	-0.513245000
C	-0.508142000	-1.178911000	-0.511831000
C	-1.868400000	-0.694985000	-0.156164000
C	-4.152307000	-0.694432000	0.459701000
C	-4.152115000	0.695453000	0.459093000
C	-3.001397000	-1.414826000	0.149665000
H	-5.062491000	1.226169000	0.704357000
H	-2.995542000	-2.496494000	0.149655000
C	-3.001011000	1.415256000	0.148413000
H	-2.994881000	2.496921000	0.147368000
C	-1.868220000	0.694835000	-0.156815000
H	-5.062823000	-1.224680000	0.705456000
O	-0.061367000	-2.287327000	-0.589800000
O	-0.060768000	2.286292000	-0.591948000
C	2.642666000	0.001836000	2.273549000
H	3.264020000	-0.891161000	2.297043000
H	3.263927000	0.894940000	2.295387000
H	1.928265000	0.002559000	3.089893000

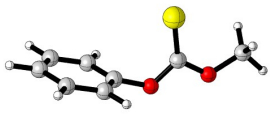
Dimethyl thionocarbonate



SCF Energy = -666.591195469
Zero-point correction = 0.093292
Thermal correction to Energy = 0.100502
Thermal correction to Enthalpy = 0.101446
Thermal correction to Gibbs Free Energy = 0.061408
Sum of electronic and zero-point Energies = -666.497903
Sum of electronic and thermal Energies = -666.490694
Sum of electronic and thermal Enthalpies = -666.489750
Sum of electronic and thermal Free Energies = -666.529787

S	0.000101000	1.450470000	0.000004000
C	-0.000009000	-0.199918000	0.000106000
O	-1.058172000	-0.978438000	0.000025000
O	1.058110000	-0.978516000	0.000027000
C	2.360946000	-0.395208000	-0.000056000
H	3.048320000	-1.235836000	-0.000106000
H	2.501816000	0.215184000	-0.890743000
H	2.501931000	0.215173000	0.890621000
C	-2.361093000	-0.395072000	-0.000055000
H	-2.501848000	0.215277000	-0.890765000
H	-3.048443000	-1.235738000	-0.000111000
H	-2.501964000	0.215255000	0.890652000

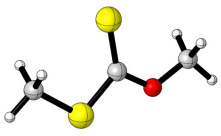
Phenyl methyl thionocarbonate



SCF Energy = -858.325007013
Zero-point correction = 0.146427
Thermal correction to Energy = 0.156451
Thermal correction to Enthalpy = 0.157395
Thermal correction to Gibbs Free Energy = 0.109368
Sum of electronic and zero-point Energies = -858.178580
Sum of electronic and thermal Energies = -858.168556
Sum of electronic and thermal Enthalpies = -858.167612
Sum of electronic and thermal Free Energies = -858.215639

S	-1.390252000	1.470711000	0.001877000
C	-1.480611000	-0.170659000	-0.000476000
O	-0.456574000	-1.016097000	-0.002195000
C	0.852670000	-0.538598000	-0.001029000
C	1.492913000	-0.352340000	1.208153000
C	1.493583000	-0.348661000	-1.209295000
C	2.819769000	0.051238000	1.202455000
C	2.820454000	0.054874000	-1.201678000
C	3.482759000	0.256639000	0.000877000
H	0.958532000	-0.518249000	2.134018000
H	0.959687000	-0.511797000	-2.135932000
H	3.334483000	0.203838000	2.142049000
H	3.335695000	0.210212000	-2.140533000
H	4.518463000	0.570554000	0.001677000
O	-2.568975000	-0.899304000	-0.001289000
C	-3.844804000	-0.255723000	0.000159000
H	-4.569658000	-1.064000000	-0.003248000
H	-3.955161000	0.356976000	0.893397000
H	-3.954020000	0.363678000	-0.888573000

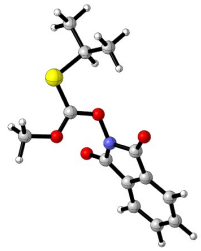
Dimethyl xanthate



SCF Energy = -989.563013246
Zero-point correction = 0.089225
Thermal correction to Energy = 0.096921
Thermal correction to Enthalpy = 0.097865
Thermal correction to Gibbs Free Energy = 0.056529
Sum of electronic and zero-point Energies = -989.473788
Sum of electronic and thermal Energies = -989.466092
Sum of electronic and thermal Enthalpies = -989.465148
Sum of electronic and thermal Free Energies = -989.506485

S	-0.428471000	1.551299000	0.000006000
C	-0.264144000	-0.080888000	0.000061000
O	-1.246051000	-0.962796000	0.000013000
S	1.232045000	-0.982222000	0.000006000
C	2.482012000	0.302460000	-0.000032000
H	3.435107000	-0.224985000	-0.000060000
H	2.399583000	0.918999000	-0.891942000
H	2.399634000	0.918997000	0.891885000
C	-2.603664000	-0.513933000	-0.000036000
H	-2.804011000	0.079800000	-0.890920000
H	-3.200234000	-1.421269000	-0.000075000
H	-2.804080000	0.079769000	0.890854000

Product of isopropyl radical addition to thionocarbonate **2f**

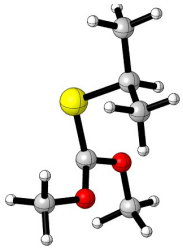


SCF Energy = -1257.60711323
Zero-point correction = 0.254840
Thermal correction to Energy = 0.273549
Thermal correction to Enthalpy = 0.274493
Thermal correction to Gibbs Free Energy = 0.204482
Sum of electronic and zero-point Energies = -1257.352274
Sum of electronic and thermal Energies = -1257.333565
Sum of electronic and thermal Enthalpies = -1257.332620
Sum of electronic and thermal Free Energies = -1257.402631

S	-3.251690000	0.548181000	-0.163544000
C	-1.574628000	0.689481000	-0.396799000
O	-1.037713000	1.633258000	-1.054187000
O	-0.802793000	-0.217036000	0.128327000
N	0.554809000	-0.032108000	-0.049285000
C	1.283721000	0.757974000	0.877460000
C	1.302777000	-1.009916000	-0.750781000
C	2.642602000	-0.691095000	-0.357186000
C	5.027881000	-0.767722000	-0.237080000
C	5.015682000	0.277164000	0.723256000
C	3.859837000	-1.247413000	-0.775468000
H	5.954589000	0.633077000	1.128600000
H	3.870290000	-2.043305000	-1.510043000
C	3.836574000	0.839100000	1.143647000
H	3.829462000	1.635603000	1.877541000
C	2.630307000	0.360676000	0.609900000
H	5.975798000	-1.189599000	-0.546622000
O	0.797412000	-1.850999000	-1.493946000
O	0.745479000	1.559833000	1.642792000
C	-3.415003000	-1.017379000	0.803701000
H	-2.654180000	-0.962230000	1.579710000
C	-3.212286000	-2.235583000	-0.079959000
C	-4.802309000	-0.955548000	1.429250000

H	-4.912260000	-0.096490000	2.090178000
H	-5.582616000	-0.921673000	0.666979000
H	-4.948882000	-1.861883000	2.017106000
H	-3.964027000	-2.272570000	-0.869181000
H	-3.322166000	-3.128557000	0.537791000
H	-2.221170000	-2.256712000	-0.530035000
C	-1.841182000	2.685898000	-1.642625000
H	-1.125480000	3.336824000	-2.129837000
H	-2.528740000	2.253171000	-2.366488000
H	-2.370163000	3.213921000	-0.851790000

Product of isopropyl radical addition to dimethyl thionocarbonate



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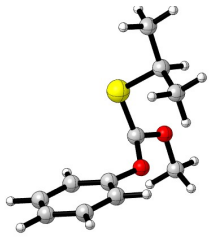
Thermal correction to Energy = 0.199197
Thermal correction to Enthalpy = 0.200142
Thermal correction to Gibbs Free Energy = 0.147284
Sum of electronic and zero-point Energies = -784.889909
Sum of electronic and thermal Energies = -784.877600
Sum of electronic and thermal Enthalpies = -784.876656
Sum of electronic and thermal Free Energies = -784.929513

S	-0.640604000	0.070832000	-1.072466000
C	0.978292000	0.121970000	-0.427139000
O	1.511761000	-0.902473000	0.288219000
O	1.364448000	1.328038000	0.043055000
C	-1.737523000	0.417075000	0.379589000
H	-1.383312000	1.359546000	0.798499000
C	-1.657352000	-0.678757000	1.428367000
C	-3.146156000	0.599060000	-0.165589000
H	-3.191489000	1.401337000	-0.902826000
H	-3.506646000	-0.320548000	-0.632736000
H	-3.826174000	0.847708000	0.651757000
H	-1.993010000	-1.632474000	1.015401000
H	-2.302157000	-0.428127000	2.274895000
H	-0.640981000	-0.802609000	1.802204000
C	2.713333000	1.448241000	0.483213000
H	3.402377000	1.076644000	-0.278247000
H	2.880259000	2.510707000	0.642804000
H	2.874452000	0.906313000	1.414925000
C	1.346395000	-2.209937000	-0.233737000
H	1.669276000	-2.255085000	-1.276040000
H	1.971022000	-2.859720000	0.374553000
H	0.304452000	-2.527433000	-0.164134000

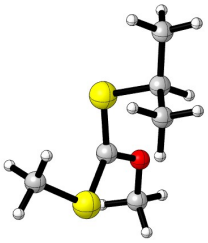
Product of isopropyl radical addition to phenyl methyl thionocarbonate



SCF Energy = -976.817152447
Zero-point correction = 0.240256
Thermal correction to Energy = 0.255301
Thermal correction to Enthalpy = 0.256246
Thermal correction to Gibbs Free Energy = 0.195720
Sum of electronic and zero-point Energies = -976.576896
Sum of electronic and thermal Energies = -976.561851
Sum of electronic and thermal Enthalpies = -976.560907
Sum of electronic and thermal Free Energies = -976.621432

S	-1.412972000	-0.307954000	-1.095233000
C	-0.719645000	1.080284000	-0.304937000
O	0.273651000	0.928038000	0.631102000
C	1.435827000	0.293832000	0.270203000
C	2.021427000	0.471675000	-0.974585000
C	2.035538000	-0.502174000	1.233265000
C	3.221537000	-0.165304000	-1.251416000
C	3.238071000	-1.128362000	0.945610000
C	3.834028000	-0.965065000	-0.297028000
H	1.541997000	1.102449000	-1.711741000
H	1.552763000	-0.625491000	2.193765000
H	3.682197000	-0.029236000	-2.221654000
H	3.707238000	-1.751703000	1.696142000
H	4.771464000	-1.457460000	-0.520090000
O	-1.576358000	2.061598000	0.027974000
C	-2.539774000	-1.050431000	0.171021000
H	-3.259124000	-0.272414000	0.428002000
C	-1.791793000	-1.497208000	1.415480000
C	-3.260147000	-2.201181000	-0.517117000
H	-3.808203000	-1.864931000	-1.398070000
H	-2.553434000	-2.975897000	-0.823117000
H	-3.972751000	-2.650639000	0.177251000
H	-1.036411000	-2.244827000	1.165285000
H	-2.494574000	-1.941550000	2.125116000
H	-1.296895000	-0.661078000	1.908238000
C	-1.004380000	3.270271000	0.525474000
H	-0.232210000	3.633161000	-0.155932000
H	-1.818878000	3.988162000	0.574762000
H	-0.578118000	3.123599000	1.517350000

Product of isopropyl radical addition to dimethyl xanthate



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Zero-point correction = 0.182939
Thermal correction to Energy = 0.195933
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Sum of electronic and zero-point Energies = -1107.876598
Sum of electronic and thermal Energies = -1107.863605
Sum of electronic and thermal Enthalpies = -1107.862660
Sum of electronic and thermal Free Energies = -1107.917710

S	-0.797486000	0.133220000	-1.019110000
C	0.767594000	0.367541000	-0.329887000
S	1.732400000	-0.896811000	0.418742000
O	1.052885000	1.645746000	0.025565000
C	-1.986972000	0.381105000	0.378852000
H	-1.739641000	1.350644000	0.812321000

C	-1.864985000	-0.706111000	1.431683000
C	-3.376396000	0.439204000	-0.238305000
H	-3.457790000	1.241868000	-0.972037000
H	-3.623928000	-0.504834000	-0.729929000
H	-4.117934000	0.613144000	0.543858000
H	-2.098431000	-1.683682000	1.004161000
H	-2.568430000	-0.512611000	2.245794000
H	-0.860553000	-0.746389000	1.853525000
C	2.407007000	2.003058000	0.271597000
H	3.046026000	1.696670000	-0.559181000
H	2.416386000	3.086329000	0.365236000
H	2.776326000	1.559087000	1.198545000
C	1.266228000	-2.340729000	-0.545068000
H	1.460088000	-2.174957000	-1.602892000
H	1.893334000	-3.153291000	-0.181214000
H	0.217982000	-2.584899000	-0.390055000

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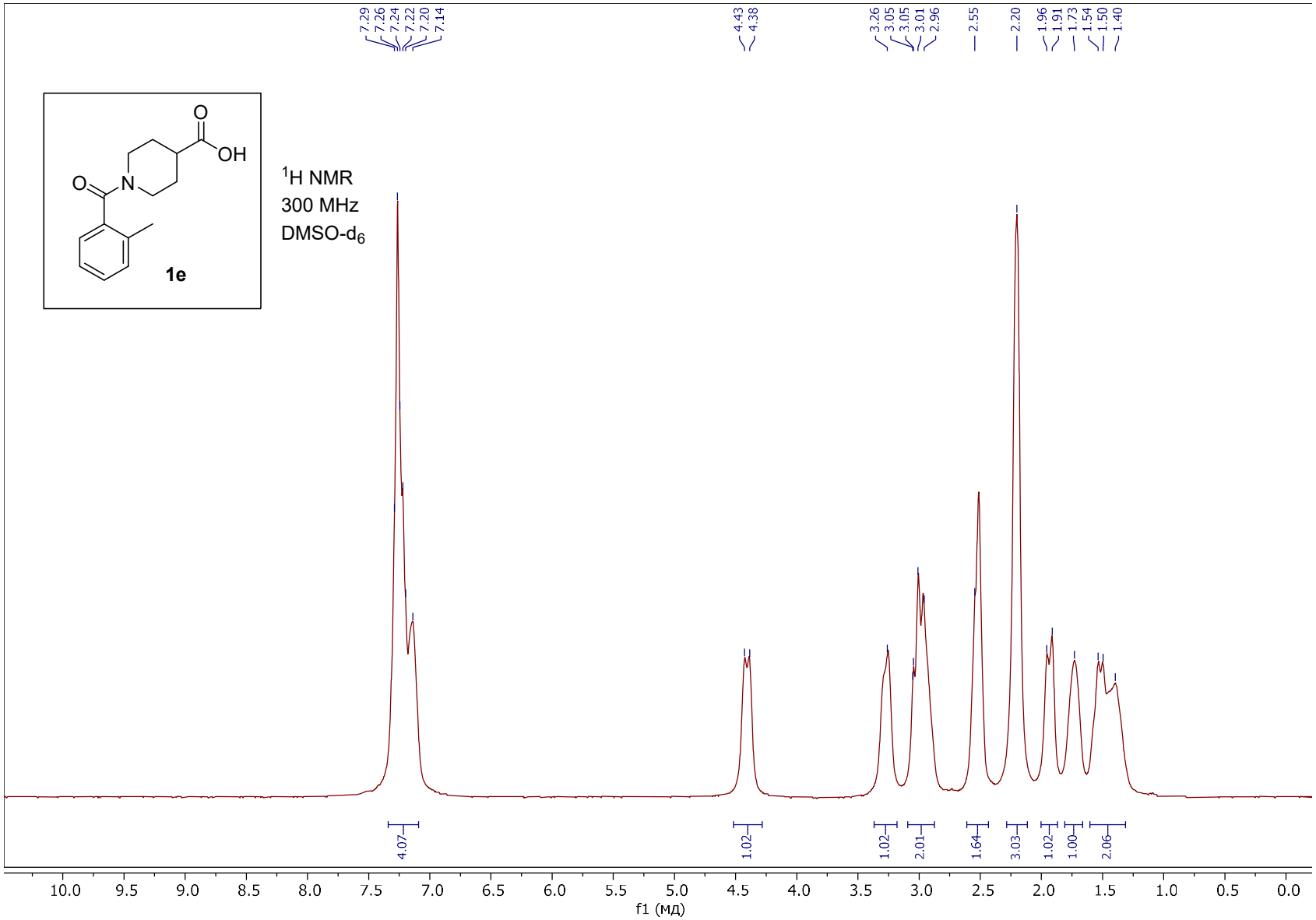
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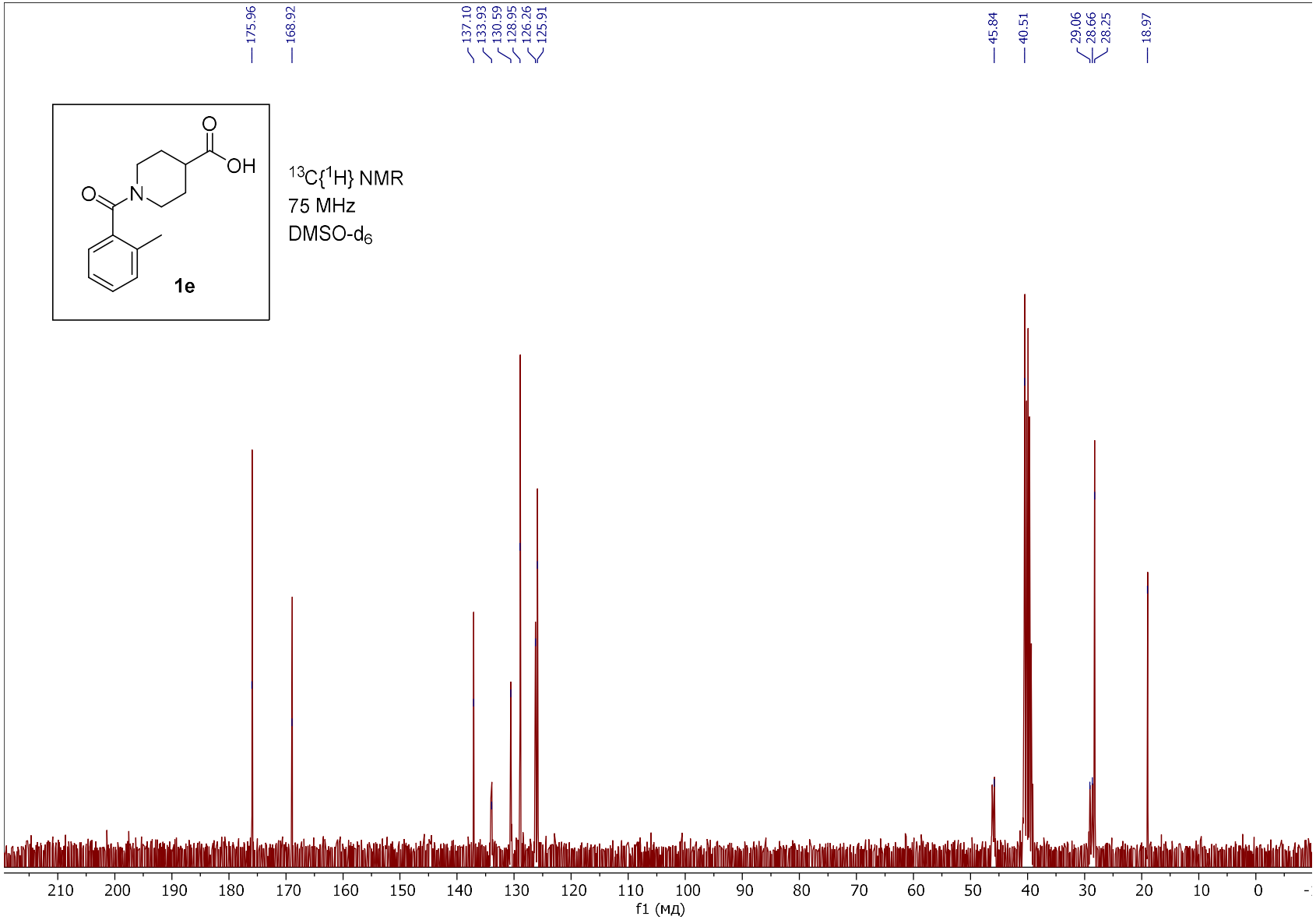
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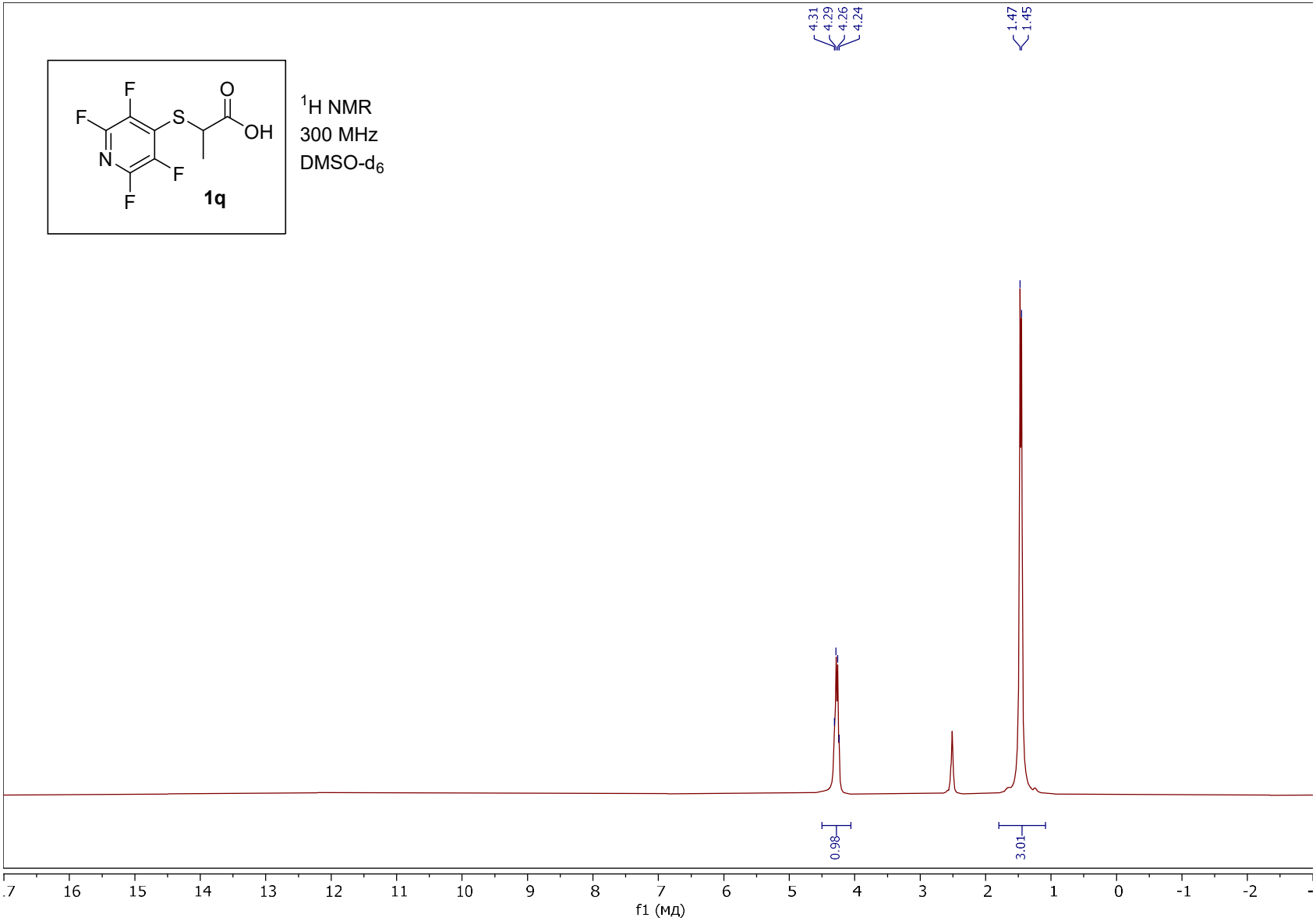
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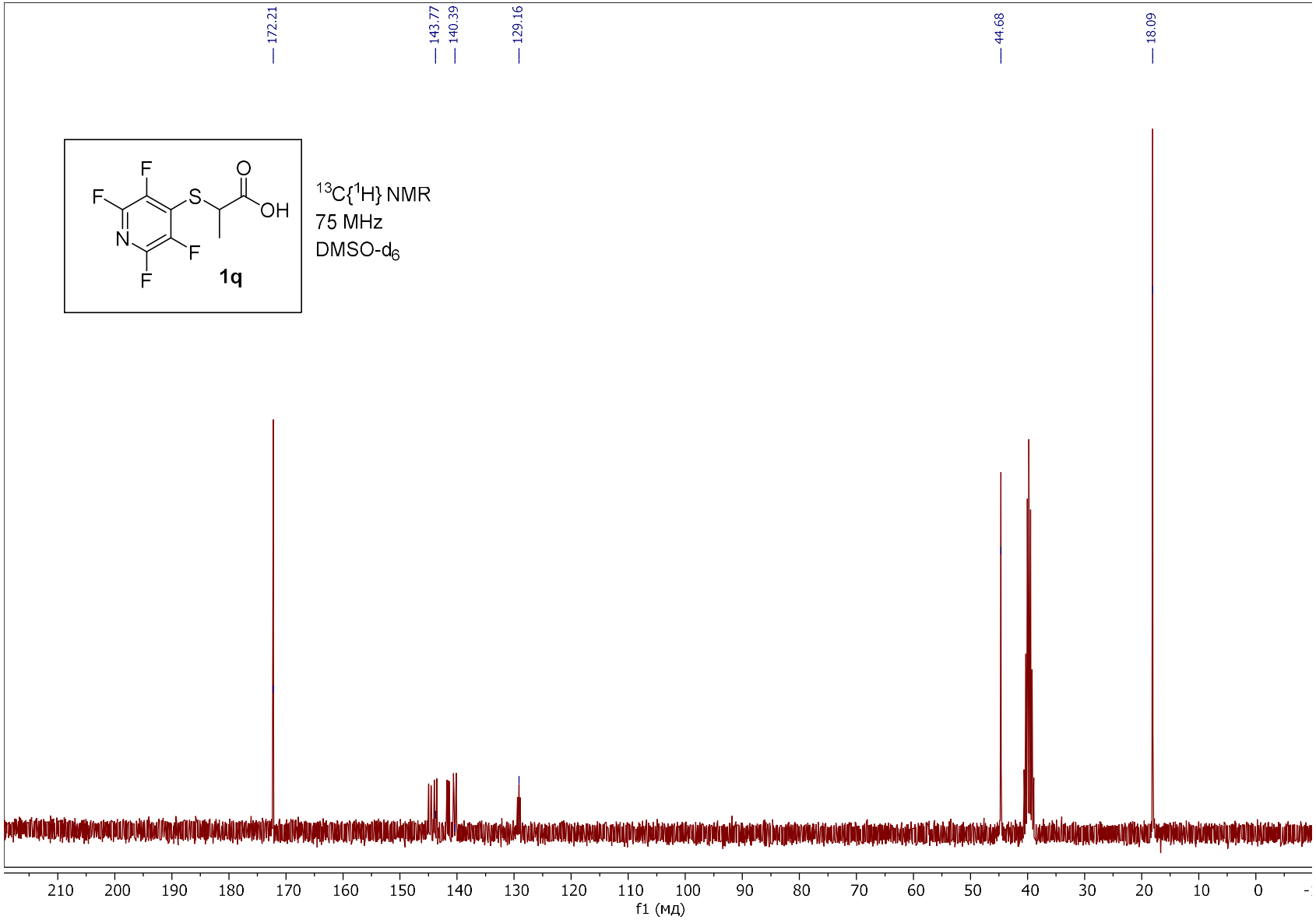
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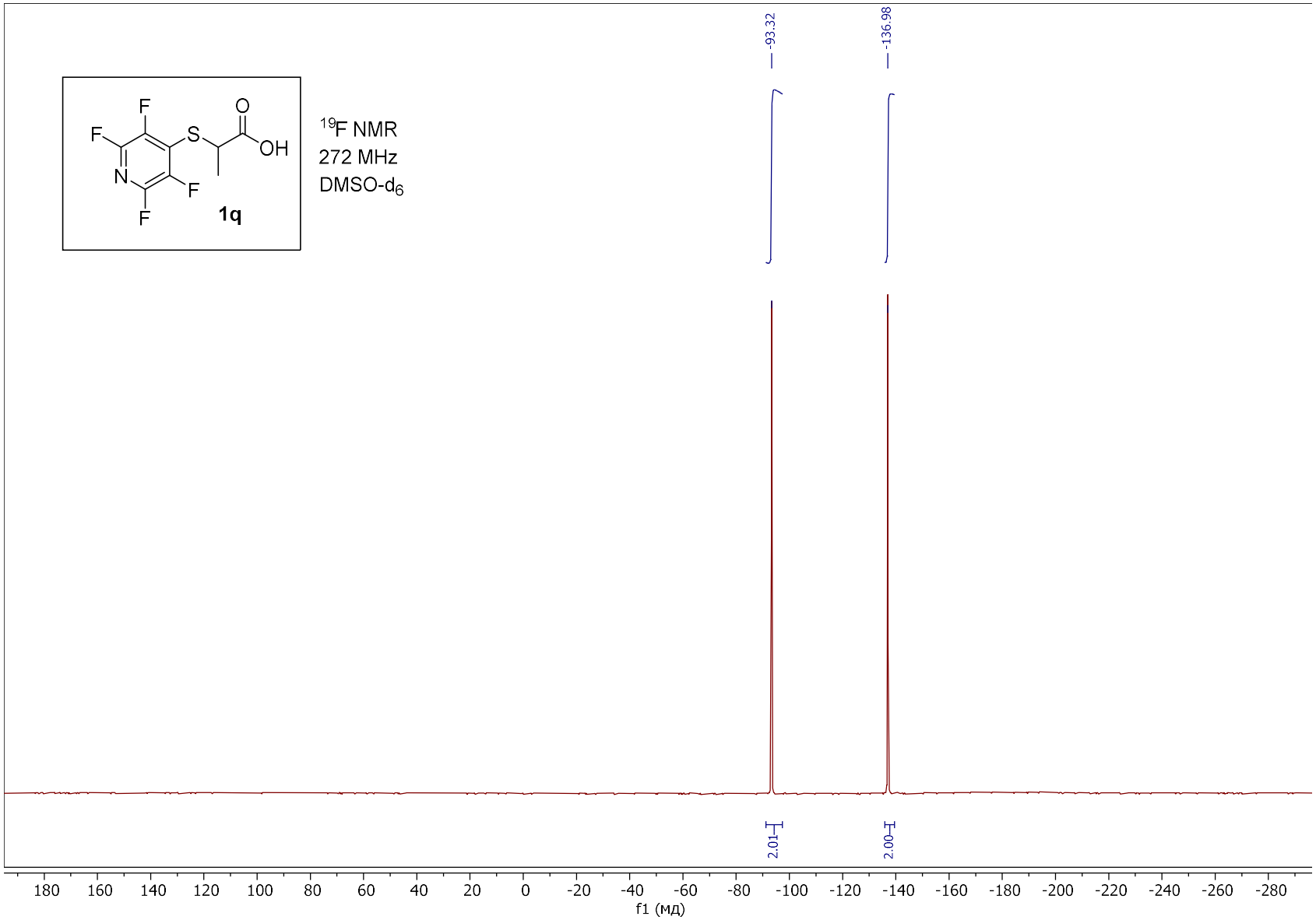
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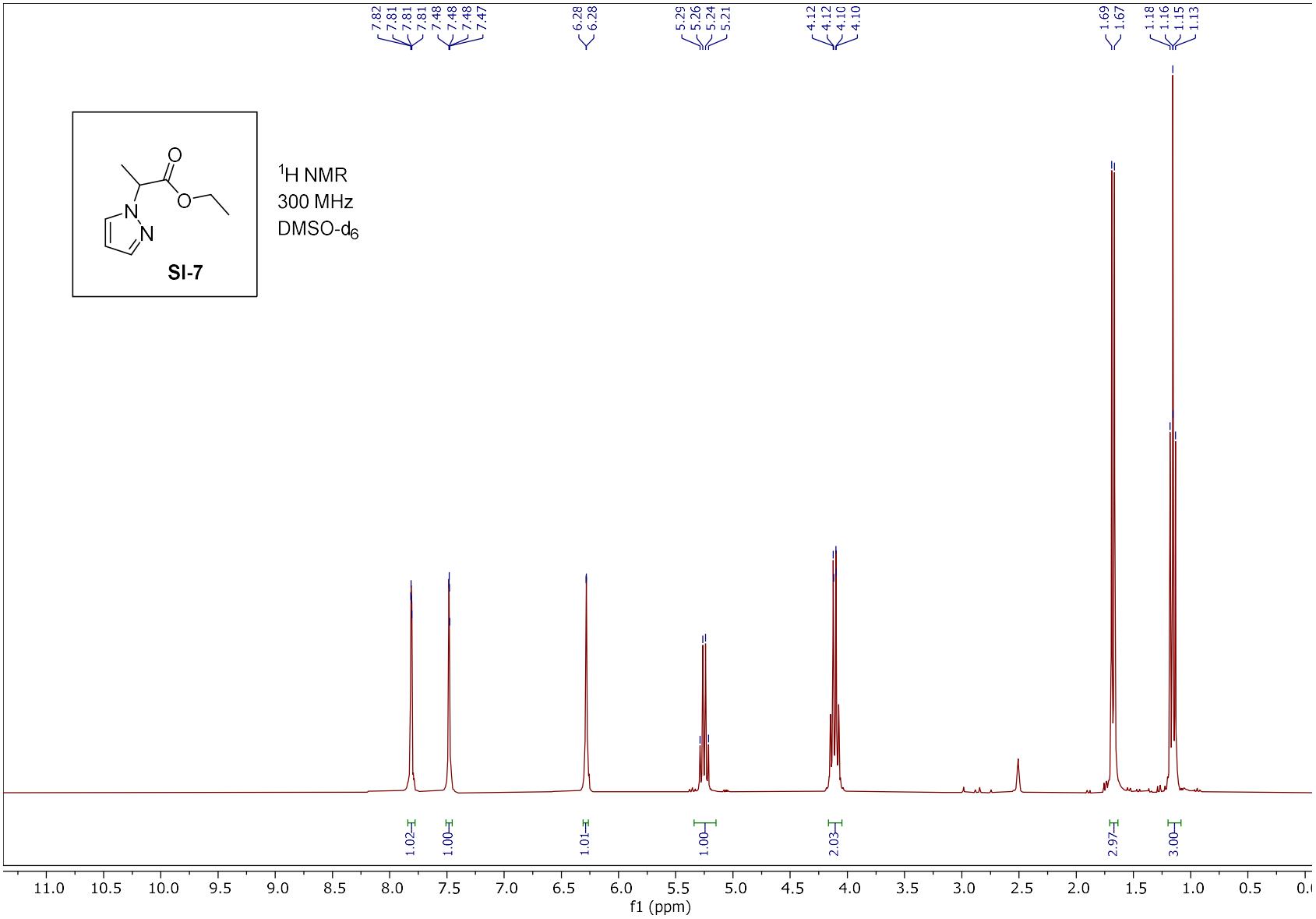
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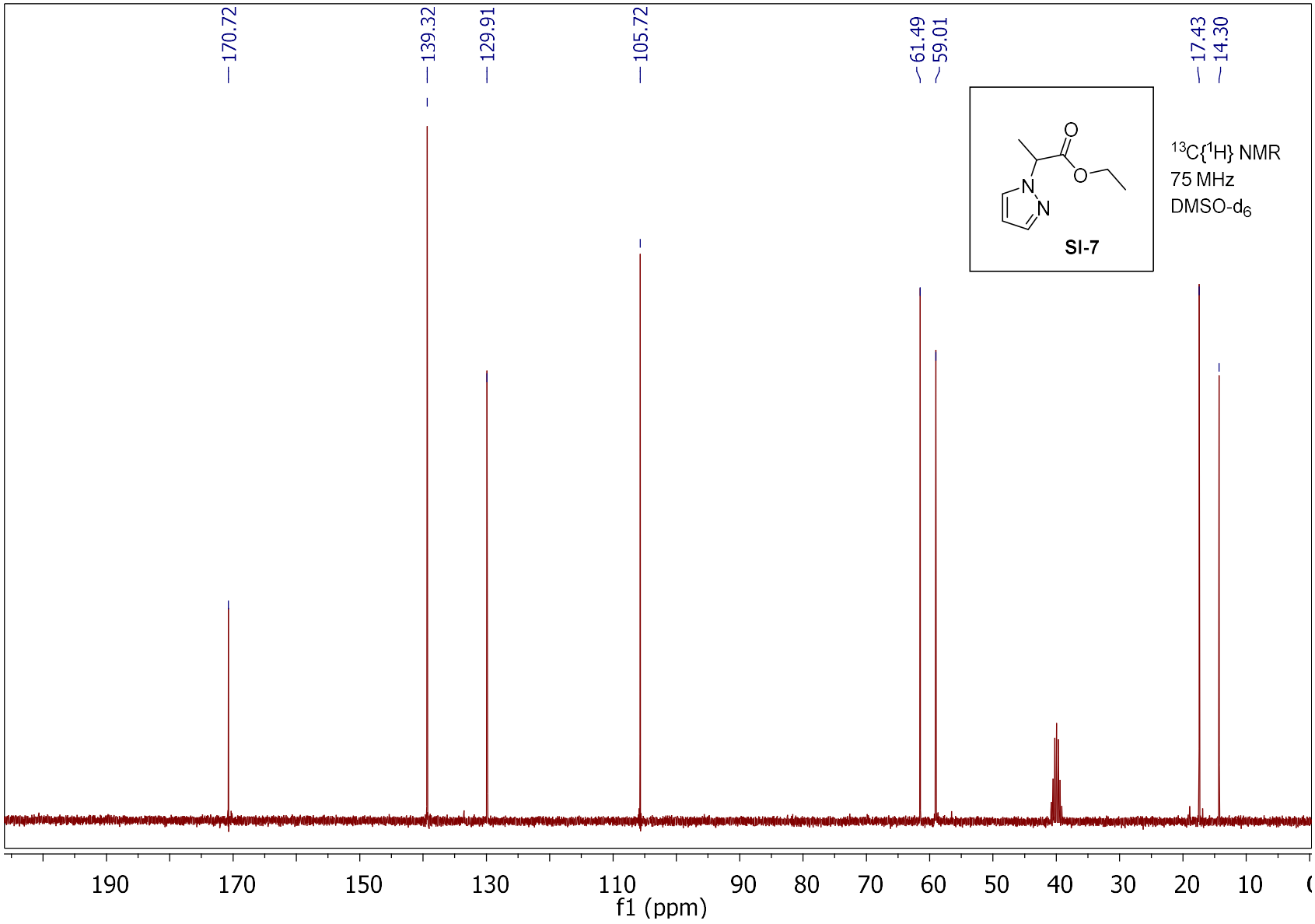
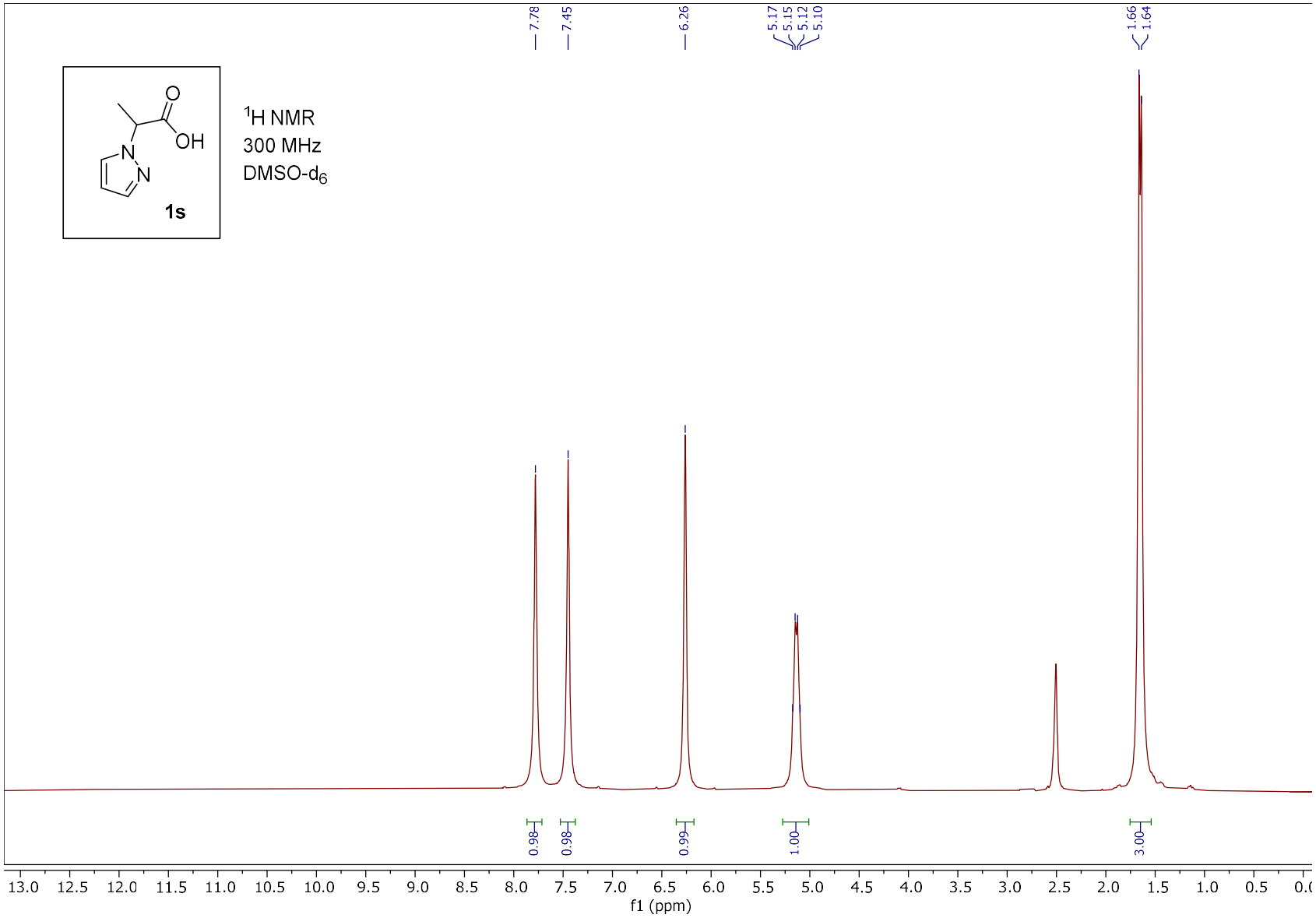
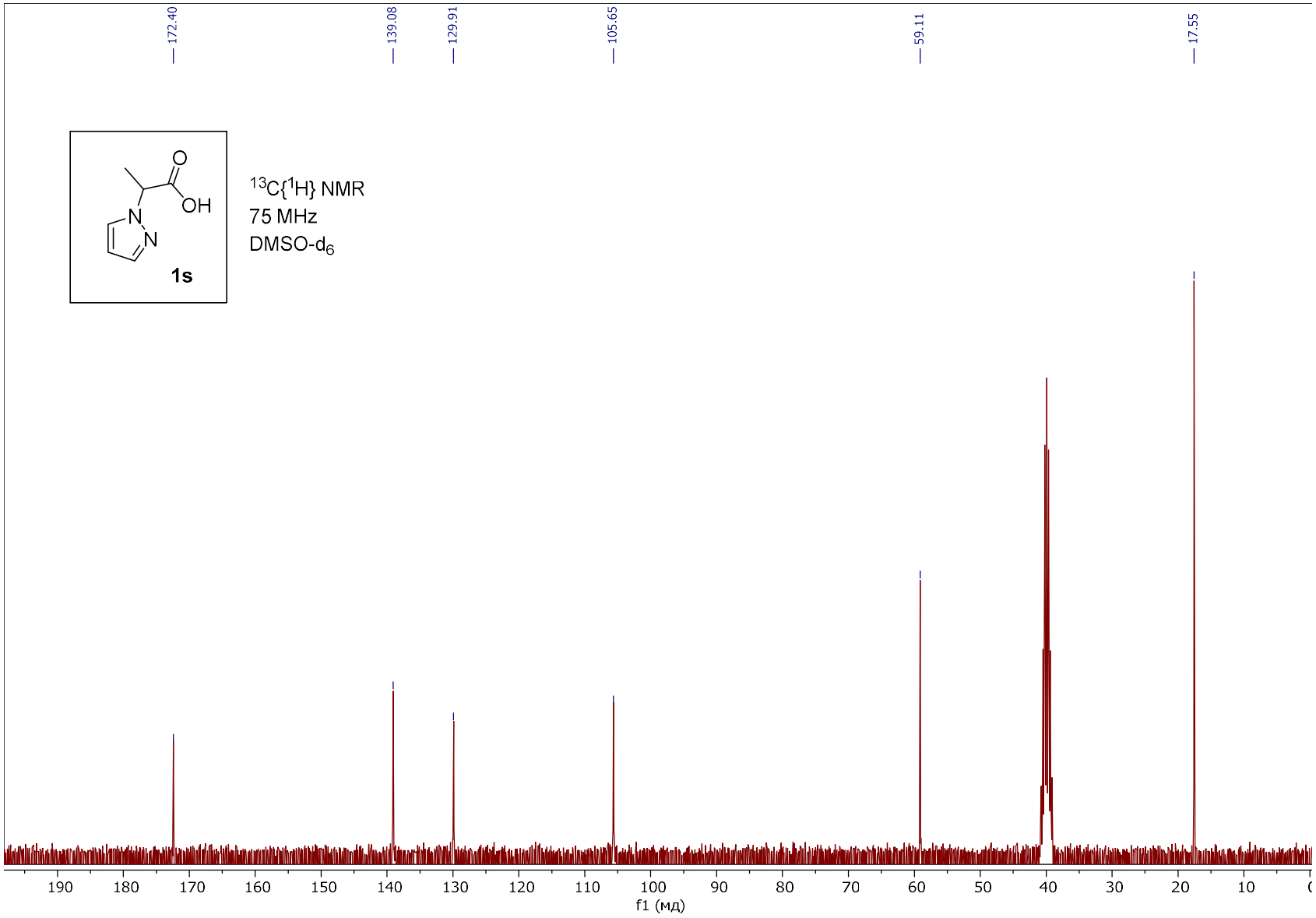
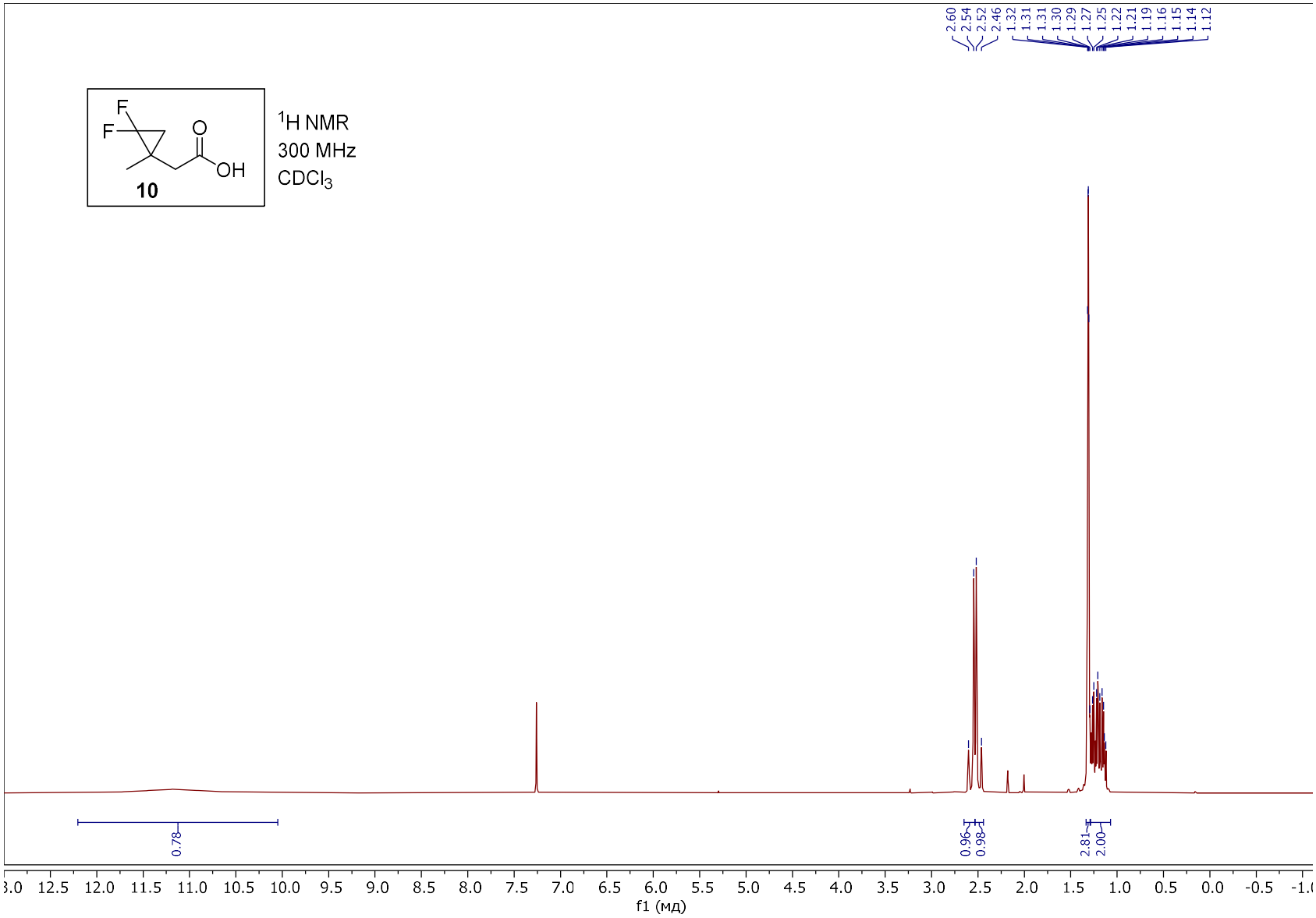
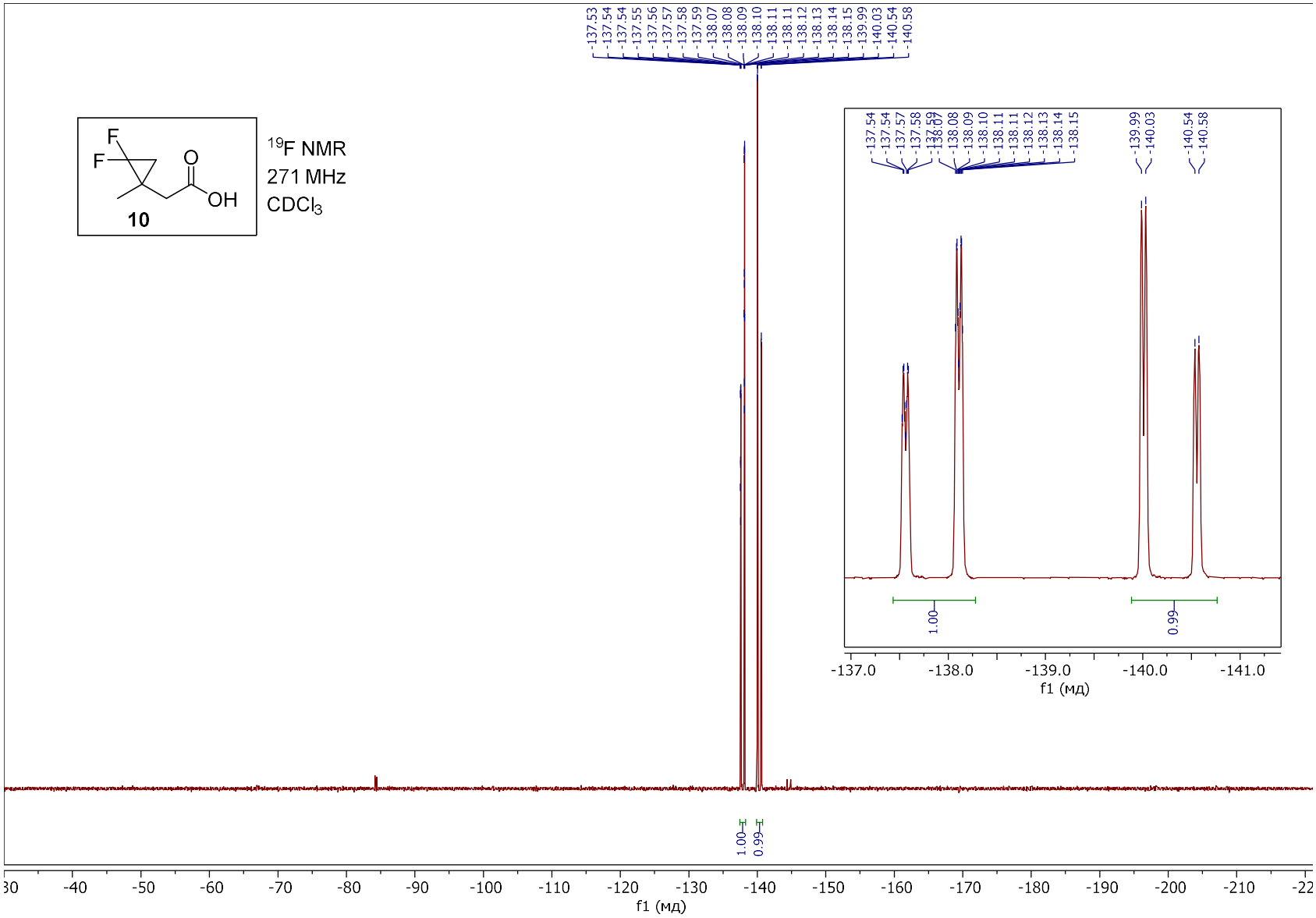
1.69
1.67
1.18
1.16
1.15
1.13
SI-7
^{1}H NMR
300 MHz
DMSO-d$_6$
1.02
1.00
1.01
1.00
2.03
2.97
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

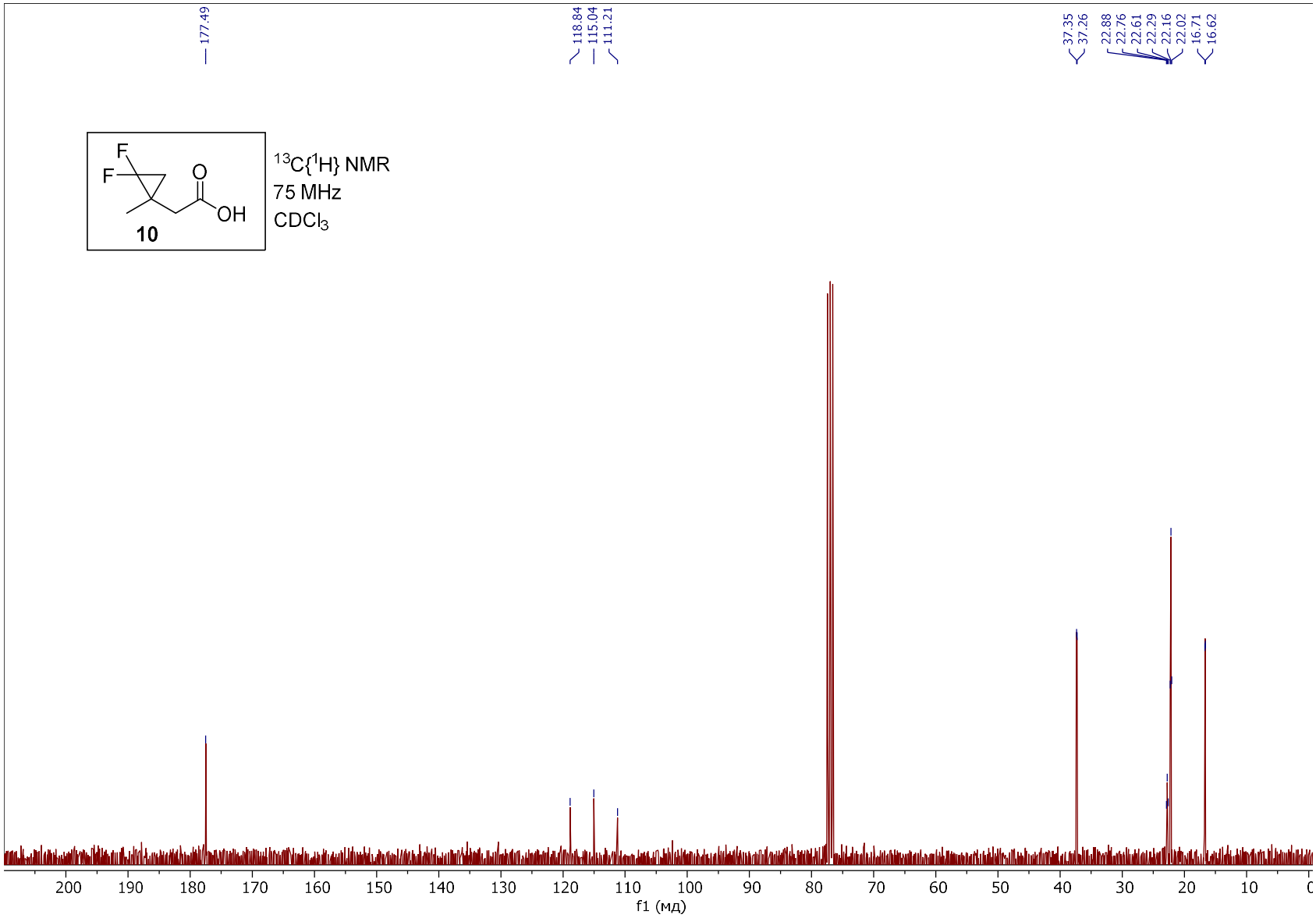

170.72
139.32
129.91
105.72
61.49
59.01
17.43
14.30
SI-7
13C{1H} NMR
75 MHz
DMSO-d6
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

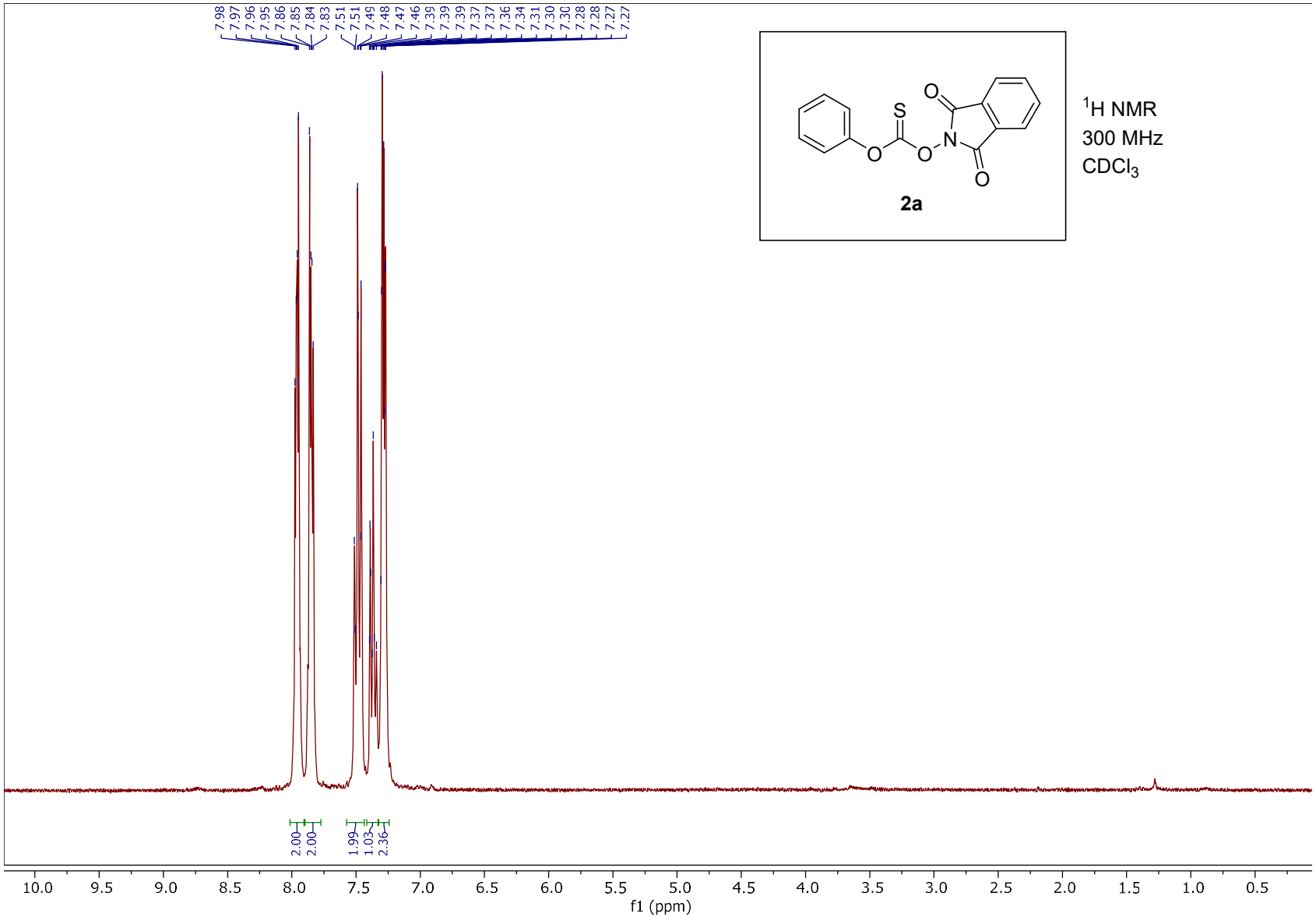

7.78
7.45
6.26
5.17
5.15
5.12
5.10
1.66
1.64
O
OH
N
N
1s
^{1}H NMR
300 MHz
DMSO-d$_6$
0.98
0.98
0.99
1.00
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

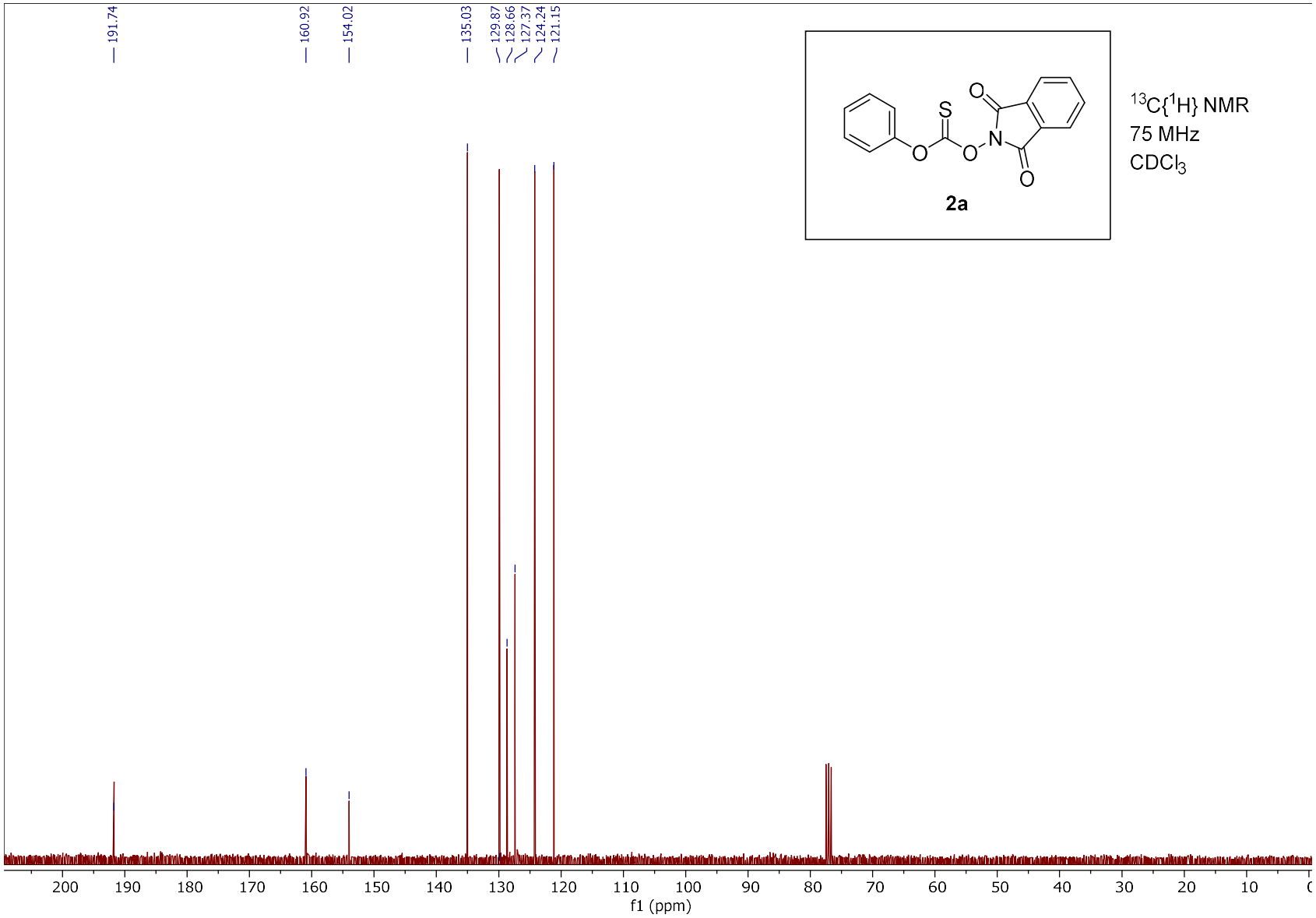

172.40
139.08
129.91
105.65
59.11
17.55
OH
N
N
1s
$^{13}C\{^{1}H\}$ NMR
75 MHz
DMSO-d_6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (мд)

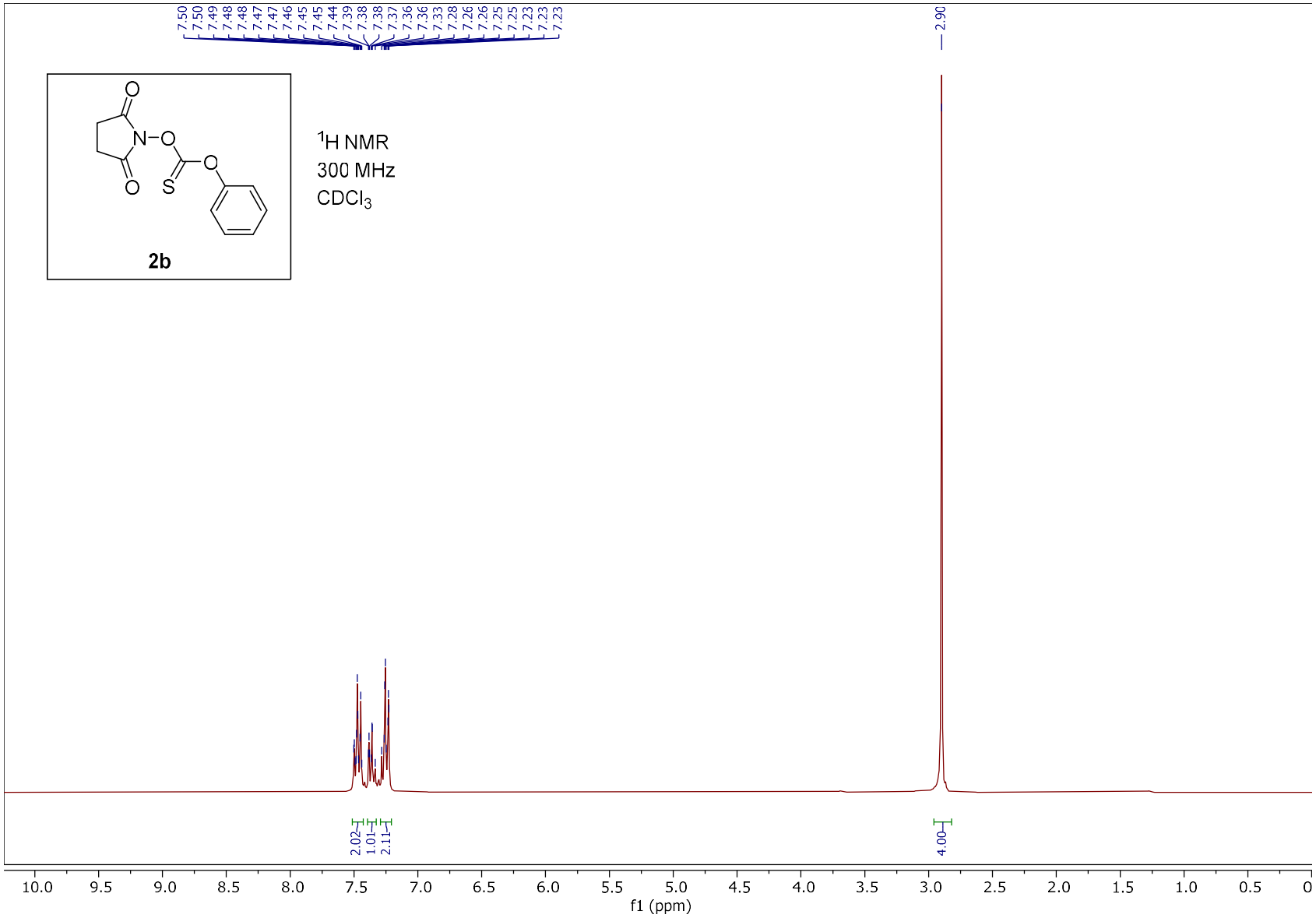

F
F
O
OH
10
1H NMR
300 MHz
CDCl3
2.60
2.54
2.52
2.46
1.32
1.31
1.31
1.30
1.29
1.27
1.25
1.22
1.21
1.19
1.16
1.15
1.14
1.12
0.78
0.96
0.98
2.81
2.00
f1 (мд)

