SUPPORTING INFORMATION

Electrochemical synthesis of CN-substituted imidazo[1,5-*a*]pyridines *via* cascade process using NH_4SCN as both electrolyte and non-trivial cyanating agent

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General materials and methods

^{1}H and ^{13}C NMR spectra were recorded on Bruker AVANCE II 300 spectrometer (300.13 and 75.48 MHz, respectively) in $CDCl_3$, DMSO-d_6, and CD_3CN. 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=7.26 ppm), ^{13}C ($CDCl_3$ δ=77.16 ppm); ^{1}H (DMSO-d_6 δ=2.50 ppm), ^{13}C (DMSO-d_6 δ=39.52 ppm); ^{1}H (CD_3CN δ=1.94 ppm), ^{13}C (CD_3CN δ=1.32 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). 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 ALUGRAM^{R} Xtra SIL G/UV_{254}). Column chromatography was performed using silica gel (0.040-0.060 mm, 60 A).

DMSO was distilled according to a standard procedure under CaH_2. NH_4SCN was dried under reduced pressure at 60 °C. DMF, DMA, CH_3CN, *p*-$TsOH \cdot H_2O$, pyridine, KI, Cs_2CO_3, $NaHCO_3$, DMAP, DBU, 2,6-lutidine, 2-pycoline, pyrazine, $NH_4OAc \cdot H_2O$, KSCN, NaSCN were purchased from commercial sources and were used as is.

Synthesis of starting compounds

Aldehydes **1a-d** and amines **2a-2r** were obtained from commercial suppliers and used without further purification**.** Imidazo[1,5-*a*]pyridine **7** [1] and *N*-benzyl-1-(pyridin-2-yl)methanimine **8** [2] were prepared according to the literature procedures.

Electrochemical cell

Glassy carbon and platinum plates from Russian commercial suppliers were used as electrodes (glassy carbon: SU-2000: TU 1916-027-27208846-01; platinum grade: AISI 304): The reactions were performed in a common chemical tube.

Before all electrochemical reactions, the electrodes were put into 5 M solution of KOH and this mixture was electrolyzed for 10 minutes at j = 200 mA/cm^2. After that, the polarity of electrodes was changed and the mixture was electrolyzed under these conditions again. Then the electrodes were washed with running water and then with acetone. All these procedures help to clean the electrodes from the impurities from the previous electrolysis.

The detailed electrochemical equipment was presented in our previous study.[3]

Determination of water content in distilled DMSO using Volumetric Karl Fischer titration.

Determination of water content in dimethyl sulfoxide (volumetric titration) was carried out accordance with the Pharmacopoeia of the Eurasian Economic Union, OFS.2.1.5.12 “Water: determination by a semi-micro method. Method A.

Reagents: solvent based on methanol ("Aqua M®-Solvent", TU2638-001-33699038-115-09 or of similar quality), K. Fischer titration reagent "HYDRANAL®-Titrant 2" ("Fluka" 34811 or of similar quality), hydranal Water Standart 10.0 for titration ("Fluka" 34849 or similar quality).

Titer setting (T): A methanol-based solvent was placed in the titration vessel and 1.0 ml of Hydranal Water Standart 10.0 was taken using disposable syringe. The syringe with water was weighted and injected into the titration cell. Then the syringe was weighted again and the mass of a sample Hydranal Water Standart was calculated based on the difference in the measuring results. Titration was carried out to the end point of titration. Based on results of titration and mass of a sample Hydranal Water Standart, the value of titre (T, mg/ml) was calculated according to the formula:

$$T = \frac{a_1 \times c_0}{V_1}$$

in which V_1 is the volume of titrant used for titration, mL;

a_1 is the mass of a sample of Hydranal Water Standart, in g;

c_0 is the water content in a sample of Hydranal Water Standart mg/g.

The value of titre was determined as the average value of at least three parallel determinations.

The test solution. Using a disposable syringe 0.5 mL of dimethyl sulfoxide was placed in titration vessels. Titration was carried out to the end point of titration.

Determination of water content in a sample, in percent, was calculated by the formula:

$$W = \frac{V \times T \times 100}{a \times 1000}$$

in which V is the volume of titrant used for titration, mL;

a_1 is the volume of sample, mL;

T is a titer, mg/mL.

According to the described procedure, at least three determinations were carried out. The average values of at least three parallel determinations were taken as the result of the analysis.

distilled DMSO according standard procedure under CaH_2

Sample weight, g	Water content in substance, %	Average water content in the substance, %	S^2	s	RSD,%
0,6250	0,0210	0,020	3,33E-07	0,0006	2,84
0,6225	0,0200				
0,7232	0,0200				

Experimental Procedures for Scheme 3

a) An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of (*E*)-*N*-benzyl-1-(pyridin-2-yl)methanimine (1.0 mmol, 196 mg, 1.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 µL, 0.5 eq.) without additives or with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.) in a 10 mL of DMSO was electrolyzed using constant current conditions at 70 ˚C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layer were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

b) An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 µL, 0.5 eq.) in a 10 mL DMSO with 3 Å MS (1.0 g); without additives or with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.), (5.0 mmol, 90 µL, 1.0 eq.) or (50.0 mmol, 900 µL, 50.0 eq.) was electrolyzed using constant current conditions at 70 ˚C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

Experimental Procedures for Table 1

Experimental Procedure for Table 1, entry 1-3

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NaSCN, KSCN or NH_4SCN (2.0 mmol, 2.0 eq.) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

Experimental Procedure for Table 1, entries 4-6

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and Cs_2CO_3, DBU or pyridine (1.0 mmol, 1.0 eq.) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

Experimental Procedure for Table 1, entry 7-11

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in a 10 mL DMSO, CH_3CN, DMF, PhCl or *n*-BuOH with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) (in the case of PhCl n-Bu_4NClO_4 (3 eq., 3.0 mmol) was added) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

Experimental Procedure for Table 1, entry 12

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2). The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in a 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) was stirred for 214 min. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was not detected.

Experimental Procedure for Table 1, entries 13-17

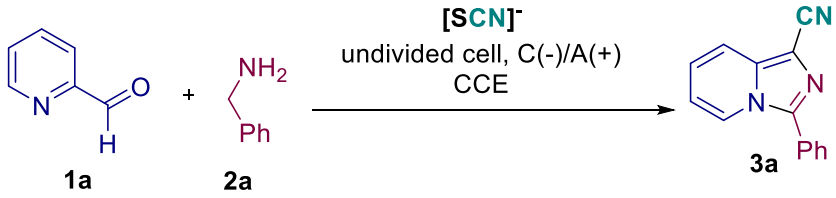
An undivided cell was equipped with platinum electrodes (3 cm^2) for each electrode (entry 13); a graphite plate anode (3 cm^2) and a platinum plate cathode (3 cm^2) (entry 14); a glassy carbon anode (3 cm^2) and a nickel foam cathode (3 cm^2) (entry 15); a glassy carbon anode (3 cm^2) and a copper plate cathode (3 cm^2) (entry 16) or a glassy carbon anode (3 cm^2) and stainless steel plate cathode (3 cm^2) (entry 17) and connected to a DC regulated power supply. The solution of

pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in a 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

Experimental Procedure for Table 1, entry 18

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in a 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA under an argon atmosphere. After that, the reaction mixture was diluted with H_2O (30 ml) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

Table S1. Detailed optimization of cyanide-functionalized imidazo[1,5-*a*]pyridine **3a** synthesis from **1a** and **2a** using thiocyanate salts as the cyanating agent.



1a **2a** **3a**

№	C(-)/A(+)	Molar ratio of **1a:2a:[SCN]**	Electrolyte	Additive (eq.)	Solvent	Current density, mA/cm^2	Current passed per **1a**, F/mol	Yield **3a**, %
1[b]	Pt/GC	1:2:4	NH_4SCN	H_2O (1), KI (2)	DMSO	20	6	30
2[b]	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	20	6	25
3	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	20	6	38
4[c]	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	20	6	26
5[d]	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	20	6	11
6	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	**30**	6	35
7	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	**10**	6	26
8	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	20	**8**	47
9	Pt/GC	1:2:4	NH_4SCN	H_2O (1)	DMSO	20	**9**	38
10	Pt/GC	**1:2:2**	NH_4SCN	H_2O (1)	DMSO	20	8	55
11	Pt/GC	**1:2:1**	NH_4SCN	H_2O (1)	DMSO	20	8	41
12	Pt/GC	1:2:2	**KSCN**	H_2O (1)	DMSO	20	8	10
13	Pt/GC	1:2:2	**NaSCN**	H_2O (1)	DMSO	20	8	13
14	Pt/GC	1:2:2	NH_4SCN	$TsOH{\cdot}H_2O$ (2), H_2O (1)	DMSO	20	8	16
15	Pt/GC	**1:1:2**	NH_4SCN	H_2O (1)	DMSO	20	8	46
16	Pt/GC	**1:3:2**	NH_4SCN	H_2O (1)	DMSO	20	8	48
19	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **Cs_2CO_3 (1)**	DMSO	20	8	9
20	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **$NaHCO_3$ (1)**	DMSO	20	8	23
21	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **Py (1)**	DMSO	20	8	63
22	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **DMAP (1)**	DMSO	20	8	52
23	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **6-lutidine (1)**	DMSO	20	8	38
24	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **2-picoline (1)**	DMSO	20	8	61
25	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **DBU (1)**	DMSO	20	8	42
26	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **Pyrazine (1)**	DMSO	20	8	37
27	Pt/GC	1:2:2	NH_4SCN	H_2O (1), **Py (0.5)**	DMSO	20	8	63
28	Pt/GC	1:2:2	NH_4SCN	Py (0.5)	**DMSO**	20	8	54
29	Pt/GC	1:2:2	NH_4SCN	**H_2O (1)**,	**DMSO**	20	8	63

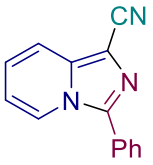
				Py (0.5)				
30	Pt/GC	1:2:2	NH_4SCN	**H_2O (5)**, Py (0.5)	**DMSO**	20	8	57
31	Pt/GC	1:2:2	NH_4SCN	**H_2O (50)**, Py (1)	**DMSO**	20	8	42
32	Pt/GC	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	**CH_3CN**	20	8	23
33	Pt/GC	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	**DMF**	20	8	26
34	Pt/GC	1:2:2	NH_4SCN	H_2O (1), Py (0.5), n-Bu_4NClO_4 (3)	**PhCl**	20	8	traces
35	Pt/GC	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	***n*-BuOH**	20	8	27
36[e]	Pt/GC	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	-	-	-
37	Pt/GC	**2:1:1**	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	24
38	**Pt/Pt**	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	61
39	**Pt/C**	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	49
40	**Ni(f)/GC**	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	43
41	**Cu/GC**	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	27
42	**SS/GC**	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	53
43[f]	Pt/GC	1:2:2	NH_4SCN	H_2O (1), Py (0.5)	DMSO	20	8	48

[a] **General reaction conditions:** undivided cell, plate anode / plate cathode (3 cm^2), constant current, **1a** (1.0 mmol, 107.0 mg), **2a** (2 mmol, 214.4 mg), **3a** (4 mmol), solvent (10.0 mL), 70 °C, air atmosphere. [b] 100 °C, [c] 50 °C, [d] 20-25 °C, [e] without electricity, [f] under Ar.

