# Supporting Information

# An environmentally benign way to 2-thiocyano-1,3-dicarbonyl compounds with high antifungal activity: a key role of solvent

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## General materials and methods

$^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra were recorded on Bruker AVANCE II 300 spectrometer (300.13, 75.48 and 282 MHz, respectively) in $CDCl_3$. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: $^{1}H$ ($CDCl_3$ δ=7.25 ppm), $^{13}C$ ($CDCl_3$ δ=77.00 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), sept (septet), m (multiplet).

High resolution mass spectra (HR-MS) were measured on a Bruker micrOTOF II instrument using electrospray ionization (ESI).[1] The measurements were performed in a positive ion mode (interface capillary voltage - 4500 V); mass range from m/z 50 to m/z 3000 Da; external calibration with Electrospray Calibrant Solution (Fluka). A syringe injection was used for all acetonitrile solutions (flow rate 3 μL/min). Nitrogen was applied as a dry gas; interface temperature was set at 180 °C.

The TLC analysis was carried out on standard silica gel chromatography plates (DC-Fertigfolien ALUGRAMR Xtra SIL G/UV254). Column chromatography was performed using silica gel (0.060-0.200 mm, 60 A, CAS 7631-86-9, Acros).

Acetic acid, HCOOH, TFA, NaSCN, KSCN, $NH_4SCN$, $Br_2$, *n*-$Bu_4NBF_4$, **1r**, **1t**, **1u** were purchased from commercial sources and were used as is. All solvents were distilled before use using standard procedures.

Starting 2-substituted 1,3-dicarbonyl compounds **1a-h,**[2] **1i,**[3] **1j-q,**[4] **1s**[5] are known compounds and were prepared accordingly literature procedures.

## Calculation of the amount of electric current

$Q = I \cdot t$

*Q* - amount of passed electric current, C (Coulomb)

*I* - electric current, A

*t* - time, sec

$Q = I \cdot t = 0.080 \cdot 120 \cdot 60 = 576\ C$

$$N = \frac{Q}{F \cdot n_r}$$

*N* - number of electrons generated in the cell per 1 molecule of dicarbonyl compound, F/mol

*Q* - amount of electricity passed, C (Coulumb)

*F* - Faraday constant, F = 96485 ($C \cdot mol^{-1}$)

$n_r$ - amount of dicarbonyl compound **1**, mol

$$N = \frac{576}{96485 \cdot 0.001} = 5.97\frac{F}{mol} \approx 6\frac{F}{mol}$$

**General Experimental Procedure for Table 1.**

A 20 mL electrolysis cell was charged with 1,3-dicarbonyl compound **1a** (1.0 mmol, 190.2 mg), $NH_4SCN$ (5.0 mmol, 380.5 mg), and solvent (10 mL). The mixture was stirred for 1-2 minutes to obtain a homogeneous solution. The platinum plate electrodes (2×1.5 cm) were inserted at a distance of 1.5 cm, and the reaction mixture was stirred at a constant current of 80 mA for 2 hours.

*in the case of $CH_3SO_3H$* – Then, $H_2O$ (30 mL) was added, the mixture was extracted with EtOAc (3×15 mL). The combined organic phase was washed with sat. $NaHCO_3$ (3×5 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 20–25 °C).

*in the other cases* - the reaction mixture was concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 40-50 °C). Then, EtOAc (30 mL) was added, the mixture was washed with $H_2O$ (3×5 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 20–25 °C).

**General Experimental Procedure for Table 2 (entry 1).**

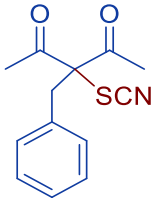
A 20 mL electrolysis cell was charged with 1,3-dicarbonyl compound **1a** (1.0 mmol, 190.2 mg), $NH_4SCN$ (5.0 mmol, 380.5 mg), and AcOH (10 mL). The mixture was stirred for 1-2 minutes to obtain a homogeneous solution. The platinum plate electrodes (2×1.5 cm) were inserted at a distance of 1.5 cm, and the reaction mixture was stirred at a constant current of 80 mA for 2 hours. Then, the reaction mixture was concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 40-50 °C). After that, the reaction mixture was transferred onto $SiO_2$ chromatographic column and product **2a** was isolated by chromatography on $SiO_2$ (PE:EtOAc = from 50:1 to 2:1).

**Experimental Procedure for Scheme 2.**

A 20 mL electrolysis cell was charged with β-dicarbonyl compound **1** (1.0 mmol), $NH_4SCN$ (5.0 mmol, 380.5 mg) and AcOH (10 mL). The mixture was stirred for 1-2 minutes to obtain a homogeneous solution. The platinum plate electrodes (2×1.5 cm) were inserted at a distance of 1.5 cm, and the reaction mixture was stirred at a constant current of 80 mA for 2 hours. Then, $CH_2Cl_2$ (30 mL) was added, the residue was filtered and washed with $CH_2Cl_2$ (2×5 mL). The combined organic phase was concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 40-50 °C). Product **2** was isolated by chromatography on $SiO_2$ (PE:EtOAc = from 50:1 to 2:1).

**Characterization of synthesized thiocyanates**

**3-Benzyl-3-thiocyanatopentane-2,4-dione, 2a** (known compound [6])

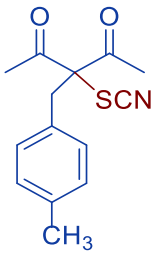



Yield 82% (202.8 mg, 0.82 mmol). Yellow solid, m.p. = 52-53 ˚C (lit.[6] 53-54 ˚C). $R_f$ = 0.30 (PE:EtOAc = 5:1).

$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 7.34 – 7.27 (m, 3H), 7.21 – 7.14 (m, 2H), 3.64 (s, 2H), 2.38 (s, 6H).

$^{13}C\{^1H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 198.3, 133.2, 129.9, 128.9, 128.2, 110.4, 83.0, 37.9, 26.7.

**3-(4-Methylbenzyl)-3-thiocyanatopentane-2,4-dione, 2b**



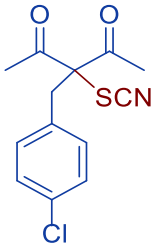

Yield 65% (169.9 mg, 0.65 mmol). Orange solid, m.p. = 91-93 ˚C. $R_f$ = 0.17 (PE:EtOAc = 5:1).

$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 7.11 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 3.60 (s, 2H), 2.37 (s, 6H), 2.32 (s, 3H).

$^{13}C\{^1H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 198.4, 138.0, 130.1, 129.7, 129.6, 110.5, 83.1, 37.6, 26.8, 21.2.

HRMS (ESI-TOF) m/z $[M+Na]^+$. Calcd for $[C_{14}H_{15}NO_2SNa]^+$: 284.0716. Found: 284.0722.

**3-(4-Chlorobenzyl)-3-thiocyanatopentane-2,4-dione, 2c** (known compound [6])




6 F/mol, 5.0 eq. $NH_4SCN$ - Yield 40% (112.7 mg, 0.40 mmol).

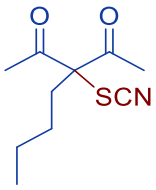
8 F/mol, 10.0 eq. $NH_4SCN$ - Yield 51% (143.7 mg, 0.51 mmol).

Orange oil. $R_f$ = 0.55 (PE:EtOAc = 2:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 7.28 (d, *J* = 8.5 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 3.60 (s, 2H), 2.37 (s, 6H).

$^{13}$C{$^{1}$H} NMR (75.48 MHz, $CDCl_3$, δ): 198.0, 134.3, 131.7, 131.20, 129.1, 110.2, 82.8, 37.3, 26.7.

**3-Butyl-3-thiocyanatopentane-2,4-dione, 2d**



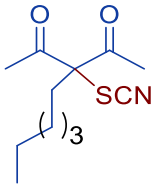

Yield 75% (160.0 mg, 0.75 mmol). Yellow oil. $R_f$ = 0.31 (PE:EtOAc = 5:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 2.35 – 2.23 (m, 8H), 1.51 – 1.35 (m, 2H), 1.32 – 1.20 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H).

$^{13}$C{$^{1}$H} NMR (75.48 MHz, $CDCl_3$, δ): 199.0, 110.2, 82.7, 32.0, 26.1, 22.6, 13.8.

HRMS (ESI-TOF) m/z $[M+Na]^+$. Calcd for $[C_{10}H_{15}NO_2SNa]^+$: 236.0716. Found: 236.0725.

**3-Hexyl-3-thiocyanatopentane-2,4-dione, 2e** (known compound [6])

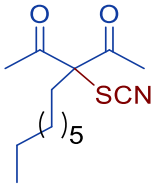



Yield 80% (193.1 mg, 0.80 mmol). Orange oil. $R_f$ = 0.41 (PE:EtOAc = 5:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 2.56 – 2.04 (m, 8H), 1.44 – 1.20 (m, 8H), 0.88 (t, *J* = 6.5 Hz, 3H).

$^{13}$C{$^{1}$H} NMR (75.48 MHz, $CDCl_3$, δ): 199.1, 110.3, 82.7, 32.2, 31.4, 29.1, 26.1, 23.9, 22.6, 14.0.

**3-Octyl-3-thiocyanatopentane-2,4-dione, 2f**



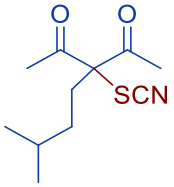

Yield 69% (185.9 mg, 0.69 mmol). Yellow oil. $R_f$ = 0.15 (PE:EtOAc = 20:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 2.34 – 2.23 (m, 8H), 1.42 – 1.20 (m, 12H), 0.87 (t, *J* = 6.7 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 199.0, 110.3, 82.7, 32.2, 31.8, 29.4, 29.23, 29.17, 26.1, 23.9, 22.7, 14.2.

HRMS (ESI-TOF) m/z $[M+NH_4]^+$. Calcd for $[C_{14}H_{27}N_2O_2S]^+$: 287.1788. Found: 287.1782.

**3-*Iso*pentyl-3-thiocyanatopentane-2,4-dione, 2g**



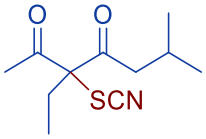

Yield 51% (116.0 mg, 0.51 mmol). Yellow oil. $R_f$ = 0.23 (PE:EtOAc = 10:1).

$^{1}H$ NMR (300.13 MHz, $CDCl_3$, δ): 2.34 – 2.23 (m, 8H), 1.71 – 1.54 (m, 1H), 1.20 – 1.10 (m, 2H), 0.93 (d, *J* = 6.6 Hz, 6H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 199.0, 110.2, 82.8, 32.8, 30.2, 28.1, 26.1, 22.4.

HRMS (ESI-TOF) m/z $[M+Na]^+$. Calcd for $[C_{11}H_{17}NO_2SNa]^+$: 250.0872. Found: 250.0879.

**3-Ethyl-6-methyl-3-thiocyanatoheptane-2,4-dione, 2h**



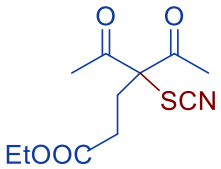

Yield 37% (84.1 mg, 0.37 mmol). Yellow oil. $R_f$ = 0.18 (PE:EtOAc = 20:1).

$^{1}H$ NMR (300.13 MHz, $CDCl_3$, δ): 2.57 – 2.45 (m, 1H), 2.42 – 2.31 (m, 2.5H), 2.27 (s, 3H), 2.29 – 2.12 (m, 1.5H), 1.00 – 0.87 (m, 9H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 200.6, 199.2, 110.4, 83.8, 47.3, 26.2, 25.6, 24.1, 22.4, 22.3, 8.3.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{11}H_{18}NO_2S]^+$: 228.1053. Found: 228.1061.

**Ethyl 4-acetyl-5-oxo-4-thiocyanatohexanoate, 2i** (known compound [6])




6 F/mol, 5.0 eq. $NH_4SCN$ - Yield 39% (100.3 mg, 0.39 mmol).

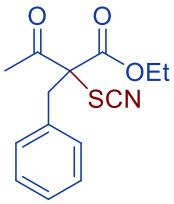
8 F/mol, 10.0 eq. $NH_4SCN$ - Yield 40% (103.0 mg, 0.40 mmol).

Yellow oil. $R_f$ = 0.57 (PE:EtOAc = 2:1).

$^{1}H$ NMR (300.13 MHz, $CDCl_3$, δ): 4.12 (q, *J* = 7.1 Hz, 2H), 2.69 – 2.62 (m, 2H), 2.41 – 2.33 (m, 2H), 2.32 (s, 6H), 1.24 (t, *J* = 7.1 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 198.5, 171.6, 109.7, 81.9, 61.3, 29.1, 27.3, 26.3, 14.3.

**Ethyl 2-benzyl-3-oxo-2-thiocyanatobutanoate, 2j**



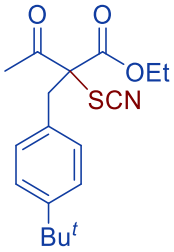

Yield 62% (172.0 mg, 0.62 mmol). Orange solid, m.p. = 74-75 °C. $R_f$ = 0.22 (PE:EtOAc = 10:1).

$^{1}H$ NMR (300.13 MHz, $CDCl_3$, δ): 7.34 – 7.28 (m, 3H), 7.24 – 7.18 (m, 2H), 4.40 – 4.22 (m, 2H), 3.64 (d, *J* = 15.1 Hz, 1H), 3.50 (d, *J* = 15.1 Hz, 1H), 2.39 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 195.7, 166.3, 133.4, 130.1, 128.7, 128.1, 109.9, 73.4, 64.2, 38.6, 25.8, 14.0.

HRMS (ESI-TOF) m/z $[M+Na]^+$. Calcd for $[C_{14}H_{15}NO_3SNa]^+$: 300.0665. Found: 300.0664.

**Ethyl 2-(4-(*tert*-butyl)benzyl)-3-oxo-2-thiocyanatobutanoate, 2k**



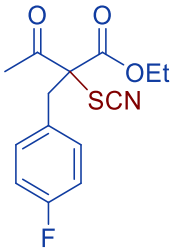

Yield 53% (176.7 mg, 0.53 mmol). Yellow oil. $R_f$ = 0.29 (PE:EtOAc = 10:1).

$^{1}H$ NMR (300.13 MHz, $CDCl_3$, δ): 7.32 (d, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 4.41 – 4.22 (m, 2H), 3.61 (d, *J* = 15.1 Hz, 1H), 3.48 (d, *J* = 15.1 Hz, 1H), 2.39 (s, 6H), 1.34 – 1.27 (m, 3H), 1.30 (s, 9H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 195.9, 166.5, 151.1, 130.3, 129.9, 125.7, 109.9, 73.5, 64.1, 38.3, 34.7, 31.4, 25.9, 14.0.

HRMS (ESI-TOF) m/z $[M+NH_4]^+$. Calcd for $[C_{18}H_{27}N_2O_3S]^+$: 351.1737. Found: 351.1742.

**Ethyl 2-(4-fluorobenzyl)-3-oxo-2-thiocyanatobutanoate, 2l**




Yield 68% (200.0 mg, 0.68 mmol). Yellow solid, m.p. = 82-84 °C. $R_f$ = 0.19 (PE:EtOAc = 10:1).

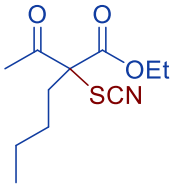
$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 7.23 – 7.12 (m, 2H), 7.05 – 6.94 (m, 2H), 4.40 – 4.22 (m, 2H), 3.61 (d, *J* = 15.2 Hz, 1H), 3.47 (d, *J* = 15.2 Hz, 1H), 2.39 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H).

$^{13}$C{$^1$H} NMR (75.48 MHz, $CDCl_3$, δ): 195.4, 166.2, 162.6 (d, *J* = 247.0 Hz), 131.8 (d, *J* = 8.1 Hz), 129.2 (d, *J* = 3.4 Hz), 115.7 (d, *J* = 21.5 Hz), 109.7, 73.3, 64.3, 37.8, 25.8, 14.0.

$^{19}$F NMR (282 MHz, $CDCl_3$, δ): -113.98 (tt, *J* = 8.5, 5.3 Hz).

HRMS (ESI-TOF) m/z [M+Na]$^+$. Calcd for $[C_{14}H_{14}FNO_3SNa]^+$: 318.0571. Found: 318.0564.

**Ethyl 2-acetyl-2-thiocyanatohexanoate, 2m** (known compound [6])




6 F/mol, 5.0 eq. $NH_4SCN$ - Yield 35% (85.2 mg, 0.35 mmol).

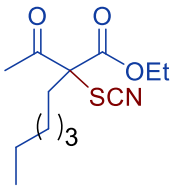
8 F/mol, 10.0 eq. $NH_4SCN$ - Yield 37% (90.0 mg, 0.37 mmol).

Yellow oil. $R_f$ = 0.15 (PE:EtOAc = 20:1).

$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 4.32 (q, *J* = 7.1 Hz, 2H), 2.39 – 2.16 (m, 2H), 2.30 (s, 3H), 1.46 – 1.25 (m, 7H), 0.93 (t, *J* = 7.1 Hz, 3H).

$^{13}$C{$^1$H} NMR (75.48 MHz, $CDCl_3$, δ): 197.1, 166.9, 109.8, 73.5, 63.9, 32.6, 26.2, 25.4, 22.5, 13.8.

**Ethyl 2-acetyl-2-thiocyanatooctanoate, 2n** (known compound [6])




6 F/mol, 5.0 eq. $NH_4SCN$ - Yield 40% (108.6 mg, 0.40 mmol).

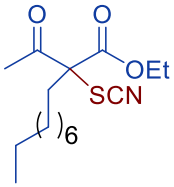
8 F/mol, 10.0 eq. $NH_4SCN$ - Yield 44% (119.4 mg, 0.44 mmol).

Yellow oil. $R_f$ = 0.18 (PE:EtOAc = 20:1).

$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 4.32 (q, *J* = 6.9 Hz, 2H), 2.38 – 2.16 (m, 5H), 1.41 – 1.21 (m, 11H), 0.88 (t, *J* = 6.9 Hz, 3H).

$^{13}$C{$^1$H} NMR (75.48 MHz, $CDCl_3$, δ): 197.1, 166.9, 109.8, 73.6, 63.9, 32.9, 31.4, 29.0, 25.4, 24.0, 22.5, 14.1, 14.0.

**Ethyl 2-acetyl-2-thiocyanatoundecanoate, 2o**



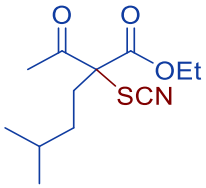

Yield 50% (156.7 mg, 0.50 mmol). Yellow oil. $R_f$ = 0.29 (PE:EtOAc = 10:1).

$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 4.33 (q, *J* = 6.9 Hz, 2H), 2.42 – 2.15 (m, 5H), 1.44 – 1.22 (m, 17H), 0.87 (t, *J* = 6.9 Hz, 3H).

$^{13}$C{$^1$H} NMR (75.13 MHz, $CDCl_3$, δ): 197.2, 167.0, 109.9, 73.6, 63.9, 33.0, 32.0, 29.5, 29.4, 29.3, 25.5, 24.1, 22.8, 14.2, 14.1.

HRMS (ESI-TOF) m/z $[M+NH_4]^+$. Calcd for $[C_{16}H_{31}N_2O_3S]^+$: 331.2050. Found: 331.2039.

**Ethyl 2-acetyl-5-methyl-2-thiocyanatohexanoate, 2p**



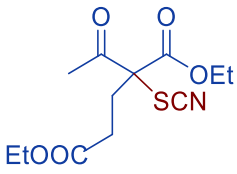

Yield 44% (113.0 mg, 0.44 mmol). Yellow oil. $R_f$ = 0.42 (PE:EtOAc = 10:1).

$^1$H NMR (300.13 MHz, $CDCl_3$, δ): 4.32 (q, *J* = 7.1 Hz, 2H), 2.38 – 2.14 (m, 5H), 1.69 – 1.53 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H), 1.27 – 1.07 (m, 2H), 0.92 (d, *J* = 6.7 Hz, 6H).

$^{13}$C{$^1$H} NMR (75.48 MHz, $CDCl_3$, δ): 197.1, 166.9, 109.8, 73.6, 63.8, 32.8, 30.9, 27.9, 25.4, 22.4, 14.0.

HRMS (ESI-TOF) m/z $[M+Na]^+$. Calcd for $[C_{12}H_{19}NO_3SNa]^+$: 280.0978. Found: 280.0969.

**Diethyl 2-acetyl-2-thiocyanatopentanedioate, 2q**




Yield 63% (181.0 mg, 0.63 mmol). Yellow oil. $R_f$ = 0.47 (PE:EtOAc = 5:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 4.38 – 4.32 (m, 2H), 4.14 (q, *J* = 7.2 Hz, 2H), 2.74 – 2.56 (m, 2H), 2.49 – 2.42 (m, 2H), 2.35 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H).

$^{13}$C{$^{1}$H} NMR (75.48 MHz, $CDCl_3$, δ): 196.5, 171.5, 166.4, 109.3, 72.6, 64.3, 61.2, 29.3, 28.2, 25.5, 14.3, 14.0.

HRMS (ESI-TOF) m/z $[M+Na]^+$. Calcd for $[C_{12}H_{17}NO_5SNa]^+$: 310.0720. Found: 310.0721.

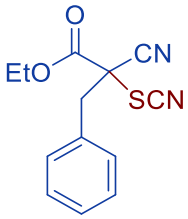
**Ethyl 2-oxo-1-thiocyanatocyclohexane-1-carboxylate, 2r** (known compound [6])


Yield 62% (141.0 mg, 0.62 mmol). Yellow oil. $R_f$ = 0.33 (PE:EtOAc = 20:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 4.35 (q, *J* = 7.1 Hz, 2H), 3.17 – 3.09 (m, 1H), 2.72 – 2.45 (m, 2H), 2.21 – 1.88 (m, 3H), 1.83 – 1.57 (m, 2H), 1.34 (t, *J* = 7.1 Hz, 3H).

$^{13}$C{$^{1}$H} NMR (75.48 MHz, $CDCl_3$, δ): 201.1, 166.4, 109.9, 68.5, 63.6, 40.3, 38.3, 26.9, 23.4, 14.0.

**Ethyl 2-cyano-3-phenyl-2-thiocyanatopropanoate, 2s**




Yield 53% (138.0 mg, 0.53 mmol). Colourless oil. $R_f$ = 0.35 (PE:EtOAc = 5:1).

$^{1}$H NMR (300.13 MHz, $CDCl_3$, δ): 7.42 – 7.27 (m, 5H), 4.42 – 4.24 (m, 2H), 3.60 (d, *J* = 13.9 Hz, 1H), 3.52 (d, *J* = 13.8 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H).

$^{13}$C{$^{1}$H} NMR (75.48 MHz, $CDCl_3$, δ): 163.12, 131.18, 130.24, 129.30, 129.19, 114.23, 107.16, 65.50, 53.76, 42.96, 13.90.

HRMS (ESI-TOF) m/z $[M+K]^+$. Calcd for $[C_{13}H_{12}N_2O_2SK]^+$: 299.0251. Found: 299.0251.

## CV study

Cyclic voltammetry (CV) was implemented on an IPC-Pro M computer-assisted potentiostat manufactured by «Econix» (scan rate error 1.0%). The starting potential was set to 0.25 mV, and the initial sweep was carried out in the positive (anode) region at a rate of 100 mV/s. Analyzed solutions were prepared in acetonitrile and contained *n*-$Bu_4NBF_4$ (0.1 M) as an supporting electrolyte and analyte (0.05 M). The experiments were performed in a 10 mL fiveneck glass conic electrochemical cell with a water jacket for thermostatting. CV curves were recorded using a three-electrode scheme. In a typical case, 10 mL of a solution was utilized. The working electrode was a disc glassy-carbon electrode (d= 3 mm, surface area ~0.07 $cm^2$). A platinum wire served as an auxiliary electrode. An $Ag/AgNO_3$ electrode was used as the reference electrode and was linked to the solution by a porous glass diaphragm. The solutions were kept under thermally controlled conditions at 15±0.5 °C and deaerated by bubbling argon. Electrochemical experiments were performed under an argon atmosphere. The working electrode was polished with figure-eight motions on a synthetic chamois leather pad using a $Cr_2O_3$-based polishing paste (~5 μm particle size) down to the mirror-like surface, and rinsed with acetonitrile. Polishing was carried before each recording of CV curve.

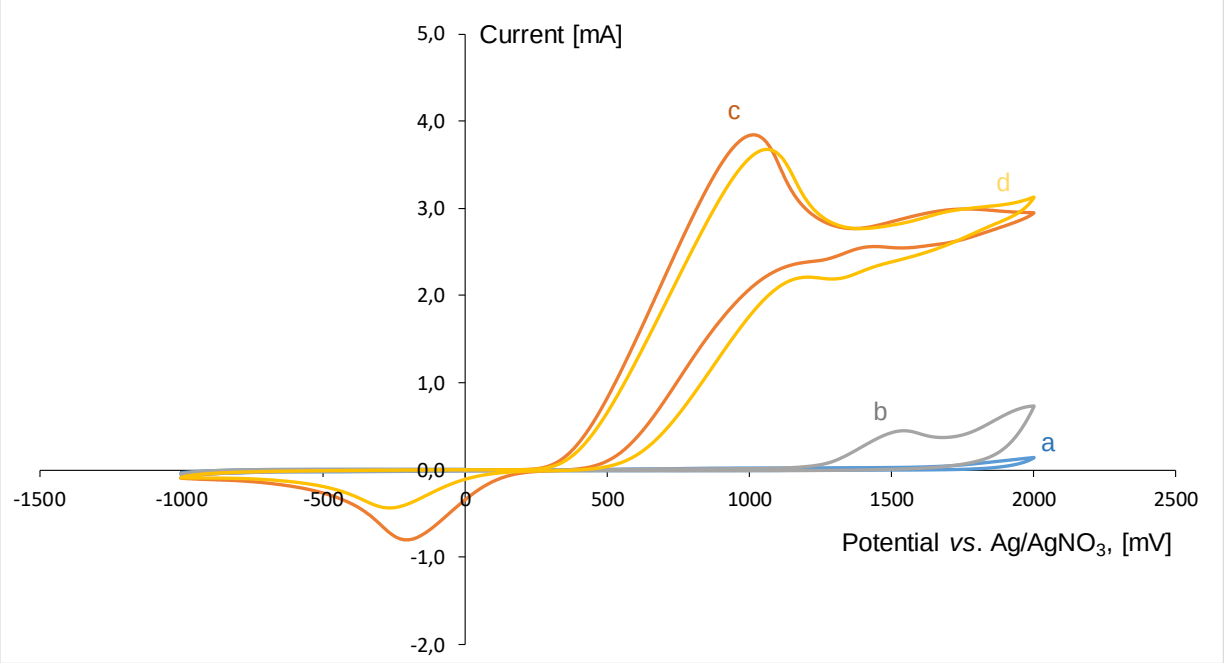



**Figure 1.** CV curve for on a working disc glassy-carbon electrode (d = 3 mm) under a scan rate of 0.1 V/s for (a) background, (b) **1a** (0.05 M), (c) $NH_4SCN$ (0.25 M), (d) mixture **1a** (0.05 M) with $NH_4SCN$ (0.25 M) in 0.1 M *n*-$Bu_4NBF_4$ in $CH_3CN$/HCOOH (8/2).

**Experimental procedures for Scheme 3. Control experiments.**

**a. Undivided cell:** A 20 mL electrolysis cell was charged with 1,3-dicarbonyl compound **1a** (1.0 mmol, 190.2 mg), $NH_4SCN$ (5.0 mmol, 380.5 mg) and 10 mL of AcOH. The mixture was stirred for 1-2 minutes to obtain a homogeneous solution. The platinum plate electrodes (2×1.5 cm) were inserted at a distance of 1.5 cm, and the reaction mixture was stirred at 40 °C at a constant current of 10 mA for 16 hours. Then, the reaction mixture was concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 40-50 °C). After that the reaction mixture was transferred onto $SiO_2$ chromatographic column and product **2a** was isolated by chromatography on $SiO_2$ (PE:EtOAc = from 50:1 to 2:1).

**Divided cell:** A divided cell was equipped with a platinum plate anode (2×1.5 cm) and a platinum plate cathode (2×1.5 cm) and connected to a DC regulated power supply. The solution of 1,3-dicarbonyl compound **1a** (1 mmol, 190.2 mg), $NH_4SCN$ (5.0 mmol, 380.5 mg) in AcOH (10 mL) (anode compartment) and solution of $NH_4SCN$ (5.0 mmol, 380.5 mg) in AcOH (10 mL) (cathode compartment) were electrolyzed using constant current conditions I = 10 mA (3.0-3.5 mA/$cm^2$) at 40 °C under magnetic stirring (6 F/mol, 16 hours). The combined organic phases (anodic and cathode compartments) were concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 20-25 °C). After that the reaction mixture was transferred onto $SiO_2$ chromatographic column and product **2a** was isolated by chromatography on $SiO_2$ (PE:EtOAc = from 50:1 to 2:1).

**b. Experiment with pre-synthesized thiocyanogen:**

KSCN (5.0 mmol, 485.9 mg) was added while stirring in 5 mL of the solvent (AcOH, $CH_3OH$, or $CH_3CN$). After dissolution of salt, $Br_2$ (2.5 mmol, 399.5 mg, 128.8 μL) was added and the mixture was stirred for 10 minutes at 20-25 °C. A solution of 1,3-dicarbonyl compound **1a** (1 mmol, 190.2 mg) in the solvent (AcOH, $CH_3OH$, or $CH_3CN$) (5 mL) was added to a yellow reaction mixture. *In the experiments 4-6 $AcONH_4$ (5.0 mmol, 385.4 mg) was also added.* The resulting reaction mixture was stirred at 40 °C for 2 hours. Then, the organic phase was concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 40-50 °C). After that, the reaction mixture was transferred onto $SiO_2$ chromatographic column and product **2a** was isolated by chromatography on $SiO_2$ (PE:EtOAc = from 50:1 to 2:1).