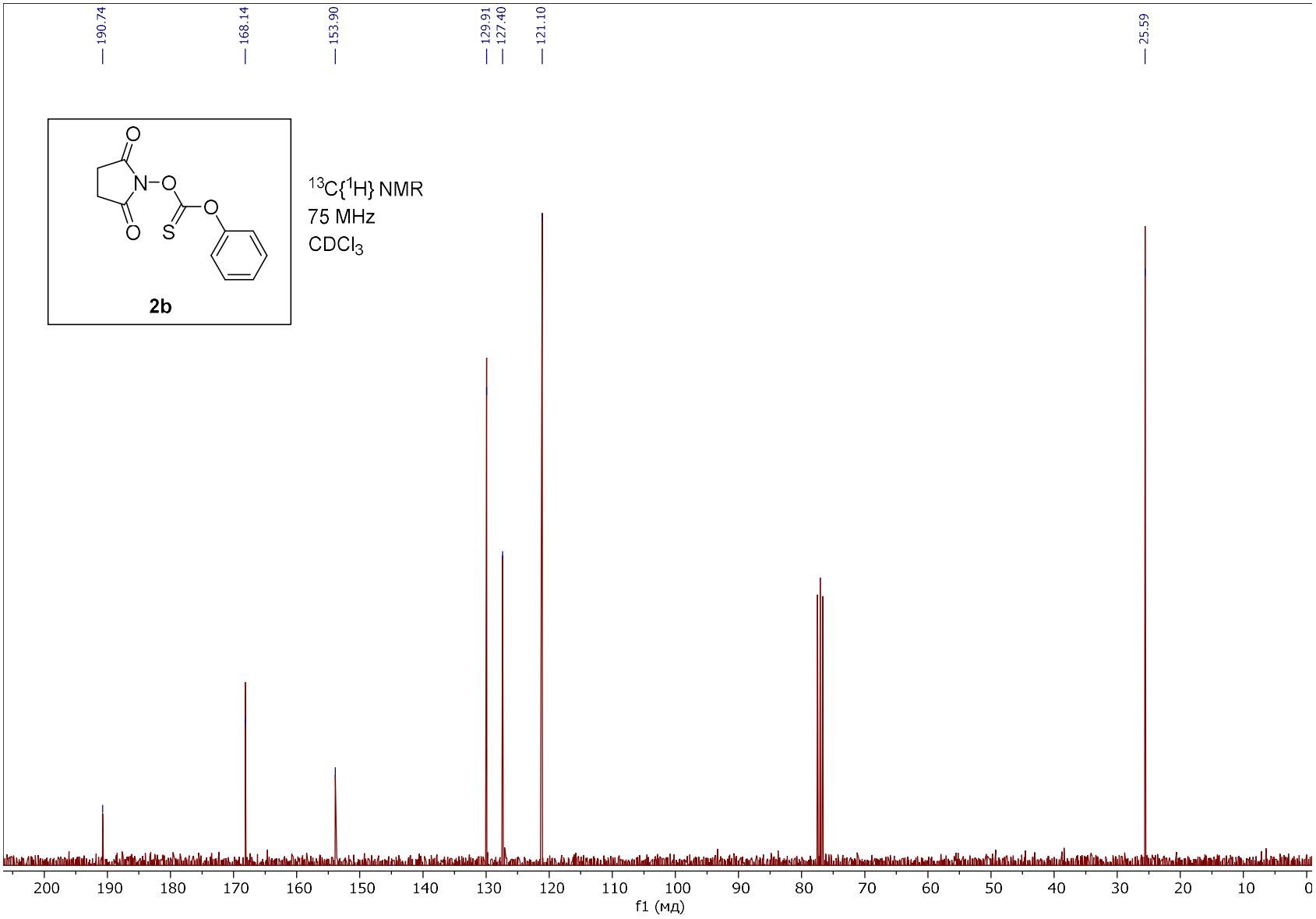

F
F
O
OH
10
19F NMR
271 MHz
CDCl3
f1 (мд)
1.00
0.99

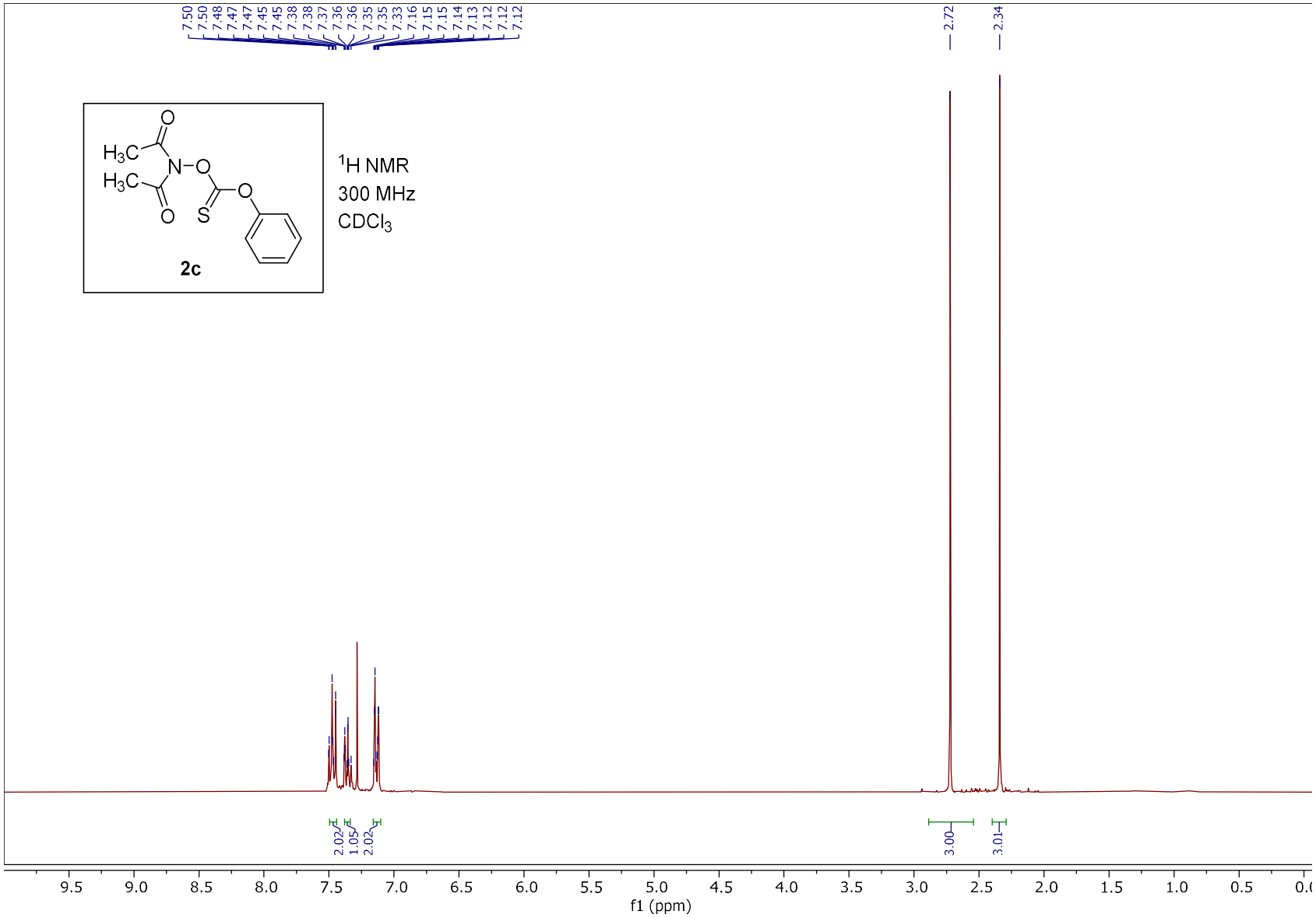

177.49
118.84
115.04
111.21
37.35
37.26
22.88
22.76
22.61
22.29
22.16
22.02
16.71
16.62
F
F
O
OH
10
13C{1H} NMR
75 MHz
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

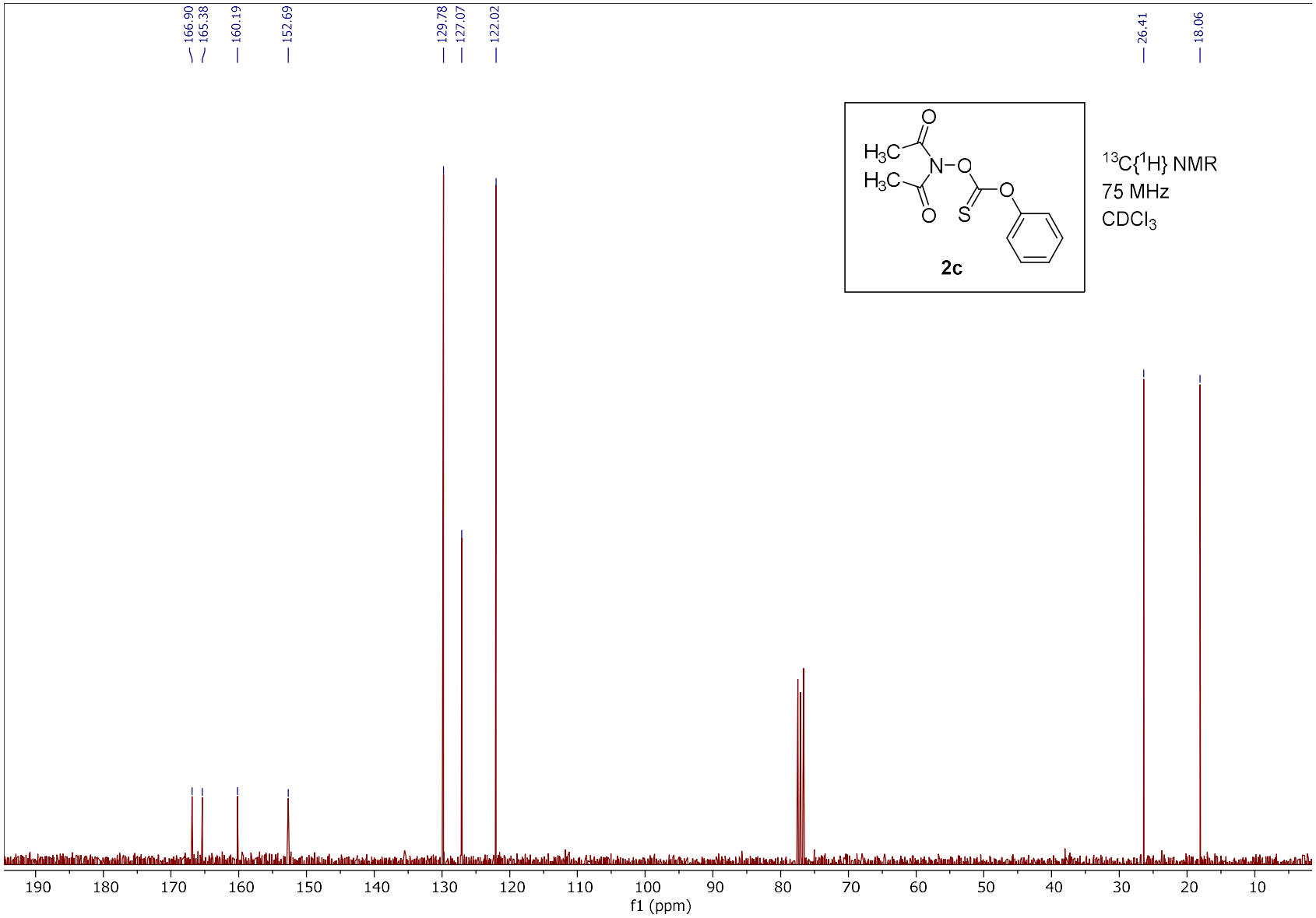

7.98
7.97
7.96
7.95
7.86
7.85
7.84
7.83
7.51
7.51
7.49
7.48
7.47
7.46
7.39
7.39
7.39
7.37
7.37
7.36
7.34
7.31
7.30
7.30
7.28
7.27
7.27
O
S
O
O
N
O
2a
1H NMR
300 MHz
CDCl3
2.00
2.00
1.99
1.03
2.36
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

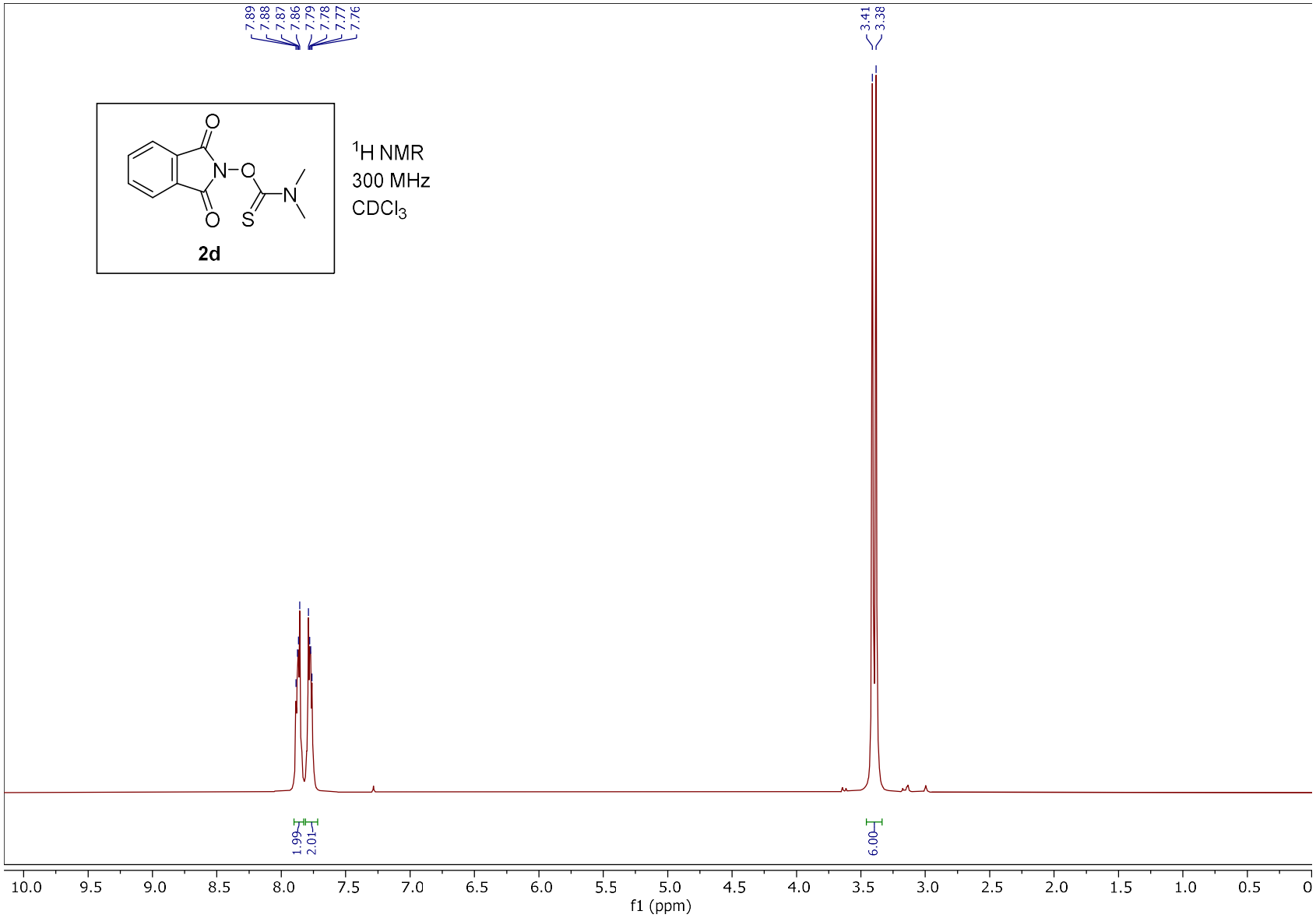

191.74
160.92
154.02
135.03
129.87
128.66
127.37
124.24
121.15
O
S
O
O
N
O
2a
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

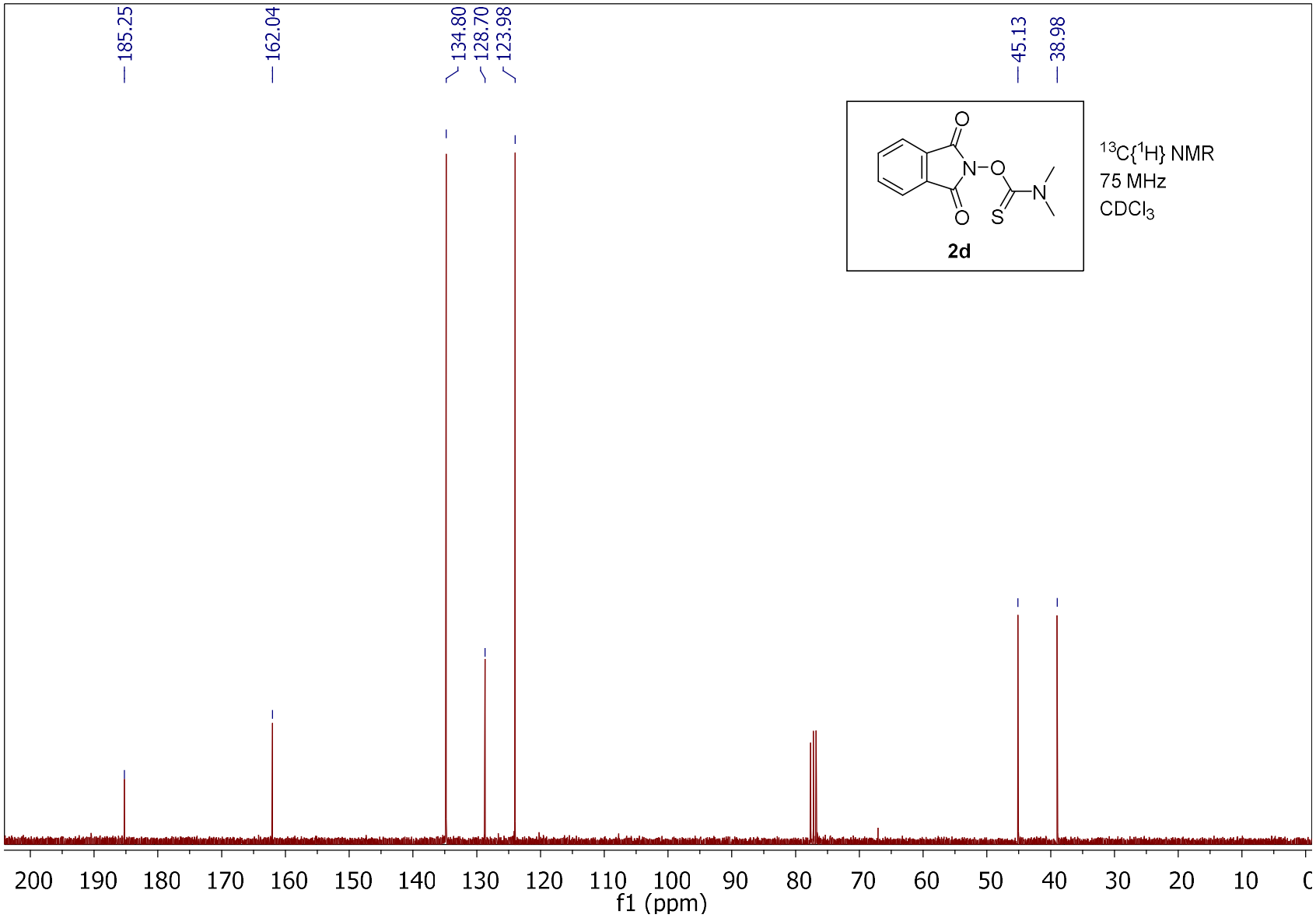

7.50
7.50
7.49
7.48
7.48
7.47
7.47
7.46
7.45
7.45
7.44
7.39
7.38
7.38
7.37
7.36
7.36
7.33
7.28
7.26
7.26
7.25
7.25
7.23
7.23
7.23
2.90
2b
1H NMR
300 MHz
CDCl3
2.02
1.01
2.11
4.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

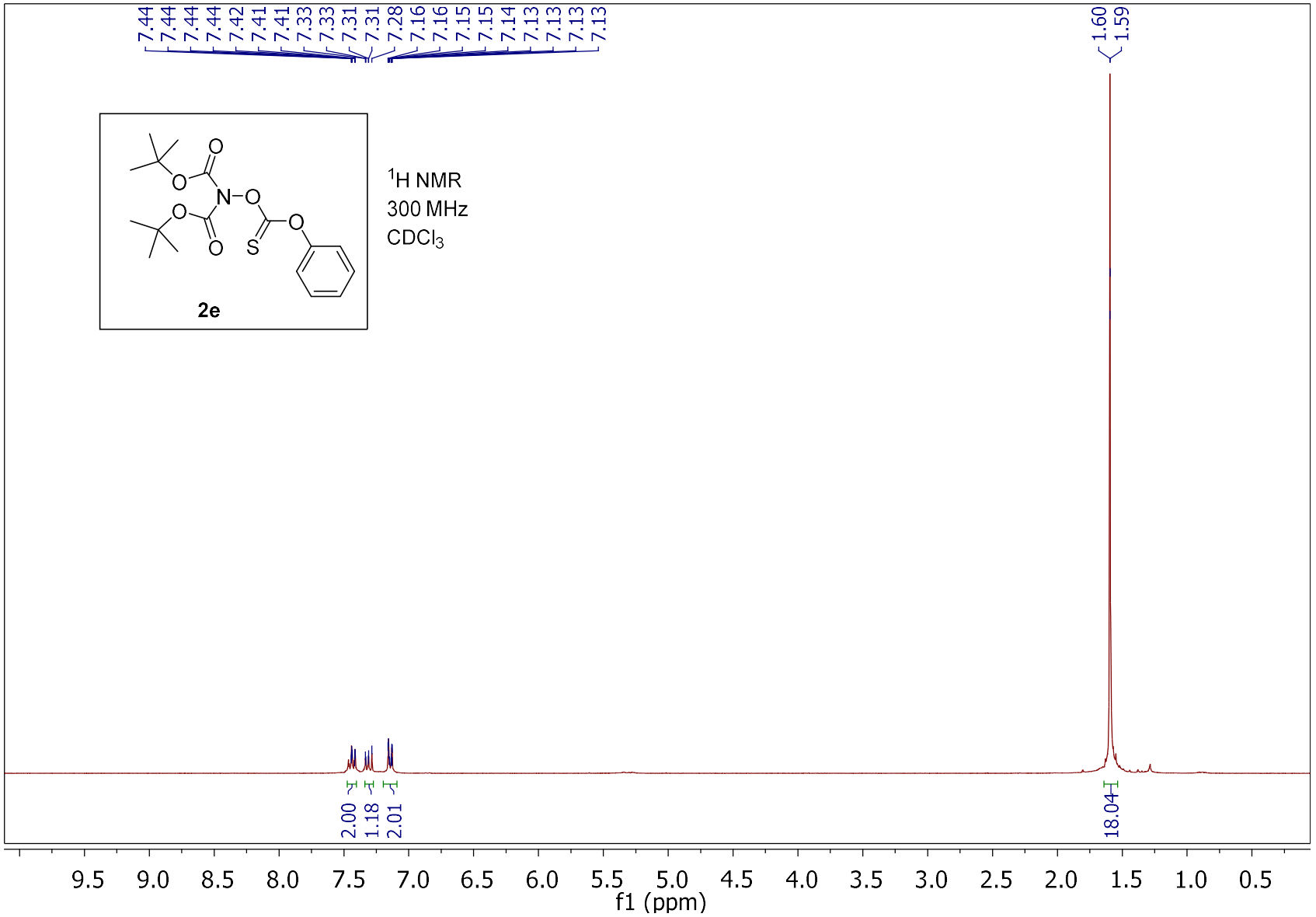

190.74
168.14
153.90
129.91
127.40
121.10
25.59
2b
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

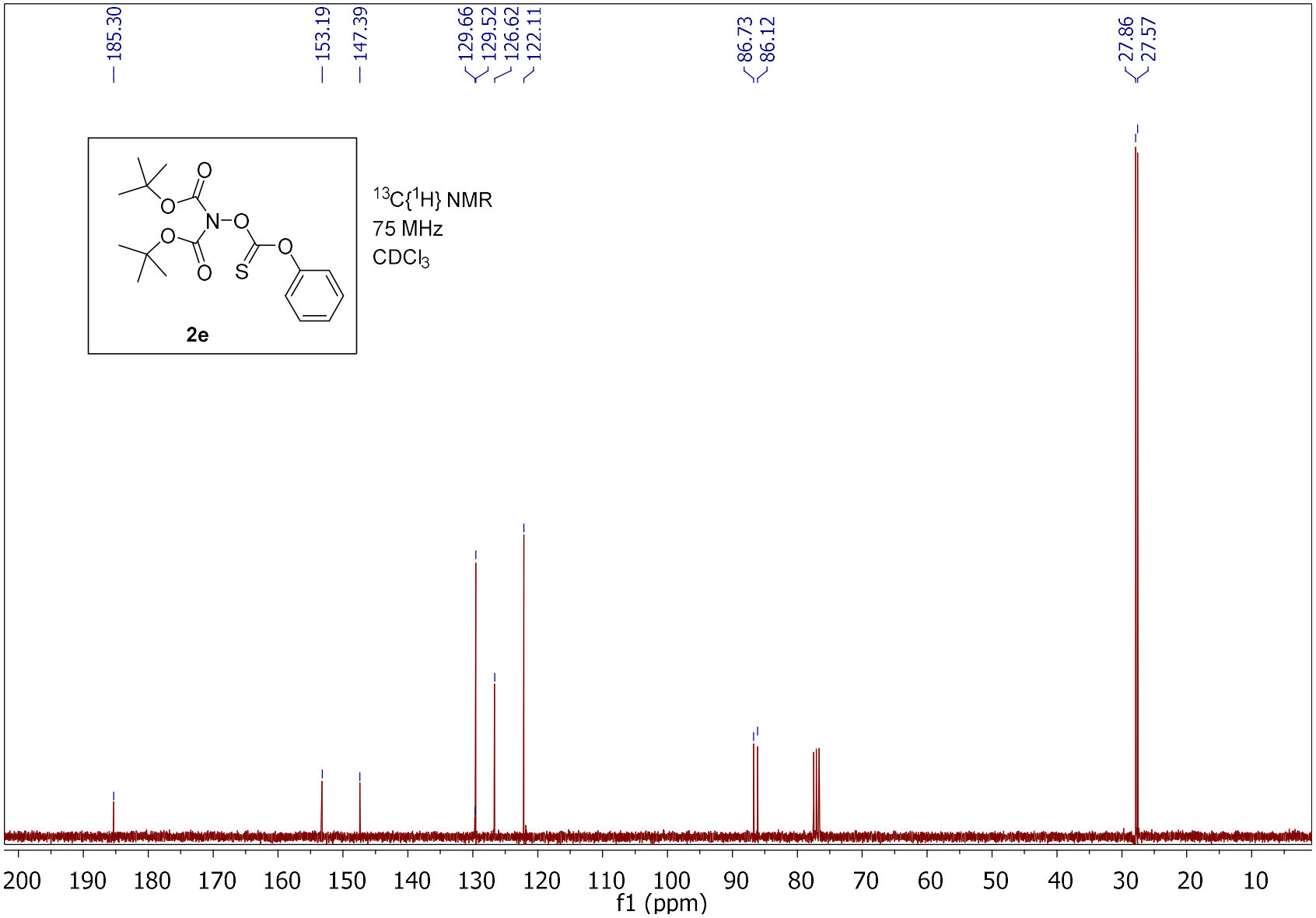

7.50
7.50
7.48
7.47
7.47
7.45
7.45
7.38
7.38
7.37
7.36
7.36
7.35
7.35
7.33
7.16
7.15
7.15
7.14
7.13
7.12
7.12
7.12
2.72
2.34
2c
1H NMR
300 MHz
CDCl3
2.02
1.05
2.02
3.00
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

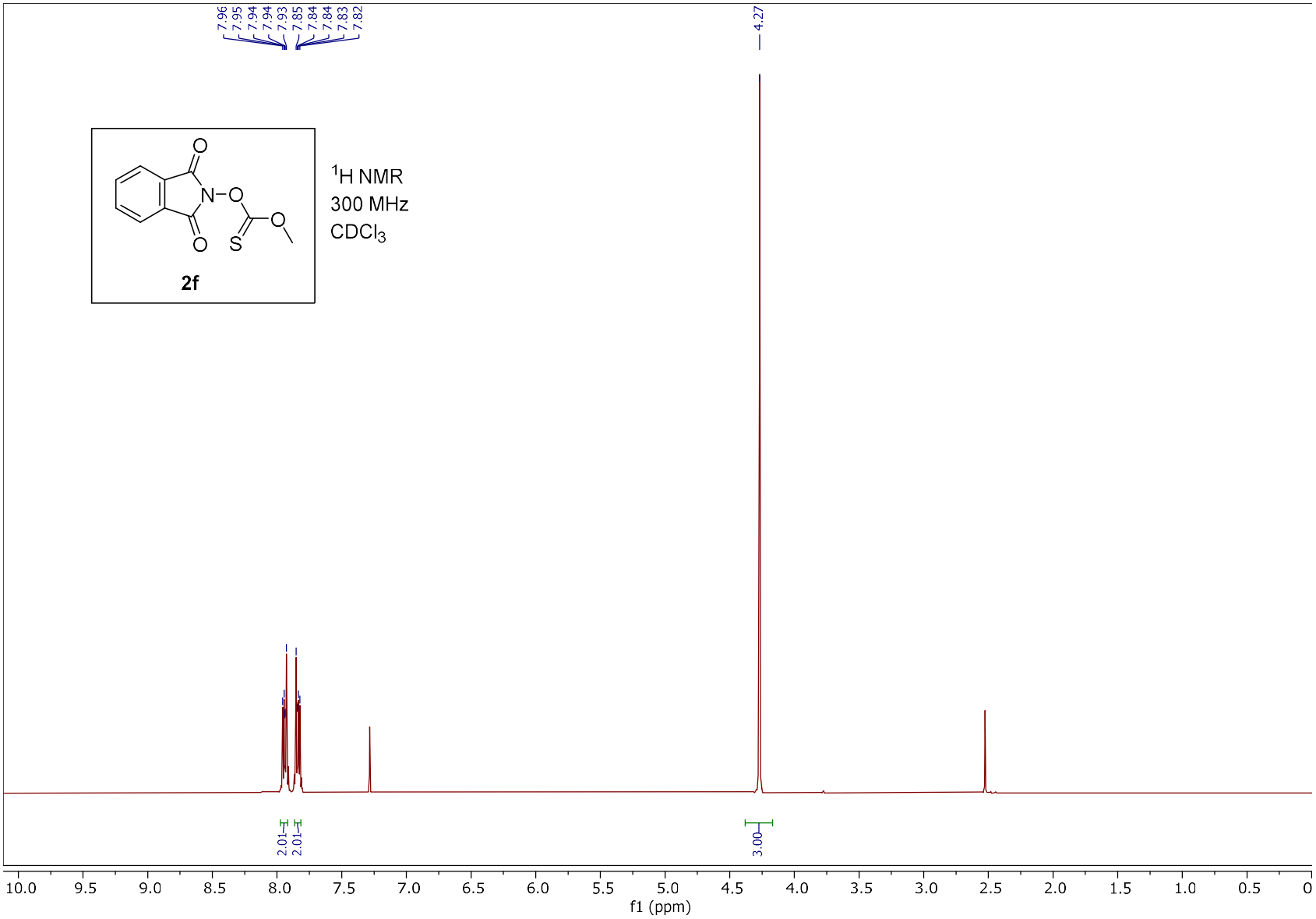

166.90
165.38
160.19
152.69
129.78
127.07
122.02
26.41
18.06
2c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

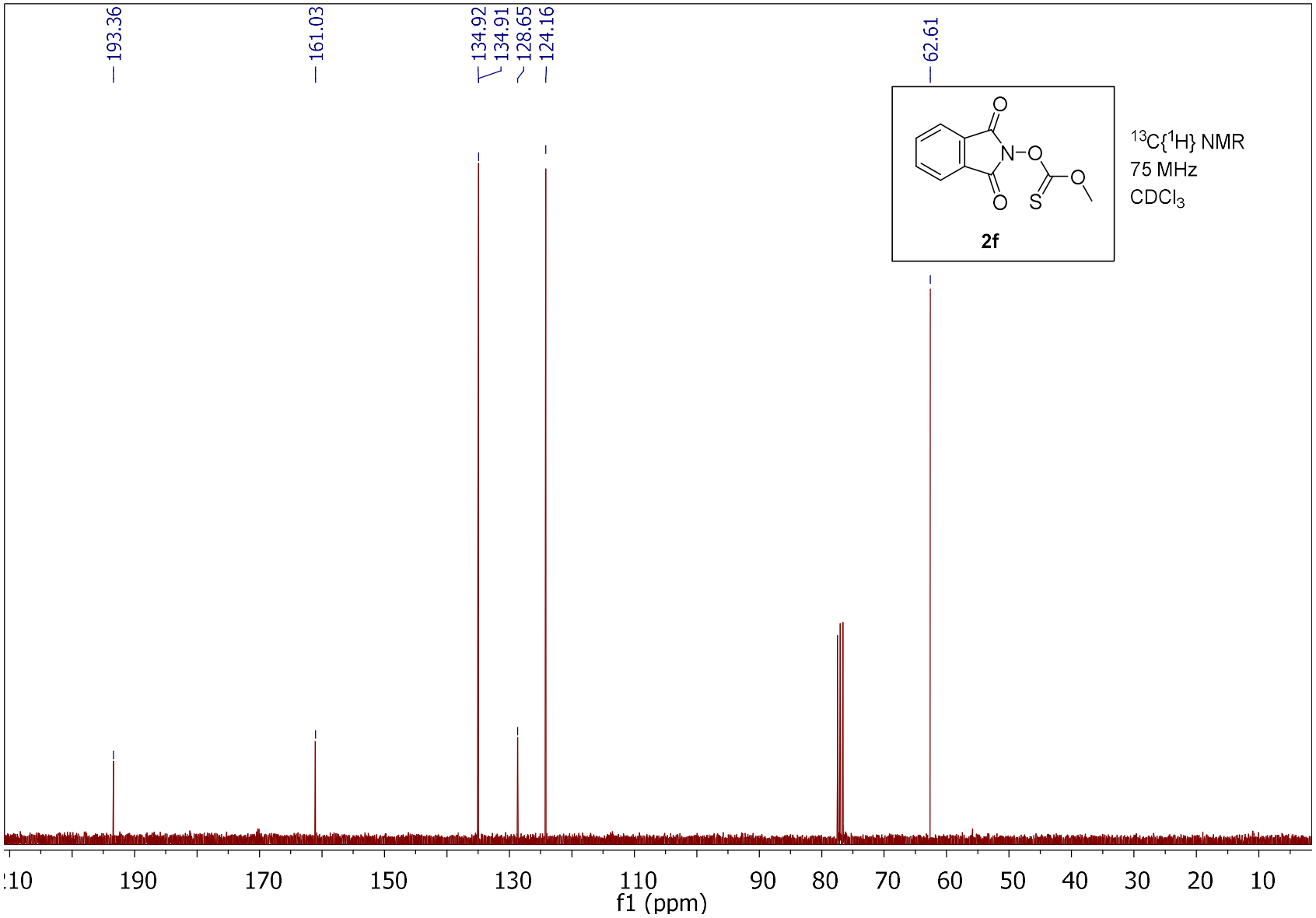

7.89
7.88
7.87
7.86
7.79
7.78
7.77
7.76
3.41
3.38
O
N
O
O
N
S
2d
^{1}H NMR
300 MHz
$CDCl_3$
1.99
2.01
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

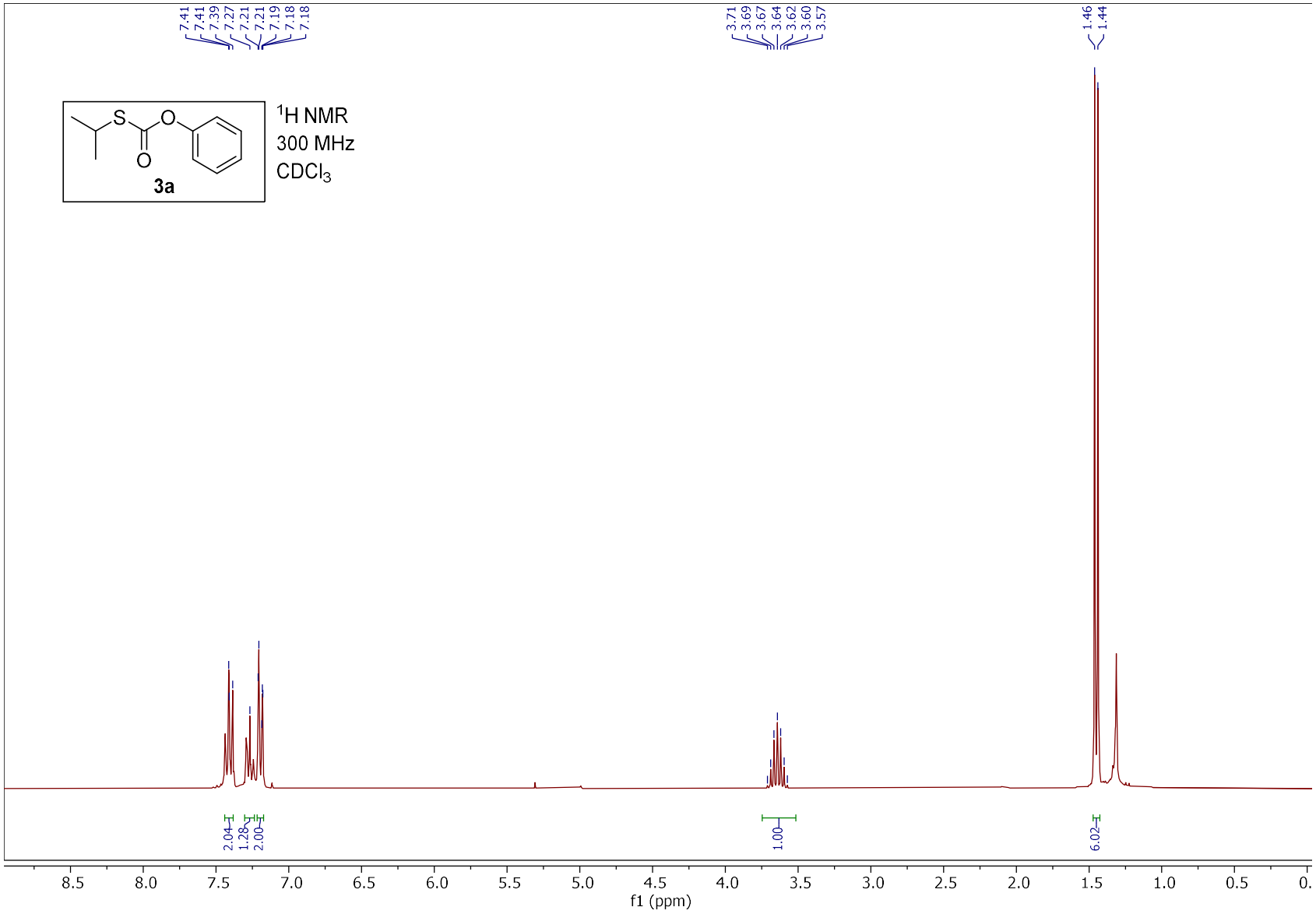

185.25
162.04
134.80
128.70
123.98
45.13
38.98
O
N
O
O
S
N
2d
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

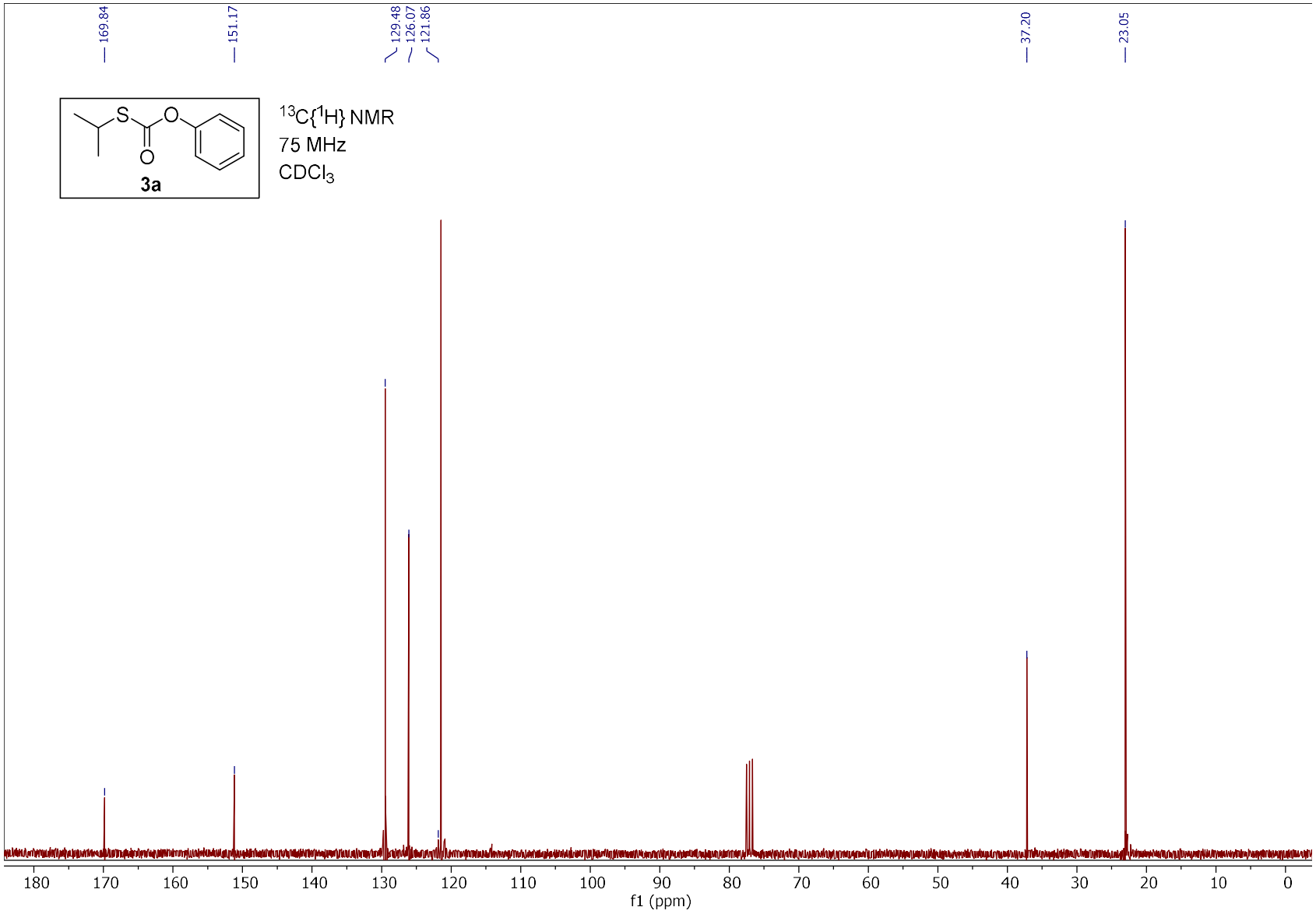

7.44
7.44
7.44
7.44
7.42
7.41
7.41
7.33
7.33
7.31
7.31
7.28
7.16
7.16
7.15
7.15
7.14
7.13
7.13
7.13
7.13
1.60
1.59
2e
1H NMR
300 MHz
CDCl3
2.00
1.18
2.01
18.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

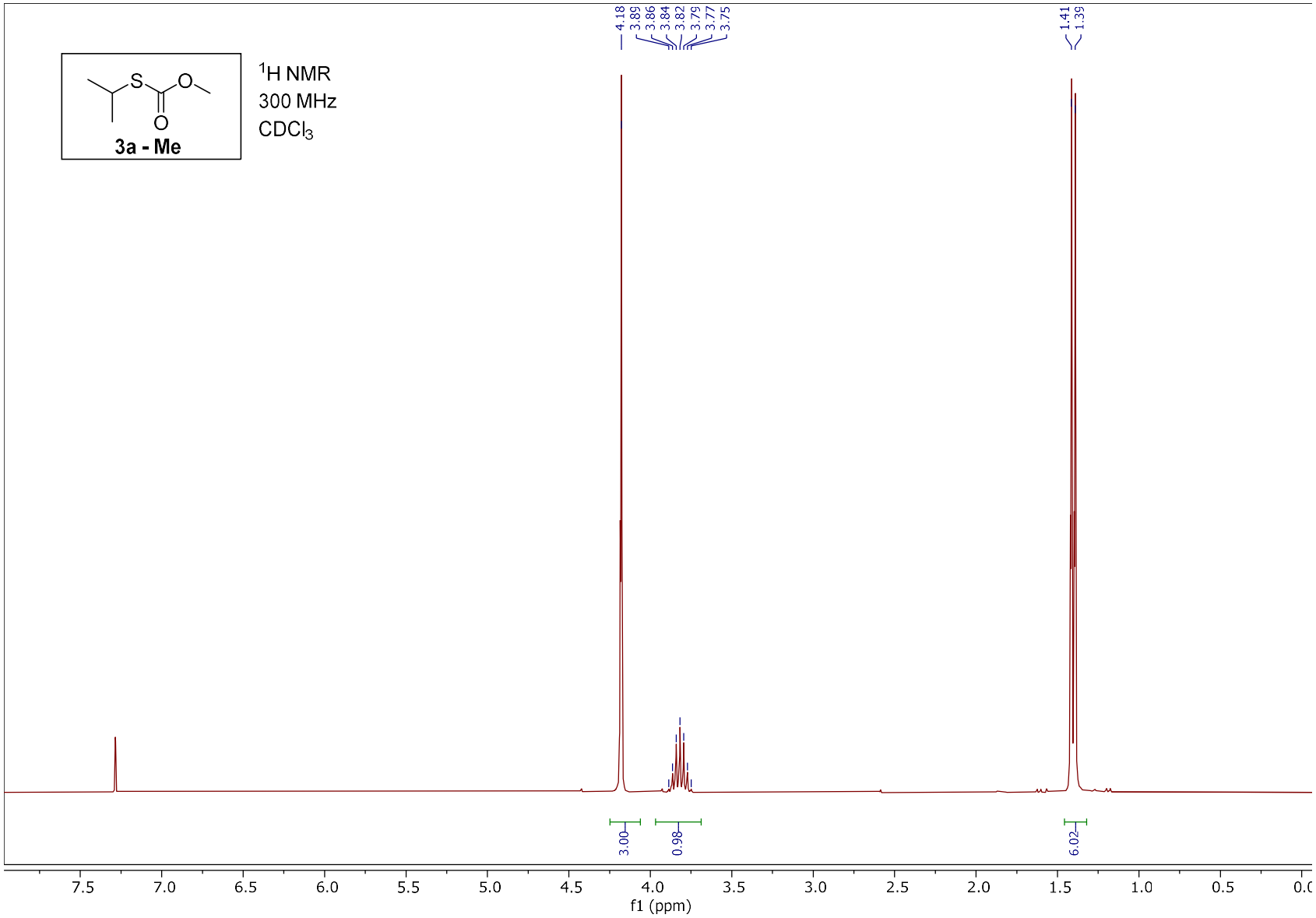

185.30
153.19
147.39
129.66
129.52
126.62
122.11
86.73
86.12
27.86
27.57
2e
13C{1H} NMR
75 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

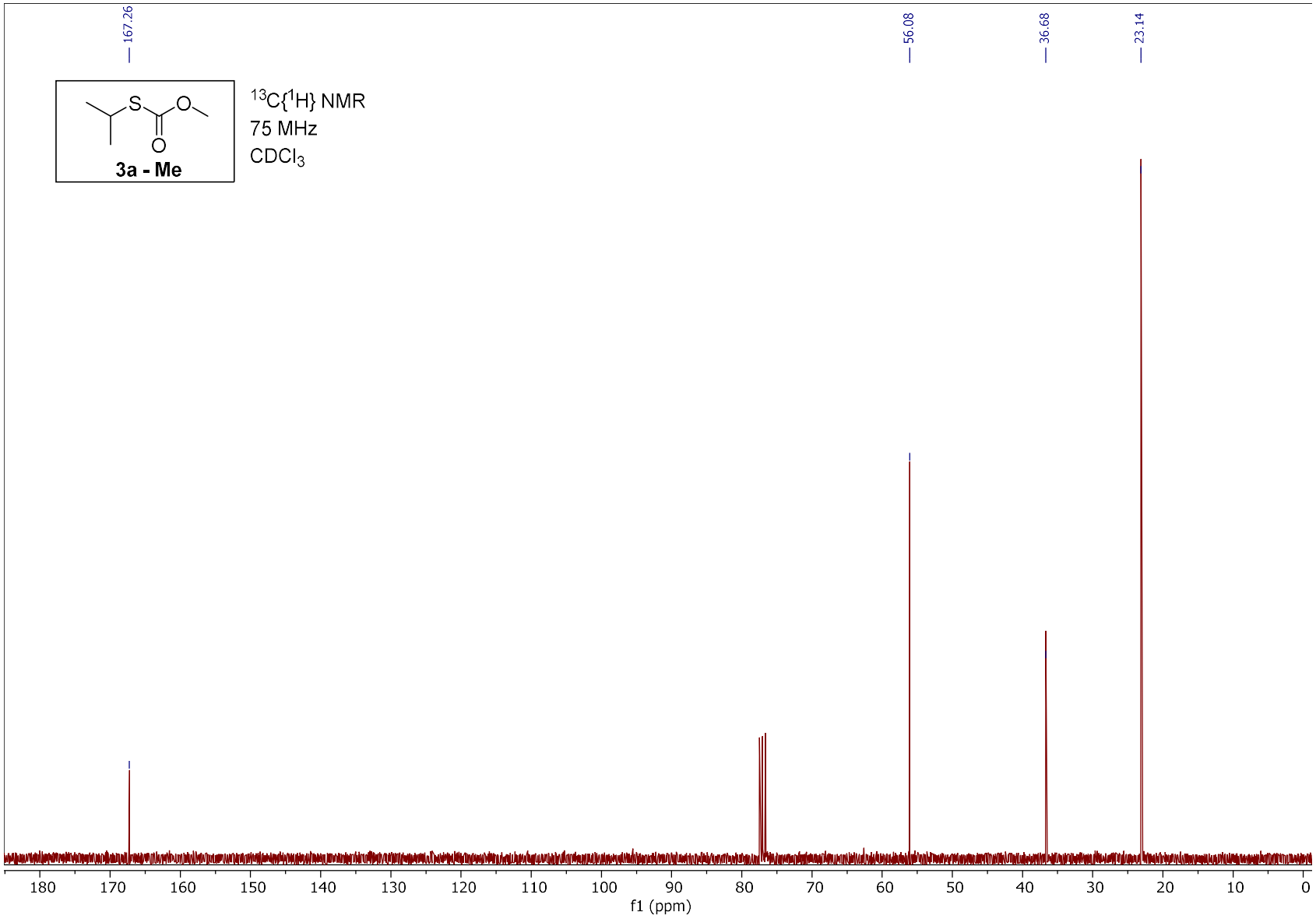

7.96
7.95
7.94
7.94
7.93
7.85
7.84
7.84
7.83
7.82
4.27
2f
^{1}H NMR
300 MHz
$CDCl_3$
2.01
2.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

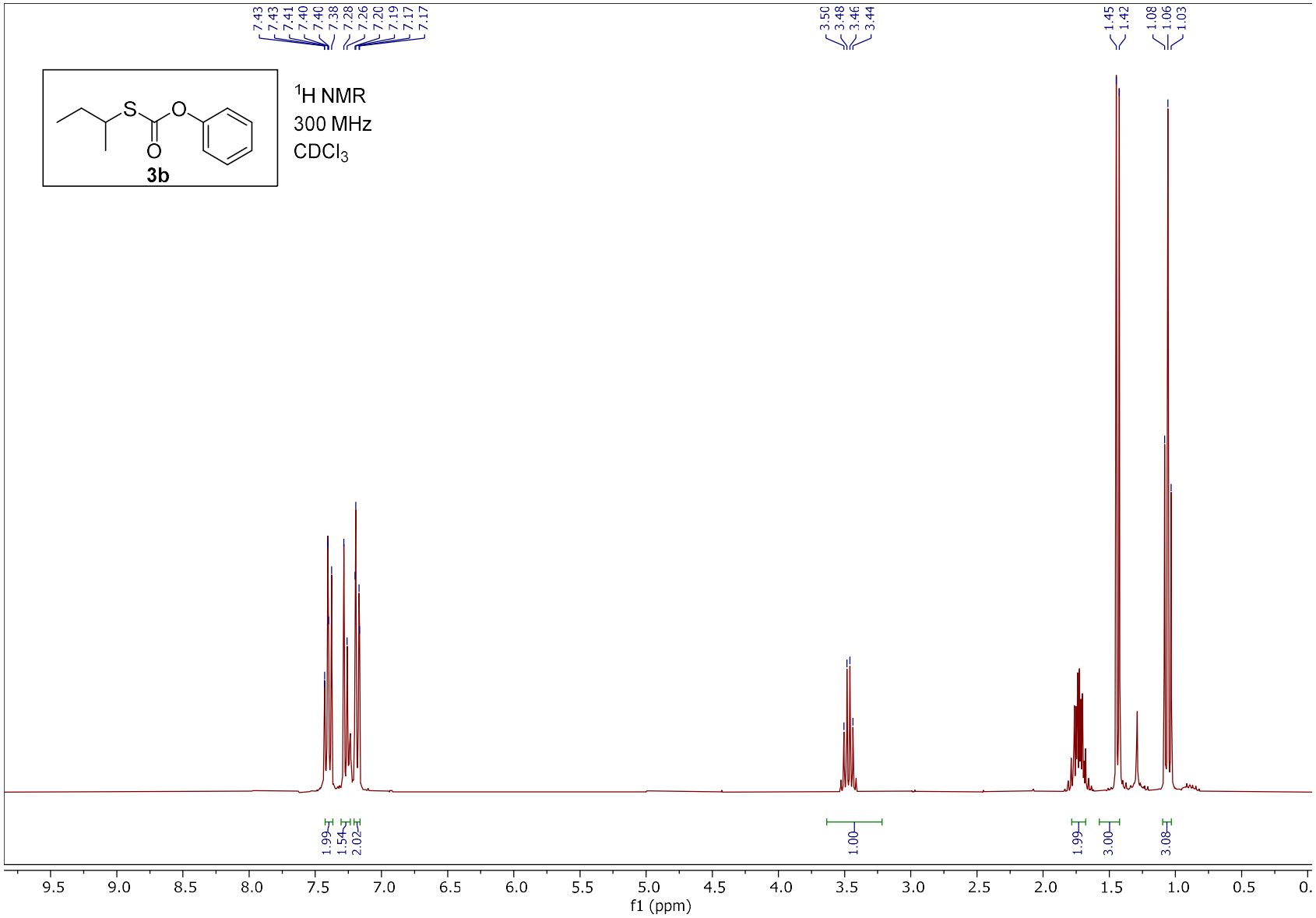

193.36
161.03
134.92
134.91
128.65
124.16
62.61
2f
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
f1 (ppm)

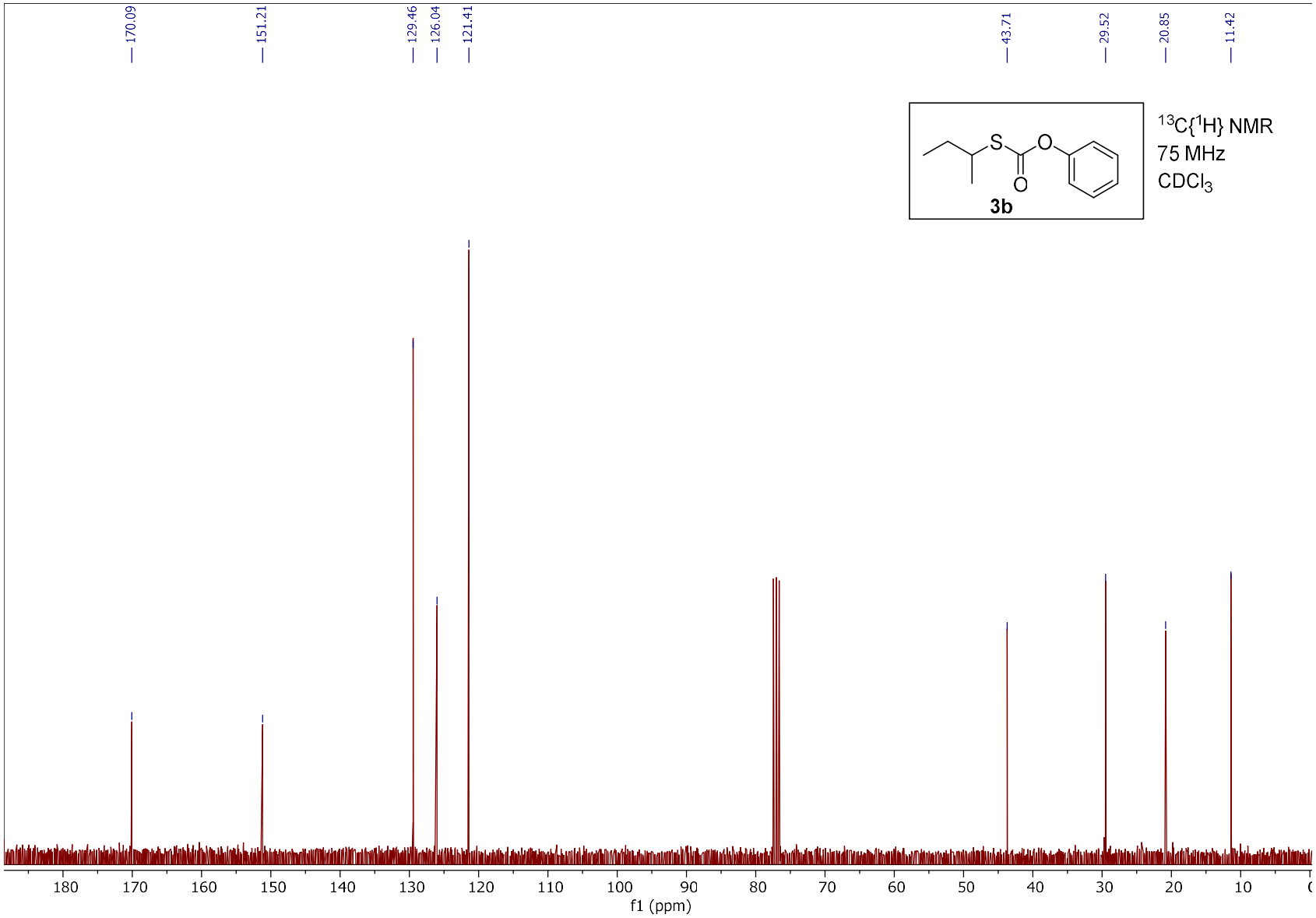

7.41
7.41
7.39
7.27
7.21
7.21
7.19
7.18
7.18
3.71
3.69
3.67
3.64
3.62
3.60
3.57
1.46
1.44
S
O
O
3a
1H NMR
300 MHz
CDCl3
2.04
1.28
2.00
1.00
6.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

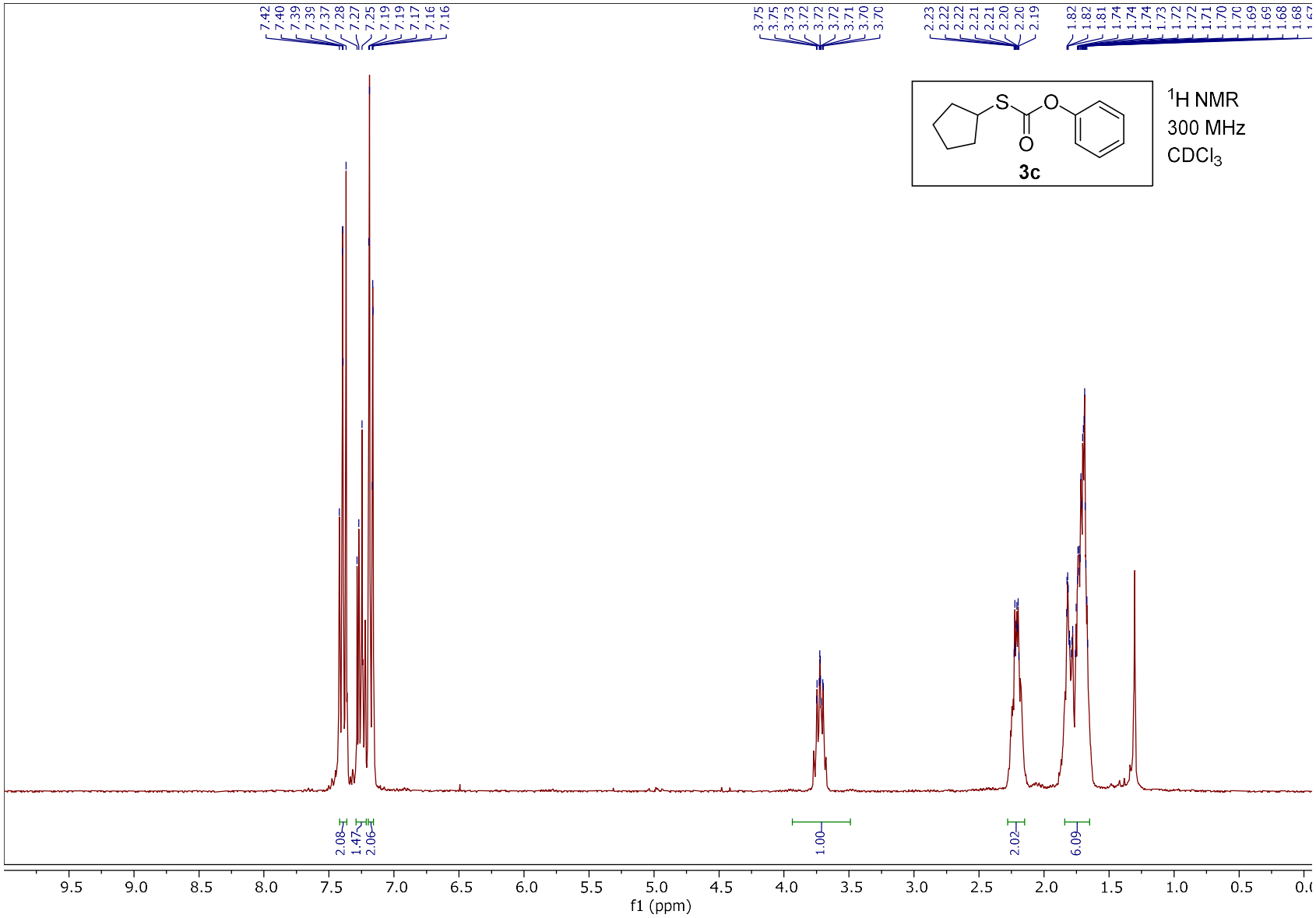

169.84
151.17
129.48
126.07
121.86
37.20
23.05
S
O
O
3a
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

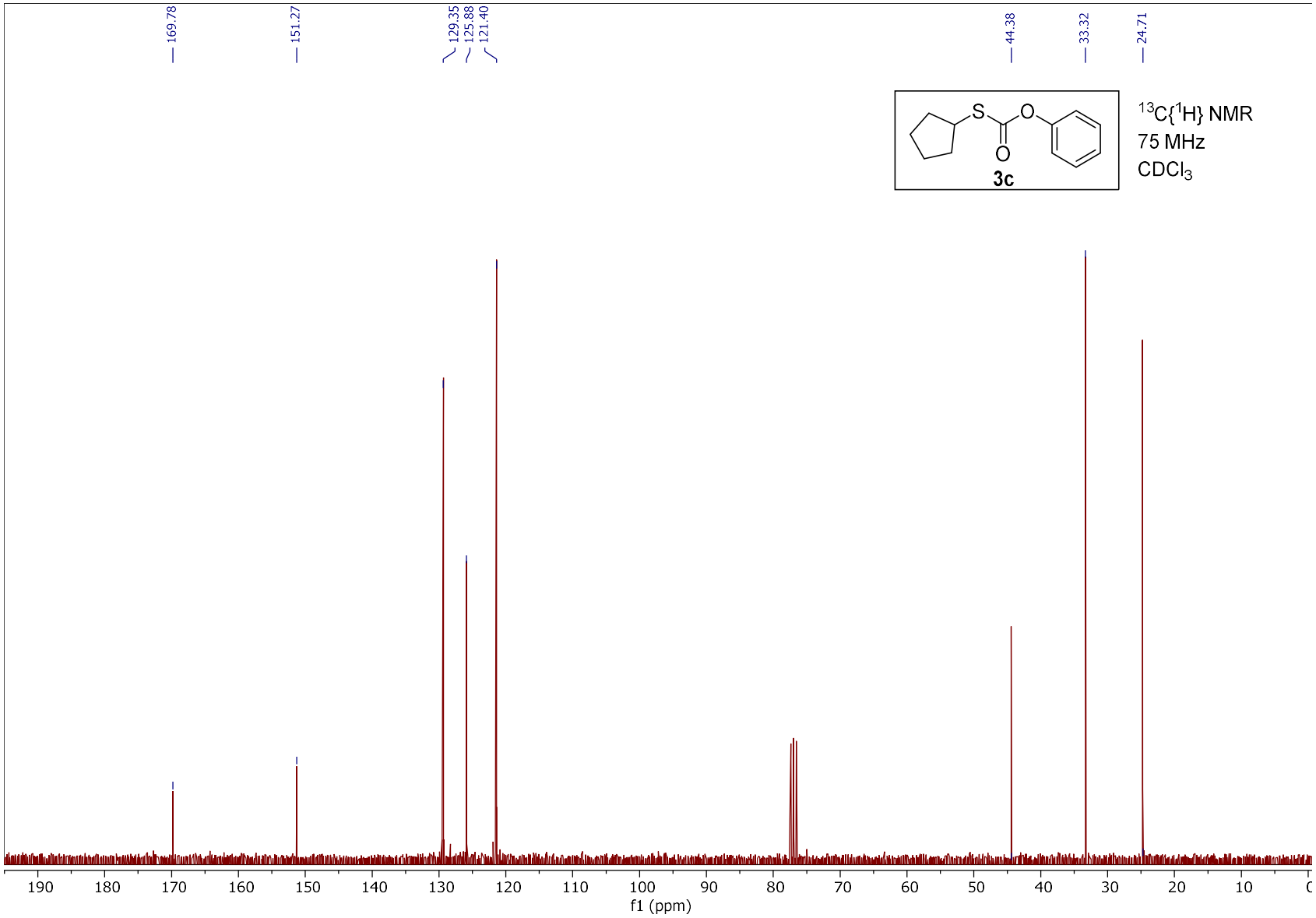

3a - Me
1H NMR
300 MHz
CDCl3
4.18
3.89
3.86
3.84
3.82
3.79
3.77
3.75
1.41
1.39
3.00
0.98
6.02
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

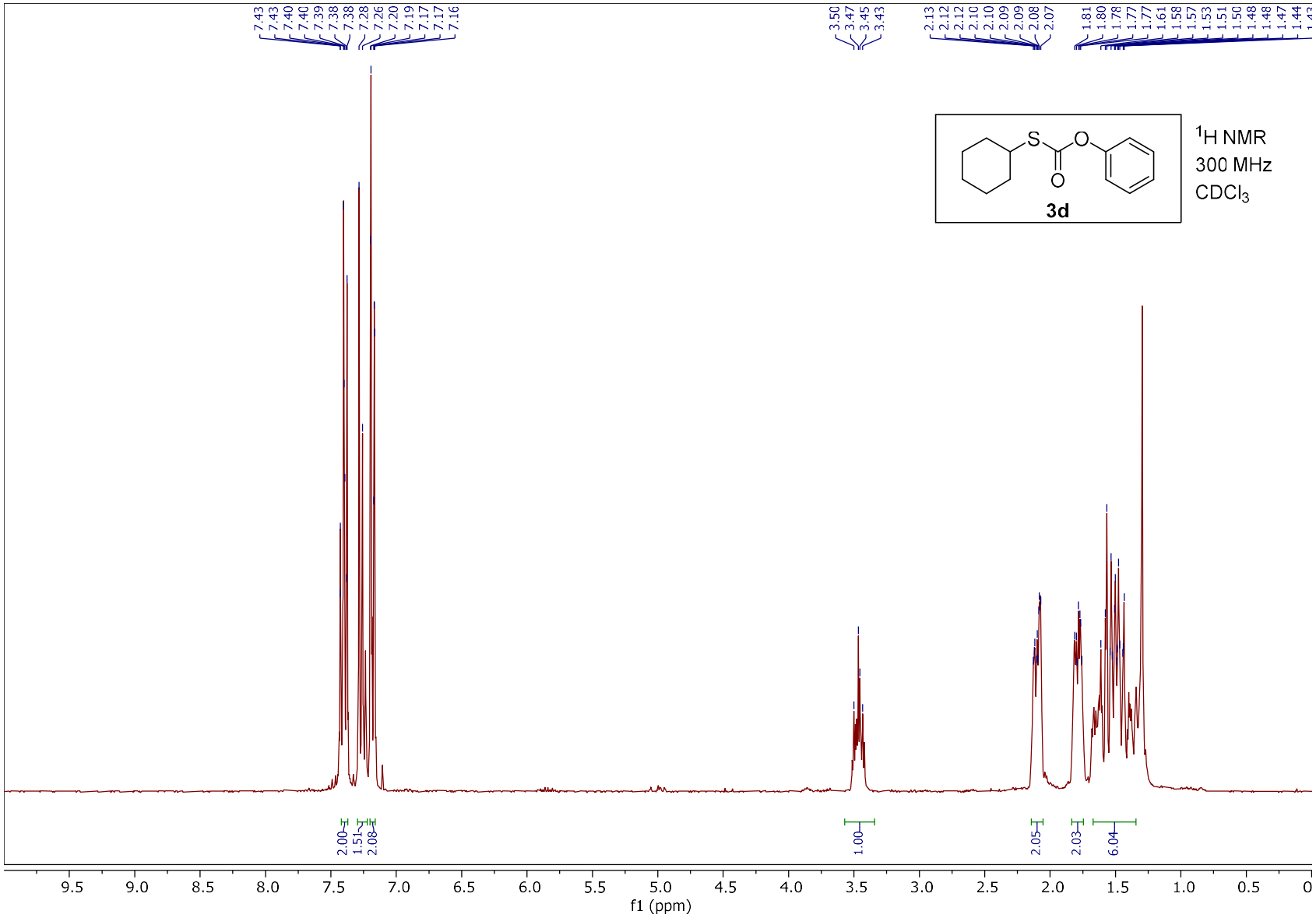

167.26
56.08
36.68
23.14
S
O
O
3a - Me
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