General Experimental Procedure for Scheme 4.

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehydes **1a-d** (1.0 mmol, 1.0 eq.), amine **2a-r** (2.0 mmol, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in a 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) was electrolyzed using constant current conditions at 70 ˚C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Products **3a-q, 3s-u** were isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1). Product **3r** was not detected.

3-Phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3a [4]



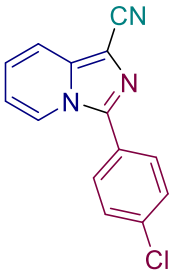
Yield 63% (138 mg, 0.63 mmol). White solid. mp = 133-134 ˚C (lit. [4] mp = 132-133 ˚C). PE/EtOAc = from 8:1 to 2:1 as eluent, R_f = 0.18 (PE/EtOAc = 5:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 8.34 (d, *J* = 7.2 Hz, 1H), 7.80 – 7.66 (m, 3H), 7.60 – 7.44 (m, 3H), 7.21 – 7.08 (m, 1H), 6.83 (t, *J* = 6.9 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 140.1, 137.7, 130.1, 129.4, 128.5, 128.4, 124.7, 123.1, 117.4, 115.5, 115.0, 103.6.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{14}H_{10}N_3]^+$: 220.0869. Found: 220.0873.

3-(4-Chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3b [4]

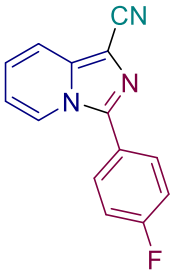


Yield 62% (157 mg, 0.62 mmol). White solid. mp = 205-206 ˚C (lit. [4] mp = 204-205 ˚C). PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.58 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.62 (d, *J* = 6.8 Hz, 1H), 8.10 – 7.77 (m, 3H), 7.76 – 7.49 (m, 2H), 7.49 – 7.22 (m, 1H), 7.20 – 6.85 (m, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 138.6, 137.6, 134.5, 130.3, 129.2, 127.0, 126.2, 124.3, 116.5, 115.6, 115.5, 101.6.

3-(4-Fluorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3c [4]



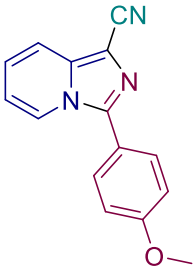
Yield 56% (132 mg, 0.56 mmol). White solid. mp = 193-194 ˚C (lit. [4] mp = 191-193 ˚C).

PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.36 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.56 (d, *J* = 7.2 Hz, 1H), 7.95 – 7.80 (m, 3H), 7.49 – 7.29 (m, 3H), 7.02 (t, *J* = 6.8 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 164.4 (d, *J* = 247.8 Hz), 138.8, 137.5, 131.0 (d, *J* = 8.4 Hz), 126.1, 124.6 (*J* = 3.3 Hz), 124.2, 116.4, 116.2 (d, *J* = 21.9 Hz), 115.6, 115.4, 101.4.

3-(4-Methoxyphenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3d [4]

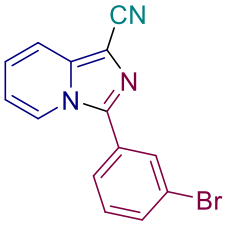


Yield 55% (137 mg, 0.55 mmol). White solid. mp = 131-133 °C (lit. [4] mp = 129-131 °C). PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.42 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.54 (d, *J* = 7.2 Hz, 1H), 7.83 (d, *J* = 9.1 Hz, 1H), 7.76 (d, *J* = 8.7 Hz, 2H), 7.32 (dd, *J* = 9.1, 6.6 Hz, 1H), 7.14 (d, *J* = 8.7 Hz, 2H), 7.00 (t, *J* = 6.6 Hz, 1H), 3.86 (s, 3H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 160.3, 139.7, 137.3, 130.0, 125.8, 124.1, 120.4, 116.4, 115.8, 115.2, 114.5, 101.1, 55.4.

3-(3-Bromophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3e [4]

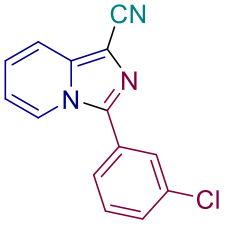


Yield 44% (131 mg, 0.44 mmol). White solid. mp = 200-201 °C (lit. [4] mp = 198-200 °C). PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.30 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 8.34 (d, *J* = 7.2 Hz, 1H), 7.93 (t, *J* = 1.7 Hz, 1H), 7.79 – 7.60 (m, 3H), 7.43 (t, *J* = 7.9 Hz, 1H), 7.19 (dd, *J* = 9.1, 6.5 Hz, 1H), 6.90 (t, *J* = 6.5 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 138.5, 137.9, 133.2, 131.5, 130.9, 130.4, 127.0, 124.9, 123.5, 122.9, 117.7, 115.4, 115.2, 104.1.

3-(3-Chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3f



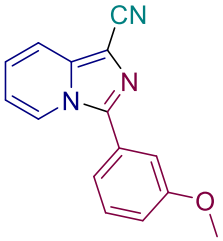
Yield 56% (142 mg, 0.56 mmol). White solid. mp = 202-203 °C. PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.32 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.65 (d, *J* = 7.1 Hz, 1H), 7.93 – 7.78 (m, 3H), 7.66 – 7.58 (m, 2H), 7.44 – 7.33 (m, 1H), 7.06 (t, *J* = 6.8 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, DMSO-d_6, δ): 138.2, 137.7, 133.8, 131.0, 130.1, 129.7, 128.2, 127.1, 126.4, 124.4, 116.4, 115.6, 115.5, 101.7.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{14}H_9ClN_3]^+$: 254.0480. Found: 254.0487.

3-(3-Methoxyphenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3g



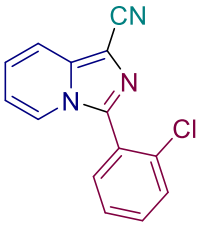
Yield 57% (142 mg, 0.57 mmol). White solid. mp = 158-160 °C. PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.36 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.63 (d, *J* = 7.2 Hz, 1H), 7.86 (d, *J* = 9.1 Hz, 1H), 7.51 (t, *J* = 7.9 Hz, 1H), 7.44 – 7.32 (m, 3H), 7.18 – 7.09 (m, 1H), 7.02 (t, *J* = 7.3 Hz, 1H), 3.84 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, DMSO-d_6, δ): 159.6, 139.5, 137.6, 130.3, 129.3, 126.1, 124.3, 120.6, 116.4, 115.9, 115.7, 115.4, 113.6, 101.4, 55.3.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{15}H_{12}N_3O]^+$: 250.0975. Found: 250.0982.

3-(2-Chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3h



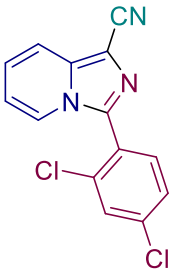
Yield 58% (147 mg, 0.58 mmol). Yellow solid. mp = 165-167 °C. PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.42 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 7.72 (t, *J* = 7.8 Hz, 2H), 7.60 – 7.36 (m, 4H), 7.25 – 7.13 (m, 1H), 6.84 (t, *J* = 7.3 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 137.5, 137.2, 134.2, 133.2, 131.9, 130.2, 127.6, 127.4, 125.0, 123.8, 117.0, 115.3, 114.6, 103.1.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{14}H_9ClN_3]^+$: 254.0480. Found: 254.0484.

3-(2,4-Dichlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3i



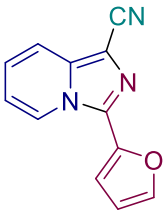
Yield 49% (141 mg, 0.49 mmol). White solid. mp = 165-167 ˚C. PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.32 (PE/EtOAc = 5:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.14 (d, *J* = 7.1 Hz, 1H), 7.97 – 7.88 (m, 2H), 7.79 – 7.62 (m, 2H), 7.41 (dd, *J* = 9.1, 6.7 Hz, 1H), 7.05 (t, *J* = 6.7 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 137.0, 136.3, 136.1, 134.7, 134.5, 129.7, 128.1, 126.5, 126.1, 124.6, 116.3, 115.4, 115.4, 101.3.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for [$C_{14}H_8Cl_2N_3$]$^+$: 288.0090. Found: 288.0086.

3-(Furan-2-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3j [4]

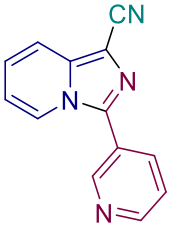


Yield 34% (71 mg, 0.34 mmol). White solid. mp = 145-146 ˚C. (lit. [4] mp = 146-147 ˚C). PE/EtOAc = from 3:1 to 2:1 as eluent, R_f = 0.14 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 8.83 (d, *J* = 7.2 Hz, 1H), 7.70 (d, *J* = 9.1 Hz, 1H), 7.62 (s, 1H), 7.23 – 7.07 (m, 2H), 6.91 (t, *J* = 6.9 Hz, 1H), 6.62 (dd, *J* = 3.3, 1.7 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 144.8, 143.2, 137.3, 132.1, 124.8, 124.7, 117.3, 115.4, 115.1, 112.2, 111.0, 103.9.

3-(Pyridin-3-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3k



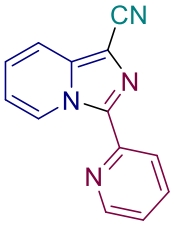
Yield 40% (88 mg, 0.40 mmol). White solid. mp = 207-208 ˚C. PE/EtOAc = from 3:1 to 2:1 as eluent, R_f = 0.27 (EtOAc).

^{1}H NMR (300.13 MHz, CD_3CN, δ): 9.00 (d, *J* = 1.6 Hz, 1H), 8.72 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.44 (d, *J* = 7.2 Hz, 1H), 8.16 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.82 – 7.72 (m, 1H), 7.61 – 7.50 (m, 1H), 7.35 – 7.23 (m, 1H), 6.95 (t, *J* = 7.4 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, CD_3CN, δ): 151.5, 150.2, 139.1, 138.5, 136.8, 126.7, 126.1, 124.8, 118.3, 117.7, 116.2, 109.1, 103.8.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{13}H_9N_4]^+$: 221.0822. Found: 221.0821.

3-(Pyridin-2-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3l



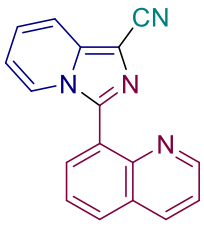
Yield 54% (119 mg, 0.54 mmol). White solid. mp = 201-203 °C. PE/EtOAc = from 5:1 to 2:1 as eluent, R_f = 0.5 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 10.13 (d, *J* = 7.3 Hz, 1H), 8.66 (d, *J* = 5.6 Hz, 1H), 8.36 (d, *J* = 8.0 Hz, 1H), 7.84 (td, *J* = 8.0, 1.8 Hz, 1H), 7.76 (d, *J* = 9.1 Hz, 1H), 7.37 – 7.19 (m, 2H), 6.96 (t, *J* = 6.9 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 149.8, 148.4, 138.6, 137.1, 136.9, 127.9, 125.6, 123.3, 122.8, 116.8, 115.5, 115.2, 103.6.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{13}H_9N_4]^+$: 221.0822. Found: 221.0830.