## Bioassay of fungicidal activity

The antifungal activities were tested according to the conventional procedure [7-9] with six phytopathogenic fungi from different taxonomic classes: *Fusarium culmorum (F.c.), Rhizoctonia solani (R.s.), Alternaria solani (A.s.), Phytophthora infestans (P.i.), and Colletotrichum coccodes (C.c.)*. The effect of the chemicals on mycelial radial growth was determined by dissolving concentration 3 mg×mL$^{-1}$ in acetone and suspending aliquots in potato-saccharose agar at 50 °C to give the concentration 30 μg×mL$^{-1}$. The final acetone concentration of both fungicide-containing and control samples was 10 mL×L$^{-1}$. Petri dishes containing 15 mL of the agar medium were inoculated by placing 2-mm micelial agar discs on the agar surface. Plates were incubated at 25 °C and radial growth was measured after 5 days. The mixed medium without a sample was used as the blank control. Three replicates of each test were carried out. The mycelium elongation diameter (mm) of fungi settlements was measured after 5 days of culture. The growth inhibition rates were calculated with the following equation: I = [(DC – DT)/DC]×100%. Here I is the growth inhibition rates (%), DC is the control settlement diameter (mm), and DT is the treatment group fungi settlement diameter (mm). The results are summarized in Table 3.

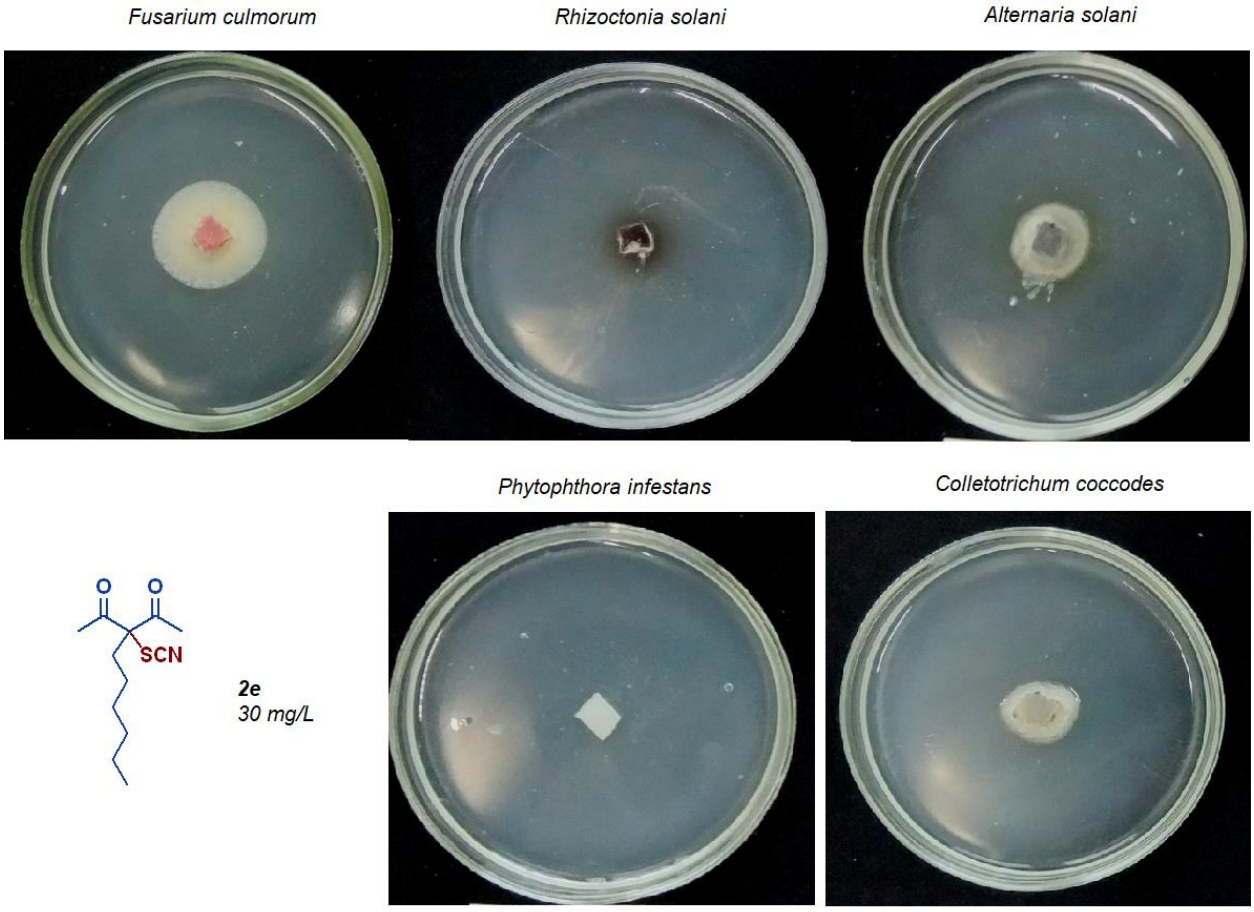



**Figure S2.** The fungicidal activity of synthesized thiocyanate **2e**.

## Translaminar activity study

The translaminar activities were tested according to the conventional procedure.[10-13]

*Chemicals and formulations*

The leader compound **2e** was compared with fluazinam (Shirlan, Syngenta, 0.4 L/ga) as a well-known contact fungicide.[14-17] The final fluazinam concentration was 2.0 g/L. Compound **2e** was formulated as 0.17 g/L solution in distilled water with the addition of 1 mL/L commercial adjuvant (Atomic) (application rate 30 g/ga).

*Plants*

Potato leaves (*Solanum tuberosum*, Arizona) were separated from plants grown in the field and brought to the laboratory for testing. One fully-expanded leaves per plant were treated and in total 10 plants were used per fungicide treatment.

*Pathogens and inoculation*

An isolate of *P. infestans* M.(161), maintained on plants in our laboratory (VNIIF, Russia), were used in this study. The pathogens were 10 day-age. Concentration of isolate *P. infestans* suspension was 20000 conidium/mL.

*Translaminar activity*

To study translaminar activity, compound **2e** and fluazinam were sprayed 24 h before the inoculation of the plants, on the adaxial (upper) leaf surface. Fungicide solutions were applied to ‘‘run-off’’ with a hand sprayer. Control seedling plants were sprayed with sterile tap water 24 h before the inoculation. After 24 h fungicide treated leaves were inoculated on the abaxial (lower) surface. A similar set of plants and leaves was treated with the same fungicides on the abaxial (lower) leaf surface and inoculated 24 h later on the same leaf surface. Inoculum on the leaves in the form of a suspension of conidia was applied locally (1-2 drops per leaf). We used a microdispenser that allows you to apply drops of 10 μL. The inoculated leaves were kept for 18 hours in a humid chamber in the dark. Then the remains of the suspension are removed from the leaves with filter paper and again placed in a humid chamber at a temperature of 20 °C. On the fourth day, the diameter of necrosis is measured, in mm. The productivity of sporulation on *P. infestans* - affected spots was assessed in points on the fifth day.[18]

**Table S2.** Severity of potato blight developed on potato leaves treated with fungicides on the adaxial (upper) or the abaxial (lower) leaf surface and inoculated on the abaxial (lower) leaf surface.

| № | Fungicide treatment | Application dose (mg/mL) | Abaxial leaf surface treatment | | Adaxial leaf surface treatment | |
|---|---|---|---|---|---|---|
| | | | Average spot growth diam-eter, mm | Points | Average spot growth diame-ter, mm | Points |
| 1 | **2e** | 0.17 | 9.8 | 4.8 | 21.2 | 10.8 |
| 2 | fluazinam | 2.0 | 0.5 | 0 | 8.6 | 4.8 |
| 3 | Control ($H_2O$) | | 22.8 | 11.4 | 23.8 | 11.4 |
| | $HCP_{0,95}$ | | 2.8 | 1.3 | 2.5 | 1.2 |

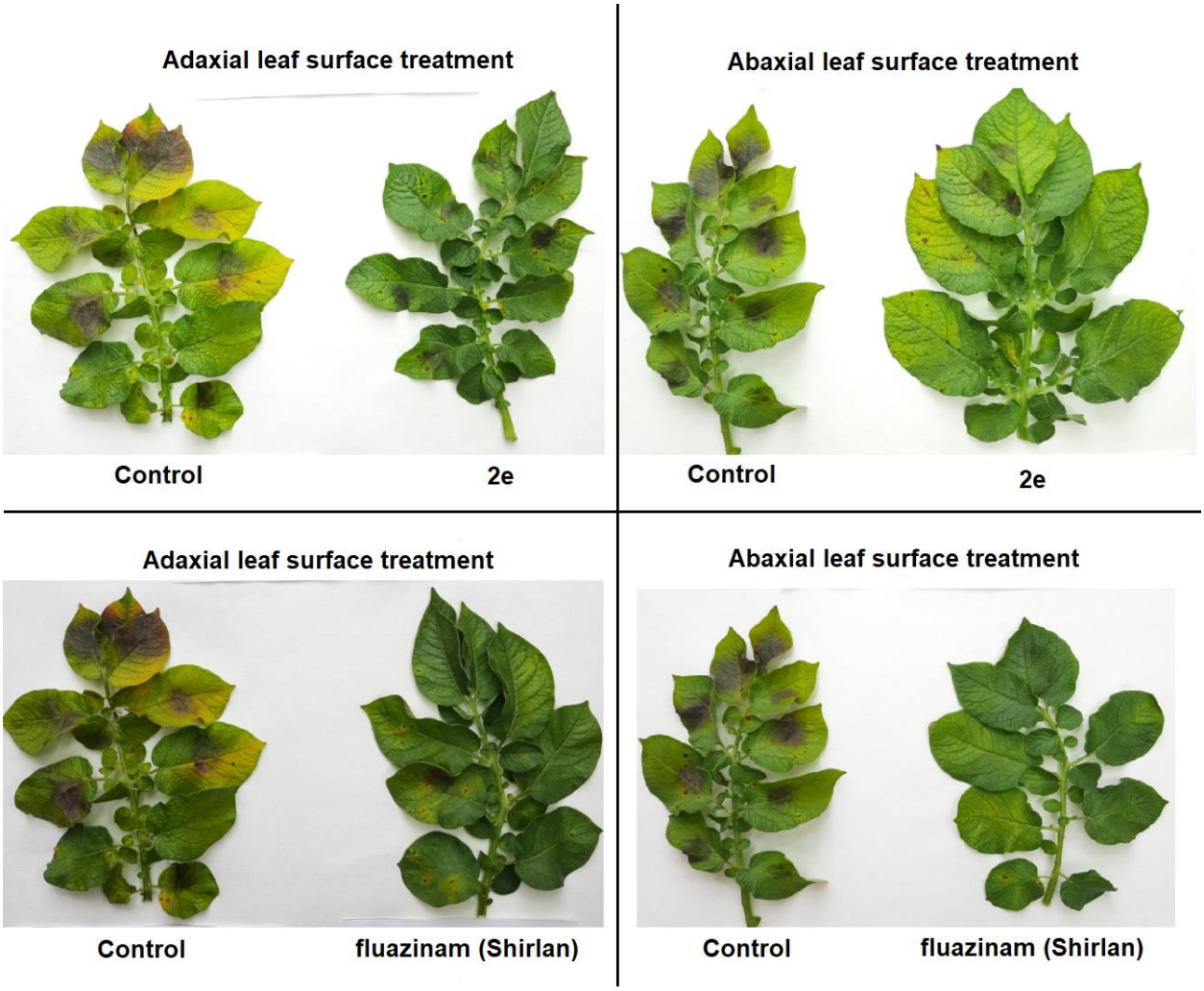



**Figure S3.** Late blight on the leaves on the 4th day after infection.

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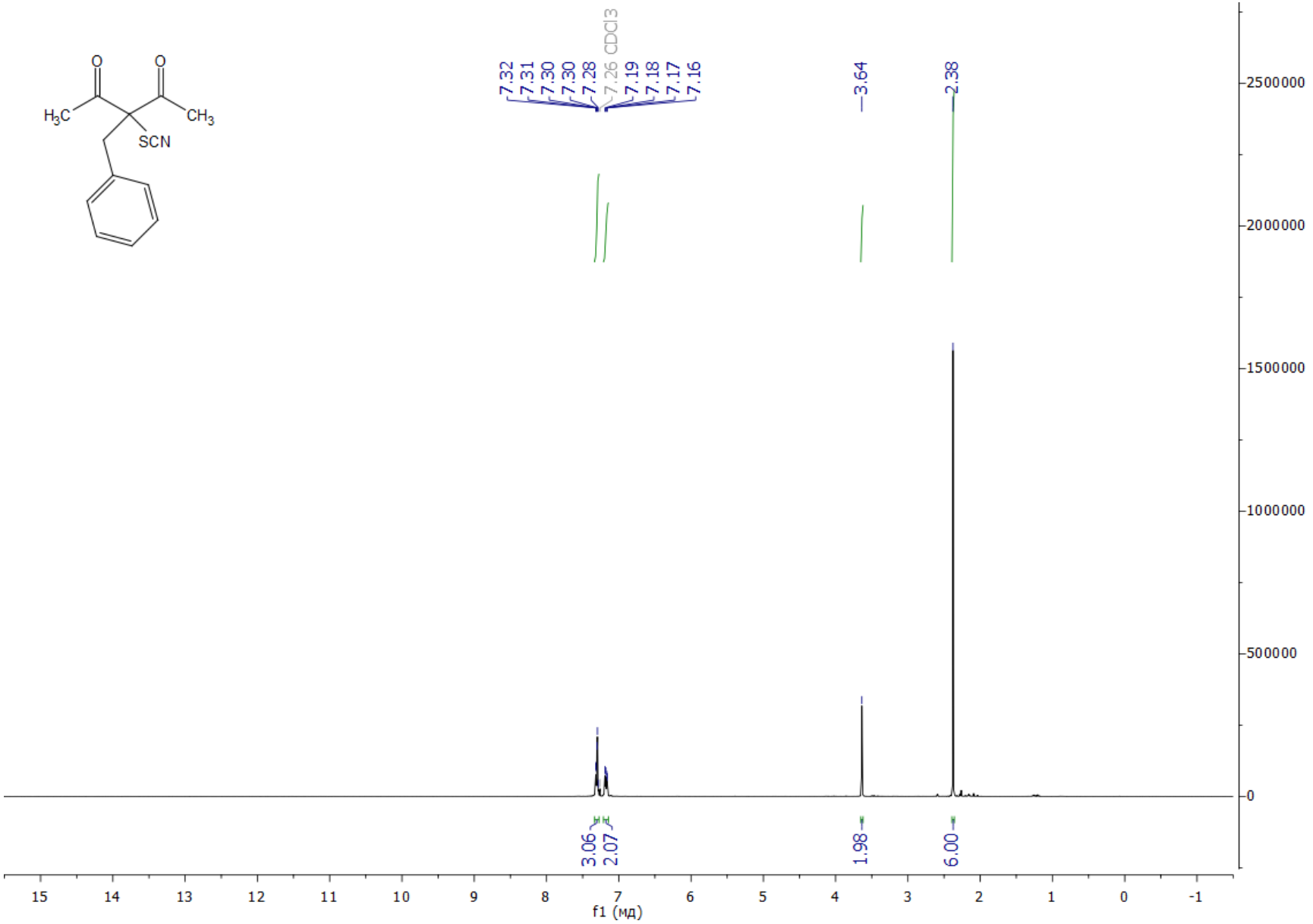
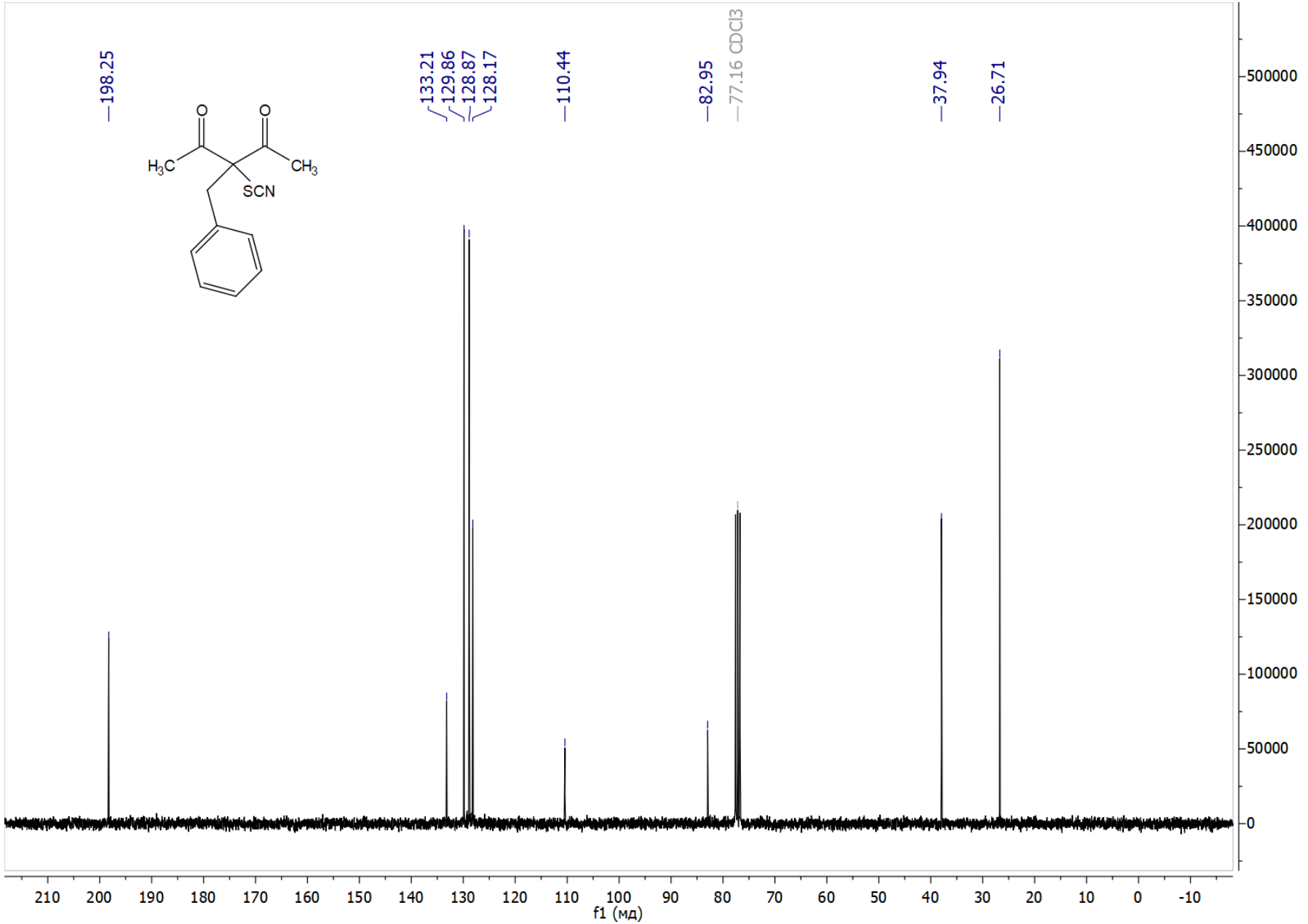
**NMR spectra of synthesized thiocyanates**

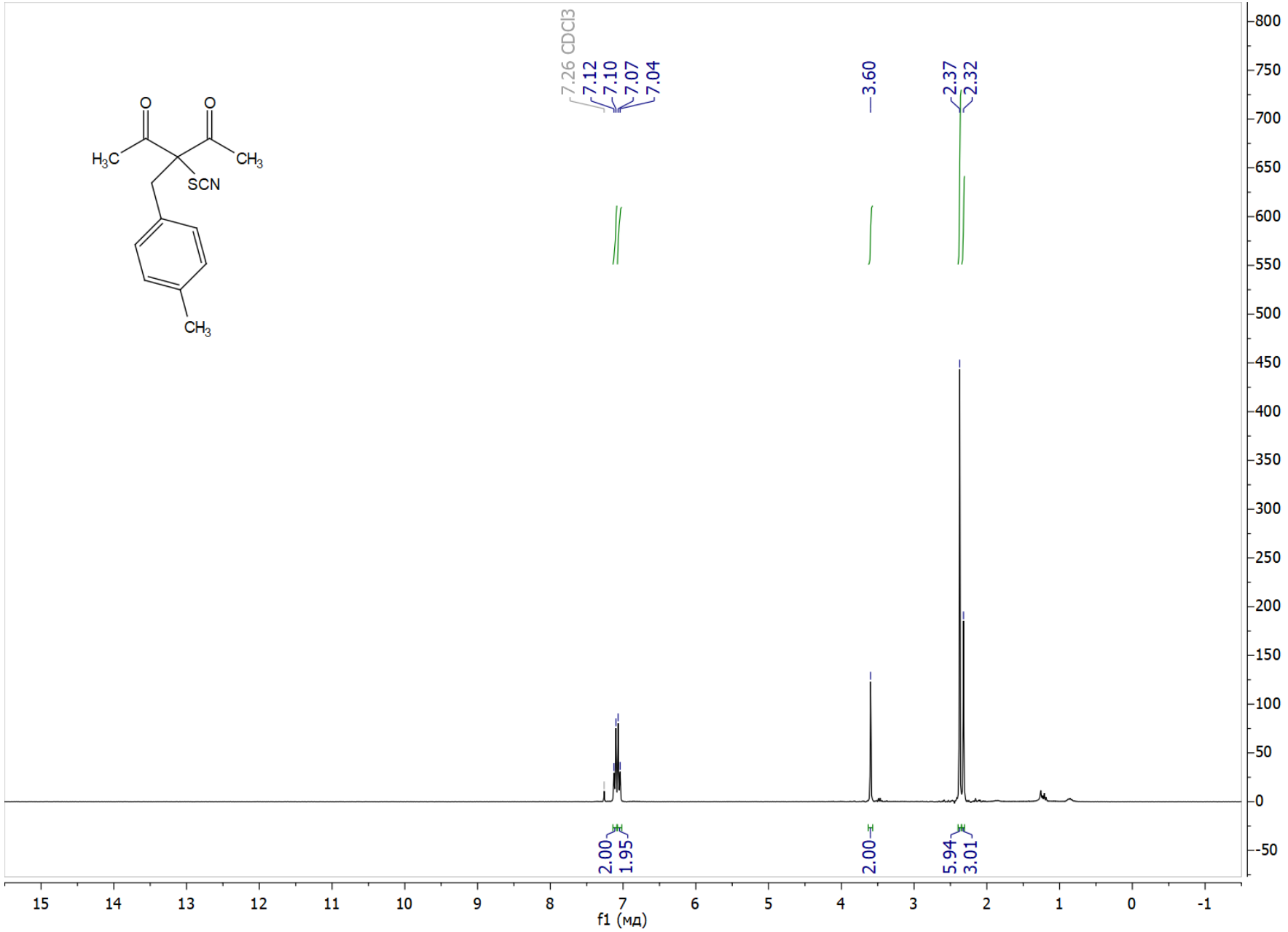
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-benzyl-3-thiocyanatopentane-2,4-dione, **2a**



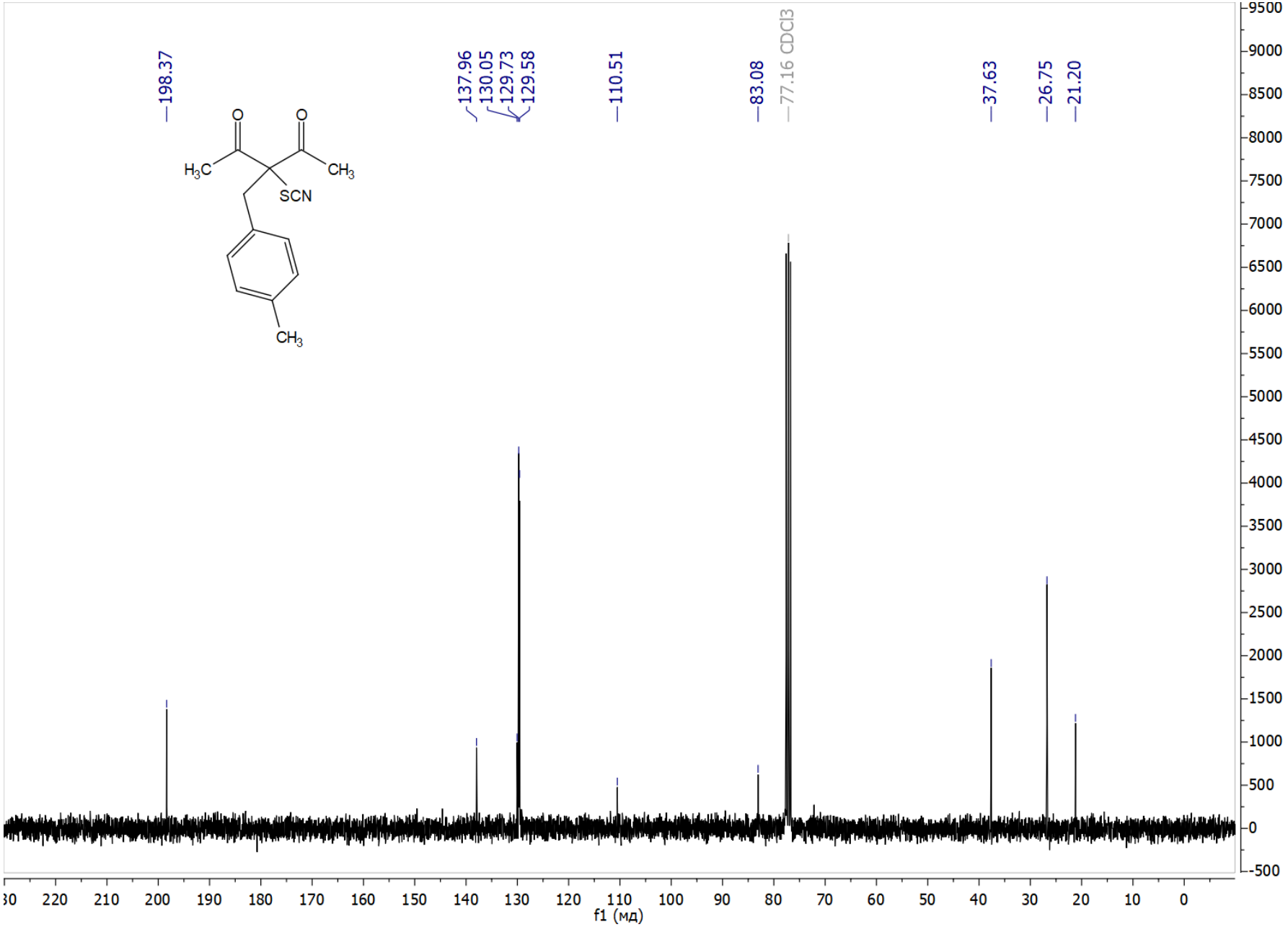
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-benzyl-3-thiocyanatopentane-2,4-dione, **2a**



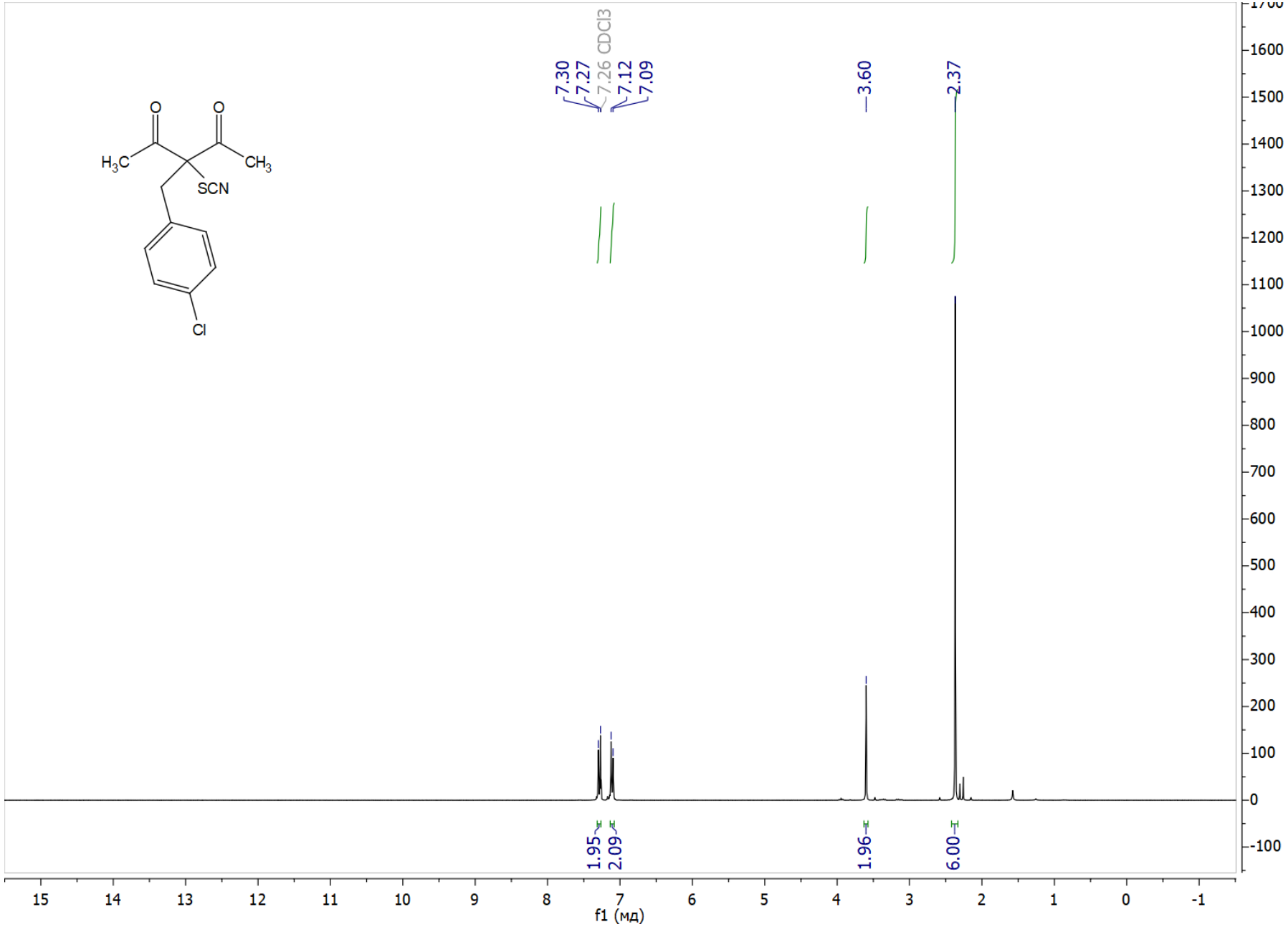
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-(4-methylbenzyl)-3-thiocyanatopentane-2,4-dione, **2b**