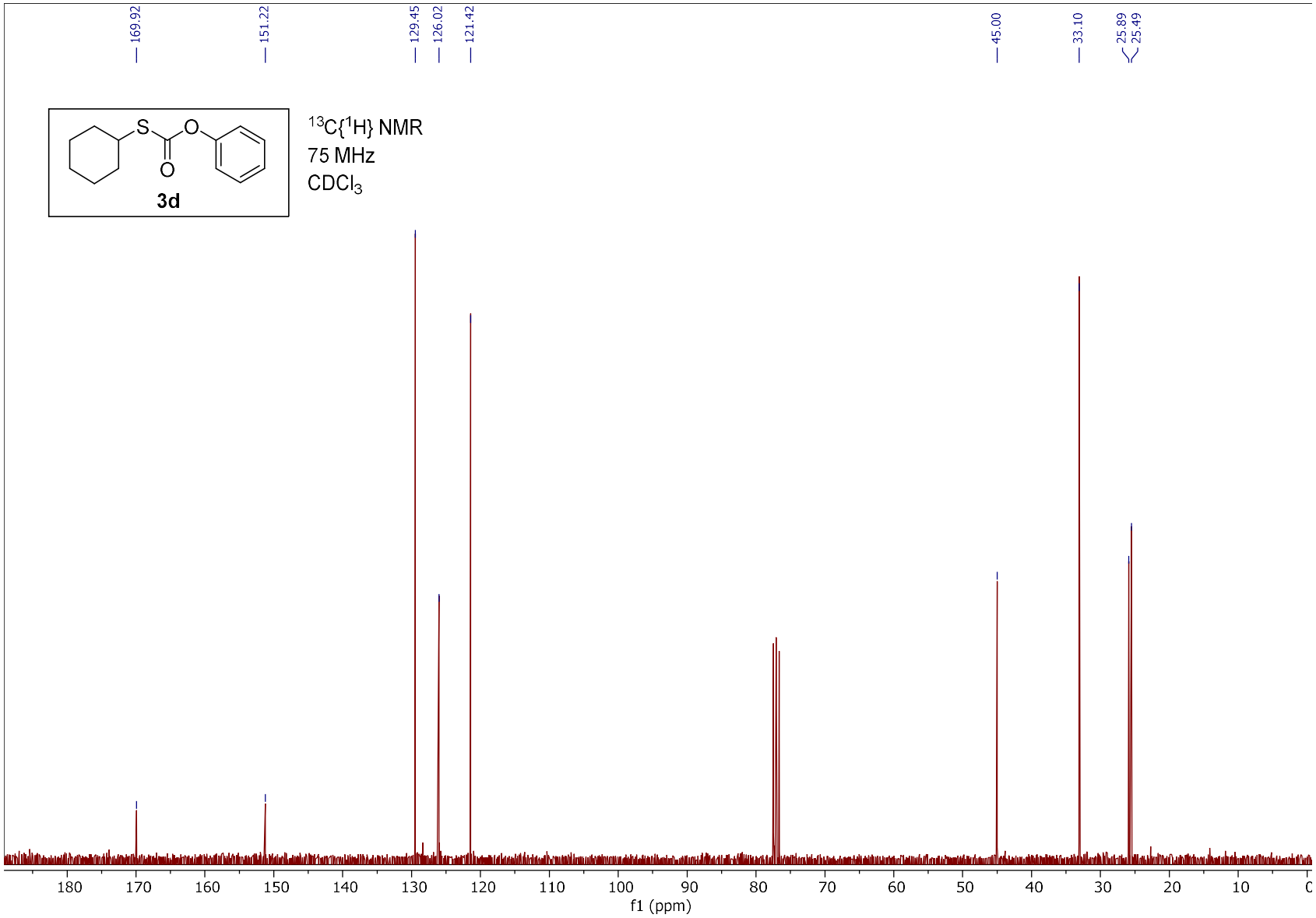

7.43
7.43
7.41
7.40
7.40
7.38
7.28
7.26
7.20
7.19
7.17
7.17
3.50
3.48
3.46
3.44
1.45
1.42
1.08
1.06
1.03
S
O
O
3b
1H NMR
300 MHz
CDCl3
1.99
1.54
2.02
1.00
1.99
3.00
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

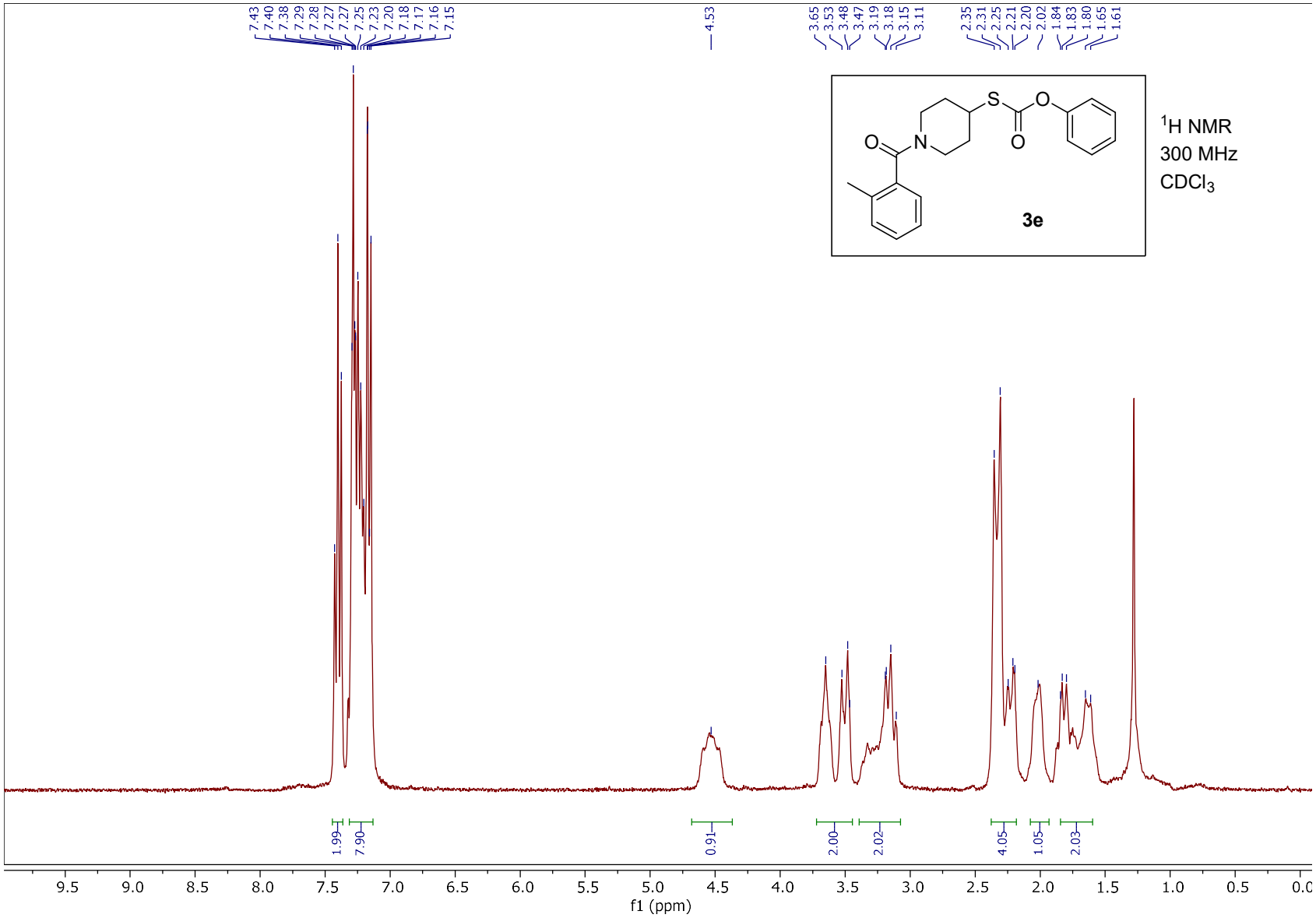

170.09
151.21
129.46
126.04
121.41
43.71
29.52
20.85
11.42
S
O
O
3b
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

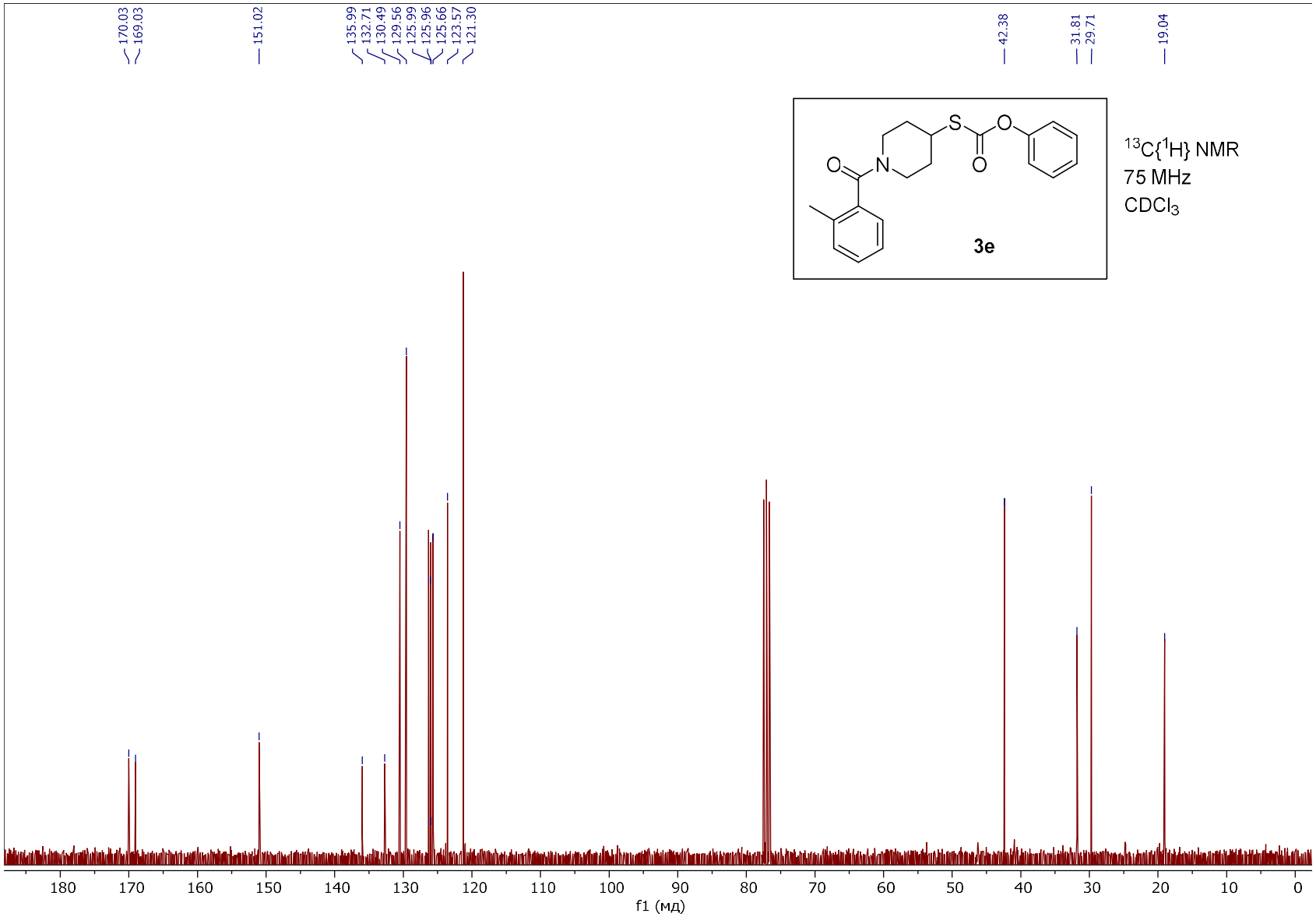

7.42
7.40
7.39
7.39
7.37
7.28
7.27
7.25
7.19
7.17
7.16
7.16
3.75
3.75
3.73
3.72
3.72
3.72
3.71
3.70
3.70
2.23
2.22
2.22
2.21
2.21
2.20
2.20
2.19
1.82
1.82
1.81
1.74
1.74
1.73
1.72
1.72
1.71
1.70
1.70
1.69
1.69
1.68
1.68
S
O
O
3c
1H NMR
300 MHz
CDCl3
2.08
1.47
2.06
1.00
2.02
6.09
9.5
9.0
8.5
8.0
7.5
7.0
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
f1 (ppm)

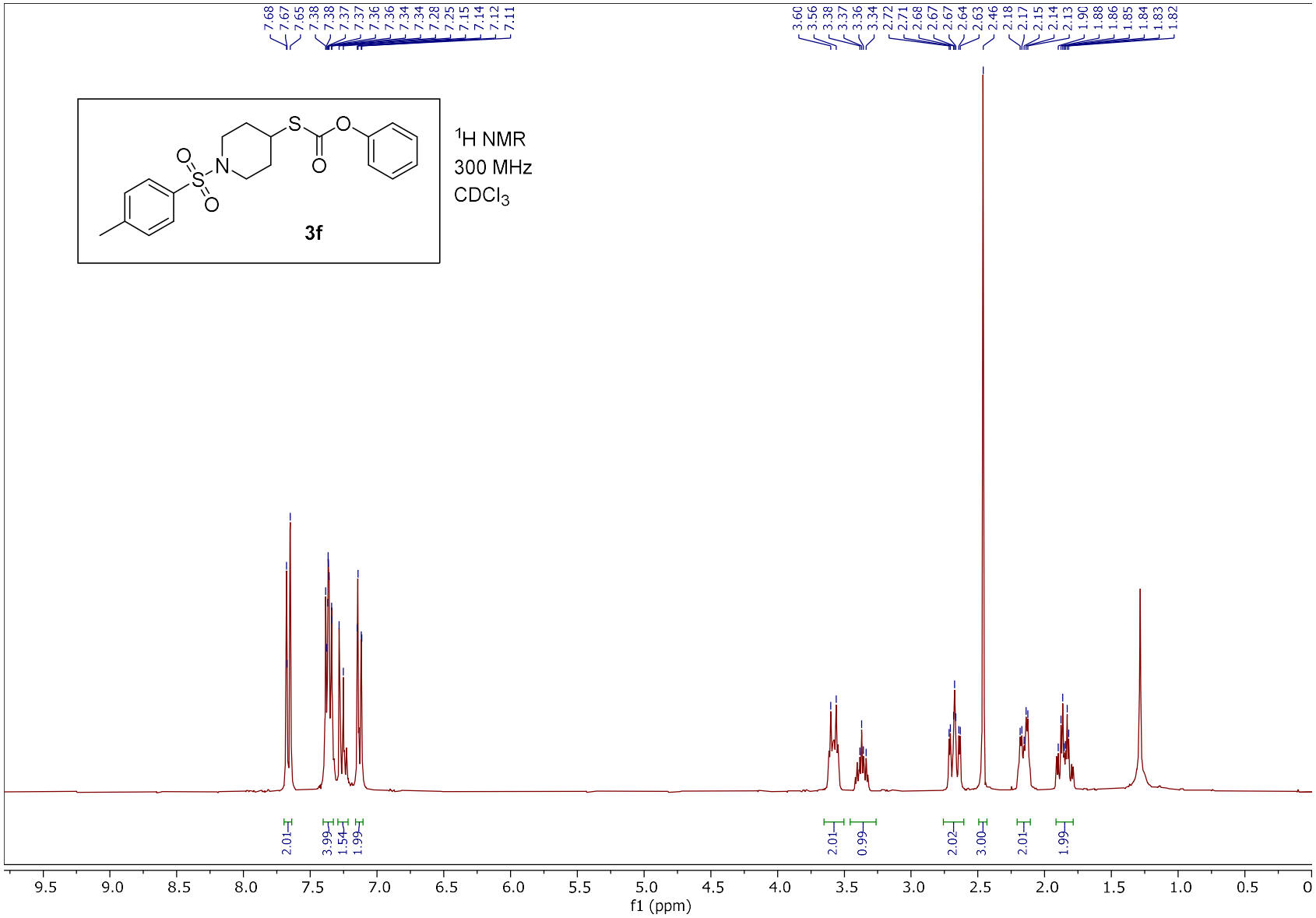

169.78
151.27
129.35
125.88
121.40
44.38
33.32
24.71
S
O
O
3c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

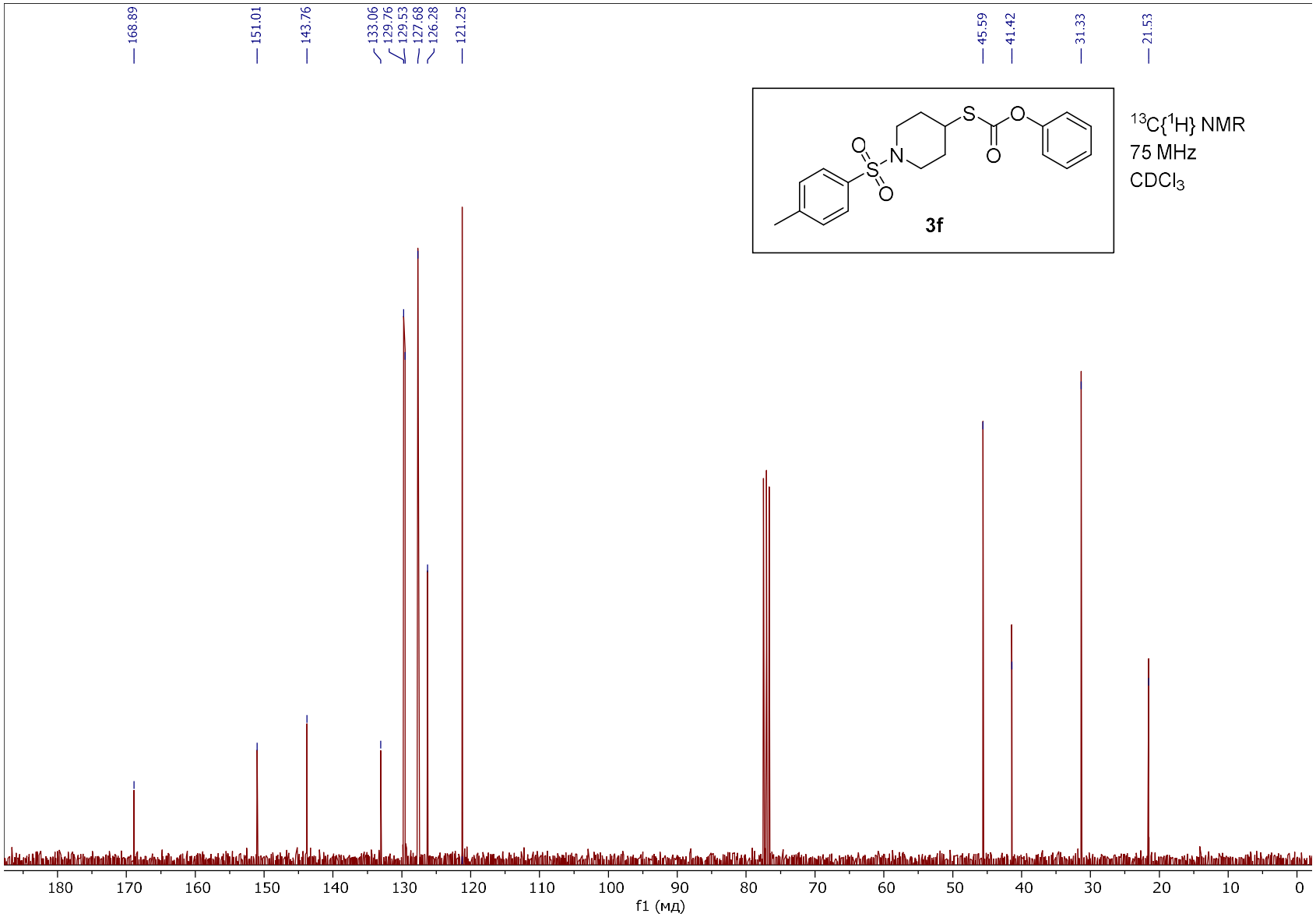

7.43
7.43
7.40
7.40
7.39
7.38
7.38
7.28
7.26
7.20
7.19
7.17
7.17
7.16
3.50
3.47
3.45
3.43
2.13
2.12
2.12
2.10
2.09
2.09
2.08
2.07
1.81
1.80
1.78
1.77
1.77
1.61
1.58
1.57
1.53
1.51
1.50
1.48
1.48
1.47
1.44
S
O
O
3d
1H NMR
300 MHz
CDCl3
2.00
1.51
2.08
1.00
2.05
2.03
6.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

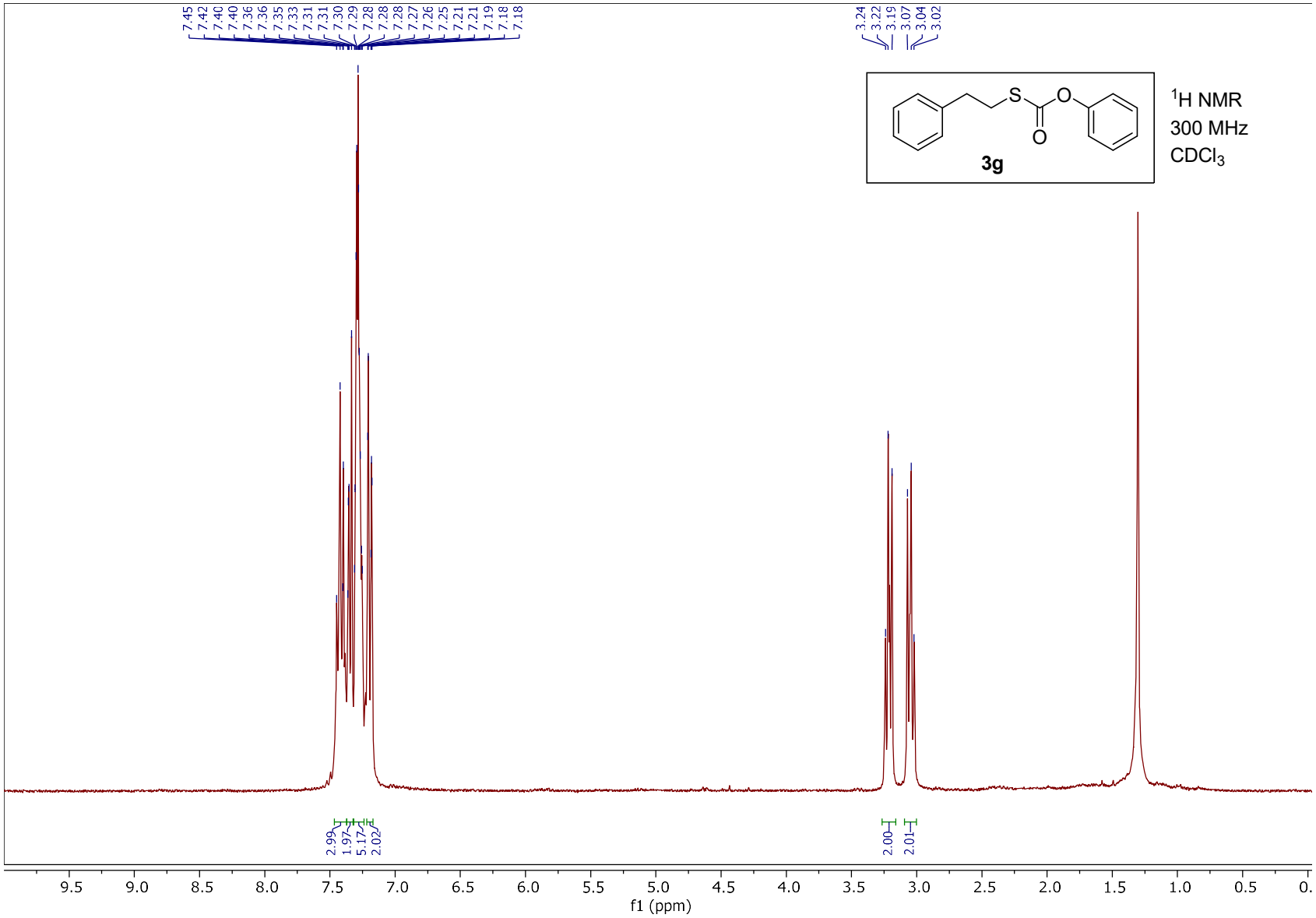

169.92
151.22
129.45
126.02
121.42
45.00
33.10
25.89
25.49
S
O
O
3d
13C{1H} NMR
75 MHz
CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

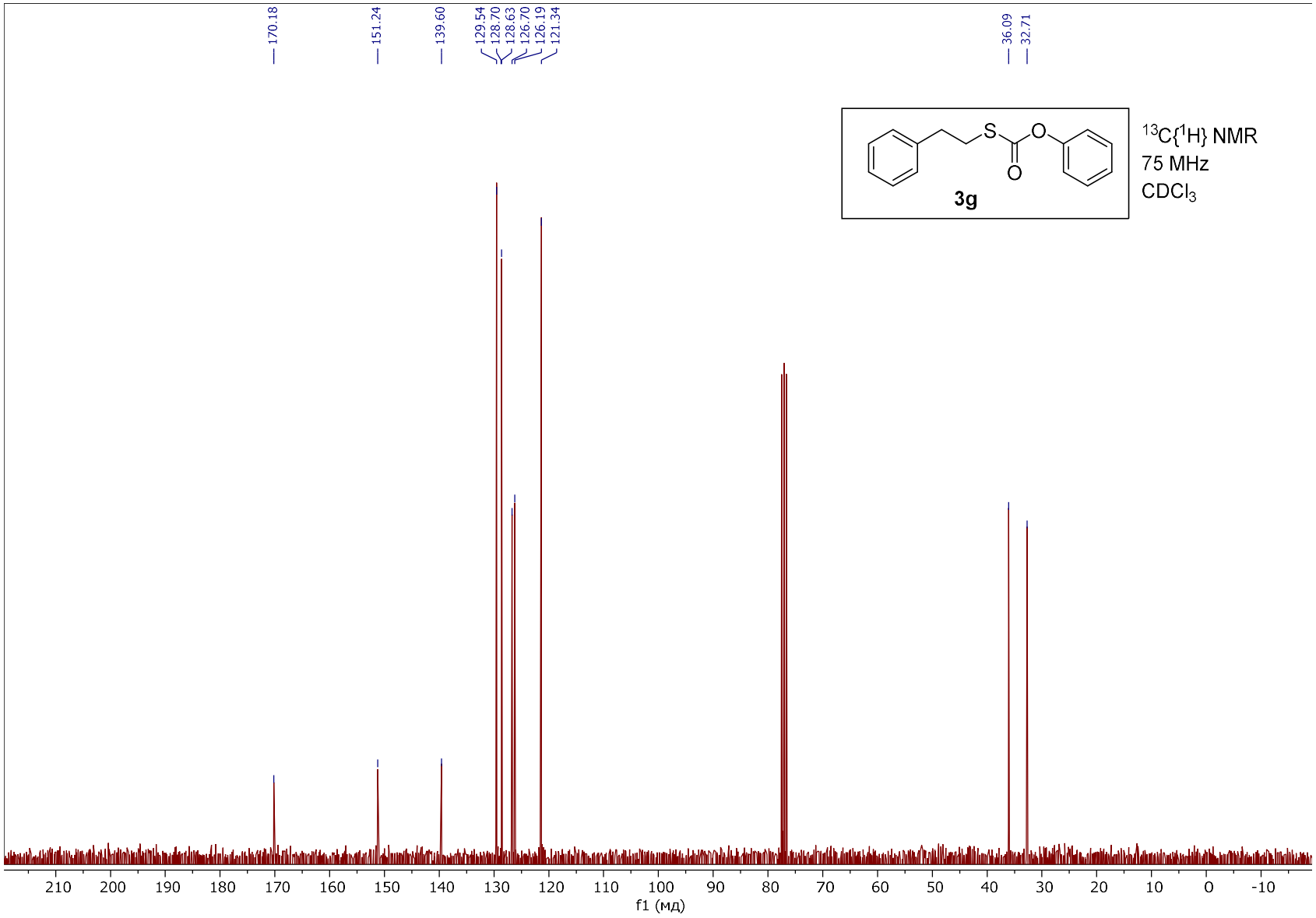

7.43
7.40
7.38
7.29
7.28
7.27
7.27
7.25
7.23
7.20
7.18
7.17
7.16
7.15
4.53
3.65
3.53
3.48
3.47
3.19
3.18
3.15
3.11
2.35
2.31
2.25
2.21
2.20
2.02
1.84
1.83
1.80
1.65
1.61
S
O
O
O
N
3e
1H NMR
300 MHz
CDCl3
1.99
7.90
0.91
2.00
2.02
4.05
1.05
2.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

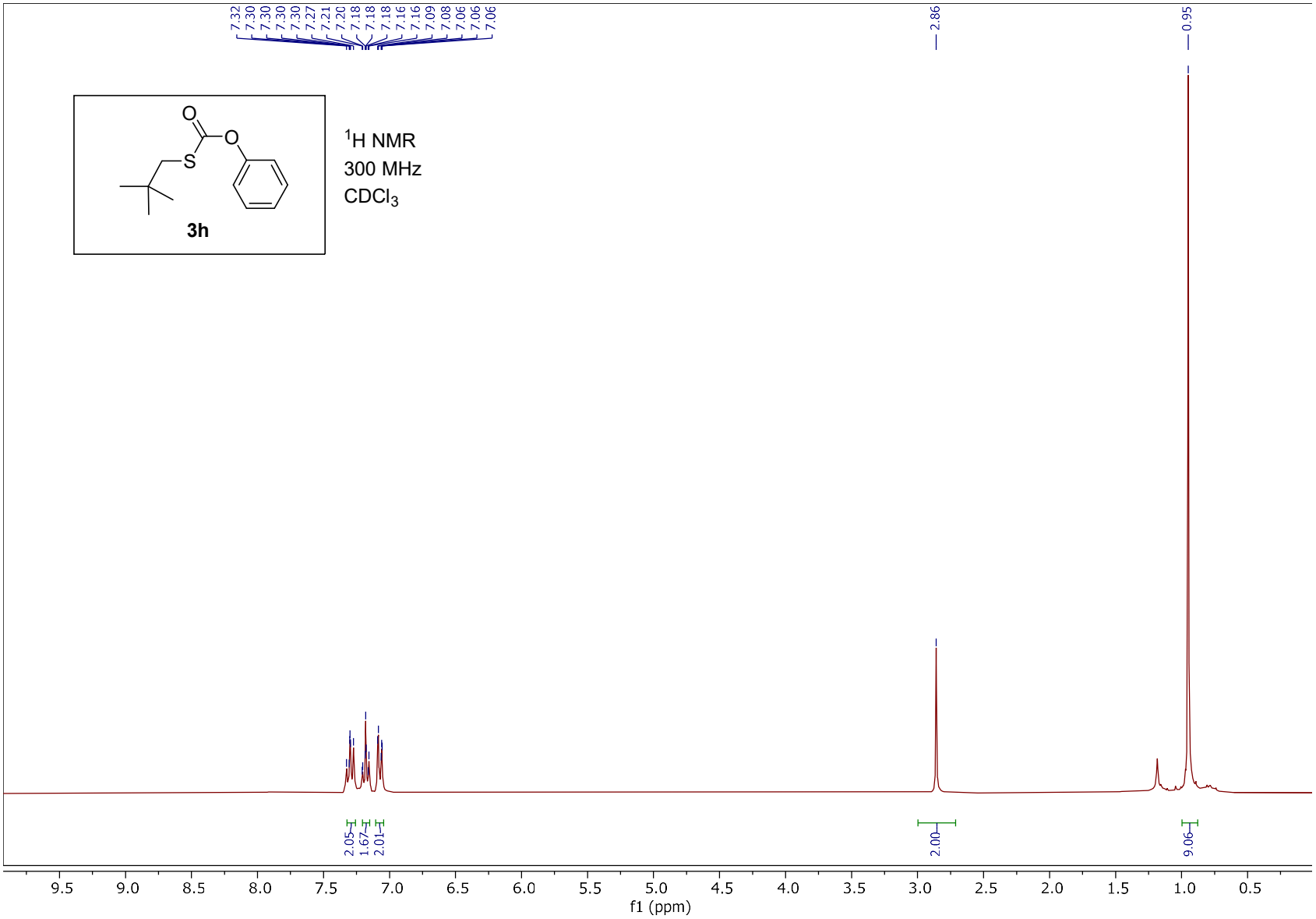

170.03
169.03
151.02
135.99
132.71
130.49
129.56
125.99
125.96
125.66
123.57
121.30
42.38
31.81
29.71
19.04
3e
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (мд)

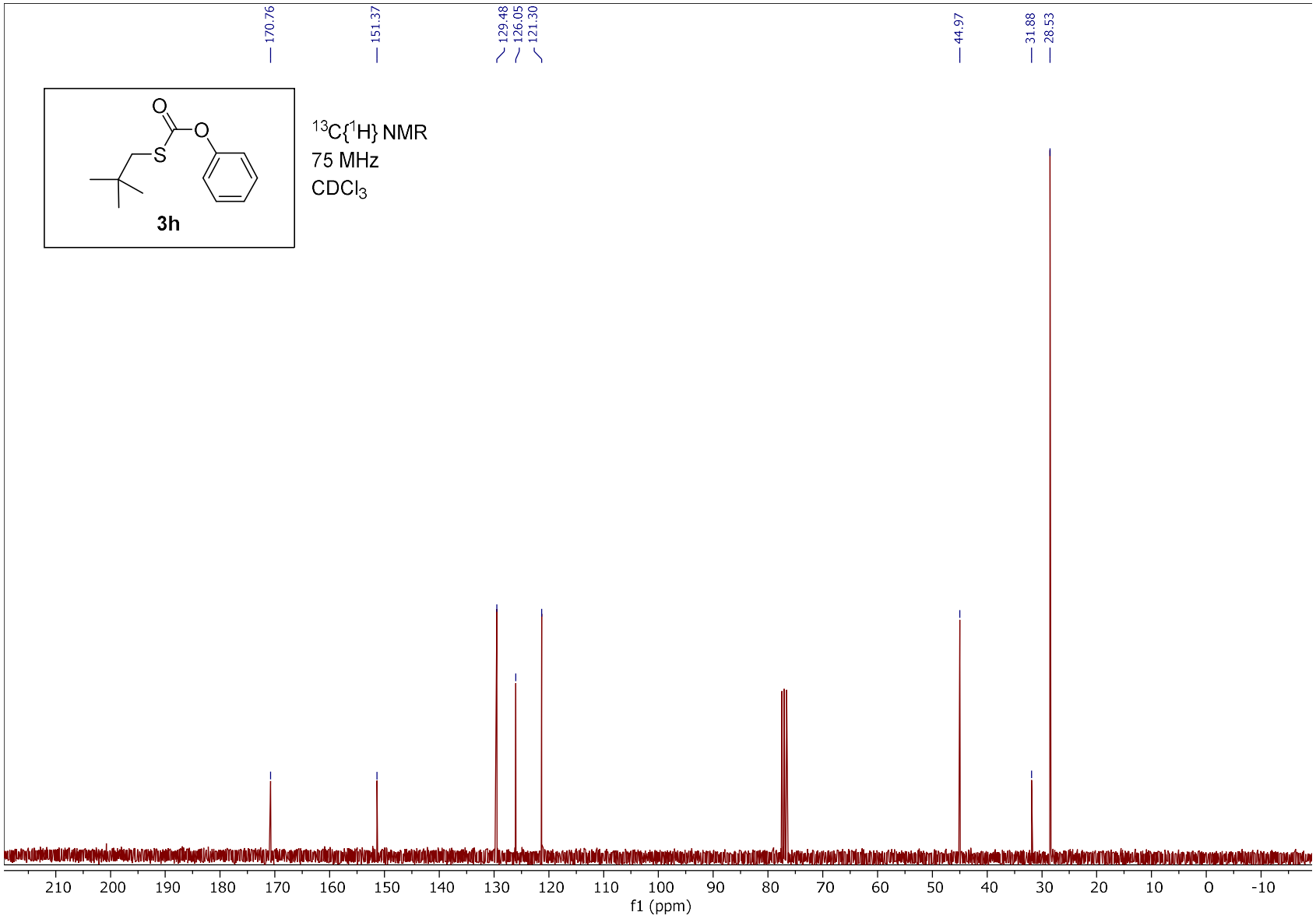

7.68
7.67
7.65
7.38
7.38
7.37
7.37
7.36
7.36
7.34
7.34
7.28
7.25
7.15
7.14
7.12
7.11
3.60
3.56
3.38
3.37
3.36
3.34
2.72
2.71
2.68
2.67
2.67
2.64
2.63
2.46
2.18
2.17
2.15
2.14
2.13
1.90
1.88
1.86
1.85
1.84
1.83
1.82
1H NMR
300 MHz
CDCl3
3f
2.01
3.99
1.54
1.99
2.01
0.99
2.02
3.00
2.01
1.99
9.5
9.0
8.5
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
f1 (ppm)

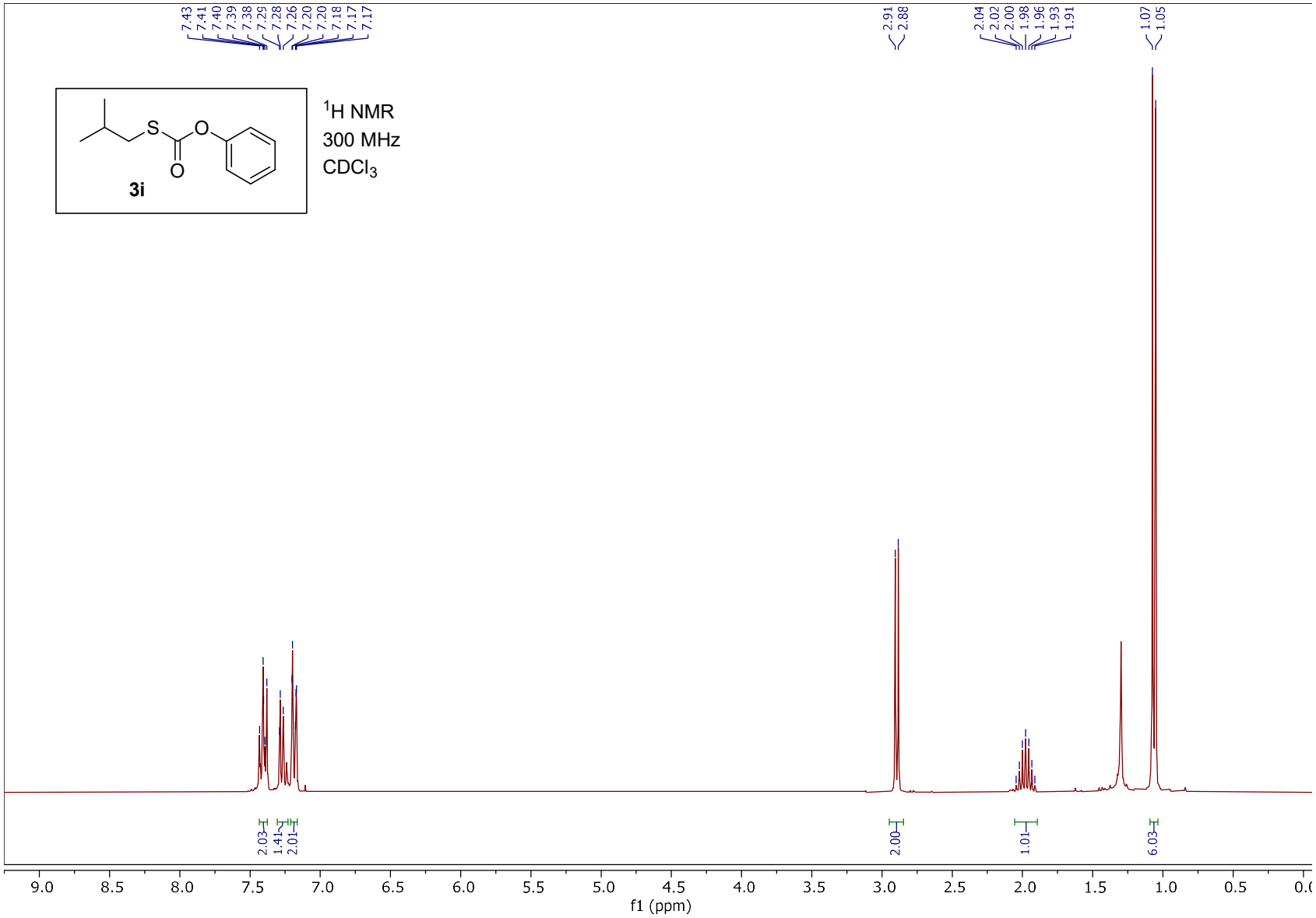

168.89
151.01
143.76
133.06
129.76
129.53
127.68
126.28
121.25
45.59
41.42
31.33
21.53
3f
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (мд)

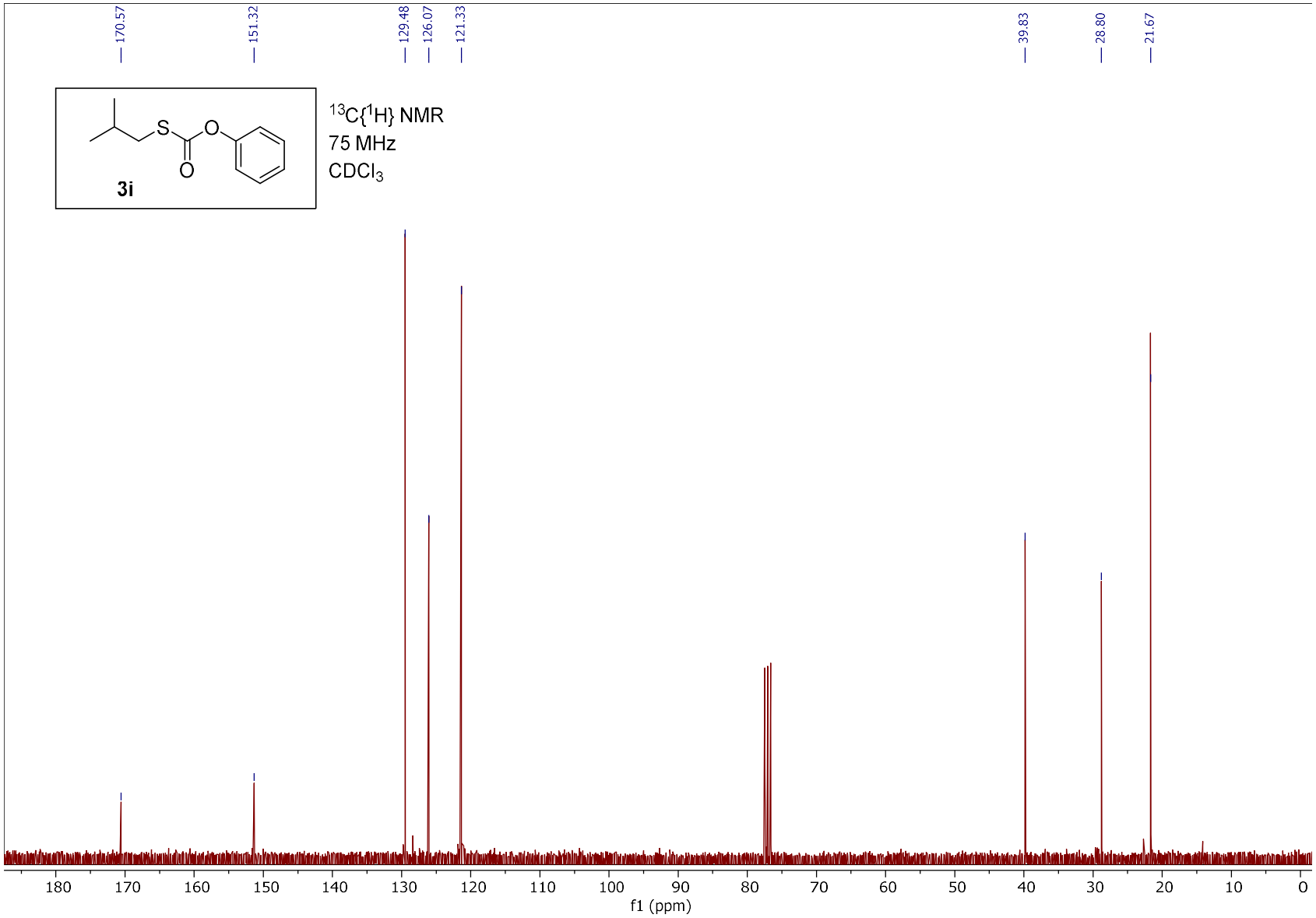

7.45
7.42
7.40
7.40
7.36
7.36
7.35
7.33
7.31
7.31
7.30
7.29
7.28
7.28
7.28
7.27
7.26
7.25
7.21
7.21
7.19
7.18
7.18
3.24
3.22
3.19
3.07
3.04
3.02
S
O
O
3g
1H NMR
300 MHz
CDCl3
2.99
1.97
5.17
2.02
2.00
2.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

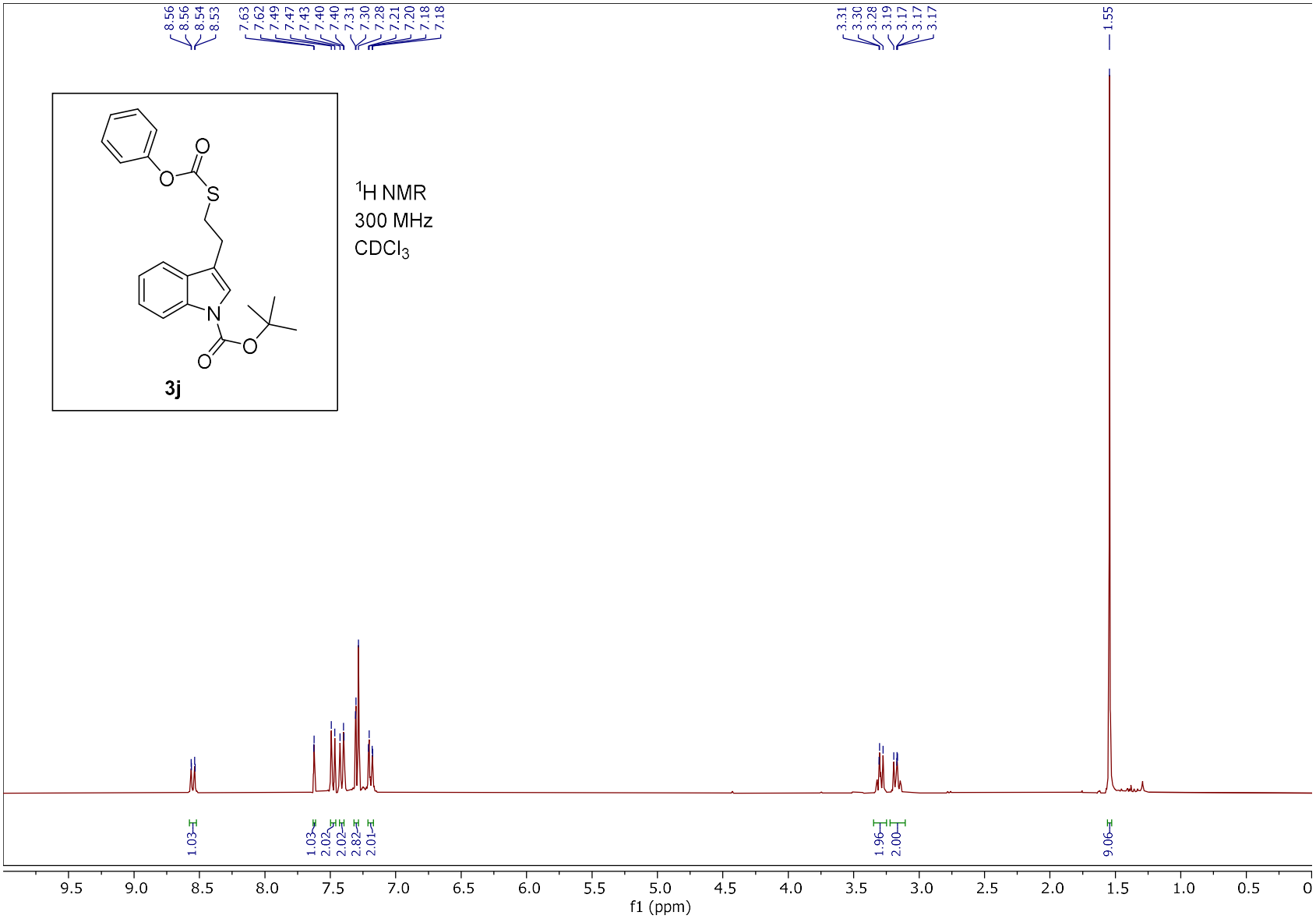

170.18
151.24
139.60
129.54
128.70
128.63
126.70
126.19
121.34
36.09
32.71
S
O
O
3g
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)

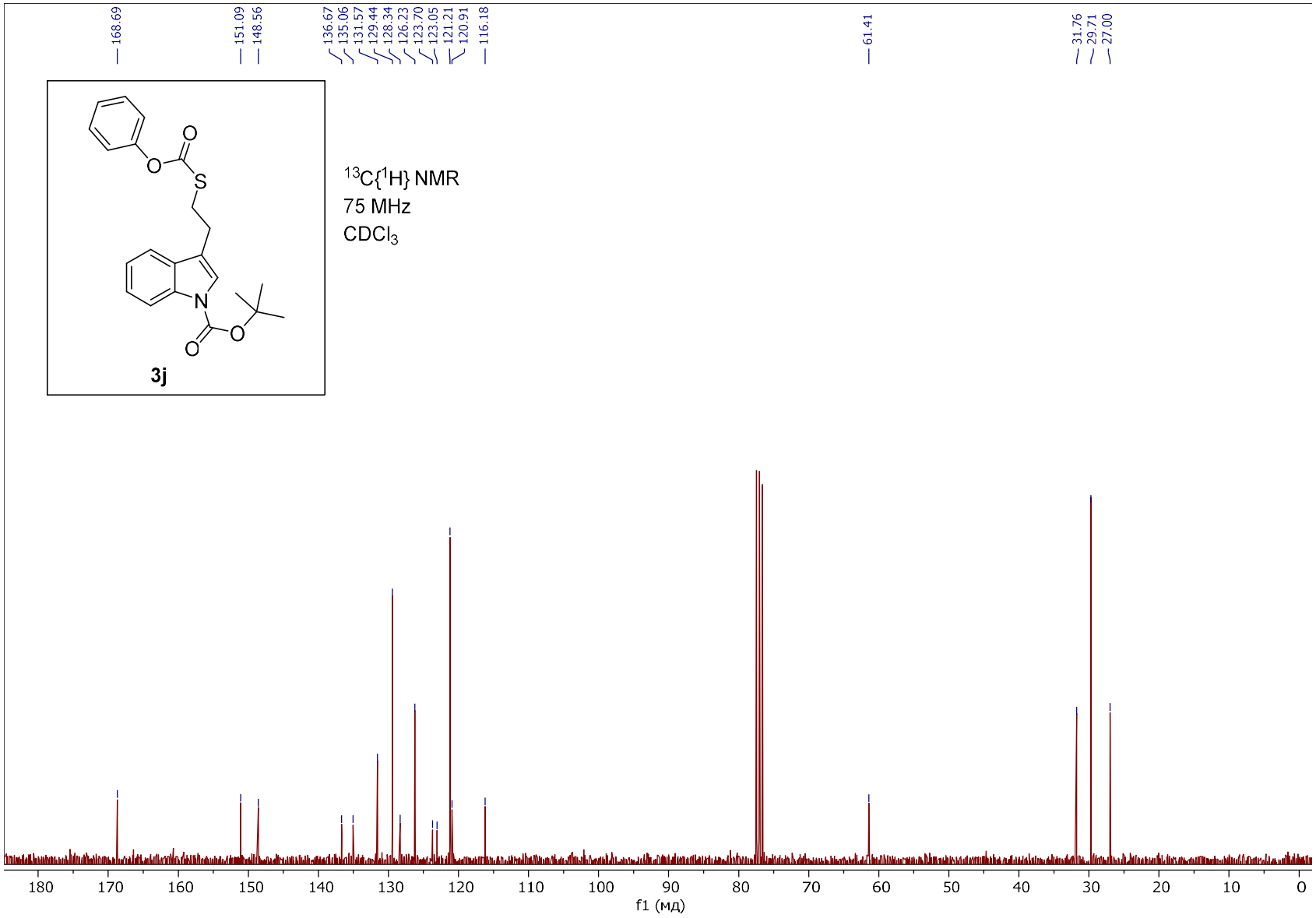

7.32
7.30
7.30
7.30
7.30
7.27
7.21
7.20
7.18
7.18
7.16
7.16
7.09
7.08
7.06
7.06
7.06
2.86
0.95
O
O
S
3h
1H NMR
300 MHz
CDCl3
2.05
1.67
2.01
2.00
9.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

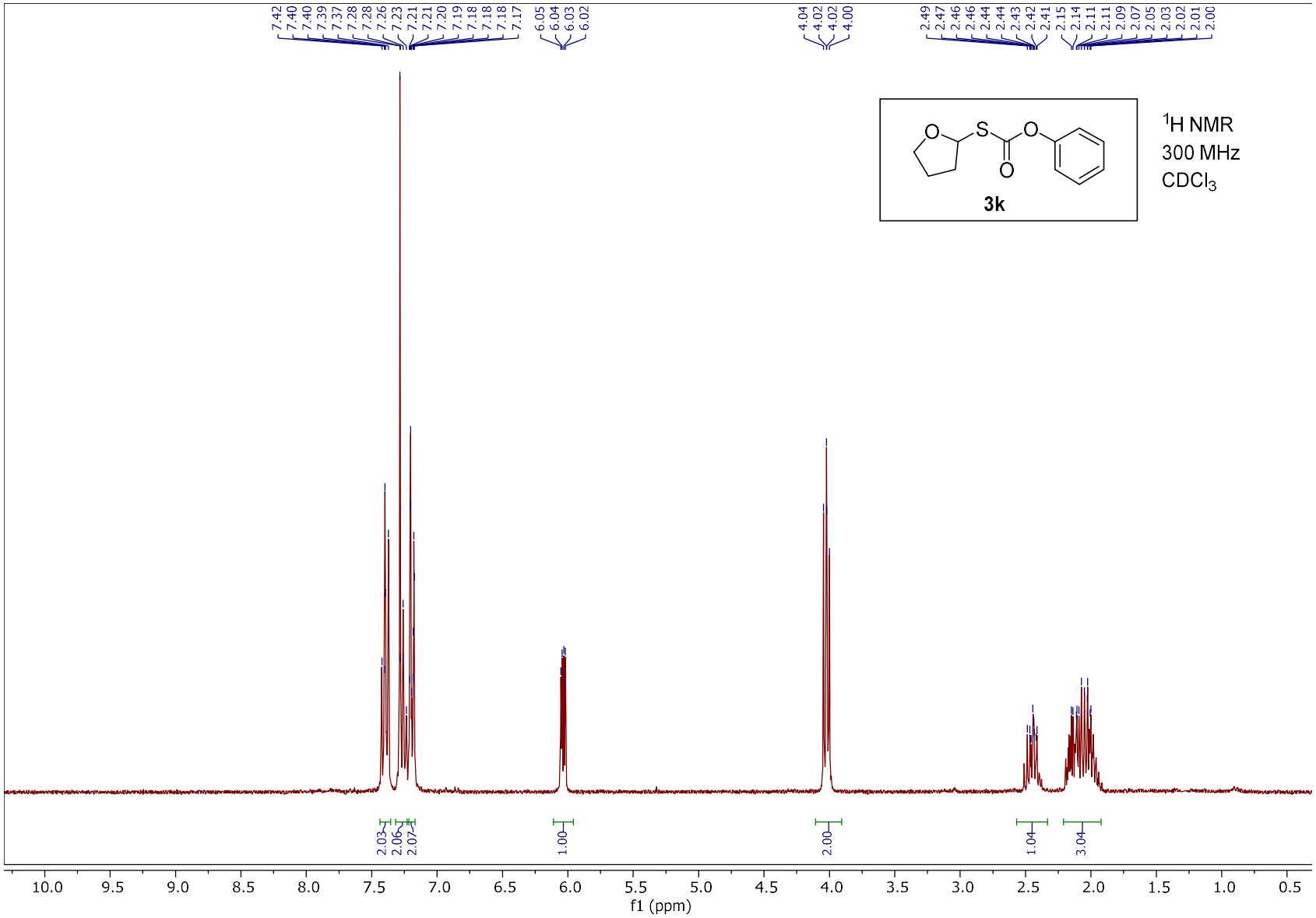

170.76
151.37
129.48
126.05
121.30
44.97
31.88
28.53
O
O
S
3h
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

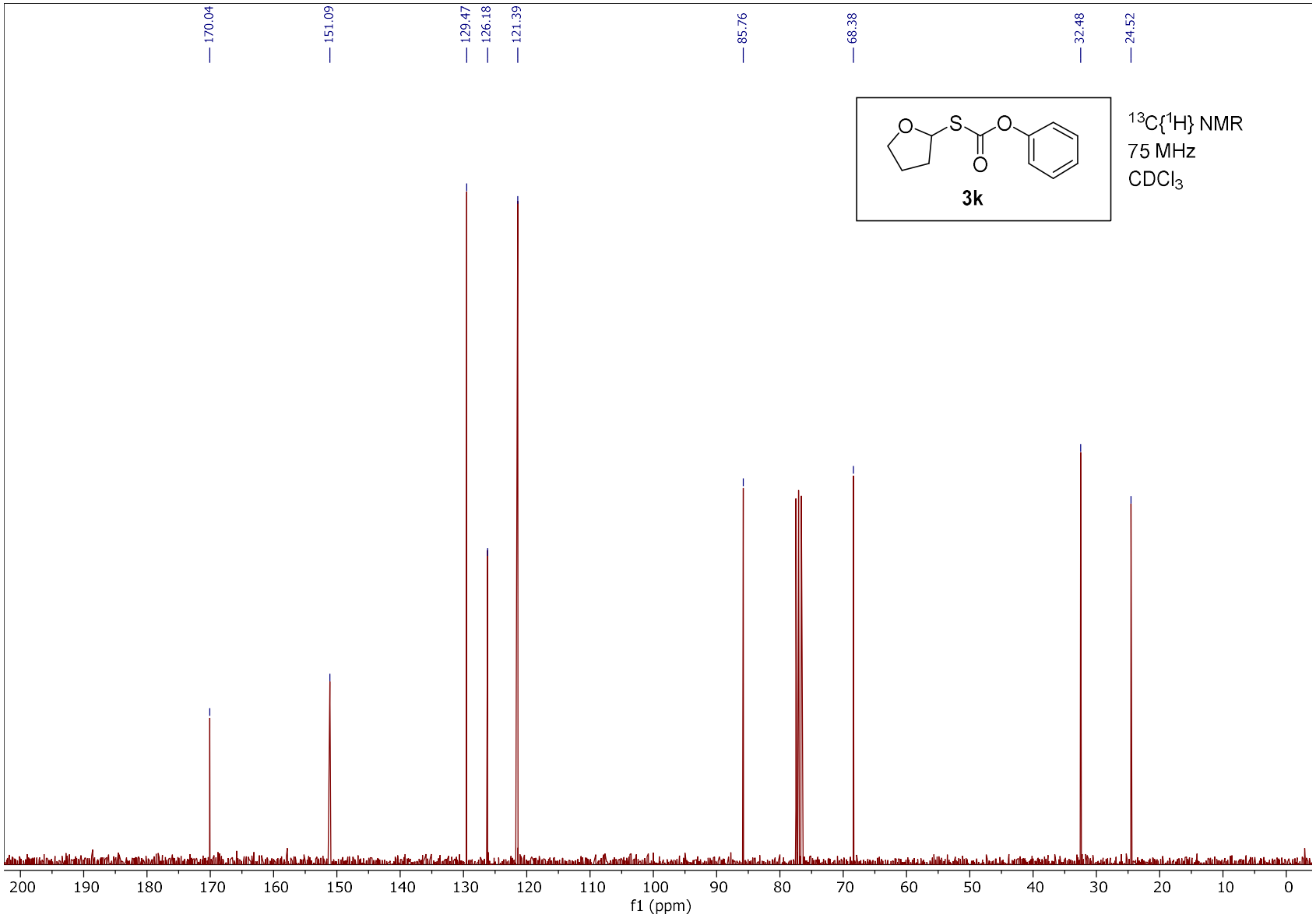

7.43
7.41
7.40
7.39
7.38
7.29
7.28
7.26
7.20
7.20
7.18
7.17
7.17
2.91
2.88
2.04
2.02
2.00
1.98
1.96
1.93
1.91
1.07
1.05
S
O
O
3i
1H NMR
300 MHz
CDCl3
2.03
1.41
2.01
2.00
1.01
6.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

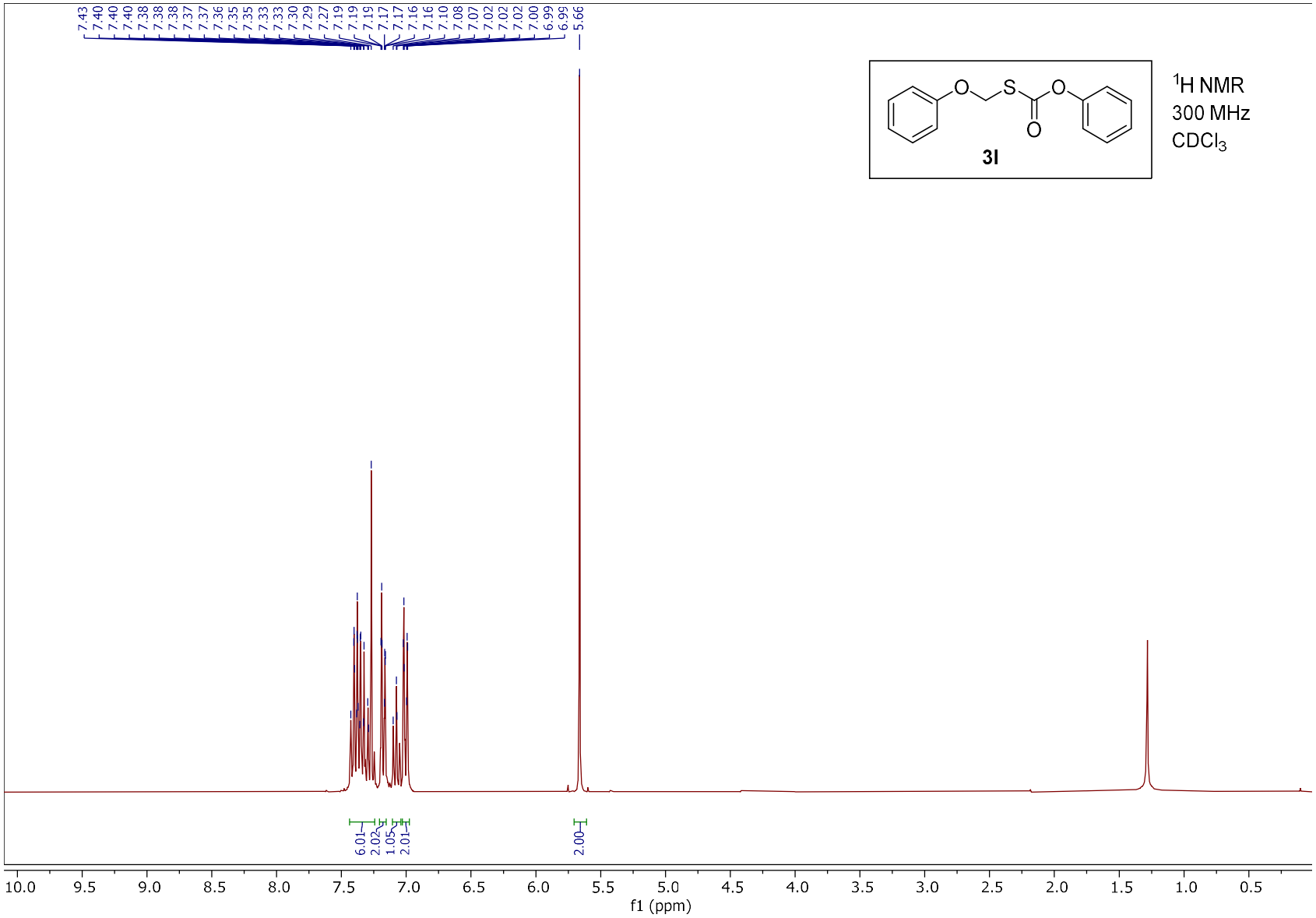

170.57
151.32
129.48
126.07
121.33
39.83
28.80
21.67
3i
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

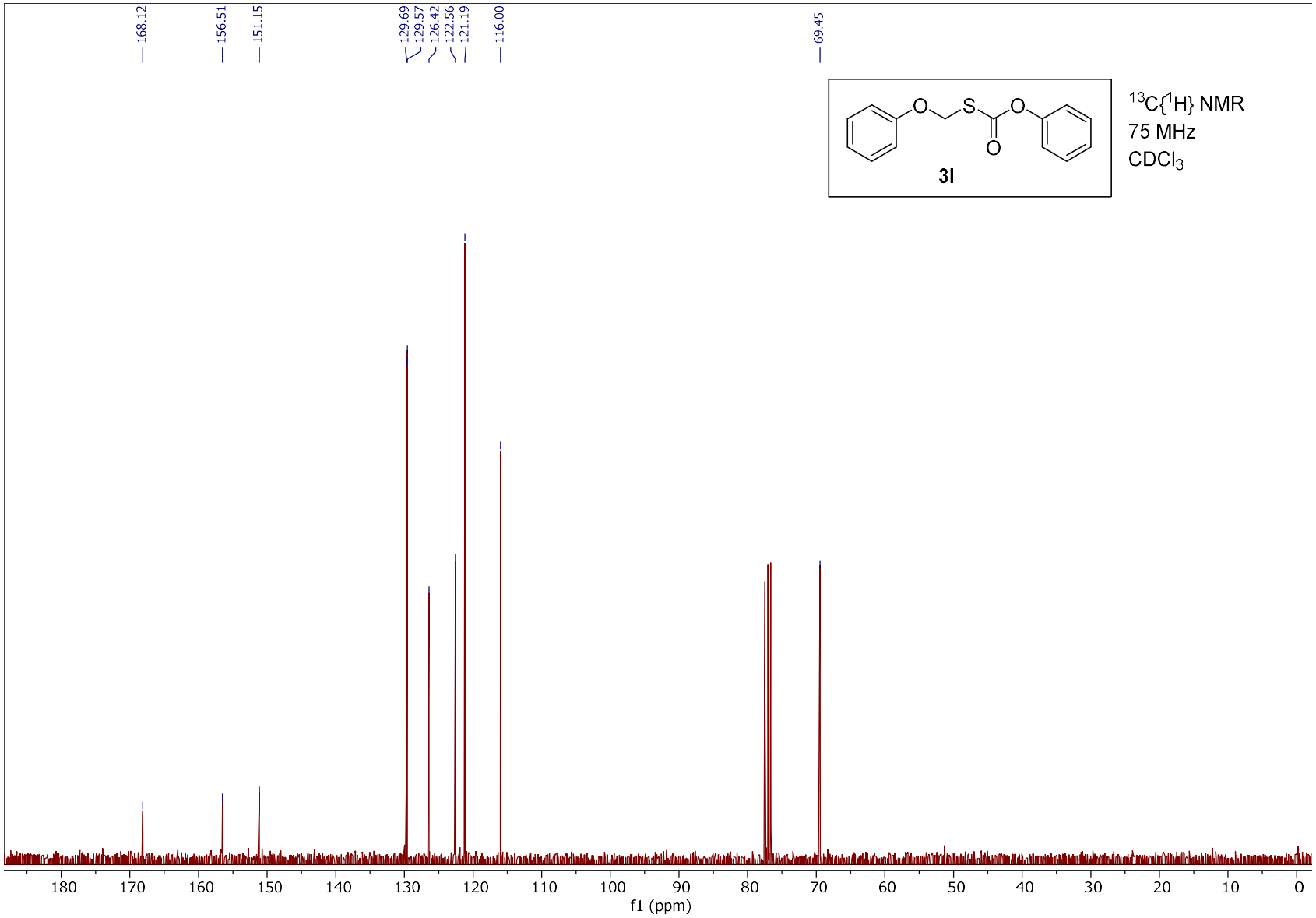

8.56
8.56
8.54
8.53
7.63
7.62
7.49
7.47
7.43
7.40
7.40
7.31
7.30
7.28
7.21
7.20
7.18
7.18
3.31
3.30
3.28
3.19
3.17
3.17
3.17
1.55
O
O
S
N
O
O
3j
1H NMR
300 MHz
CDCl3
1.03
1.03
2.02
2.02
2.82
2.01
1.96
2.00
9.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

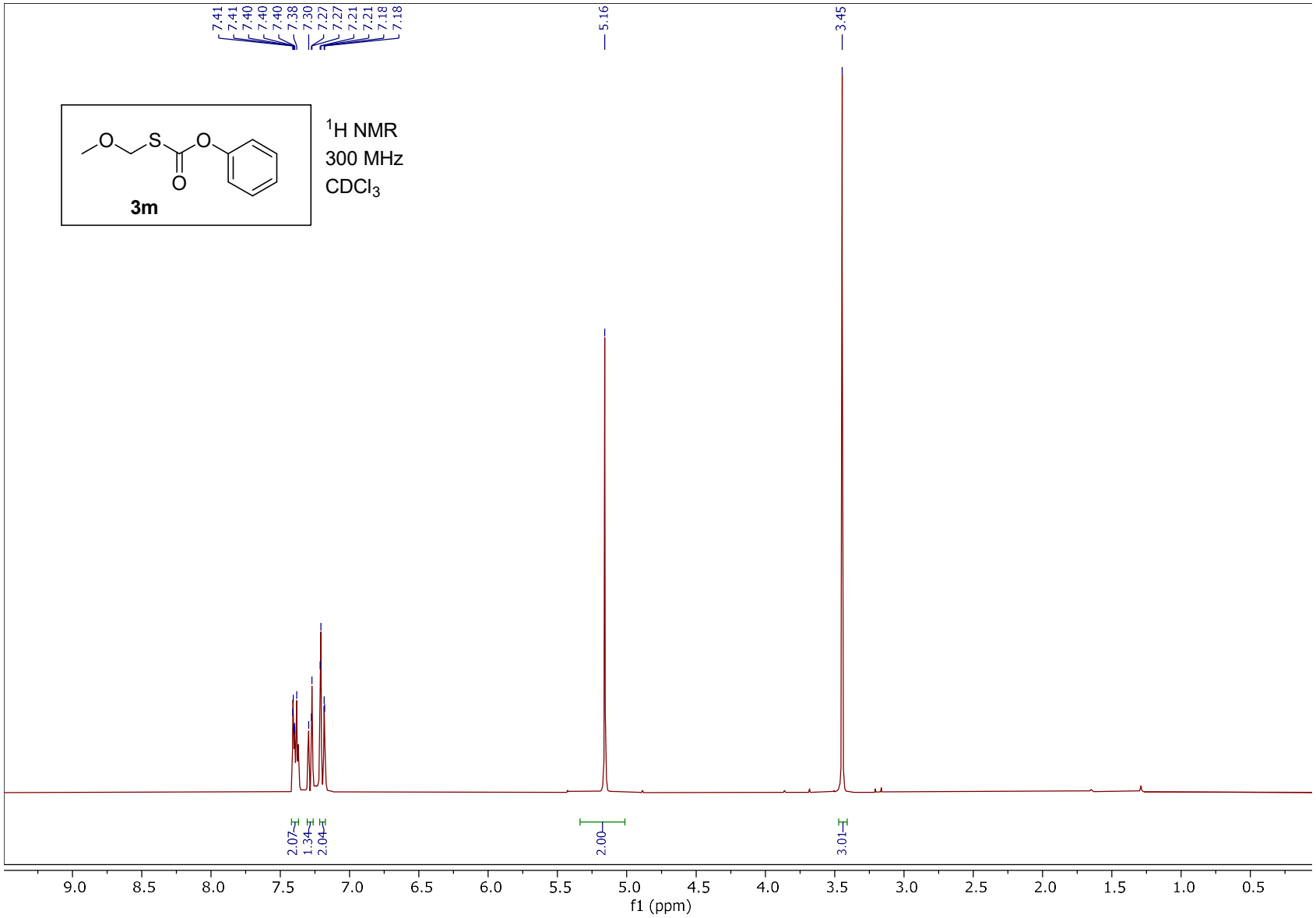

168.69
151.09
148.56
136.67
135.06
131.57
129.44
128.34
126.23
123.70
123.05
121.21
120.91
116.18
61.41
31.76
29.71
27.00
O
O
S
N
O
O
3j
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (мд)