3-(Quinolin-8-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3m



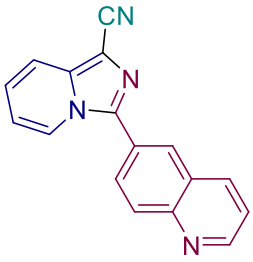
Yield 48% (130 mg, 0.48 mmol). White solid. mp = 262-263 °C (decomp.). PE/EtOAc 1:1 as eluent, R_f = 0.11 (EtOAc).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.88 – 8.80 (m, 1H), 8.57 (dd, *J* = 8.4, 1.6 Hz, 1H), 8.34 – 8.24 (m, 1H), 8.08 (dd, *J* = 7.1, 1.3 Hz, 1H), 7.91 (d, *J* = 9.1 Hz, 1H), 7.88 – 7.76 (m, 2H), 7.66 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.43 – 7.32 (m, 1H), 6.89 (t, *J* = 7.3 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75.48 MHz, DMSO-d_6, δ): 151.2, 145.4, 139.2, 137.3, 137.0, 131.0, 128.4, 128.2, 127.1, 126.6, 126.1, 125.8, 122.2, 116.0, 115.9, 114.2, 101.0.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{17}H_{11}N_4]^+$: 271.0978. Found: 271.0988.

3-(Quinolin-6-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3n



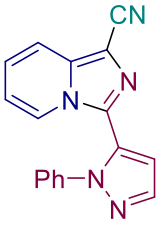
Yield 44% (119 mg, 0.44 mmol). White solid. mp = 243-245 °C (decomp.). PE/EtOAc 1:1 as eluent, R_f = 0.13 (EtOAc).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 9.02 – 8.95 (m, 1H), 8.88 – 8.79 (m, 1H), 8.56 – 8.46 (m, 2H), 8.22 – 8.15 (m, 2H), 7.90 (d, *J* = 8.7 Hz, 1H), 7.68 – 7.59 (m, 1H), 7.45 – 7.34 (m, 1H), 7.14 – 7.05 (m, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 151.7, 147.7, 139.0, 137.8, 136.7, 134.6, 129.8, 129.3, 127.9, 127.8, 126.3, 126.0, 124.5, 122.3, 116.5, 115.6, 101.9.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{17}H_{11}N_4]^+$: 271.0978. Found: 271.0980.

3-(1-Phenyl-1H-pyrazol-5-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3o



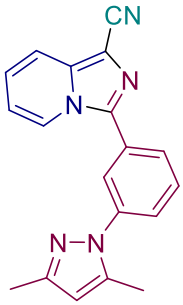
Yield 54% (154 mg, 0.54 mmol). White solid. mp = 168-170 °C. PE/EtOAc 3:1 to 1:1 as eluent, R_f = 0.20 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.26 (d, *J* = 7.1 Hz, 1H), 8.01 (d, *J* = 1.8 Hz, 1H), 7.88 (d, *J* = 9.1 Hz, 1H), 7.44 – 7.28 (m, 4H), 7.32 – 7.19 (m, 2H), 7.13 (d, *J* = 1.8 Hz, 1H), 7.01 (t, *J* = 6.8 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 140.8, 139.3, 137.1, 129.9, 129.3, 129.1, 127.9, 126.8, 124.3, 123.7, 116.2, 115.7, 115.2, 111.1, 101.8.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{17}H_{12}N_5]^+$: 286.1087. Found: 286.1084.

3-(3-(3,5-Dimethyl-1*H*-pyrazol-1-yl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3p



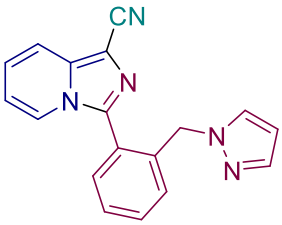
Yield 57% (179 mg, 0.57 mmol). White solid. mp = 187-188 ˚C. PE/EtOAc 2:1 to 1:1 as eluent, R_f = 0.10 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): δ 8.64 (d, J = 7.2 Hz, 1H), 8.05 – 7.78 (m, 3H), 7.70 (d, J = 5.2 Hz, 2H), 7.38 (dd, J = 9.0, 6.5 Hz, 1H), 7.07 (t, J = 6.9 Hz, 1H), 6.11 (s, 1H), 2.38 (s, 3H), 2.20 (s, 3H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 148.3, 140.3, 139.5, 138.9, 137.7, 130.0, 129.0, 126.6, 126.3, 124.9, 124.3, 123.6, 116.5, 115.6, 115.6, 107.7, 101.6, 13.3, 12.3.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{19}H_{16}N_5]^+$: 314.1400. Found: 314.1393.

3-(2-((1H-Pyrazol-1-yl)methyl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3q



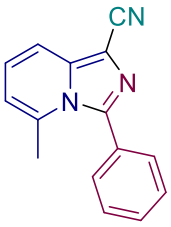
Yield 66% (198 mg, 0.66 mmol). White solid. mp = 157-158 ˚C. PE/EtOAc 2:1 to 1:1 as eluent, R_f = 0.10 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, DMSO-d_6, δ): 8.01 (d, J = 7.1 Hz, 1H), 7.86 (d, J = 9.1 Hz, 1H), 7.69 – 7.44 (m, 4H), 7.41 – 7.29 (m, 1H), 7.30 – 7.20 (m, 2H), 6.93 (t, J = 6.8 Hz, 1H), 6.06 (t, J = 2.0 Hz, 1H), 5.37 (s, 2H).

^{13}C{^{1}H} NMR (75.48 MHz, DMSO-d_6, δ): 139.0, 138.1, 137.7, 137.0, 130.5, 130.3, 130.1, 129.4, 128.2, 126.5, 126.2, 124.0, 116.1, 115.9, 115.0, 105.1, 100.9, 52.3.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{18}H_{14}N_5]^+$: 300.1244. Found: 300.1244.

5-Methyl-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3s [4]

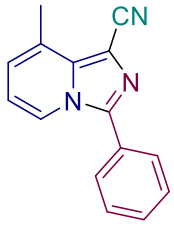


Yield 48% (112 mg, 0.48 mmol). White solid. mp = 143-144 ˚C (lit. [4] mp = 141-143 ˚C). PE/EtOAc 5:1 to 2:1 as eluent, R_f = 0.44 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 7.54 (d, J = 9.0 Hz, 1H), 7.51 – 7.35 (m, 5H), 7.04 (dd, J = 9.0, 6.7 Hz, 1H), 6.53 (d, J = 6.7 Hz, 1H), 2.12 (s, 3H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 140.7, 138.9, 135.3, 131.9, 130.9, 129.9, 127.7, 125.0, 115.7, 115.5, 114.9, 102.5, 21.7.

8-Methyl-3-phenylimidazo[1,5-a]pyridine-1-carbonitrile, 3t



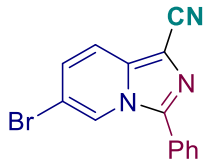
Yield 47% (109 mg, 0.47 mmol). White solid. mp = 190-192 ˚C. PE/EtOAc 5:1 to 2:1 as eluent, R_f = 0.4 (PE/EtOAc = 2:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): δ 8.20 (d, *J* = 7.1 Hz, 1H), 7.73 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.60 – 7.46 (m, 3H), 6.87 (d, *J* = 6.7 Hz, 1H), 6.73 (t, *J* = 6.9 Hz, 1H), 2.73 (s, 3H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 140.3, 137.6, 130.0, 129.2, 128.7, 128.6, 124.0, 120.9, 117.0, 115.1, 103.1, 18.2.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{15}H_{12}N_3]^+$: 234.1026. Found: 234.1035.

6-Bromo-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3u [4]

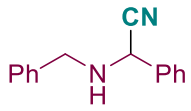


Yield 43% (198 mg, 0.43 mmol). White solid. mp = 176-177 ˚C (lit. [4] mp = 177-179 ˚C). PE/EtOAc 5:1 to 2:1 as eluent, R_f = 0.24 (PE/EtOAc = 5:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 8.46 (s, 1H), 7.78 – 7.68 (m, 2H), 7.67 – 7.53 (m, 4H), 7.19 (d, *J* = 8.5 Hz, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 140.2, 135.9, 130.5, 129.6, 128.6, 128.1, 127.9, 122.9, 118.1, 114.8, 110.6, 105.0.

2-(Benzylamino)-2-phenylacetonitrile, 4 [5]



Yield 15% (34 mg, 0.15 mmol). Yellow oil. PE/EtOAc 10:1 to 5:1 as eluent, R_f = 0.23 (n-pentane/EtOAc = 20:1).

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 7.55 (d, *J* = 6.1 Hz, 2H), 7.44 – 7.27 (m, 8H), 4.76 (s, 1H), 4.08 (d, *J* = 12.9 Hz, 1H), 3.97 (d, *J* = 12.9 Hz, 1H), 1.88 (br. s, 1H).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 138.3, 134.9, 129.2, 129.1, 128.8, 128.5, 127.8, 127.4, 118.9, 53.6, 51.4.

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{15}H_{15}N_2]^+$: 223.1230. Found: 223.1222.

Experimental Procedure for Scale-Up Electrosynthesis.

Gram scale synthesis was carried out in a sandwich-type cell. An undivided cell was equipped with a glassy carbon anode (15 cm^2) (total surface area was 30 cm^2) and two platinum plate cathode (5 cm^2) (total surface area was 10 cm^2) and connected to a DC regulated power supply (cathodes were wired in parallel). The solution of pyridine-2-carboxaldehyde **1a** (9.3 mmol, 1.0 g, 1.0 eq.), amine **2a** (18.6 mmol, 2.0 g, 2.0 eq.), NH_4SCN (18.6 mmol, 1.41 g, 2.0 eq.), and pyridine (4.6 mmol, 363 mg, 0.5 eq.) in a 90 mL of DMSO with H_2O (9.3 mmol, 167.0 μL, 1.0 eq.) was electrolyzed using constant current conditions at 70 ˚C under magnetic stirring for 3 h 20 min with I = 600 mA (j_{anode} = 20 mA/cm^2). After that, the reaction mixture was diluted with H_2O (250 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×250 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** 53% (1080 mg, 4.93 mmol) was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

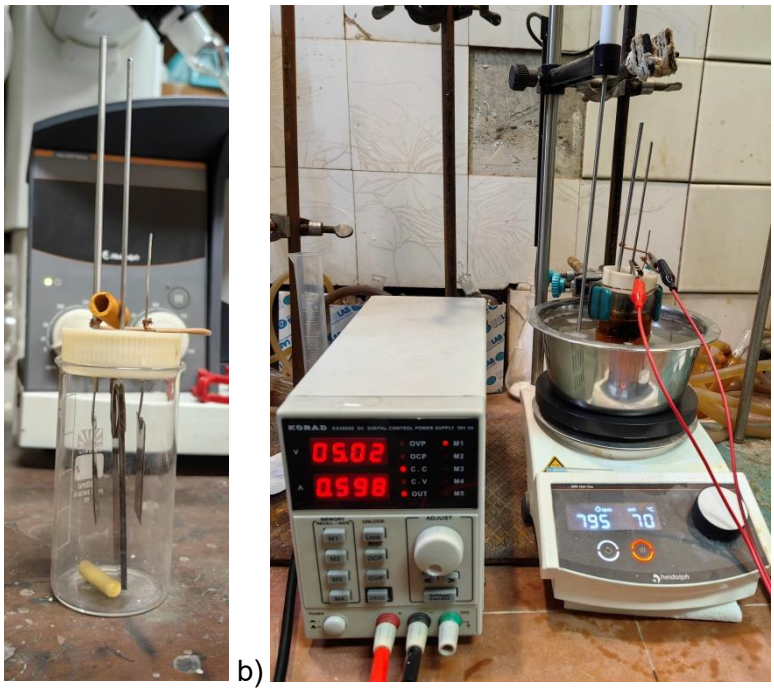


Figure S1. Equipment employed for gram-scale synthesis in the present work
a) a sandwich-type cell; b) the model reaction for gram-scale synthesis.