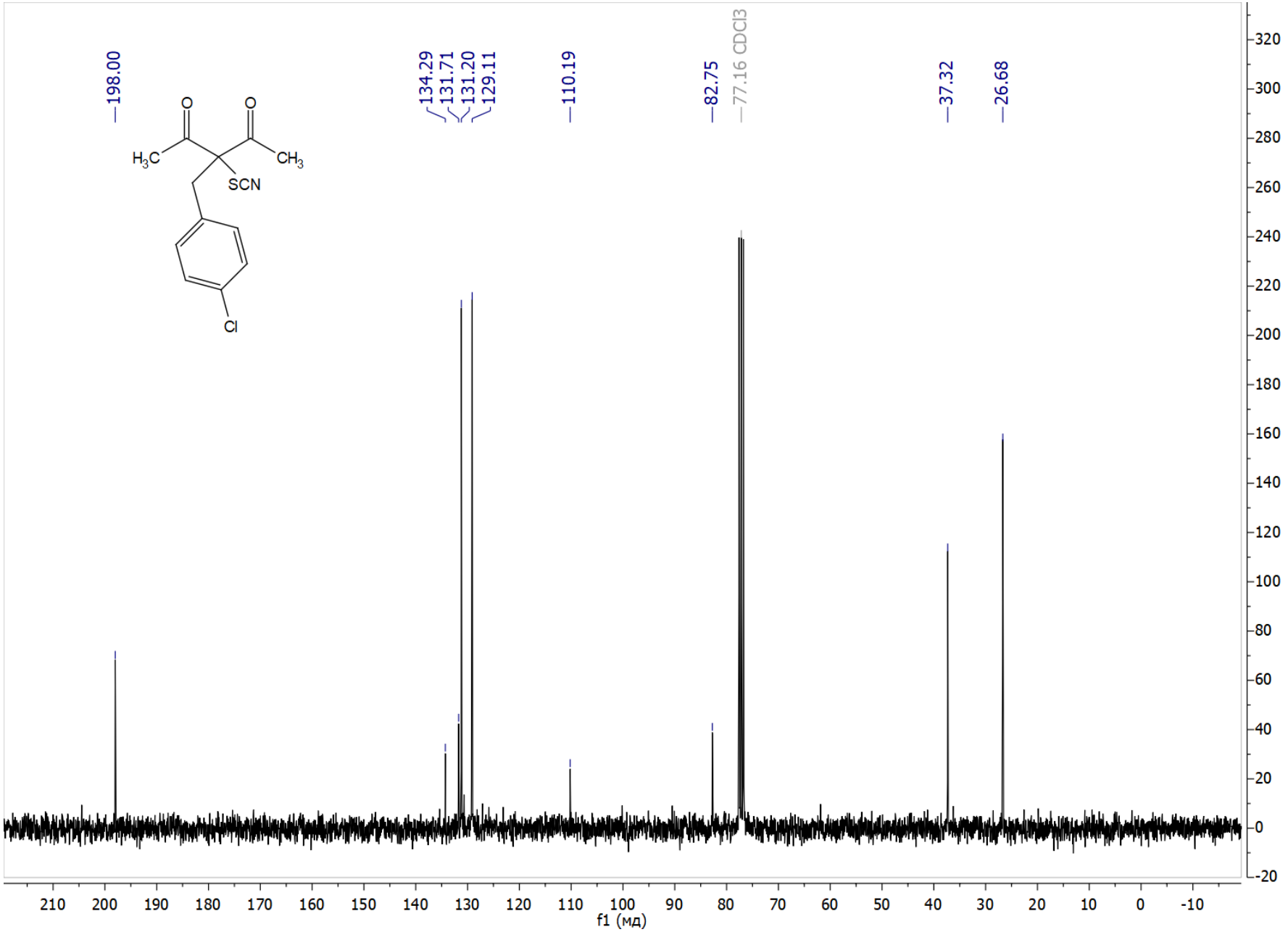
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-(4-methylbenzyl)-3-thiocyanatopentane-2,4-dione, **2b**



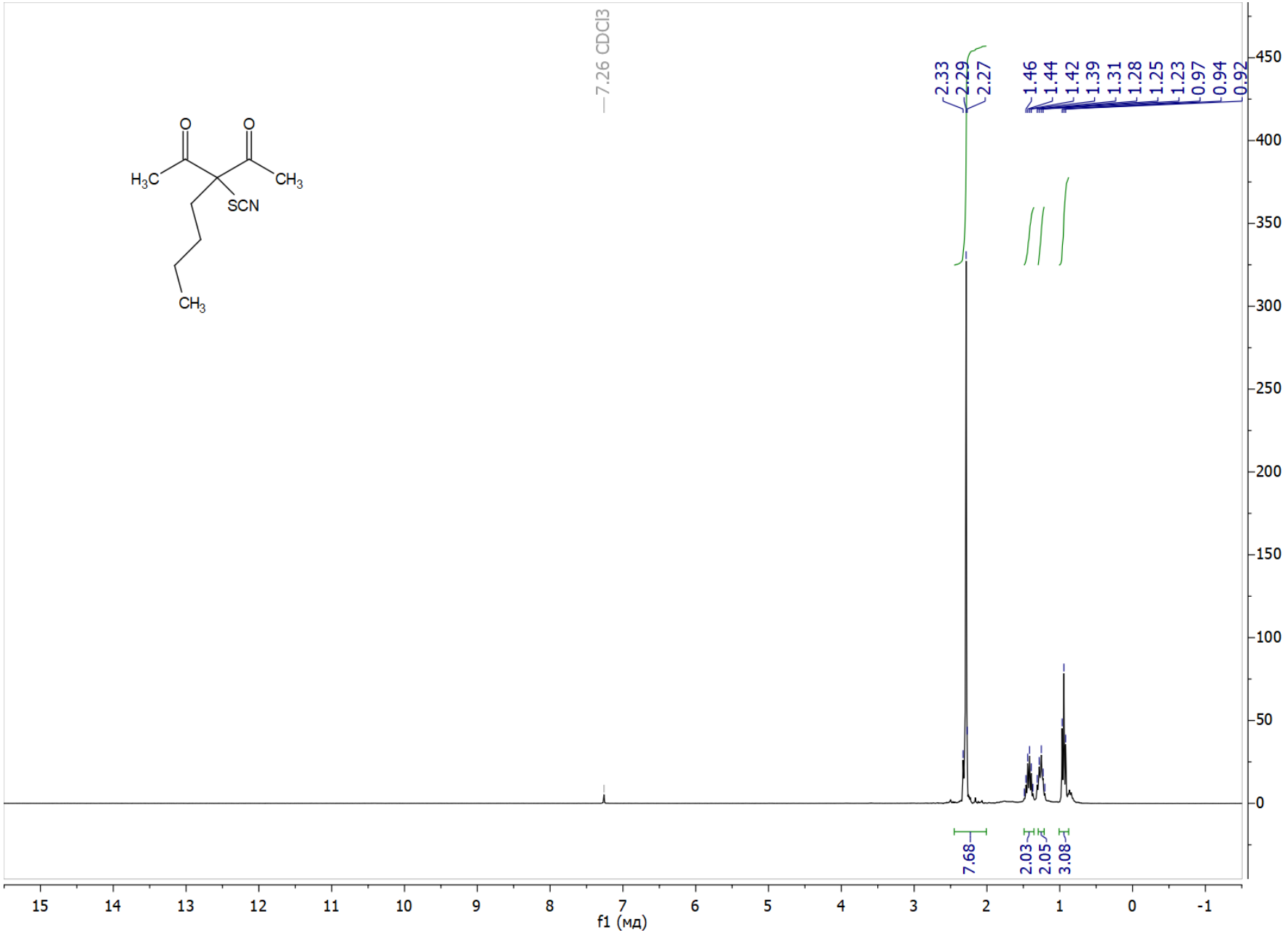
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-(4-chlorobenzyl)-3-thiocyanatopentane-2,4-dione, **2c**



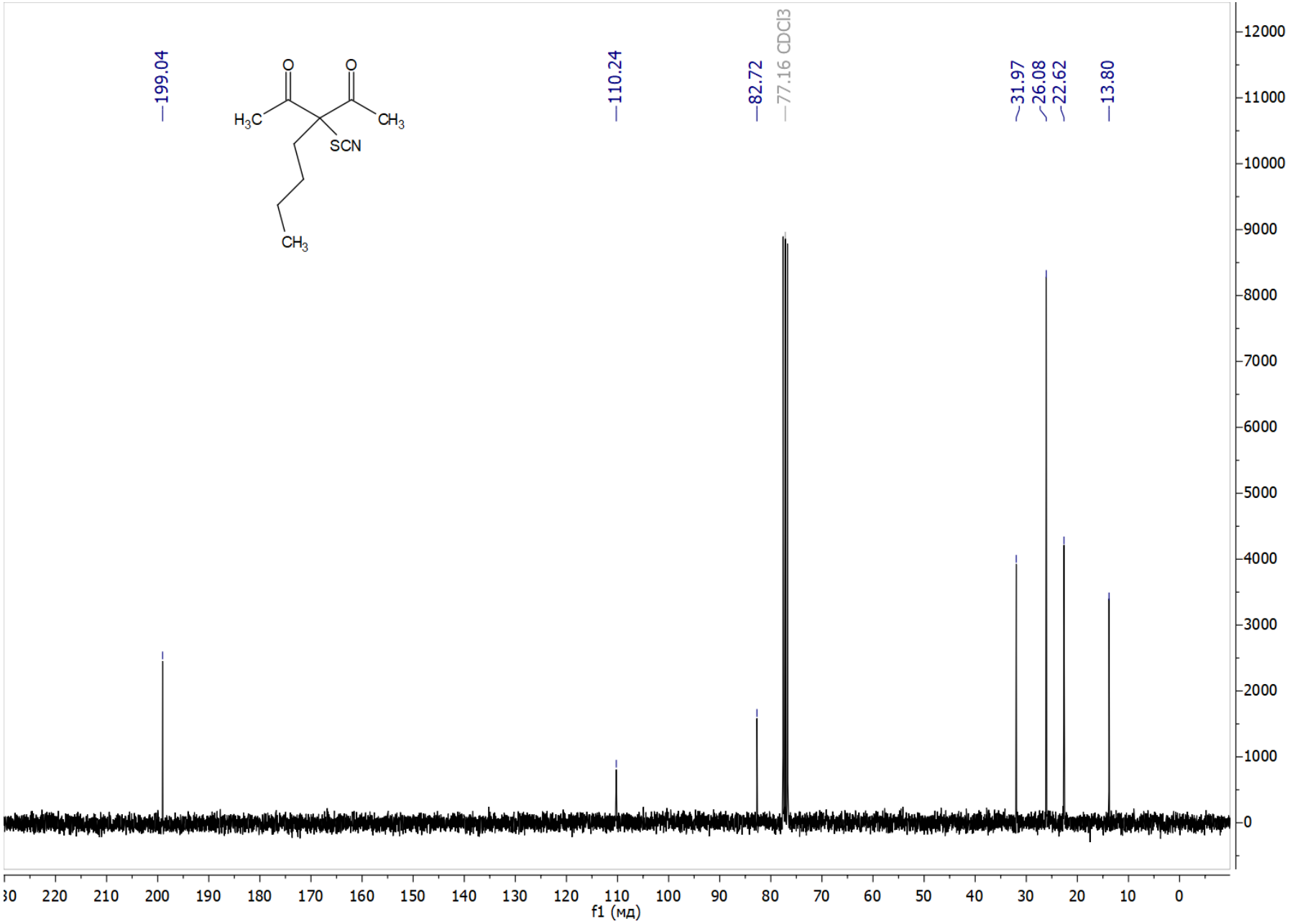
$^{13}C$ NMR (75.48 MHz, $CDCl_3$) spectrum of 3-(4-chlorobenzyl)-3-thiocyanatopentane-2,4-dione, **2c**



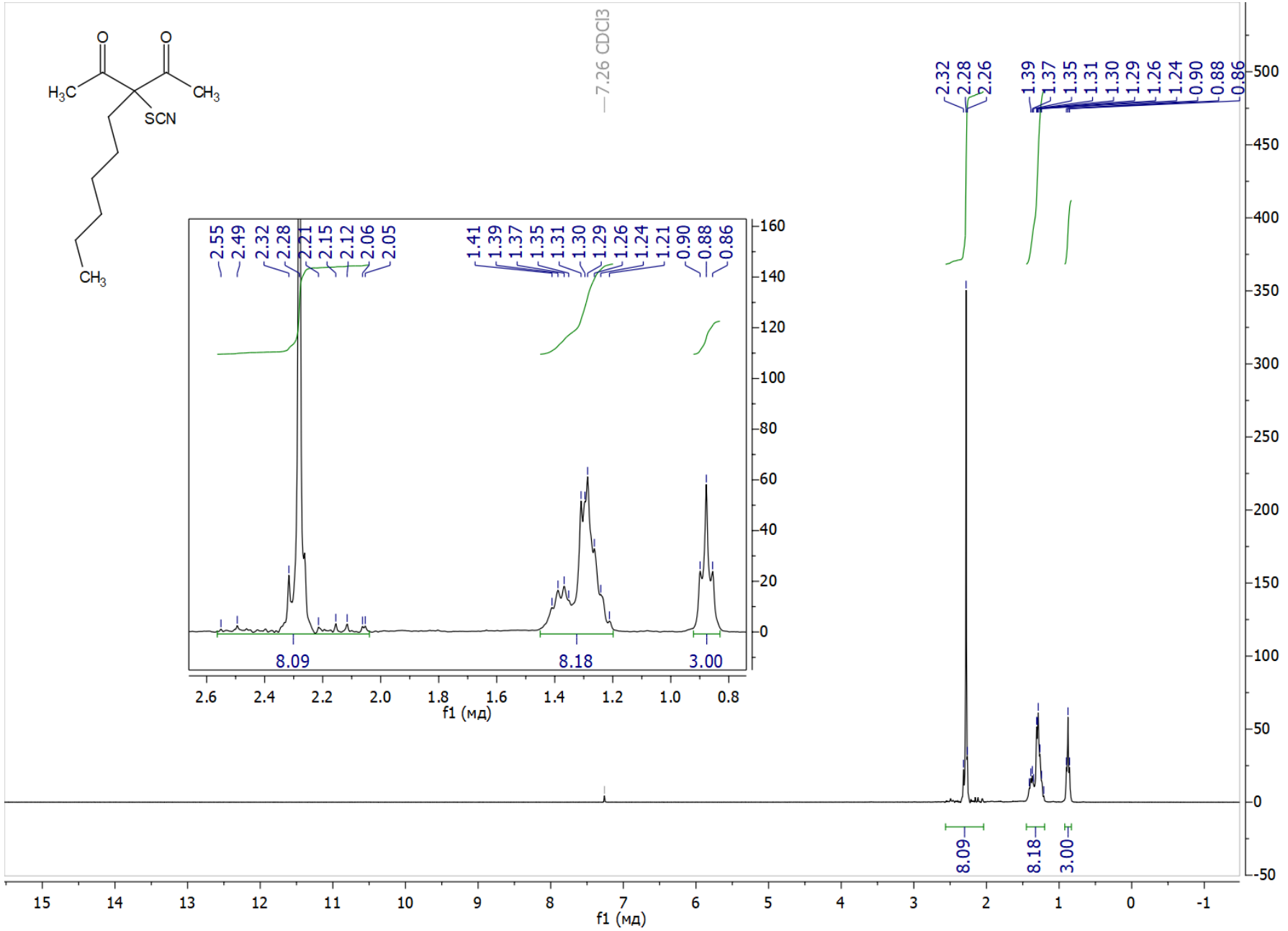
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-butyl-3-thiocyanatopentane-2,4-dione, **2d**



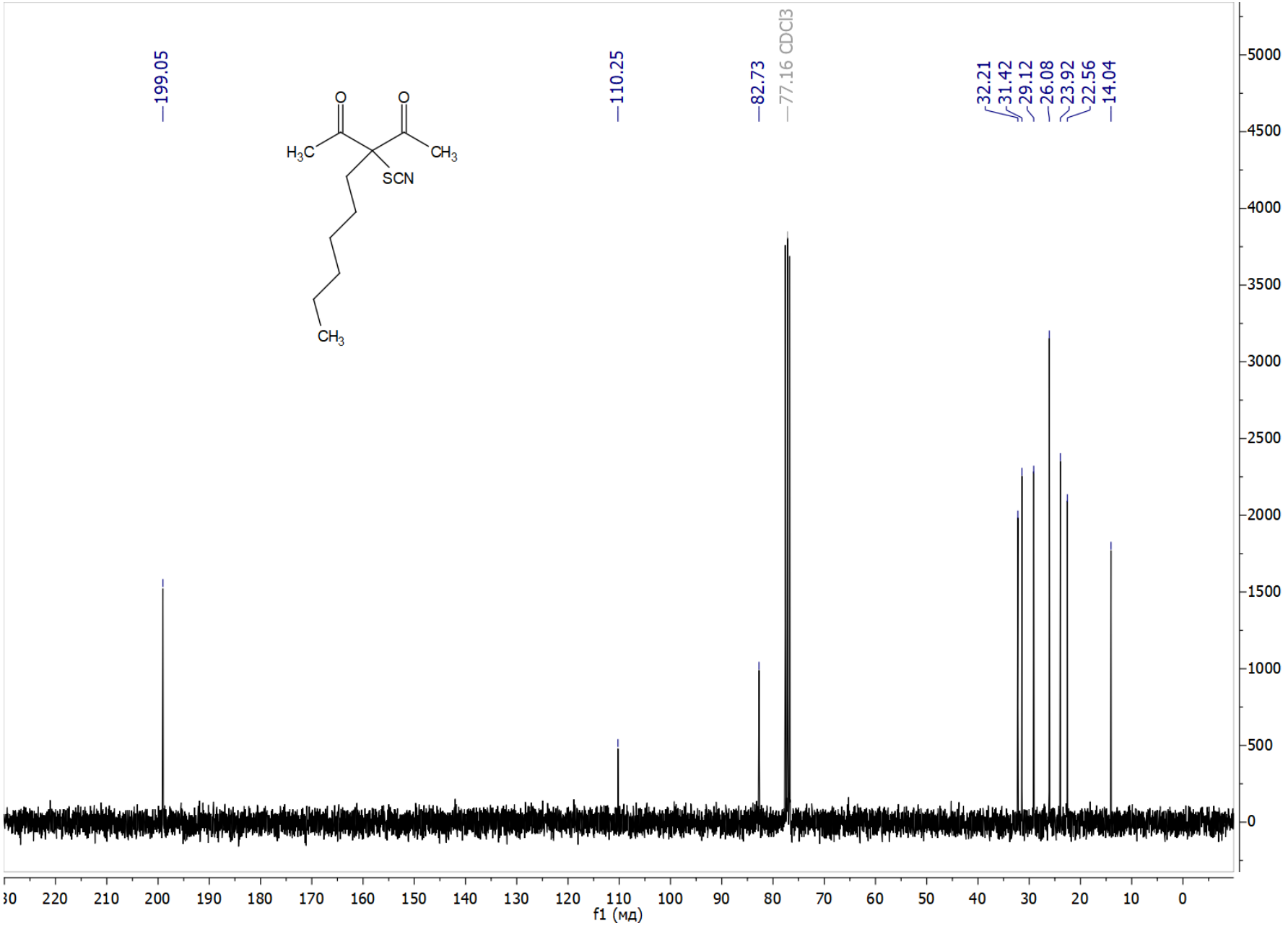
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-butyl-3-thiocyanatopentane-2,4-dione, **2d**



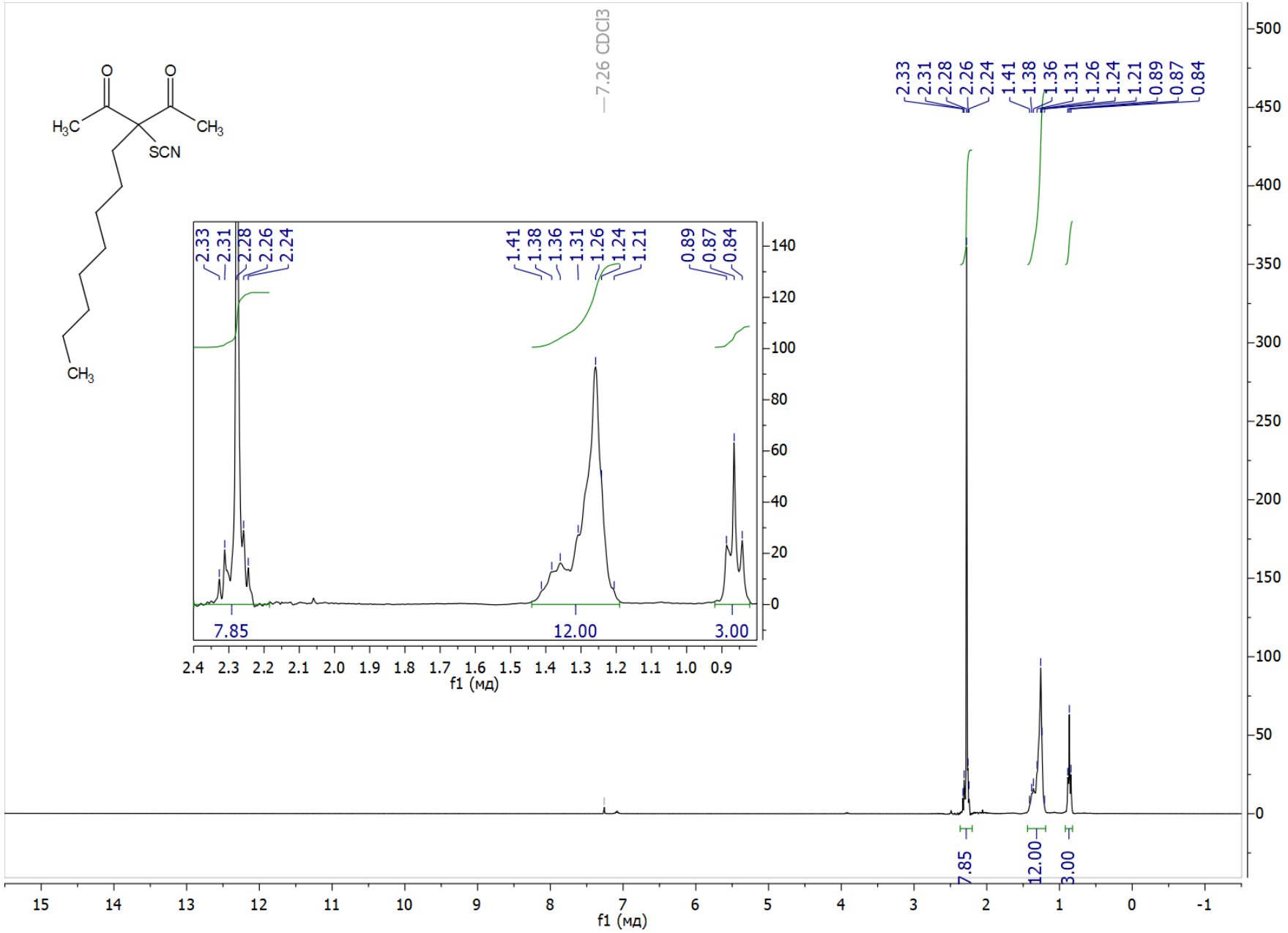
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-hexyl-3-thiocyanatopentane-2,4-dione, **2e**



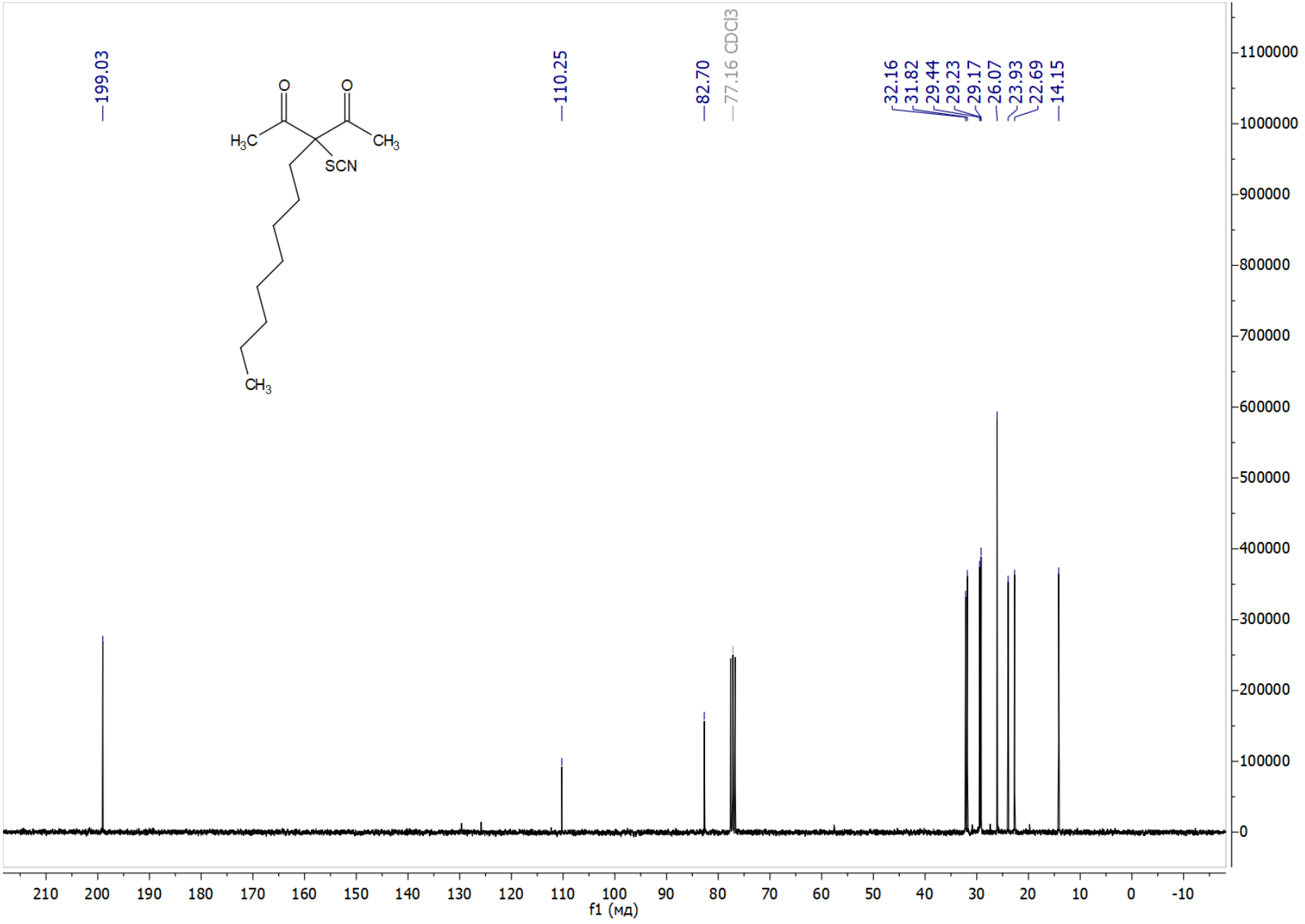
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-hexyl-3-thiocyanatopentane-2,4-dione, **2e**



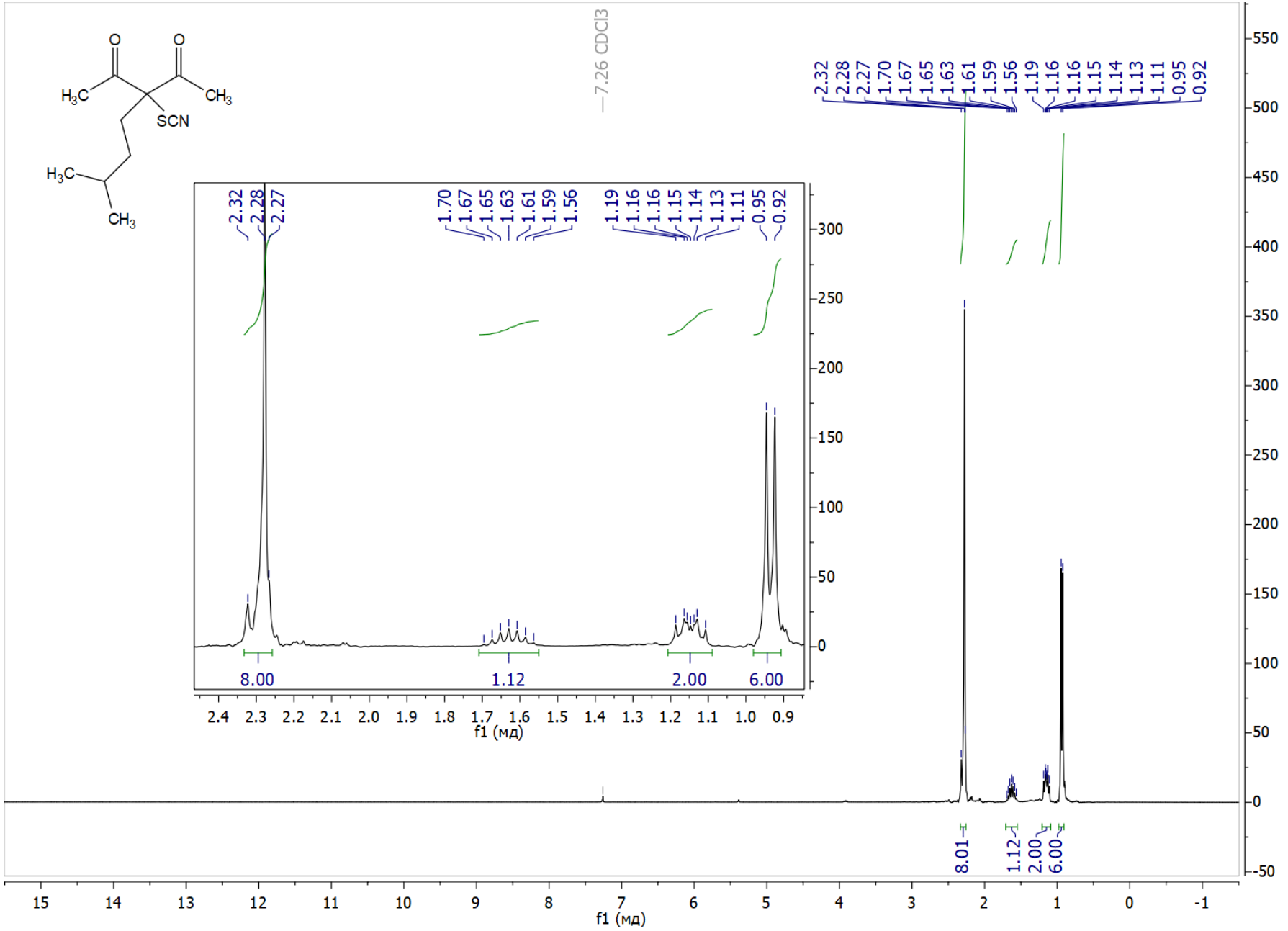
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-octyl-3-thiocyanatopentane-2,4-dione, **2f**