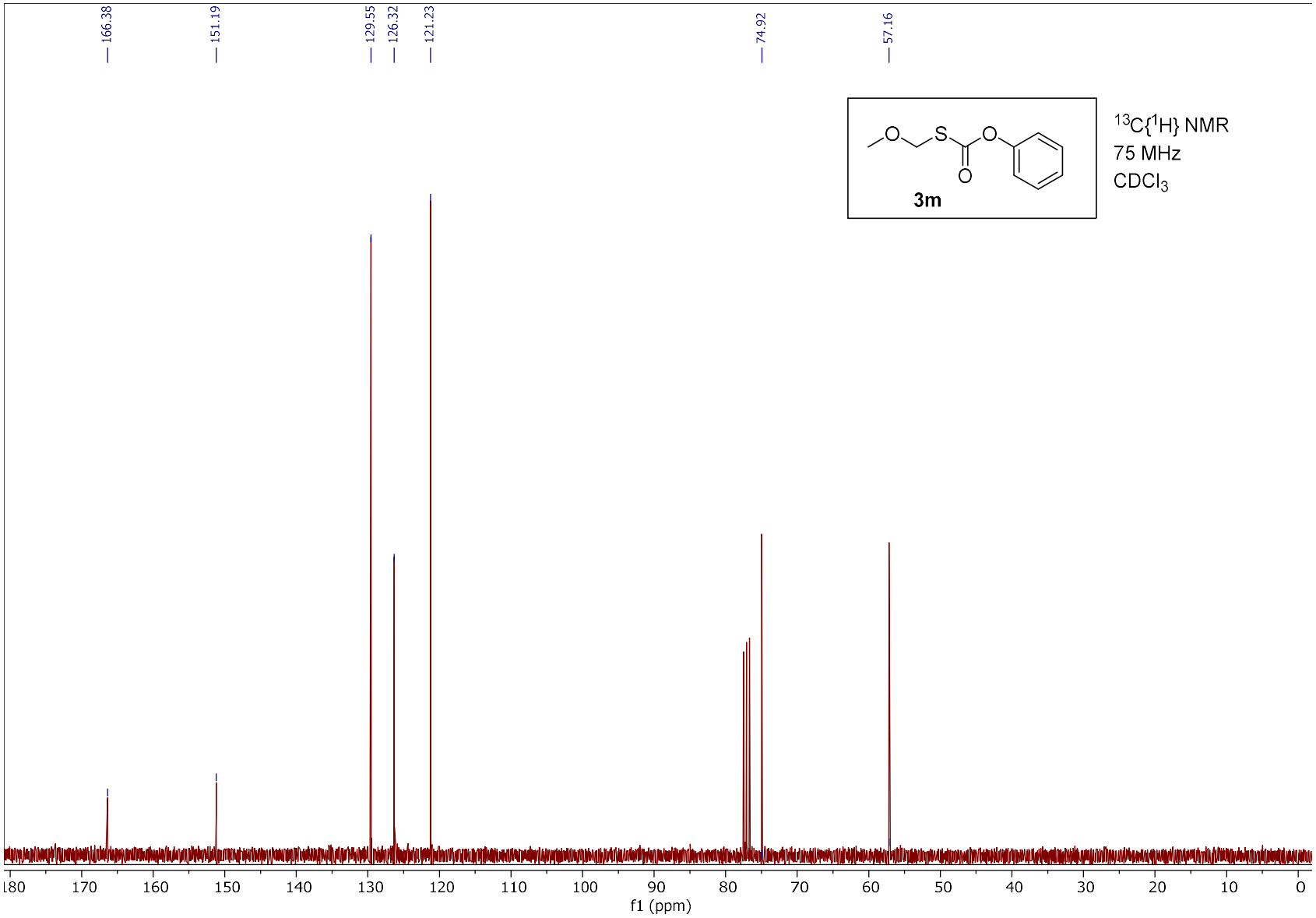

7.42 7.40 7.40 7.39 7.37 7.28 7.28 7.26 7.23 7.21 7.21 7.20 7.19 7.18 7.18 7.17
6.05 6.04 6.03 6.02
4.04 4.02 4.02 4.00
2.49 2.47 2.46 2.46 2.44 2.44 2.43 2.42 2.41 2.15 2.14 2.11 2.11 2.09 2.07 2.05 2.03 2.02 2.01 2.00
O S O O
3k
1H NMR
300 MHz
CDCl3
2.03 2.06 2.07 1.00 2.00 1.04 3.04
10.0 9.5 9.0 8.5 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
f1 (ppm)

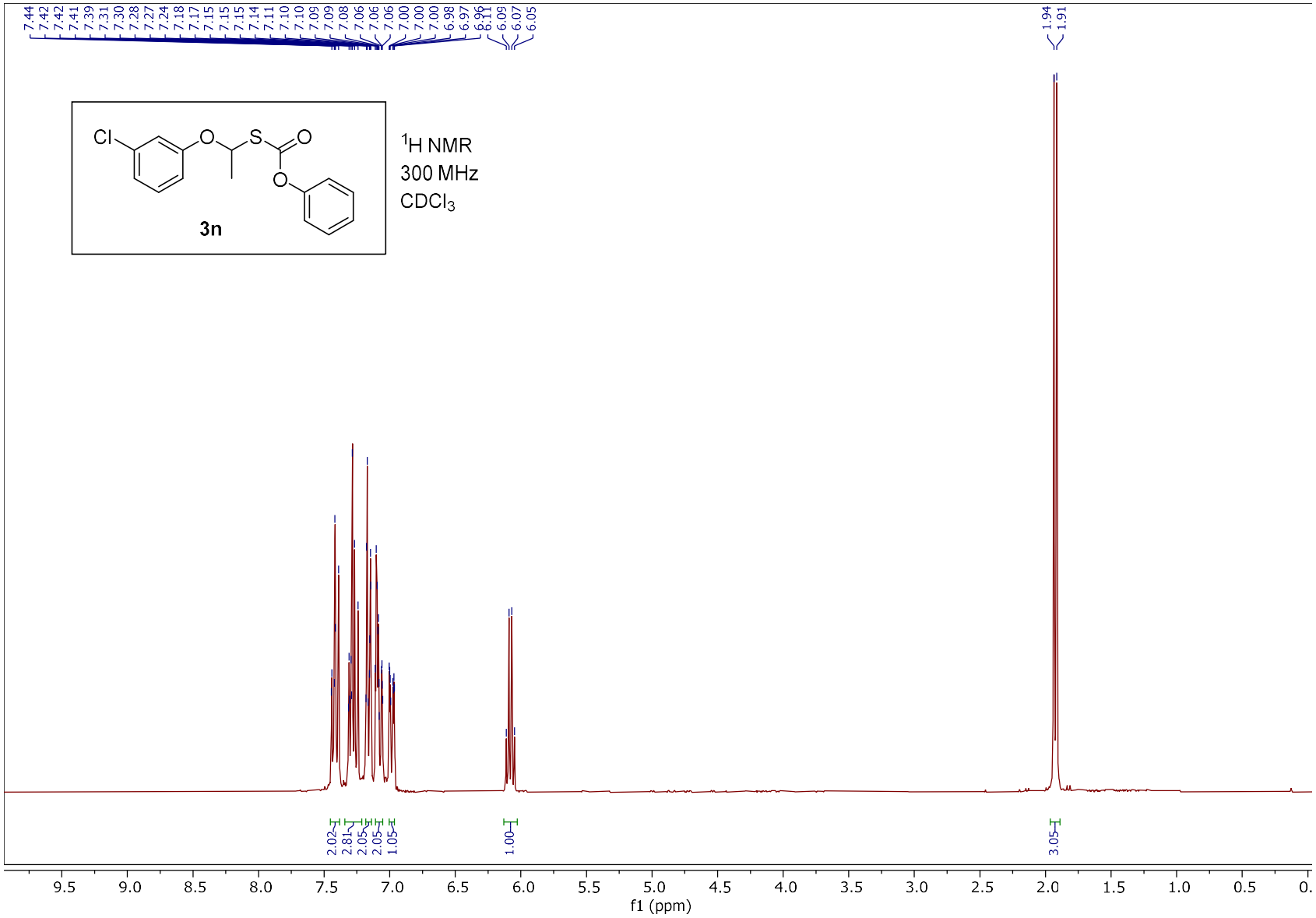

170.04
151.09
129.47
126.18
121.39
85.76
68.38
32.48
24.52
O
S
O
O
3k
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

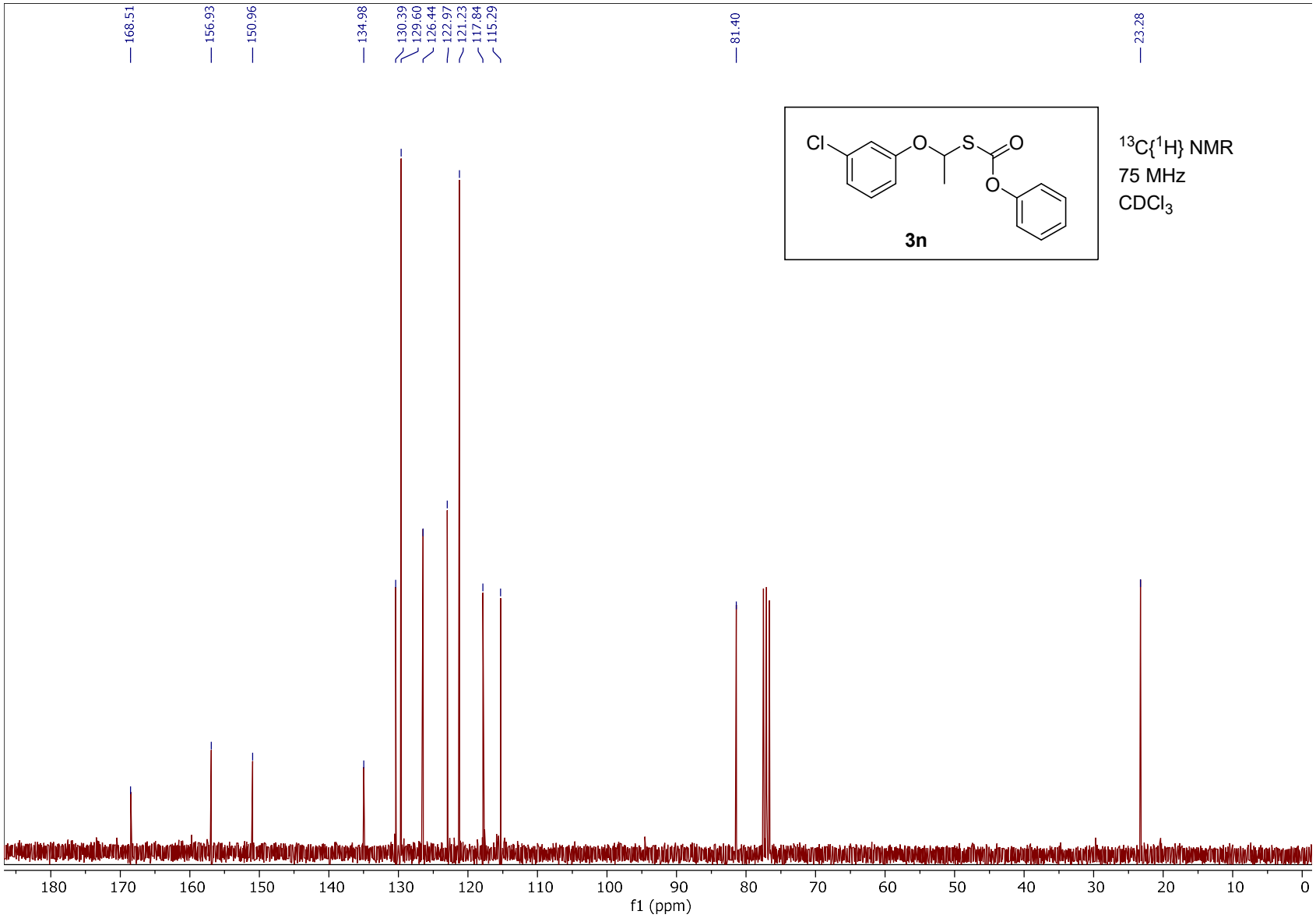

7.43
7.40
7.40
7.40
7.38
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.33
7.33
7.30
7.29
7.27
7.19
7.19
7.19
7.17
7.17
7.16
7.16
7.10
7.08
7.07
7.02
7.02
7.02
7.00
6.99
6.99
5.66
O
S
O
O
3l
1H NMR
300 MHz
CDCl3
6.01
2.02
1.05
2.01
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

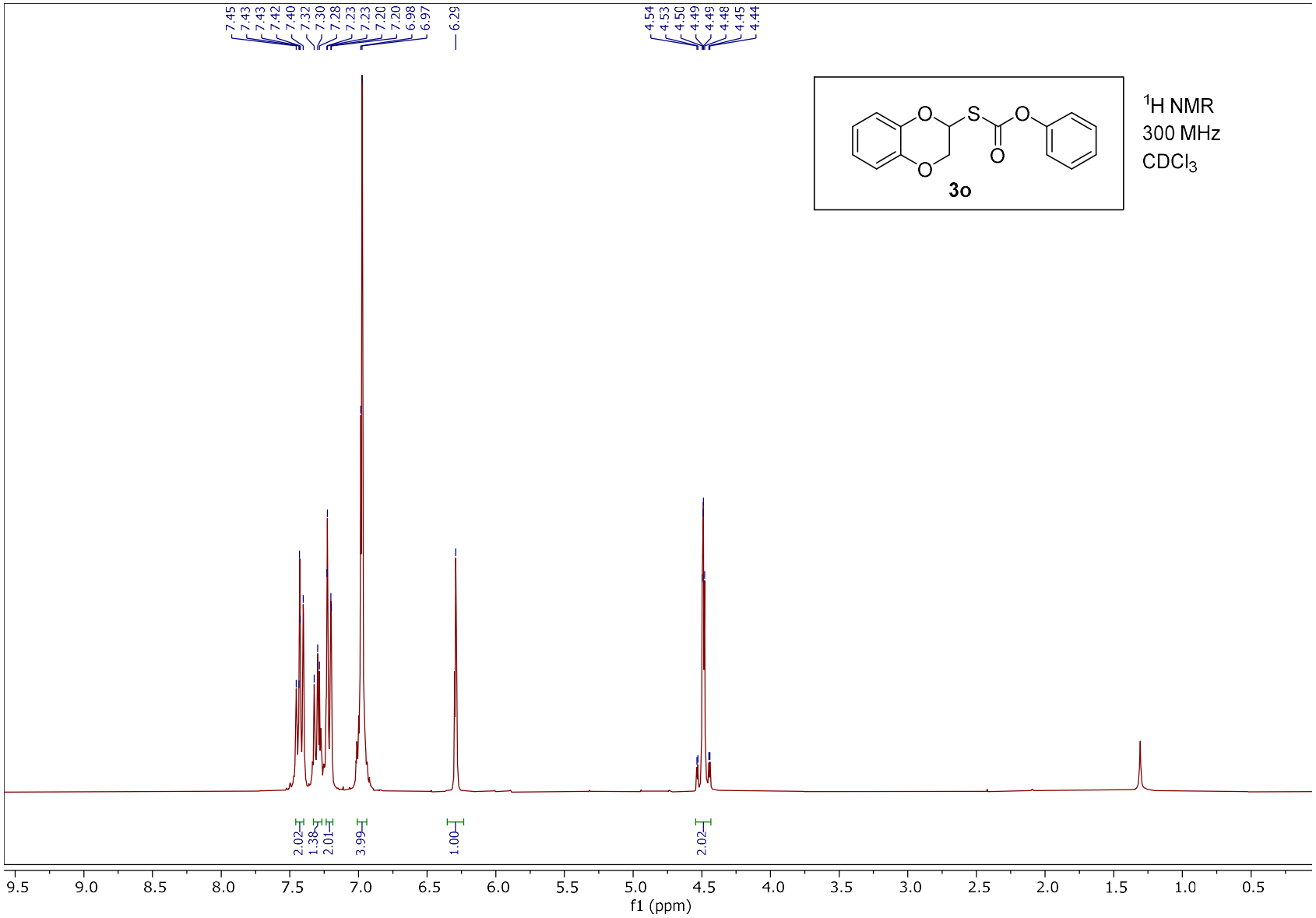

168.12
156.51
151.15
129.69
129.57
126.42
122.56
121.19
116.00
69.45
O
S
O
O
3l
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

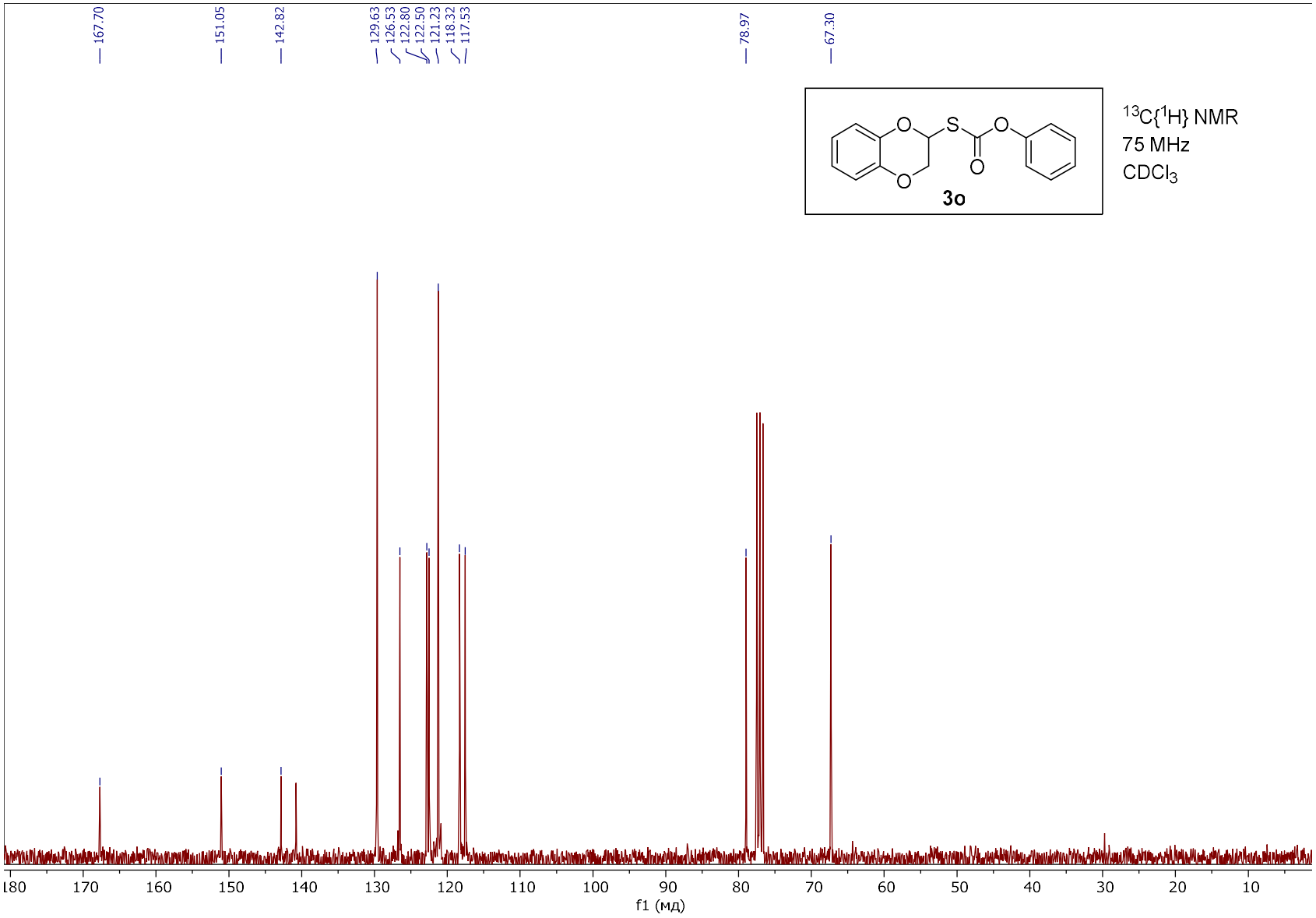

7.41
7.41
7.40
7.40
7.40
7.38
7.30
7.27
7.27
7.21
7.21
7.18
7.18
5.16
3.45
O
S
O
O
3m
1H NMR
300 MHz
CDCl3
2.07
1.34
2.04
2.00
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

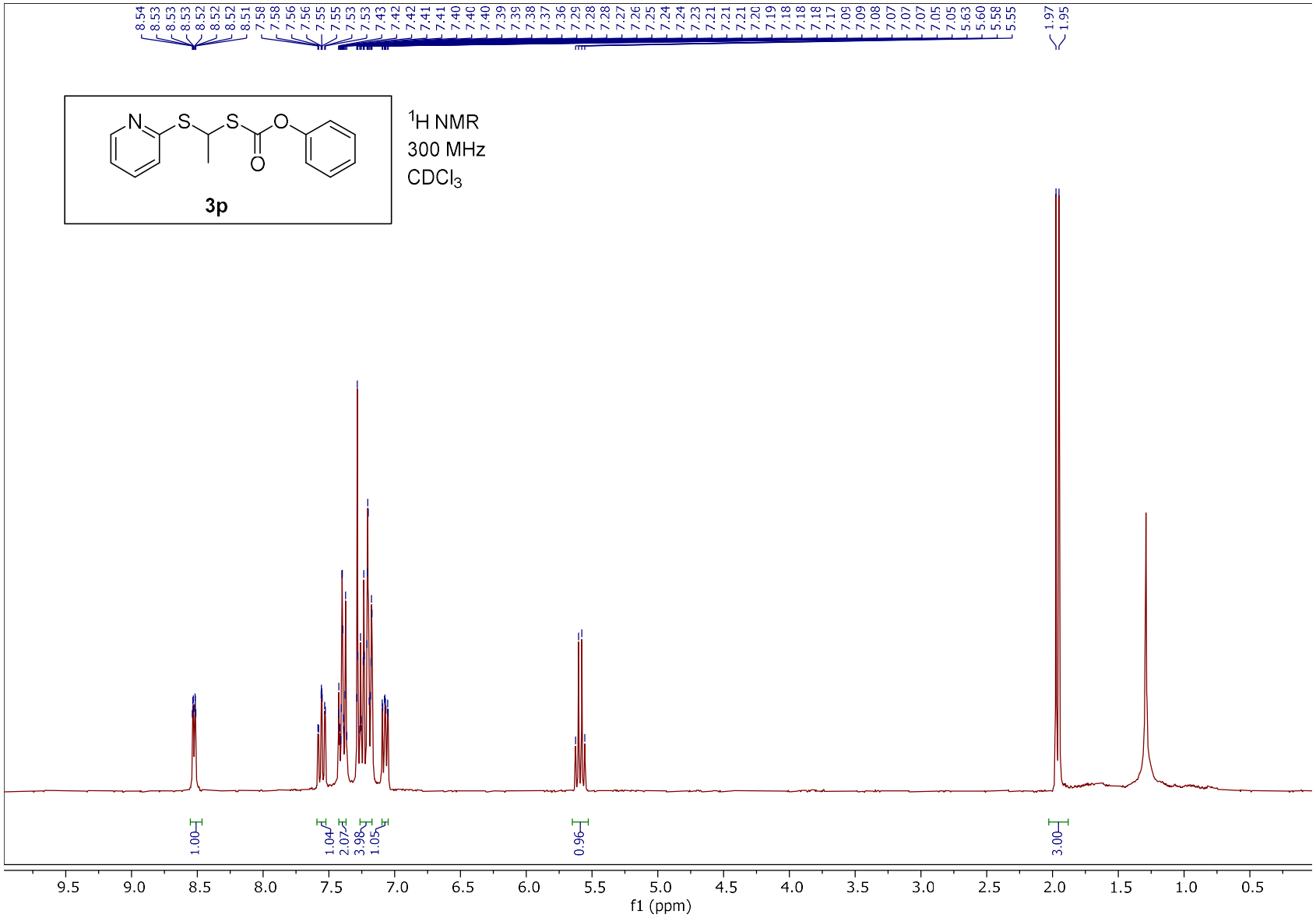

166.38
151.19
129.55
126.32
121.23
74.92
57.16
O
S
O
O
3m
13C{1H} NMR
75 MHz
CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

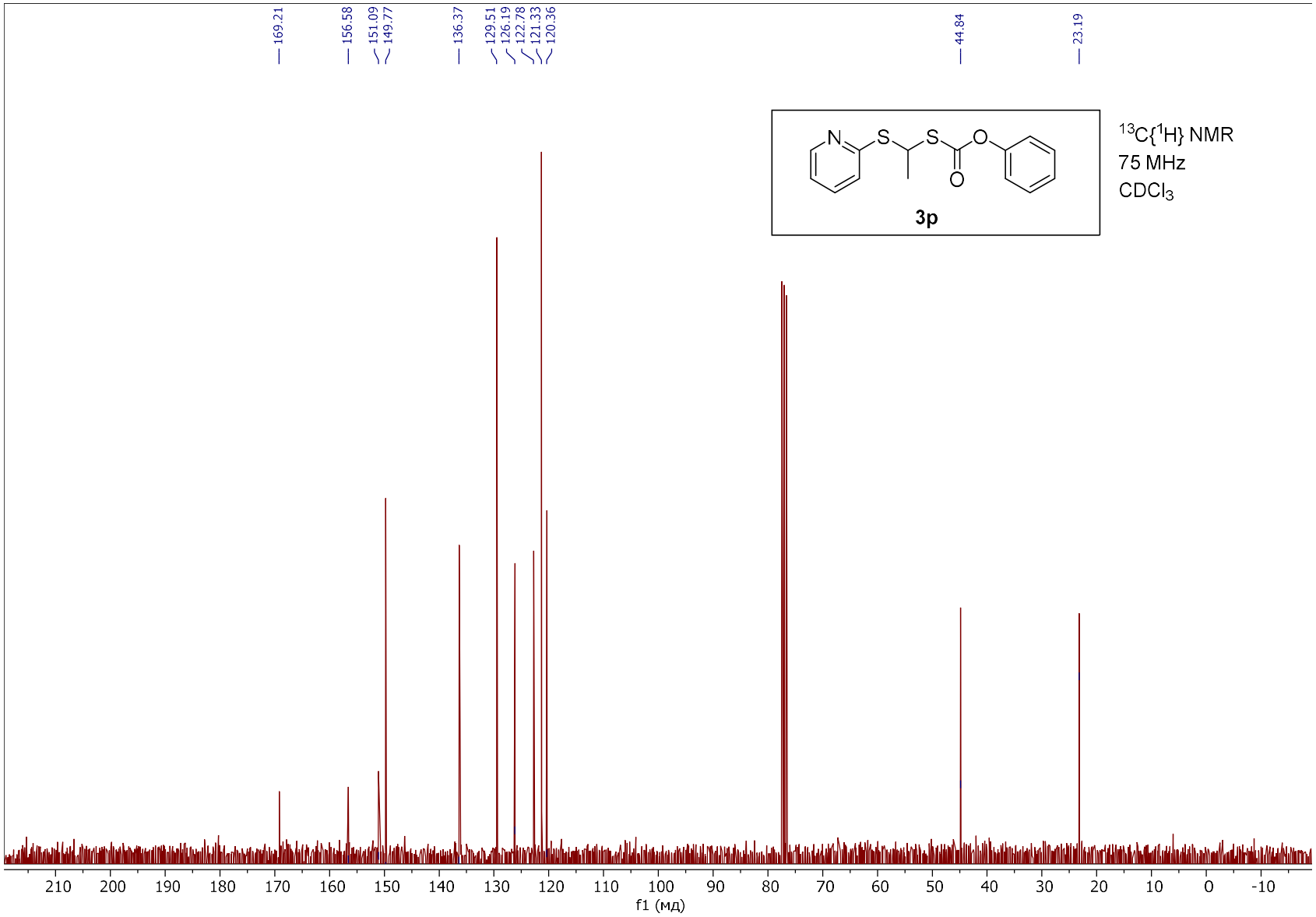

7.44
7.42
7.42
7.41
7.39
7.31
7.30
7.28
7.27
7.24
7.18
7.17
7.15
7.15
7.15
7.14
7.11
7.10
7.10
7.09
7.09
7.08
7.06
7.06
7.06
7.00
7.00
7.00
6.98
6.97
6.96
6.11
6.09
6.07
6.05
1.94
1.91
Cl
O
S
O
O
3n
1H NMR
300 MHz
CDCl3
2.02
2.81
2.05
2.05
1.05
1.00
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

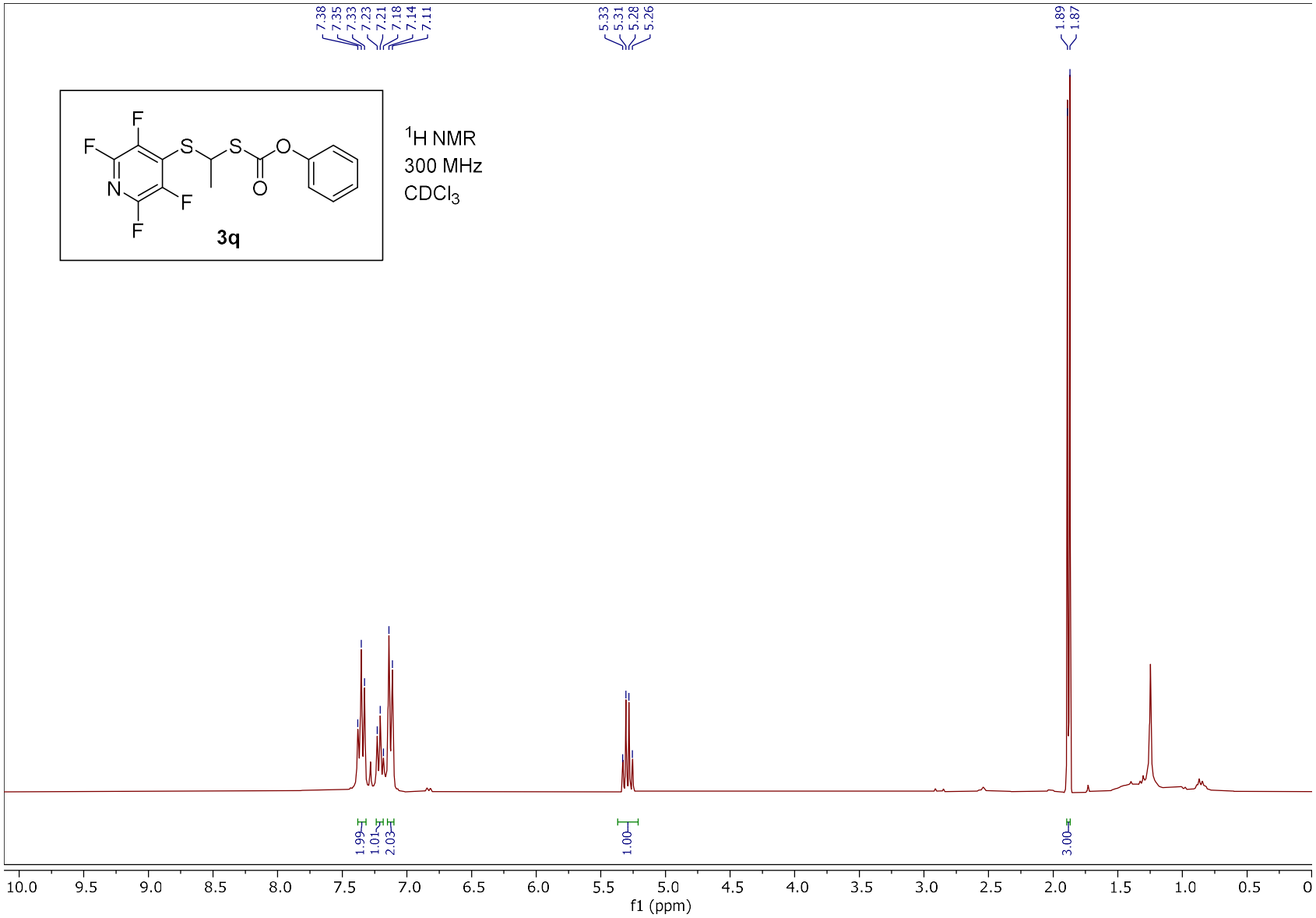

168.51
156.93
150.96
134.98
130.39
129.60
126.44
122.97
121.23
117.84
115.29
81.40
23.28
Cl
O
S
O
O
3n
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

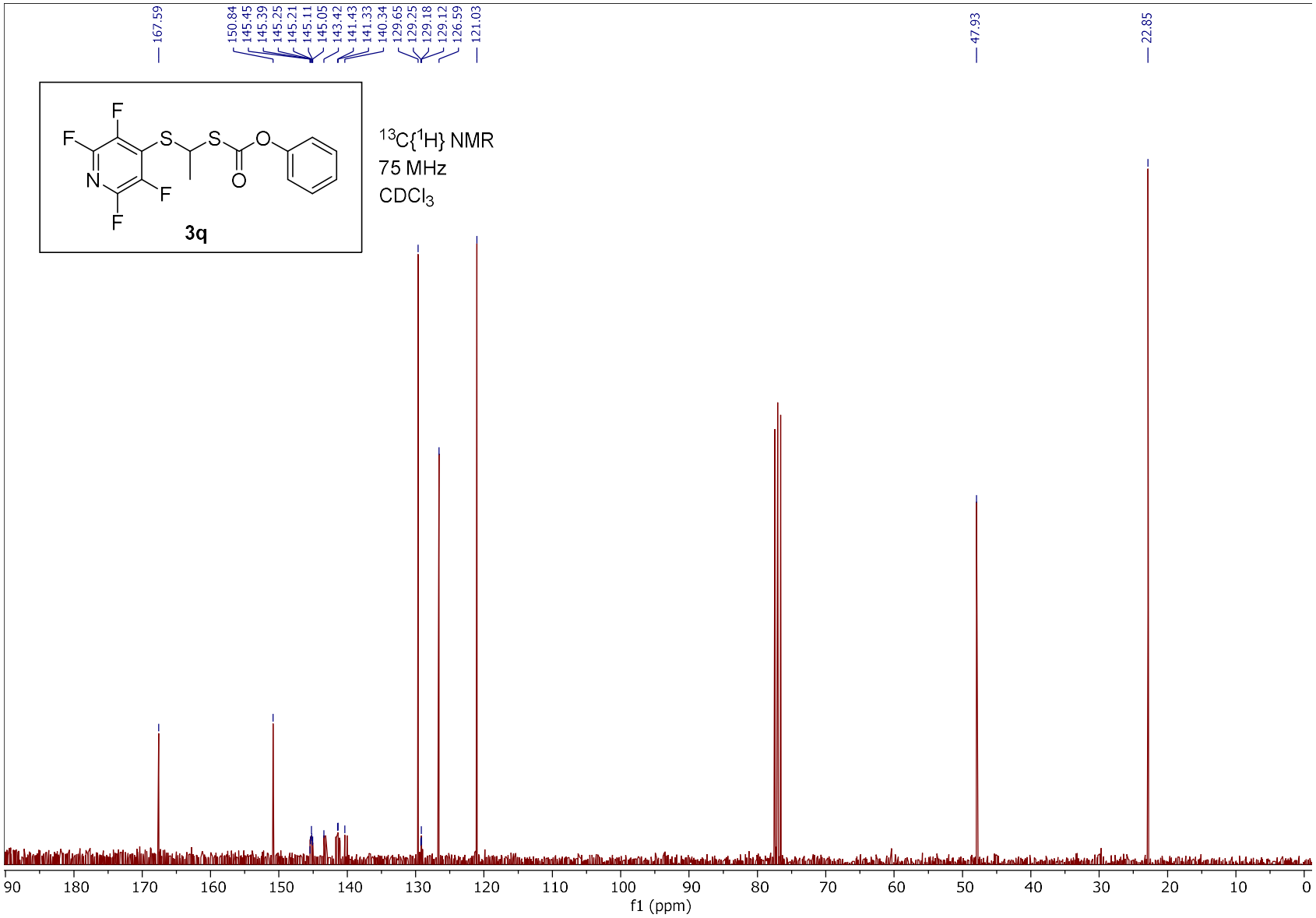

7.45
7.43
7.43
7.42
7.40
7.32
7.30
7.28
7.23
7.23
7.20
7.20
6.98
6.97
6.29
4.54
4.53
4.50
4.49
4.49
4.48
4.45
4.44
O
S
O
O
O
3o
^{1}H NMR
300 MHz
$CDCl_3$
2.02
1.38
2.01
3.99
1.00
2.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

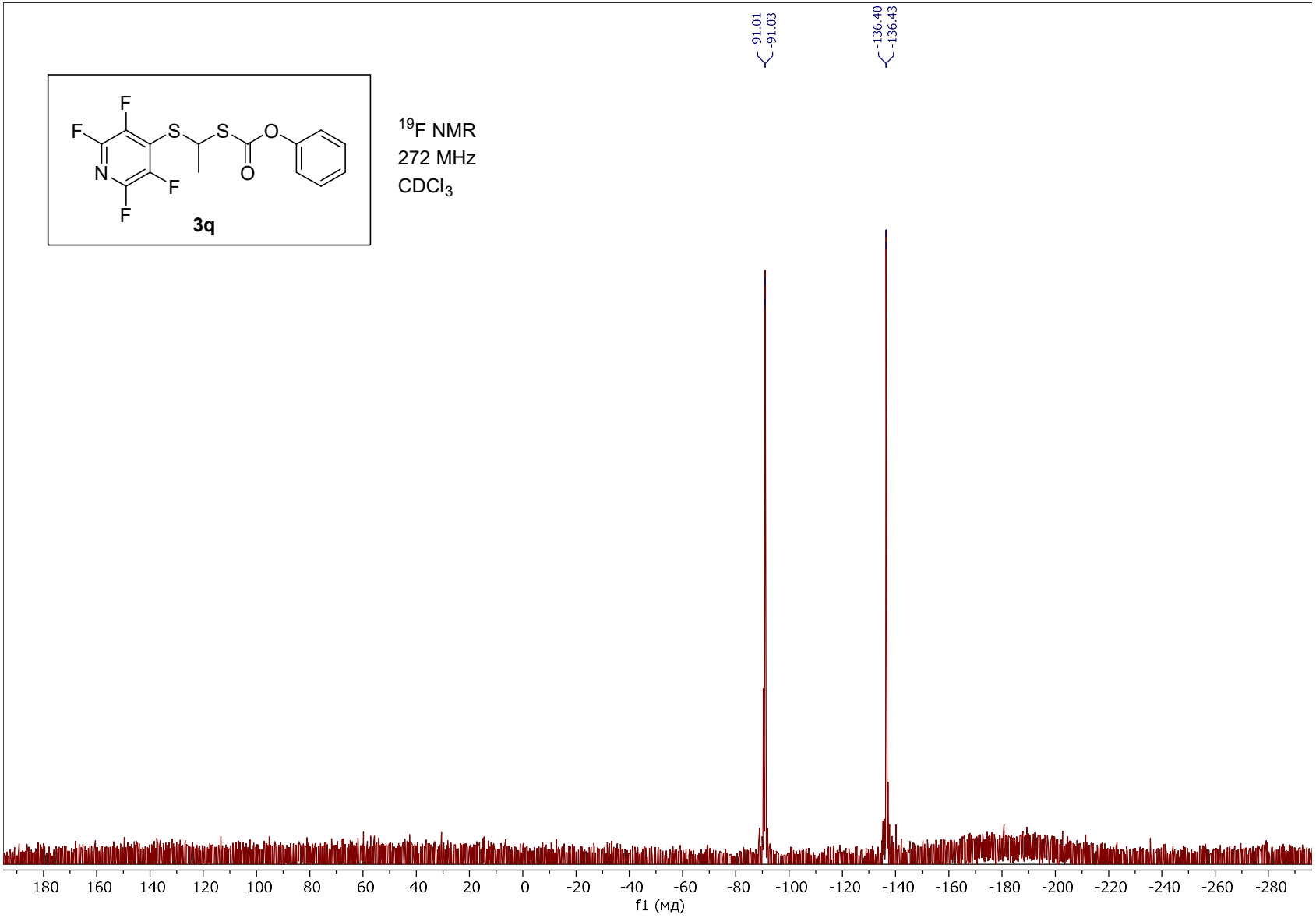

167.70
151.05
142.82
129.63
126.53
122.80
122.50
121.23
118.32
117.53
78.97
67.30
O
S
O
O
O
3o
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

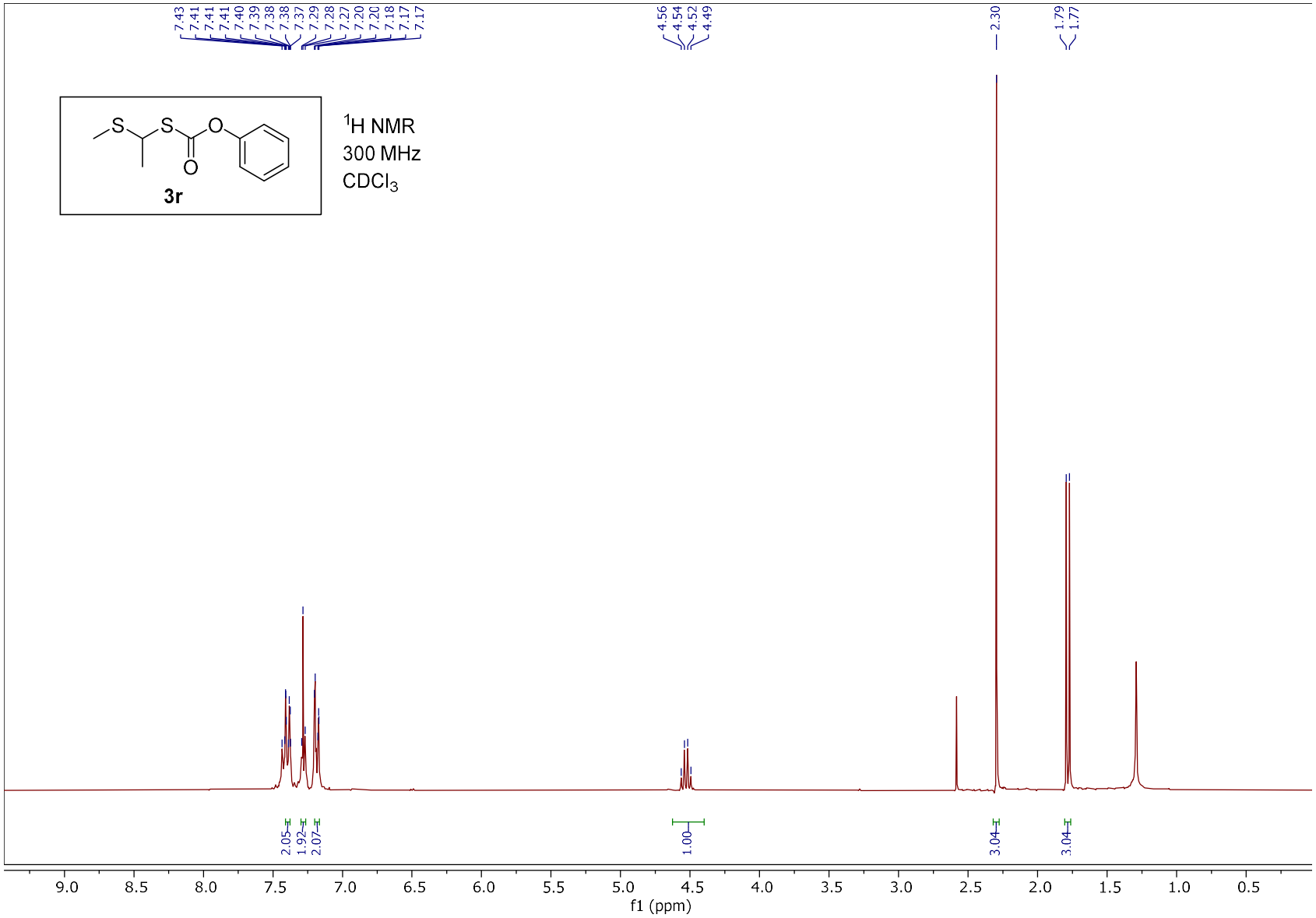

8.54 8.53 8.53 8.53 8.52 8.52 8.52 8.51 7.58 7.58 7.56 7.56 7.55 7.55 7.53 7.53 7.43 7.42 7.42 7.41 7.41 7.40 7.40 7.40 7.39 7.39 7.38 7.37 7.36 7.29 7.28 7.28 7.27 7.26 7.25 7.24 7.24 7.23 7.21 7.21 7.21 7.20 7.19 7.18 7.18 7.17 7.09 7.09 7.08 7.07 7.07 7.07 7.05 7.05 5.63 5.60 5.58 5.55 1.97 1.95
N S S O O
3p
^{1}H NMR
300 MHz
$CDCl_3$
1.00 1.04 2.07 3.98 1.05 0.96 3.00
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
f1 (ppm)

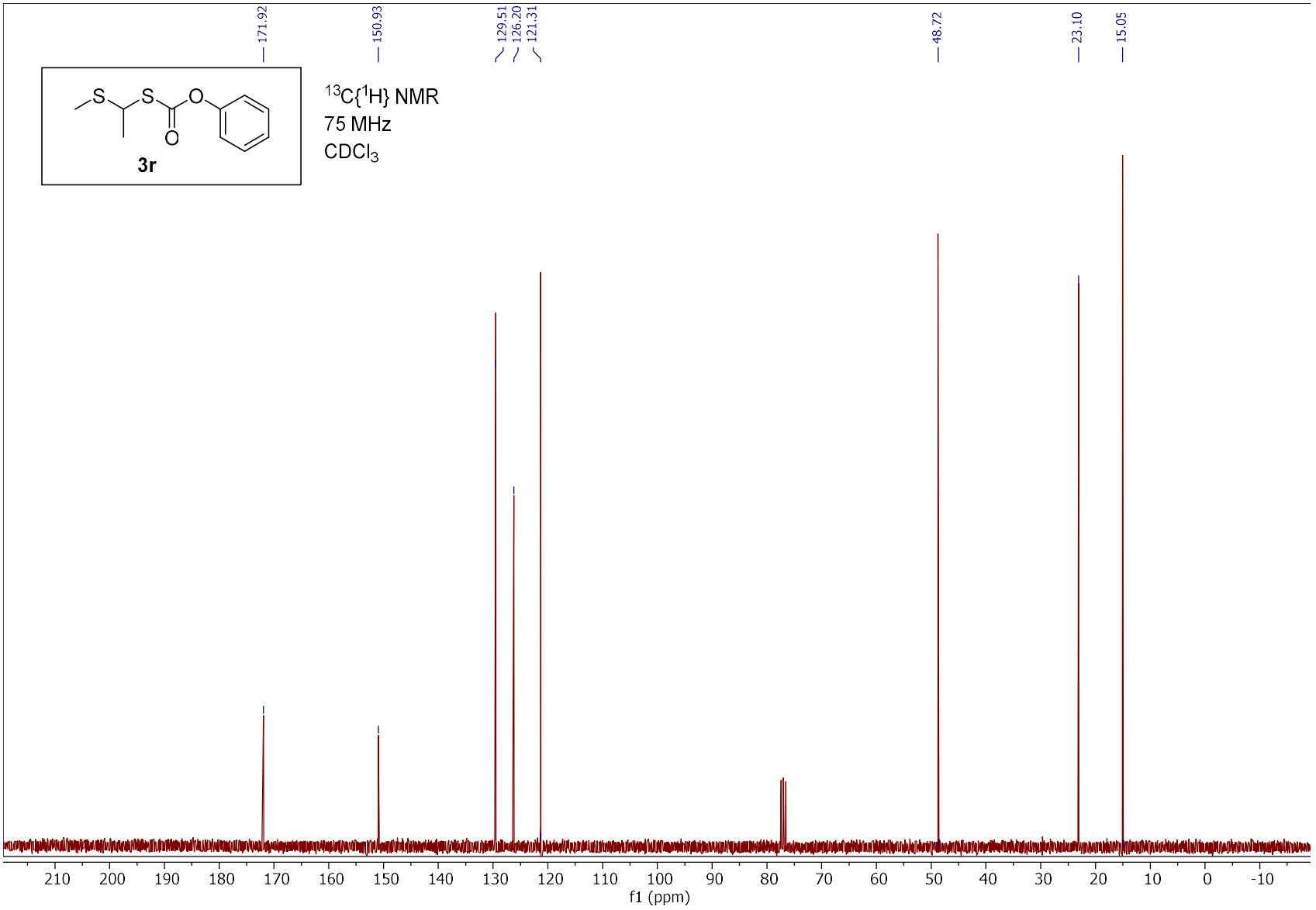

169.21
156.58
151.09
149.77
136.37
129.51
126.19
122.78
121.33
120.36
44.84
23.19
N
S
S
O
O
3p
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)

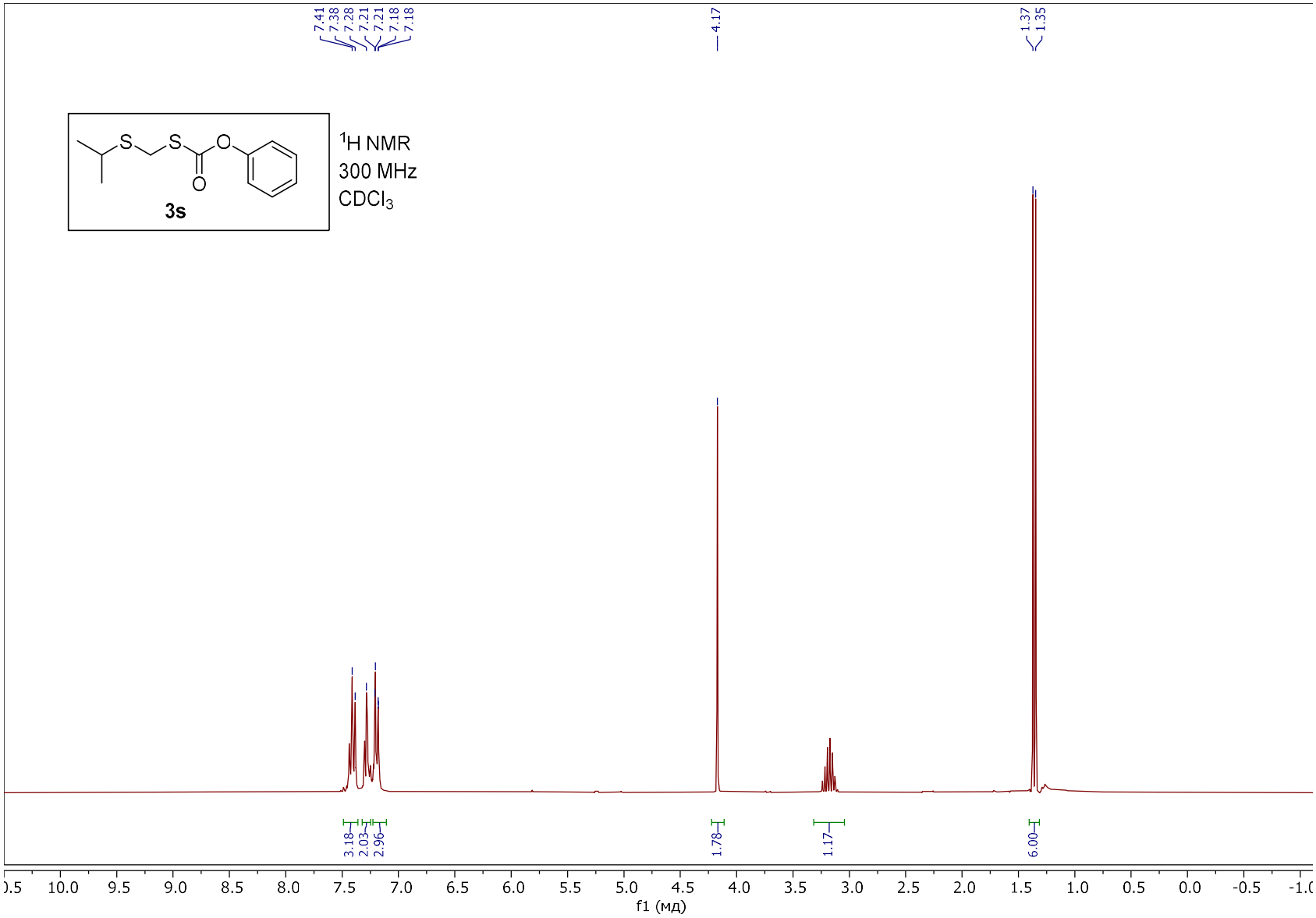

7.38
7.35
7.33
7.23
7.21
7.18
7.14
7.11
5.33
5.31
5.28
5.26
1.89
1.87
F
F
N
F
F
S
S
O
O
3q
^{1}H NMR
300 MHz
$CDCl_3$
1.99
1.01
2.03
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

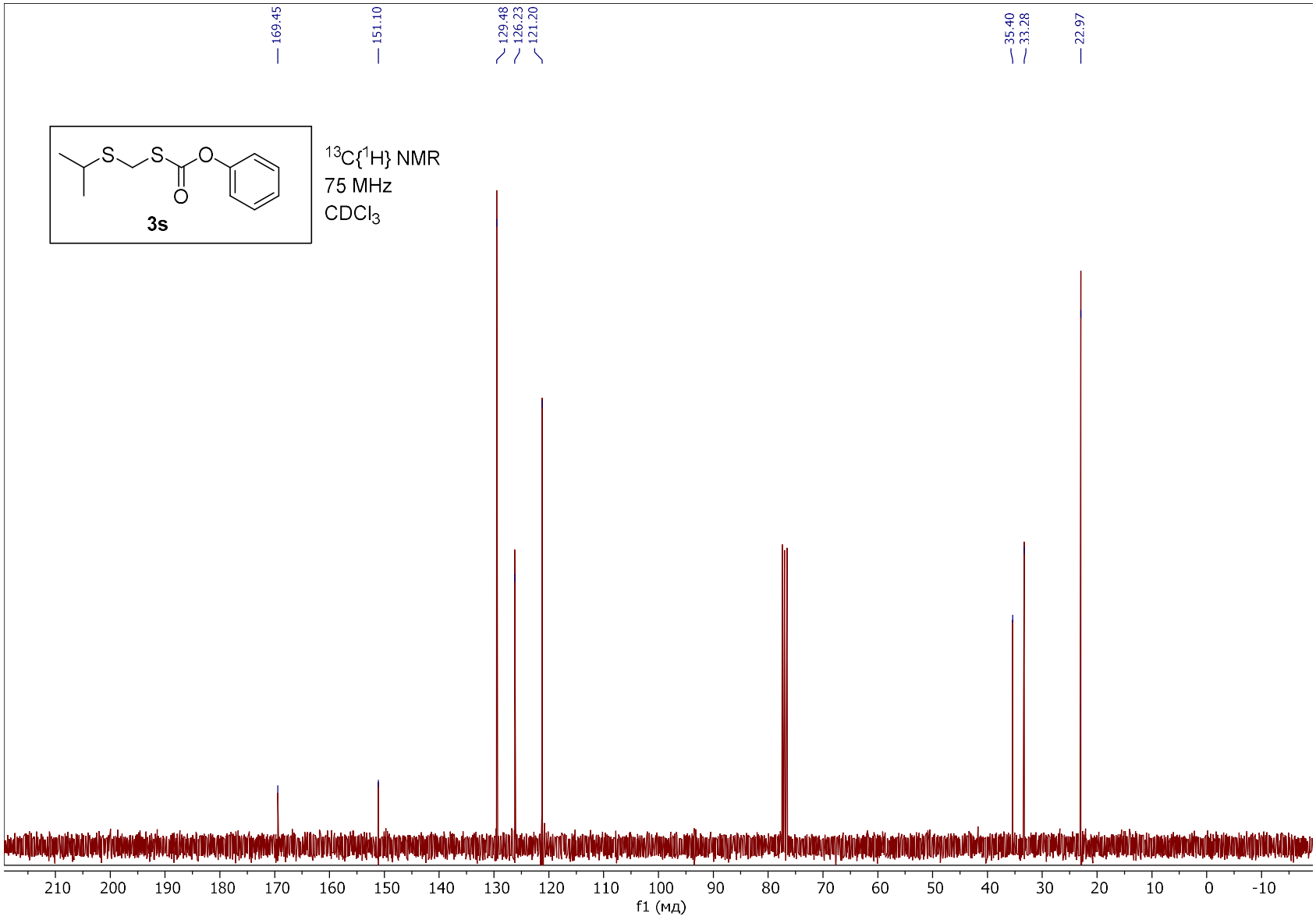

167.59
150.84
145.45
145.39
145.25
145.21
145.11
145.05
143.42
141.43
141.33
140.34
129.65
129.25
129.18
129.12
126.59
121.03
47.93
22.85
F
F
S
S
O
N
F
O
F
3q
13C{1H} NMR
75 MHz
CDCl3
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

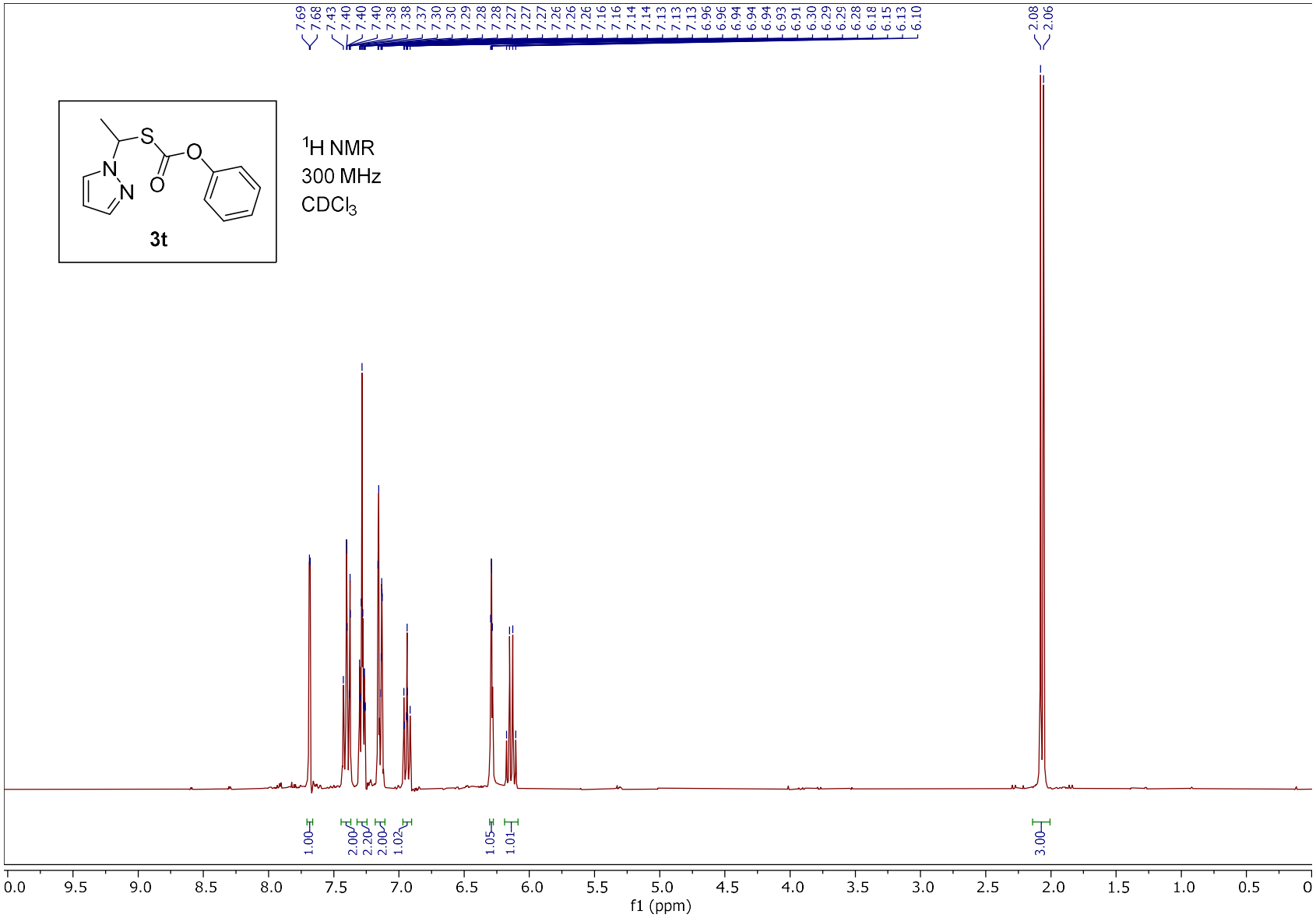

-91.01
-91.03
-136.40
-136.43
F
F
S
S
O
N
F
O
F
3q
19F NMR
272 MHz
CDCl3
180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280
f1 (мд)

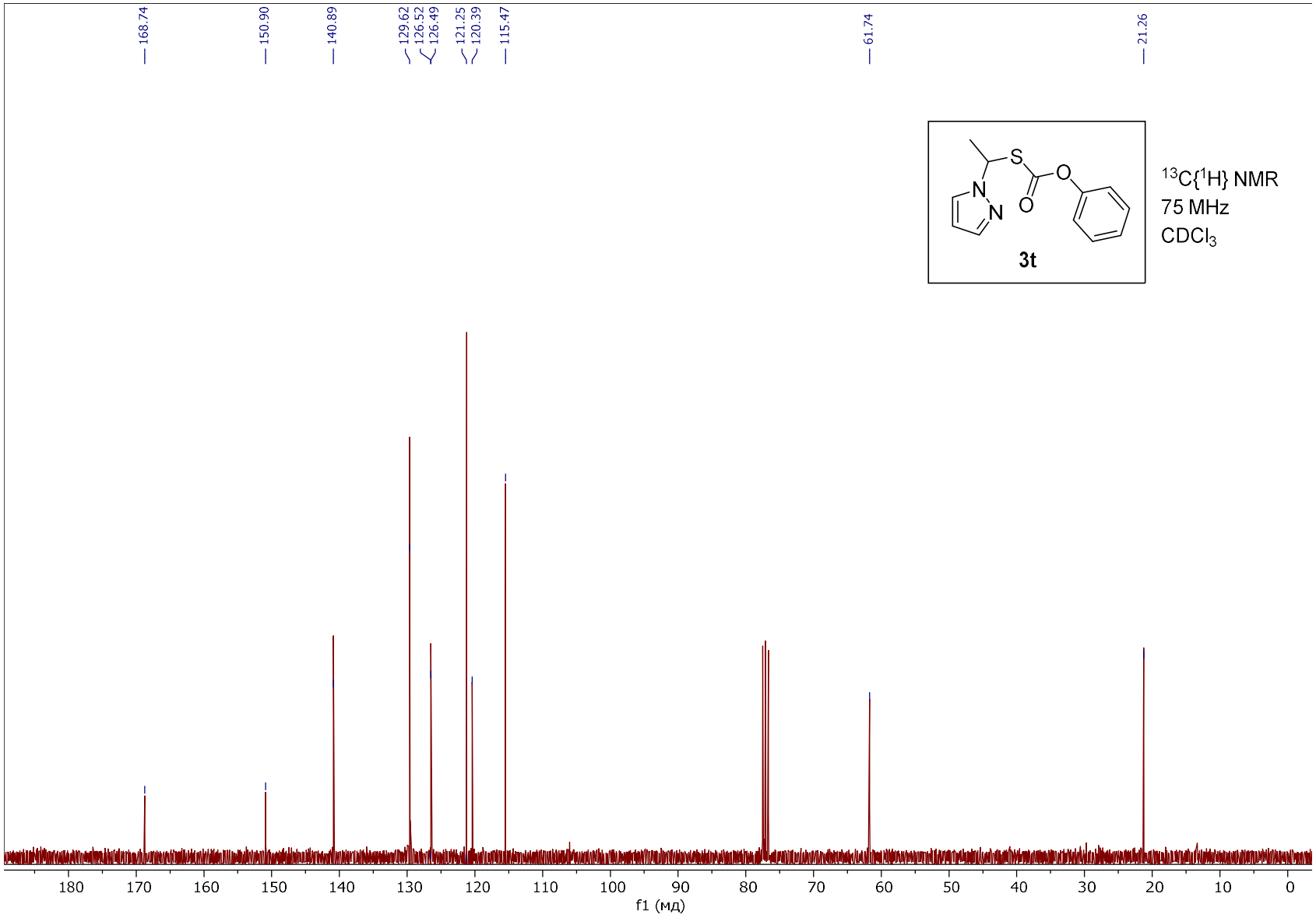

7.43
7.41
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.29
7.28
7.27
7.20
7.20
7.18
7.17
7.17
4.56
4.54
4.52
4.49
2.30
1.79
1.77
S
S
O
O
3r
1H NMR
300 MHz
CDCl3
2.05
1.92
2.07
1.00
3.04
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

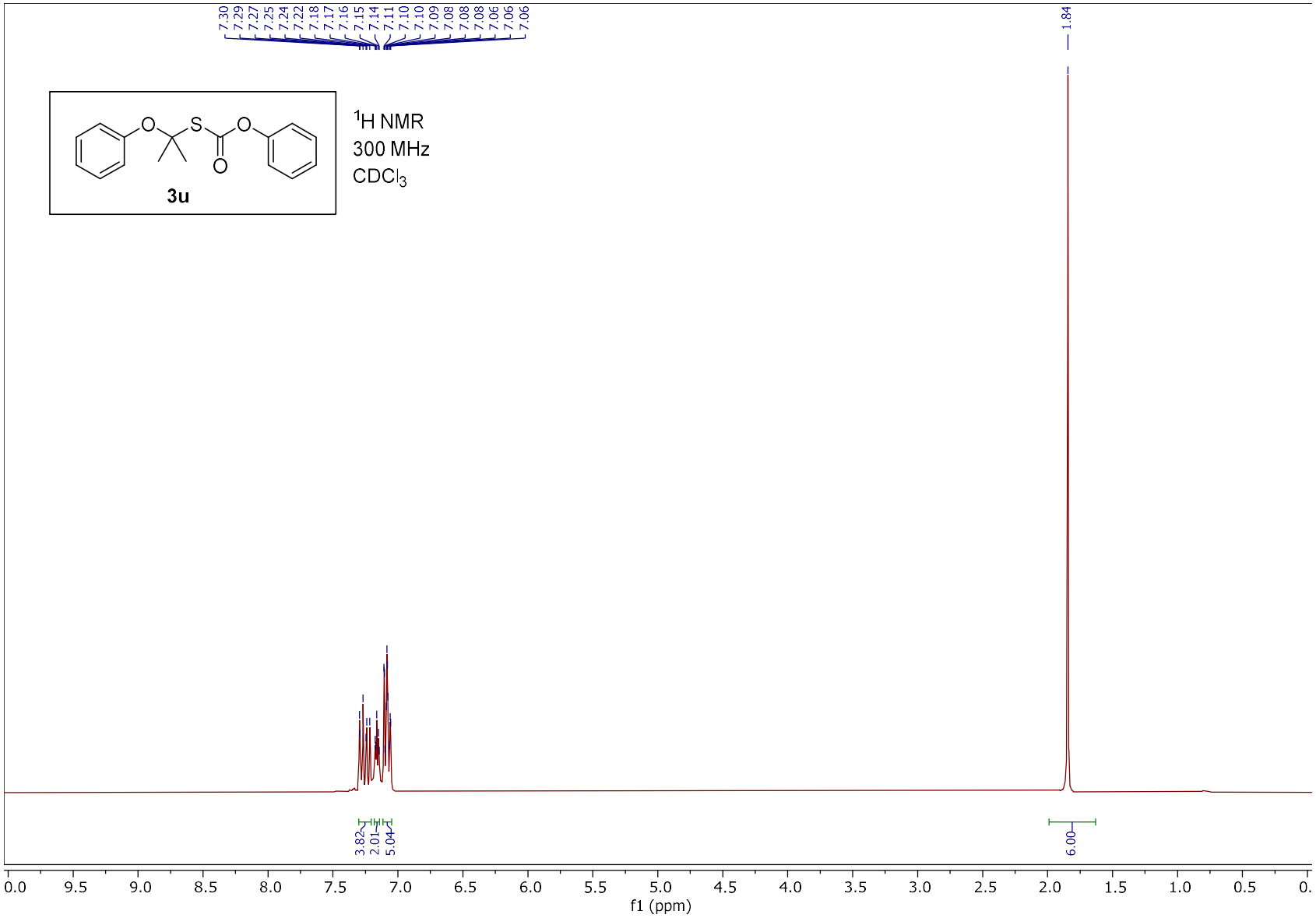

171.92
150.93
129.51
126.20
121.31
48.72
23.10
15.05
S
S
O
O
3r
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

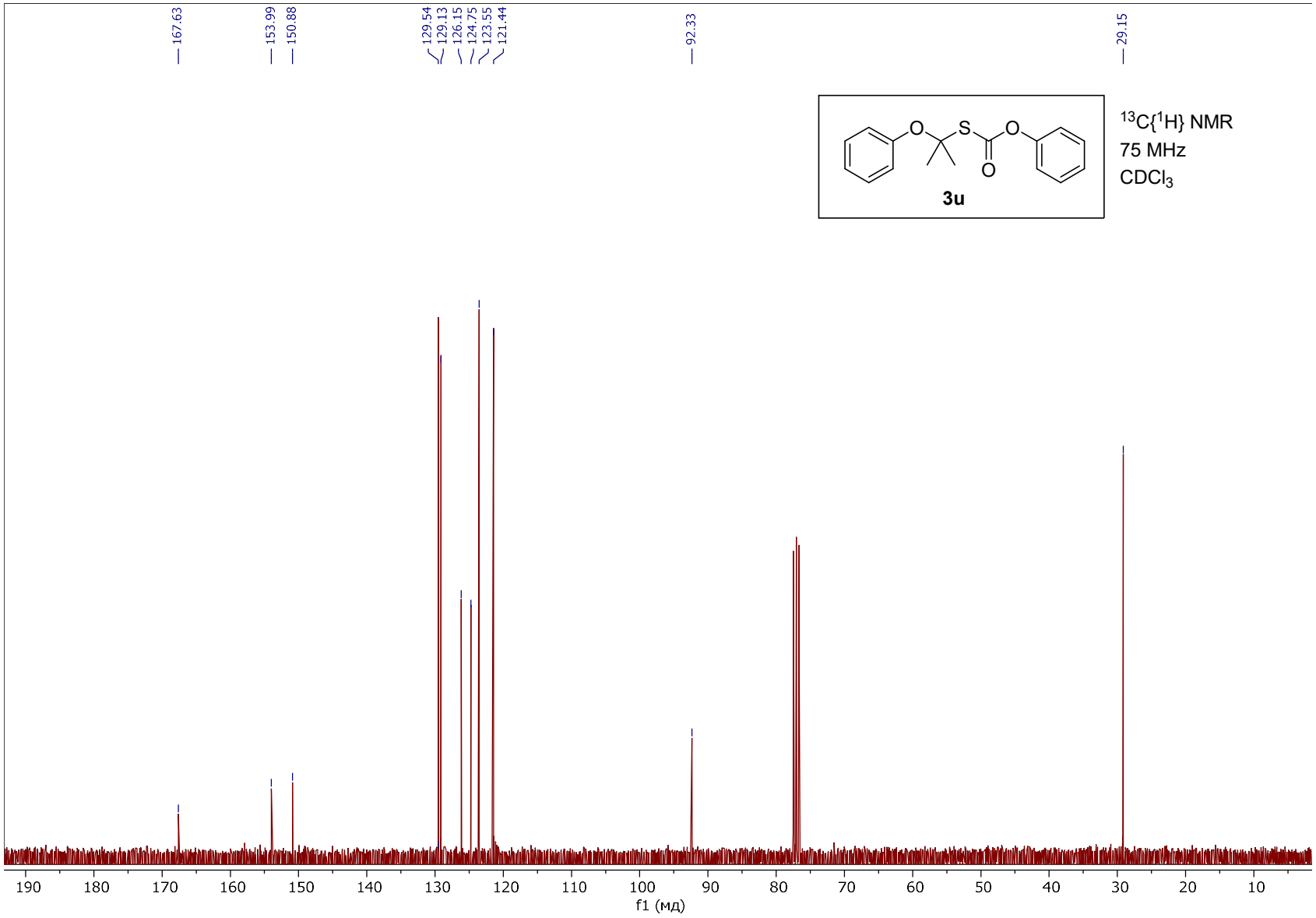

7.41
7.38
7.28
7.21
7.21
7.18
7.18
4.17
1.37
1.35
S
S
O
O
3s
1H NMR
300 MHz
CDCl3
3.18
2.03
2.96
1.78
1.17
6.00
f1 (мд)