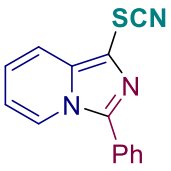
Experimental Procedures for Scheme 5.

a) To generate thiocyanogen, bromine (2.0 mmol, 319 mg, 103 μL) was added to the solution of sodium thiocyanate (4.0 mmol, 324 mg) in DMSO (3 mL) at 20-25 °C under stirring. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in a 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.) was added to the resulting solution of thiocyanogen at 20-25 °C under stirring. The reaction mixture was stirring for 214 min. at 70 °C. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL).

Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Products **5** and **6** were isolated by chromatography on SiO_2 (PE:EtOAc = from 4:1 to 2:1). Product **3a** was not detected.

b) An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of 3-phenylimidazo[1,5-*a*]pyridine **7** (1.0 mmol, 194 mg, 1.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 µL, 0.5 eq.) in a 10 mL of DMSO with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **5** was isolated as a white solid. mp = 107-108 °C. (lit. [5] mp = 105-106 °C). The isolated yield of **5** was 42% (106 mg, 0.42 mmol, PE:EtOAc = from 4:1 to 2:1 as an eluent). R_f = 0.26 (PE/EtOAc = 5:1).

3-Phenyl-1-thiocyanatoimidazo[1,5-*a*]pyridine, 5 [5]



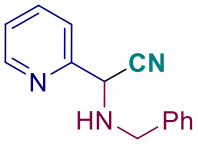
^1H NMR (300.13 MHz, $CDCl_3$, δ): 8.32 (d, *J* = 7.1 Hz, 1H), 7.81 – 7.68 (m, 3H), 7.61 – 7.46 (m, 3H), 7.09 (dd, *J* = 8.9, 6.7 Hz, 1H), 6.78 (t, *J* = 7.1 Hz, 1H).

$^{13}C\{^1H\}$ NMR (75.48 MHz, $CDCl_3$, δ): 140.3, 135.4, 129.8, 129.3, 128.8, 128.4, 123.4, 122.8, 117.4, 114.5, 110.6, 108.2.

HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{14}H_{10}N_3S]^+$: 252.0590. Found: 252.0600.

c) An oven-dried reaction vessel was charged with *N*-benzyl-1-(pyridin-2-yl)methanimine **8** (1.0 mmol, 196 mg, 1.0 eq.) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.). TMSCN (2.0 mmol, 259 µL, 2.0 eq.) was added, and the mixture was further stirred at room temperature for 6 h. After completion of the reaction (TLC), the reaction mixture was quenched with water (30 mL) and extracted with ethyl acetate (2×30 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **9** was isolated by chromatography on SiO_2 PE/EtOAc 5:1 to 2:1) as an yellow oil. The isolated yield of **9** was 60% (134 mg, 0.60 mmol).

2-(Benzylamino)-2-(pyridin-2-yl)acetonitrile, 9 [4]



^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 8.63 (d, *J* = 4.3 Hz, 1H), 7.75 (t, *J* = 7.7 Hz, 1H), 7.52 – 7.27 (m, 7H), 4.81 (s, 1H), 4.13 (d, *J* = 12.9 Hz, 1H), 3.99 (d, *J* = 12.9 Hz, 1H), 2.51 (br. s, 1 H).
^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 153.9, 150.0, 138.1, 137.5, 128.8, 128.6, 127.8, 124.0, 122.2, 118.3, 55.1, 51.6.

d) An oven-dried reaction vessel was charged with **9** (0.5 mmol, 112 mg, 1.0 eq) in DMSO (10 mL) with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.), and the mixture was stirred at 70 °C for 3.5 h. After completion of the reaction (TLC), the reaction mixture was quenched with water (30 mL) and extracted with ethyl acetate (2×30 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Products **3a** and **10** were isolated by chromatography on SiO_2 PE/EtOAc 5:1 to 2:1). The isolated yield **3a** was 60% (134 mg, 0.60 mmol). Product **10** was isolated as an yellow oil. The isolated yield **10** was 50% (53 mg, 0.25 mmol). (R_f = 0.33 (PE/EtOAc = 2:1).

N-benzylpicolinamide, 10 [6]

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): δ 8.57 – 8.48 (m, 1H), 8.37 (br.s, 1H), 8.29 – 8.19 (m, 1H), 7.86 (td, *J* = 7.7, 1.7 Hz, 1H), 7.44 (dd, *J* = 4.8, 1.2 Hz, 1H), 7.39-7.33 (m, 4H), 7-33-7.27 (m, 1H), 4.68 (d, *J* = 6.1 Hz, 2H).
^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 164.4, 150.0, 148.2, 138.4, 137.5, 128.9, 128.0, 127.6, 126.4, 122.5, 43.7.
HRMS (ESI-TOF) m/z $[M+H]^+$. Calcd for $[C_{13}H_{13}N_2O]^+$: 213.1022. Found: 213.1029.

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of 2-(benzylamino)-2-(pyridin-2-yl)acetonitrile**, 9** (0.5 mmol, 112 mg, 1.0 eq.), NH_4SCN (0.5 mmol, 38 mg, 1.0 eq.) and pyridine (0.25 mmol, 19 mg, 20.0 µL, 0.5 eq.) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 60 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

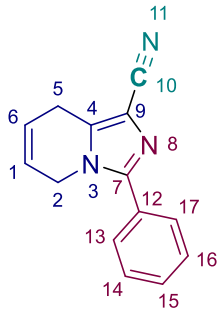
Experimental Procedures for Scheme 6.

a) A divided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. Anodic space: The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), pyridine (0.5 mmol, 39 mg, 40.0 µL, 0.5 eq.), and supporting electrolyte *n*-Bu_4NBF_4 (1.0 mmol, 329 mg) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.). Cathodic space: NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.) and supporting electrolyte *n*-Bu_4NBF_4 (1.0 mmol, 329 mg) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.). The solutions were electrolyzed using constant current conditions at 20-25 °C under magnetic stirring for 322 min. with I = 40 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), NH_4SCN (2.0 mmol, 152 mg, 2.0 eq.), pyridine (0.5 mmol, 39 mg, 40.0 µL, 0.5 eq.), and supporting electrolyte *n*-Bu_4NBF_4 (1.0 mmol, 329 mg) in 10 mL of with H_2O (1.0 mmol, 18.0 µL, 1.0 eq.), was electrolyzed using constant current conditions at 20-25 °C under magnetic stirring for 322 min. with I = 40 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was isolated by chromatography on SiO_2 (PE:EtOAc = from 8:1 to 2:1).

b) An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of 3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile **3a** (0.5 mmol, 109 mg, 1.0 eq.), NH_4SCN (1.0 mmol, 76 mg, 2.0 eq.), and pyridine (0.25 mmol, 19 mg, 20.0 µL, 0.5 eq.) in 5 mL of DMSO with H_2O (0.5 mmol, 9.0 µL, 1.0 eq.) was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 107 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (15 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×15 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **11** was isolated by chromatography on SiO_2 (PE:EtOAc = from 5:1 to 2:1).

3-Phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11



56% (124 mg, 0.28 mmol, PE/EtOAc 5:1 to 2:1 as eluent). R_f = 0.16 (PE/EtOAc = 4:1).

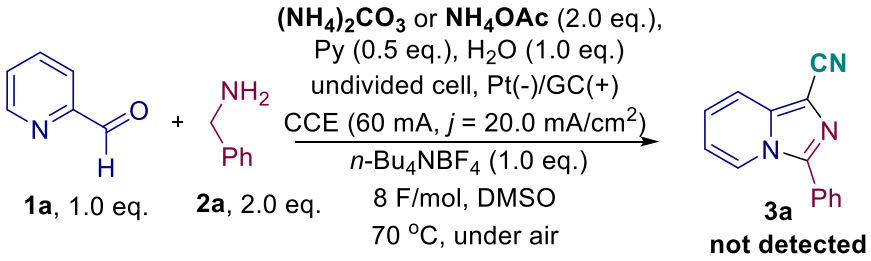
White solid. mp = 154-155 °C.

^{1}H NMR (300.13 MHz, $CDCl_3$, δ): 7.71 – 7.56 (m, 2H, *H13,17*), 7.54 – 7.39 (m, 3H, *H14-16*), 6.13 – 5.99 (m, 1H, *H6*), 5.97 – 5.84 (m, 1H, *H1*), 4.72 – 4.53 (m, 2H, *H2*), 3.67 – 3.49 (m, 2H, *H5*).

^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$, δ): 147.47 (*C7*), 136.68 (*C4*), 129.78 (*C15*), 129.21 (*C12*), 128.94 (*C14-16*), 128.68 (*C13,17*), 121.28 (*C6*), 115.24 (*C10*), 109.77 (*C9*), 44.72 (*C2*), 22.12 (*C5*).

HRMS (ESI-TOF) m/z [M+H]$^+$. Calcd for $[C_{14}H_{12}N_3]^+$: 222.1026. Found: 222.1035.

Experimental procedures for electrolysis of the starting substrates under optimal conditions with NH_4OAc or $(NH_4)_2CO_3$.



1a, 1.0 eq. **2a**, 2.0 eq. **3a** **not detected**

An undivided cell was equipped with a glassy carbon anode (3 cm^2) and a platinum plate cathode (3 cm^2) and connected to a DC regulated power supply. The solution of pyridine-2-carboxaldehyde **1a** (1.0 mmol, 107 mg, 1.0 eq.), benzylamine **2a** (2.0 mmol, 214 mg, 2.0 eq.), $NH_4OAc{\cdot}H_2O$ (2.0 mmol, 154 mg, 2.0 eq.) or $(NH_4)_2CO_3$ (2.0 mmol, 192 mg, 2.0 eq.), and pyridine (0.5 mmol, 39 mg, 40.0 μL, 0.5 eq.) in 10 mL of DMSO with H_2O (1.0 mmol, 18.0 μL, 1.0 eq.), was electrolyzed using constant current conditions at 70 °C under magnetic stirring for 214 min. with I = 60 mA. After that, the reaction mixture was diluted with H_2O (30 mL) and washed with mixture of PE and ethyl acetate (1:1) (2×30 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure using a rotary evaporator (15-20 mmHg), (bath temperature, ca. 30–40 °C). Product **3a** was not detected.