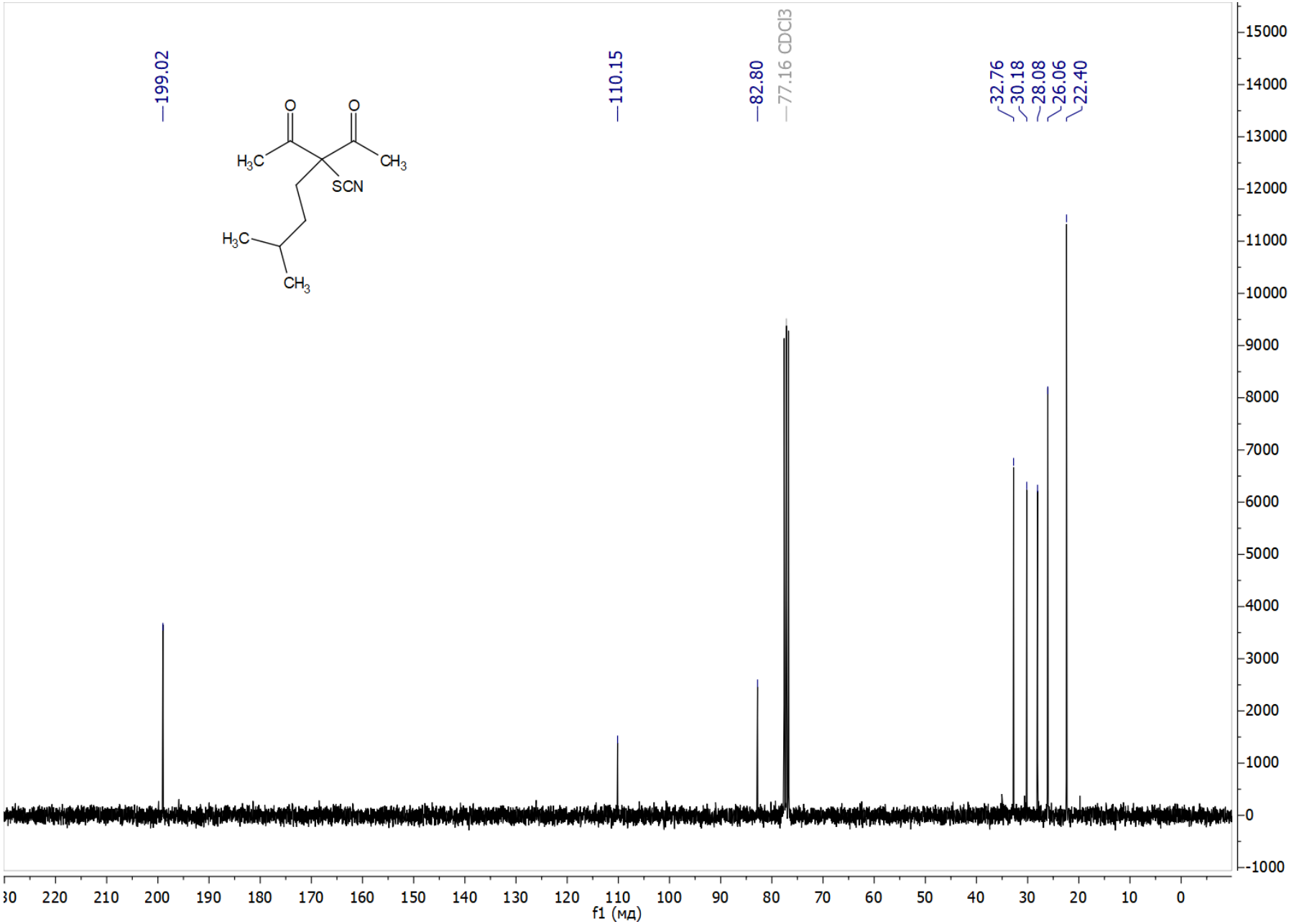
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-octyl-3-thiocyanatopentane-2,4-dione, **2f**



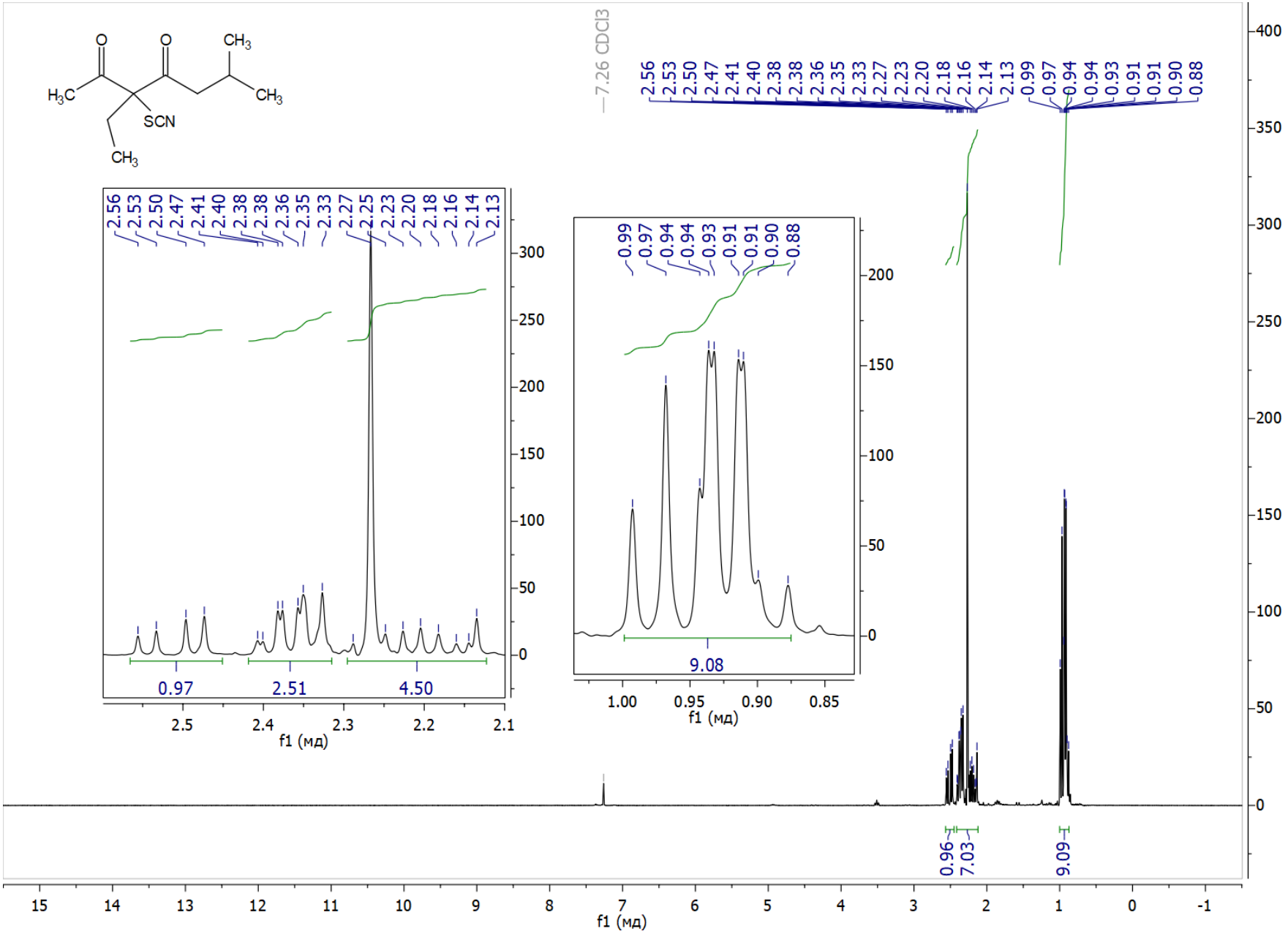
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-*iso*pentyl-3-thiocyanatopentane-2,4-dione, **2g**



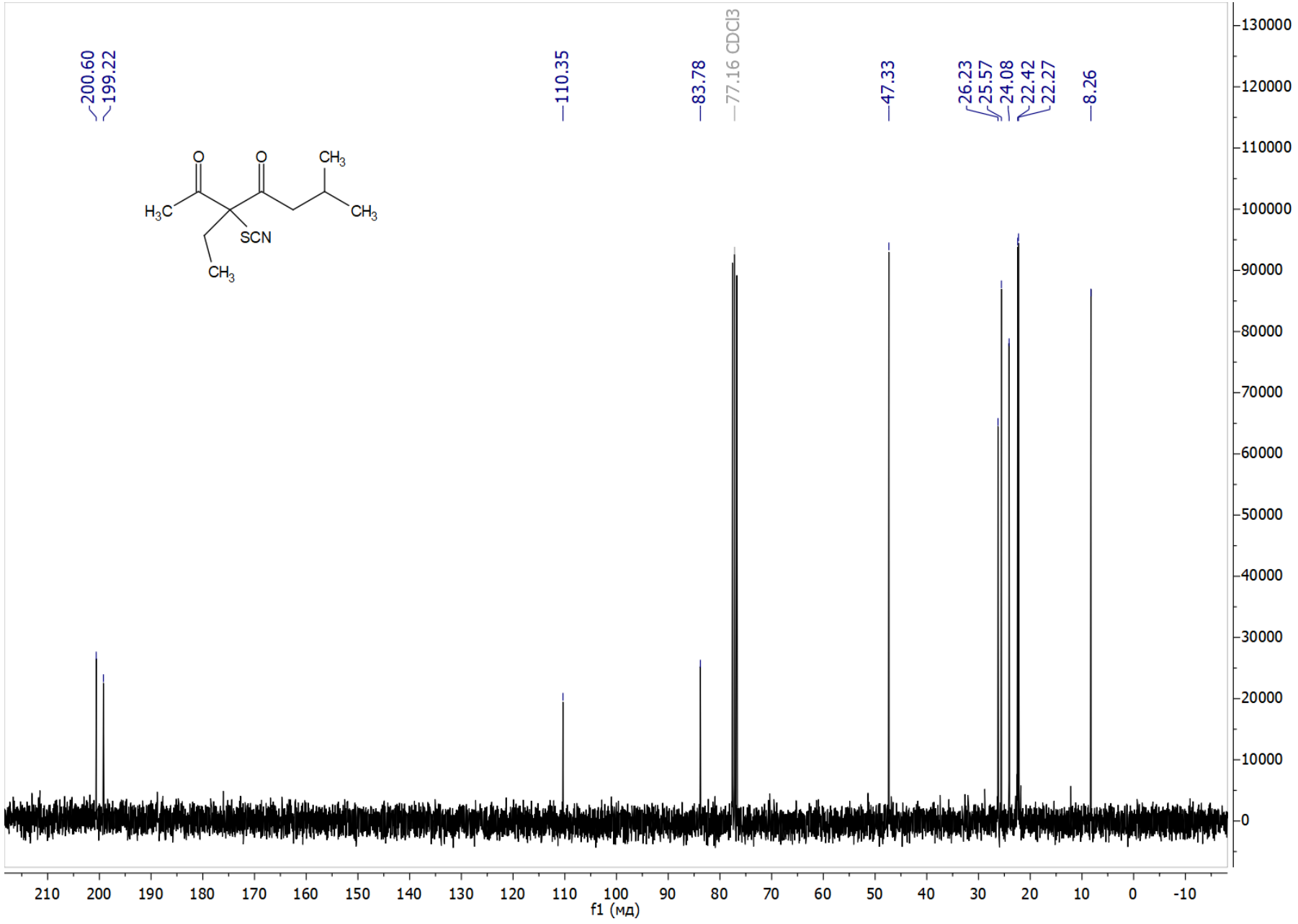
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-*iso*pentyl-3-thiocyanatopentane-2,4-dione, **2g**



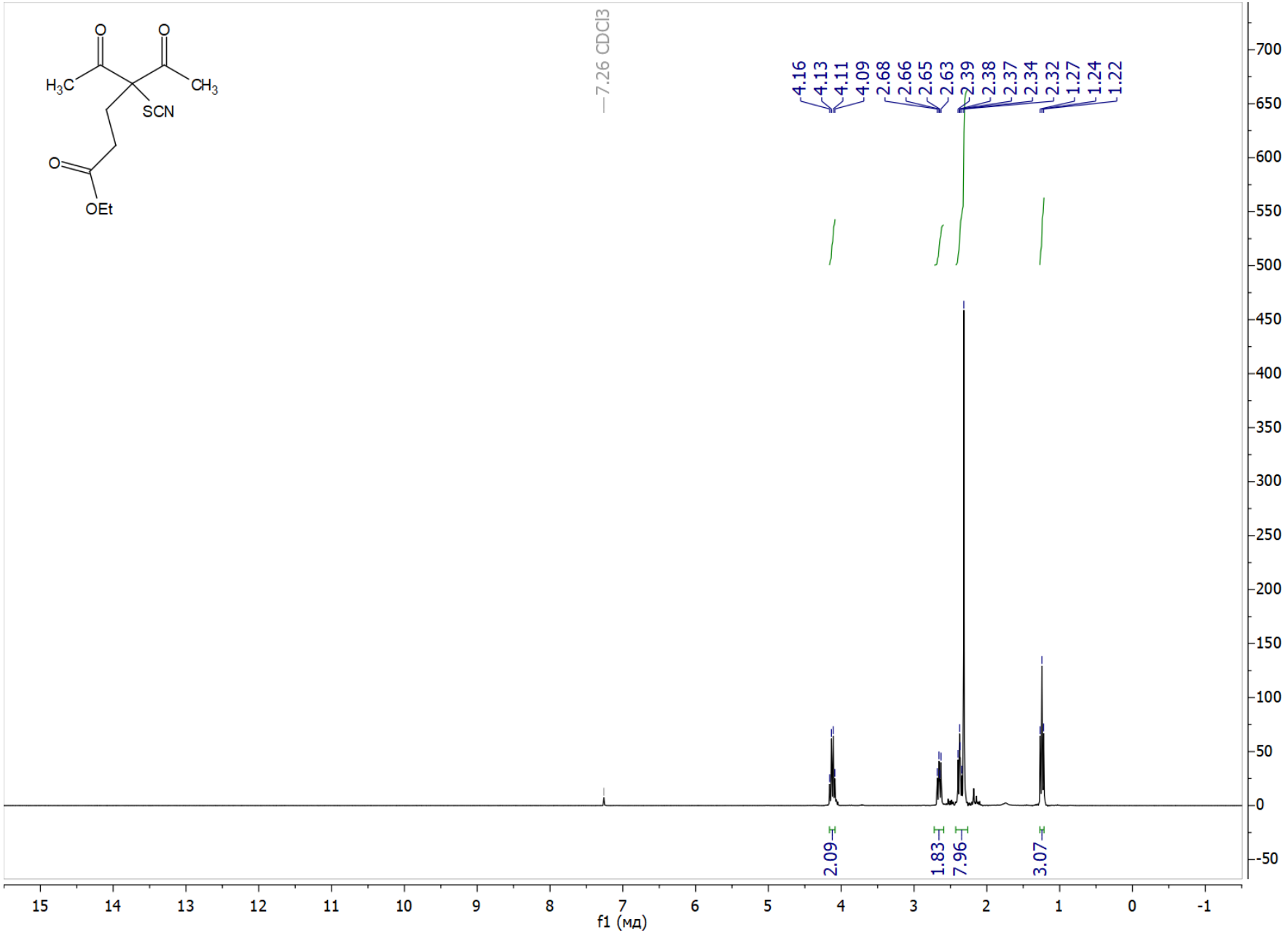
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of 3-ethyl-6-methyl-3-thiocyanatoheptane-2,4-dione, **2h**



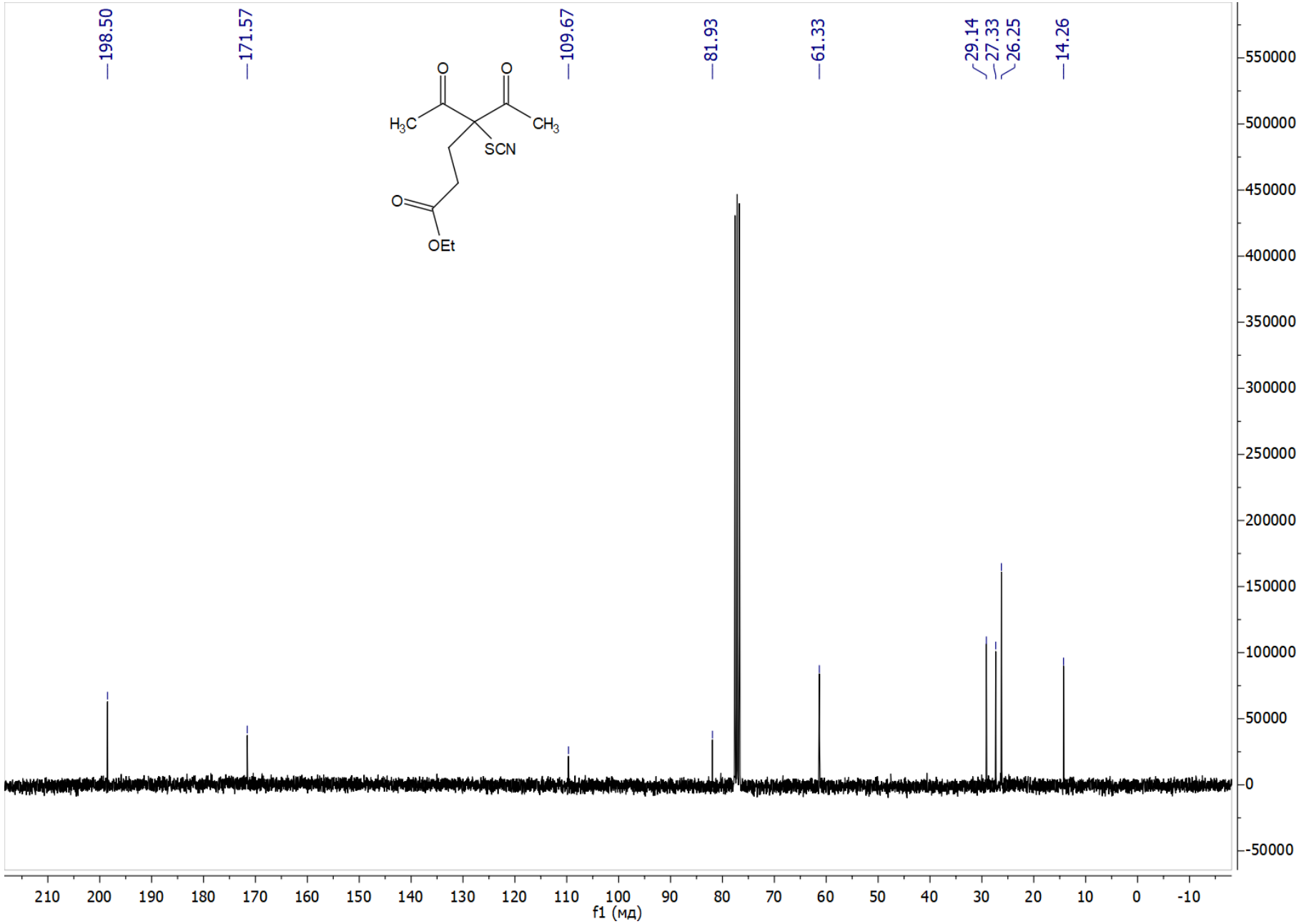
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of 3-ethyl-6-methyl-3-thiocyanatoheptane-2,4-dione, **2h**



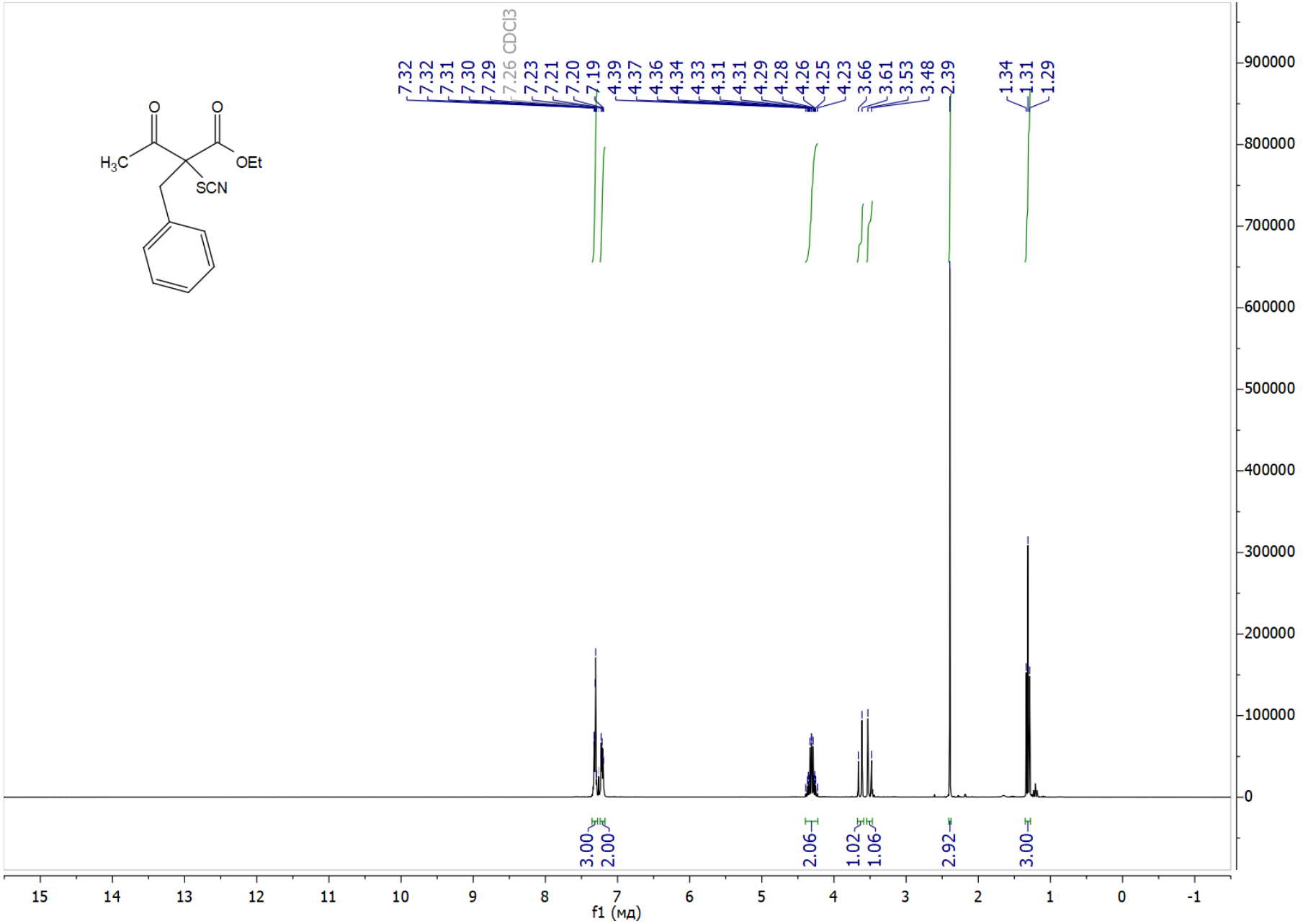
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 4-acetyl-5-oxo-4-thiocyanatohexanoate, **2i**



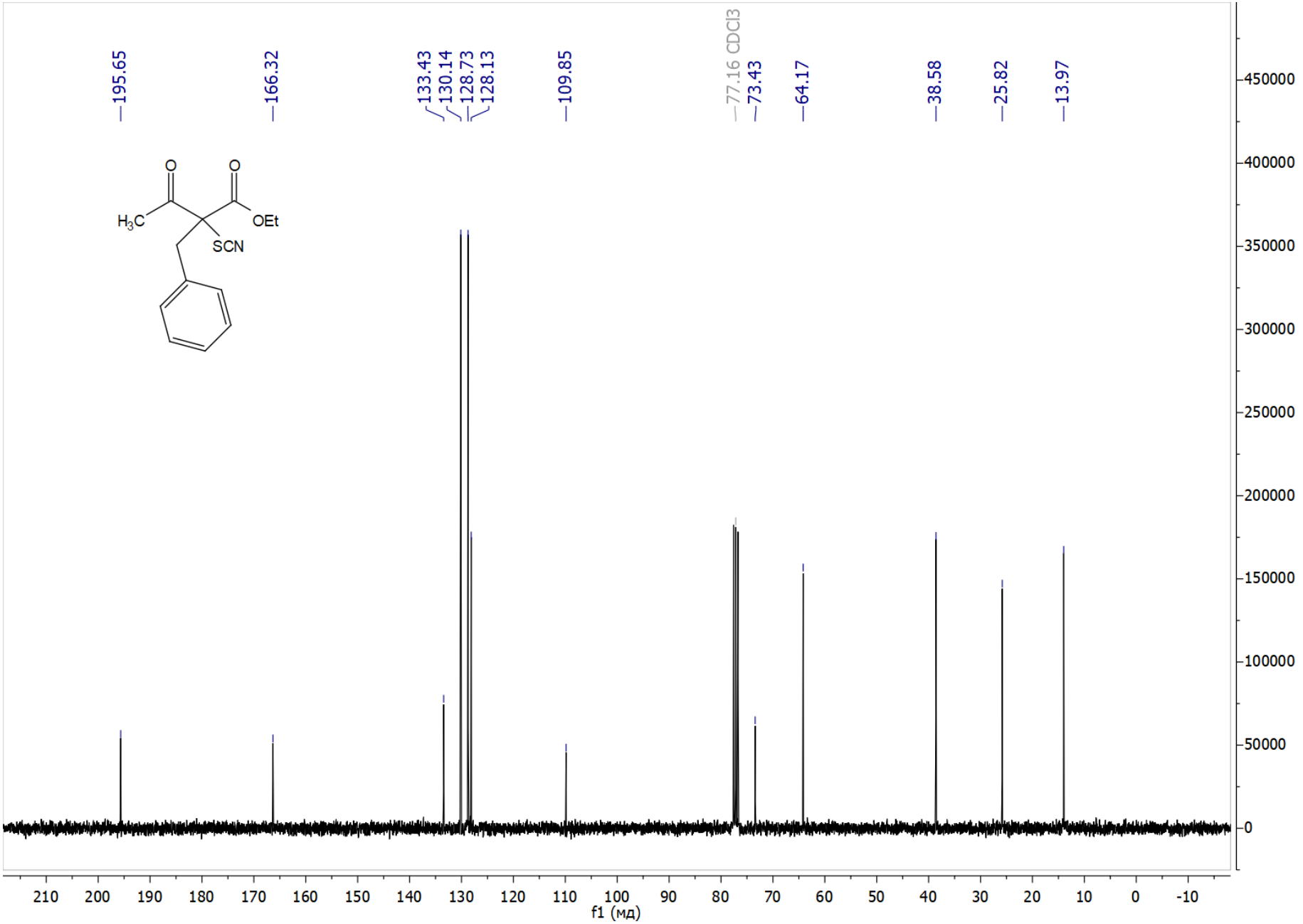
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 4-acetyl-5-oxo-4-thiocyanatohexanoate, **2i**



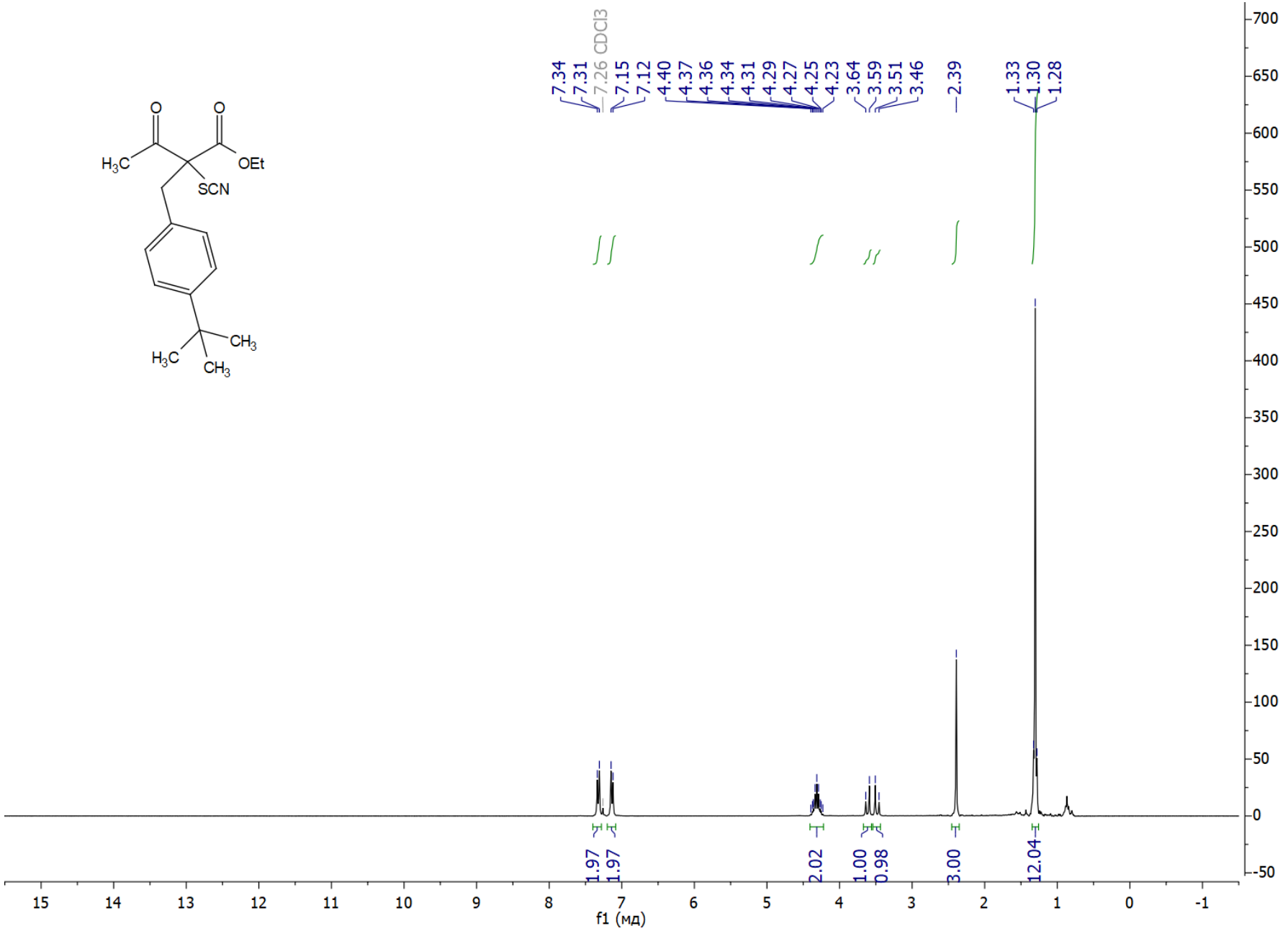
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-benzyl-3-oxo-2-thiocyanatobutanoate, **2j**