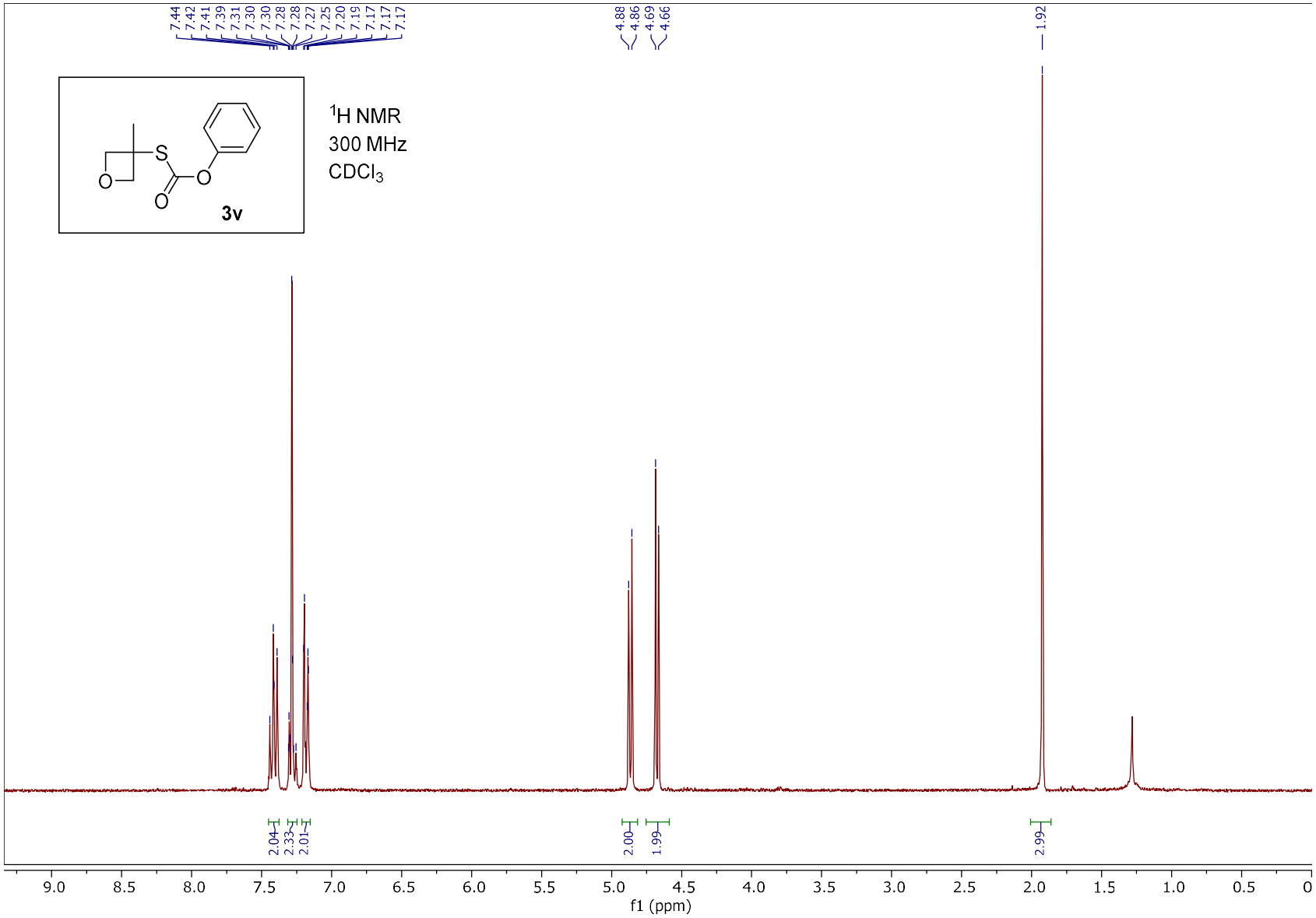

169.45
151.10
129.48
126.23
121.20
35.40
33.28
22.97
3s
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)

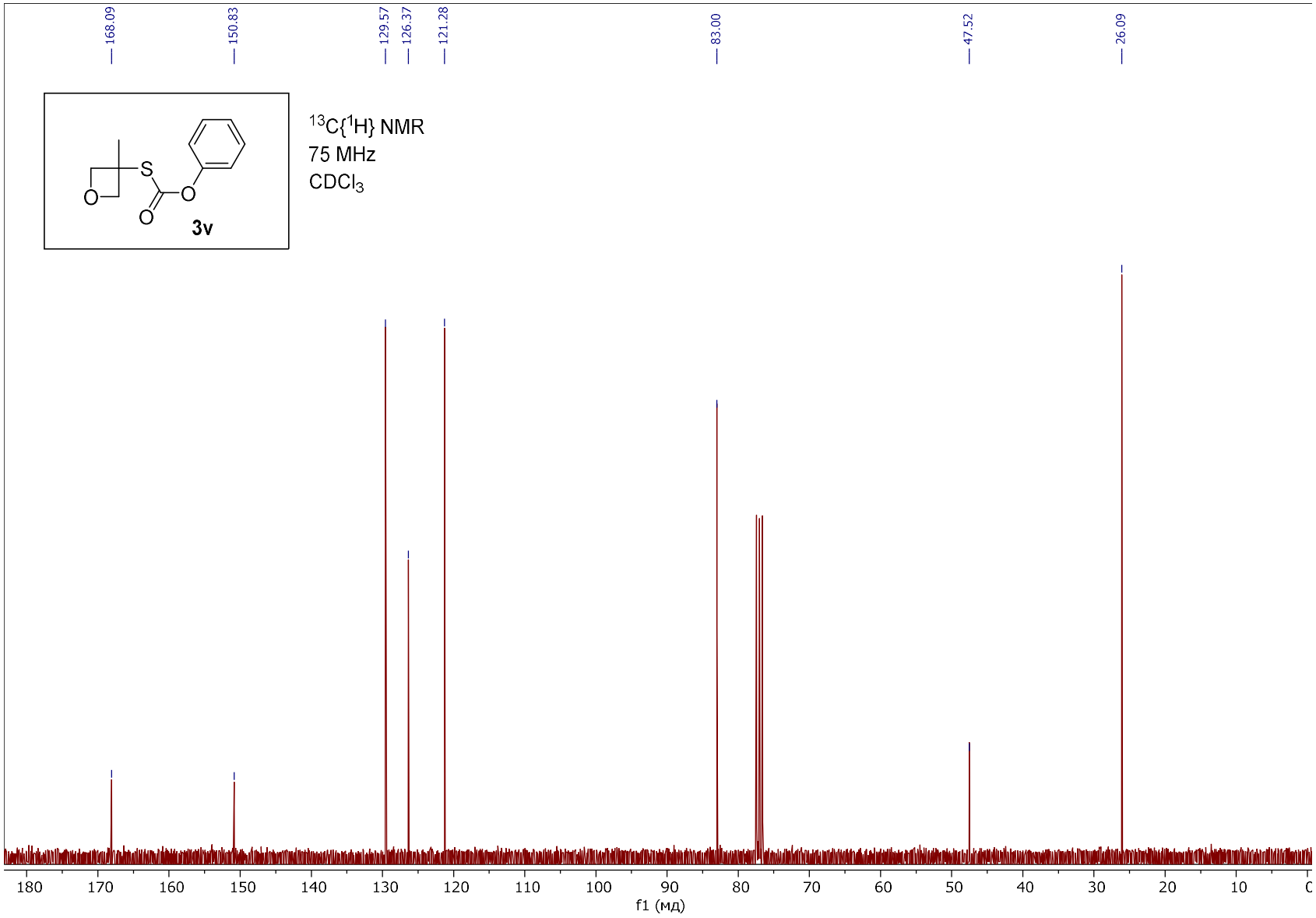

7.69
7.68
7.43
7.40
7.40
7.40
7.38
7.38
7.37
7.30
7.30
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.26
7.26
7.16
7.14
7.14
7.13
7.13
7.13
6.96
6.96
6.94
6.94
6.94
6.93
6.91
6.30
6.29
6.29
6.28
6.18
6.15
6.13
6.10
2.08
2.06
S
O
N
N
O
3t
1H NMR
300 MHz
CDCl3
1.00
2.00
2.20
2.00
1.02
1.05
1.01
3.00
0.0
9.5
9.0
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
f1 (ppm)

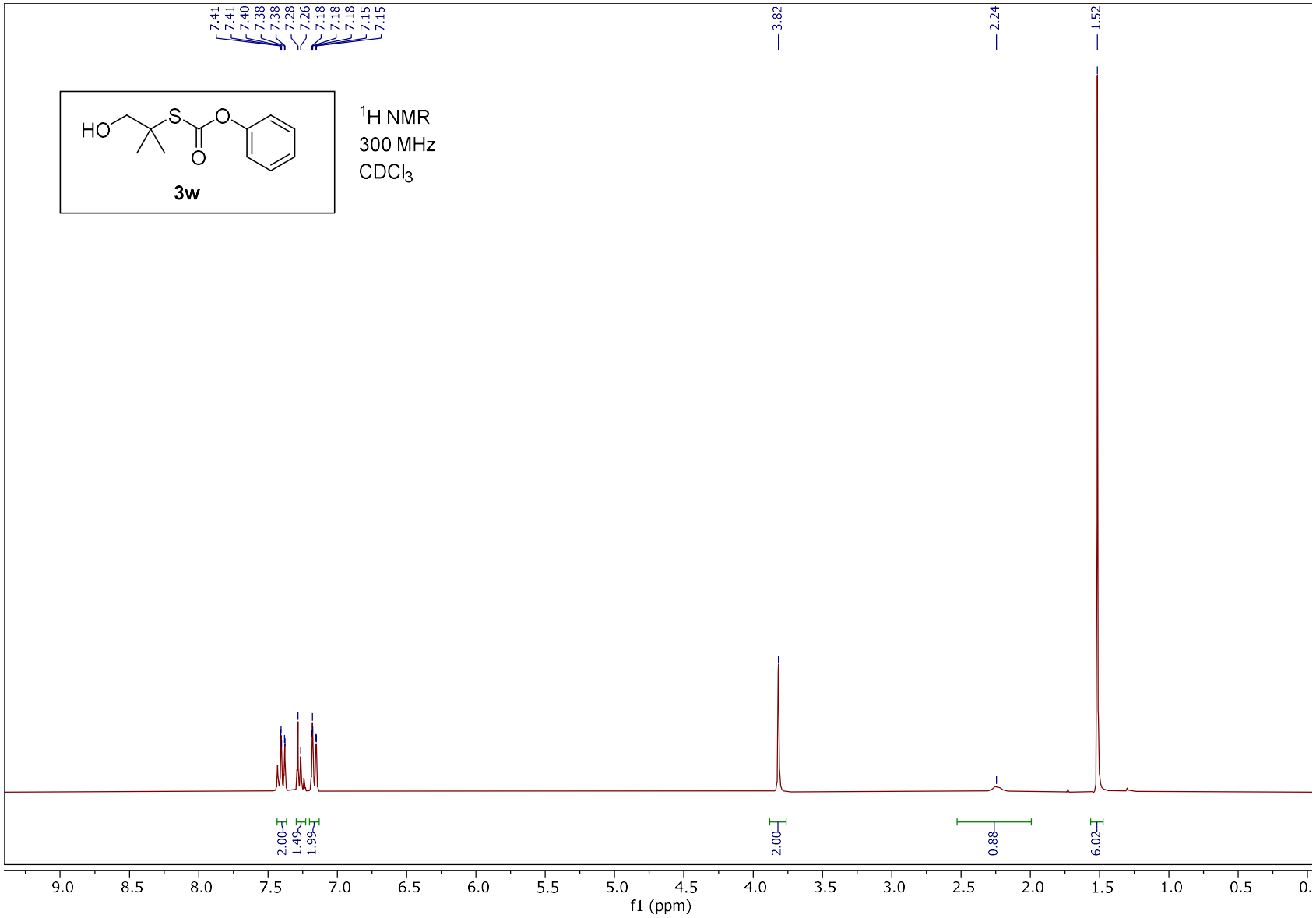

168.74
150.90
140.89
129.62
126.52
126.49
121.25
120.39
115.47
61.74
21.26
S
N
N
O
O
3t
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (мд)

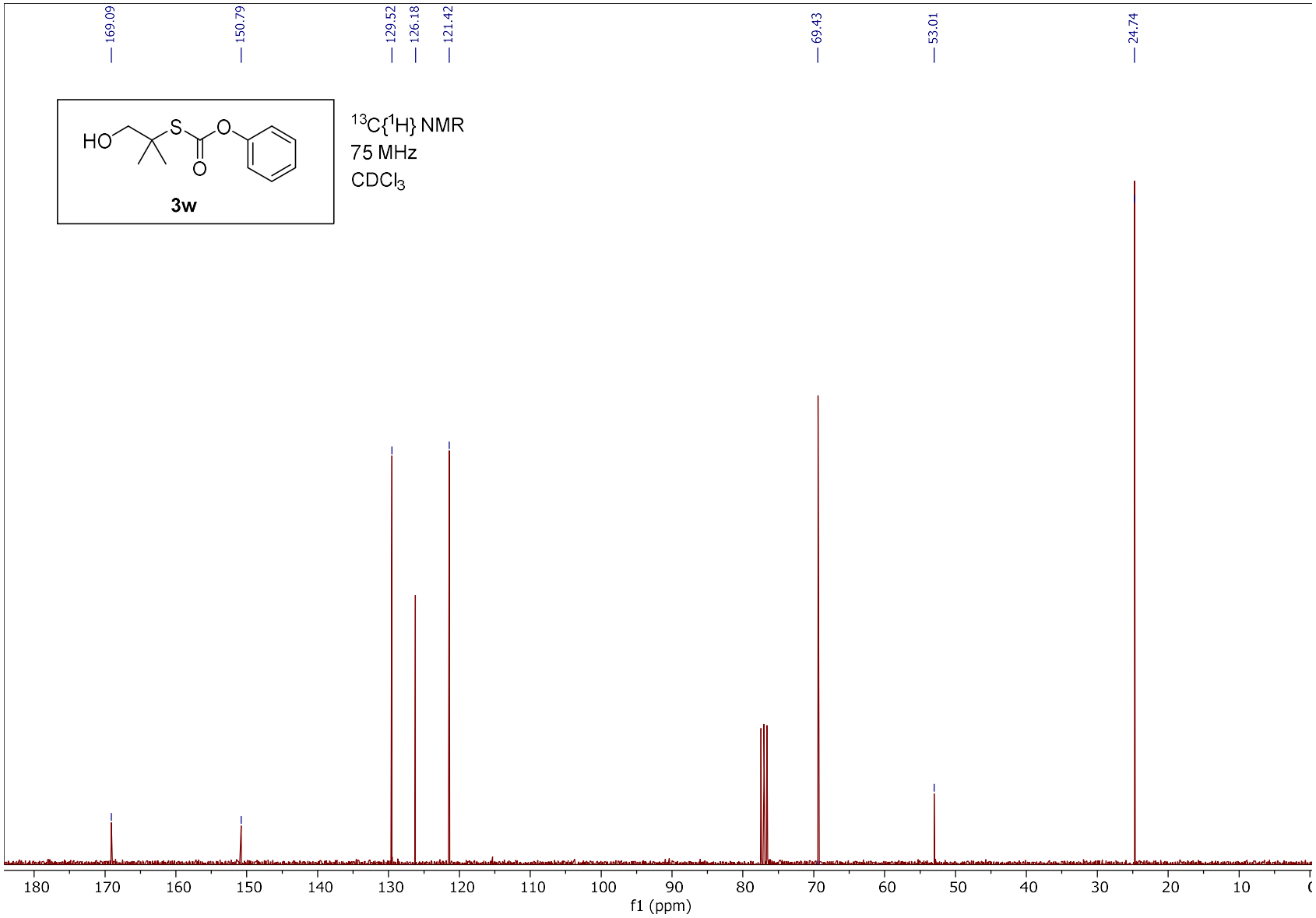

7.30
7.29
7.27
7.25
7.24
7.22
7.18
7.17
7.16
7.15
7.14
7.11
7.10
7.10
7.09
7.08
7.08
7.08
7.06
7.06
7.06
1.84
O
S
O
O
3u
^{1}H NMR
300 MHz
$CDCl_3$
3.82
2.01
5.04
6.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

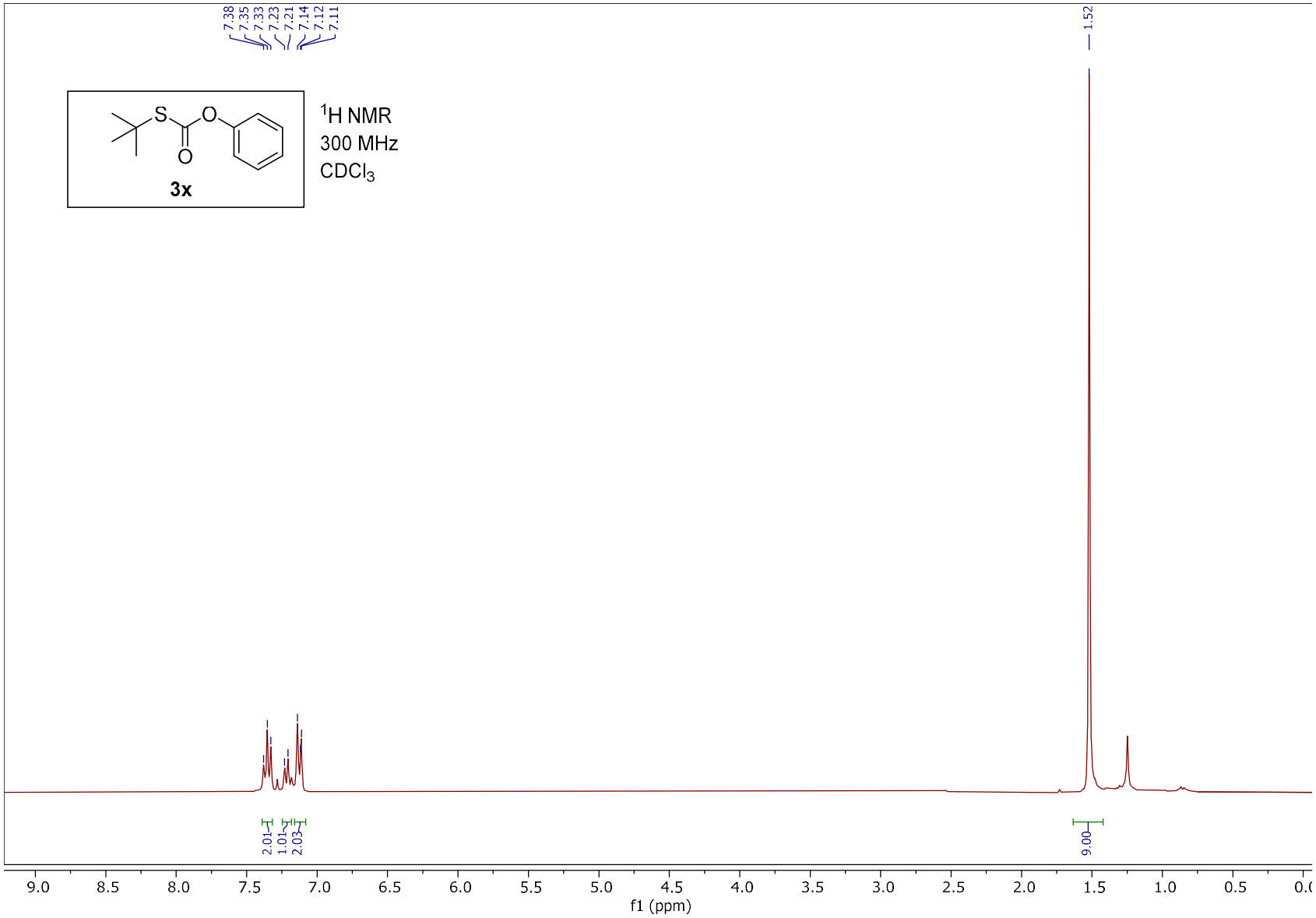

167.63
153.99
150.88
129.54
129.13
126.15
124.75
123.55
121.44
92.33
29.15
O
S
O
O
3u
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

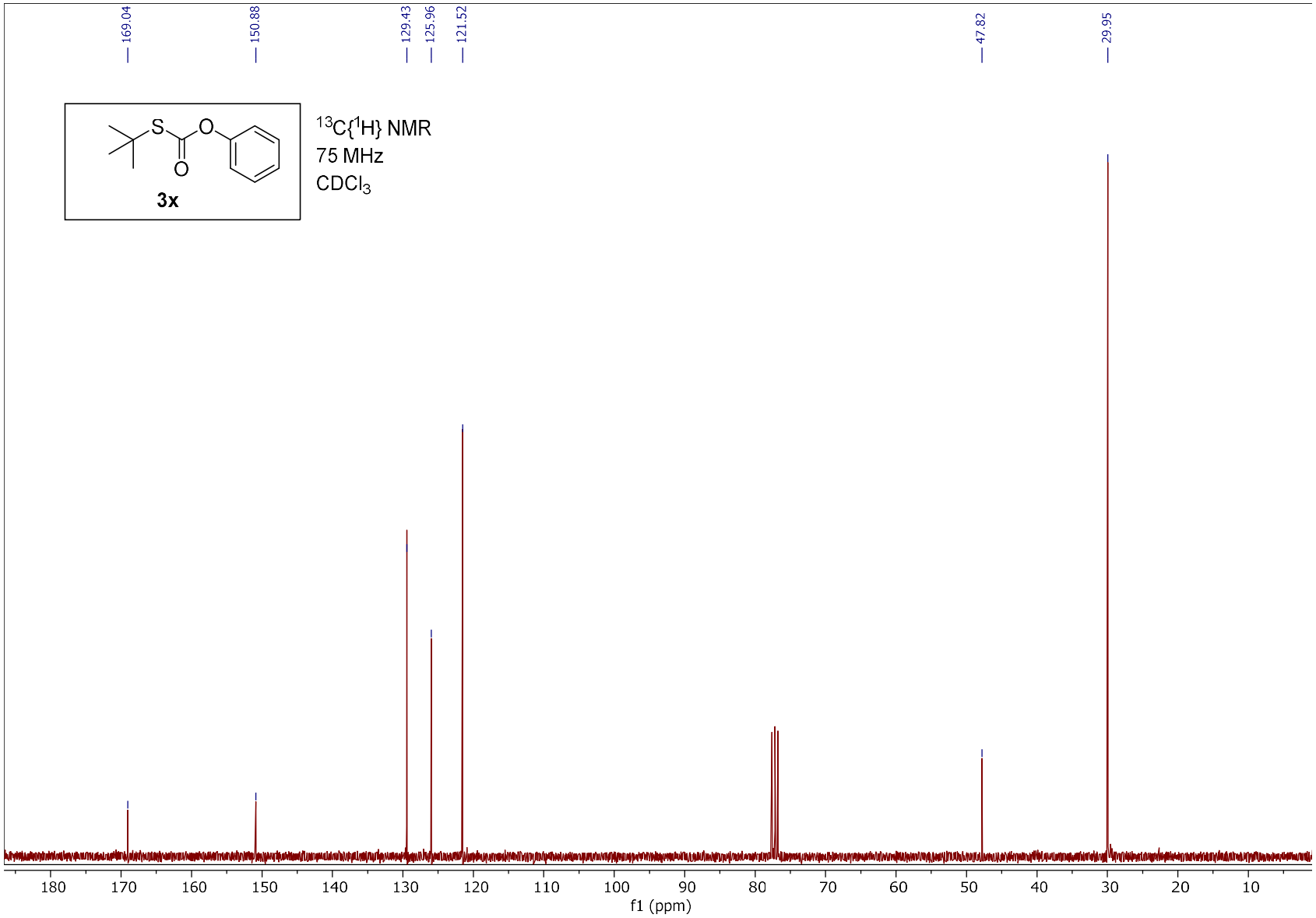

7.44
7.42
7.41
7.39
7.31
7.30
7.30
7.28
7.28
7.27
7.25
7.20
7.19
7.17
7.17
7.17
4.88
4.86
4.69
4.66
1.92
S
O
O
O
3v
1H NMR
300 MHz
CDCl3
2.04
2.33
2.01
2.00
1.99
2.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

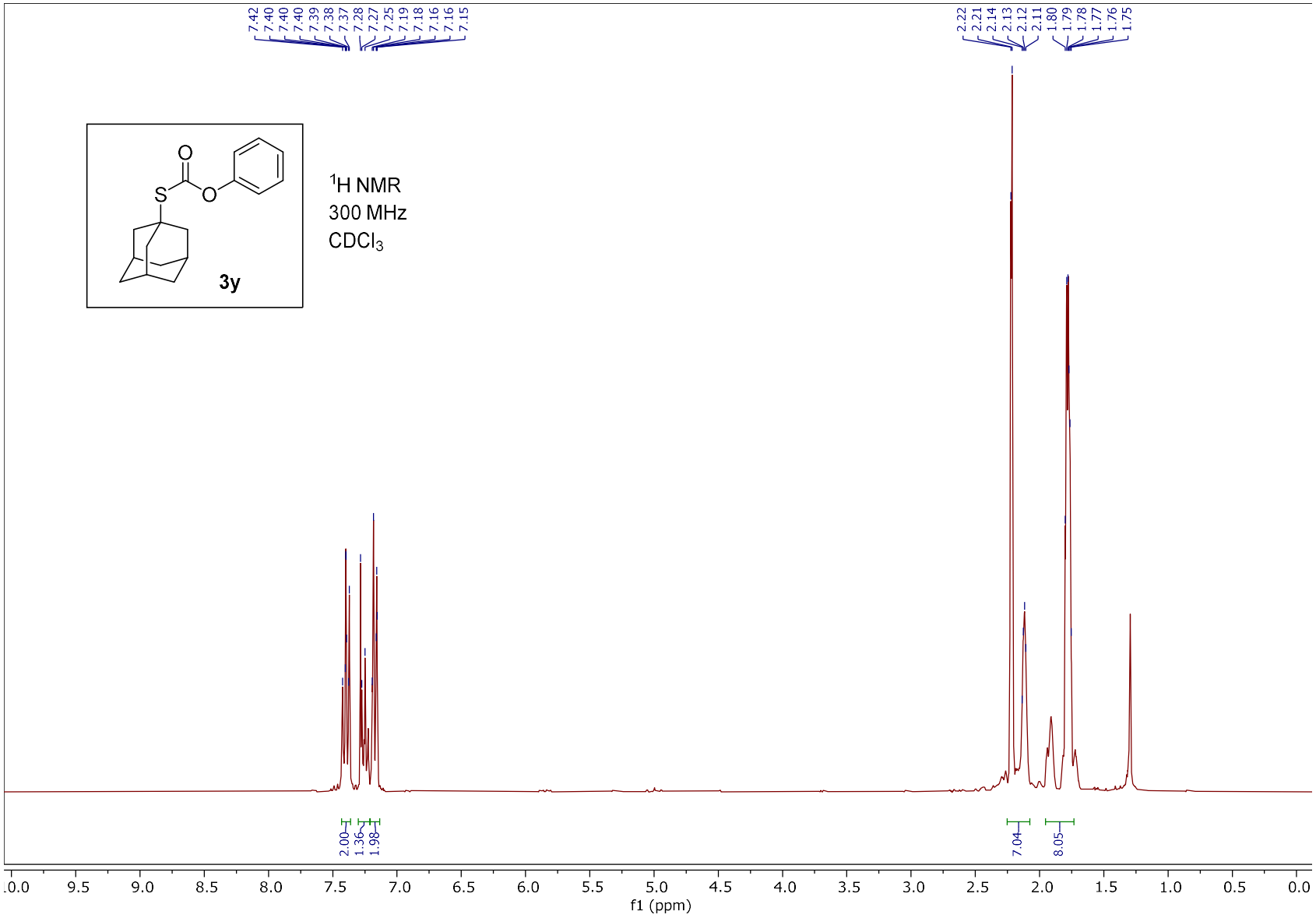

168.09
150.83
129.57
126.37
121.28
83.00
47.52
26.09
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
3v
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

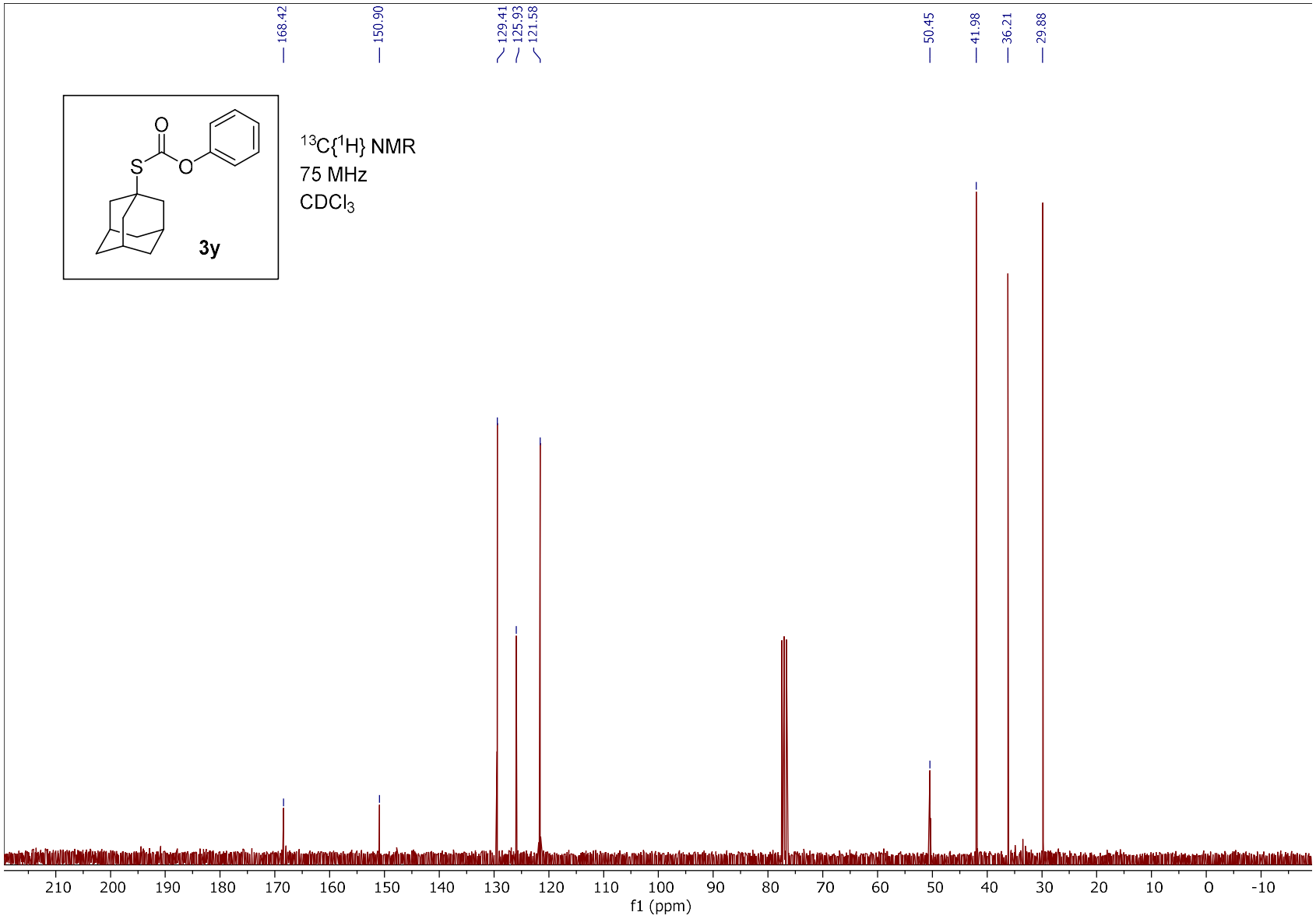

7.41
7.41
7.40
7.38
7.38
7.28
7.26
7.18
7.18
7.18
7.15
7.15
3.82
2.24
1.52
HO
S
O
O
3w
1H NMR
300 MHz
CDCl3
2.00
1.49
1.99
2.00
0.88
6.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

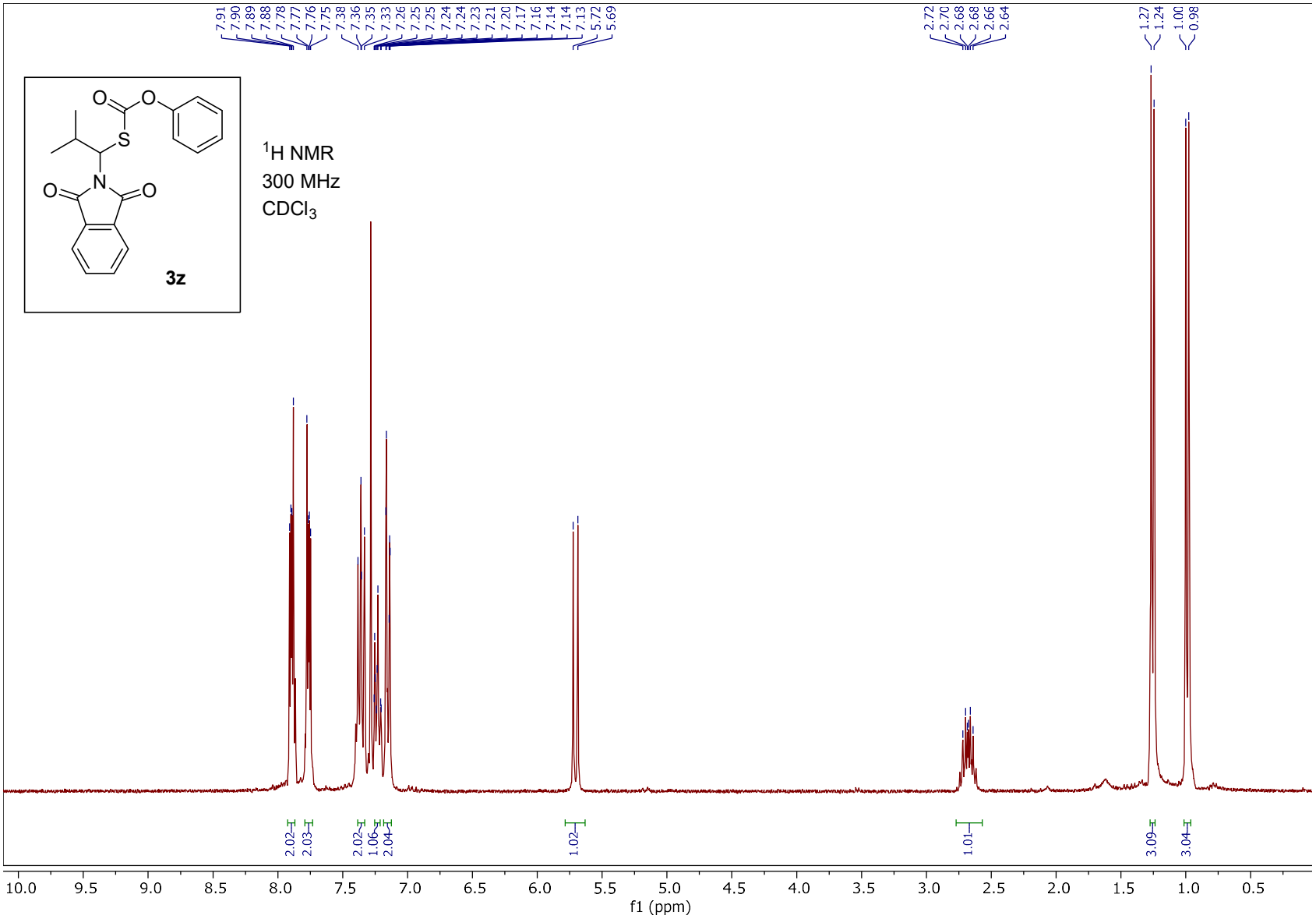

169.09
150.79
129.52
126.18
121.42
69.43
53.01
24.74
HO
S
O
O
3w
13C{1H} NMR
75 MHz
CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

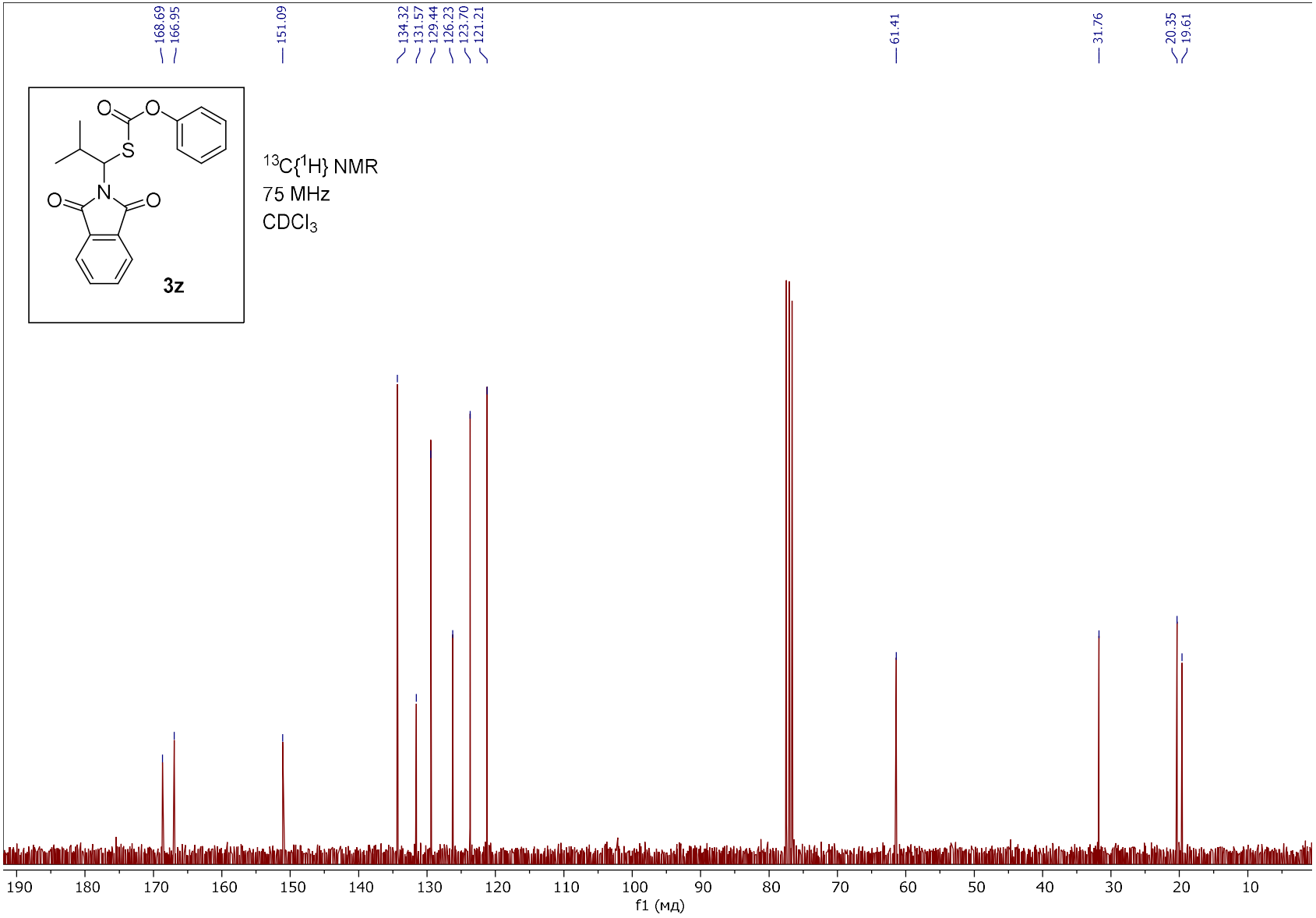

7.38
7.35
7.33
7.23
7.21
7.14
7.12
7.11
1.52
S
O
O
3x
^{1}H NMR
300 MHz
$CDCl_3$
2.01
1.01
2.03
9.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

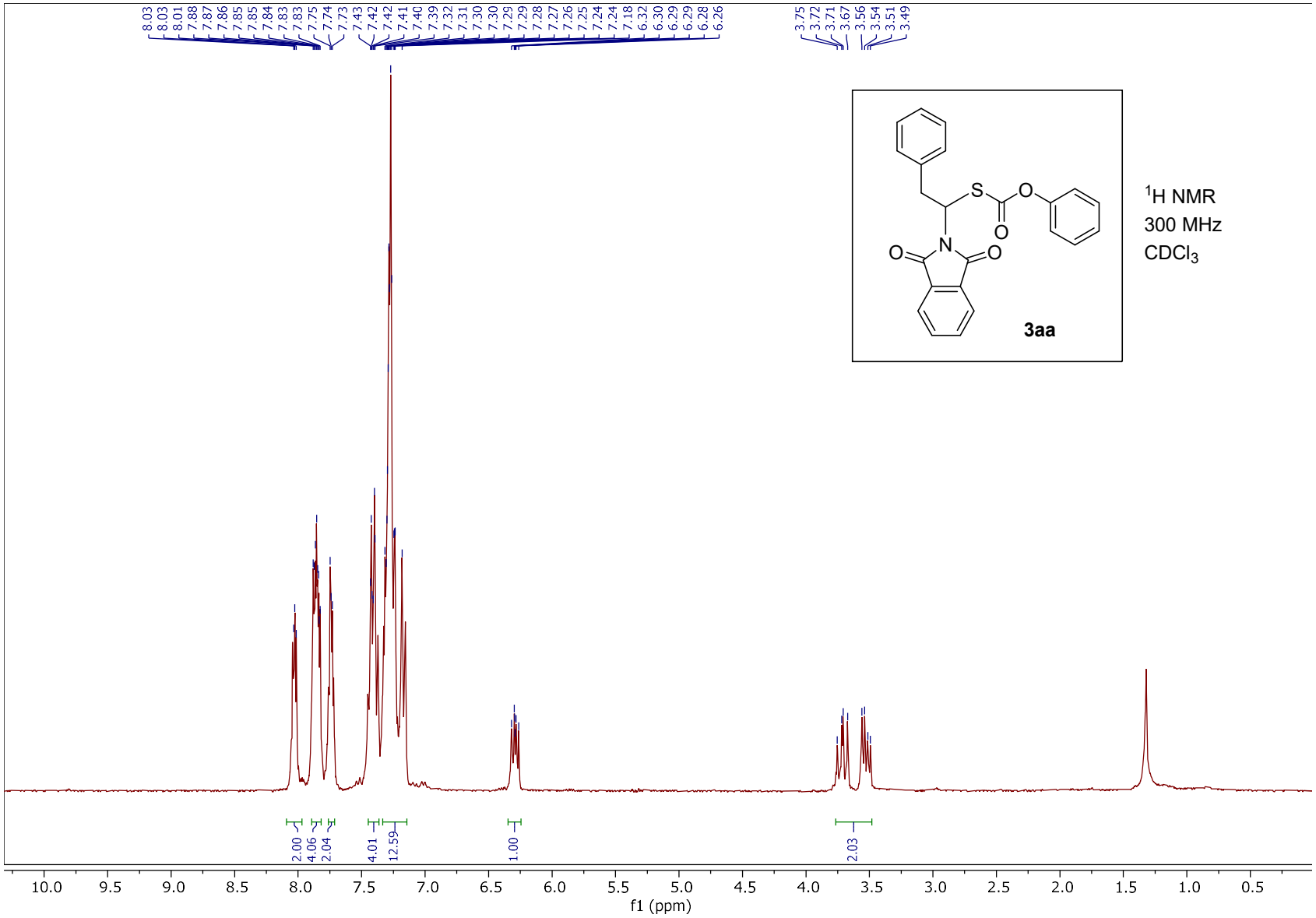

169.04
150.88
129.43
125.96
121.52
47.82
29.95
S
O
O
3x
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

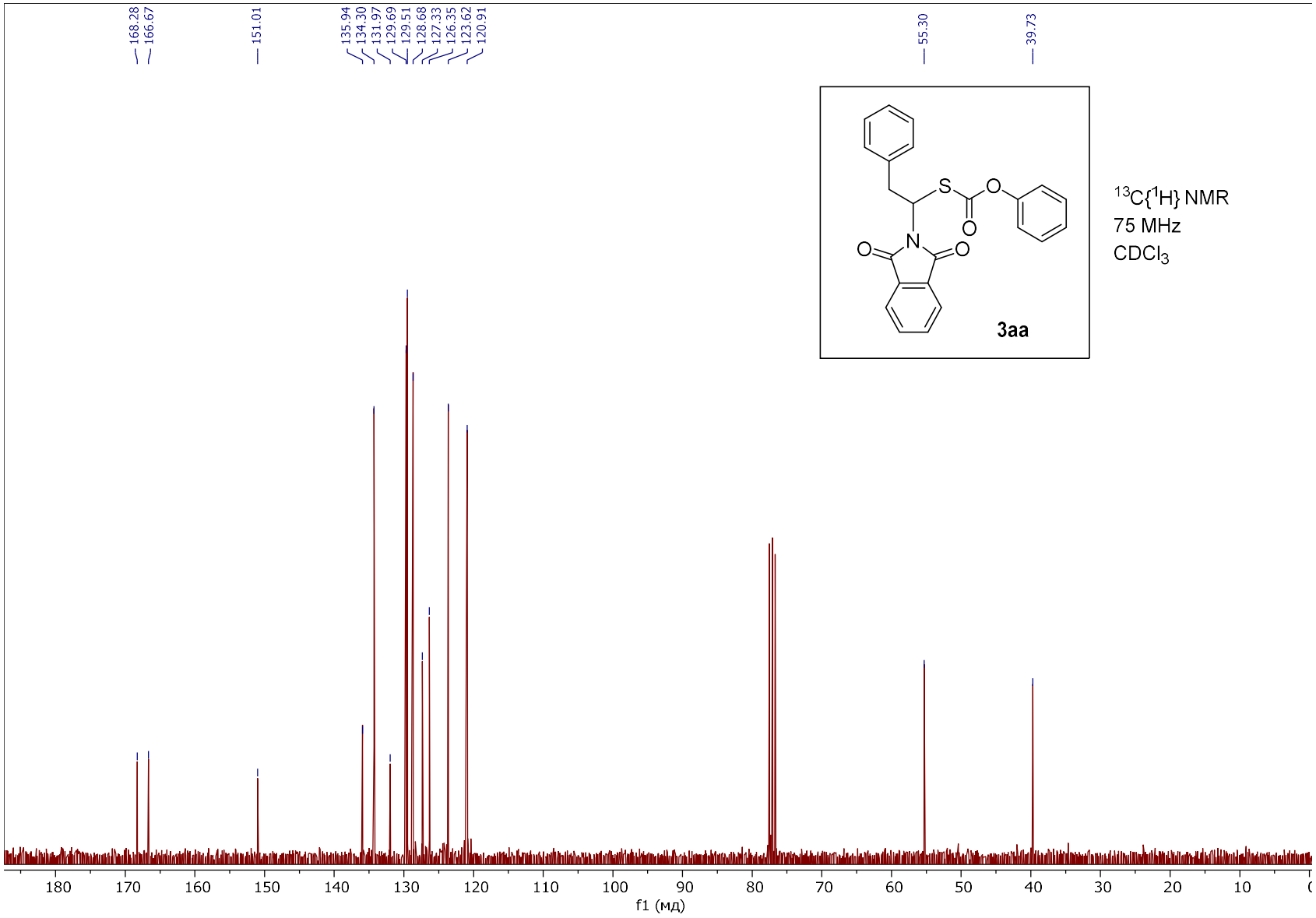

7.42
7.40
7.40
7.40
7.39
7.38
7.37
7.28
7.27
7.25
7.19
7.18
7.16
7.16
7.15
2.22
2.21
2.14
2.13
2.12
2.11
1.80
1.79
1.78
1.77
1.76
1.75
O
S
O
3y
1H NMR
300 MHz
CDCl3
2.00
1.36
1.98
7.04
8.05
.0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

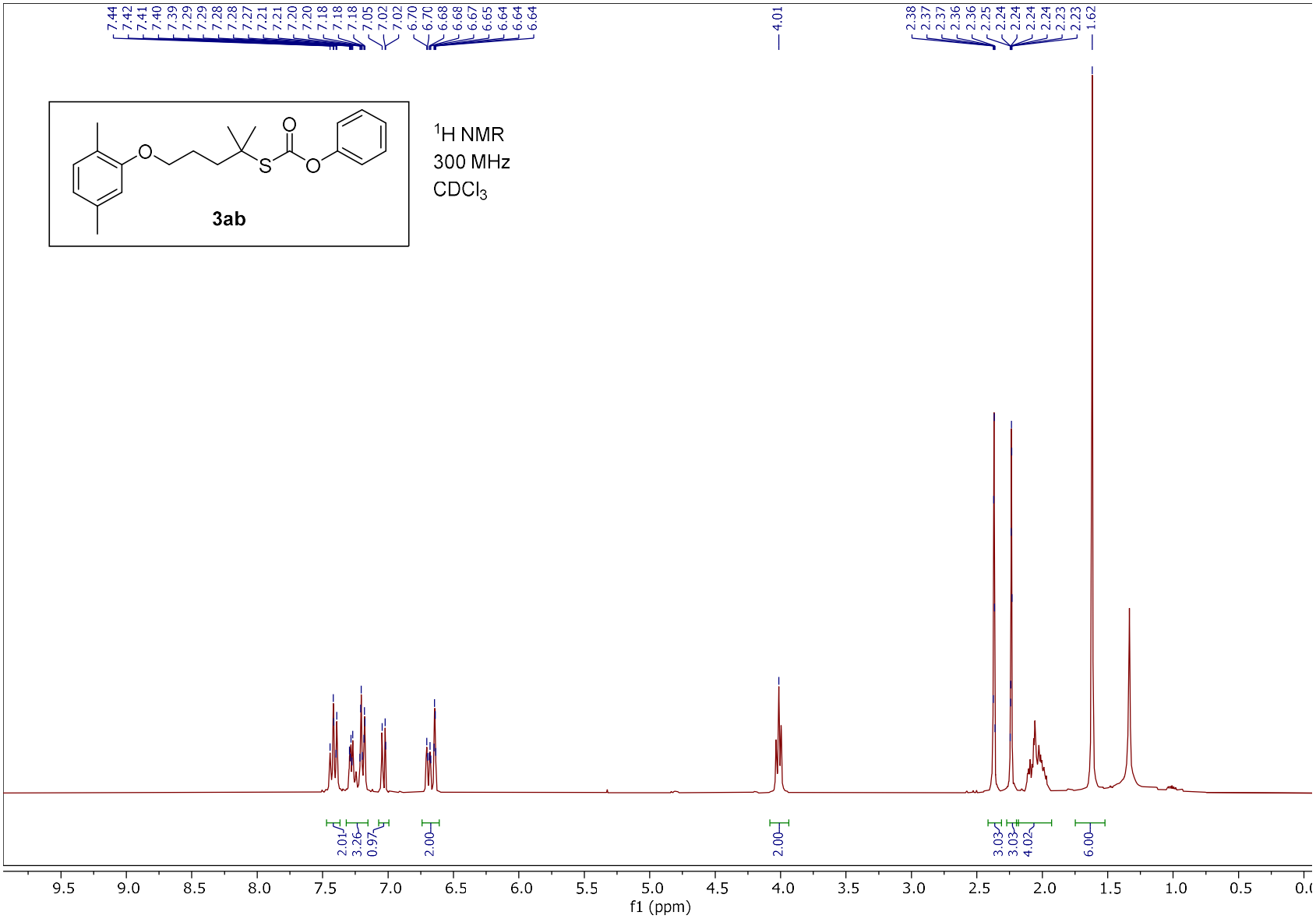

168.42
150.90
129.41
125.93
121.58
50.45
41.98
36.21
29.88
O
S
O
3y
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

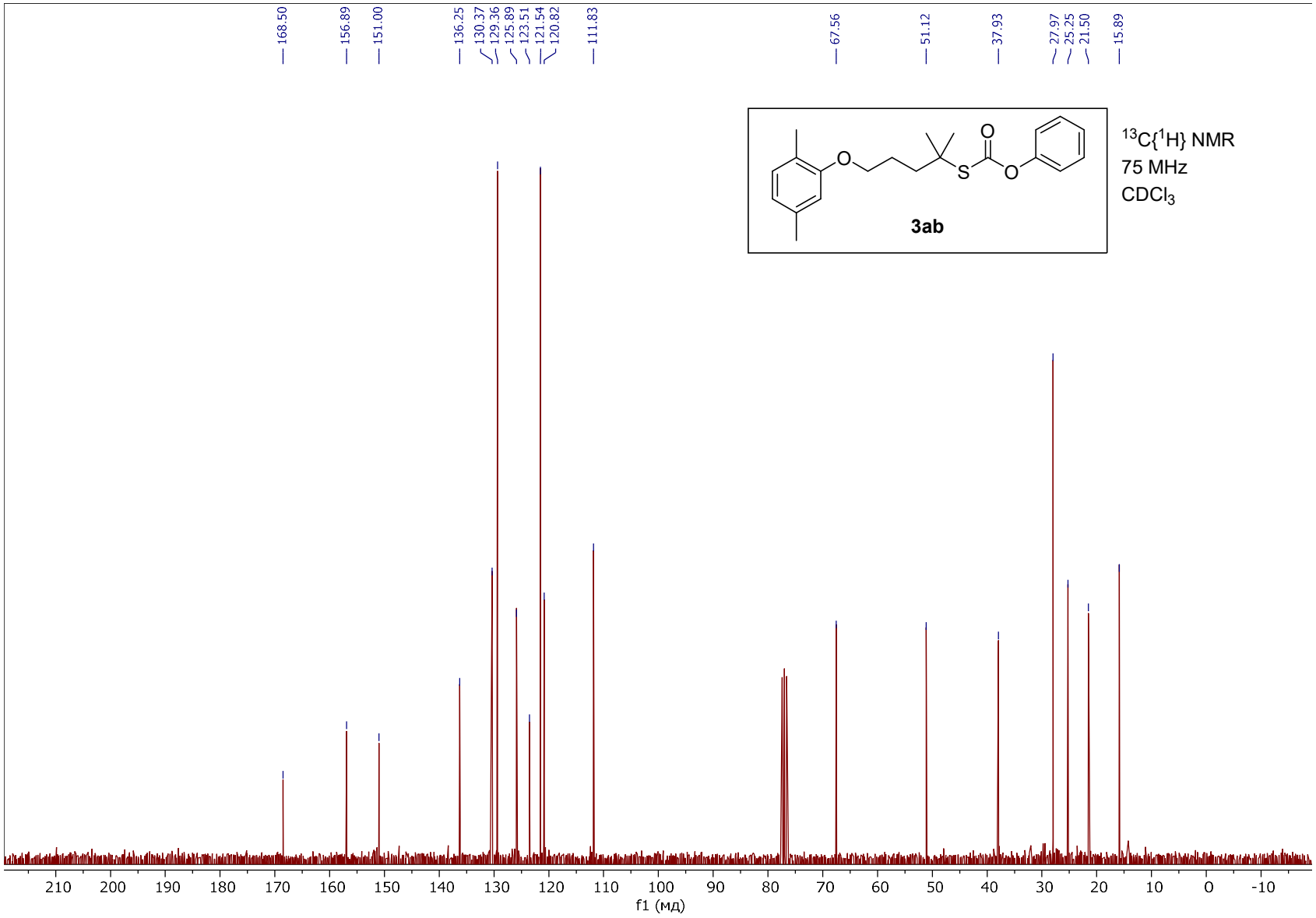

7.91
7.90
7.89
7.88
7.78
7.77
7.76
7.75
7.38
7.36
7.35
7.33
7.26
7.25
7.25
7.24
7.24
7.23
7.21
7.20
7.17
7.16
7.14
7.14
7.13
5.72
5.69
2.72
2.70
2.68
2.68
2.66
2.64
1.27
1.24
1.00
0.98
O
O
S
N
O
O
3z
1H NMR
300 MHz
CDCl3
2.02
2.03
2.02
1.06
2.04
1.02
1.01
3.09
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

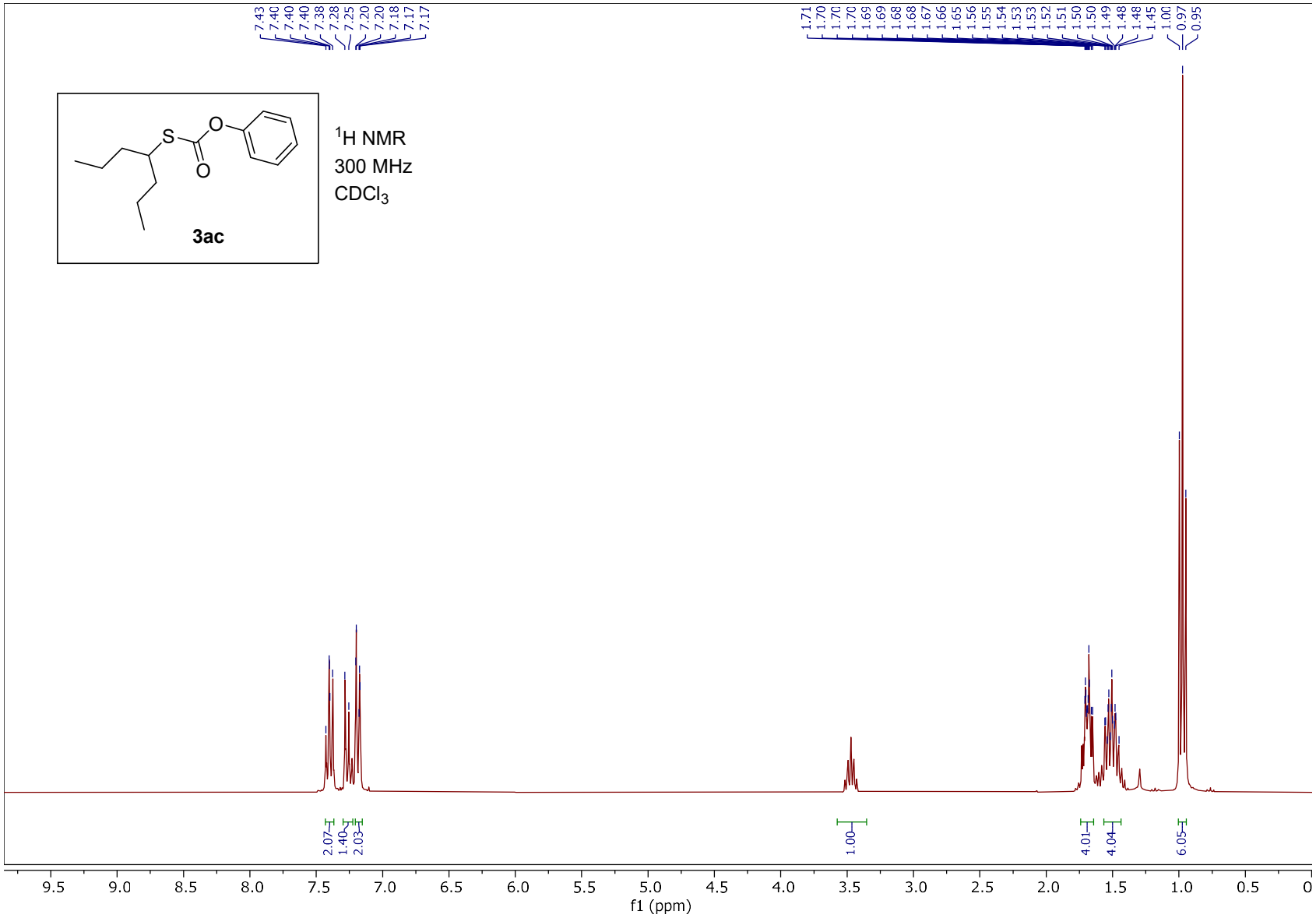

168.69
166.95
151.09
134.32
131.57
129.44
126.23
123.70
121.21
61.41
31.76
20.35
19.61
O
O
S
N
O
O
3z
13C{1H} NMR
75 MHz
CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

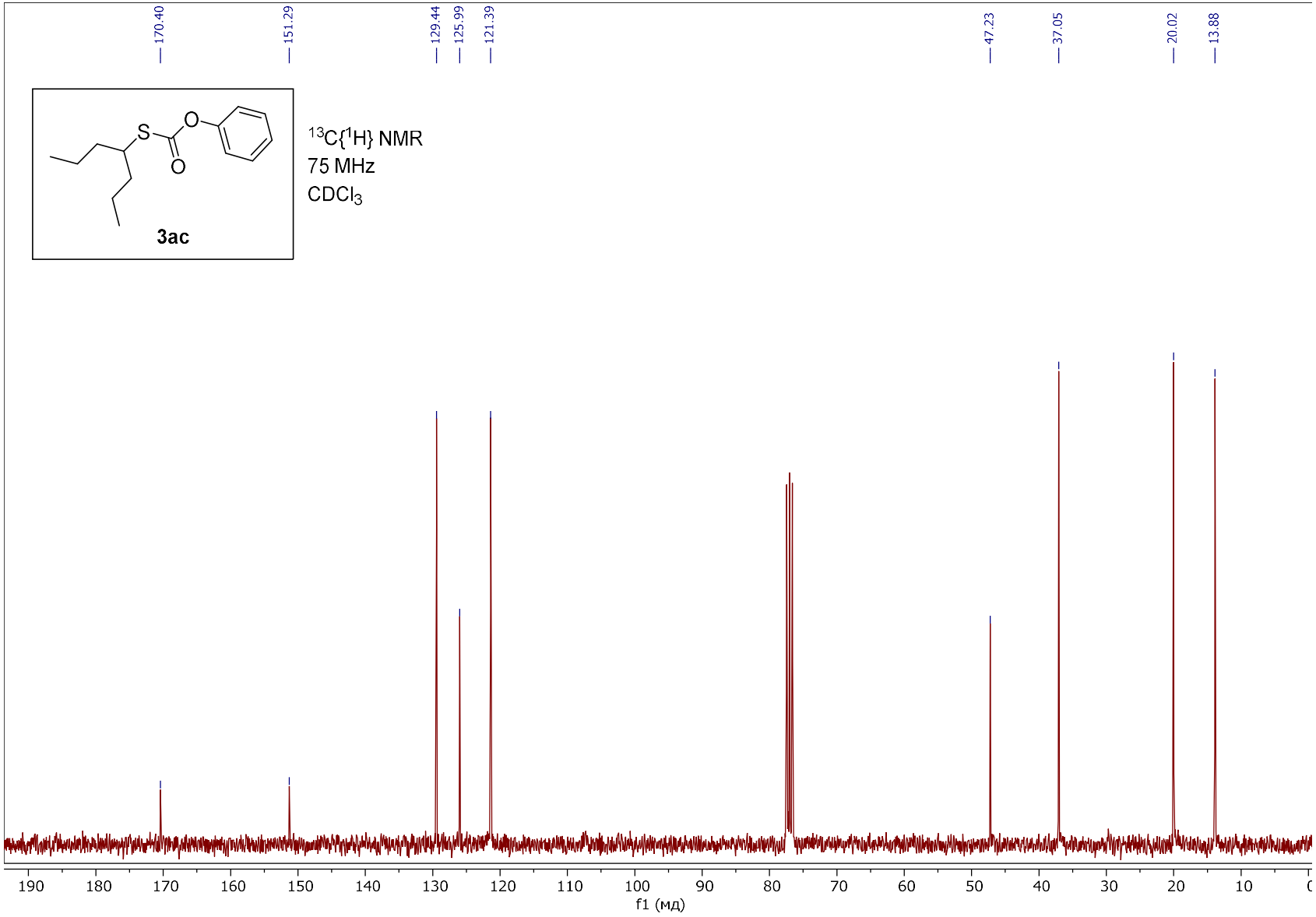

8.03 8.03 8.01 7.88 7.87 7.86 7.85 7.85 7.84 7.83 7.83 7.75 7.74 7.73 7.43 7.42 7.42 7.41 7.40 7.39 7.32 7.31 7.30 7.30 7.29 7.29 7.28 7.27 7.26 7.25 7.24 7.24 7.18 6.32 6.30 6.29 6.29 6.28 6.26
3.75 3.72 3.71 3.67 3.56 3.54 3.51 3.49
S
O
O
N
O
O
3aa
^{1}H NMR
300 MHz
$CDCl_3$
2.00 4.06 2.04 4.01 12.59 1.00 2.03
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
f1 (ppm)

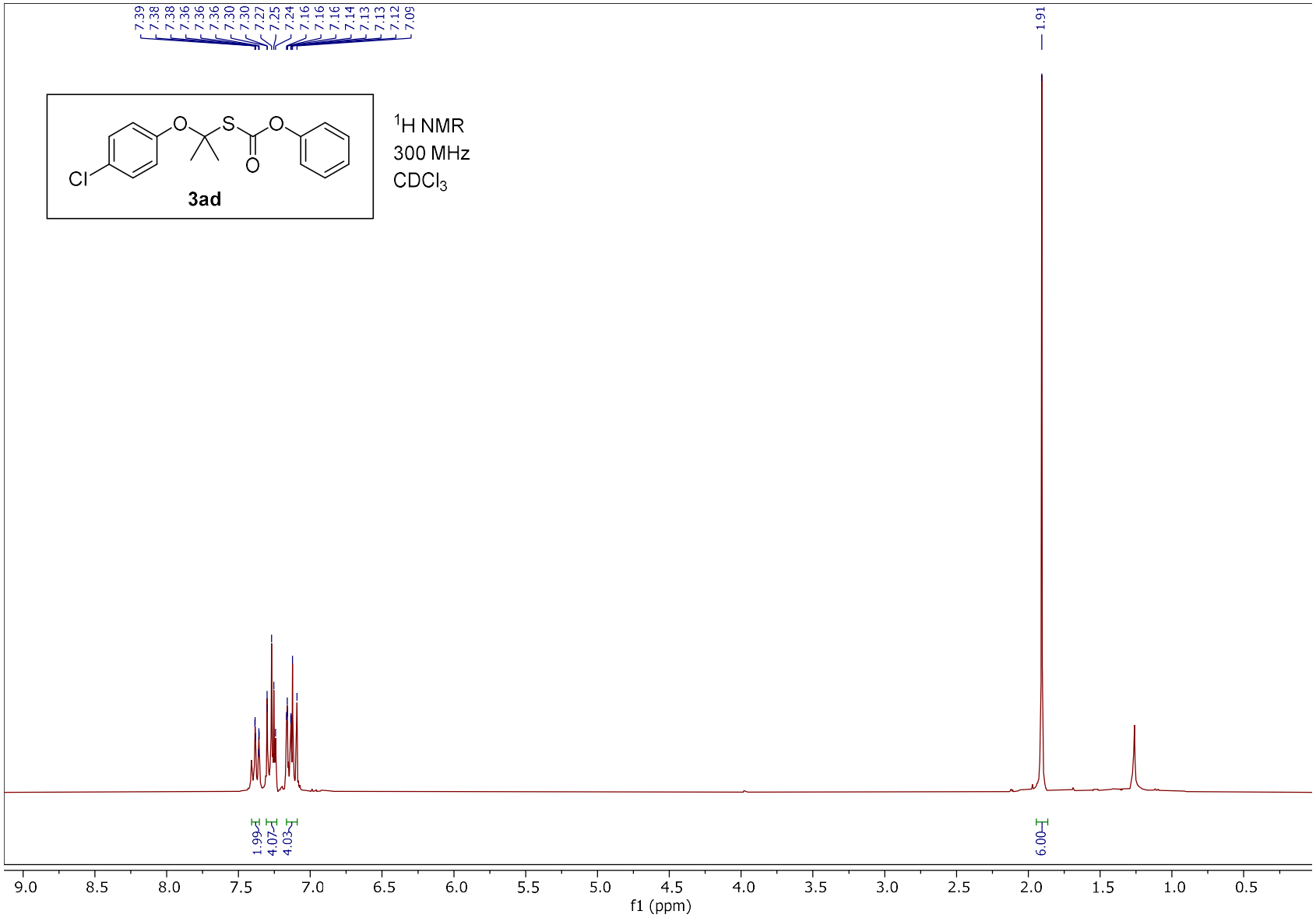

168.28
166.67
151.01
135.94
134.30
131.97
129.69
129.51
128.68
127.33
126.35
123.62
120.91
55.30
39.73
S
O
O
N
O
O
3aa
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

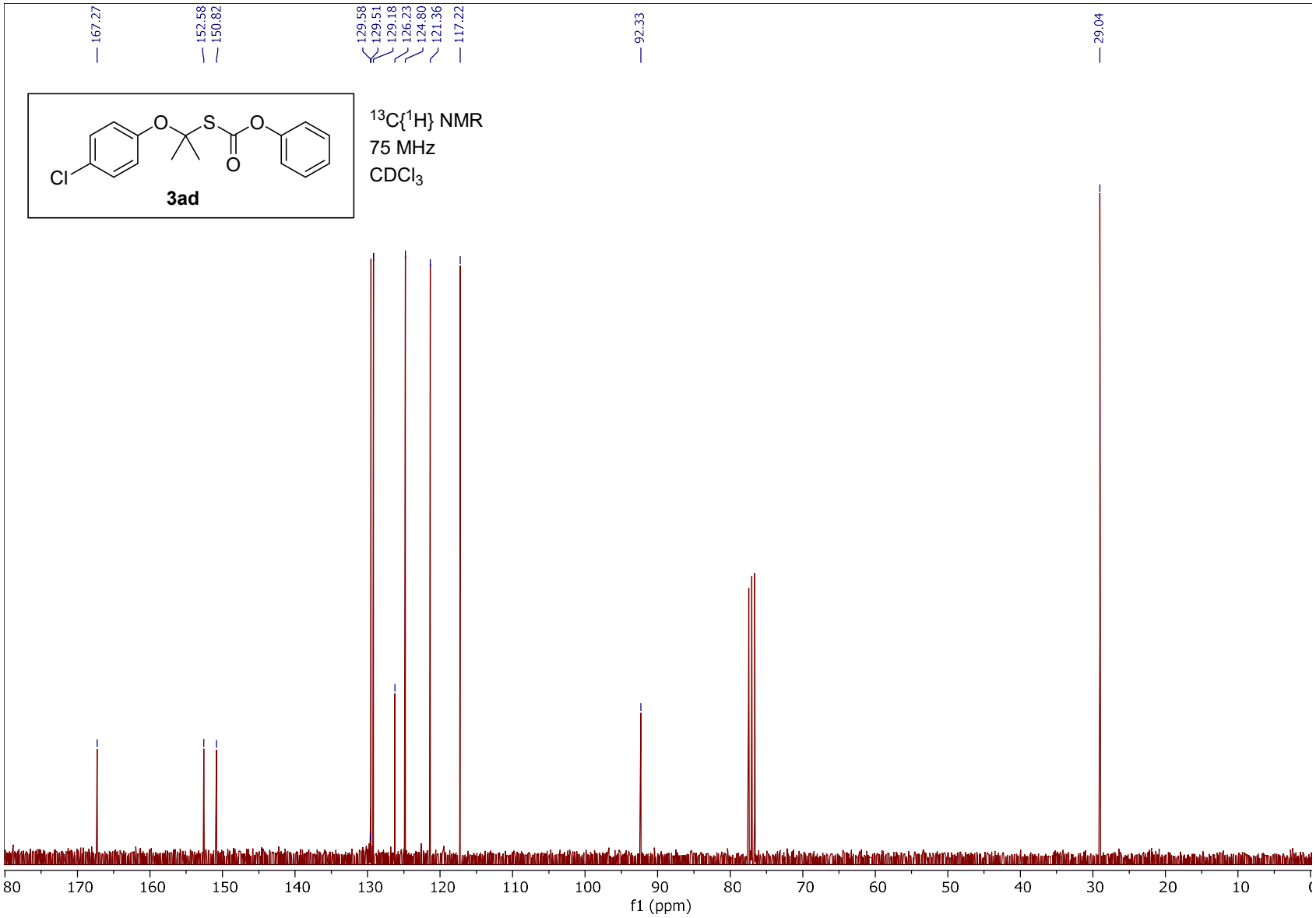

7.44
7.42
7.41
7.40
7.39
7.29
7.29
7.28
7.28
7.27
7.21
7.21
7.20
7.20
7.18
7.18
7.18
7.05
7.02
7.02
6.70
6.70
6.68
6.68
6.67
6.65
6.64
6.64
6.64
4.01
2.38
2.37
2.37
2.36
2.36
2.25
2.24
2.24
2.24
2.24
2.23
1.62
O
O
S
O
3ab
1H NMR
300 MHz
CDCl3
2.01
3.26
0.97
2.00
2.00
3.03
3.03
4.02
6.00
9.5
9.0
8.5
8.0
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
f1 (ppm)