CV-study

Cyclic voltammetry (CV) was implemented on an IPC-Pro M computer-assisted potentiostat manufactured by «Econix» (scan rate error 1.0%, potential setting 0.25 mV; scan rate 50-250 mV s^{-1}). Analyzed solutions were prepared in 5 ml DMSO with 0.1 M H_2O and contained *n*-Bu_4NClO_4 (0.1 M) as the supporting electrolyte and analyte (0.1 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 argon bubbling. 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.

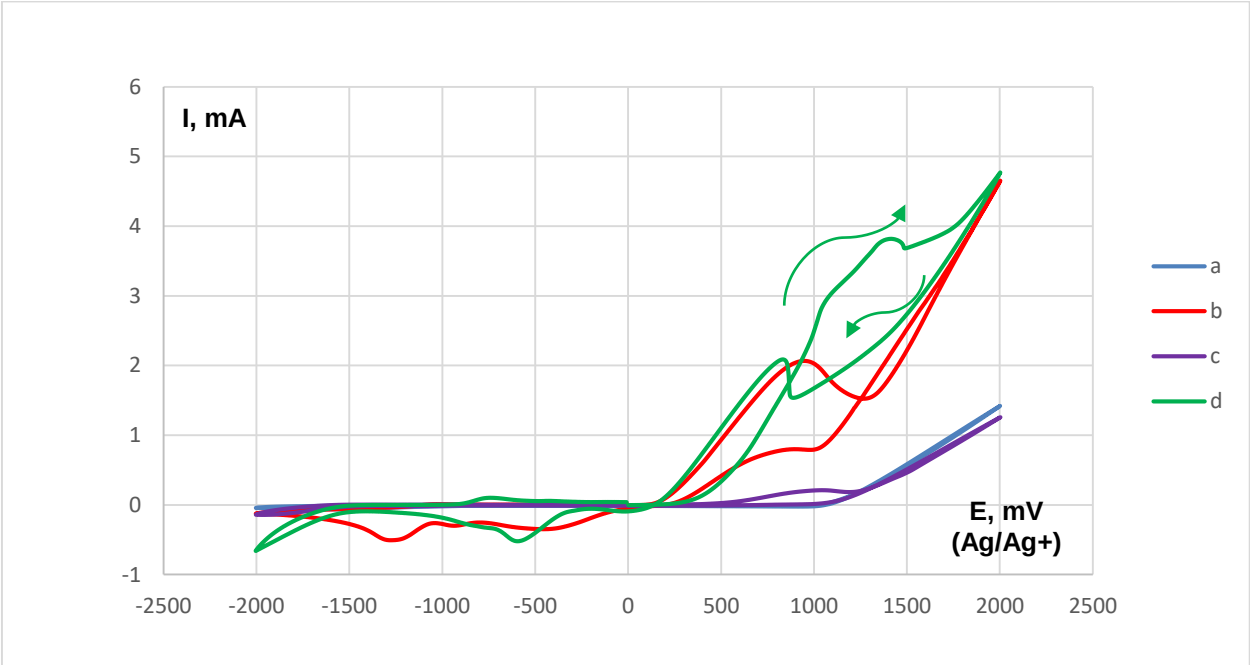


Figure S2. CV curves for the corresponding solutions on a working glassy-carbon electrode (d = 3 mm) under a scan rate of 0.1 V/s at 20 °C. (a) 0.1 M *n*-Bu_4NClO_4 solution (b) 0.2 M solution of NH_4SCN; (c) 0.1 M solution of aldehyde **1a** and 0.2 M solution of amine **2a**; (d) 0.1 M solution of aldehyde **1a**, 0.2 M solution of amine **2a** and 0.2 M solution of NH_4SCN in 0.1 M *n*-Bu_4NClO_4 solution in DMSO with 0.1 M H_2O.

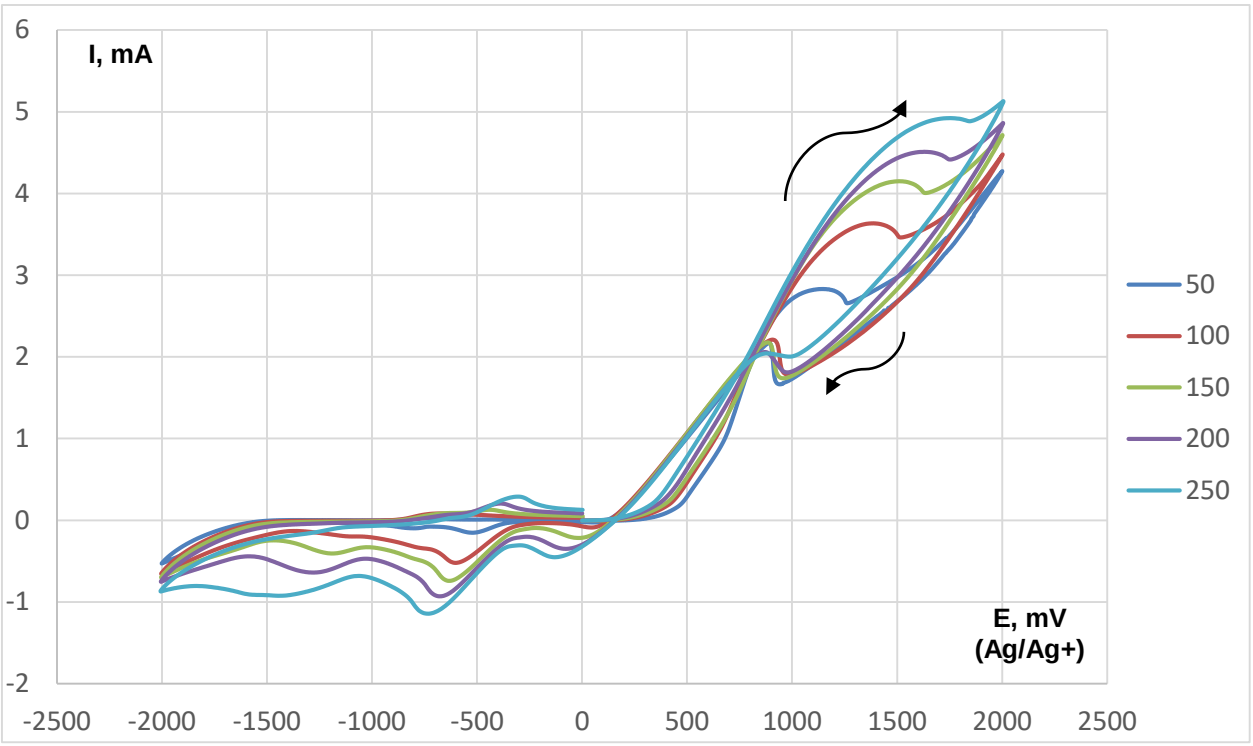


Figure S3. CV curves for the reaction mixture on a working glassy-carbon electrode (d = 3 mm) under different scan rates from 50 mV/s to 250 mV/s at 20 °C. Reaction mixture contains 0.1 M solution of aldehyde **1a**, 0.2 M solution of amine **2a** and 0.2 M solution of NH_4SCN in 0.1 M *n*-Bu_4NClO_4 solution in DMSO with 0.1 M H_2O.

Bioassay of fungicidal activity

The antifungal activities were tested according to the conventional procedure [7-9] with six phytopathogenic fungi from different taxonomic classes: *S. sclerotiorum (S.s.)*, *F. oxysporum (F.o.)*, *F. moniliforme (F.m.)*, *B. sorokiniana (B.s.)*, *R. solani (R.s.)*, and *V. inaequalis (V.i.)*. The effect of the chemicals on mycelial radial growth was determined by dissolving concentration 3 $mg \times mL^{-1}$ in acetone and suspending aliquots in potato-saccharose agar at 50 °C to give the concentration 30 $\mu g \times mL^{-1}$. The final acetone concentration of both fungicide-containing and control samples was 10 $mL \times L^{-1}$. 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 72 h. The mixed medium without 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 72 h of culture. The growth inhibition rates were calculated with the following equation: $I = [(DC - DT)/DC] \times 100\%$. 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 2.

X-ray study

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[10]. The structure was solved by direct methods using SHELXT[11] and refined on *F*[11] using SHELXL-2018[12] in the OLEX2 program.[13] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. Locations of hydrogen atoms (H4A, H4B, H7A and H7B) were found from the electron density-difference map; these hydrogen atoms were refined with individual isotropic displacement parameters. All other hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

CCDC 2290138 contains the supplementary crystallographic data for **11**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures.

Sample preparation: compound **11** was dissolved in EtOAc and crystallized by vapor diffusion of petroleum ether.

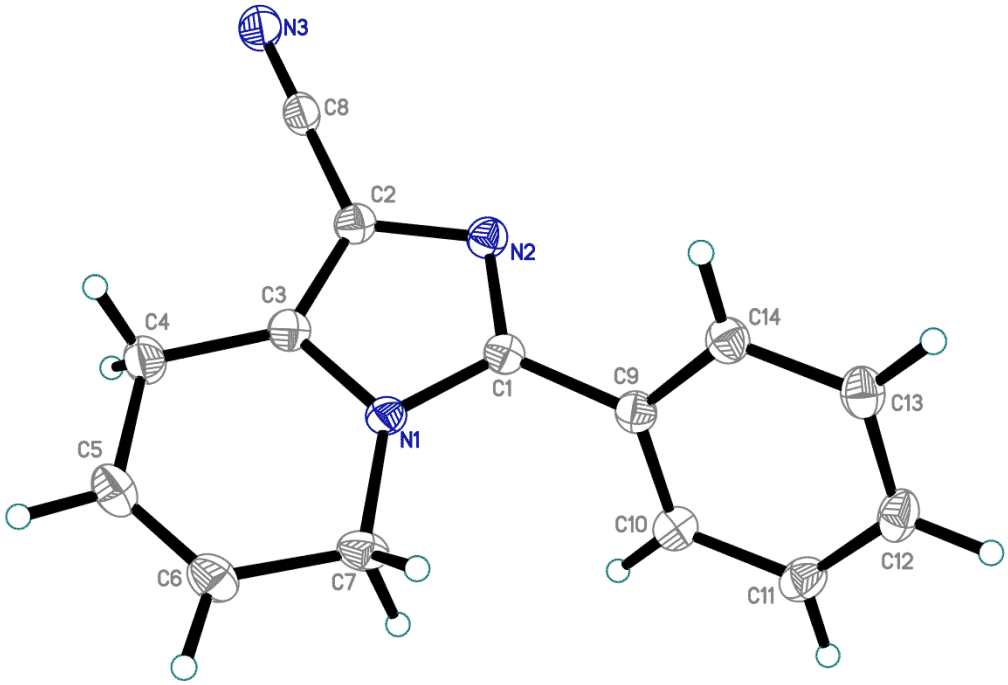


Figure S4. Molecular structure of **11** presented in thermal ellipsoids (P = 50%).