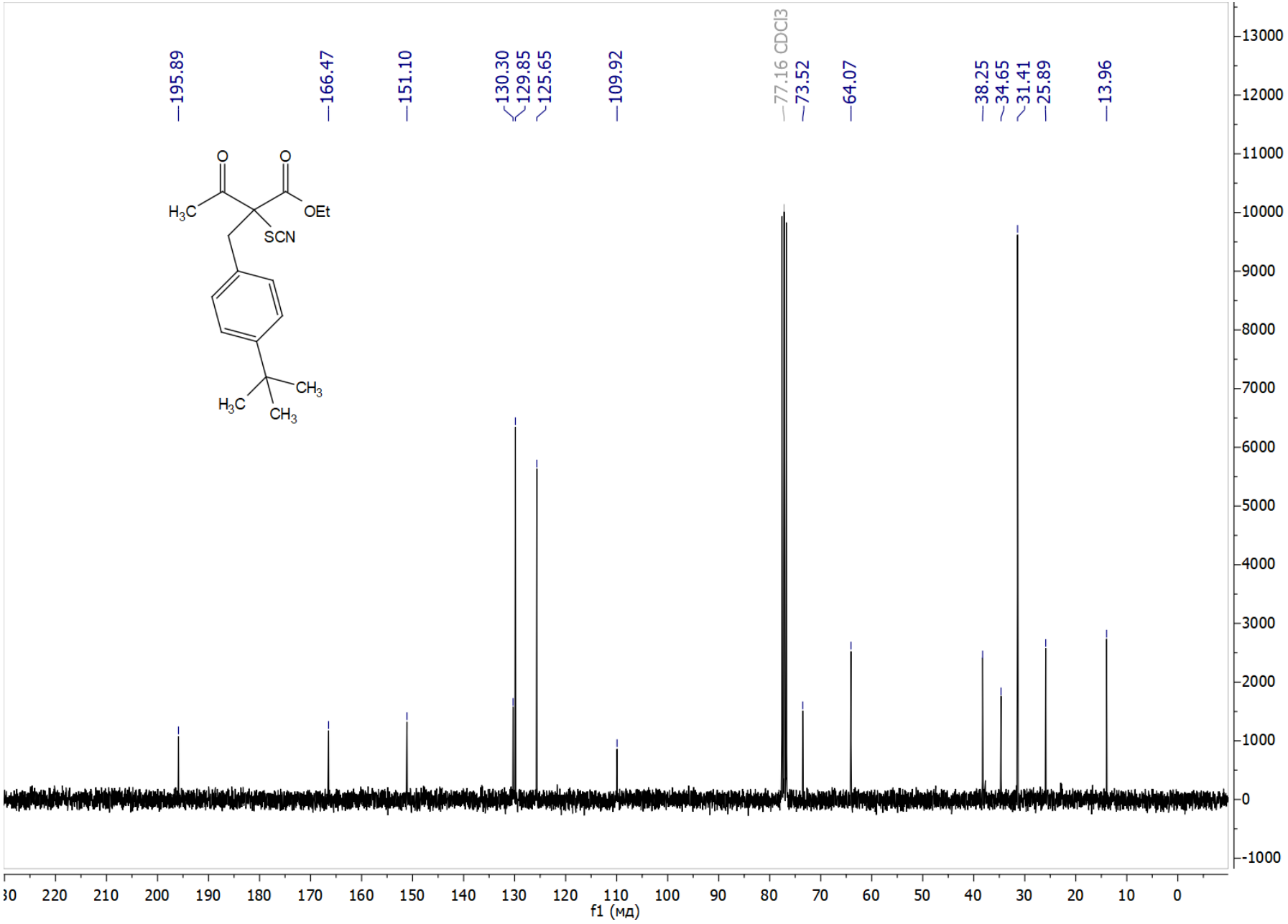
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-benzyl-3-oxo-2-thiocyanatobutanoate, **2j**



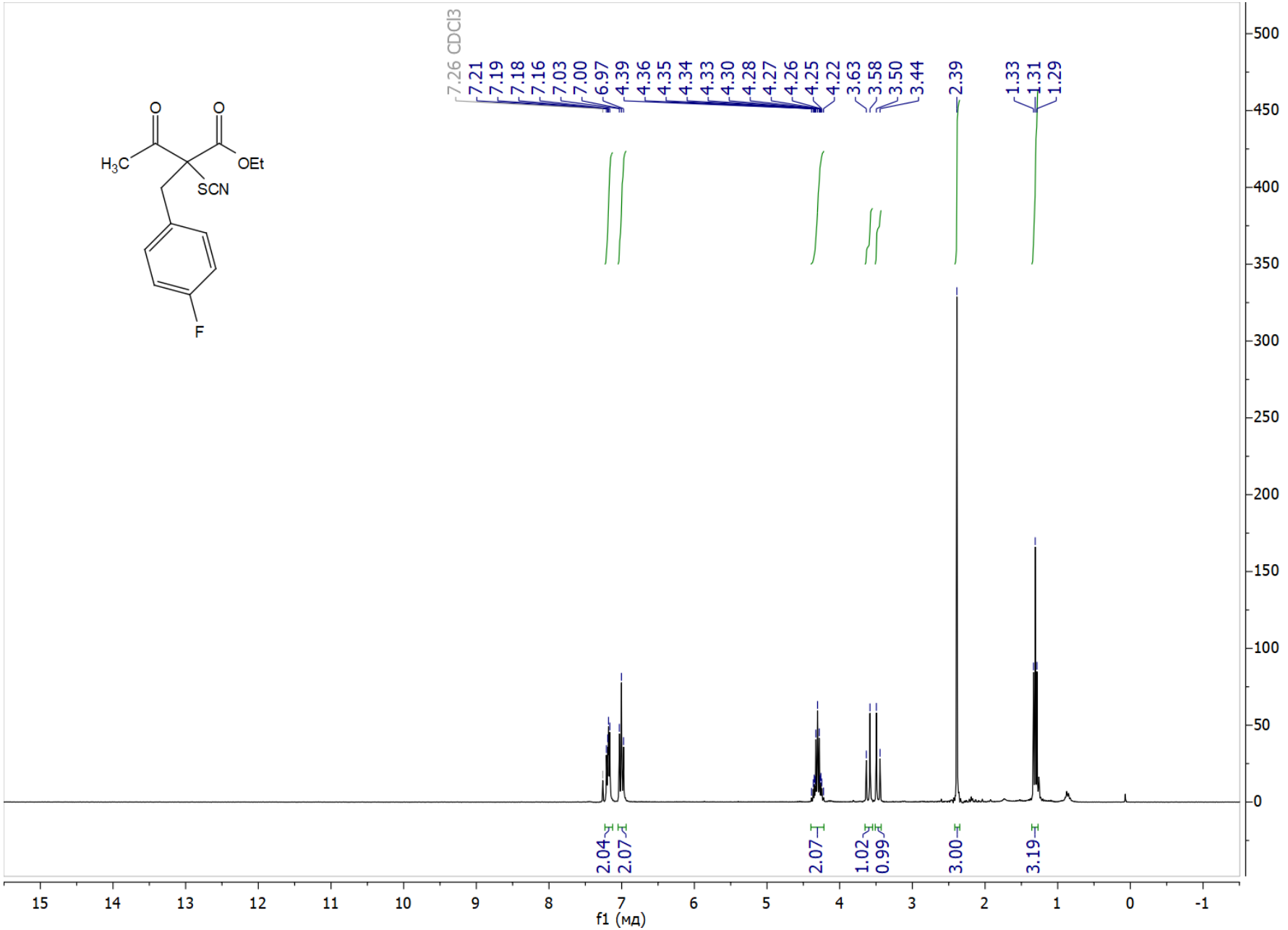
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-(4-(*tert*-butyl)benzyl)-3-oxo-2-thiocyanatobutanoate, **2k**



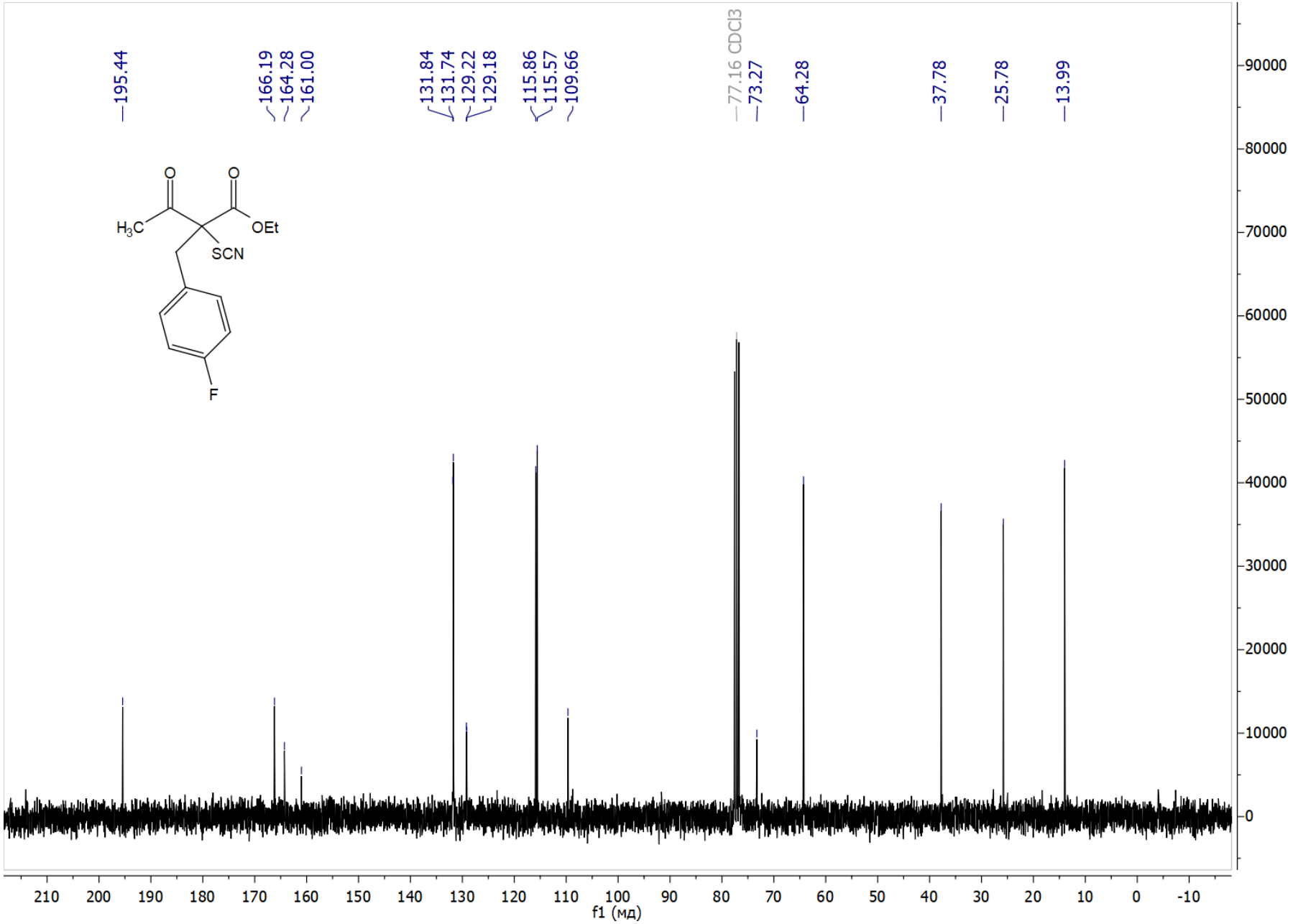
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-(4-(*tert*-butyl)benzyl)-3-oxo-2-thiocyanatobutanoate, **2k**



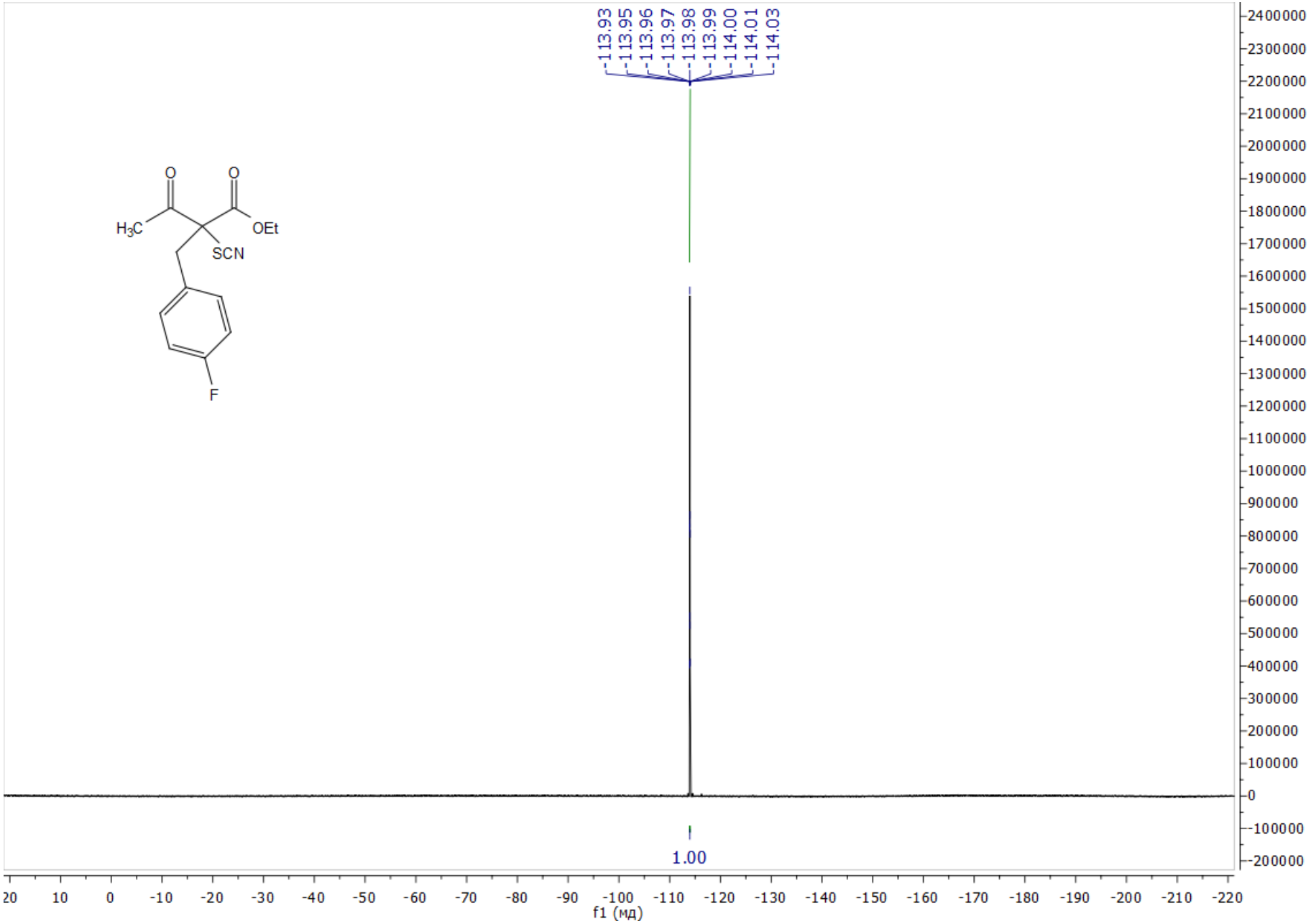
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-(4-fluorobenzyl)-3-oxo-2-thiocyanatobutanoate, **2l**



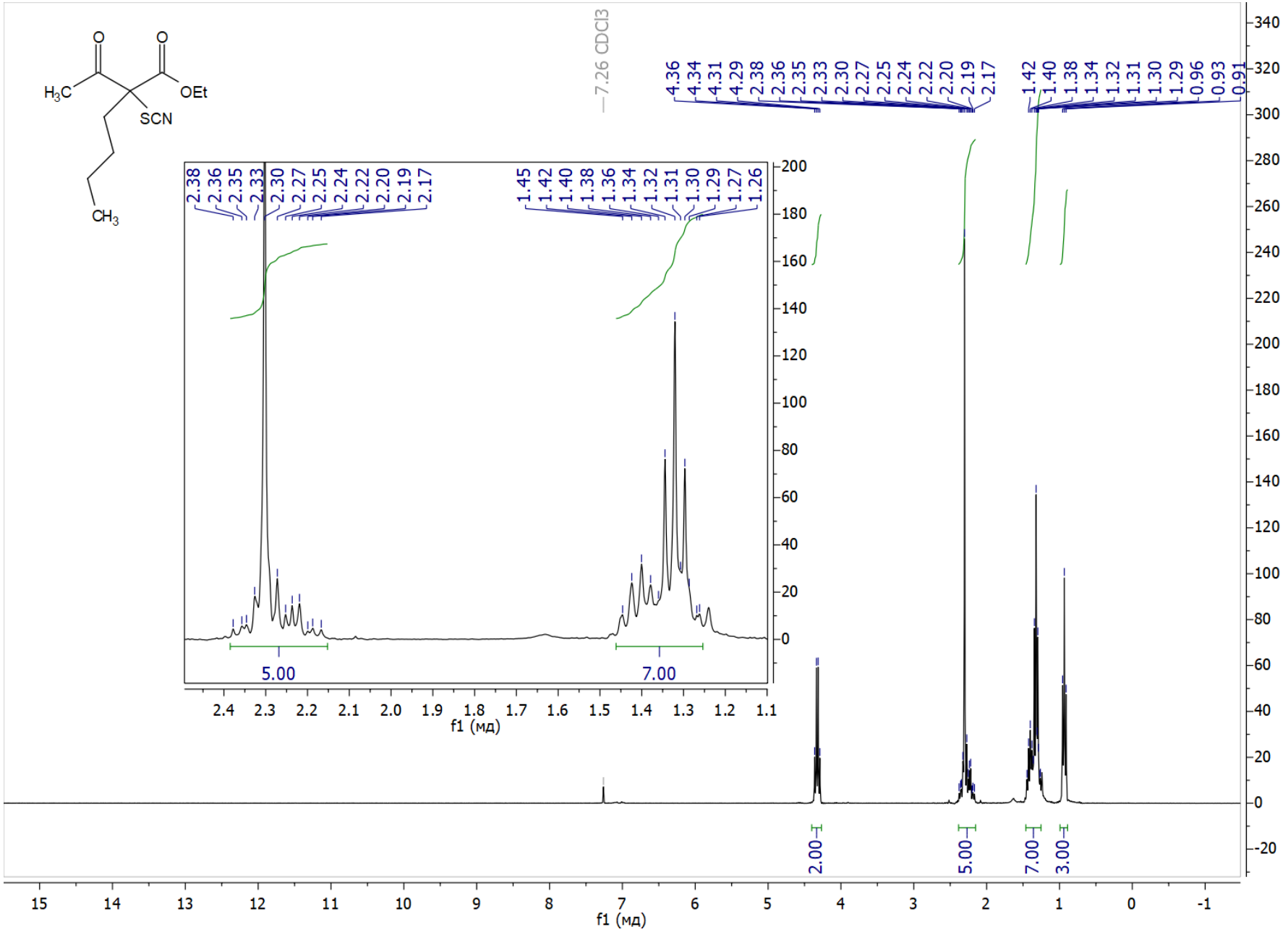
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-(4-fluorobenzyl)-3-oxo-2-thiocyanatobutanoate, **2l**



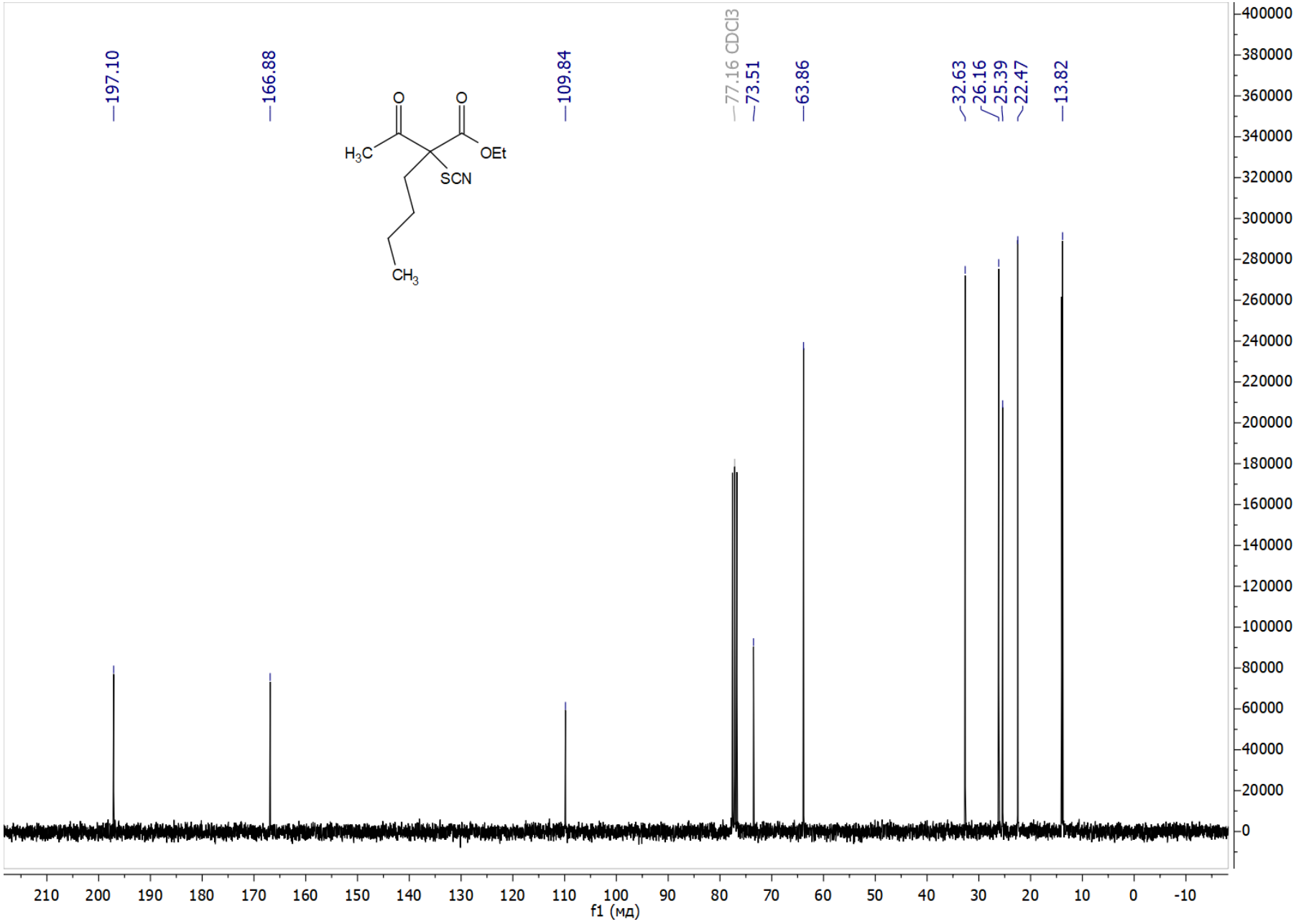
$^{19}$F NMR (282 MHz, $CDCl_3$) spectrum of ethyl 2-(4-fluorobenzyl)-3-oxo-2-thiocyanatobutanoate, **2l**



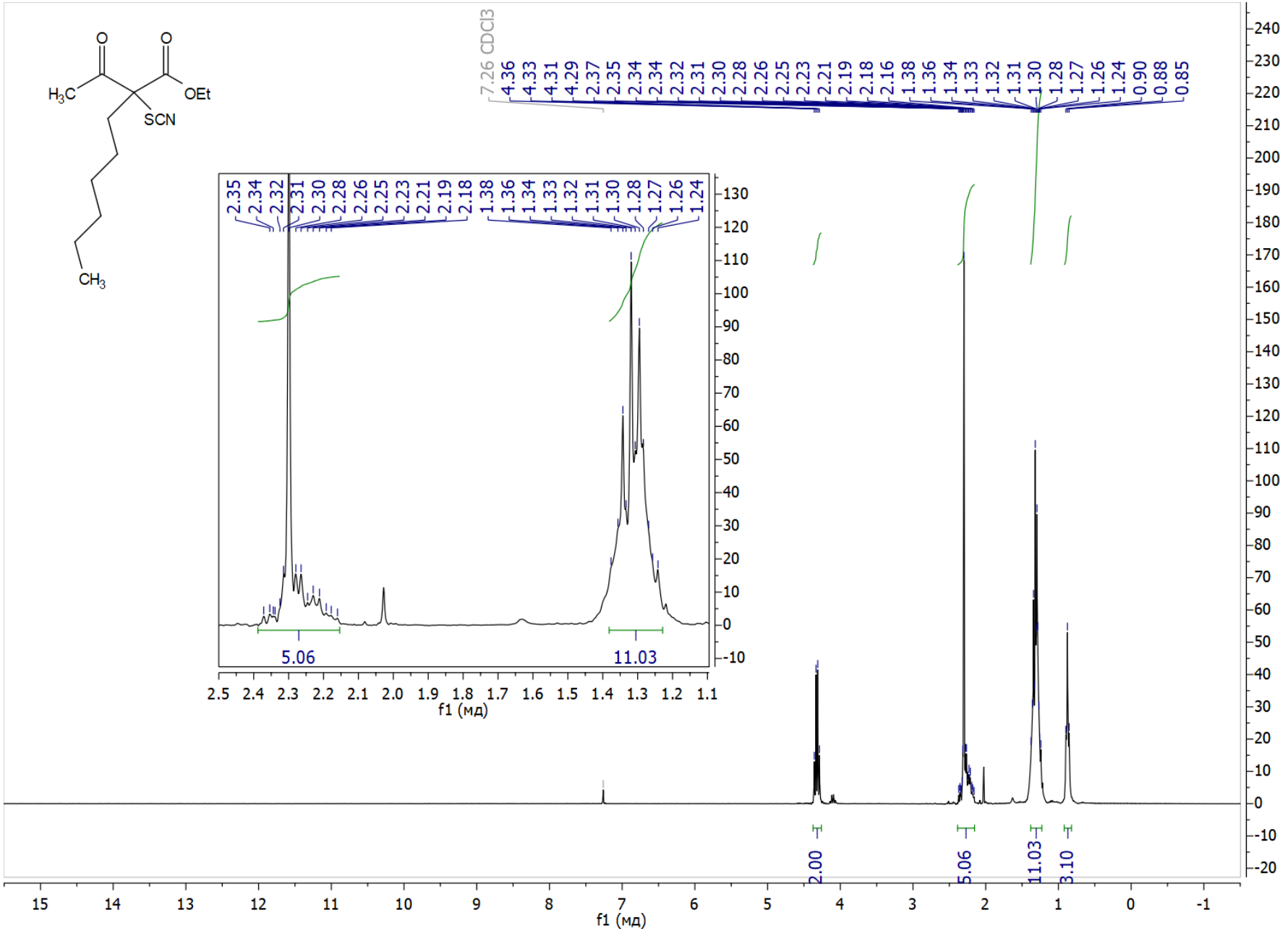
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-2-thiocyanatohexanoate, **2m**