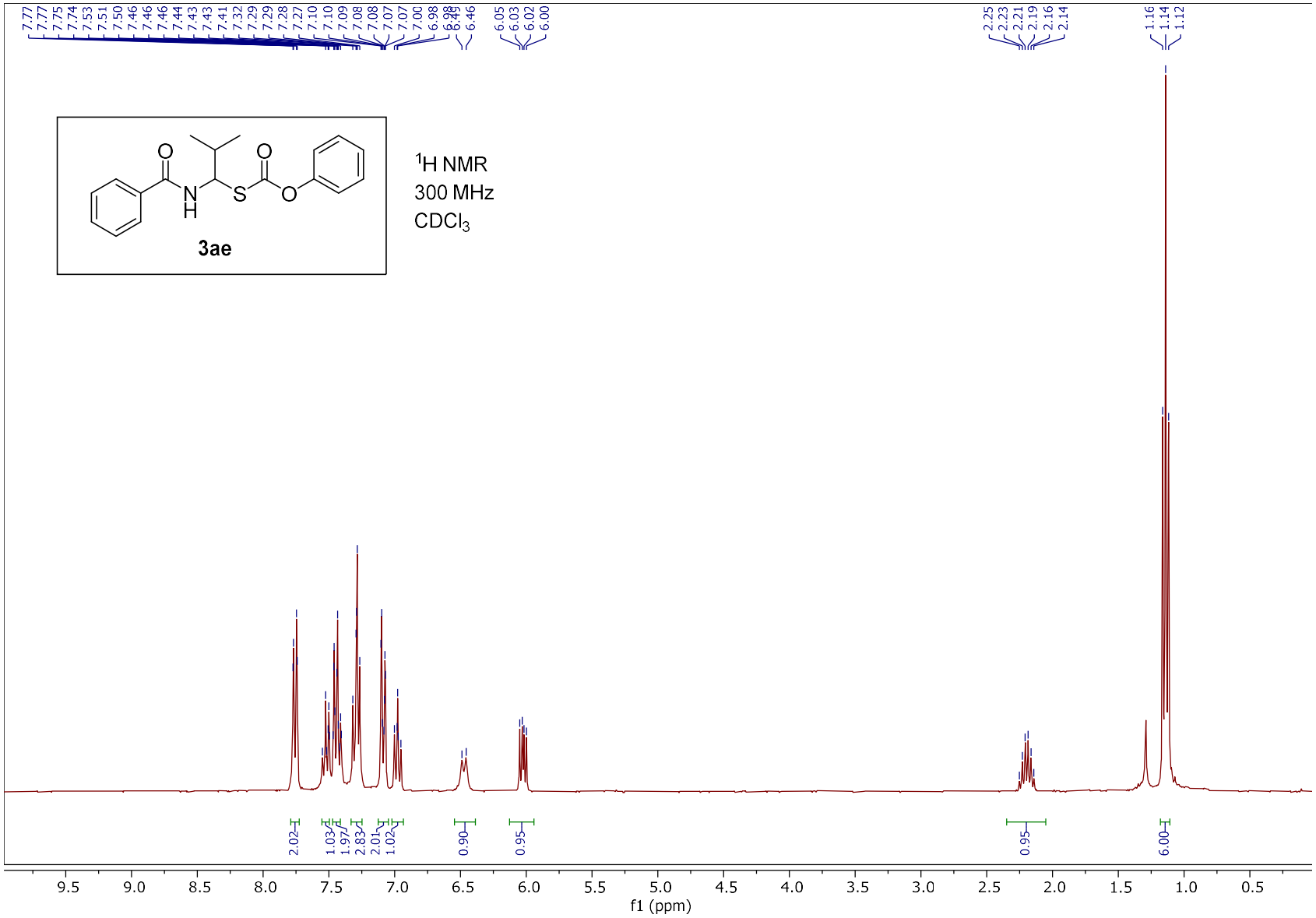

168.50
156.89
151.00
136.25
130.37
129.36
125.89
123.51
121.54
120.82
111.83
67.56
51.12
37.93
27.97
25.25
21.50
15.89
O
O
S
O
3ab
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)

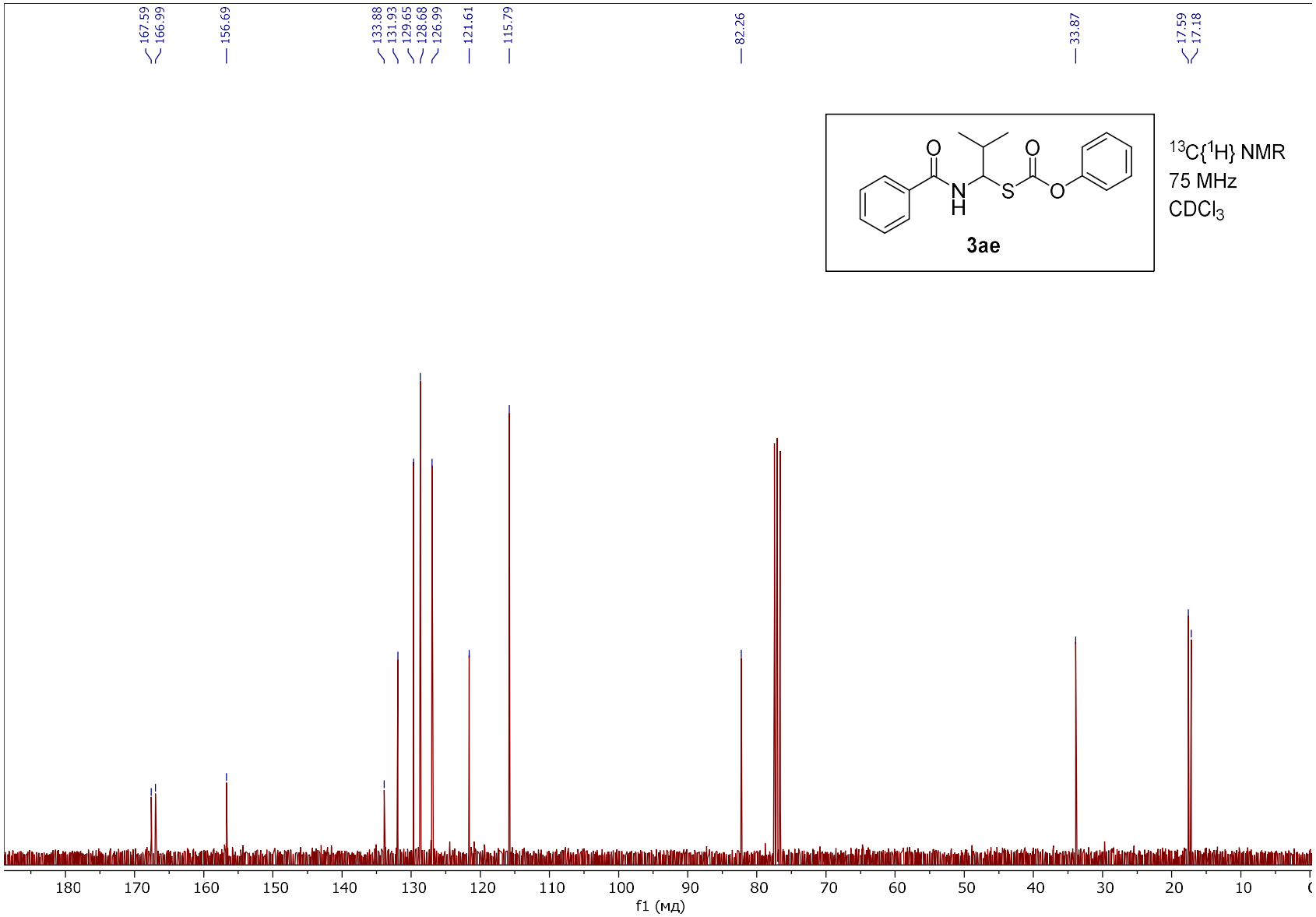

7.43
7.40
7.40
7.40
7.38
7.28
7.25
7.20
7.20
7.18
7.17
7.17
1.71
1.70
1.70
1.70
1.69
1.69
1.68
1.68
1.67
1.66
1.65
1.56
1.55
1.54
1.53
1.53
1.52
1.51
1.50
1.50
1.49
1.48
1.48
1.45
1.00
0.97
0.95
S
O
O
3ac
1H NMR
300 MHz
CDCl3
2.07
1.40
2.03
1.00
4.01
4.04
6.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

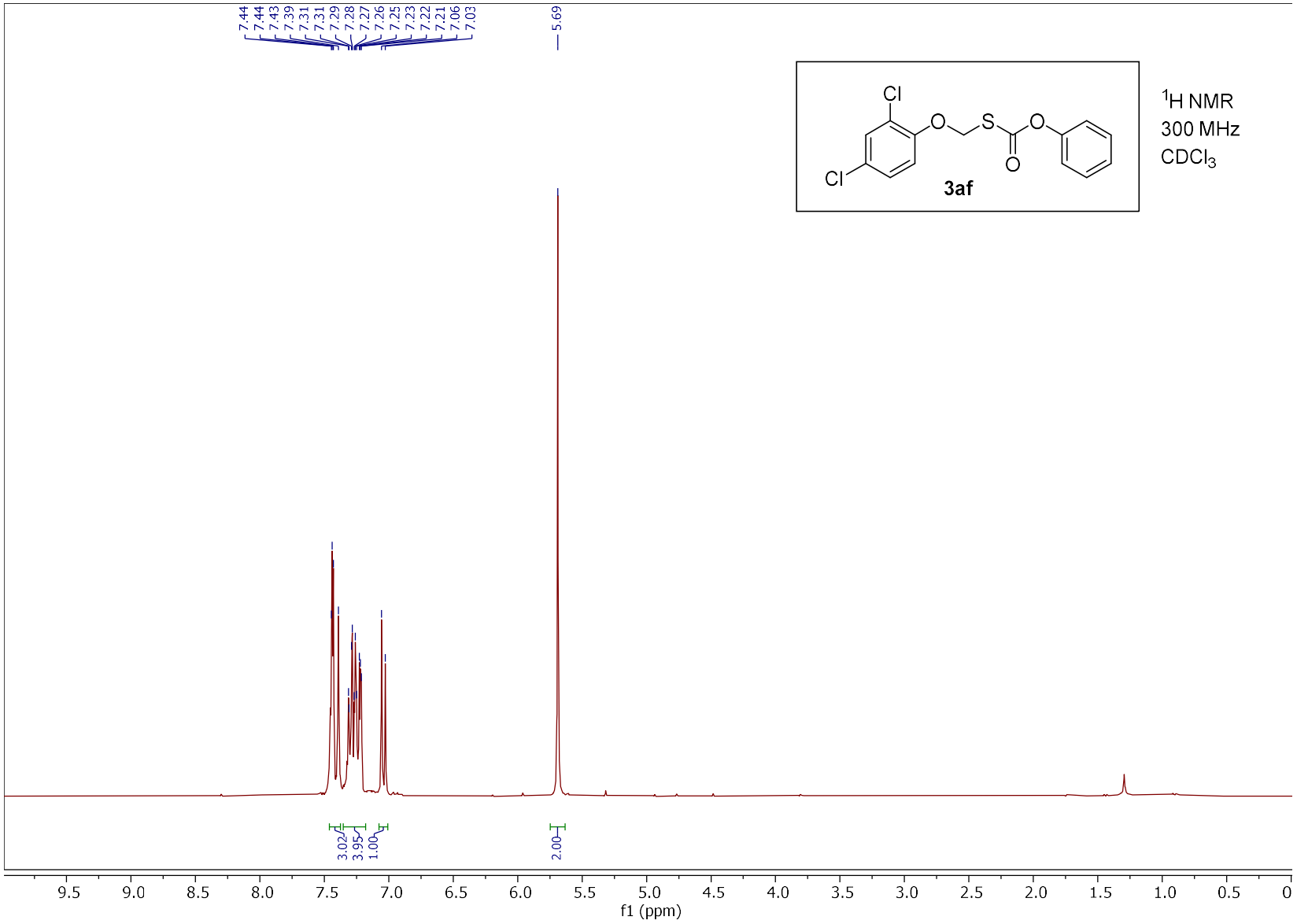

170.40
151.29
129.44
125.99
121.39
47.23
37.05
20.02
13.88
S
O
O
3ac
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

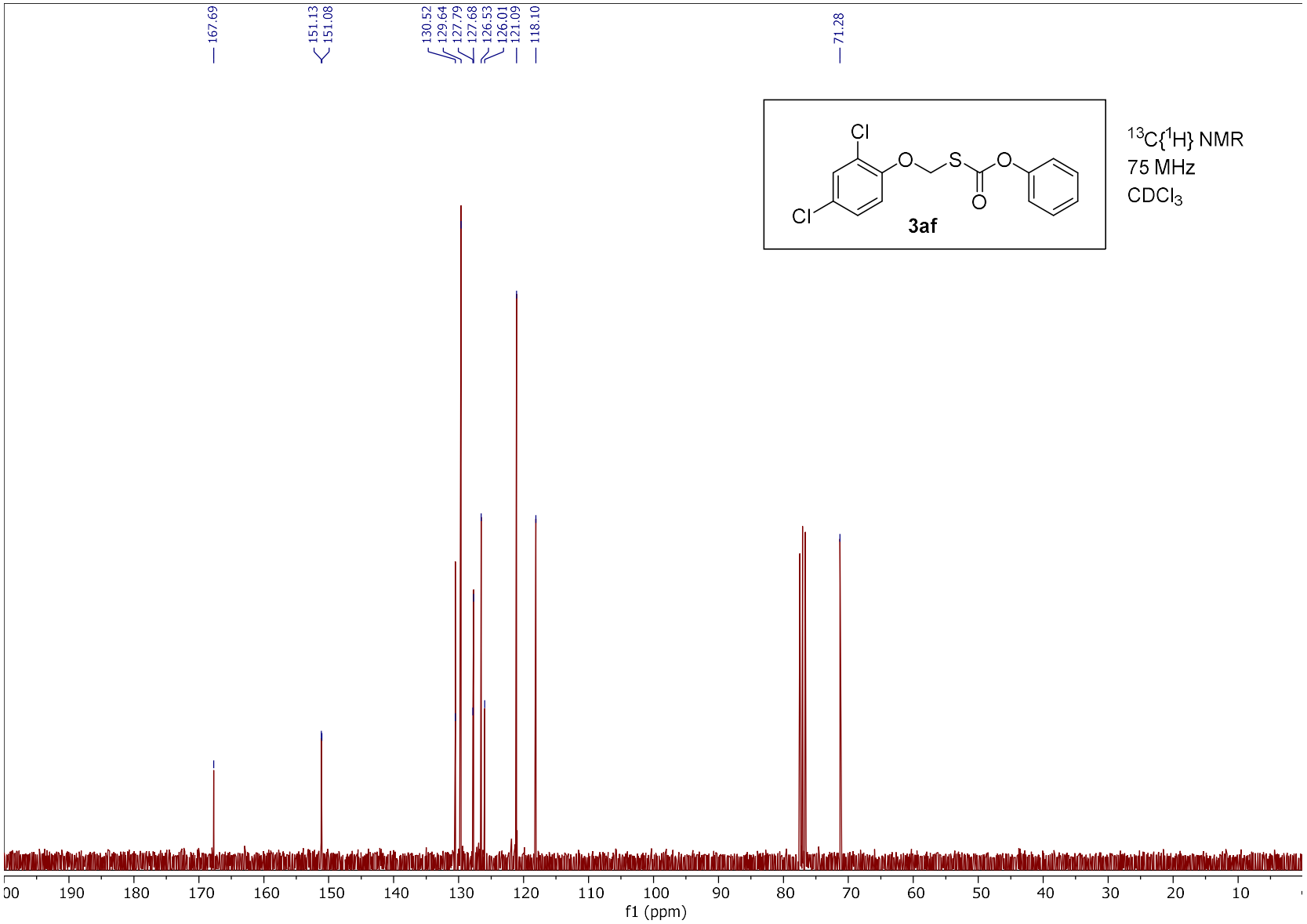

7.39
7.38
7.38
7.36
7.36
7.36
7.30
7.30
7.27
7.25
7.24
7.16
7.16
7.16
7.14
7.13
7.12
7.09
1.91
Cl
O
S
O
O
3ad
^{1}H NMR
300 MHz
$CDCl_3$
1.99
4.07
4.03
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

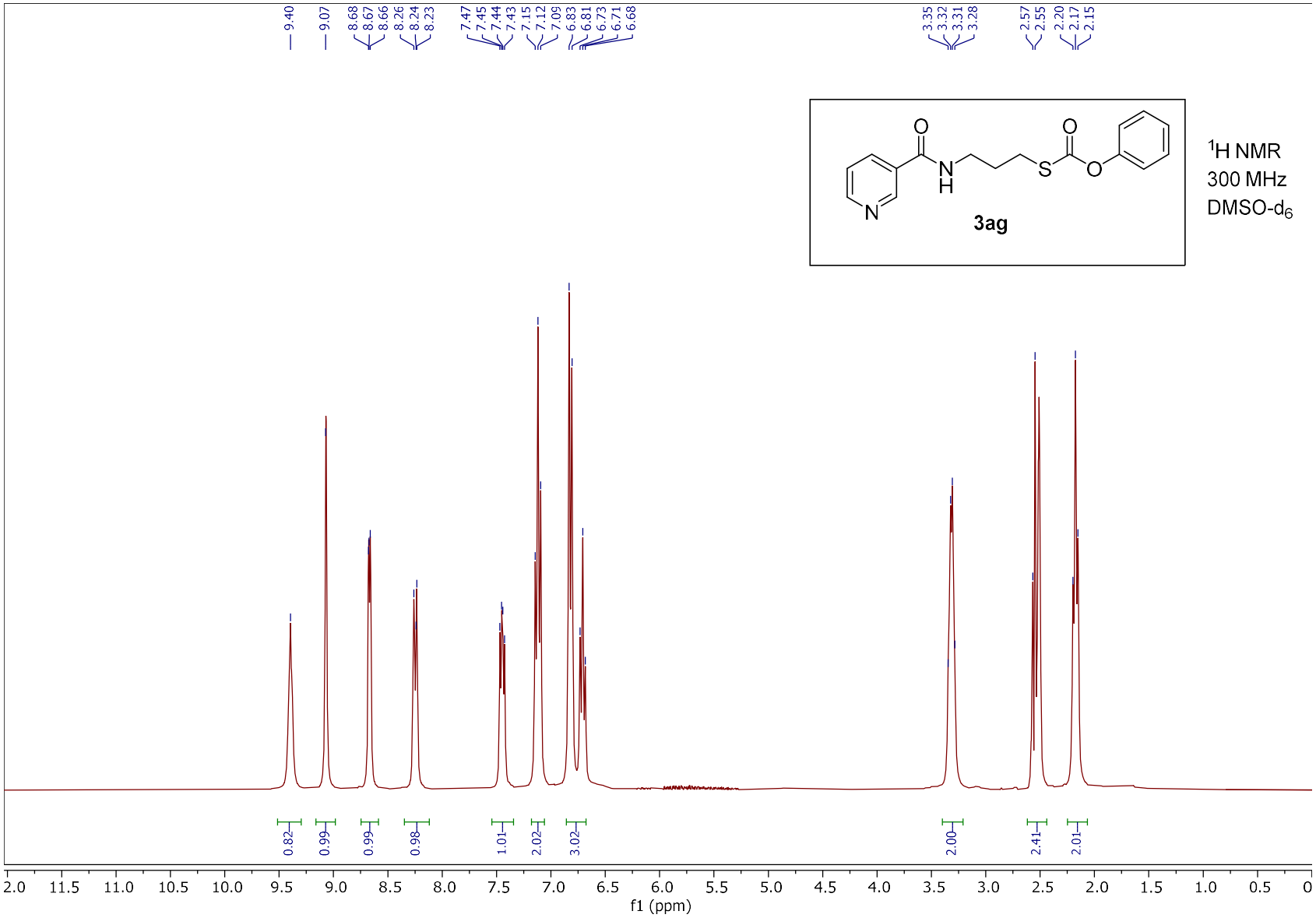

167.27
152.58
150.82
129.58
129.51
129.18
126.23
124.80
121.36
117.22
92.33
29.04
Cl
O
S
O
O
3ad
13C{1H} NMR
75 MHz
CDCl3
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

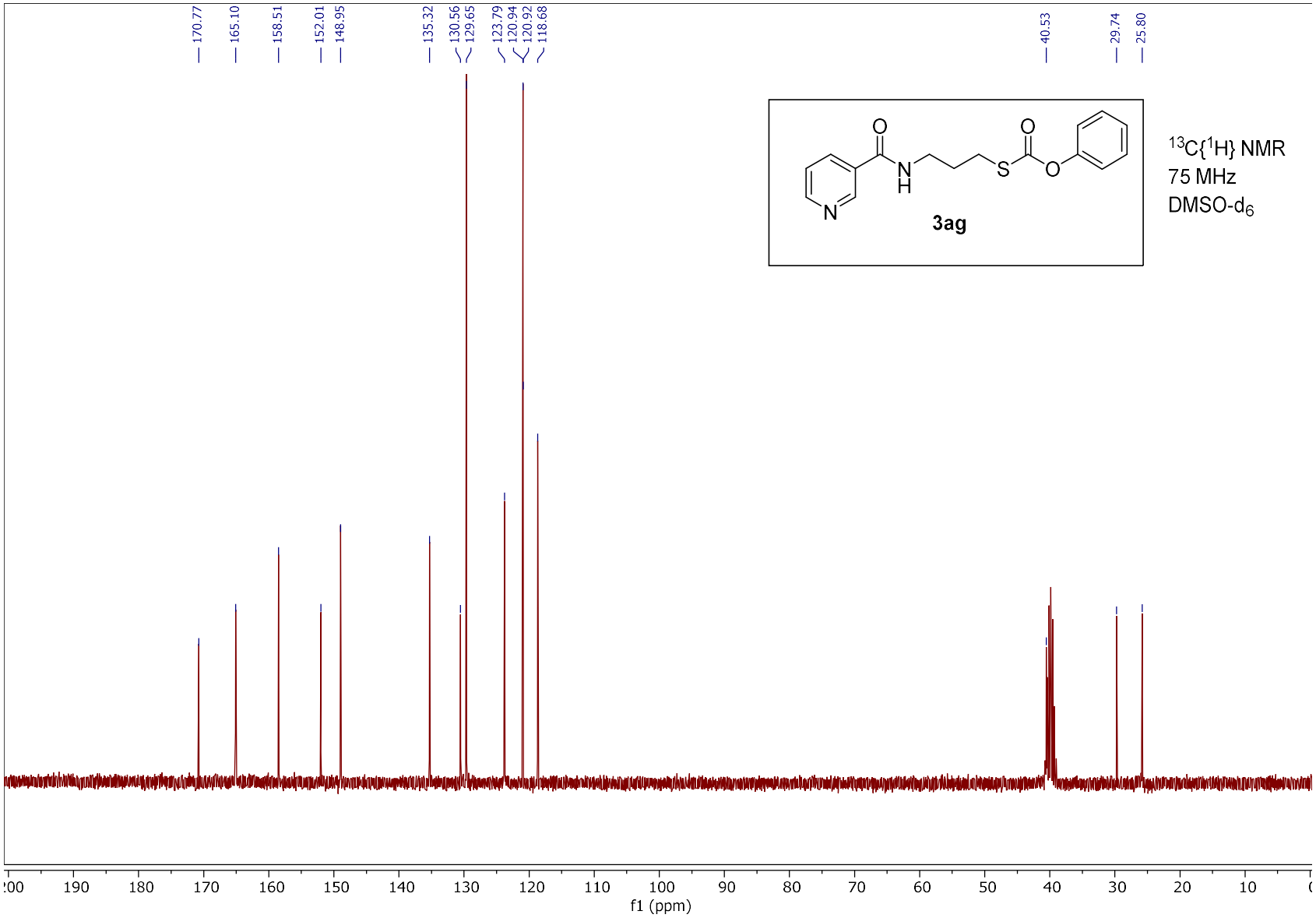

7.77
7.77
7.75
7.74
7.53
7.51
7.50
7.46
7.46
7.46
7.44
7.43
7.43
7.41
7.32
7.29
7.29
7.28
7.27
7.10
7.10
7.09
7.08
7.08
7.07
7.07
7.00
6.98
6.46
6.05
6.03
6.02
6.00
2.25
2.23
2.21
2.19
2.16
2.14
1.16
1.14
1.12
O
O
N
H
S
O
3ae
1H NMR
300 MHz
CDCl3
2.02
1.03
1.97
2.83
2.01
1.02
0.90
0.95
0.95
6.00
9.5
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
f1 (ppm)

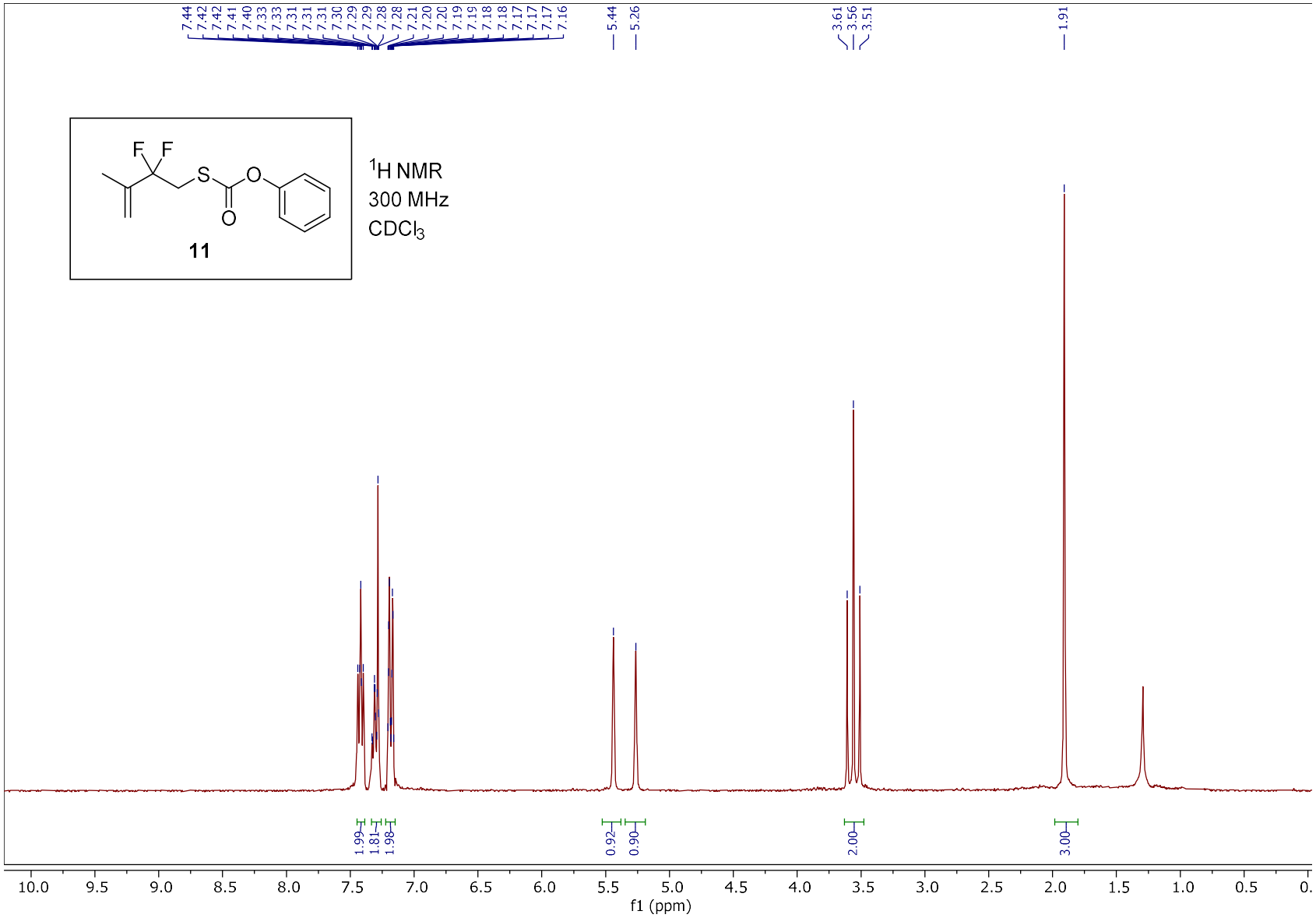

167.59
166.99
156.69
133.88
131.93
129.65
128.68
126.99
121.61
115.79
82.26
33.87
17.59
17.18
O
O
N
H
S
O
3ae
13C{1H} NMR
75 MHz
CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

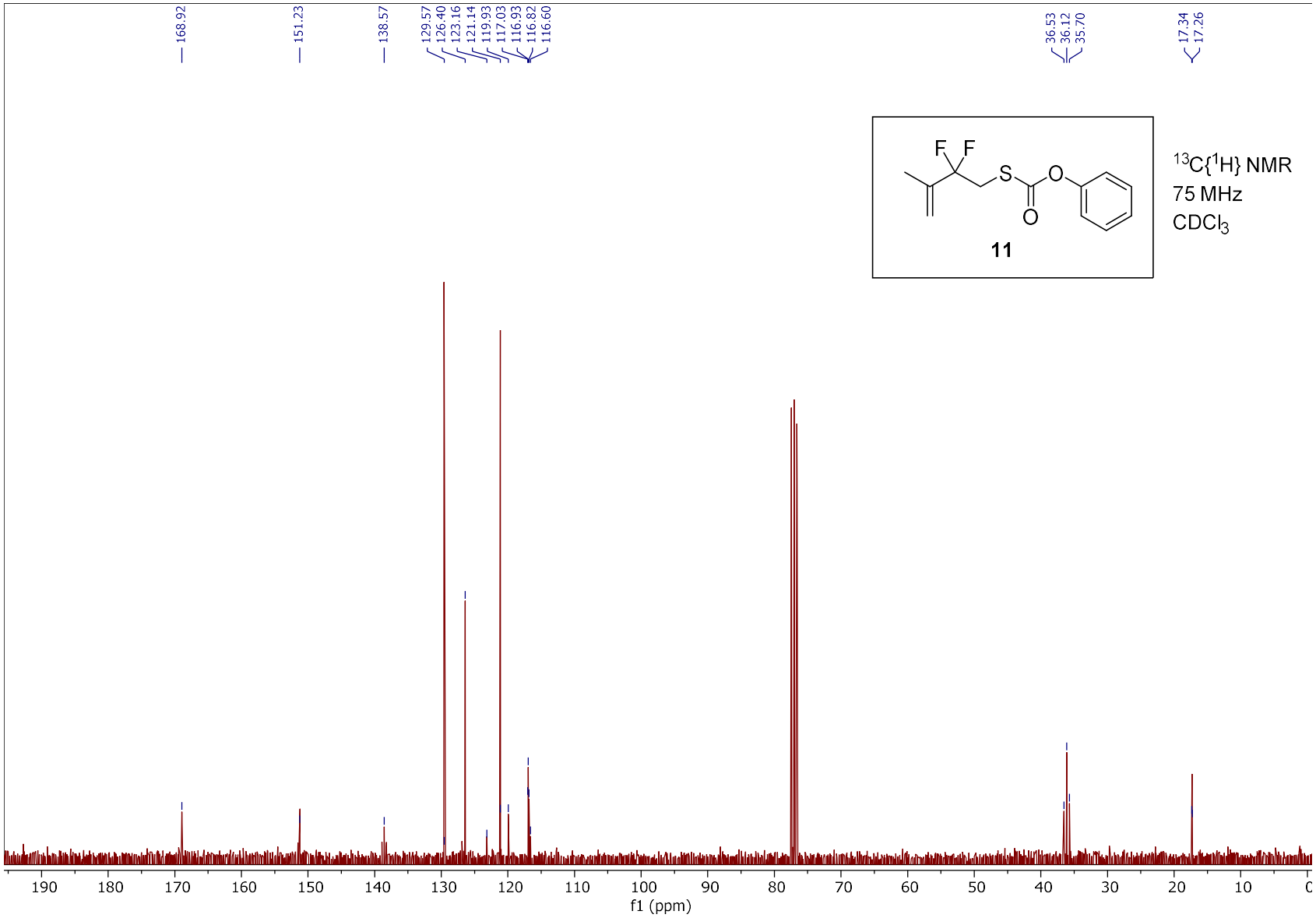

7.44
7.44
7.43
7.39
7.31
7.31
7.29
7.28
7.27
7.26
7.25
7.23
7.22
7.21
7.06
7.03
5.69
Cl
O
S
O
Cl
O
3af
1H NMR
300 MHz
CDCl3
3.02
3.95
1.00
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

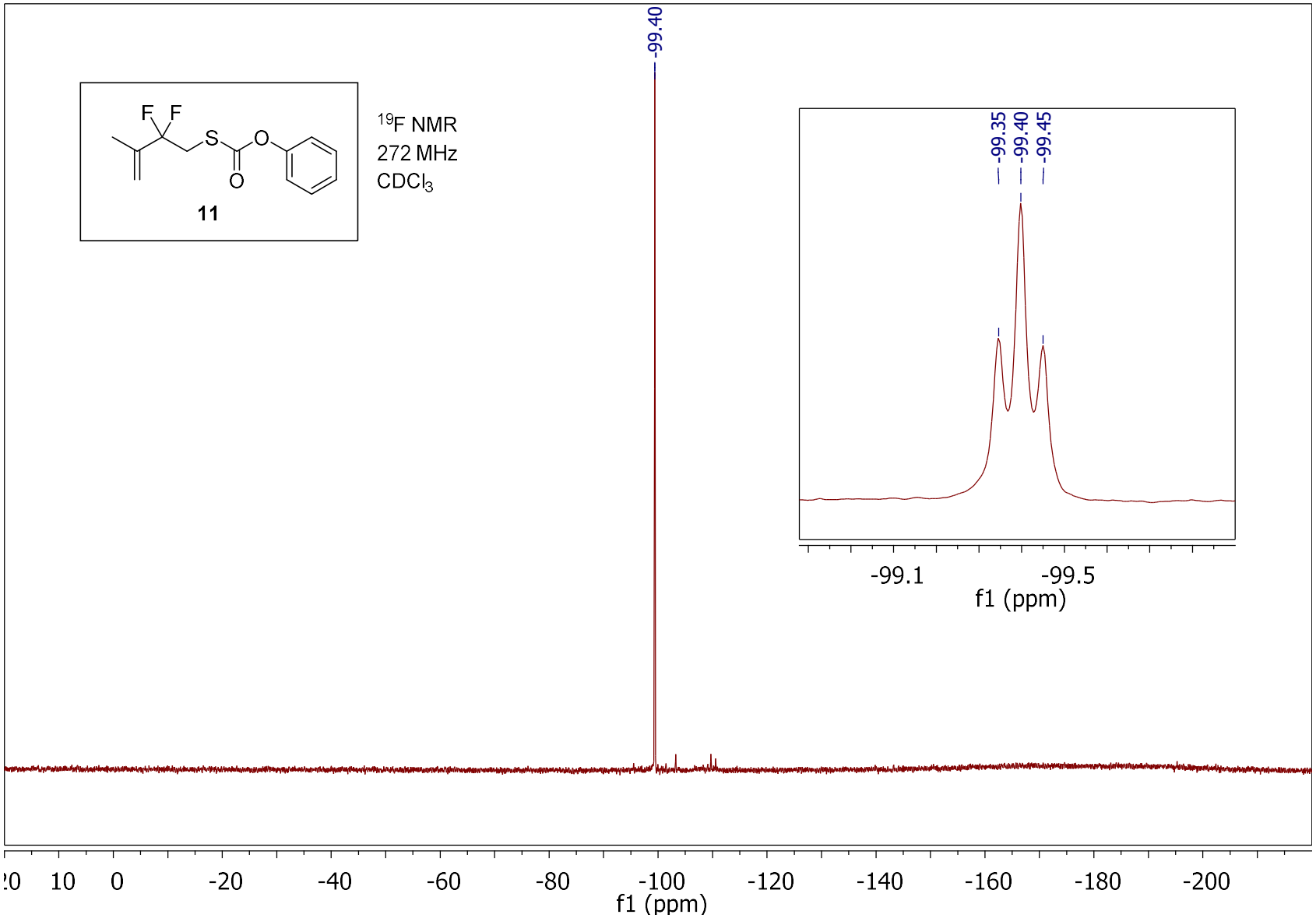

167.69
151.13
151.08
130.52
129.64
127.79
127.68
126.53
126.01
121.09
118.10
71.28
Cl
Cl
O
S
O
O
3af
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
f1 (ppm)

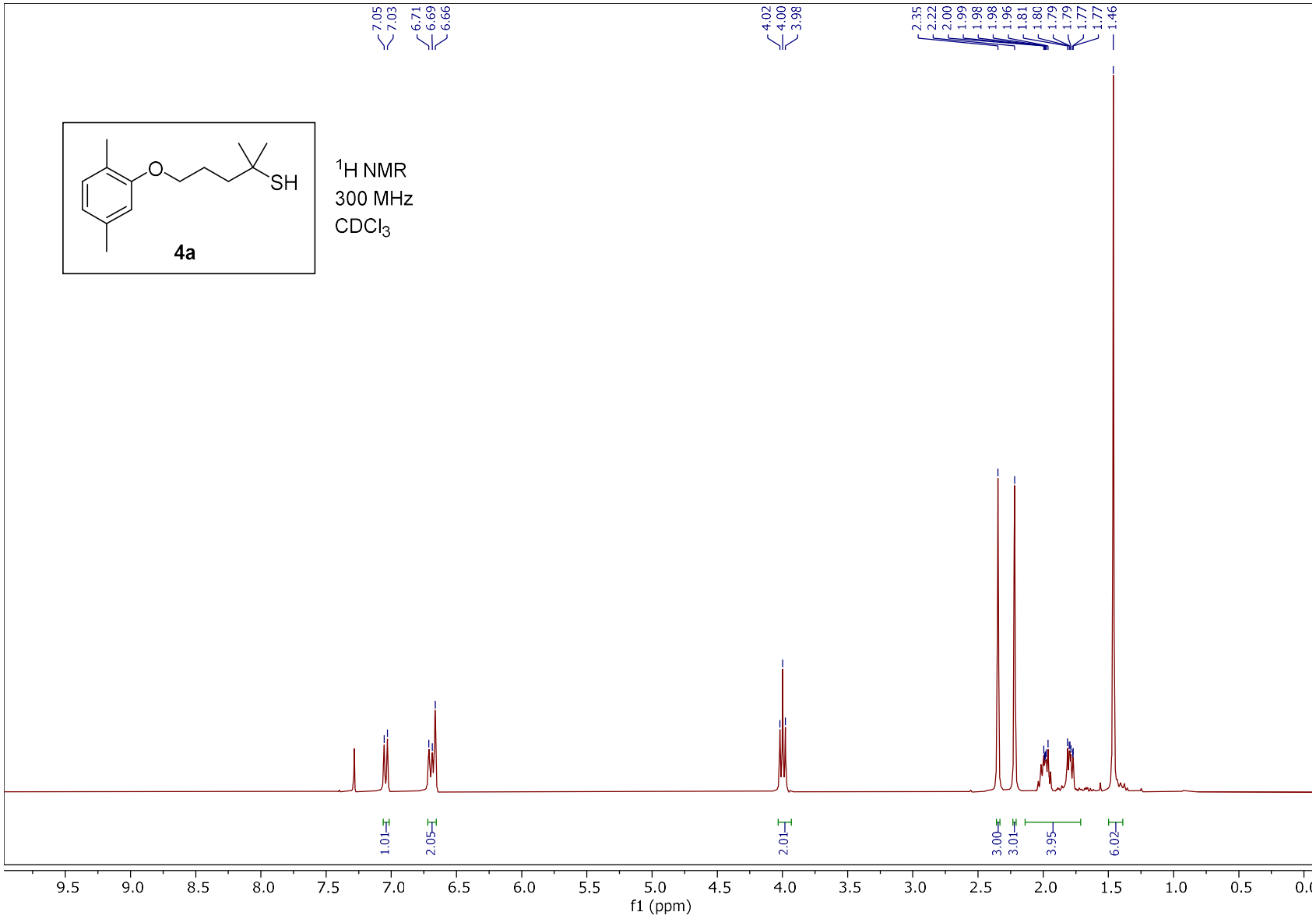

9.40
9.07
8.68
8.67
8.66
8.26
8.24
8.23
7.47
7.45
7.44
7.43
7.15
7.12
7.09
6.83
6.81
6.73
6.71
6.68
3.35
3.32
3.31
3.28
2.57
2.55
2.20
2.17
2.15
O
O
N
H
S
O
N
3ag
1H NMR
300 MHz
DMSO-d6
0.82
0.99
0.99
0.98
1.01
2.02
3.02
2.00
2.41
2.01
2.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

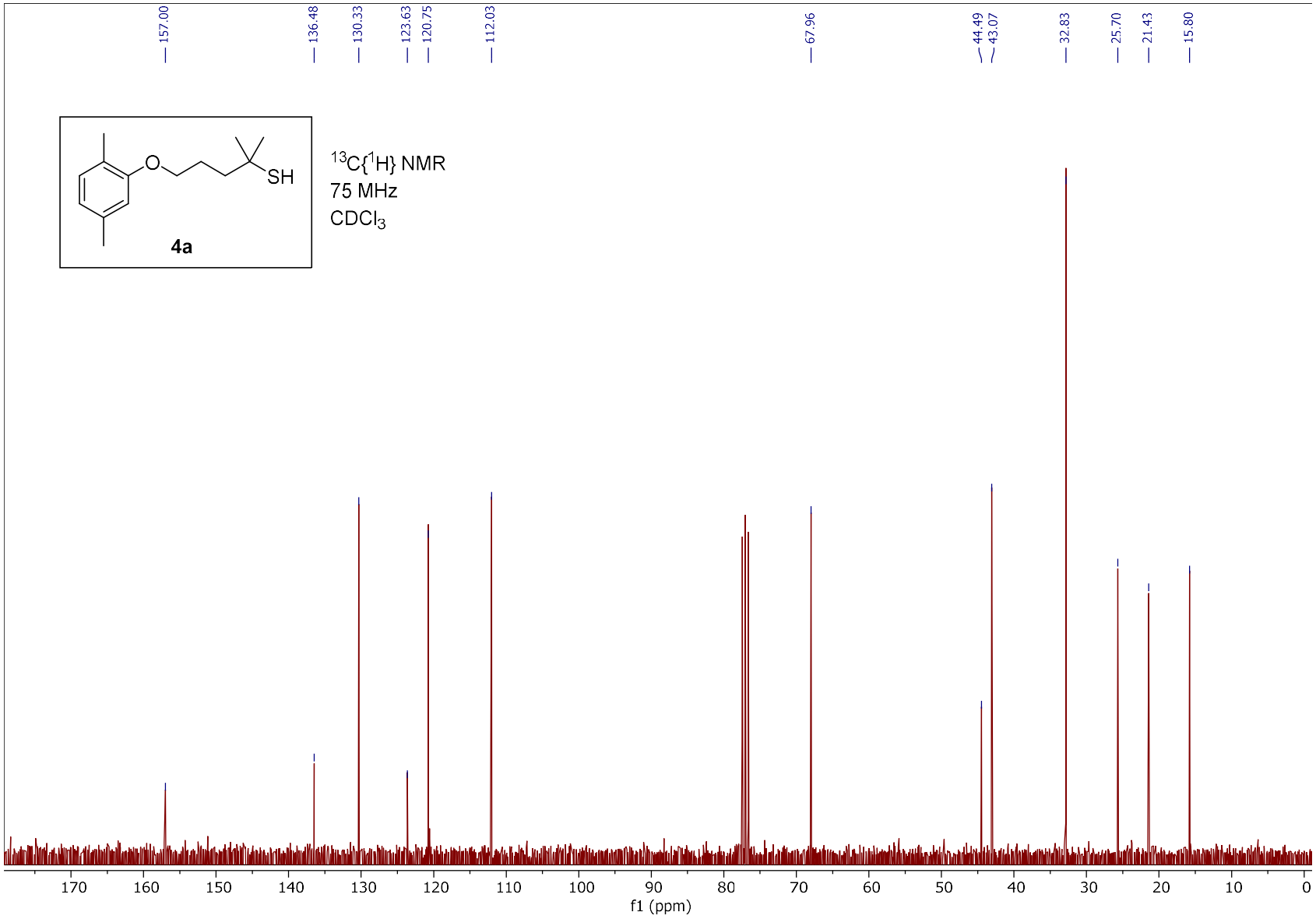

170.77
165.10
158.51
152.01
148.95
135.32
130.56
129.65
123.79
120.94
120.92
118.68
40.53
29.74
25.80
O
O
N
H
S
O
N
3ag
13C{1H} NMR
75 MHz
DMSO-d6
f1 (ppm)

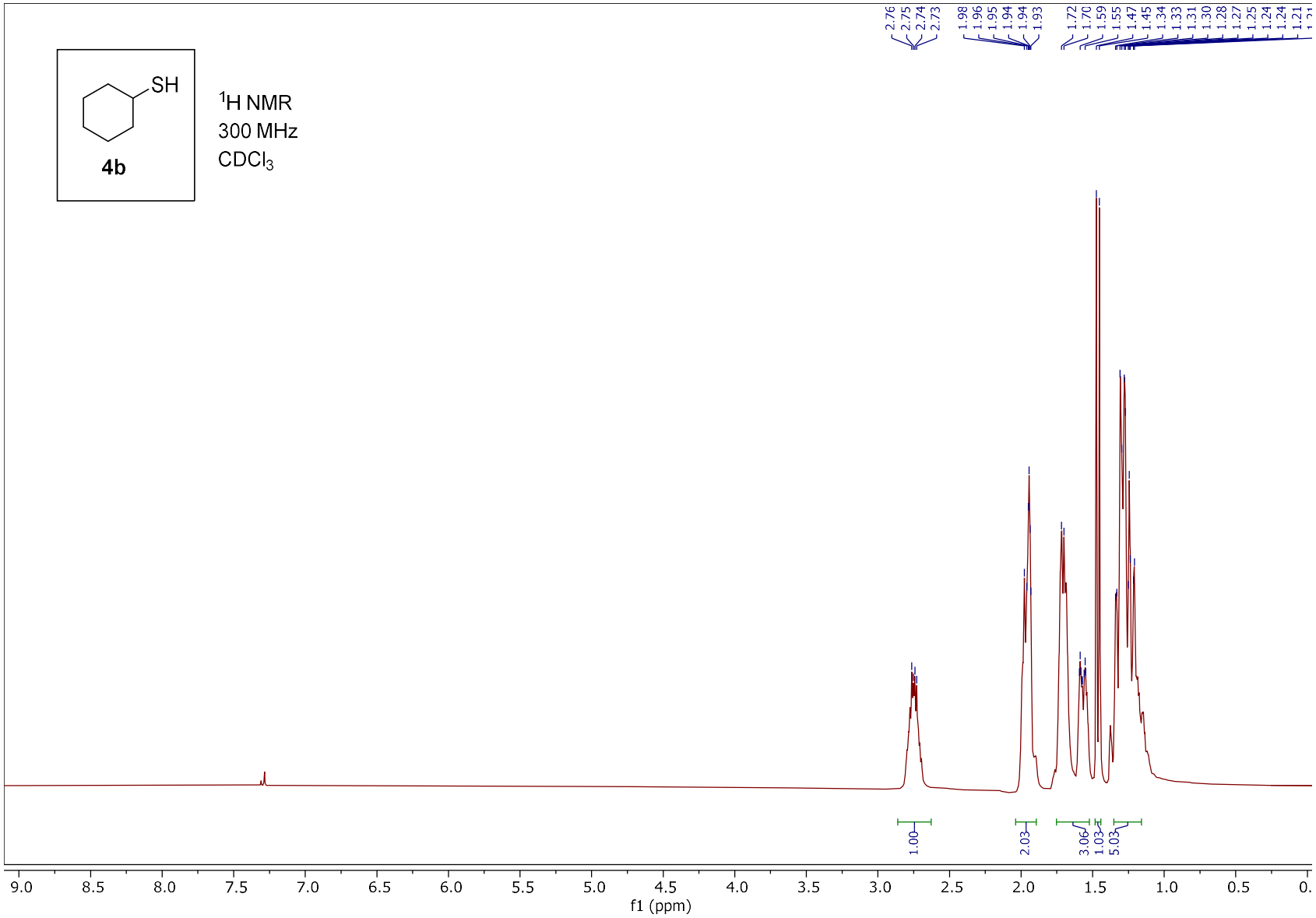

7.44
7.42
7.42
7.41
7.40
7.33
7.33
7.31
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.17
7.17
7.17
7.16
5.44
5.26
3.61
3.56
3.51
1.91
F F
S
O
O
11
1H NMR
300 MHz
CDCl3
1.99
1.81
1.98
0.92
0.90
2.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

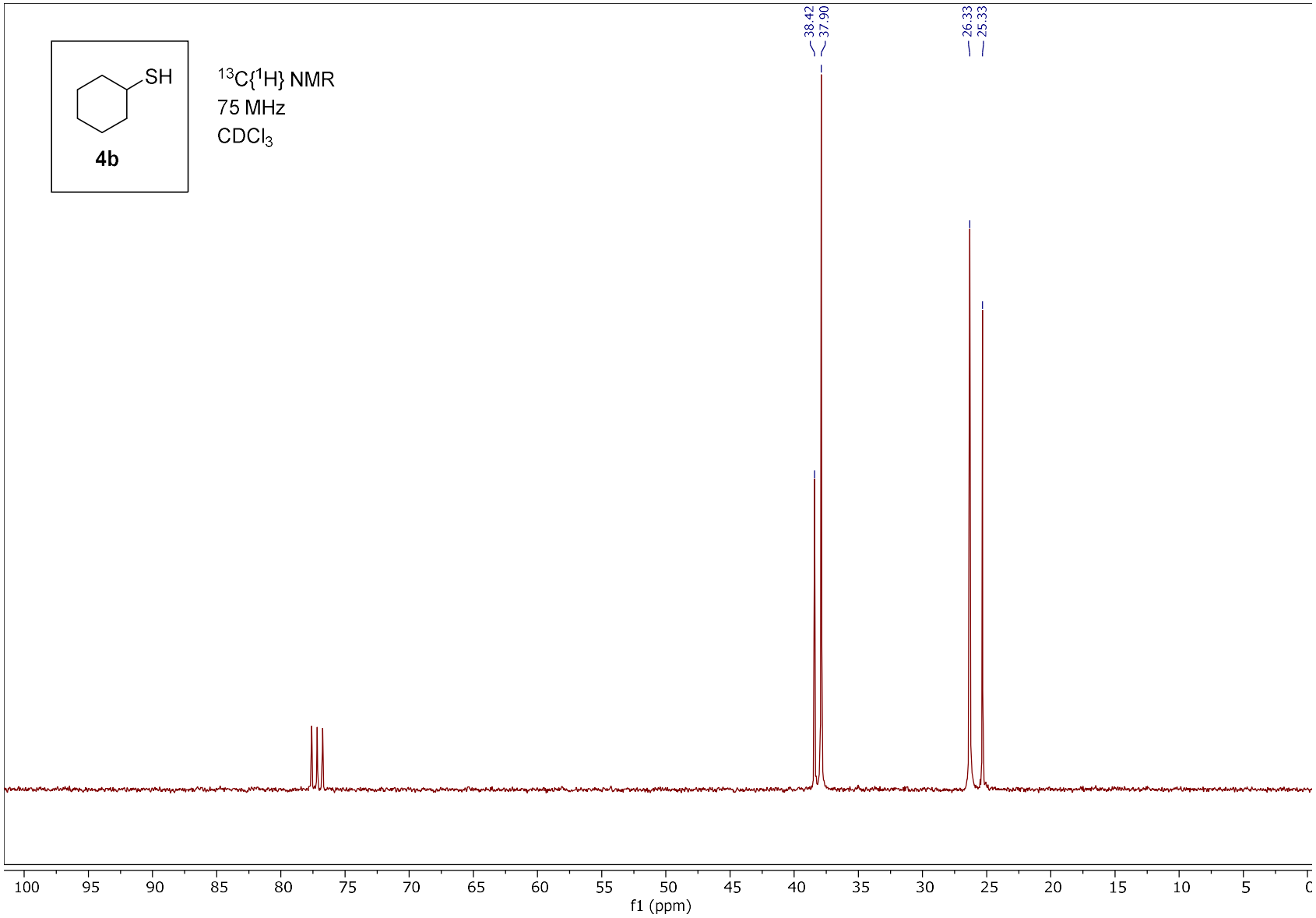

168.92
151.23
138.57
129.57
126.40
123.16
121.14
119.93
117.03
116.93
116.82
116.60
36.53
36.12
35.70
17.34
17.26
F F
S
O
O
11
13C{1H} NMR
75 MHz
CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

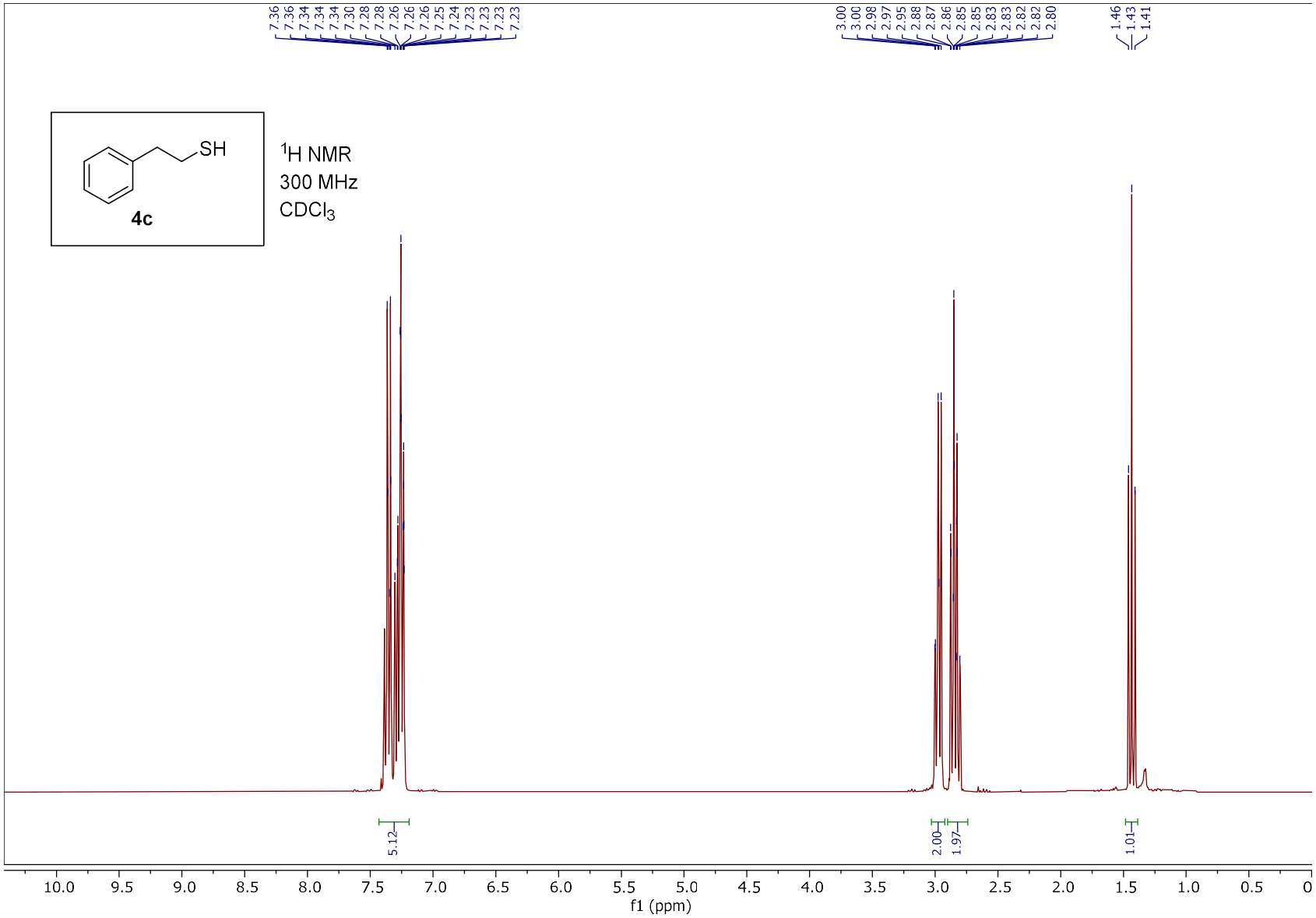

-99.40
F F
S
O
O
11
19F NMR
272 MHz
CDCl3
-99.35
-99.40
-99.45
-99.1
-99.5
f1 (ppm)
10
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

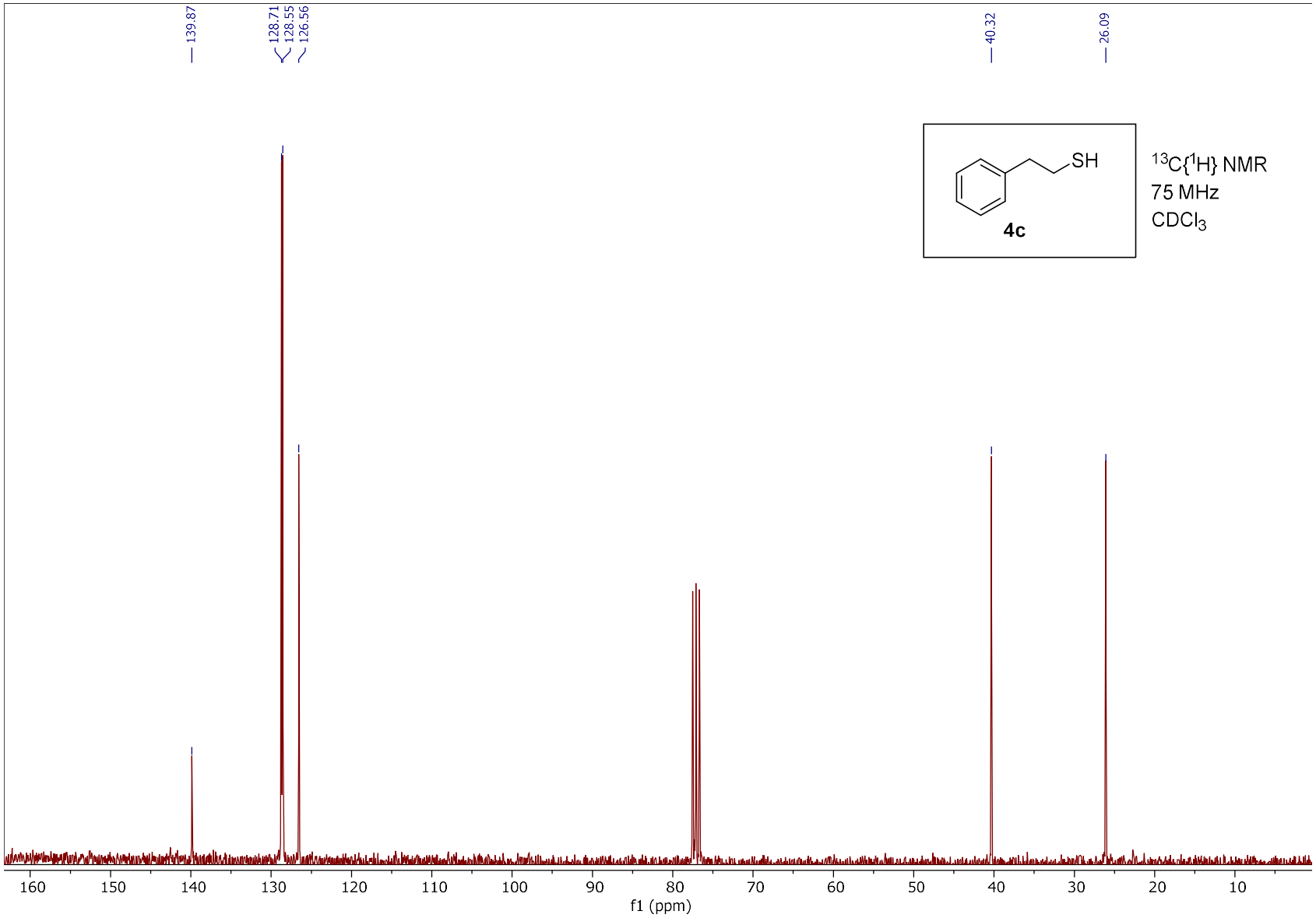

7.05
7.03
6.71
6.69
6.66
4.02
4.00
3.98
2.35
2.22
2.00
1.99
1.98
1.98
1.96
1.81
1.80
1.79
1.79
1.77
1.77
1.46
O
SH
4a
1H NMR
300 MHz
CDCl3
1.01
2.05
2.01
3.00
3.01
3.95
6.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

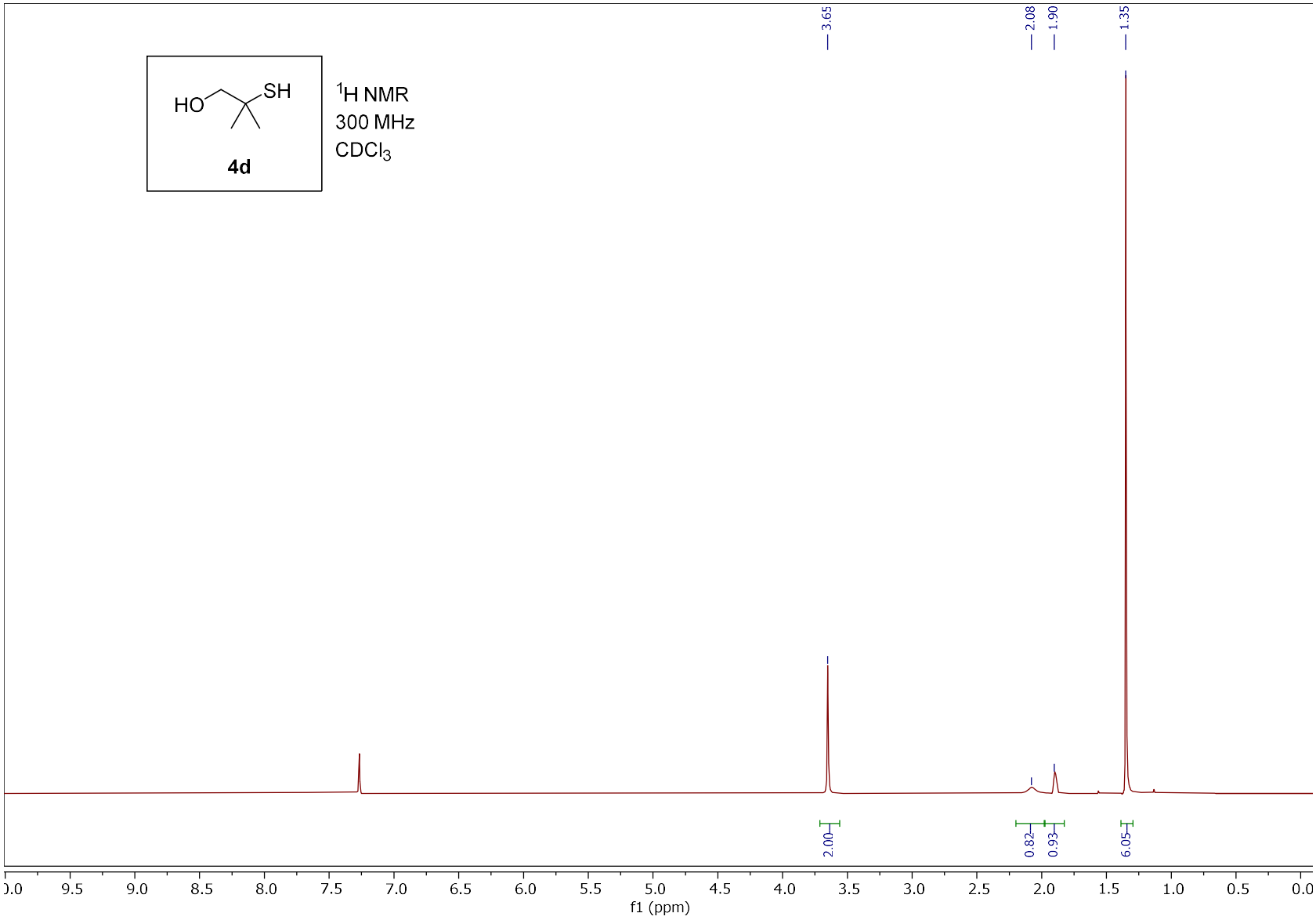

157.00
136.48
130.33
123.63
120.75
112.03
67.96
44.49
43.07
32.83
25.70
21.43
15.80
O
SH
4a
13C{1H} NMR
75 MHz
CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

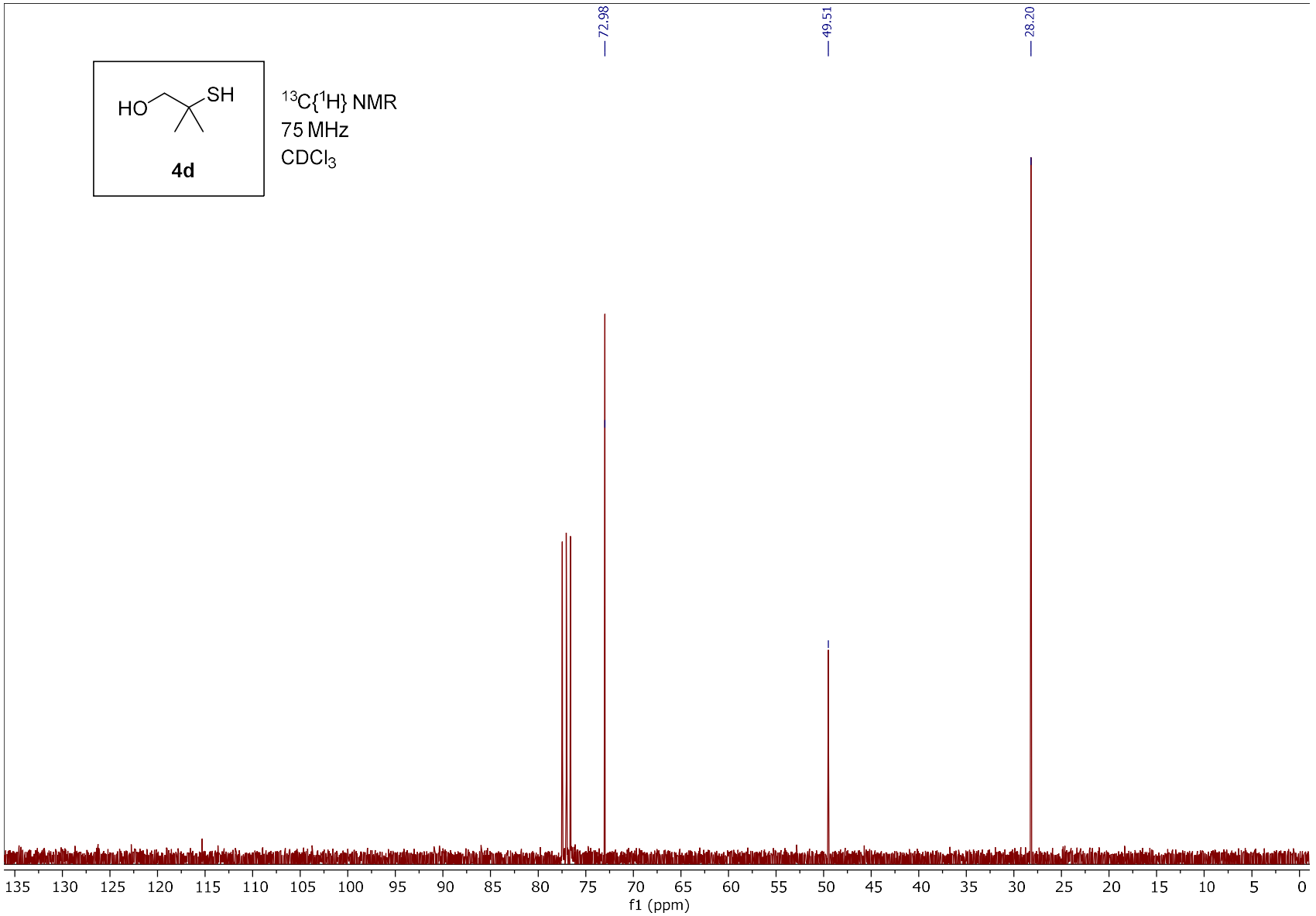

SH
4b
1H NMR
300 MHz
CDCl3
2.76
2.75
2.74
2.73
1.98
1.96
1.95
1.94
1.94
1.93
1.72
1.70
1.59
1.55
1.47
1.45
1.34
1.33
1.31
1.30
1.28
1.27
1.25
1.24
1.24
1.21
1.00
2.03
3.06
1.03
5.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