Table S2. Crystal data and structure refinement for 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile **(11)**

Identification code	**11**	
Empirical formula	C14 H11 N3	
Formula weight	221.26	
Temperature	100.0(3) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 5.76010(10) Å	a= 90°.
	b = 16.4872(3) Å	b= 102.0990(10)°.
	c = 11.6145(2) Å	g = 90°.
Volume	1078.50(3) $Å^3$	
Z	4	
Density (calculated)	1.363 g/cm^3	
Absorption coefficient	0.662 mm^{-1}	
F(000)	464	
Crystal size	0.12 x 0.05 x 0.03 mm^3	
Theta range for data collection	5.366 to 77.086°.	
Index ranges	-4<=h<=7, -20<=k<=20, -14<=l<=14	
Reflections collected	5838	
Independent reflections	1451 [R(int) = 0.0305]	
Observed reflections	1435	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.51018	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1451 / 2 / 170	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0328, wR2 = 0.0857	
R indices (all data)	R1 = 0.0330, wR2 = 0.0859	
Absolute structure parameter	-0.4(5)	
Largest diff. peak and hole	0.242 and -0.164 e.$Å^{-3}$	

Table S3. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for compound (**11**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	7196(3)	2842(1)	5002(1)	17(1)
N(2)	3955(3)	3600(1)	4439(2)	18(1)
N(3)	-143(3)	2504(1)	2356(2)	26(1)
C(1)	6095(3)	3564(1)	5124(2)	17(1)
C(2)	3692(4)	2860(1)	3862(2)	18(1)

C(3)	5667(4)	2379(1)	4210(2)	18(1)
C(4)	6203(4)	1528(1)	3927(2)	24(1)
C(5)	8449(4)	1229(1)	4689(2)	24(1)
C(6)	9910(4)	1694(1)	5457(2)	24(1)
C(7)	9506(4)	2565(1)	5671(2)	21(1)
C(8)	1571(4)	2662(1)	3029(2)	20(1)
C(9)	7128(3)	4200(1)	5978(2)	18(1)
C(10)	9287(4)	4579(1)	5954(2)	21(1)
C(11)	10150(4)	5184(1)	6778(2)	23(1)
C(12)	8881(4)	5402(1)	7622(2)	22(1)
C(13)	6726(4)	5030(1)	7642(2)	22(1)
C(14)	5846(4)	4433(1)	6822(2)	19(1)

Table S4. Bond lengths [Å] and angles [°] for compound (**11**).

N(1)-C(1)	1.370(2)
N(1)-C(3)	1.365(3)
N(1)-C(7)	1.466(3)
N(2)-C(1)	1.321(2)
N(2)-C(2)	1.385(3)
N(3)-C(8)	1.153(3)
C(1)-C(9)	1.480(3)
C(2)-C(3)	1.375(3)
C(2)-C(8)	1.428(3)
C(3)-C(4)	1.488(3)
C(4)-H(4A)	0.99(4)
C(4)-H(4B)	1.01(4)
C(4)-C(5)	1.491(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.333(3)
C(6)-H(6)	0.9500
C(6)-C(7)	1.484(3)
C(7)-H(7A)	1.03(3)
C(7)-H(7B)	0.97(3)
C(9)-C(10)	1.397(3)
C(9)-C(14)	1.399(3)
C(10)-H(10)	0.9500
C(10)-C(11)	1.399(3)
C(11)-H(11)	0.9500
C(11)-C(12)	1.388(3)
C(12)-H(12)	0.9500
C(12)-C(13)	1.389(3)

C(13)-H(13)	0.9500
C(13)-C(14)	1.389(3)
C(14)-H(14)	0.9500

C(1)-N(1)-C(7)	127.16(17)
C(3)-N(1)-C(1)	107.94(16)
C(3)-N(1)-C(7)	124.66(18)
C(1)-N(2)-C(2)	104.17(16)
N(1)-C(1)-C(9)	123.72(17)
N(2)-C(1)-N(1)	111.76(17)
N(2)-C(1)-C(9)	124.41(17)
N(2)-C(2)-C(8)	121.30(19)
C(3)-C(2)-N(2)	111.45(18)
C(3)-C(2)-C(8)	127.25(18)
N(1)-C(3)-C(2)	104.66(17)
N(1)-C(3)-C(4)	122.77(18)
C(2)-C(3)-C(4)	132.47(19)
C(3)-C(4)-H(4A)	110(2)
C(3)-C(4)-H(4B)	109(2)
C(3)-C(4)-C(5)	112.09(18)
H(4A)-C(4)-H(4B)	110(3)
C(5)-C(4)-H(4A)	107(2)
C(5)-C(4)-H(4B)	108(2)
C(4)-C(5)-H(5)	118.2
C(6)-C(5)-C(4)	123.6(2)
C(6)-C(5)-H(5)	118.2
C(5)-C(6)-H(6)	117.6
C(5)-C(6)-C(7)	124.7(2)
C(7)-C(6)-H(6)	117.6
N(1)-C(7)-C(6)	111.68(18)
N(1)-C(7)-H(7A)	113.2(18)
N(1)-C(7)-H(7B)	111.6(18)
C(6)-C(7)-H(7A)	108.2(18)
C(6)-C(7)-H(7B)	109.9(17)
H(7A)-C(7)-H(7B)	102(3)
N(3)-C(8)-C(2)	179.9(3)
C(10)-C(9)-C(1)	122.60(17)
C(10)-C(9)-C(14)	119.55(18)
C(14)-C(9)-C(1)	117.84(17)
C(9)-C(10)-H(10)	120.1

C(9)-C(10)-C(11)	119.73(19)
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-C(10)	120.25(19)
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-H(12)	119.9
C(11)-C(12)-C(13)	120.13(18)
C(13)-C(12)-H(12)	119.9
C(12)-C(13)-H(13)	120.0
C(12)-C(13)-C(14)	120.03(19)
C(14)-C(13)-H(13)	120.0
C(9)-C(14)-H(14)	119.8
C(13)-C(14)-C(9)	120.30(19)
C(13)-C(14)-H(14)	119.8

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound (**11**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	16(1)	19(1)	16(1)	-2(1)	1(1)	1(1)
N(2)	19(1)	19(1)	18(1)	0(1)	3(1)	0(1)
N(3)	23(1)	24(1)	27(1)	-4(1)	-2(1)	2(1)
C(1)	18(1)	18(1)	15(1)	1(1)	5(1)	0(1)
C(2)	18(1)	21(1)	16(1)	-1(1)	3(1)	-1(1)
C(3)	19(1)	22(1)	14(1)	-1(1)	4(1)	0(1)
C(4)	24(1)	22(1)	24(1)	-4(1)	-1(1)	4(1)
C(5)	28(1)	21(1)	25(1)	2(1)	5(1)	7(1)
C(6)	23(1)	25(1)	22(1)	4(1)	2(1)	6(1)
C(7)	17(1)	28(1)	18(1)	1(1)	1(1)	4(1)
C(8)	21(1)	17(1)	21(1)	-2(1)	4(1)	2(1)
C(9)	19(1)	17(1)	17(1)	1(1)	1(1)	2(1)
C(10)	21(1)	22(1)	20(1)	1(1)	4(1)	-1(1)
C(11)	21(1)	20(1)	25(1)	2(1)	2(1)	-4(1)
C(12)	29(1)	15(1)	20(1)	-1(1)	0(1)	0(1)
C(13)	26(1)	18(1)	21(1)	0(1)	5(1)	2(1)
C(14)	21(1)	17(1)	20(1)	1(1)	5(1)	0(1)

Table S6. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 x10^3$) for compound (**11**).

	x	y	z	U(eq)
H(4A)	4910(60)	1160(20)	4060(30)	37(8)
H(4B)	6360(70)	1490(20)	3080(40)	54(10)
H(5)	8863	675	4624	29
H(6)	11310	1450	5900	28
H(7A)	10910(60)	2890(19)	5490(30)	33(8)
H(7B)	9670(50)	2662(17)	6510(30)	26(7)
H(10)	10165	4427	5381	25
H(11)	11610	5446	6759	27
H(12)	9488	5806	8188	26
H(13)	5854	5183	8217	26
H(14)	4366	4182	6834	23

Table S7. Torsion angles [°] for compound (**11**).

N(1)-C(1)-C(9)-C(10)	60.5(3)
N(1)-C(1)-C(9)-C(14)	-120.7(2)
N(1)-C(3)-C(4)-C(5)	5.7(3)
N(2)-C(1)-C(9)-C(10)	-123.7(2)
N(2)-C(1)-C(9)-C(14)	55.1(2)
N(2)-C(2)-C(3)-N(1)	-1.2(2)
N(2)-C(2)-C(3)-C(4)	175.0(2)
C(1)-N(1)-C(3)-C(2)	1.4(2)
C(1)-N(1)-C(3)-C(4)	-175.32(18)
C(1)-N(1)-C(7)-C(6)	169.06(18)
C(1)-N(2)-C(2)-C(3)	0.5(2)
C(1)-N(2)-C(2)-C(8)	179.99(18)
C(1)-C(9)-C(10)-C(11)	179.15(17)
C(1)-C(9)-C(14)-C(13)	-179.71(17)
C(2)-N(2)-C(1)-N(1)	0.4(2)

C(2)-N(2)-C(1)-C(9)	-175.88(17)
C(2)-C(3)-C(4)-C(5)	-169.9(2)
C(3)-N(1)-C(1)-N(2)	-1.2(2)
C(3)-N(1)-C(1)-C(9)	175.15(17)
C(3)-N(1)-C(7)-C(6)	-4.7(3)
C(3)-C(4)-C(5)-C(6)	-5.8(3)
C(4)-C(5)-C(6)-C(7)	0.6(4)
C(5)-C(6)-C(7)-N(1)	4.7(3)
C(7)-N(1)-C(1)-N(2)	-175.73(18)
C(7)-N(1)-C(1)-C(9)	0.6(3)
C(7)-N(1)-C(3)-C(2)	176.11(18)
C(7)-N(1)-C(3)-C(4)	-0.6(3)
C(8)-C(2)-C(3)-N(1)	179.4(2)
C(8)-C(2)-C(3)-C(4)	-4.4(4)
C(9)-C(10)-C(11)-C(12)	0.6(3)
C(10)-C(9)-C(14)-C(13)	-0.9(3)
C(10)-C(11)-C(12)-C(13)	-1.1(3)
C(11)-C(12)-C(13)-C(14)	0.6(3)
C(12)-C(13)-C(14)-C(9)	0.4(3)
C(14)-C(9)-C(10)-C(11)	0.4(3)