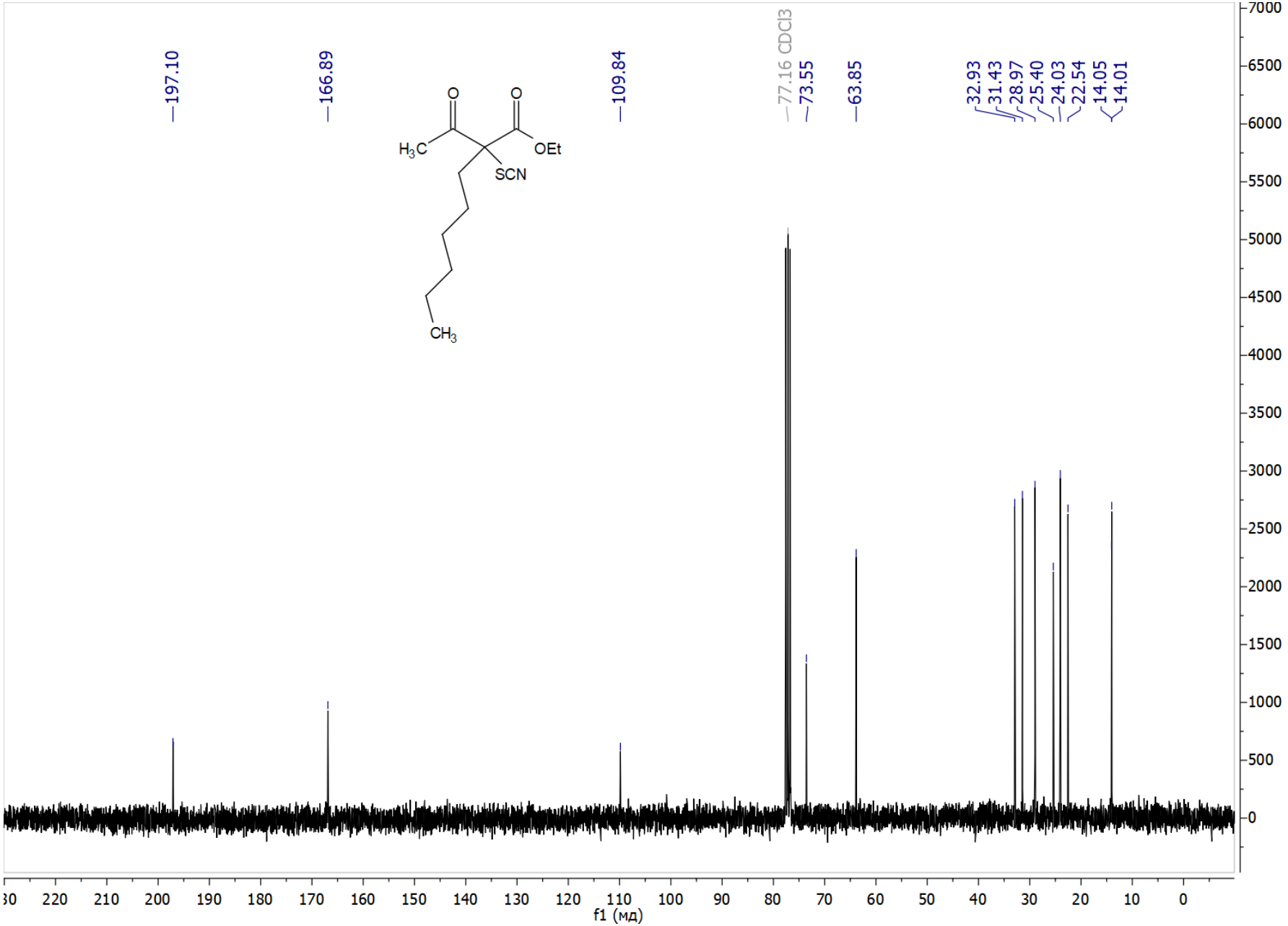
$^{13}C$ NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-2-thiocyanatohexanoate, **2m**



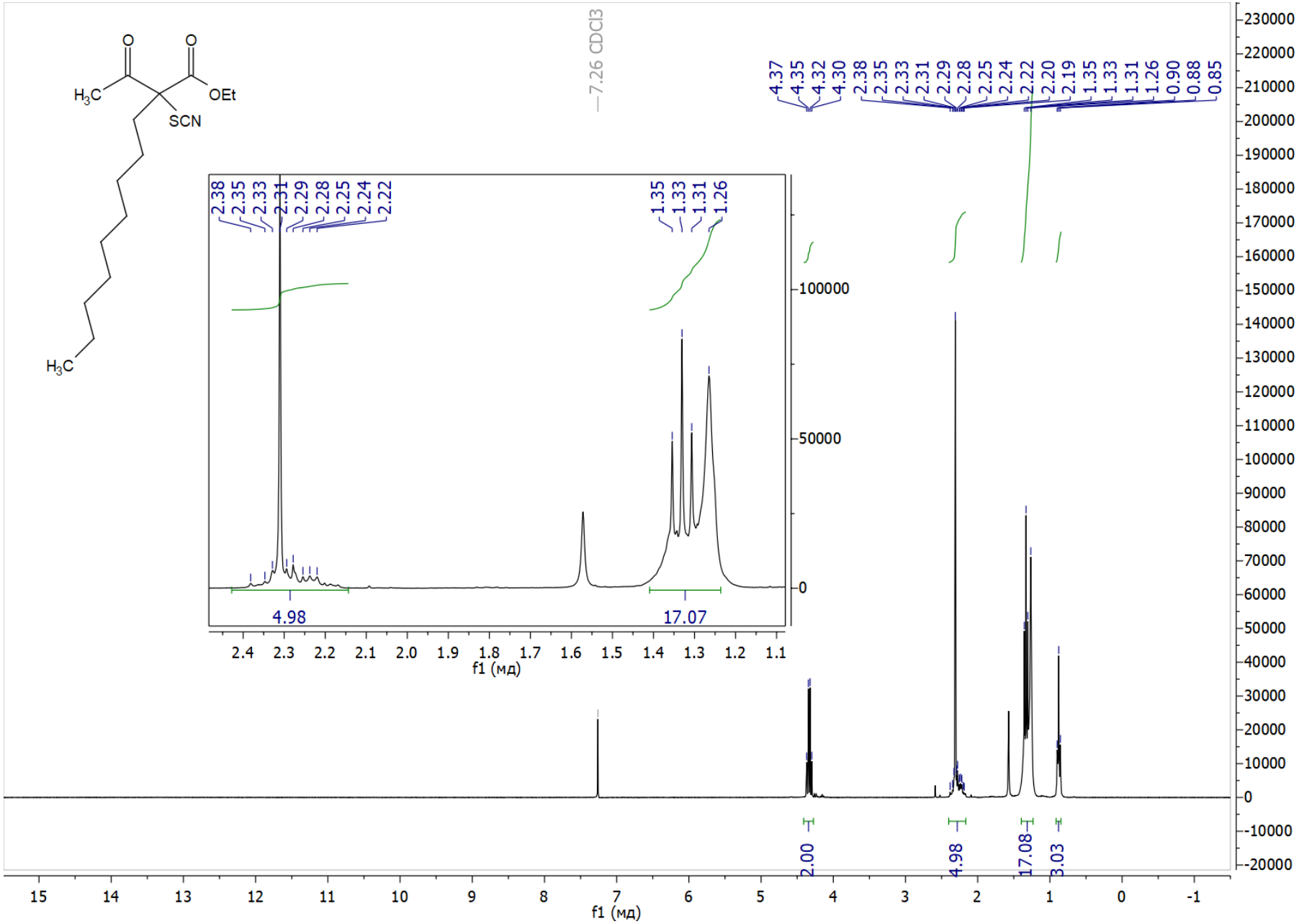
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-2-thiocyanatooctanoate, **2n**



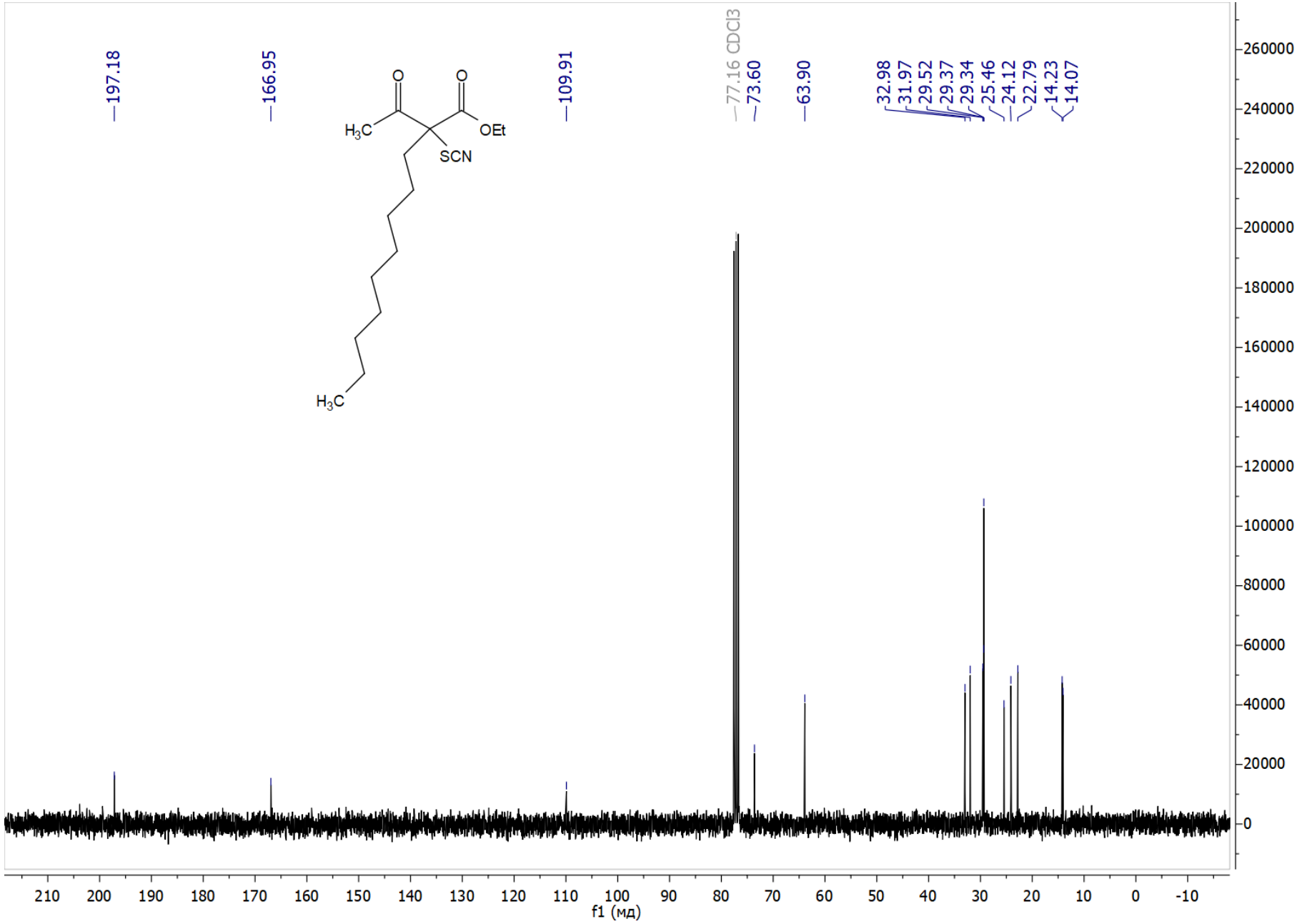
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-2-thiocyanatooctanoate, **2n**



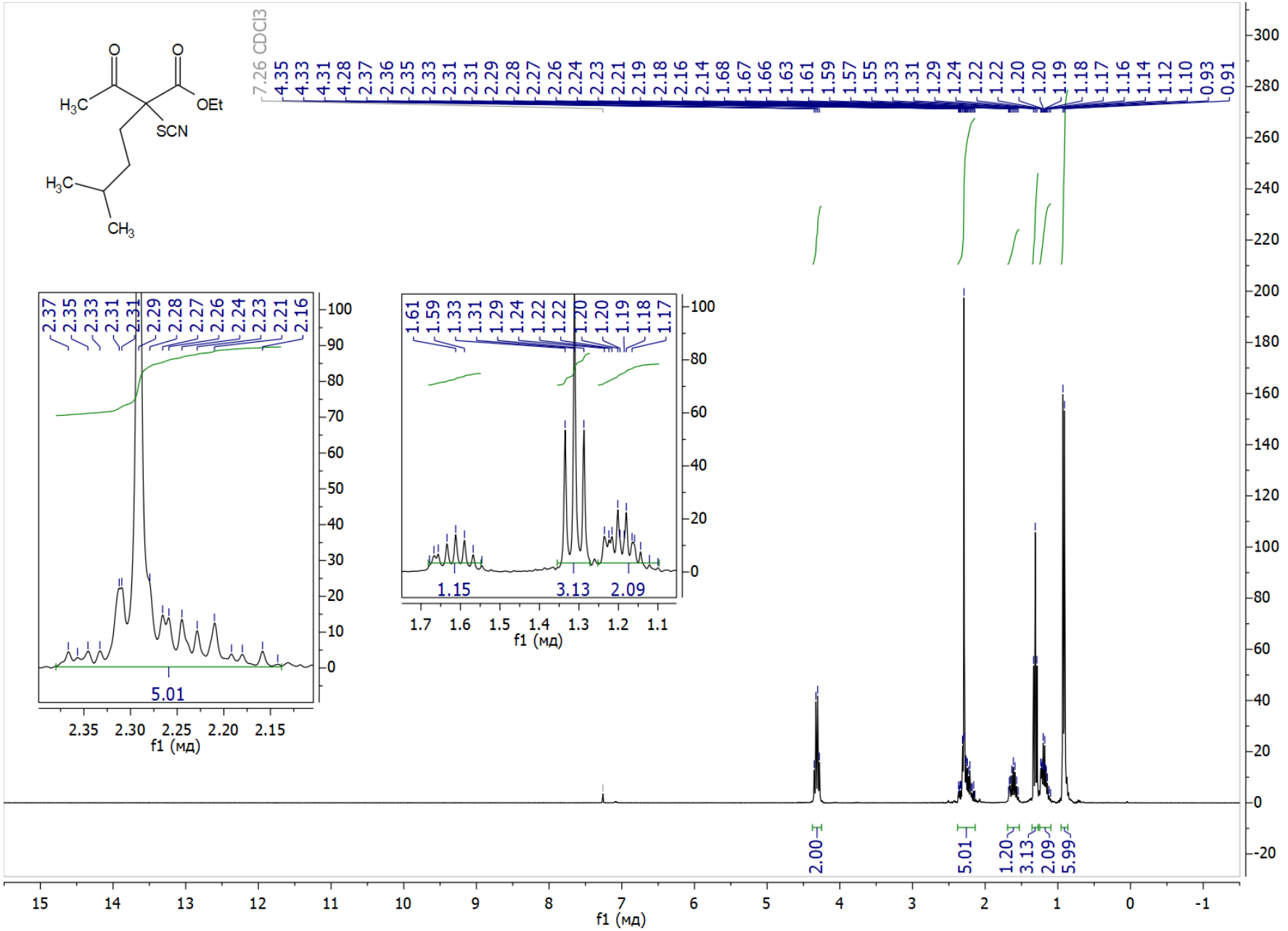
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-2-thiocyanatoundecanoate, **2o**



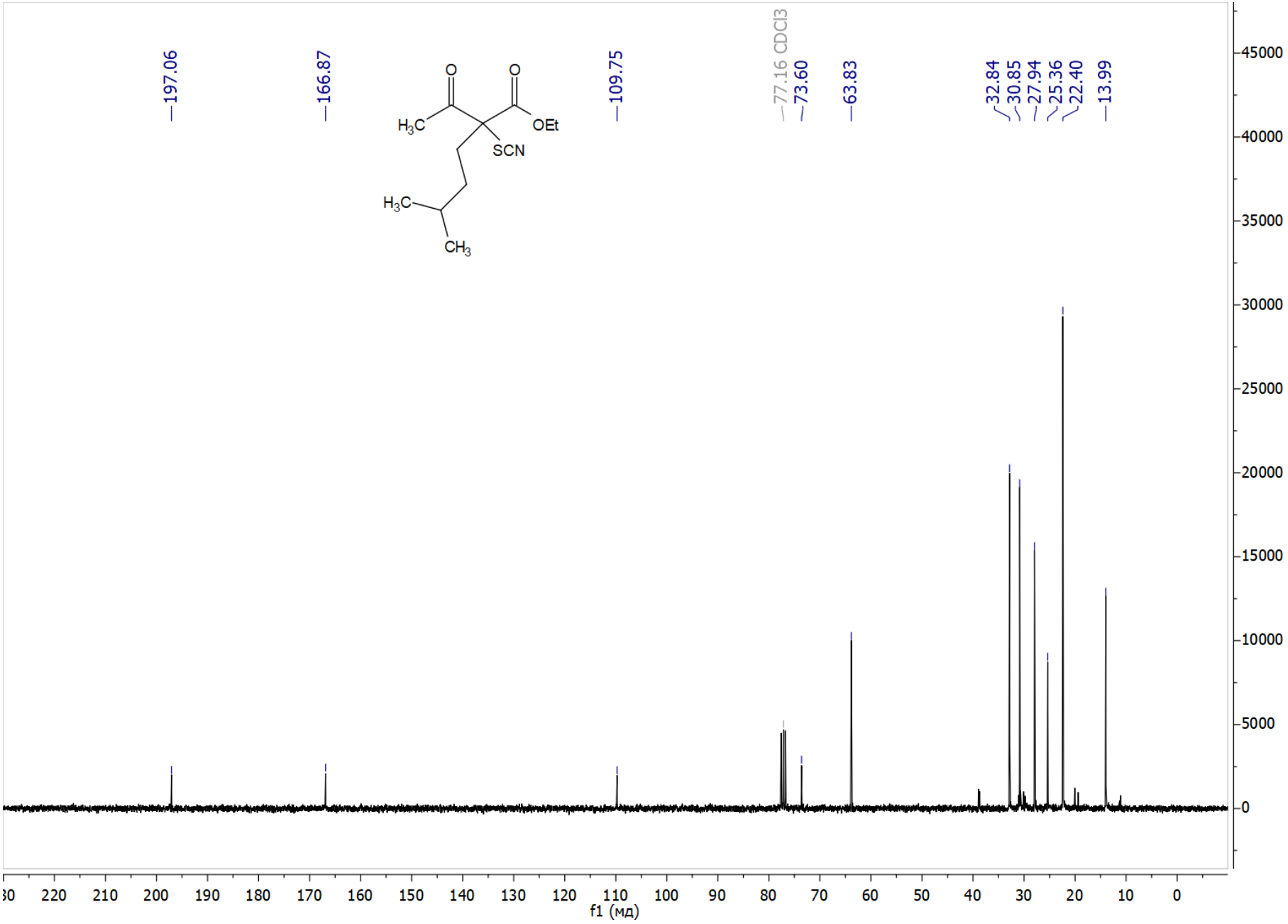
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-2-thiocyanatoundecanoate, **2o**



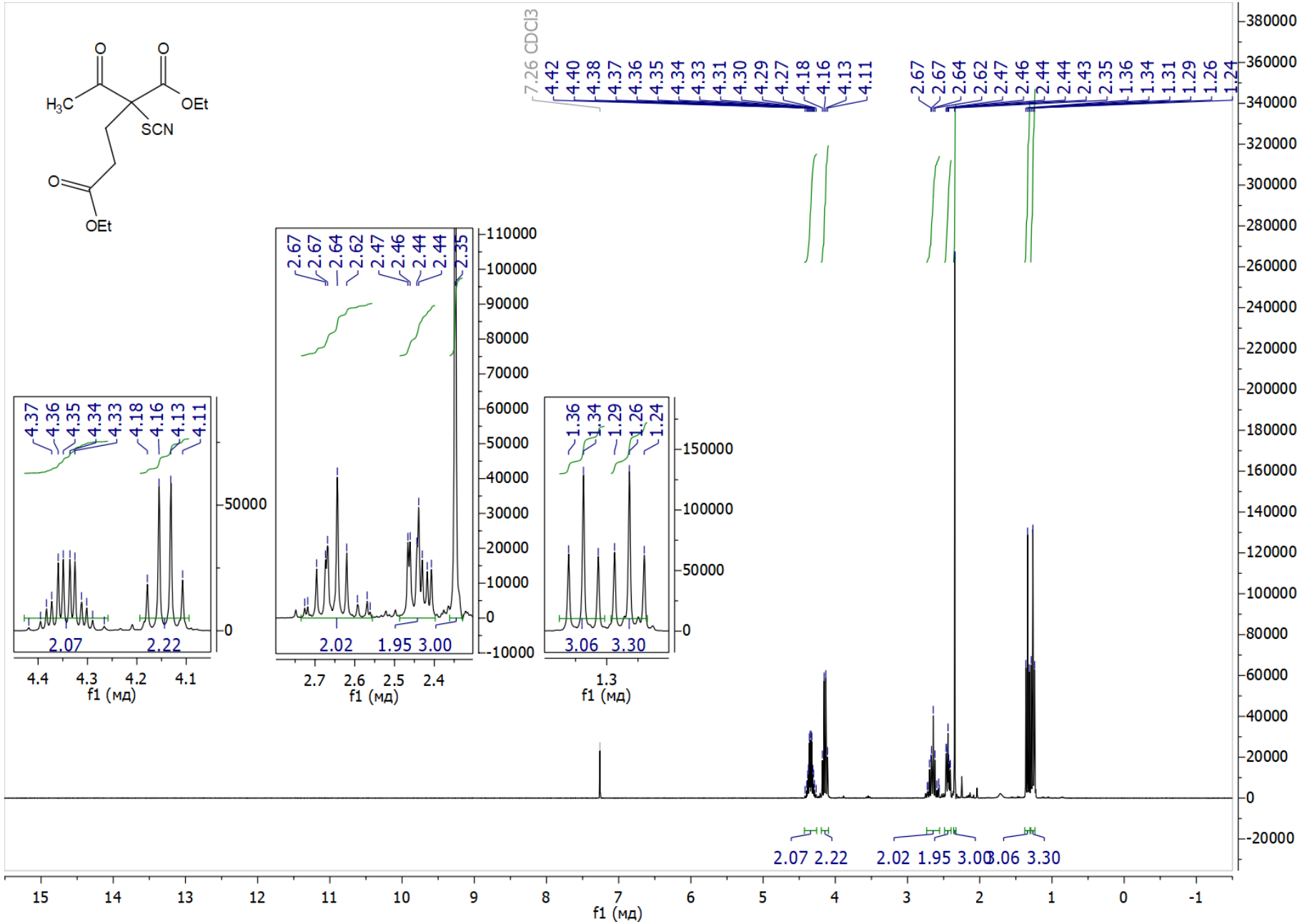
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-5-methyl-2-thiocyanatohexanoate, **2p**



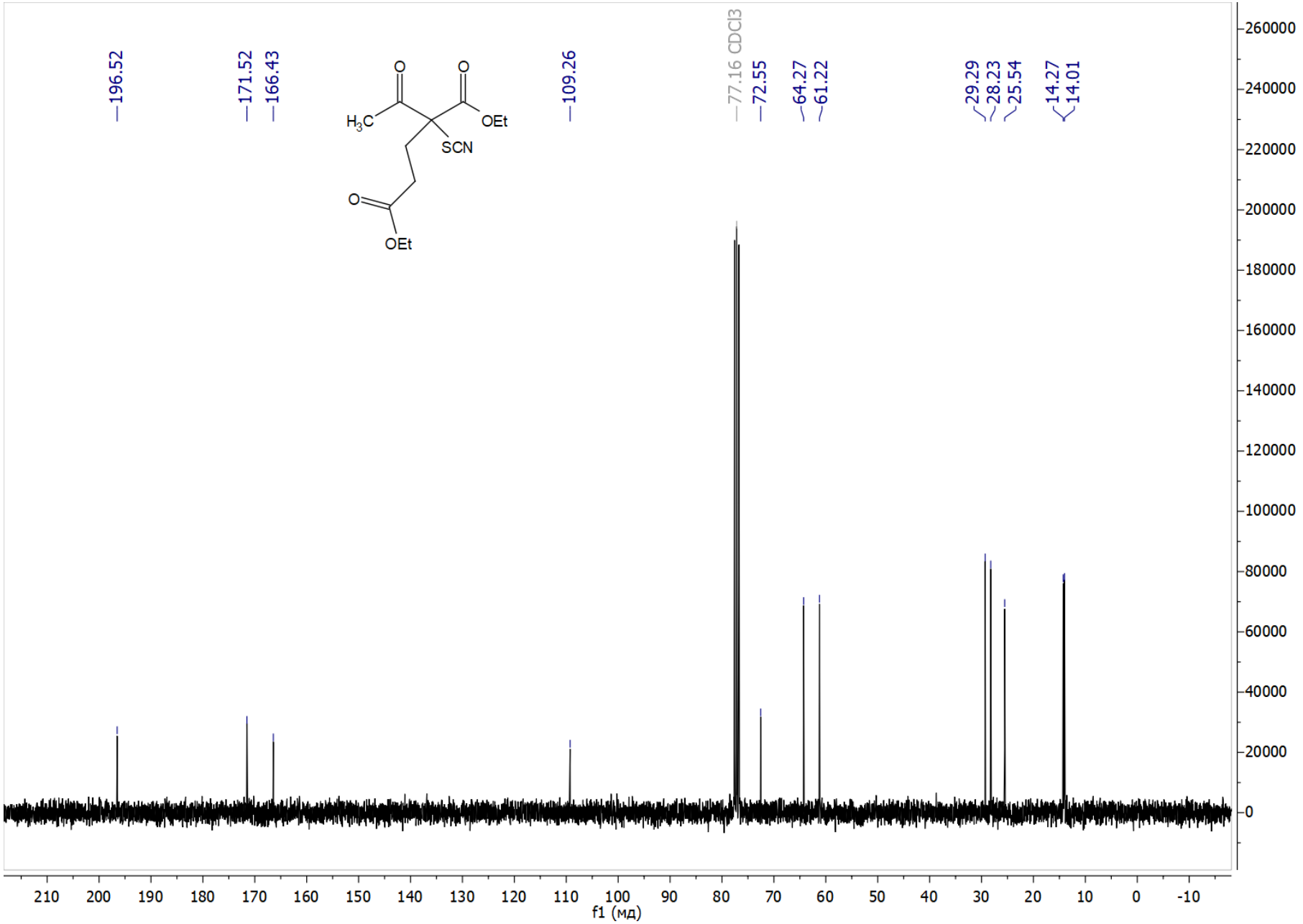
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-acetyl-5-methyl-2-thiocyanatohexanoate, **2p**



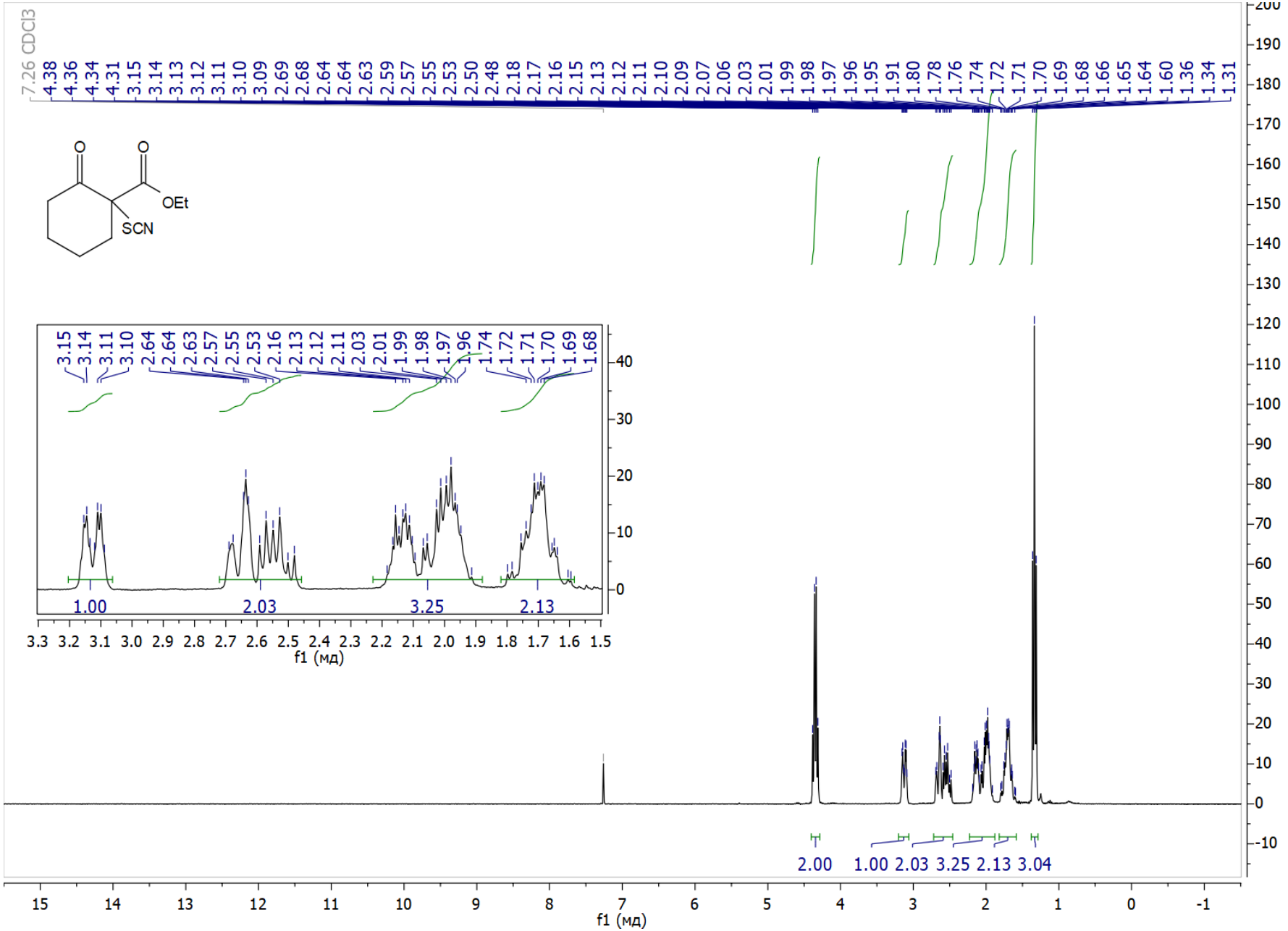
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of diethyl 2-acetyl-2-thiocyanatopentanedioate, **2q**