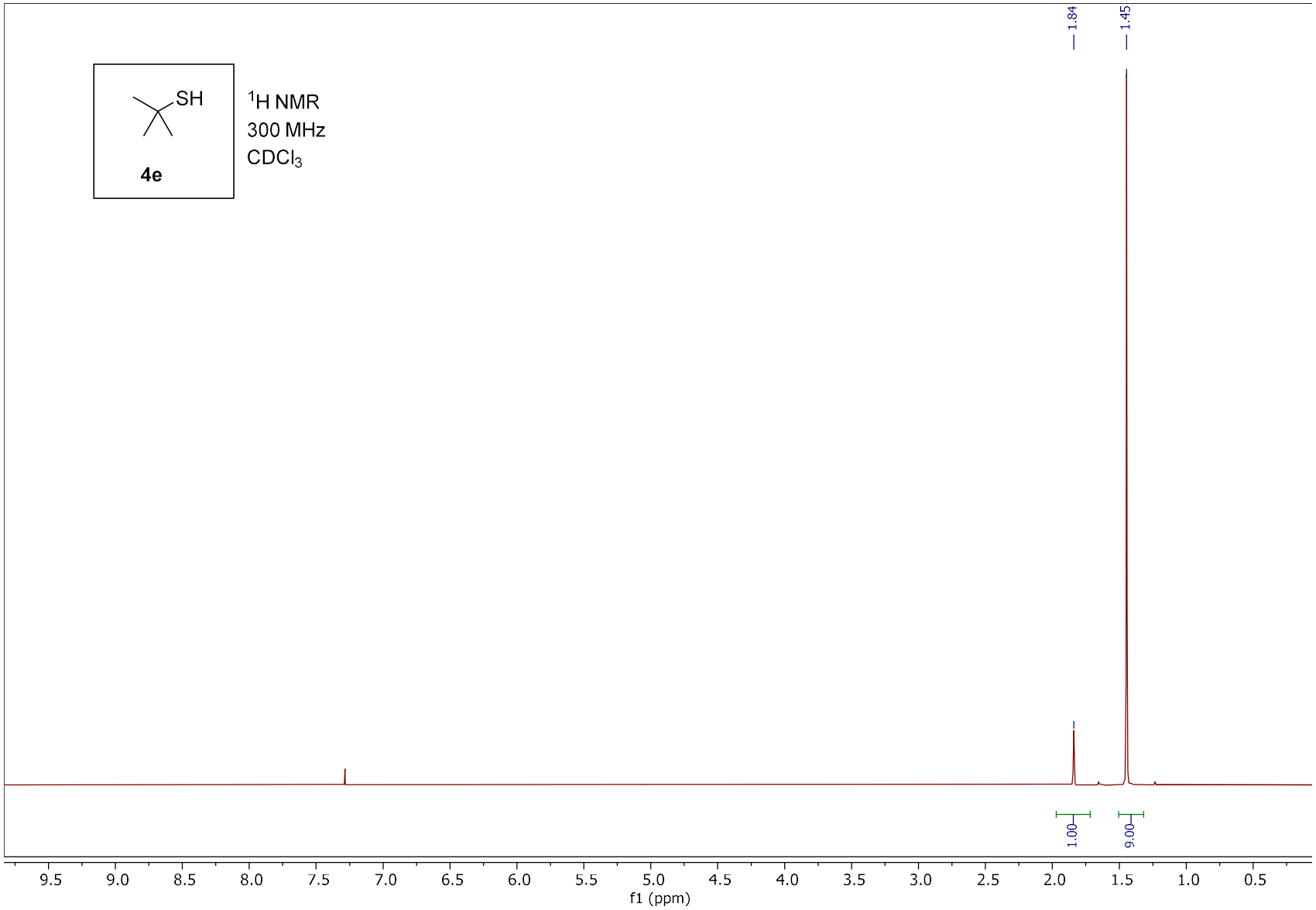

SH
4b
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
38.42
37.90
26.33
25.33
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

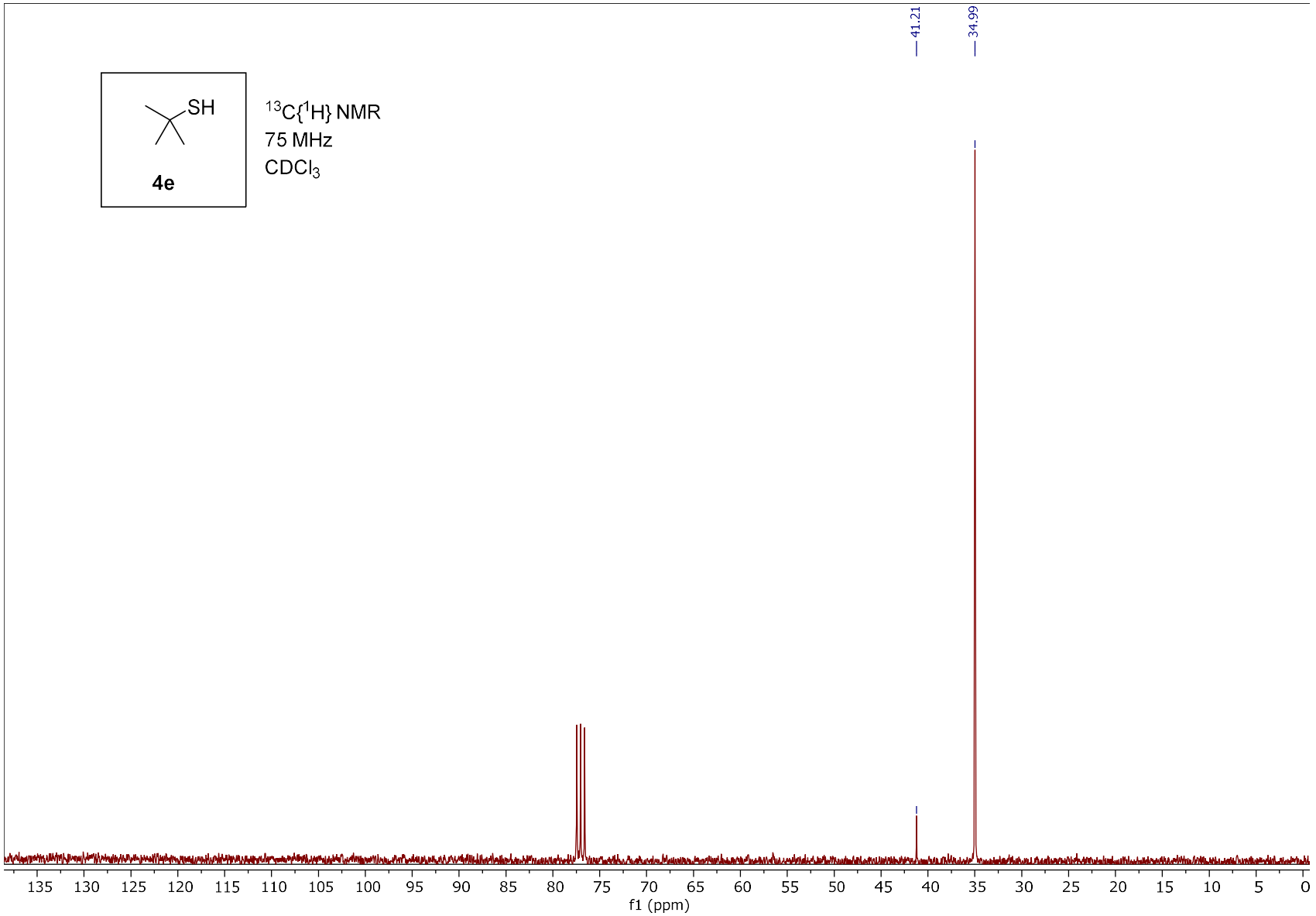

7.36
7.36
7.34
7.34
7.34
7.30
7.28
7.28
7.26
7.26
7.26
7.25
7.24
7.23
7.23
7.23
3.00
3.00
2.98
2.97
2.95
2.88
2.87
2.86
2.85
2.85
2.83
2.83
2.82
2.82
2.80
1.46
1.43
1.41
SH
4c
1H NMR
300 MHz
CDCl3
5.12
2.00
1.97
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

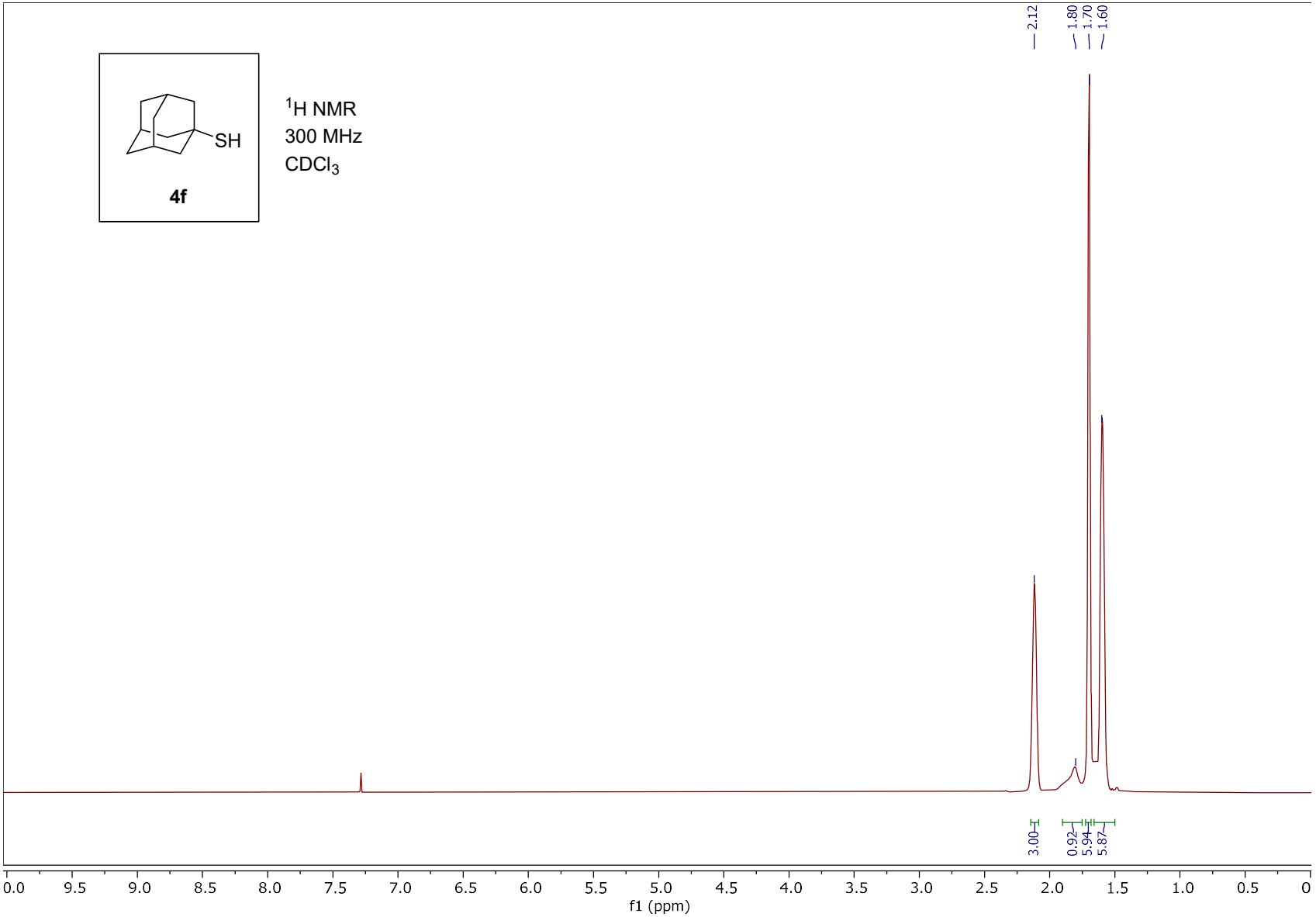

139.87
128.71
128.55
126.56
40.32
26.09
SH
4c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

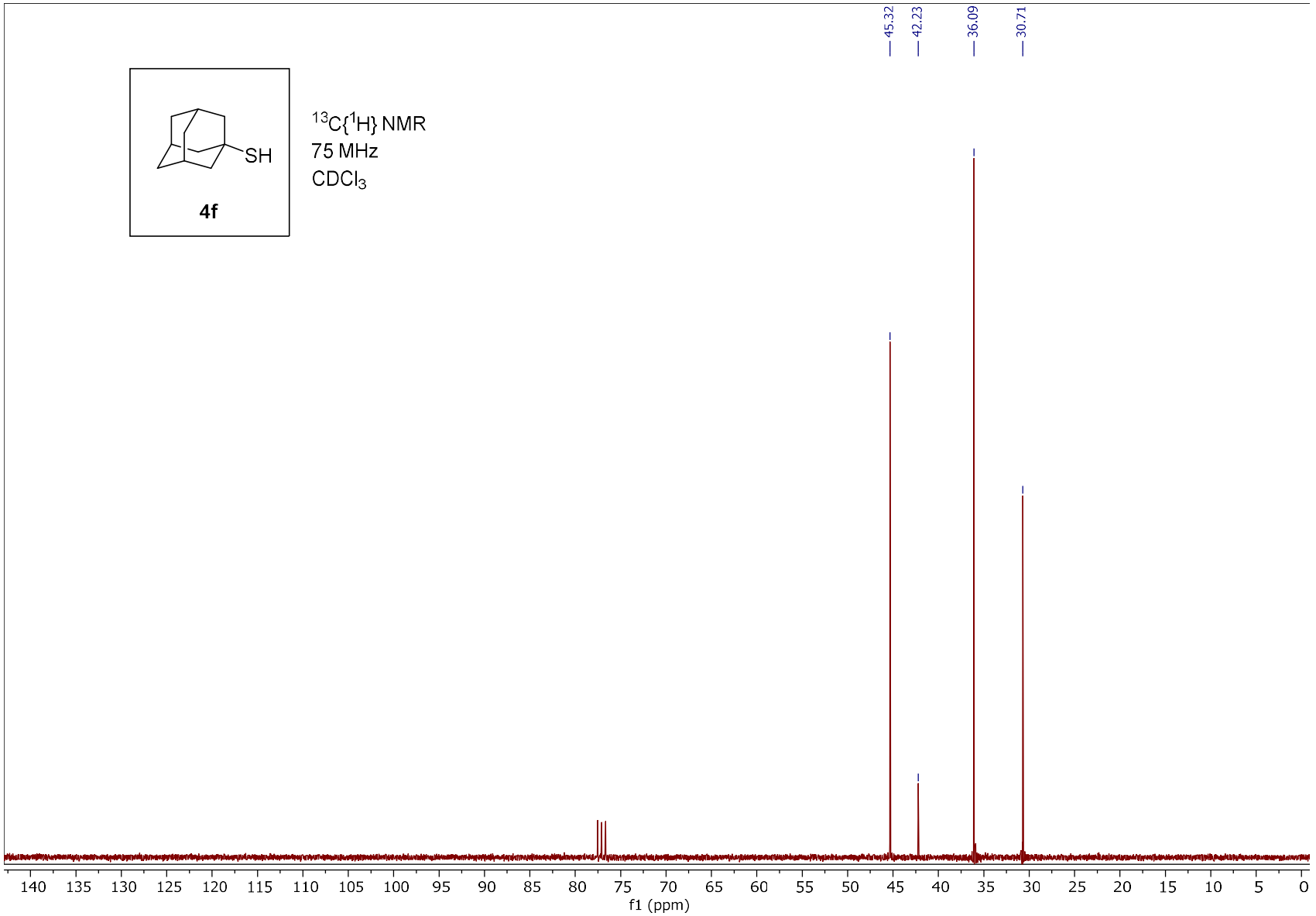

HO
SH
4d
^{1}H NMR
300 MHz
$CDCl_3$
3.65
2.08
1.90
1.35
2.00
0.82
0.93
6.05
f1 (ppm)

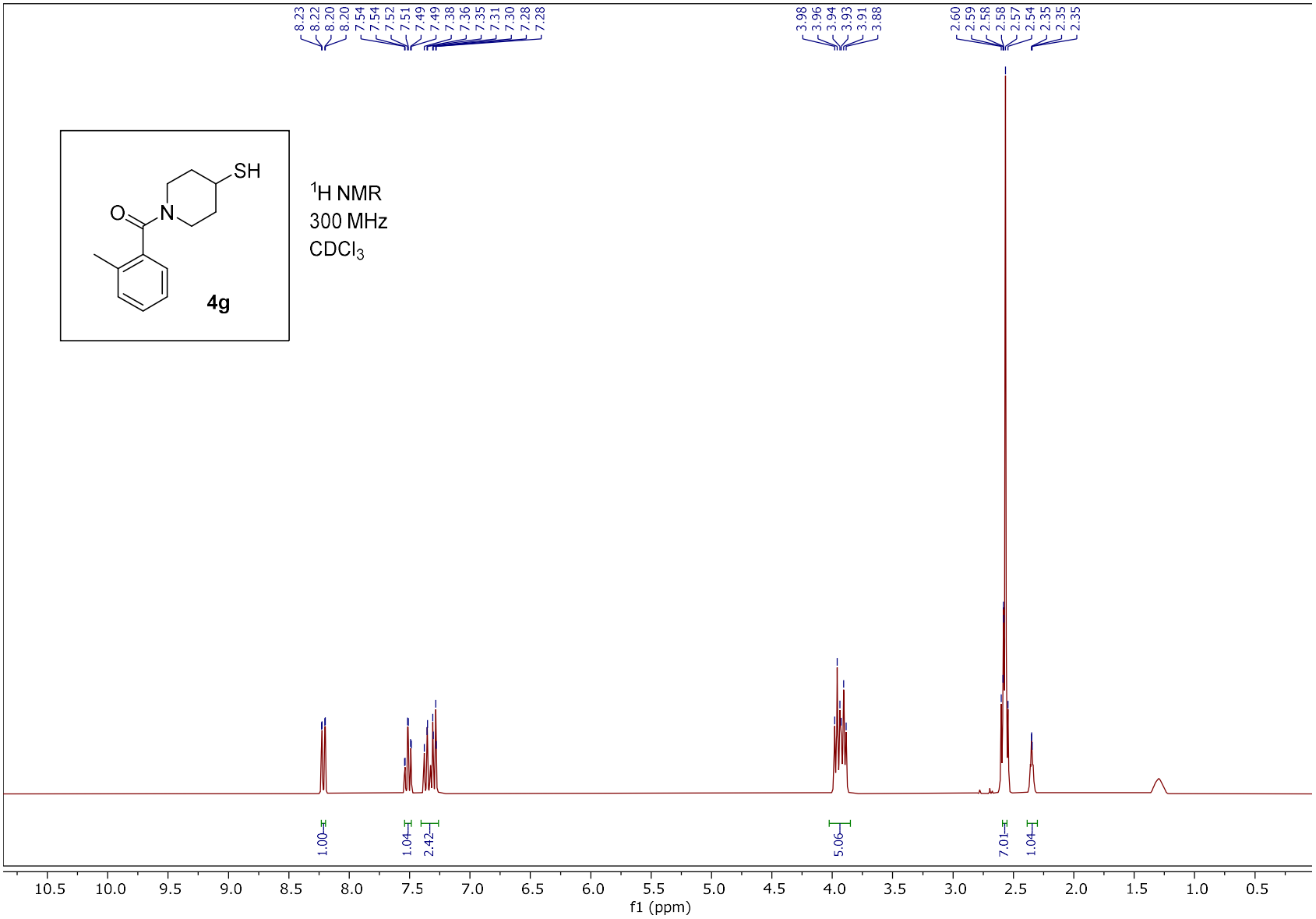

72.98
49.51
28.20
HO
SH
4d
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

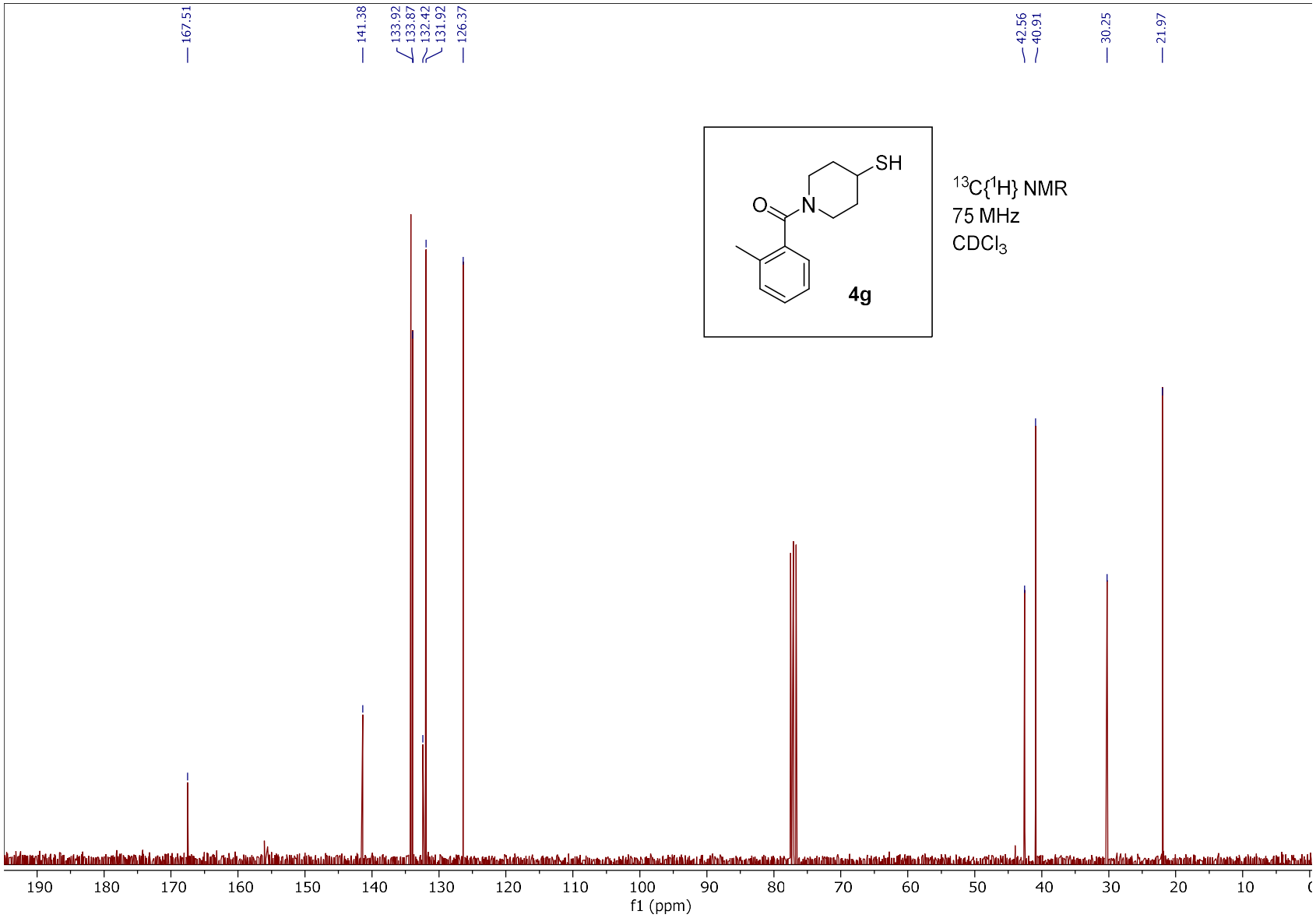

SH
4e
1H NMR
300 MHz
CDCl3
1.84
1.45
1.00
9.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

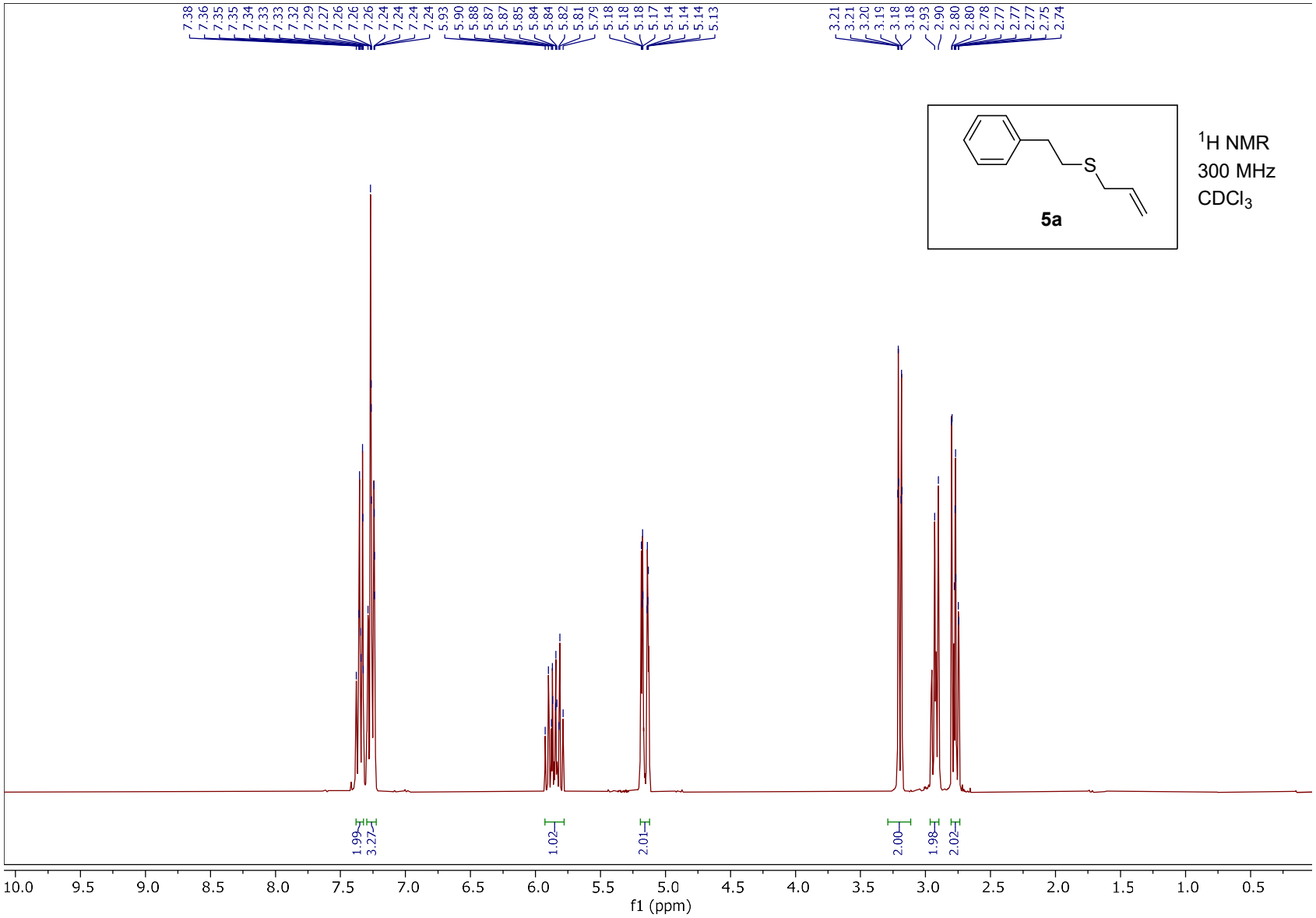

SH
4e
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
41.21
34.99
135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

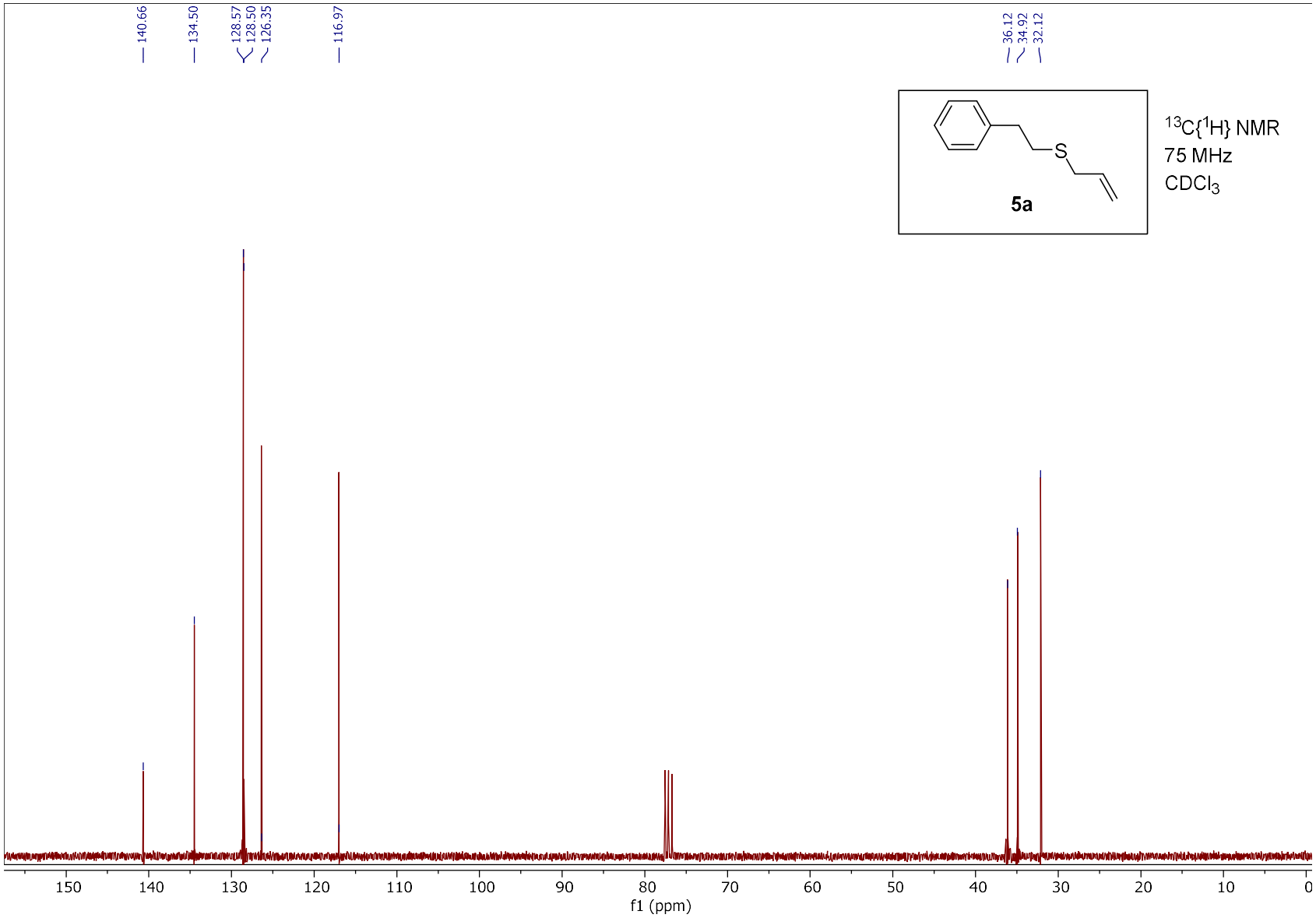

SH
4f
1H NMR
300 MHz
CDCl3
2.12
1.80
1.70
1.60
3.00
0.92
5.94
5.87
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

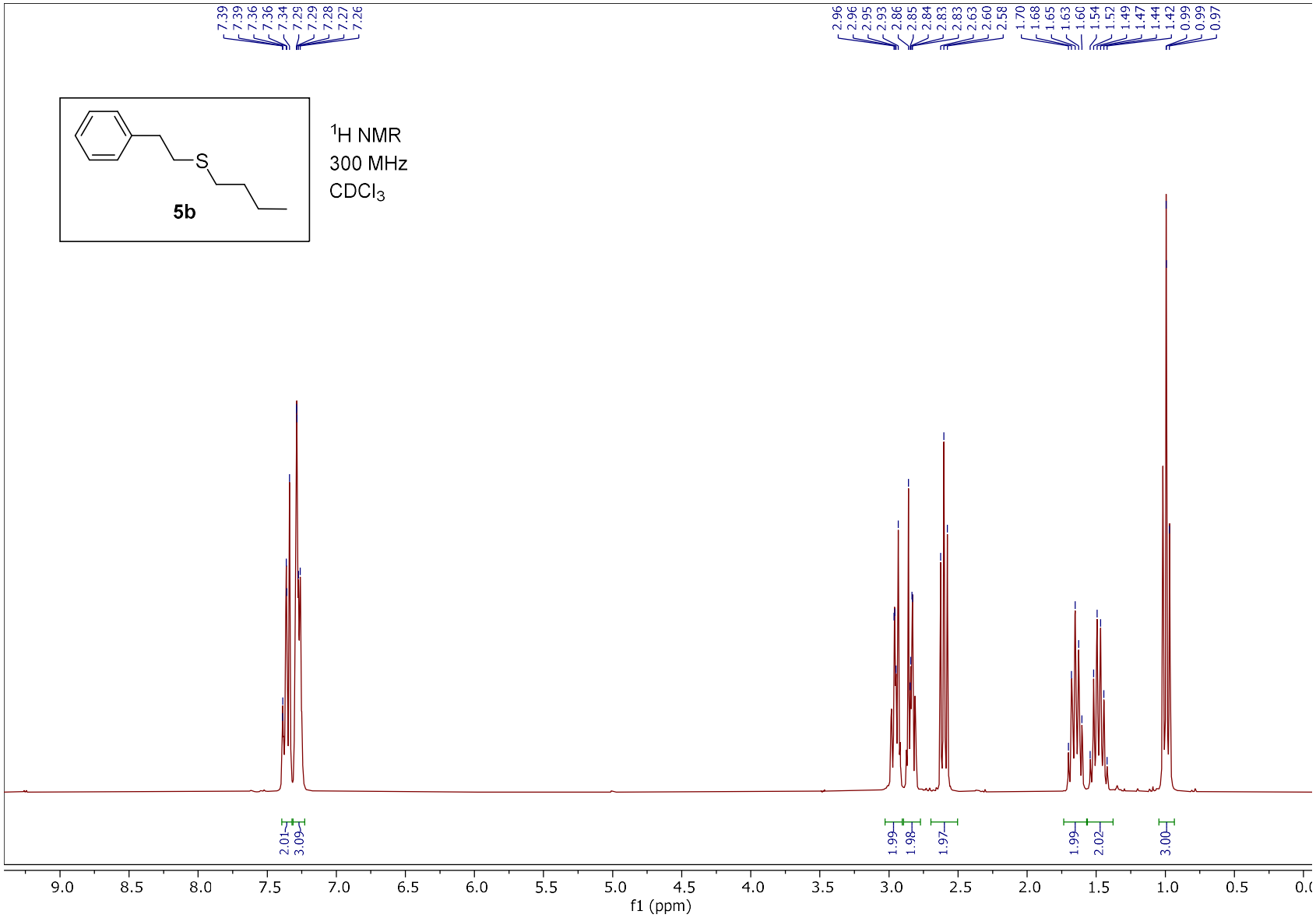

SH
4f
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
45.32
42.23
36.09
30.71
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

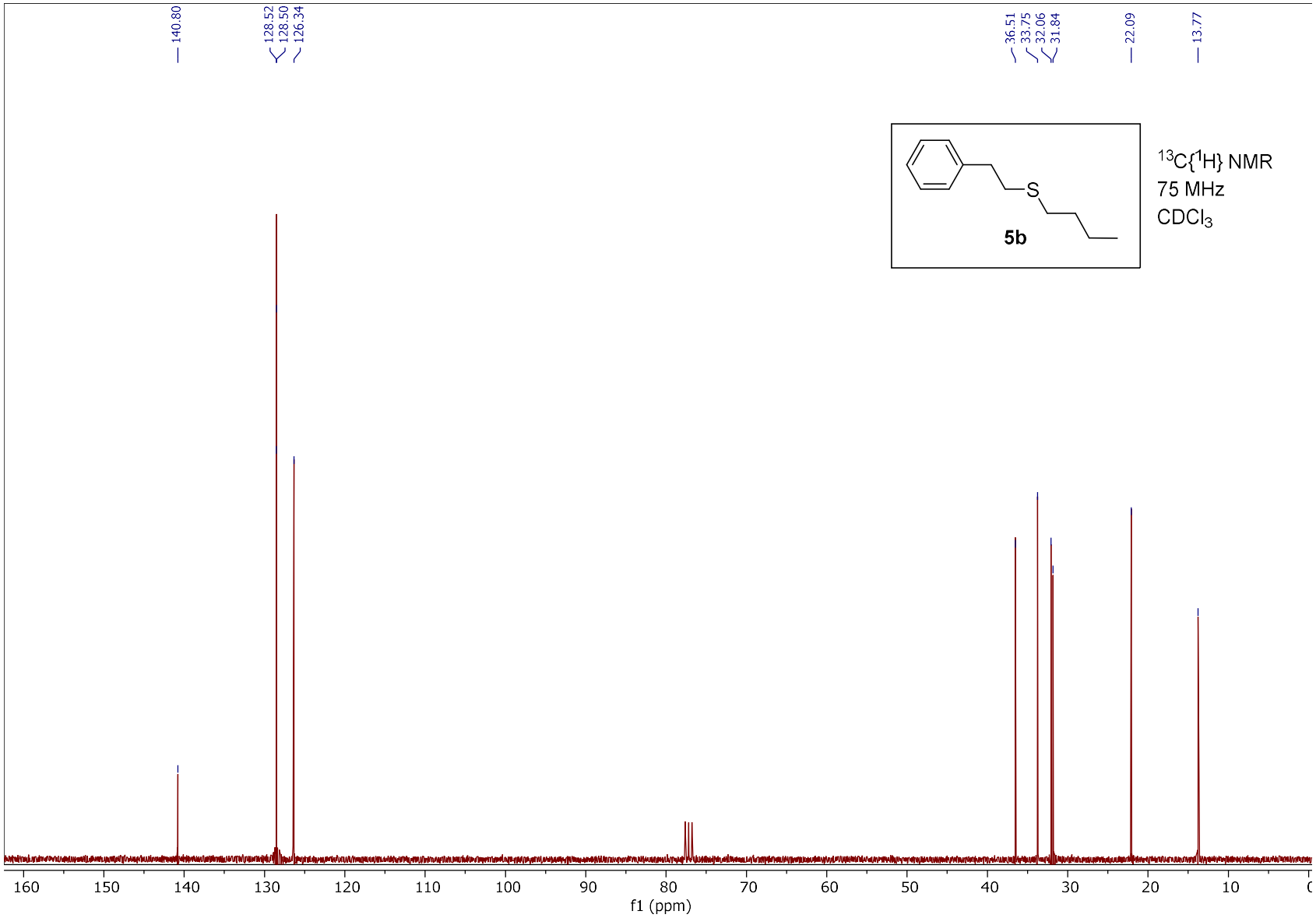

8.23
8.22
8.20
8.20
7.54
7.54
7.52
7.51
7.49
7.49
7.38
7.36
7.35
7.31
7.30
7.28
7.28
3.98
3.96
3.94
3.93
3.91
3.88
2.60
2.59
2.58
2.58
2.57
2.54
2.35
2.35
2.35
SH
O
N
4g
1H NMR
300 MHz
CDCl3
1.00
1.04
2.42
5.06
7.01
1.04
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

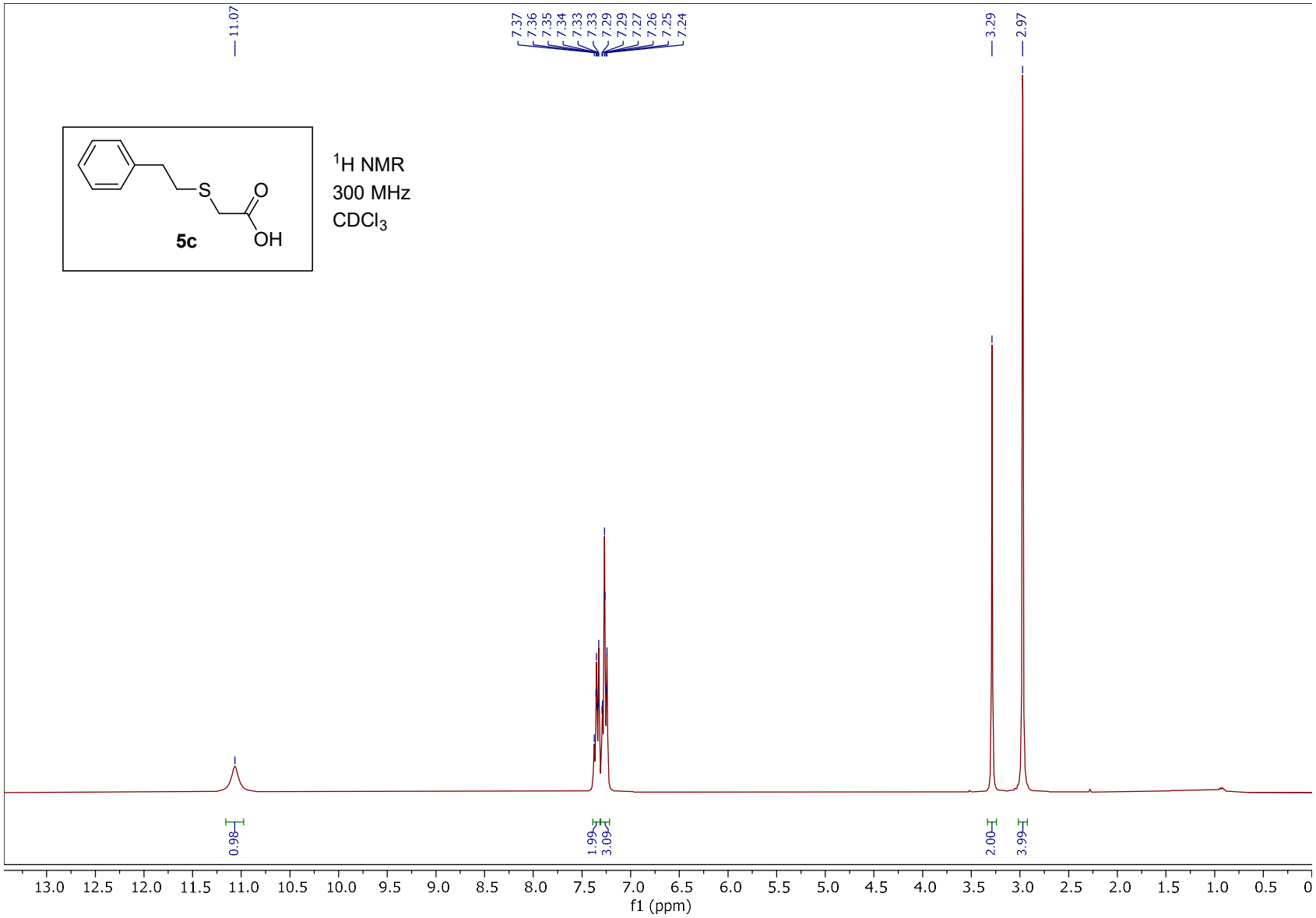

167.51
141.38
133.92
133.87
132.42
131.92
126.37
42.56
40.91
30.25
21.97
SH
O
N
4g
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

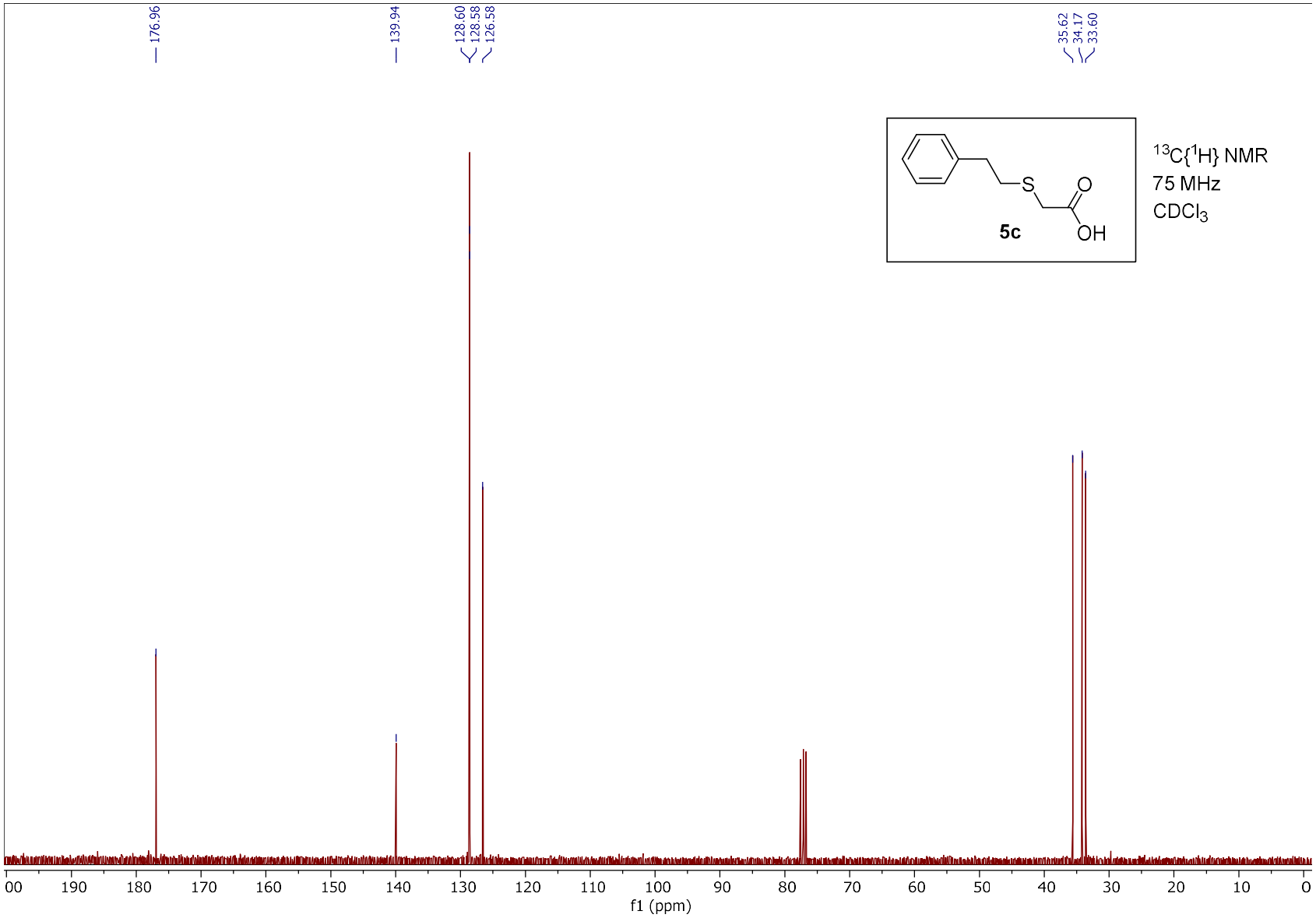

7.38 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.29 7.27 7.26 7.26 7.26 7.24 7.24 7.24 7.24
5.93 5.90 5.88 5.87 5.87 5.85 5.84 5.84 5.82 5.81 5.79
5.18 5.18 5.17 5.14 5.14 5.14 5.13
3.21 3.21 3.20 3.19 3.18 3.18 2.93 2.90 2.80 2.80 2.78 2.77 2.77 2.77 2.75 2.74
S
5a
1H NMR
300 MHz
CDCl3
1.99 3.27 1.02 2.01 2.00 1.98 2.02
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
f1 (ppm)

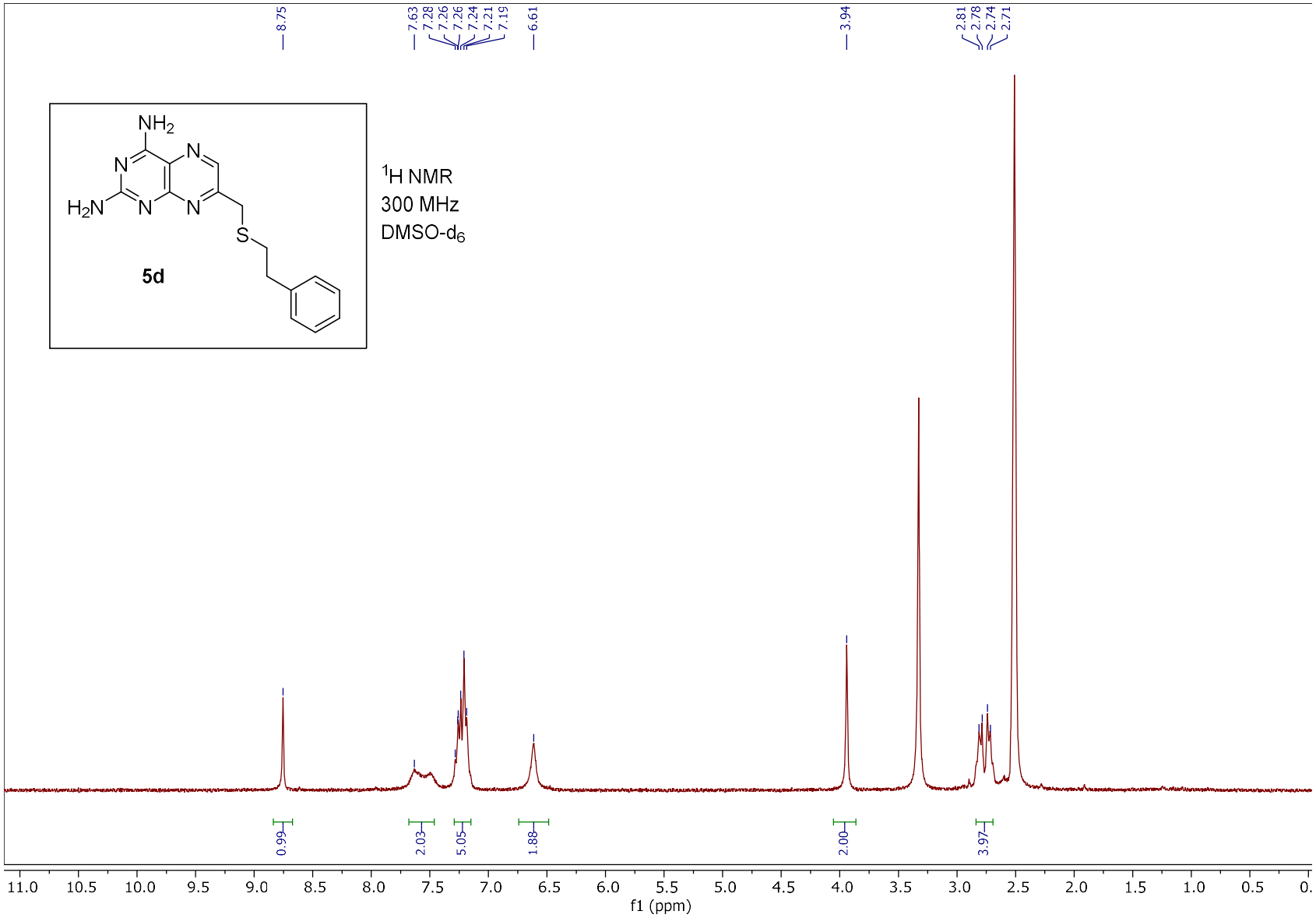

140.66
134.50
128.57
128.50
126.35
116.97
36.12
34.92
32.12
S
5a
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

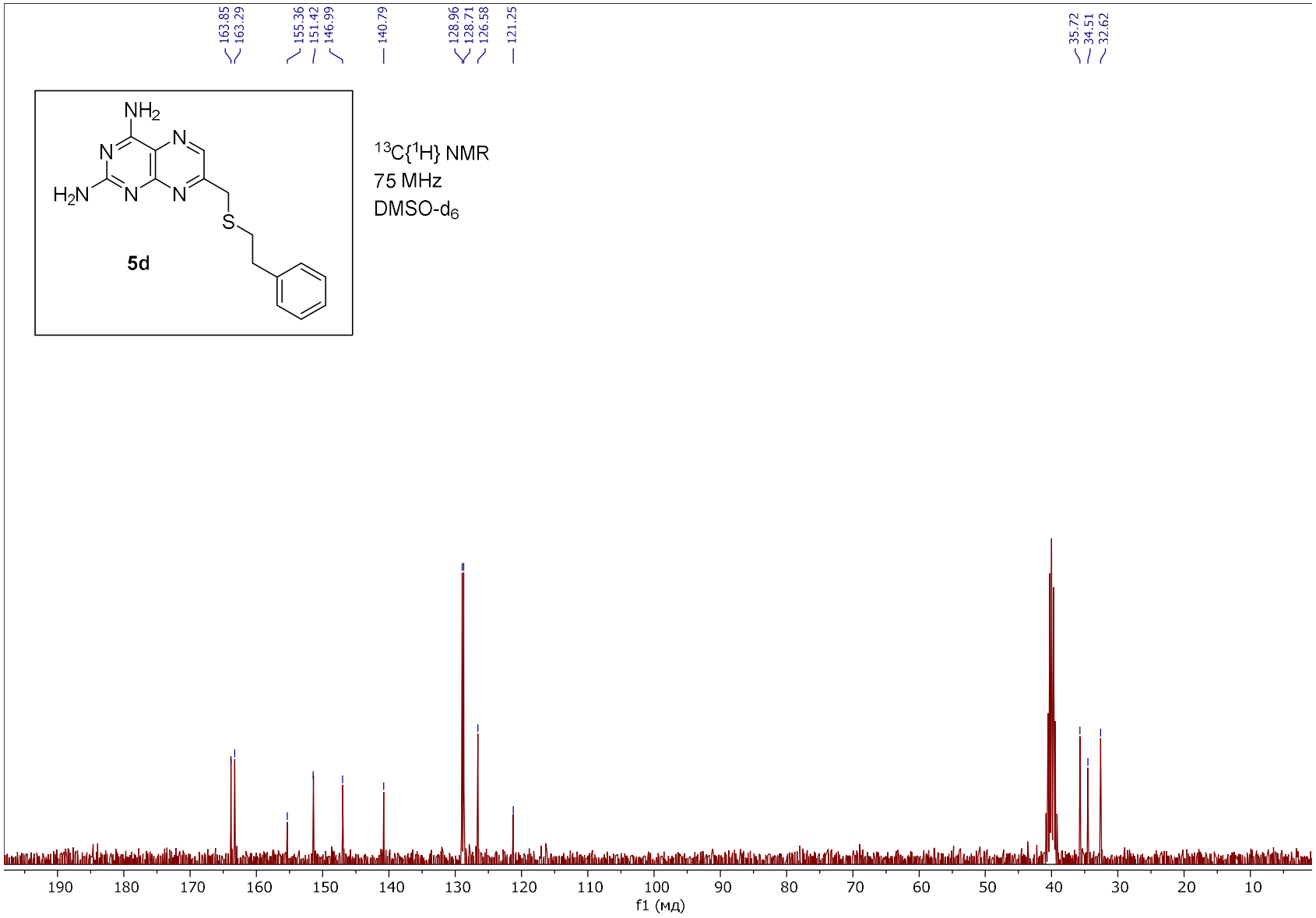

7.39
7.39
7.36
7.36
7.34
7.29
7.29
7.28
7.27
7.26
2.96
2.96
2.95
2.93
2.86
2.85
2.84
2.83
2.83
2.63
2.60
2.58
1.70
1.68
1.65
1.63
1.60
1.54
1.52
1.49
1.47
1.44
1.42
0.99
0.99
0.97
S
5b
1H NMR
300 MHz
CDCl3
2.01
3.09
1.99
1.98
1.97
1.99
2.02
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

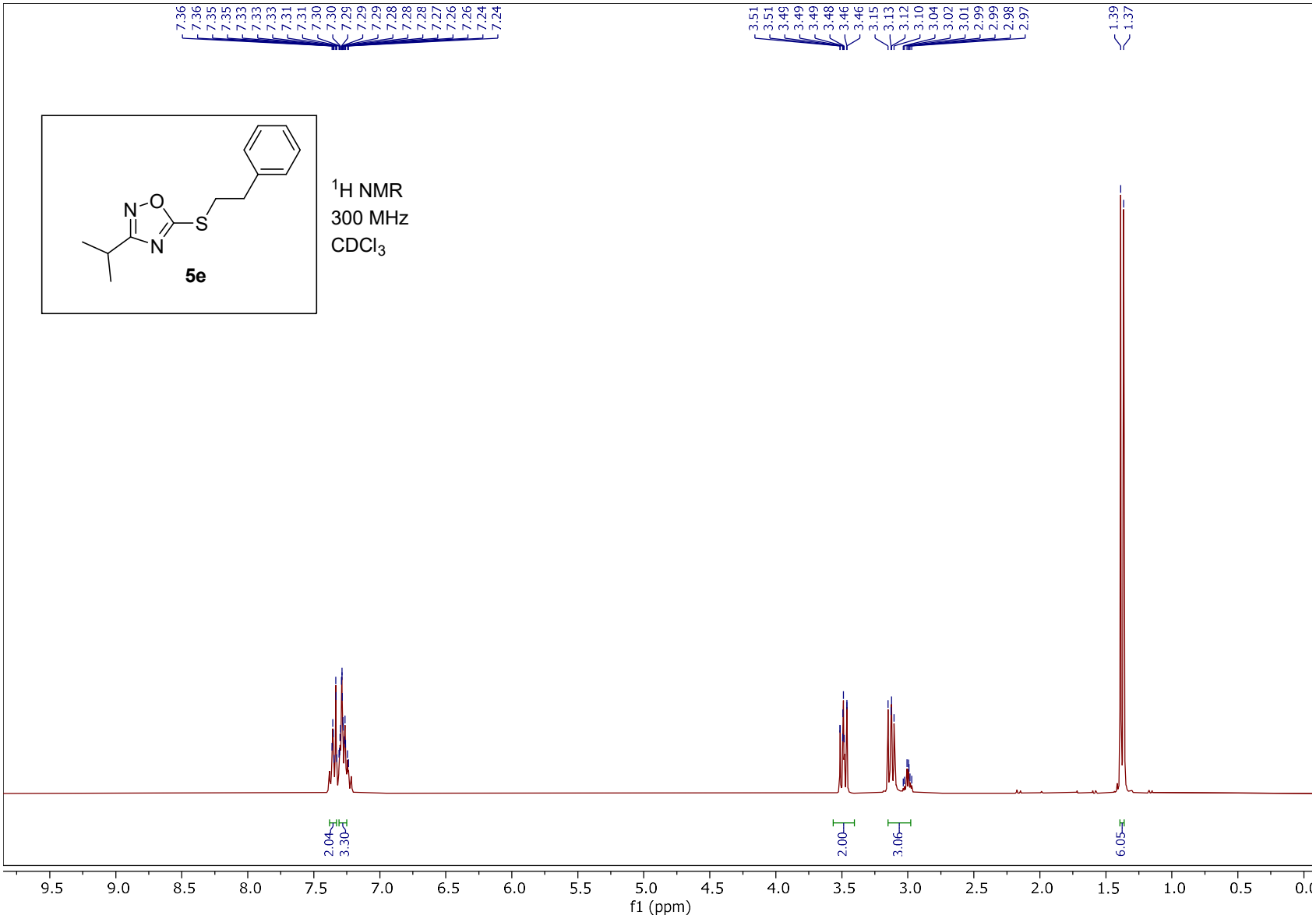

140.80
128.52
128.50
126.34
36.51
33.75
32.06
31.84
22.09
13.77
S
5b
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

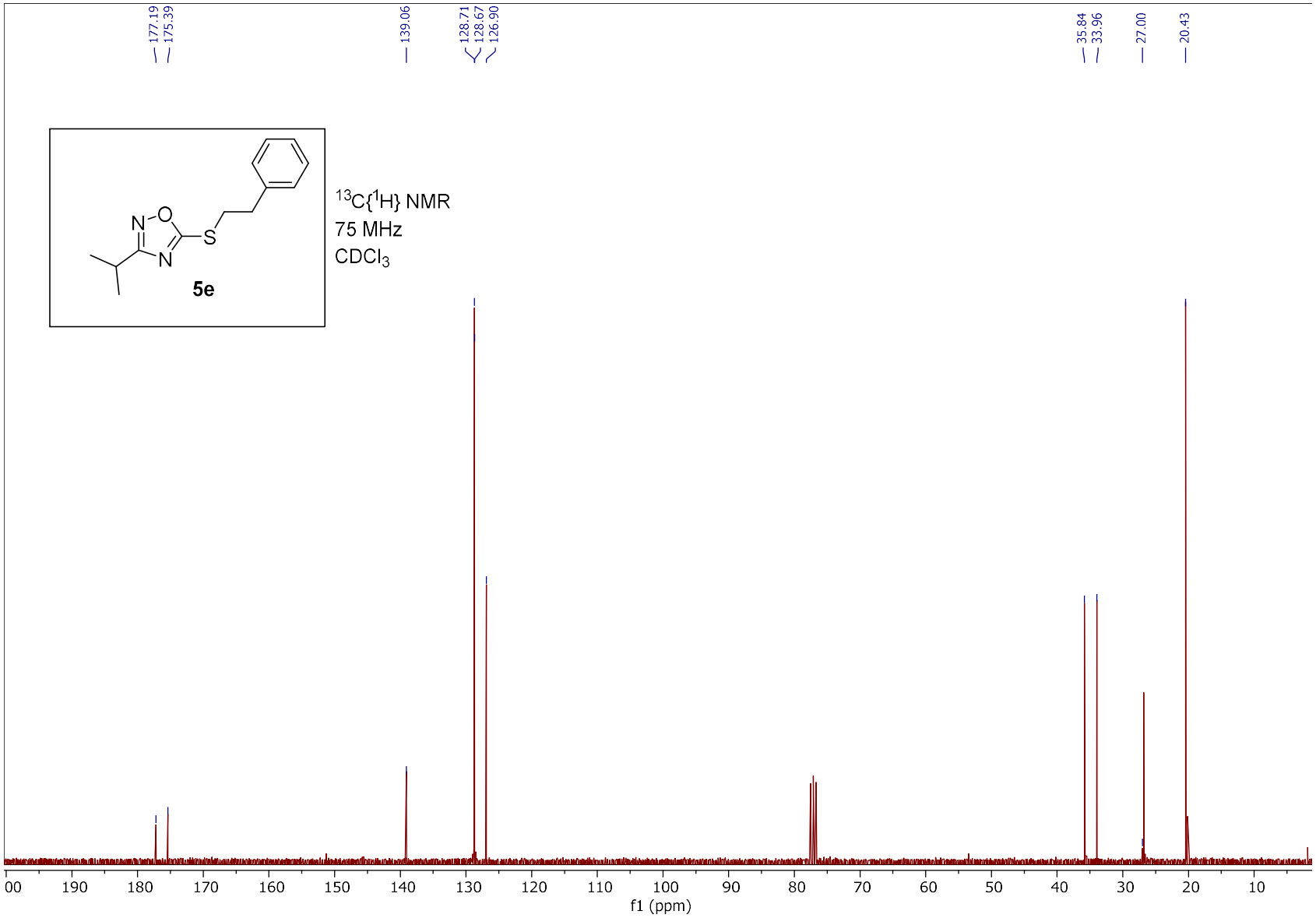

11.07
7.37
7.36
7.35
7.34
7.33
7.33
7.29
7.29
7.27
7.26
7.25
7.24
3.29
2.97
S
O
OH
5c
1H NMR
300 MHz
CDCl3
0.98
1.99
3.09
2.00
3.99
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

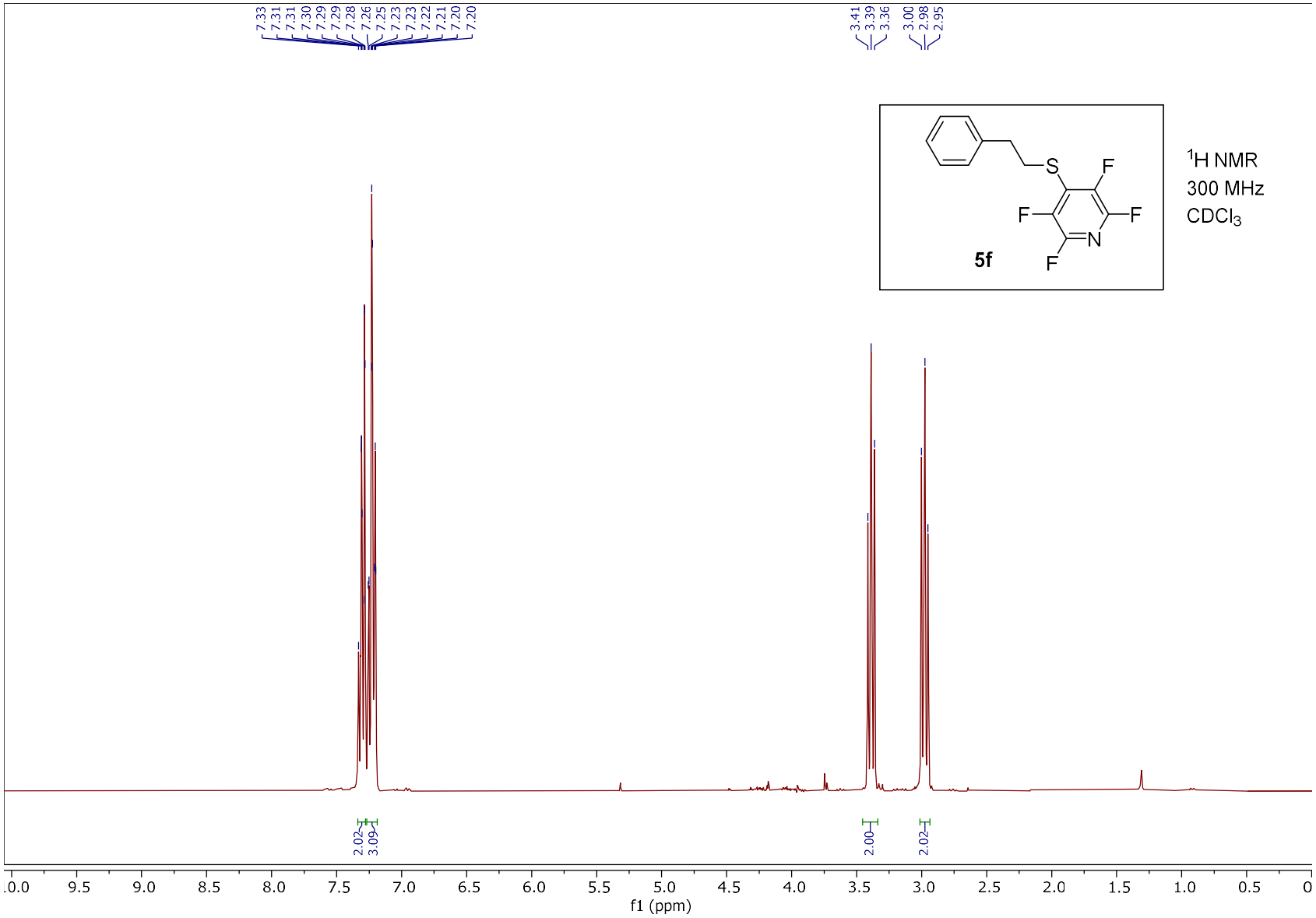

176.96
139.94
128.60
128.58
126.58
35.62
34.17
33.60
S
O
OH
5c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

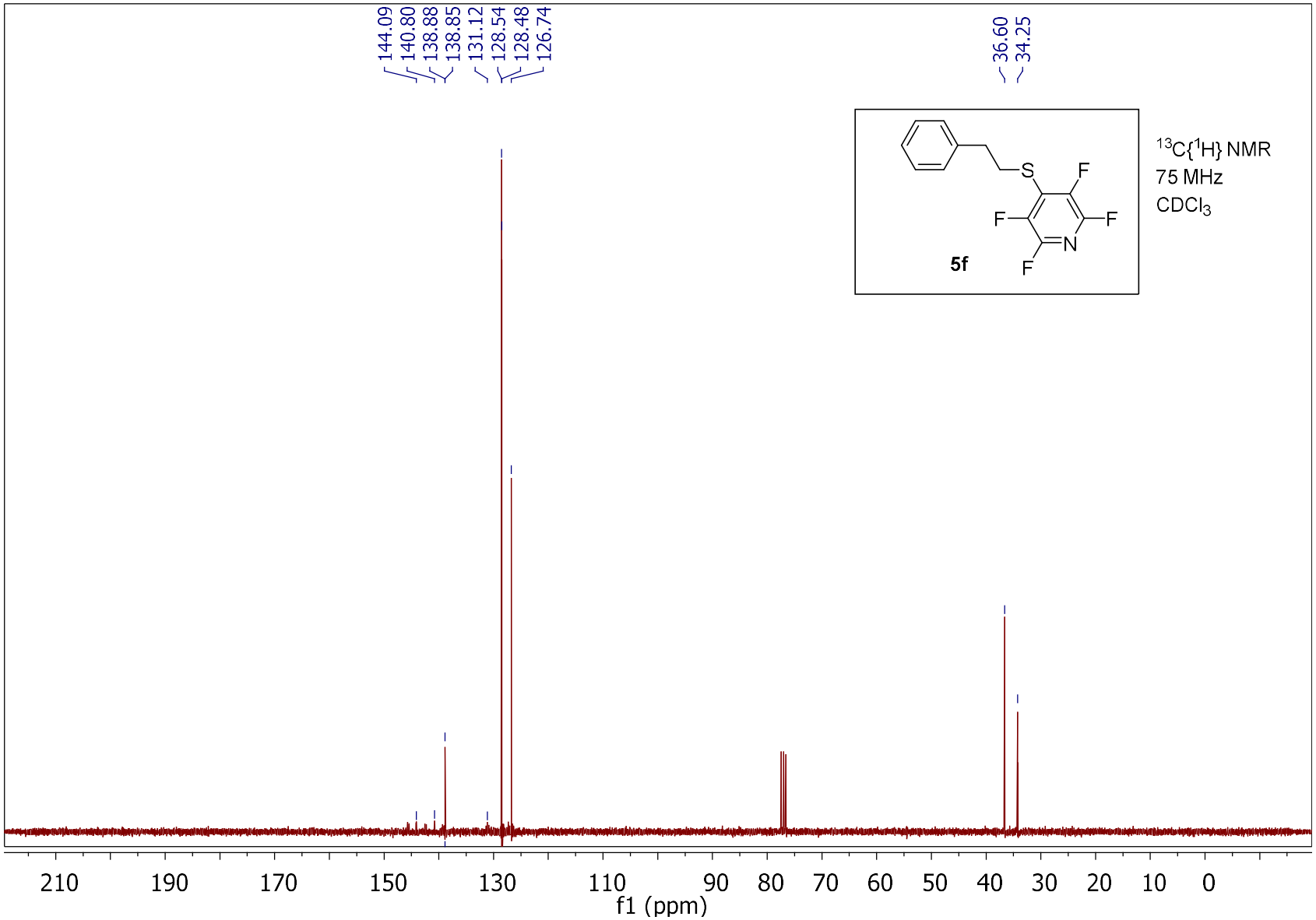

8.75
7.63
7.28
7.26
7.26
7.24
7.21
7.19
6.61
3.94
2.81
2.78
2.74
2.71
NH2
N
N
H2N
N
N
S
5d
1H NMR
300 MHz
DMSO-d6
0.99
2.03
5.05
1.88
2.00
3.97
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