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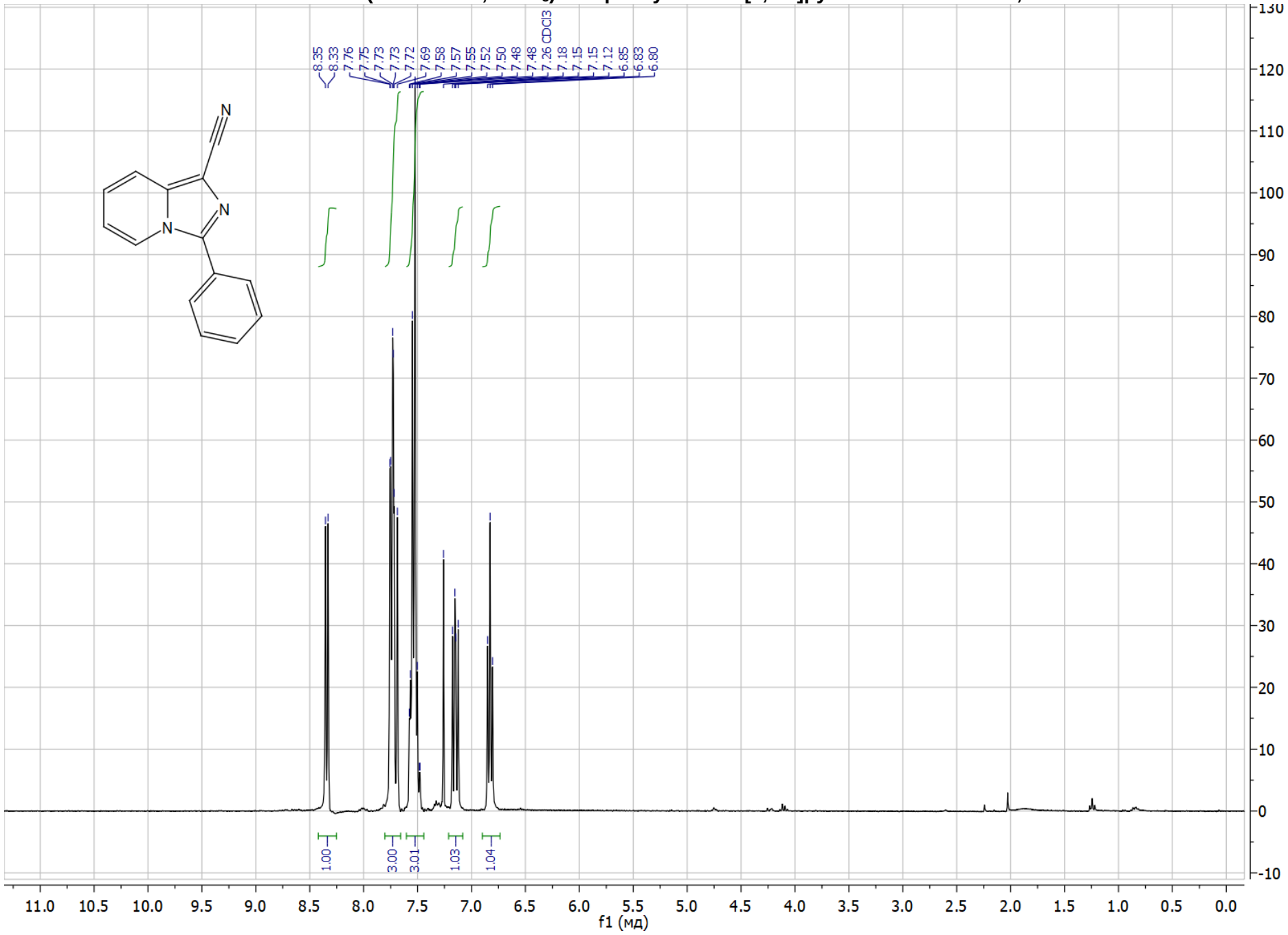
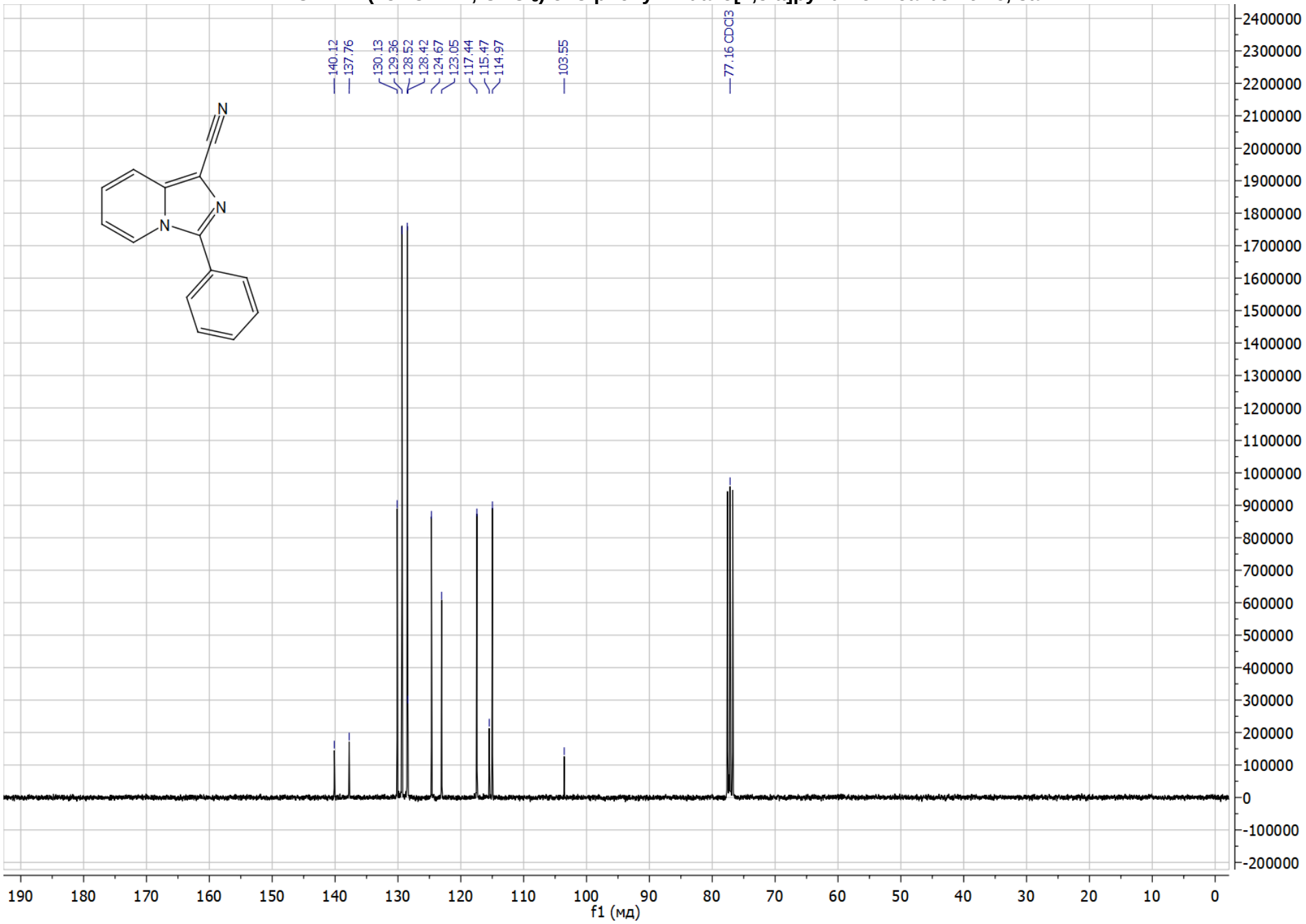
NMR spectra of the synthesized compounds

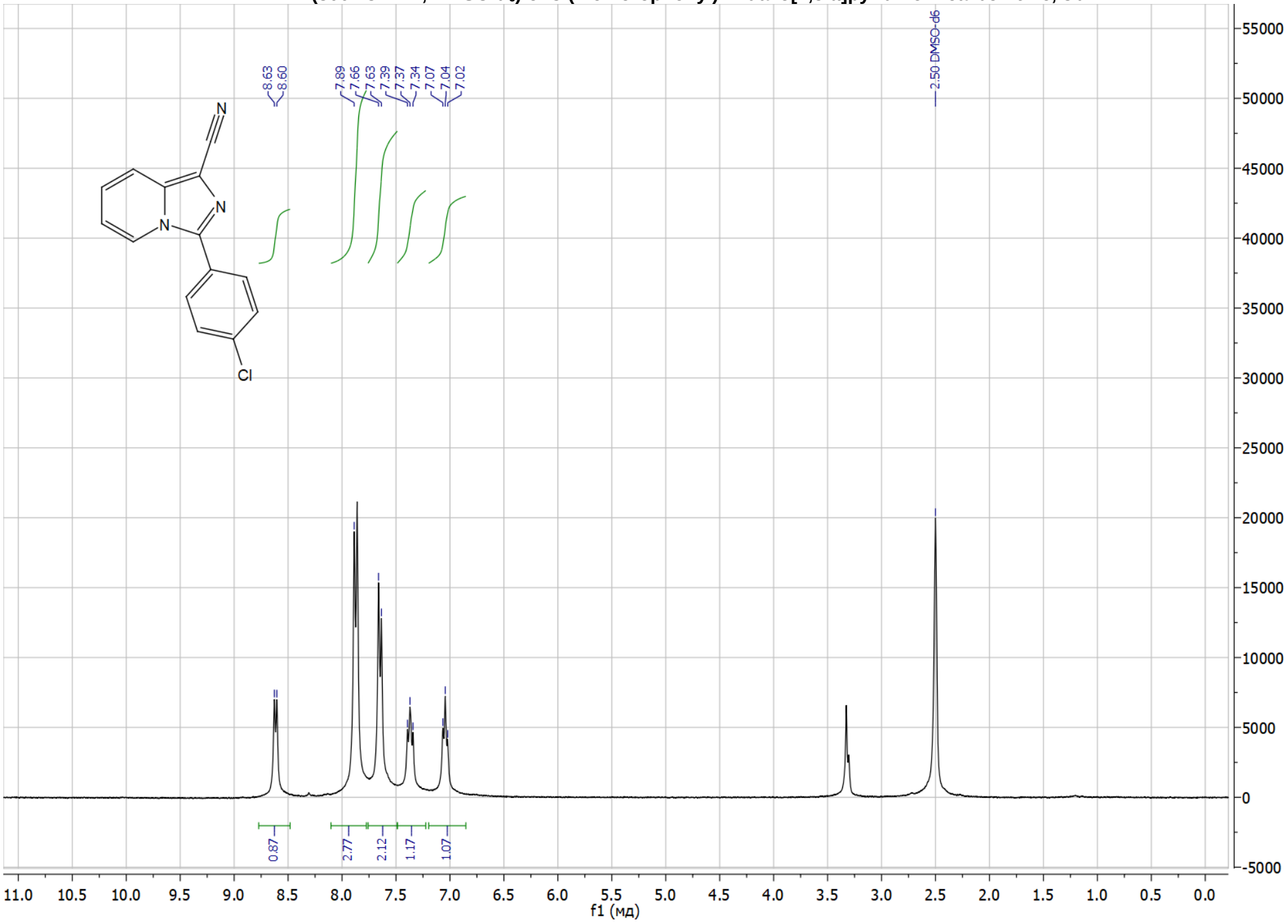
^{1}H NMR (300.13 MHz, $CDCl_3$) of 3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3a



^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3a



^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(4-chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3b