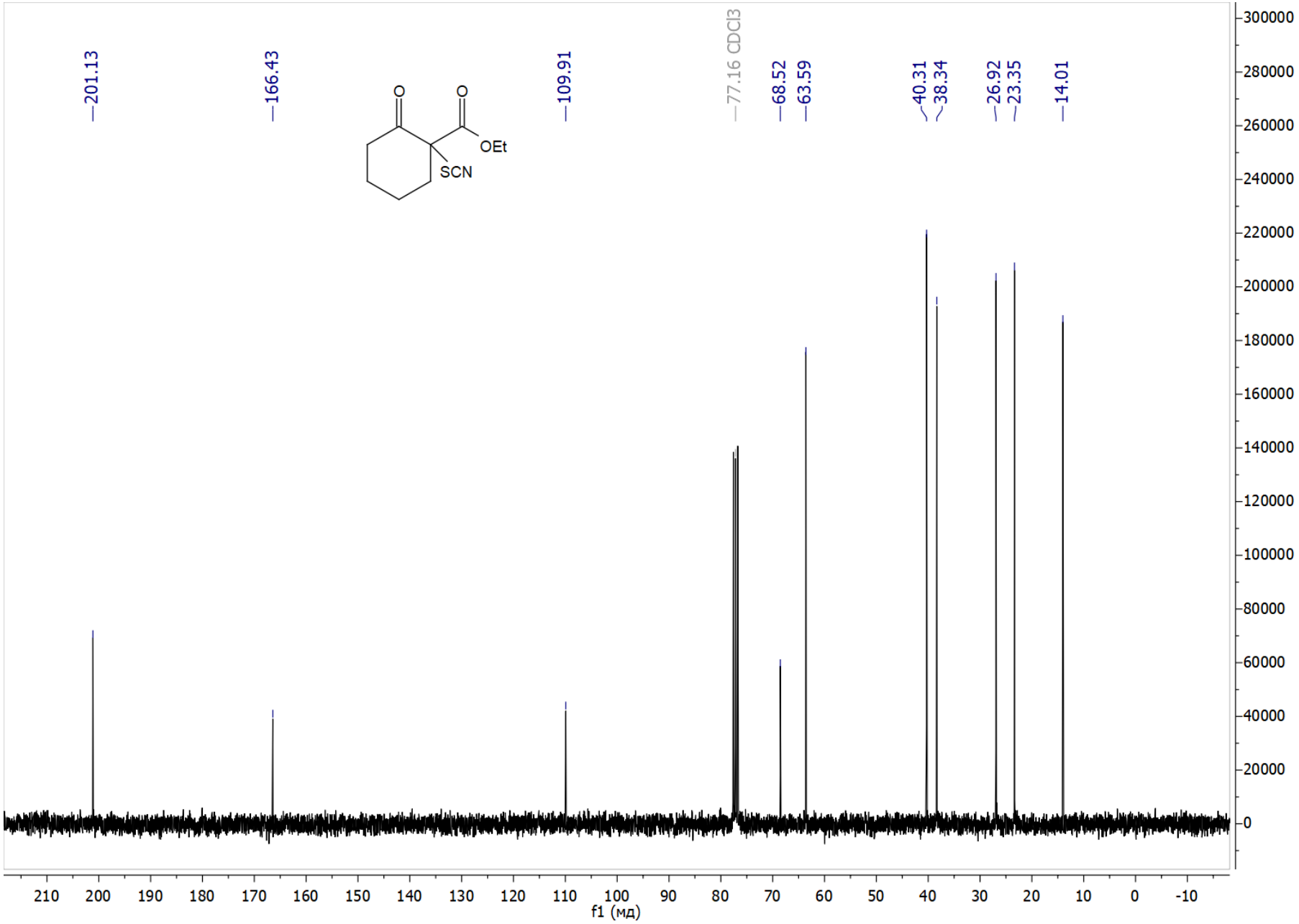
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of diethyl 2-acetyl-2-thiocyanatopentanedioate, **2q**



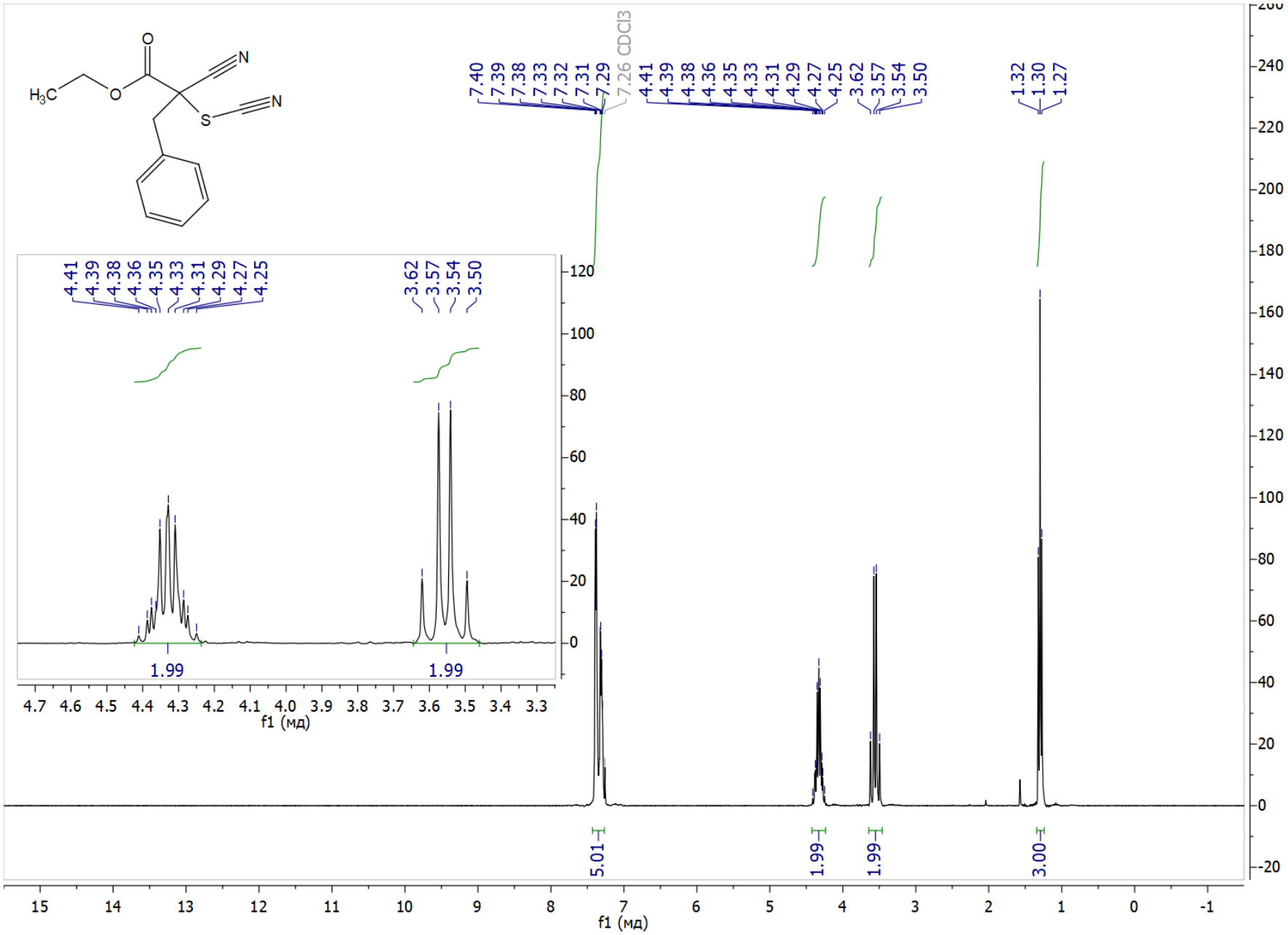
$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-oxo-1-thiocyanatocyclohexane-1-carboxylate, **2r**



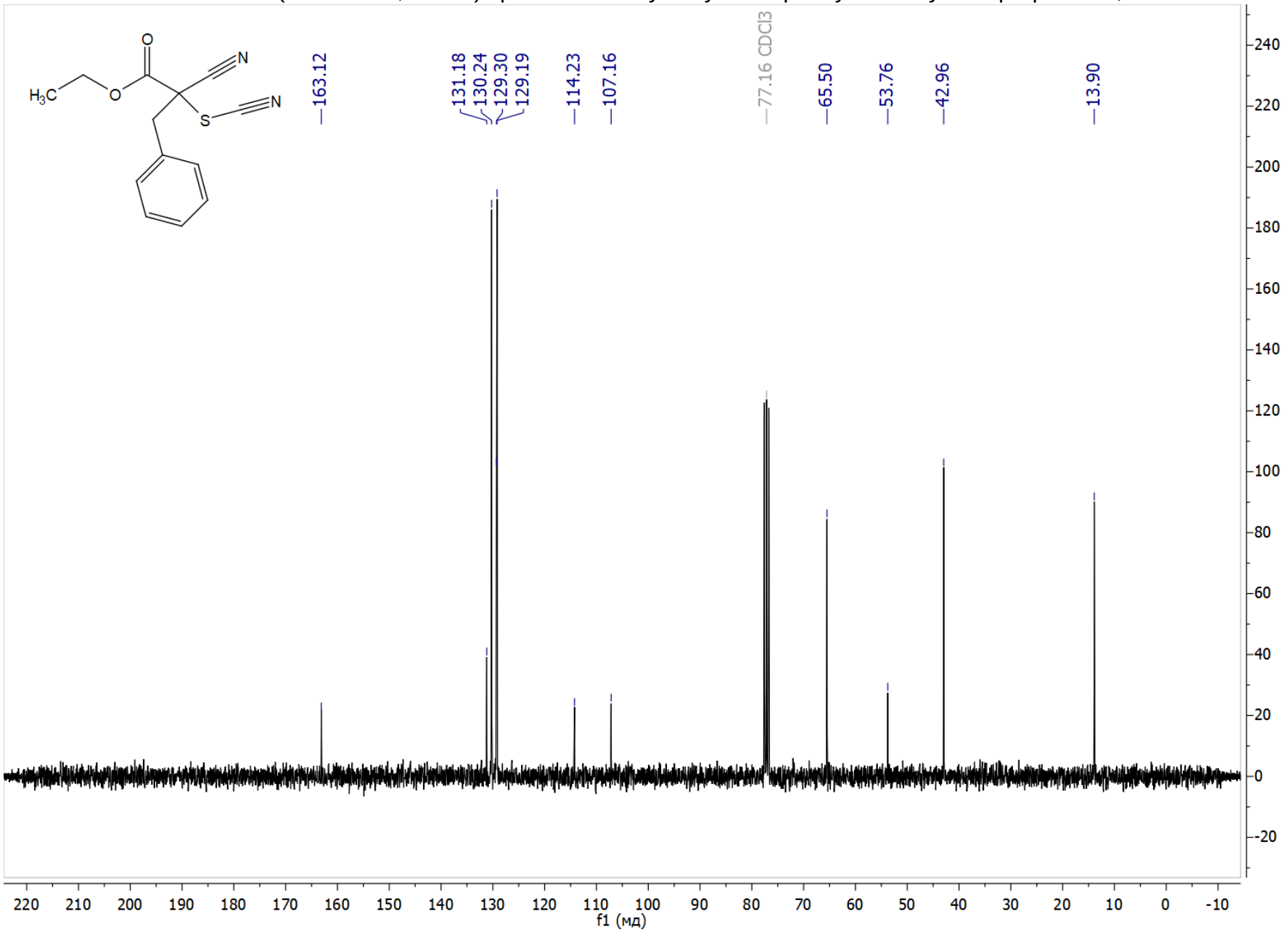
$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-oxo-1-thiocyanatocyclohexane-1-carboxylate, **2r**



$^{1}$H NMR (300.13 MHz, $CDCl_3$) spectrum of ethyl 2-cyano-3-phenyl-2-thiocyanatopropanoate, **2s**



$^{13}$C NMR (75.48 MHz, $CDCl_3$) spectrum of ethyl 2-cyano-3-phenyl-2-thiocyanatopropanoate, **2s**



**HRMS spectra of synthesized thiocyanates**

HRMS spectrum of 3-(4-methylbenzyl)-3-thiocyanatopentane-2,4-dione, **2b**

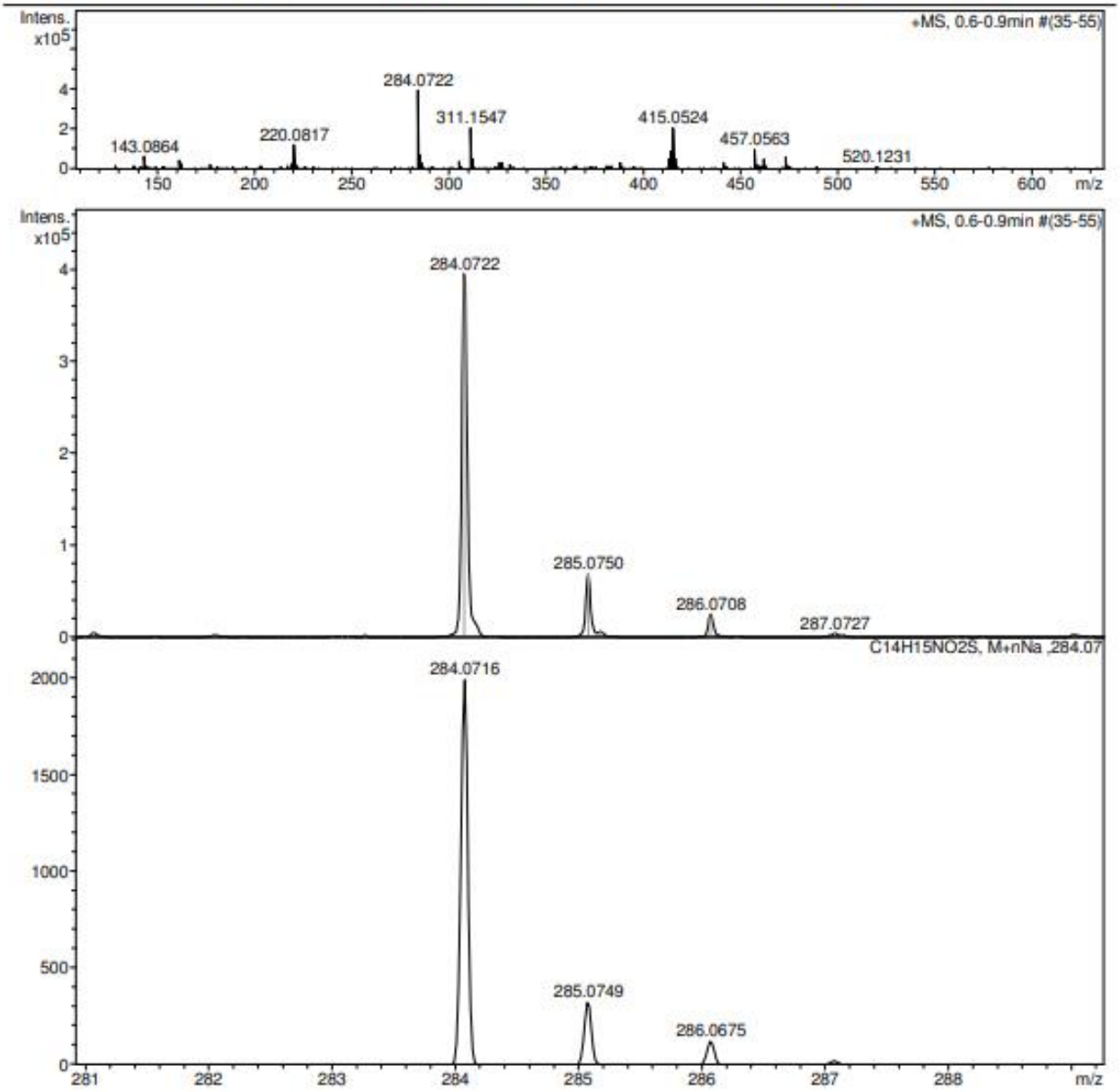
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1004025.d | Acquisition Date | 04.10.2022 19:24:38 |
| Method | tune_50-1600_pos_15_12.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil469 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C14H15NO2S mH 262.0896 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1600 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |




Bruker Compass DataAnalysis 4.0 printed: 04.10.2022 19:29:07 Page 1 of 1

HRMS spectrum of 3-butyl-3-thiocyanatopentane-2,4-dione, **2d**

# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1004021.d | Acquisition Date | 04.10.2022 18:44:05 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil462 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C10H15NO2S mH 214.0896 clb added CH3CN | | |

**Acquisition Parameter**

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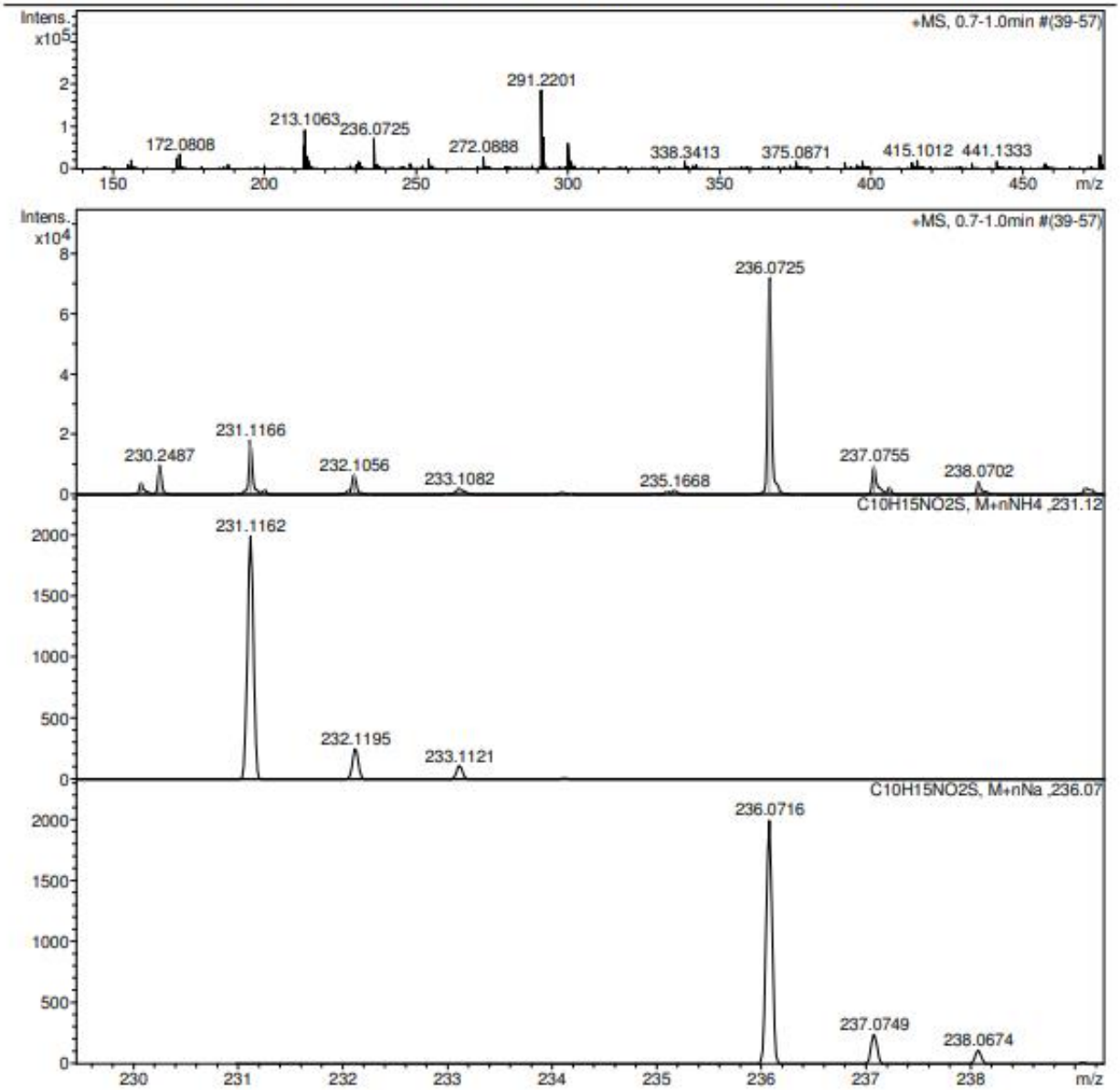
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |



HRMS spectrum of 3-octyl-3-thiocyanatopentane-2,4-dione, **2f**

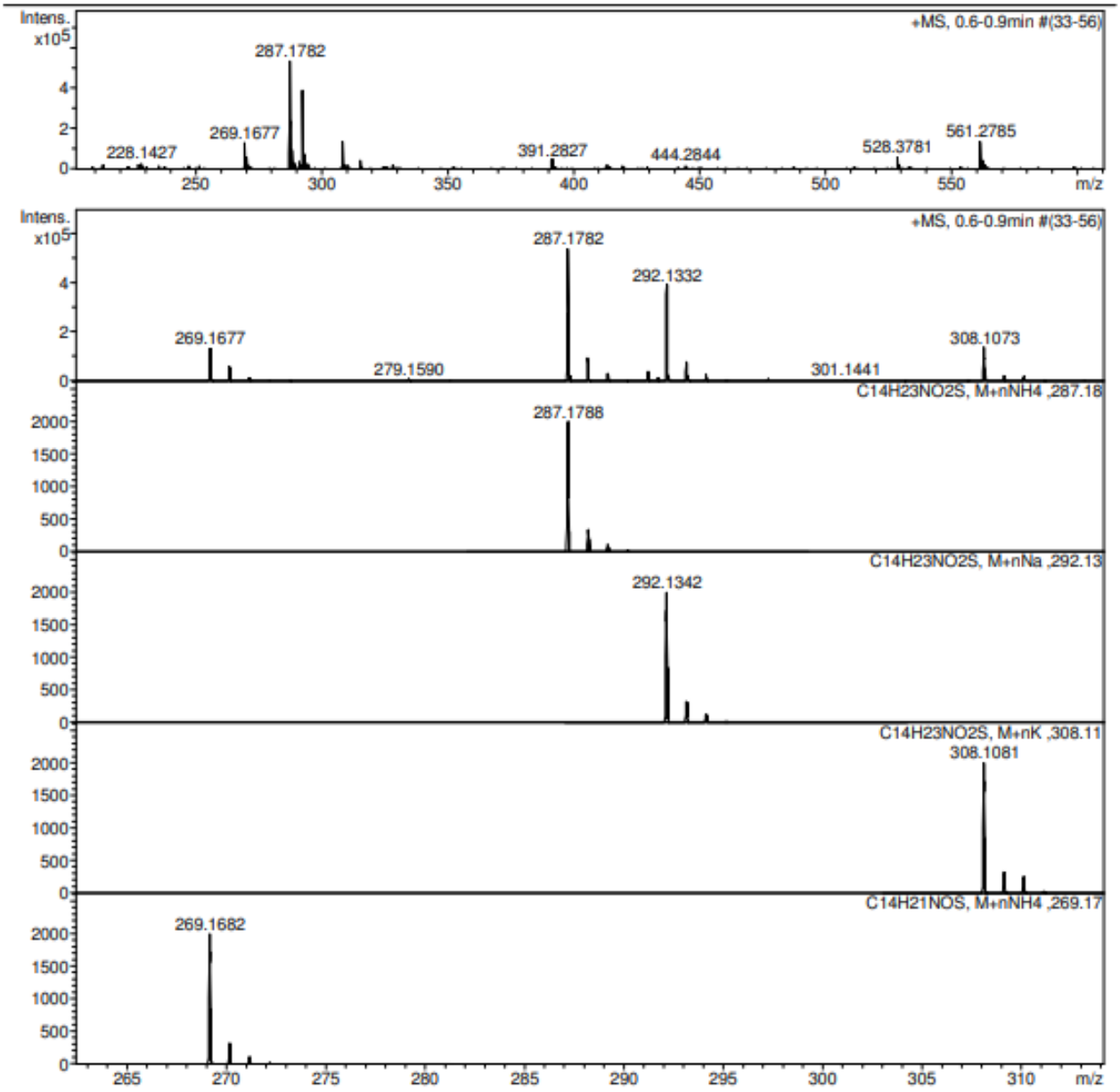
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1004022.d | | |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil475 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C14H23NO2S mH 270.1522 clb added CH3CN | Acquisition Date | 04.10.2022 18:50:47 |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |



HRMS spectrum of 3-*iso*pentyl-3-thiocyanatopentane-2,4-dione, **2g**

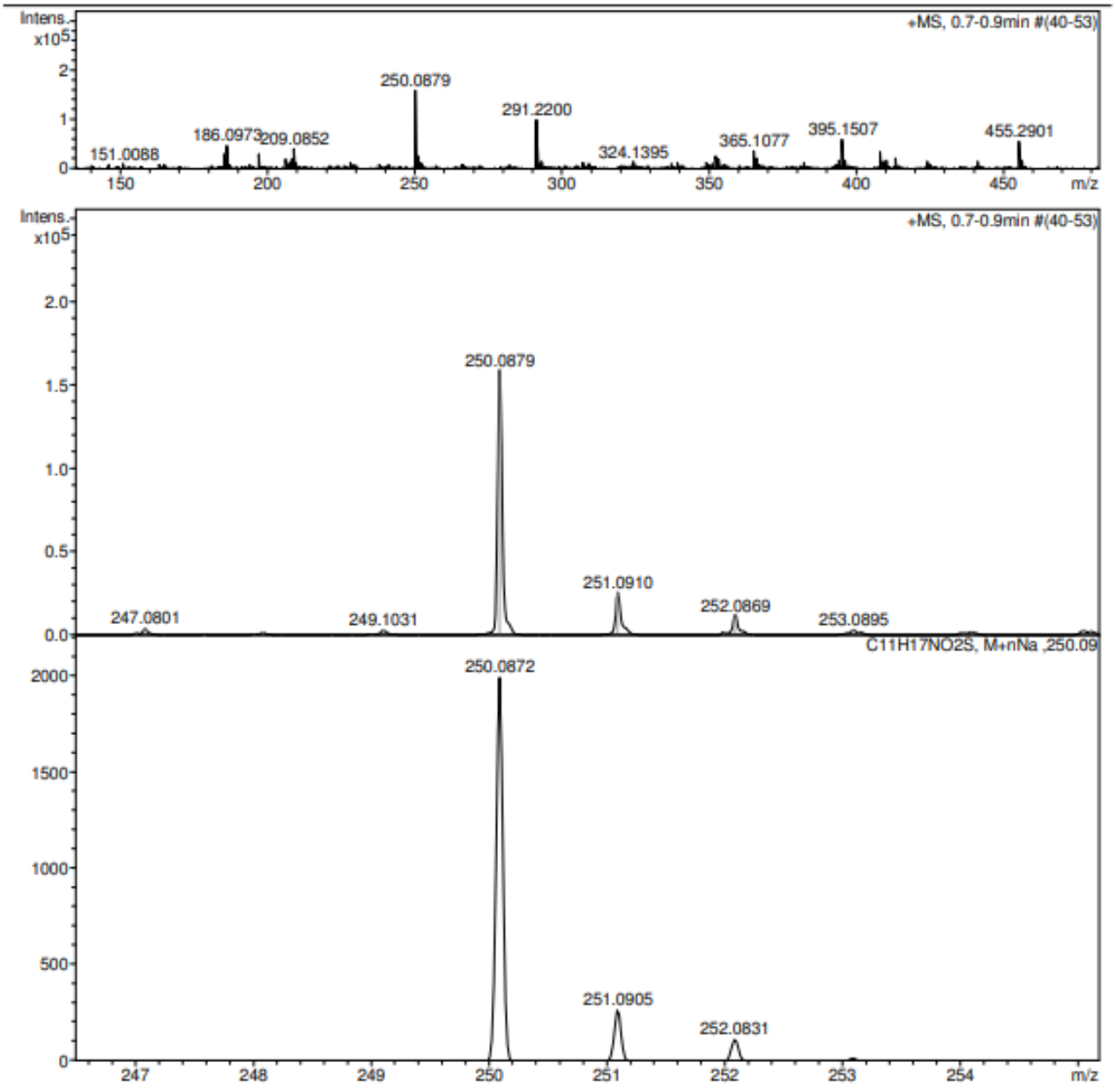
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1004024.d | Acquisition Date | 04.10.2022 19:10:32 |
| Method | tune_50-1600_pos_15_12.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil413 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C11H17NO2S mH 228.1052 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1600 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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HRMS spectrum of 3-ethyl-6-methyl-3-thiocyanatoheptane-2,4-dione, **2h**

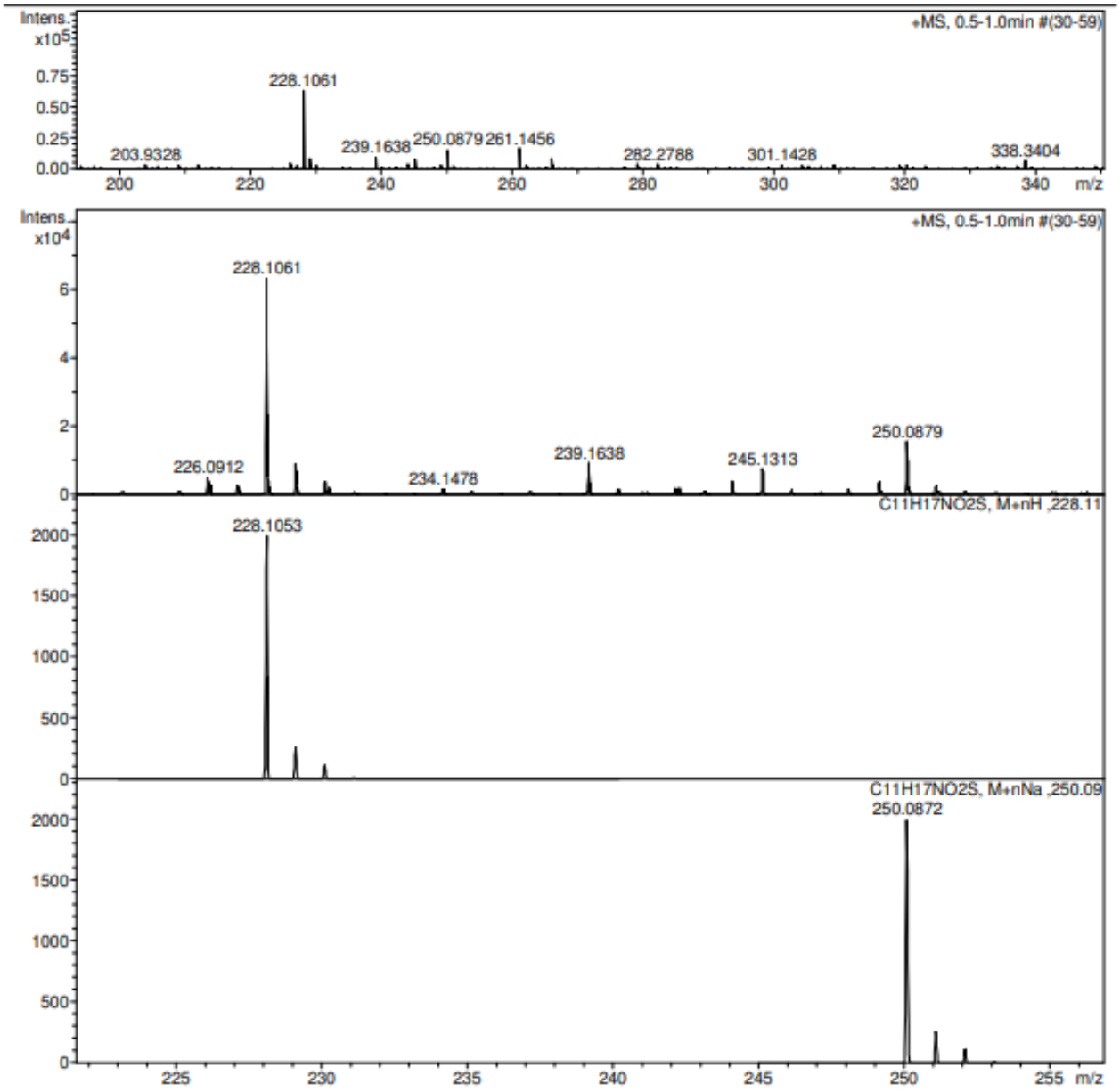
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1006007.d | Acquisition Date | 06.10.2022 10:40:22 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil427 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C11H17NO2S mH228.1052 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |