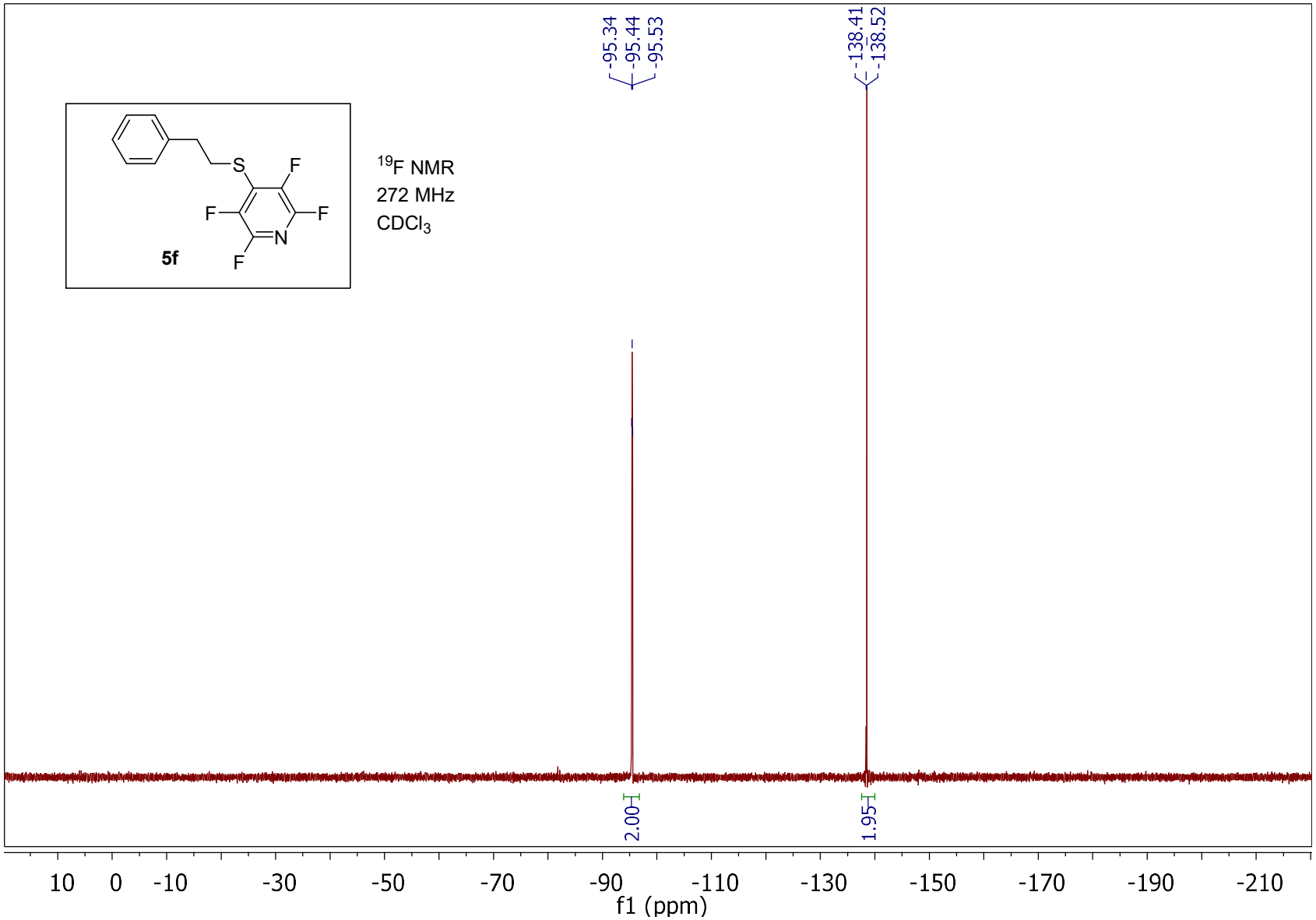

163.85
163.29
155.36
151.42
146.99
140.79
128.96
128.71
126.58
121.25
35.72
34.51
32.62
NH2
N
N
H2N
N
N
S
5d
13C{1H} NMR
75 MHz
DMSO-d6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

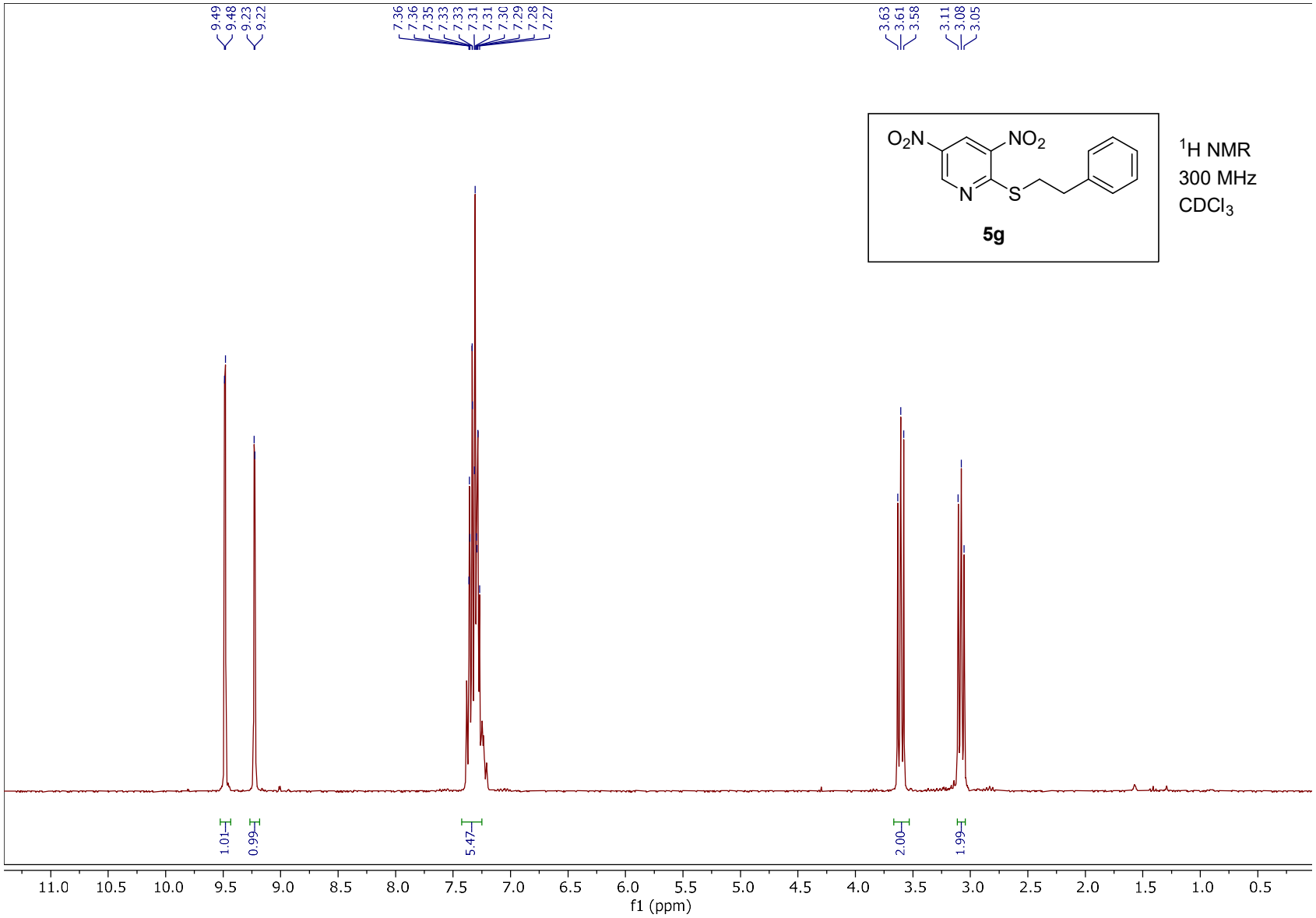

7.36
7.36
7.35
7.35
7.33
7.33
7.33
7.31
7.31
7.30
7.30
7.29
7.29
7.29
7.28
7.28
7.28
7.27
7.26
7.26
7.24
7.24
3.51
3.51
3.49
3.49
3.49
3.48
3.46
3.46
3.15
3.13
3.12
3.10
3.04
3.02
3.01
2.99
2.99
2.98
2.97
1.39
1.37
N
O
S
N
5e
1H NMR
300 MHz
CDCl3
2.04
3.30
2.00
3.06
6.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

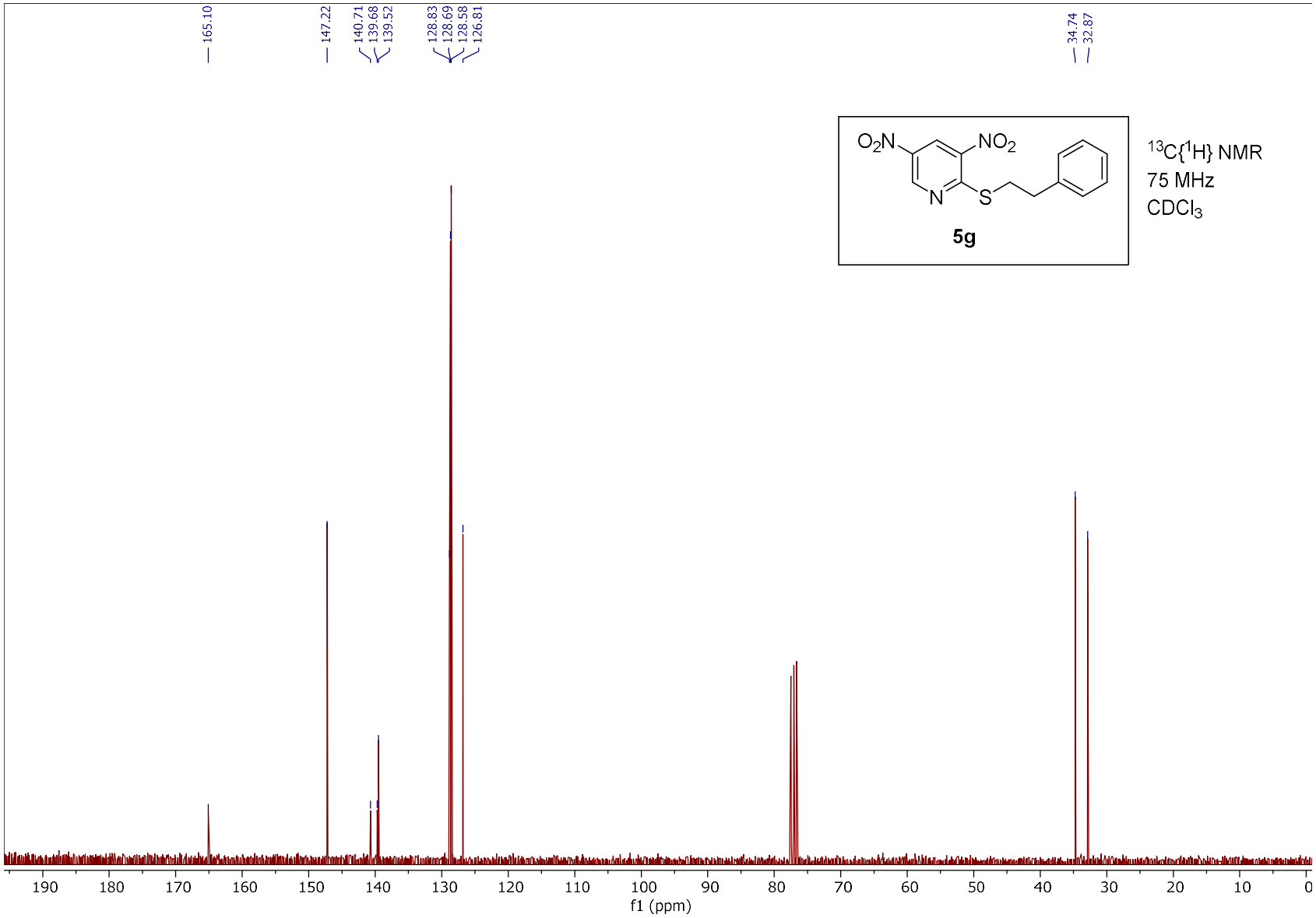

177.19
175.39
139.06
128.71
128.67
126.90
35.84
33.96
27.00
20.43
5e
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
f1 (ppm)

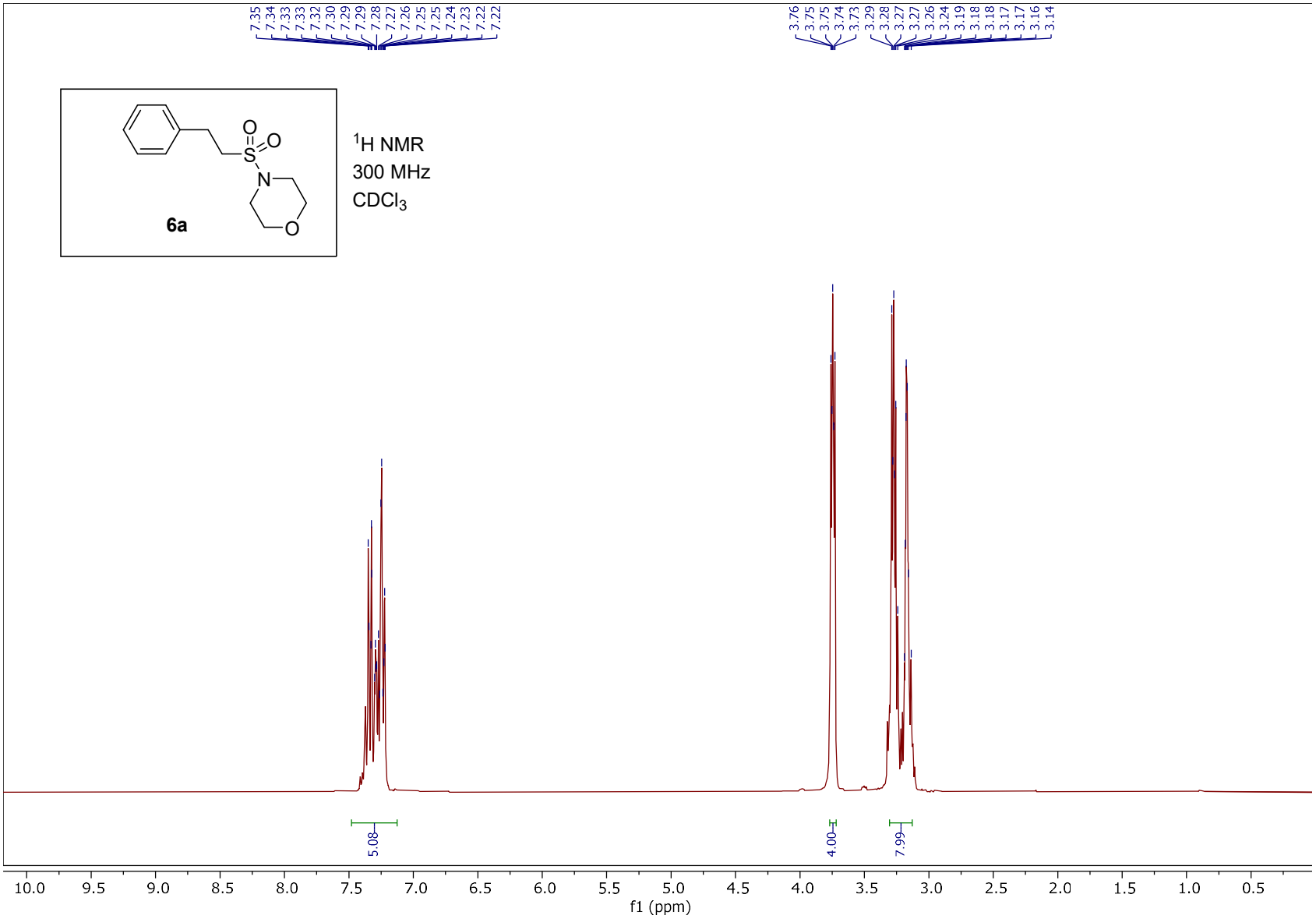

7.33
7.31
7.31
7.30
7.29
7.29
7.28
7.26
7.25
7.23
7.23
7.22
7.21
7.20
7.20
3.41
3.39
3.36
3.00
2.98
2.95
S
F
F
F
N
F
5f
1H NMR
300 MHz
CDCl3
2.02
3.09
2.00
2.02
f1 (ppm)

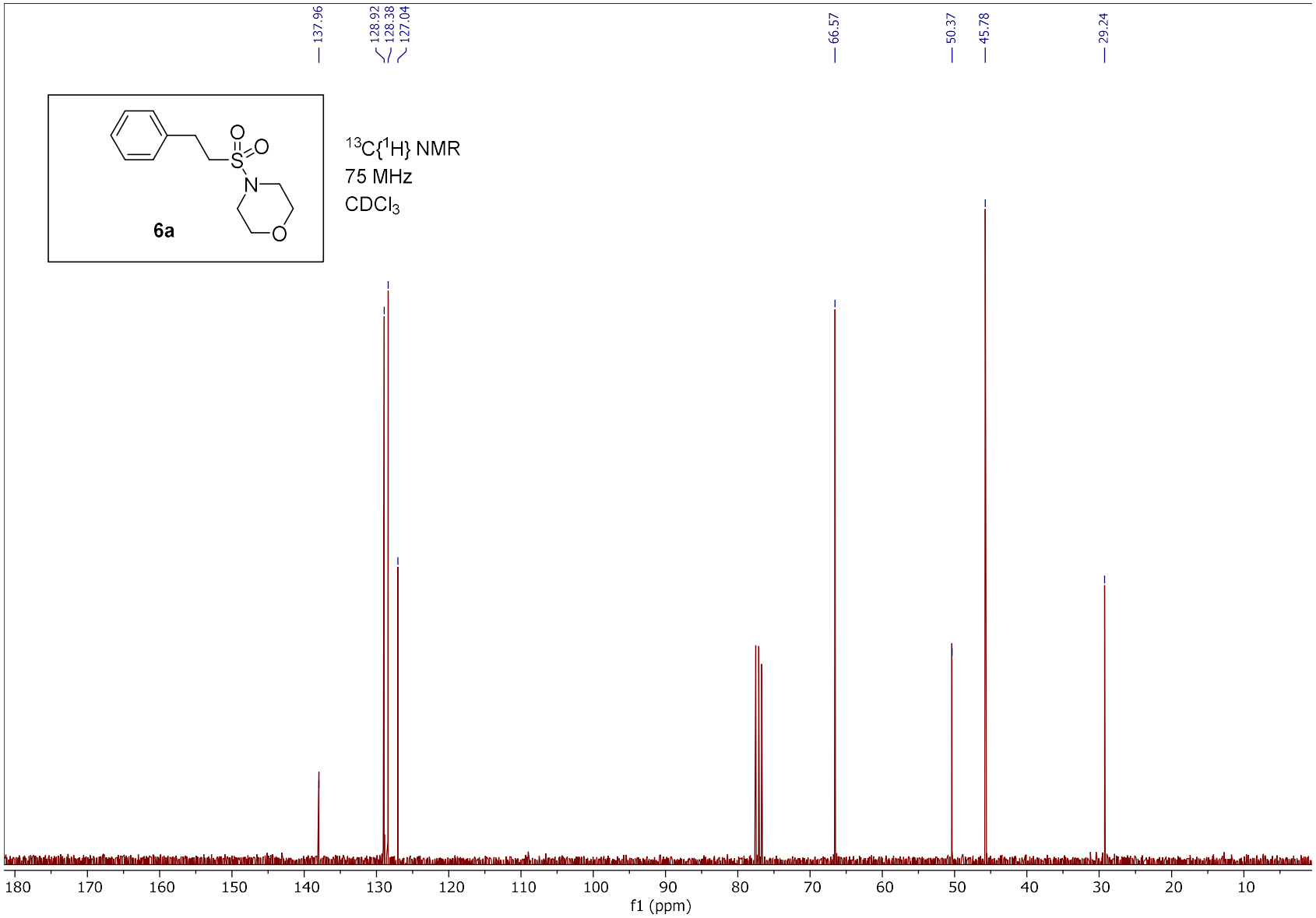

144.09
140.80
138.88
138.85
131.12
128.54
128.48
126.74
36.60
34.25
S
F
F
F
F
N
5f
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

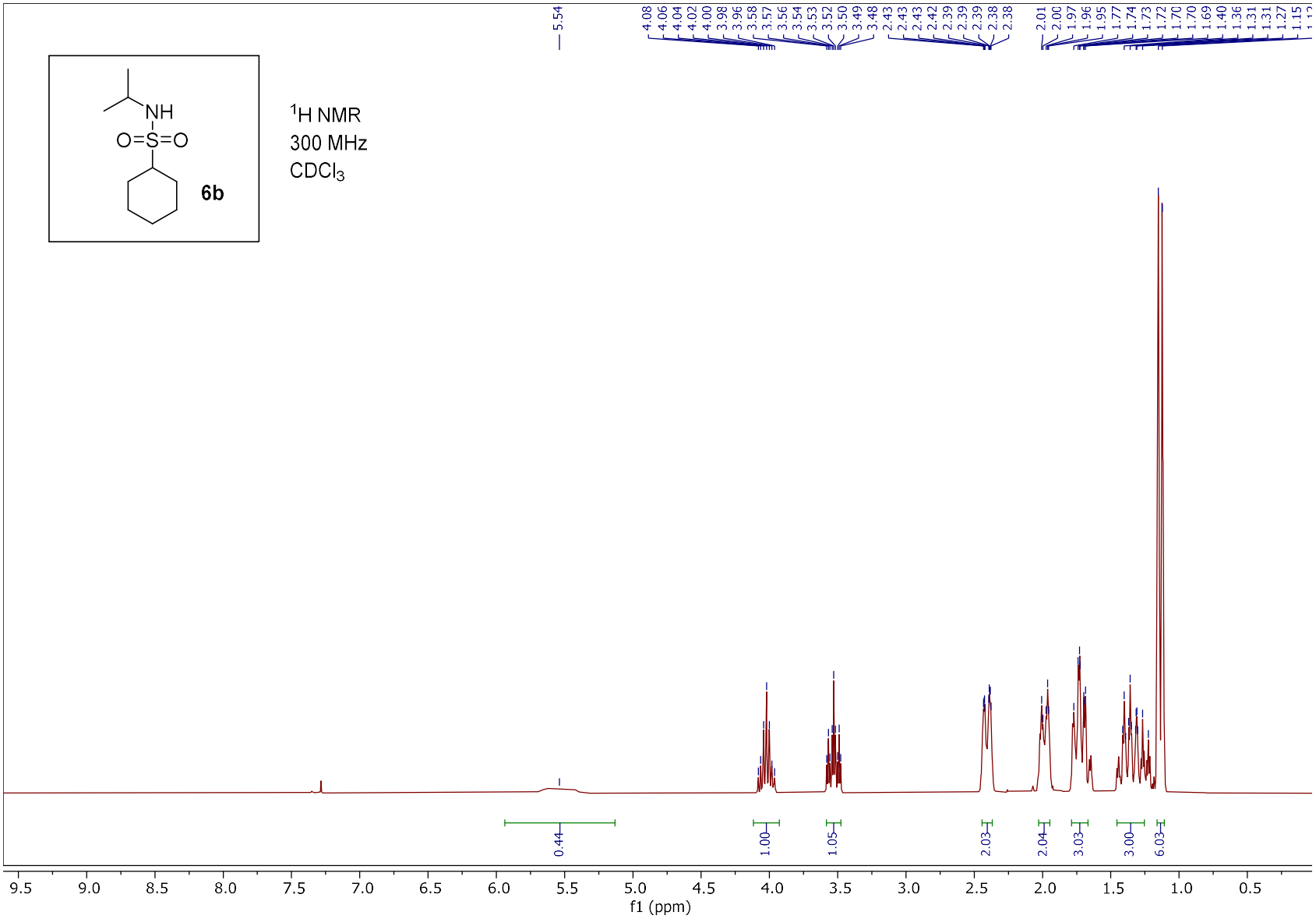

-95.34
-95.44
-95.53
-138.41
-138.52
S
F
F
F
N
F
5f
19F NMR
272 MHz
CDCl3
2.00
1.95
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

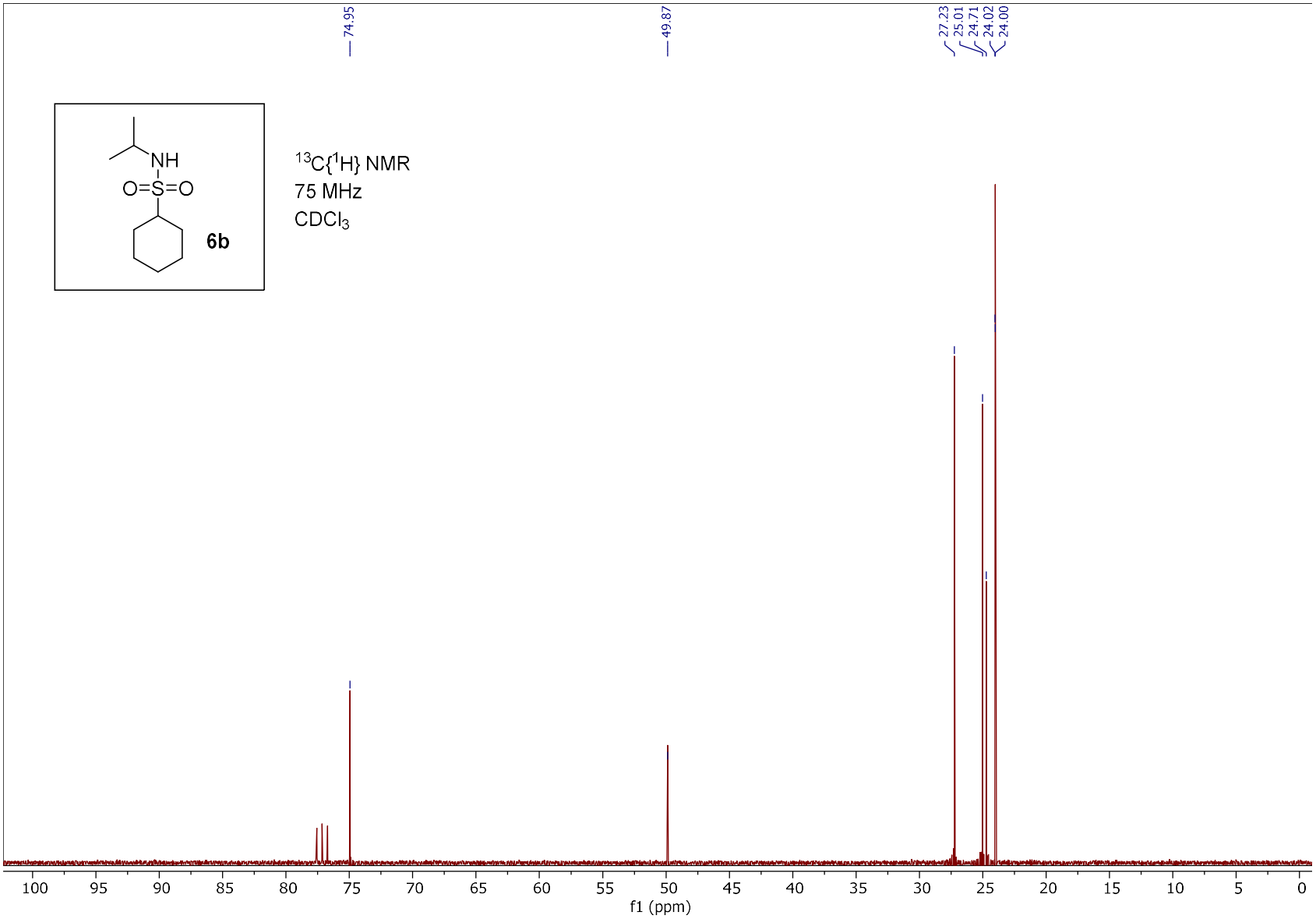

9.49
9.48
9.23
9.22
7.36
7.36
7.35
7.33
7.33
7.31
7.31
7.30
7.29
7.28
7.27
3.63
3.61
3.58
3.11
3.08
3.05
O2N
NO2
N
S
5g
1H NMR
300 MHz
CDCl3
1.01
0.99
5.47
2.00
1.99
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

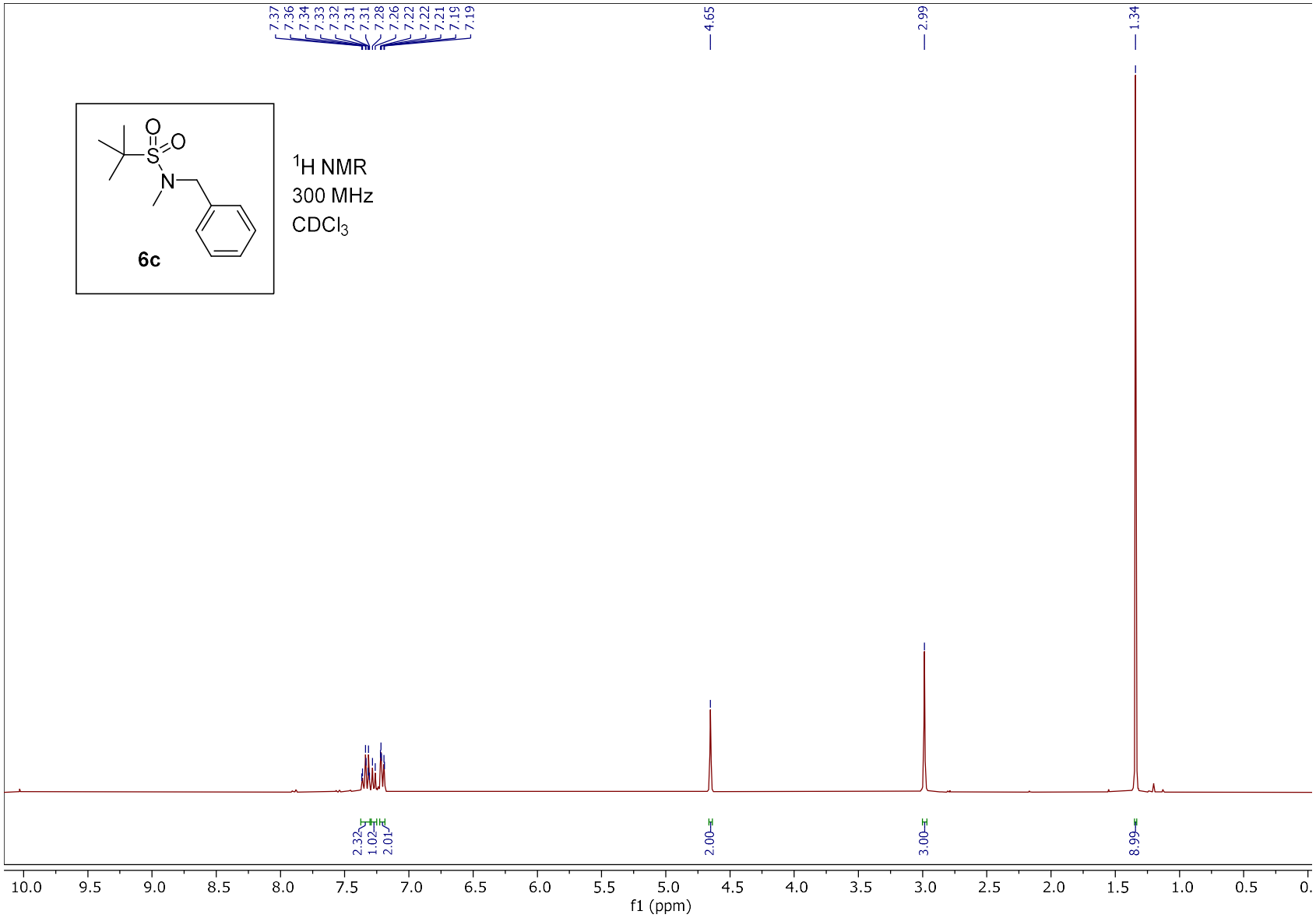

165.10
147.22
140.71
139.68
139.52
128.83
128.69
128.58
126.81
34.74
32.87
O2N
NO2
N
S
5g
13C{1H} NMR
75 MHz
CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

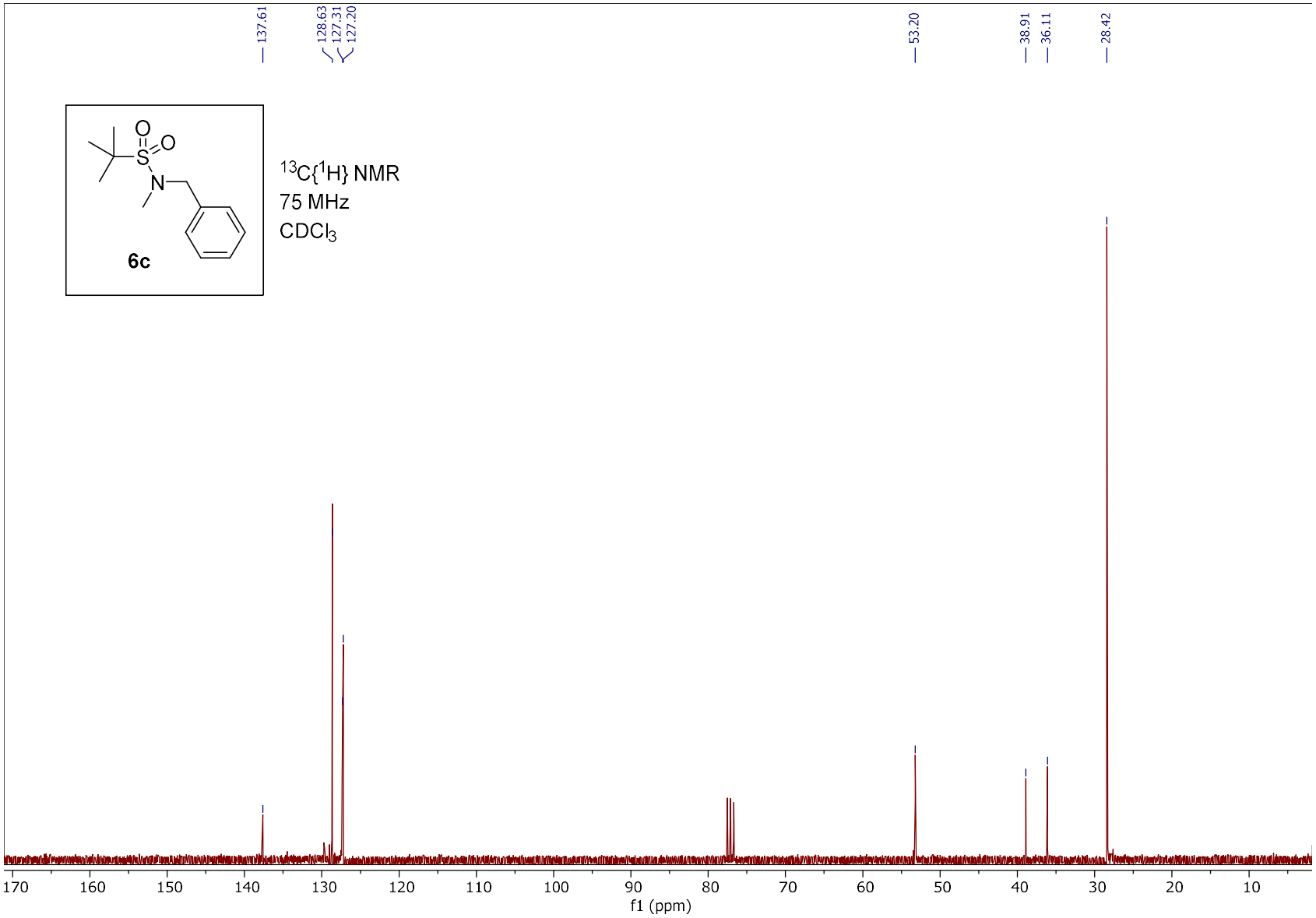

7.35
7.34
7.33
7.33
7.32
7.30
7.29
7.29
7.28
7.27
7.26
7.25
7.25
7.24
7.23
7.22
7.22
3.76
3.75
3.75
3.74
3.73
3.29
3.28
3.27
3.27
3.26
3.24
3.19
3.18
3.18
3.17
3.17
3.16
3.14
O
O
S
N
O
6a
1H NMR
300 MHz
CDCl3
5.08
4.00
7.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

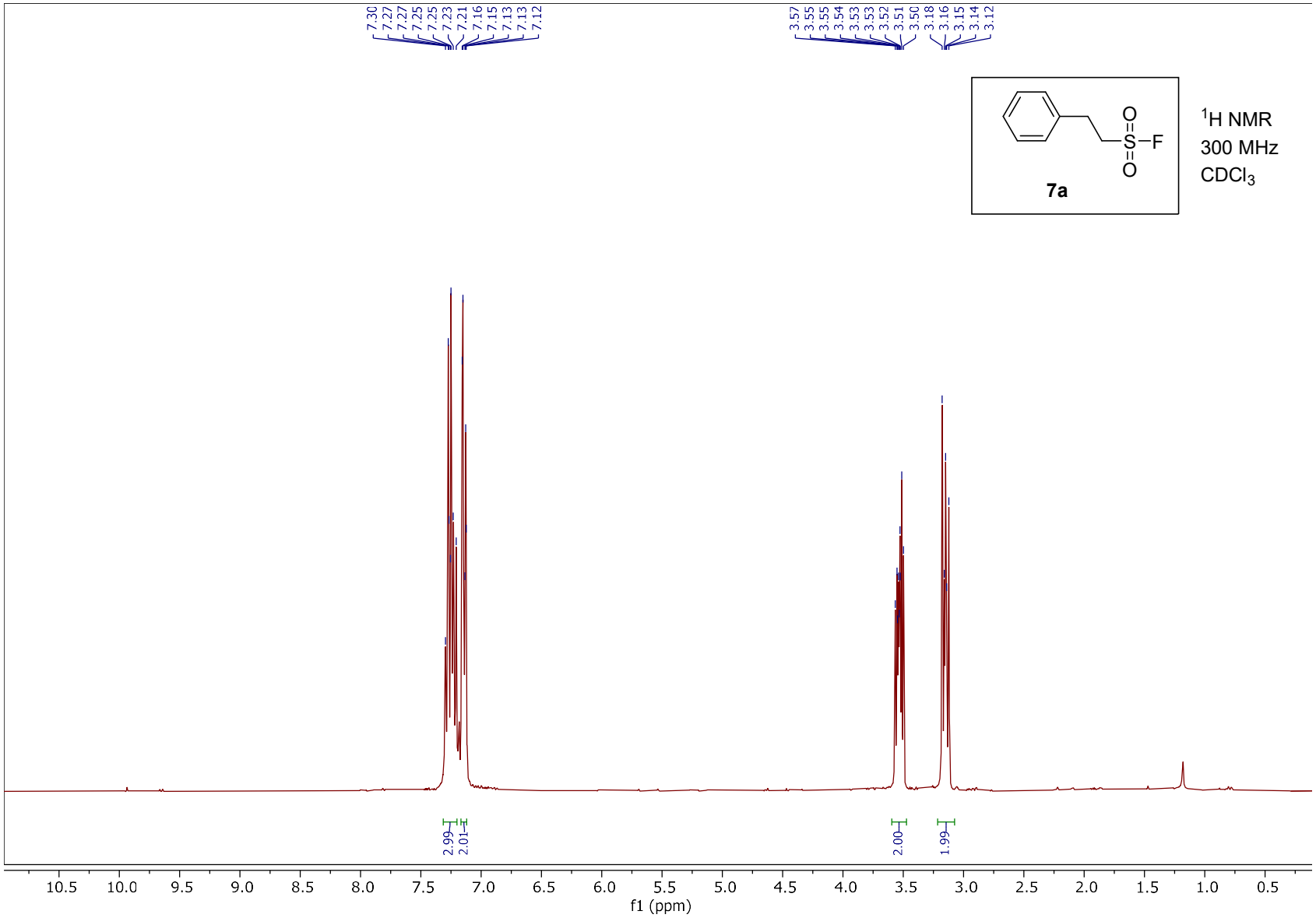

137.96
128.92
128.38
127.04
66.57
50.37
45.78
29.24
6a
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

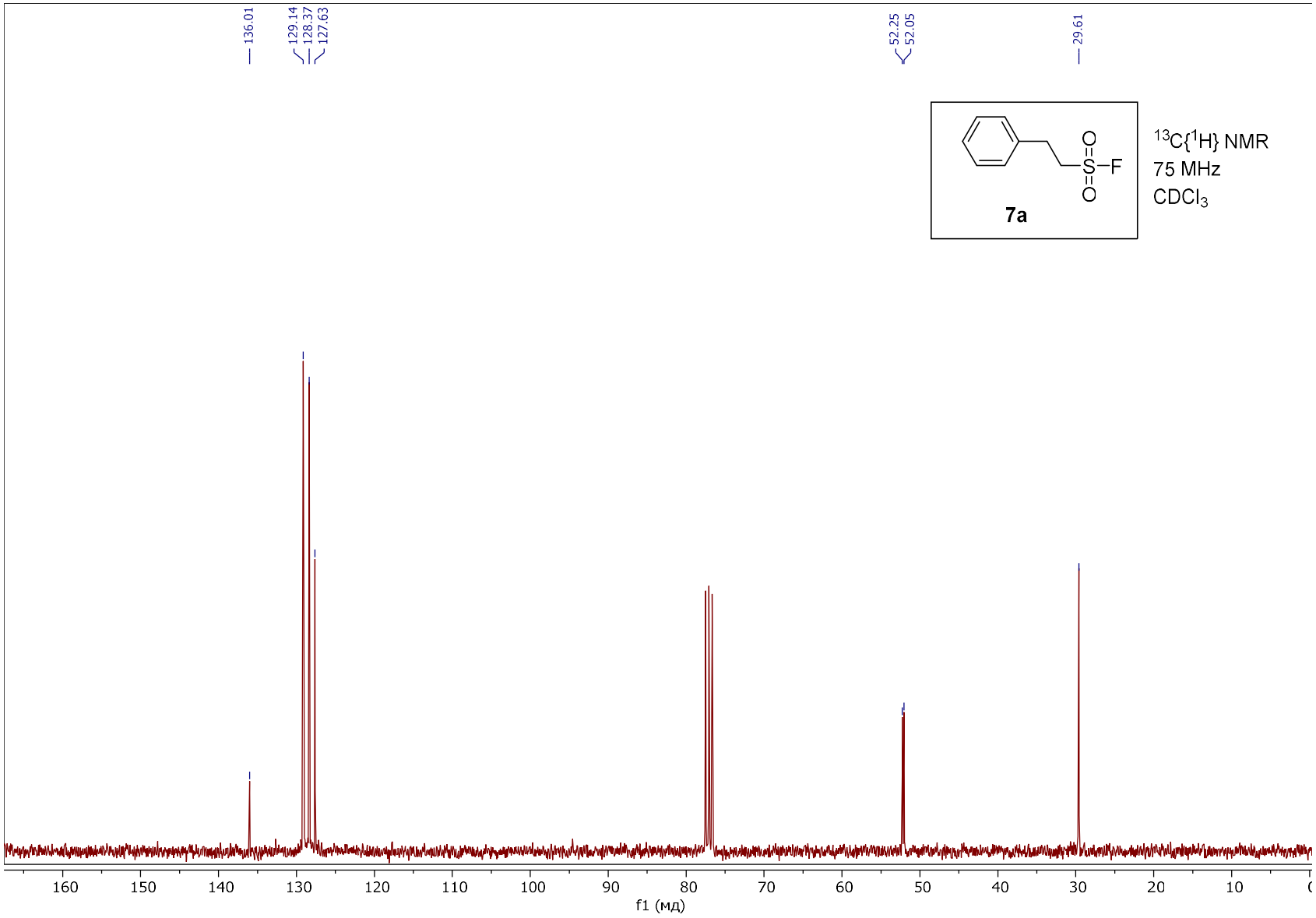

NH
O=S=O
6b
^{1}H NMR
300 MHz
$CDCl_3$
5.54
4.08
4.06
4.04
4.02
4.00
3.98
3.96
3.58
3.57
3.56
3.54
3.53
3.52
3.50
3.49
3.48
2.43
2.43
2.42
2.39
2.39
2.38
2.38
2.01
2.00
1.97
1.96
1.95
1.77
1.74
1.73
1.72
1.70
1.70
1.69
1.40
1.36
1.31
1.31
1.27
1.15
0.44
1.00
1.05
2.03
2.04
3.03
3.00
6.03
9.5
9.0
8.5
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
f1 (ppm)

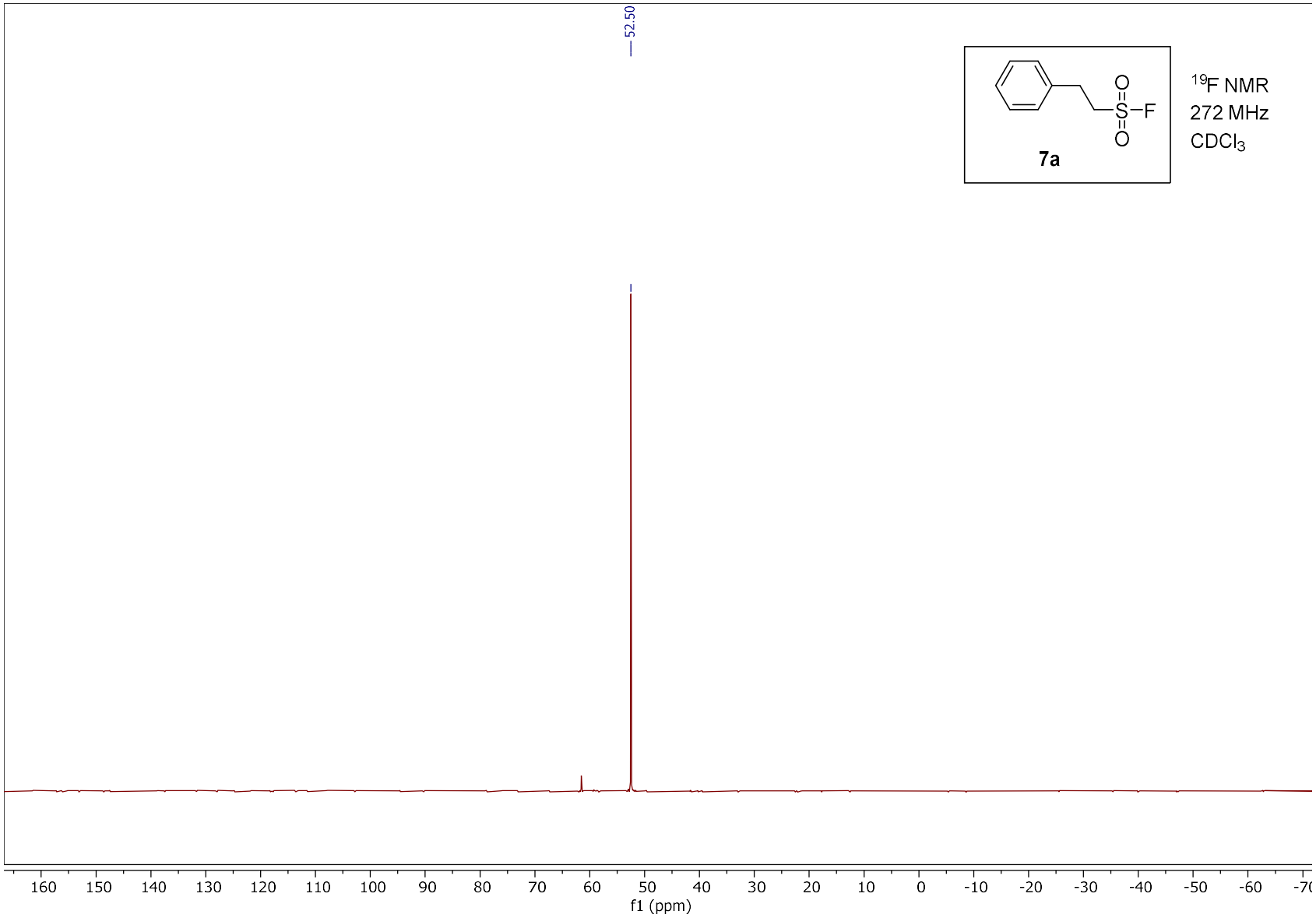

74.95
49.87
27.23
25.01
24.71
24.02
24.00
NH
O=S=O
6b
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

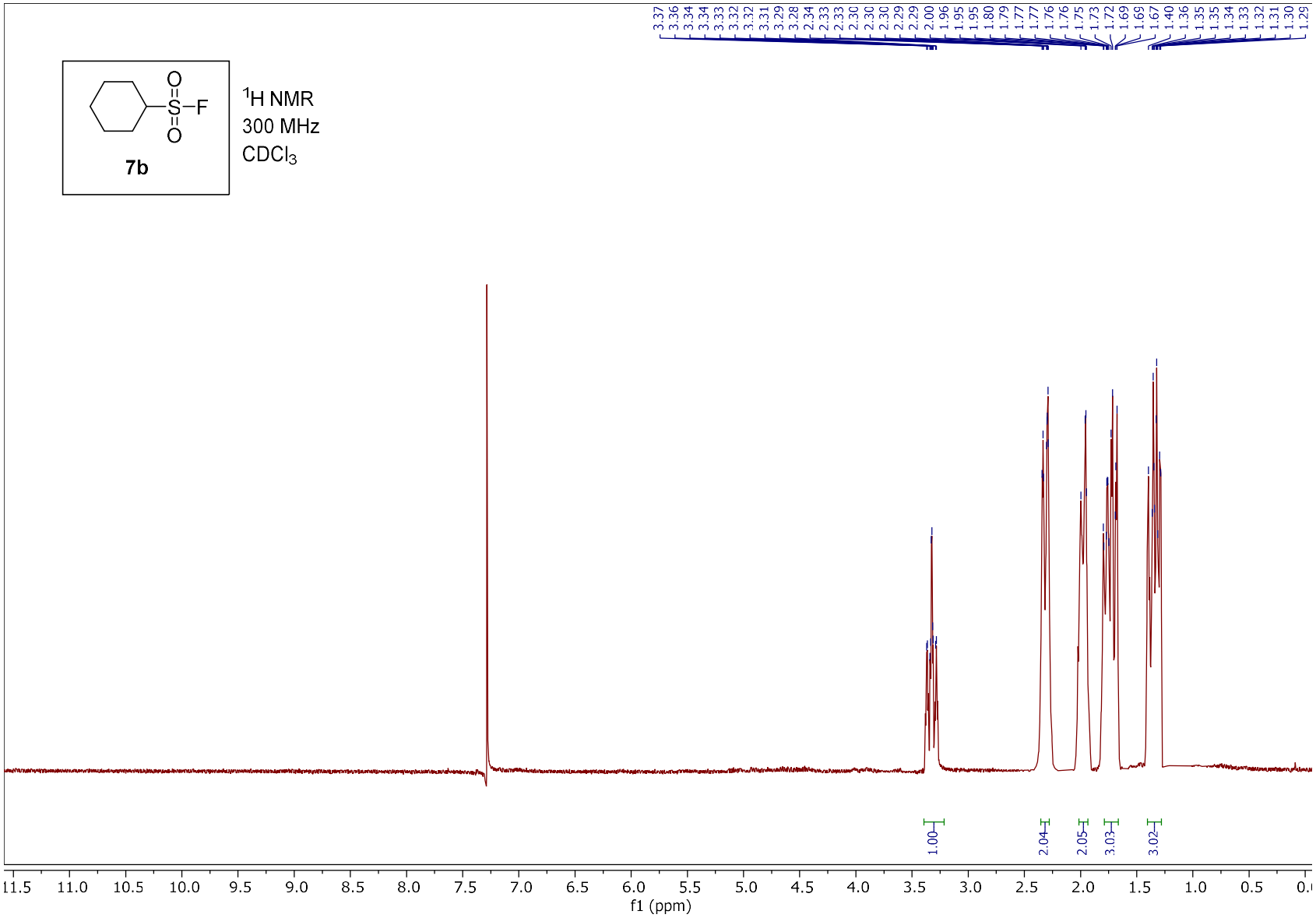

7.37
7.36
7.34
7.33
7.32
7.31
7.31
7.28
7.26
7.22
7.22
7.21
7.19
7.19
4.65
2.99
1.34
6c
1H NMR
300 MHz
CDCl3
2.32
1.02
2.01
2.00
3.00
8.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

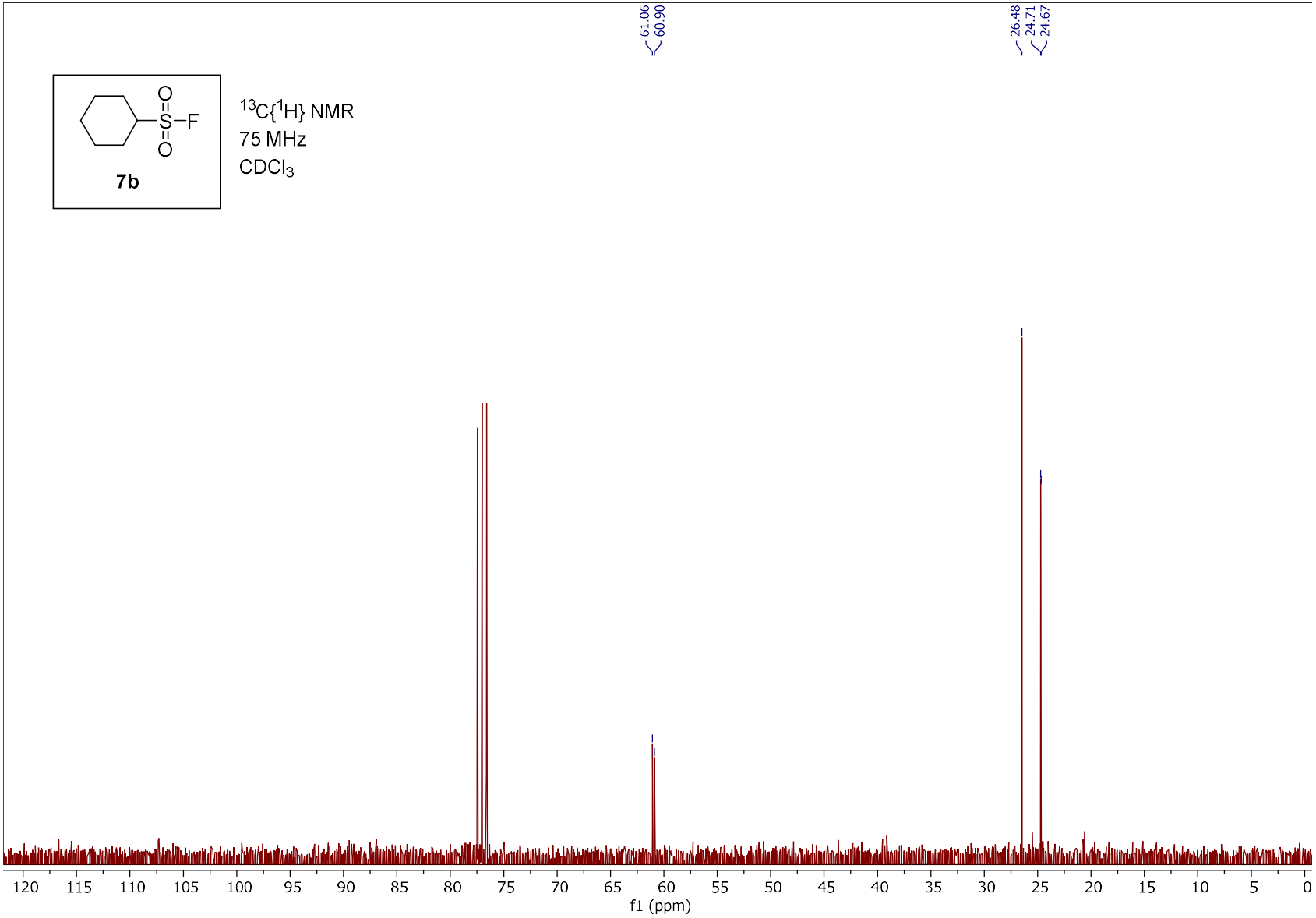

137.61
128.63
127.31
127.20
53.20
38.91
36.11
28.42
6c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

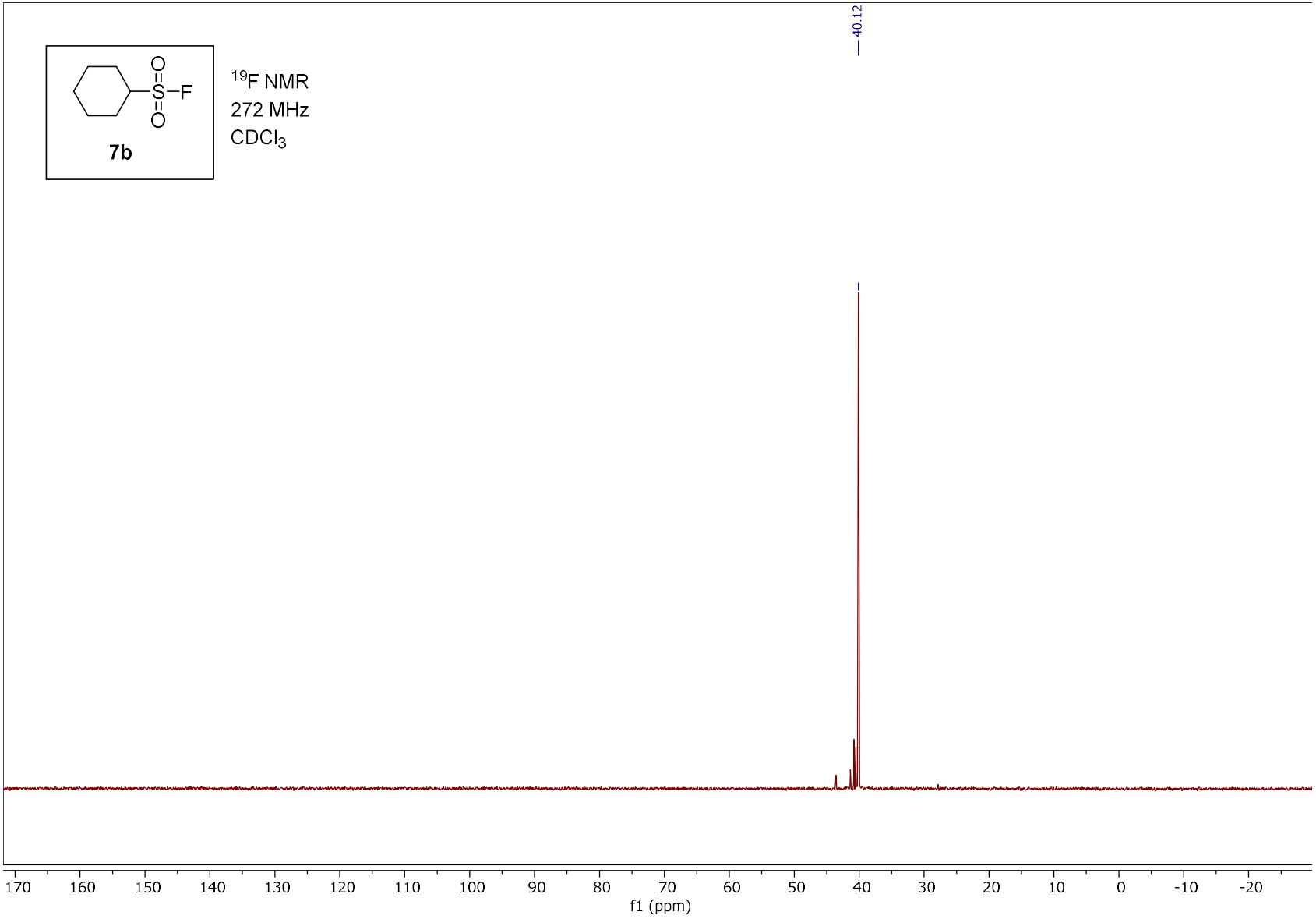

7.30
7.27
7.27
7.25
7.25
7.23
7.21
7.16
7.15
7.13
7.13
7.12
3.57
3.55
3.55
3.54
3.53
3.53
3.52
3.51
3.50
3.18
3.16
3.15
3.14
3.12
7a
^{1}H NMR
300 MHz
$CDCl_3$
2.99
2.01
2.00
1.99
f1 (ppm)

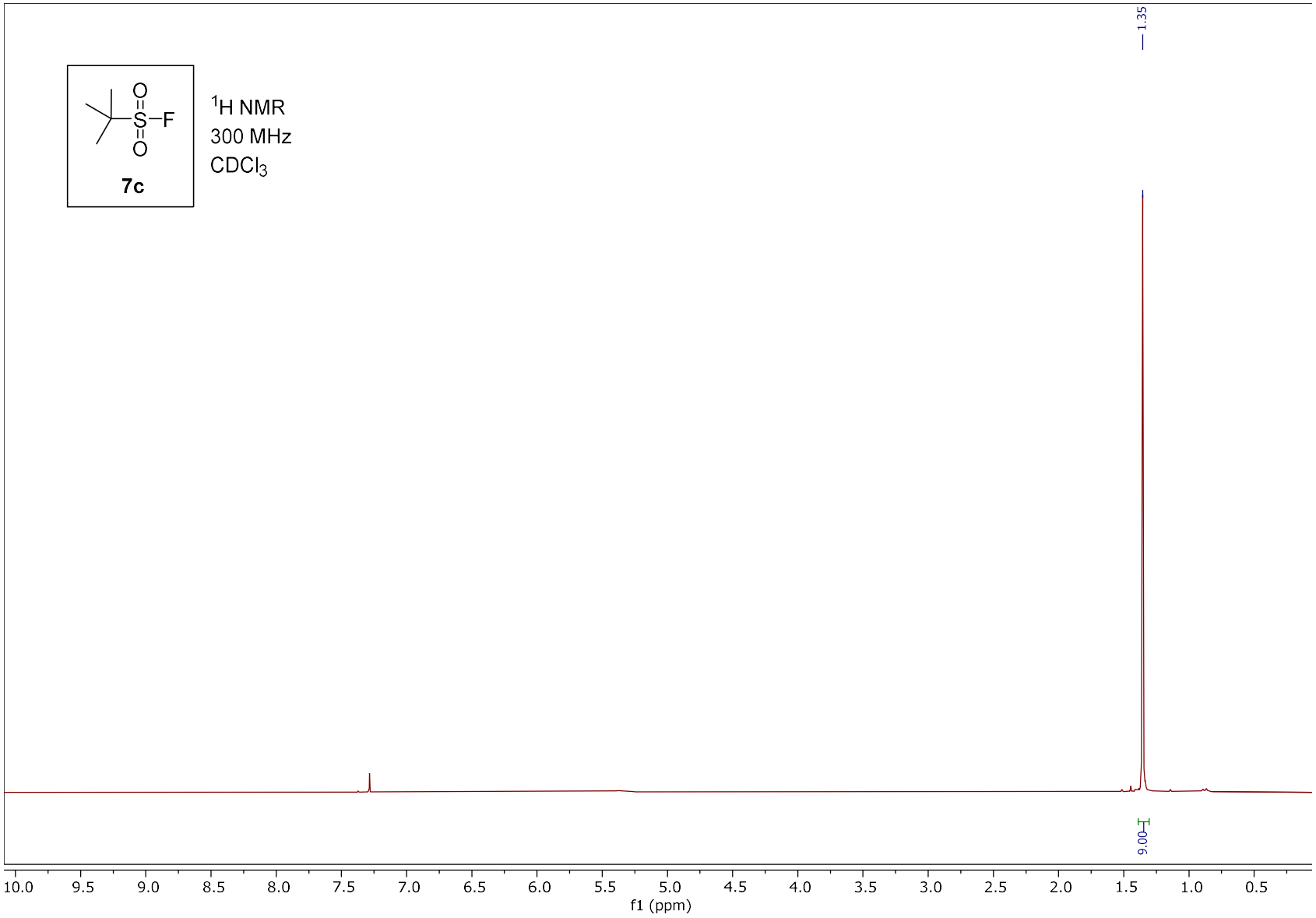

136.01
129.14
128.37
127.63
52.25
52.05
29.61
7a
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

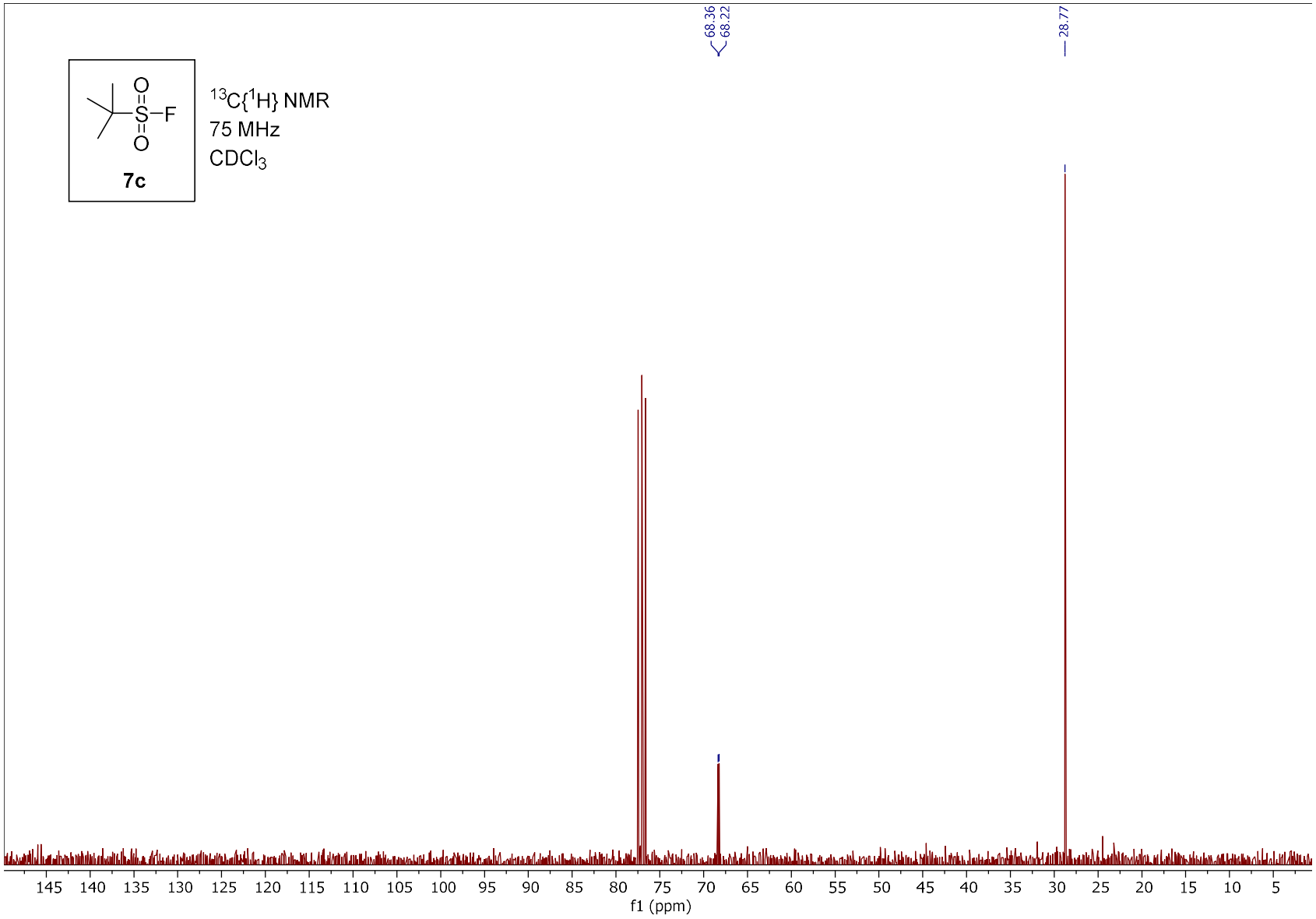

52.50
7a
19F NMR
272 MHz
CDCl3
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)

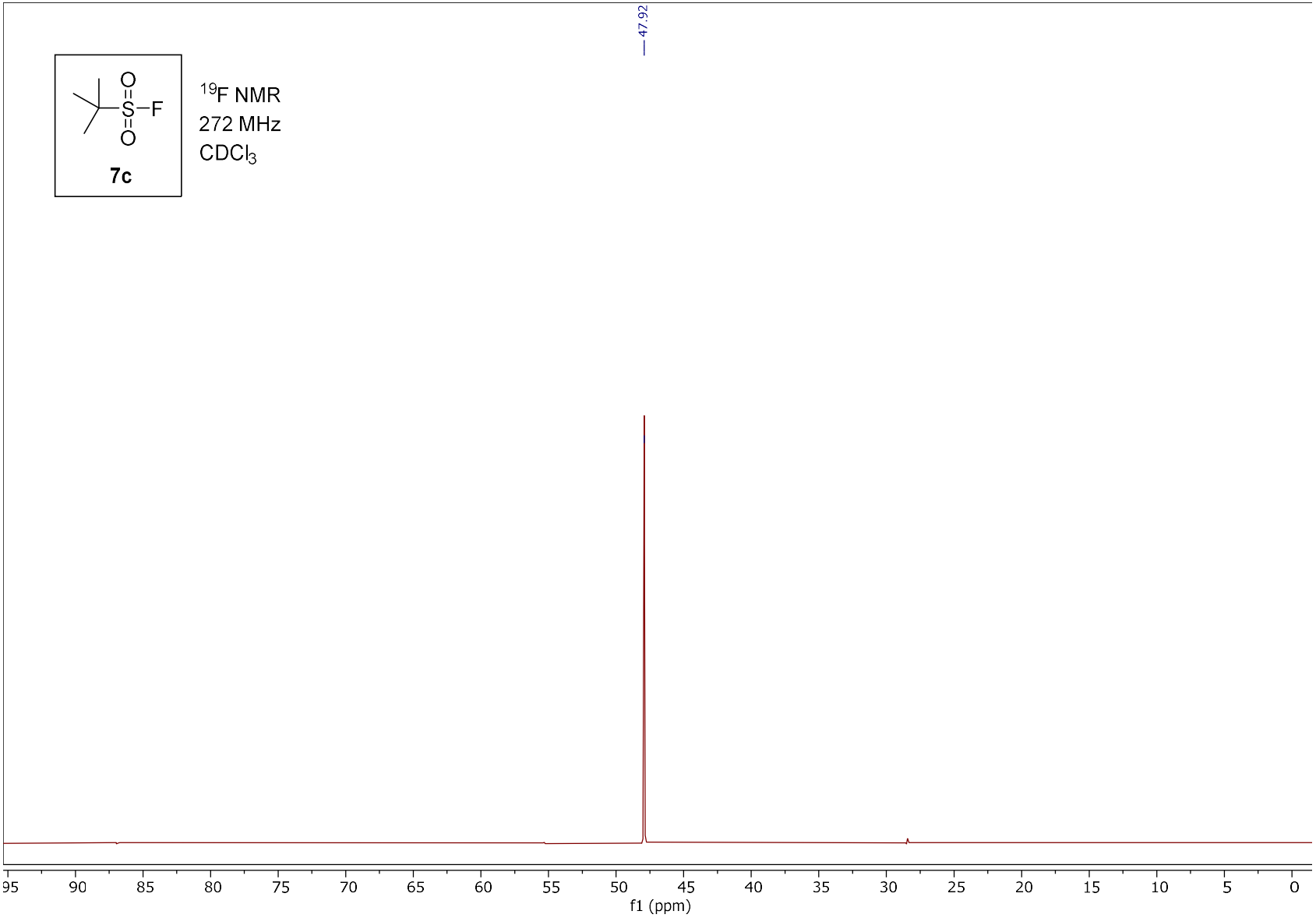

7b
^{1}H NMR
300 MHz
$CDCl_3$
3.37 3.36 3.34 3.34 3.33 3.32 3.31 3.29 3.28 2.34 2.33 2.33 2.30 2.30 2.30 2.29 2.29 2.00 1.96 1.95 1.95 1.80 1.79 1.77 1.77 1.76 1.76 1.75 1.73 1.72 1.69 1.69 1.67 1.40 1.36 1.35 1.35 1.34 1.33 1.32 1.31 1.30 1.29
1.00
2.04
2.05
3.03
3.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 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
f1 (ppm)


61.06
60.90
26.48
24.71
24.67
7b
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


40.12
7b
19F NMR
272 MHz
CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


7c
1H NMR
300 MHz
CDCl3
1.35
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
f1 (ppm)


68.36
68.22
28.77
7c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
f1 (ppm)


47.92
7c
19F NMR
272 MHz
CDCl3
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)