HRMS spectrum of ethyl 2-benzyl-3-oxo-2-thiocyanatobutanoate, **2j**

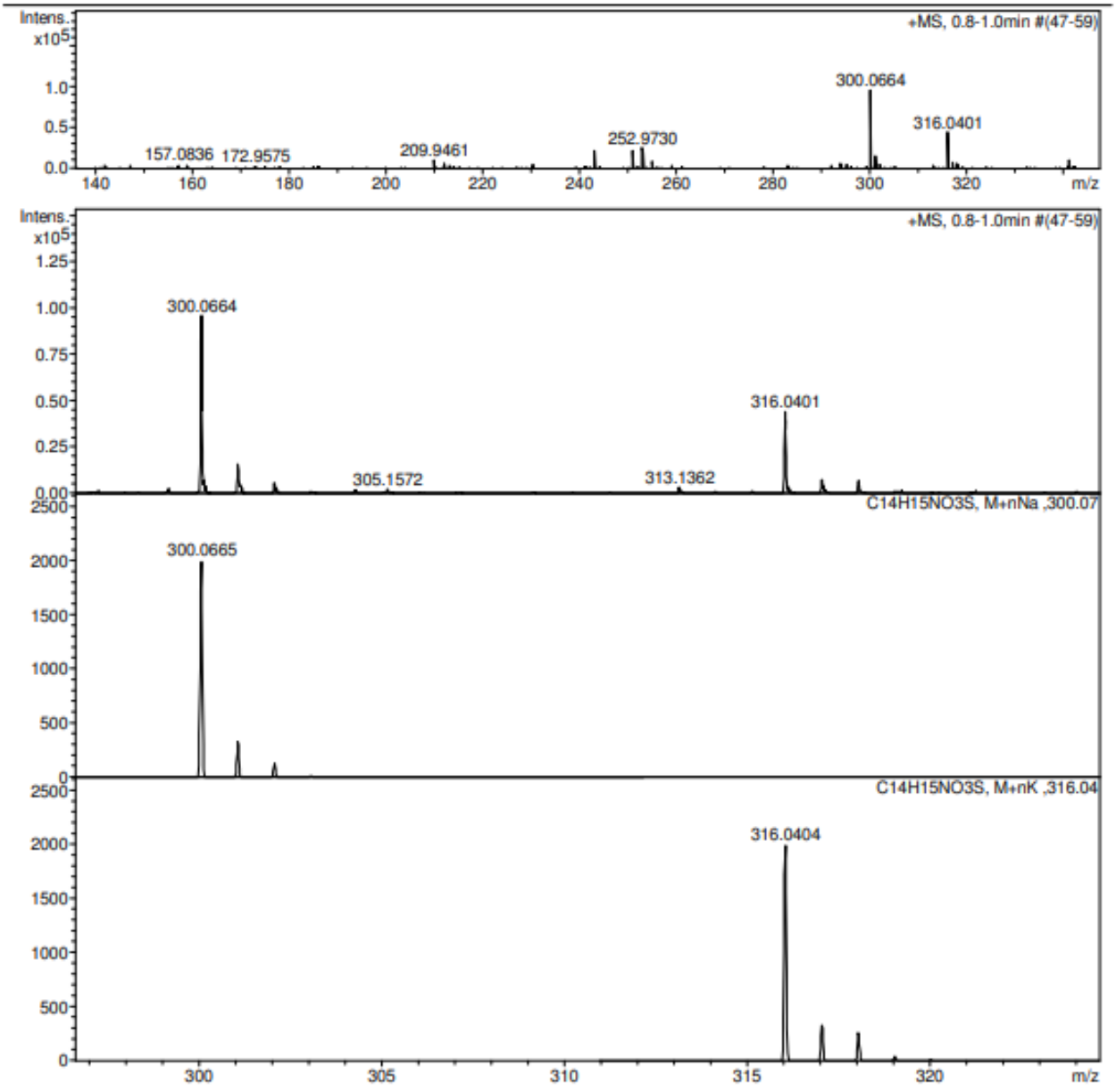
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1006009.d | Acquisition Date | 06.10.2022 10:57:52 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil477 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C14H15NO3S mH278.0845 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |




Bruker Compass DataAnalysis 4.0 printed: 06.10.2022 11:02:42 Page 1 of 1

HRMS spectrum of ethyl 2-(4-(*tert*-butyl)benzyl)-3-oxo-2-thiocyanatobutanoate, **2k**

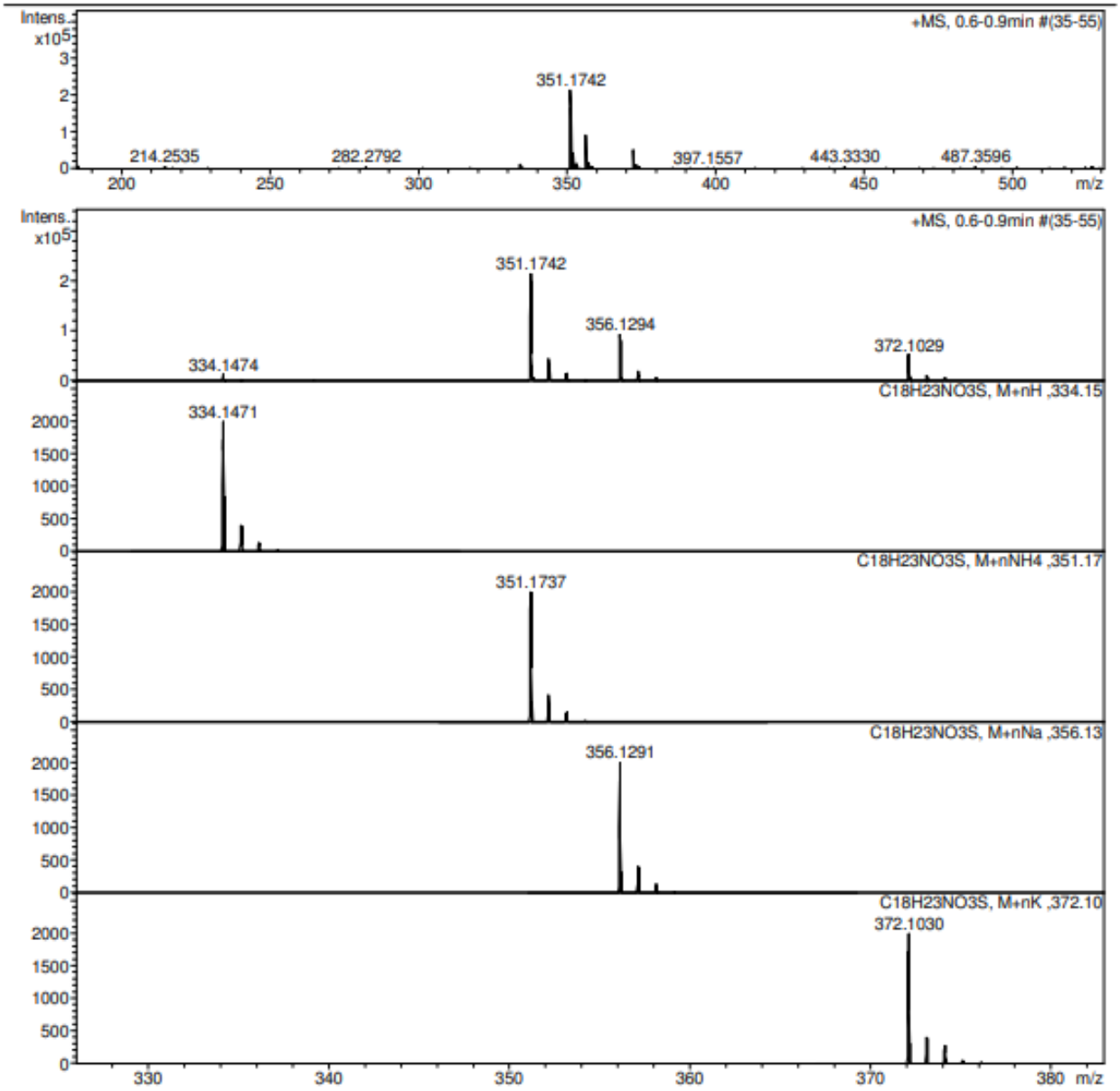
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1006006.d | Acquisition Date | 06.10.2022 10:36:02 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil410 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C18H23NO3S mH334.1471 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |




Bruker Compass DataAnalysis 4.0 printed: 06.10.2022 10:38:29 Page 1 of 1

HRMS spectrum of ethyl 2-(4-fluorobenzyl)-3-oxo-2-thiocyanatobutanoate, **2l**

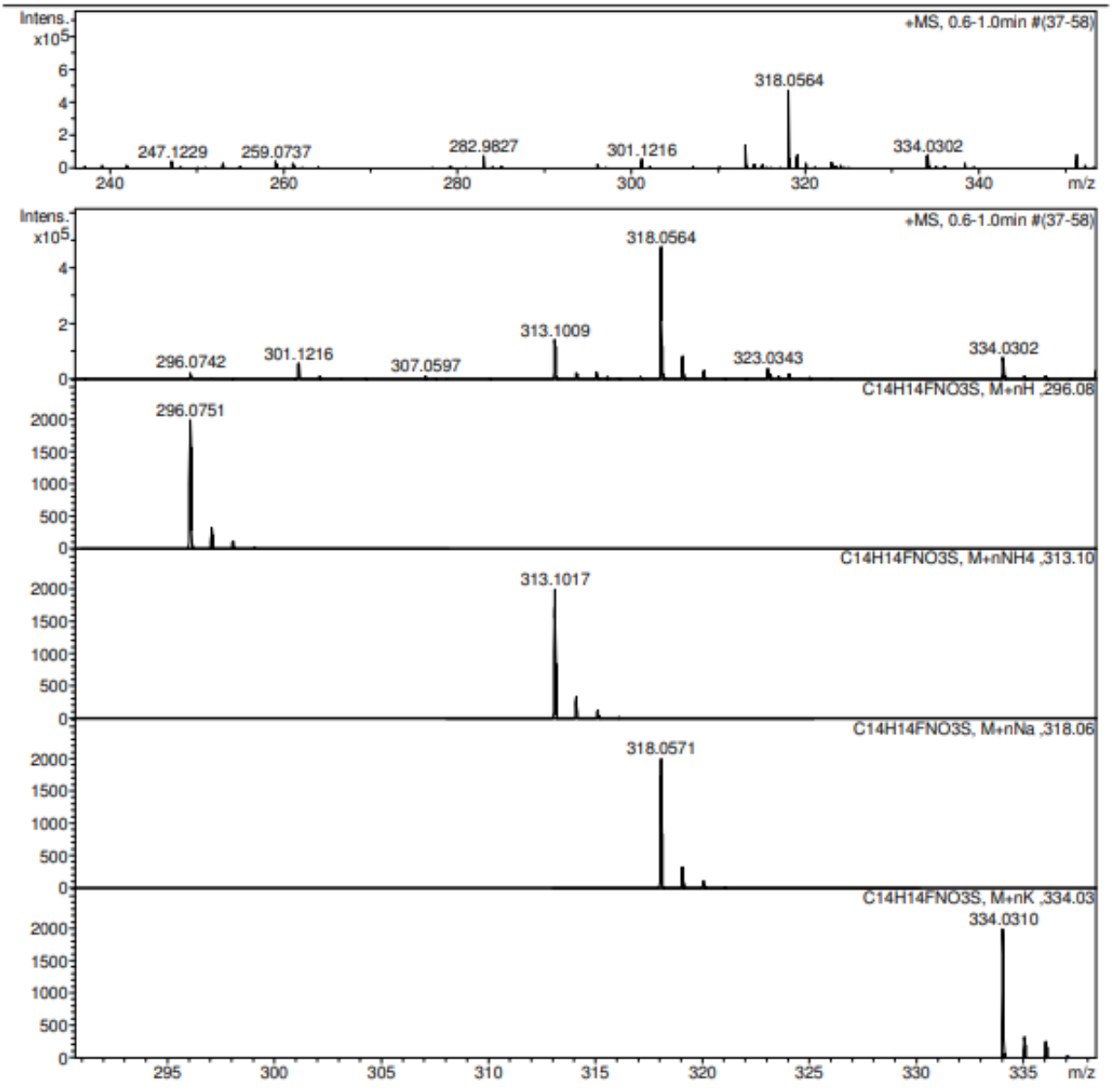
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1006008.d | Acquisition Date | 06.10.2022 10:50:08 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil456 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C14H14FNO3S mH296.0751 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |



HRMS spectrum of ethyl 2-acetyl-2-thiocyanatoundecanoate, **2o**

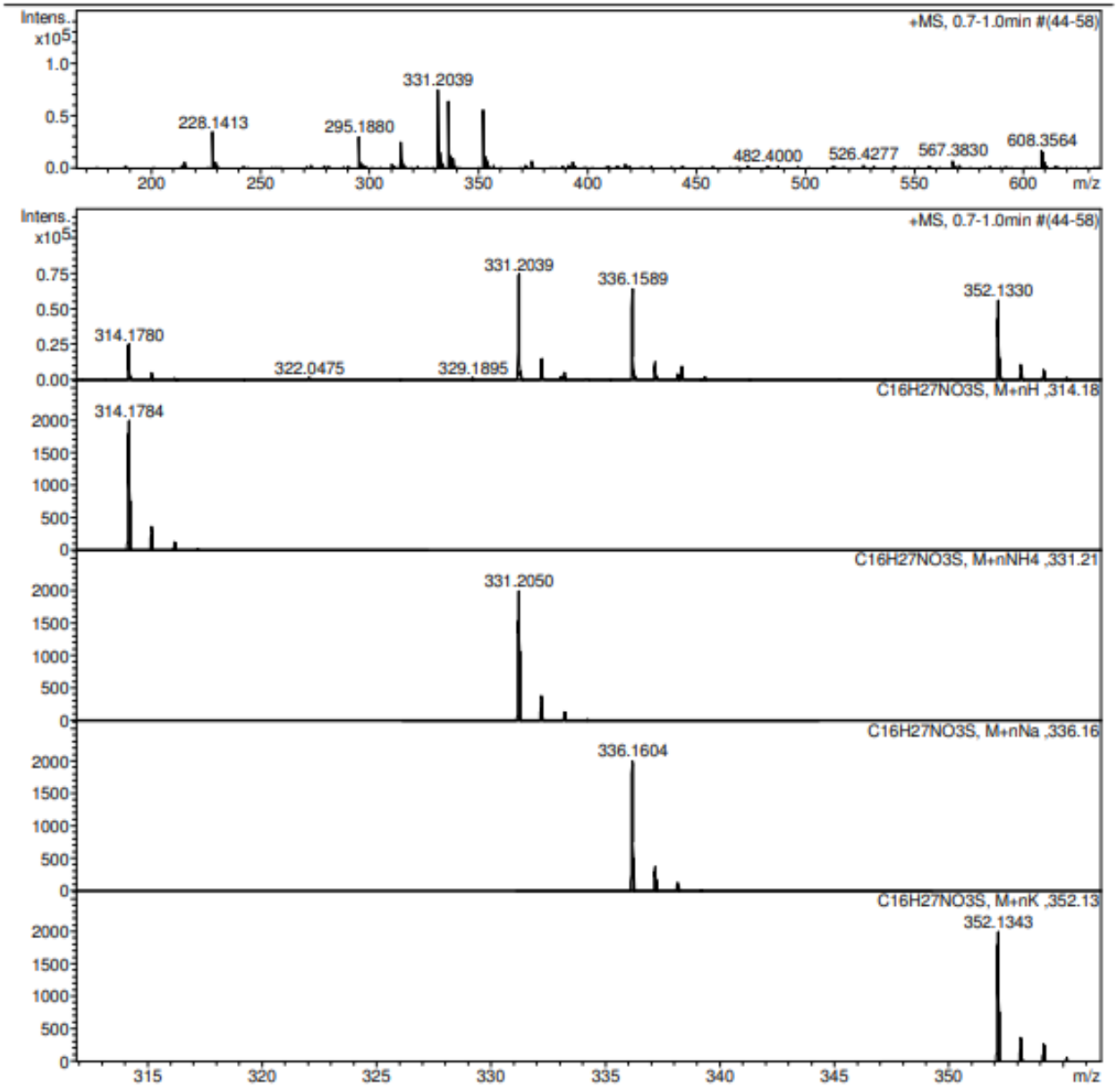
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1101023.d | Acquisition Date | 01.11.2022 15:23:10 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN SE-83 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C16H27NO3S mH314.1784 calibrant added, CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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HRMS spectrum of ethyl 2-acetyl-5-methyl-2-thiocyanatohexanoate, **2p**

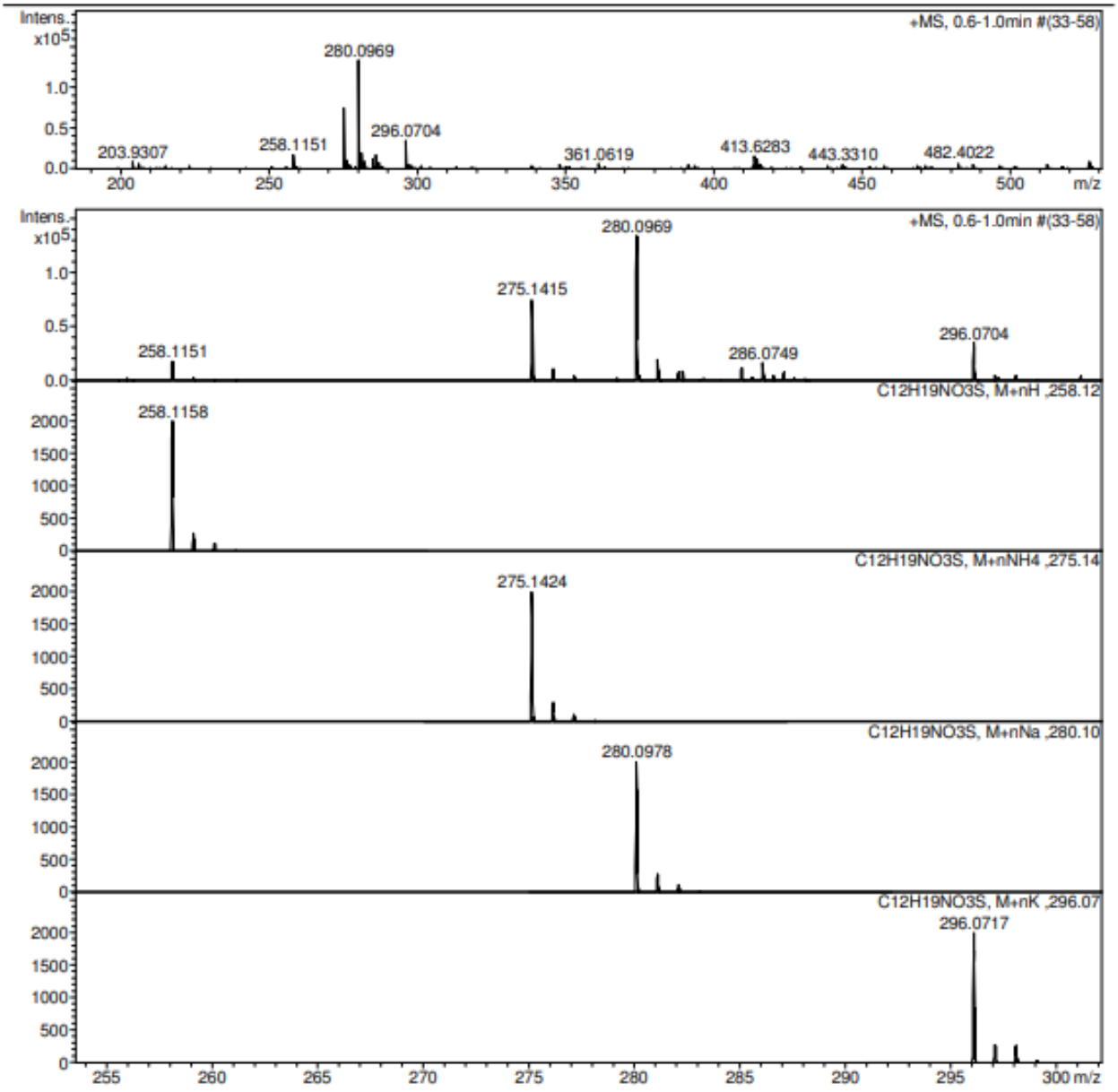
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1006005.d | Acquisition Date | 06.10.2022 10:25:10 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil384 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C12H19NO3S mH258.1158 clb added CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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HRMS spectrum of diethyl 2-acetyl-2-thiocyanatopentanedioate, **2q**

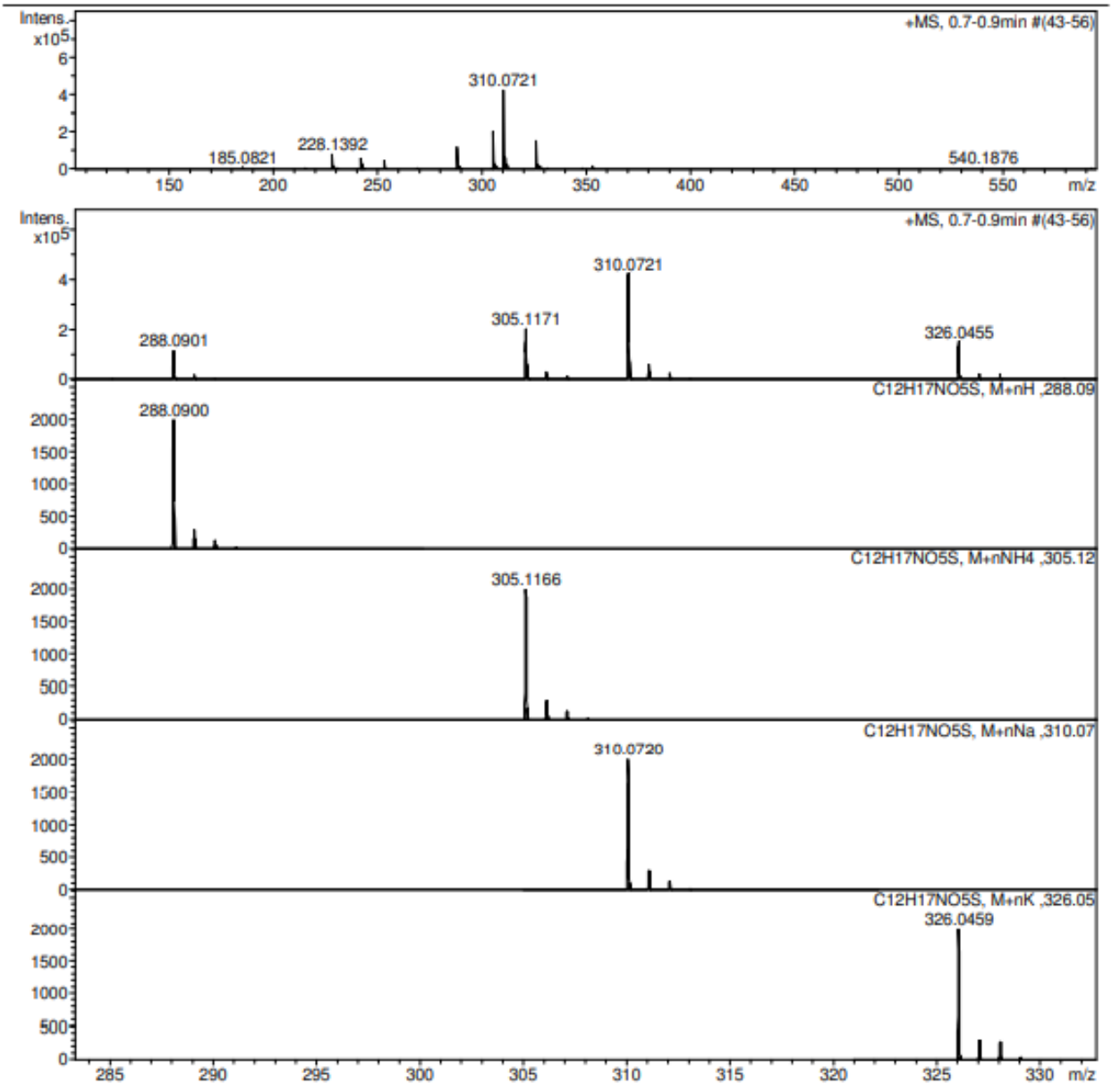
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Kolotyrkina\2022\Kirillov\1101022.d | Acquisition Date | 01.11.2022 15:17:29 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN SE-76 | Instrument / Ser# | micrOTOF 10248 |
| Comment | C12H17NO5S mH289.0900 calibrant added, CH3CN | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 2500 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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HRMS spectrum of ethyl 2-cyano-3-phenyl-2-thiocyanatopropanoate, **2s**

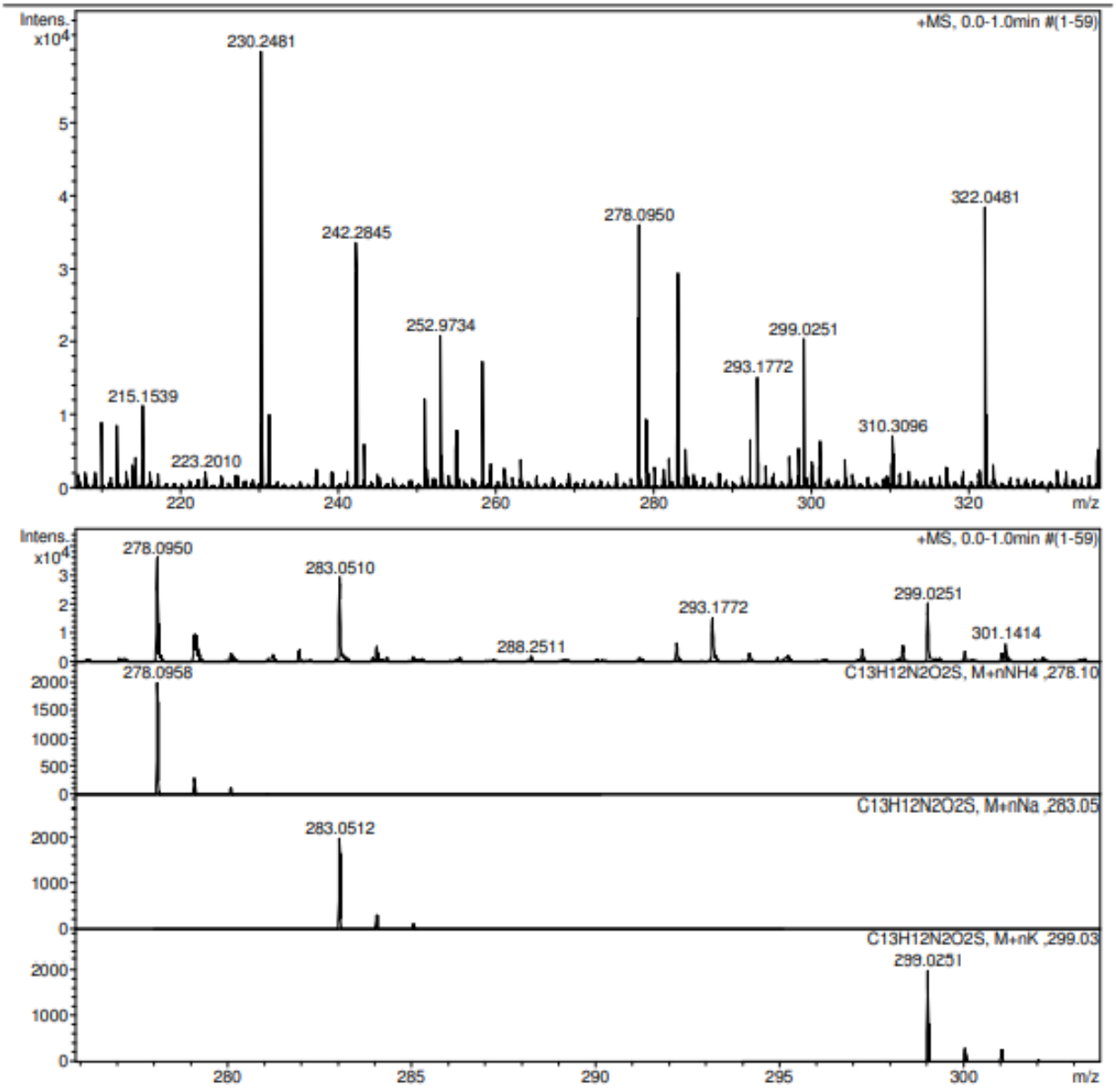
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\Chizhov\Terentiev\Kirillov\pil632_&clblow.d | Acquisition Date | 27.01.2023 16:36:52 |
| Method | tune_low.m | Operator | BDAL@DE |
| Sample Name | /TERN Pil632 | Instrument / Ser# | micrOTOF 10248 |
| Comment | CH3CN 100 %, dil. 20, calibrant added | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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