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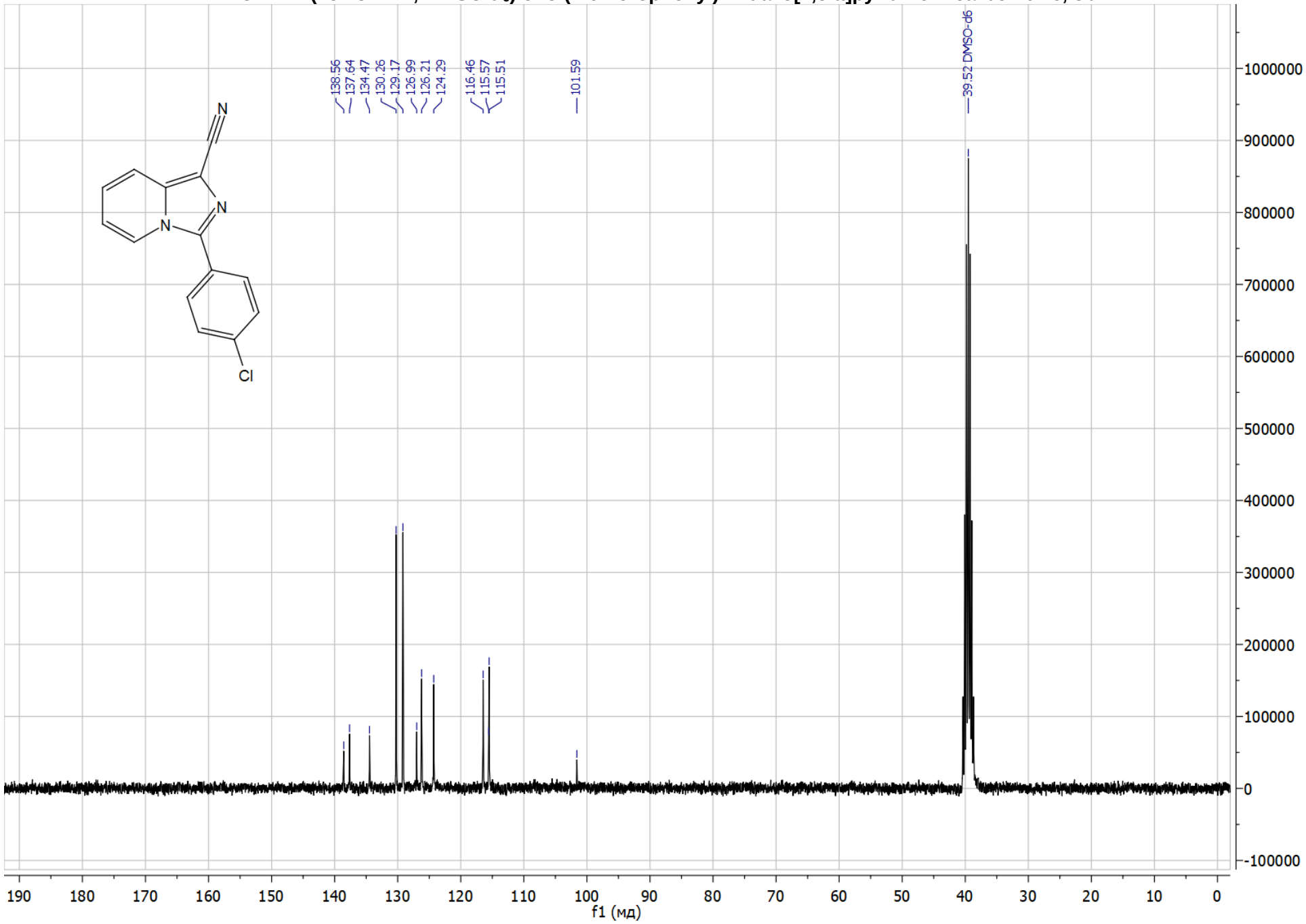

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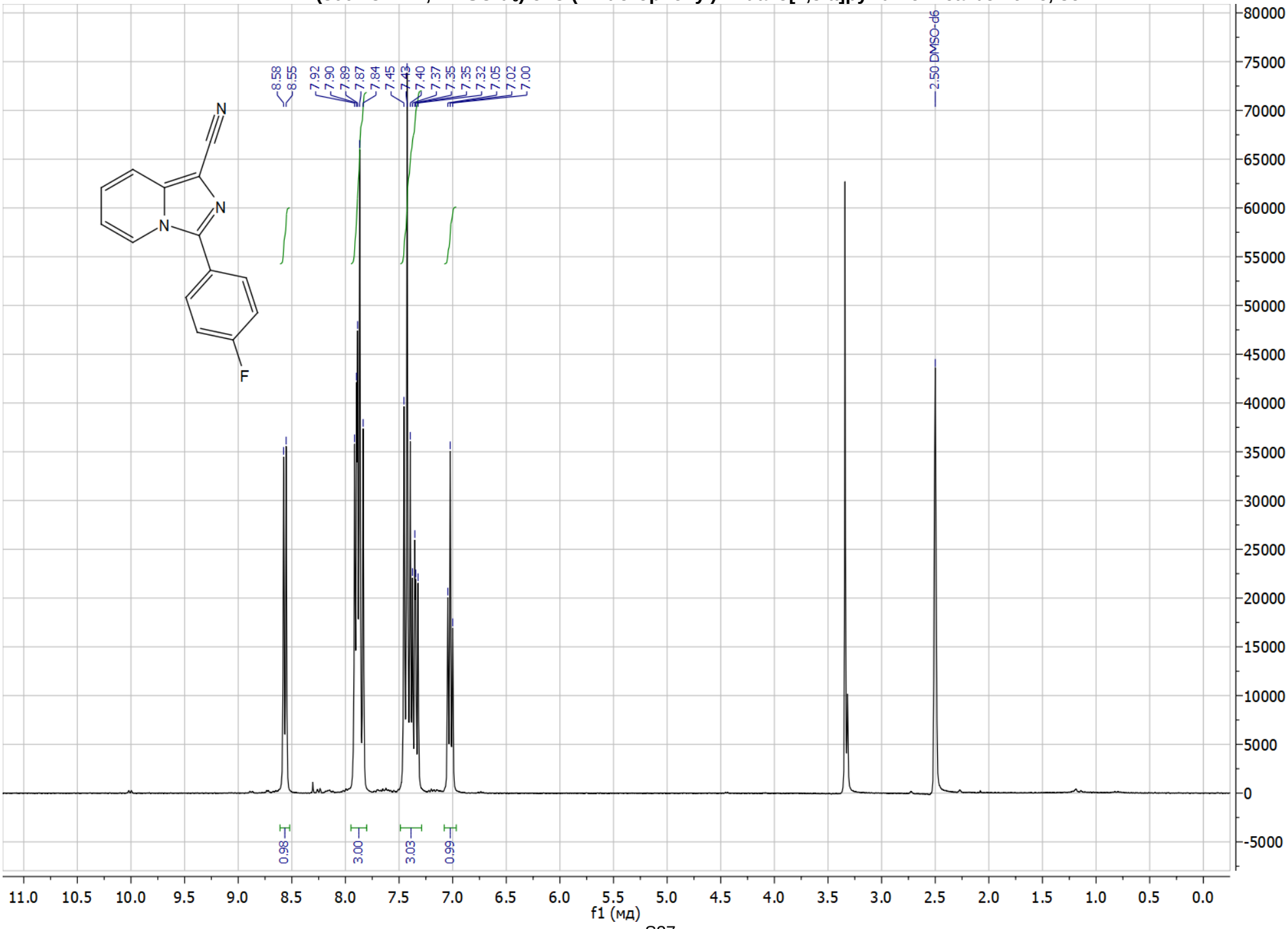

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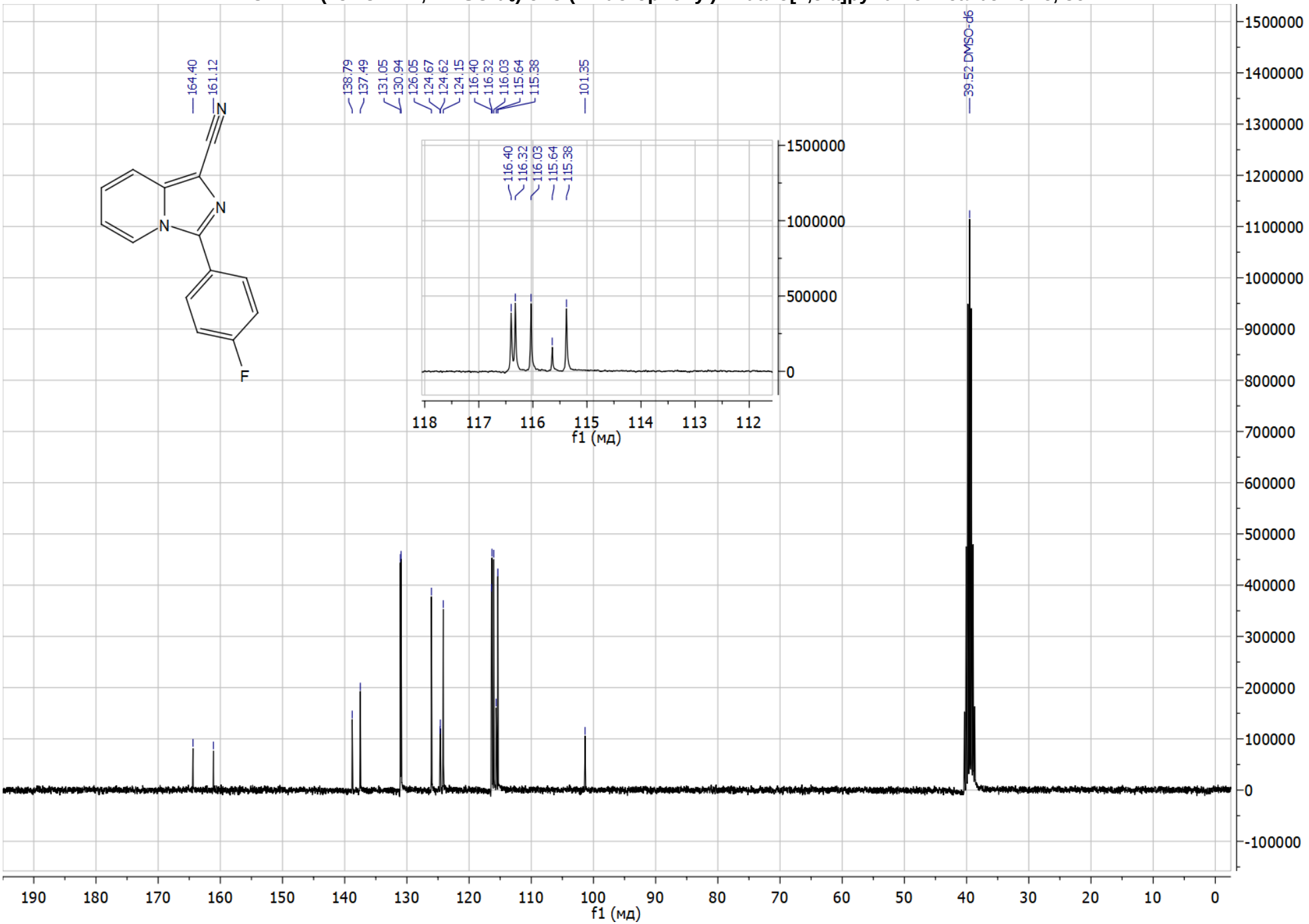

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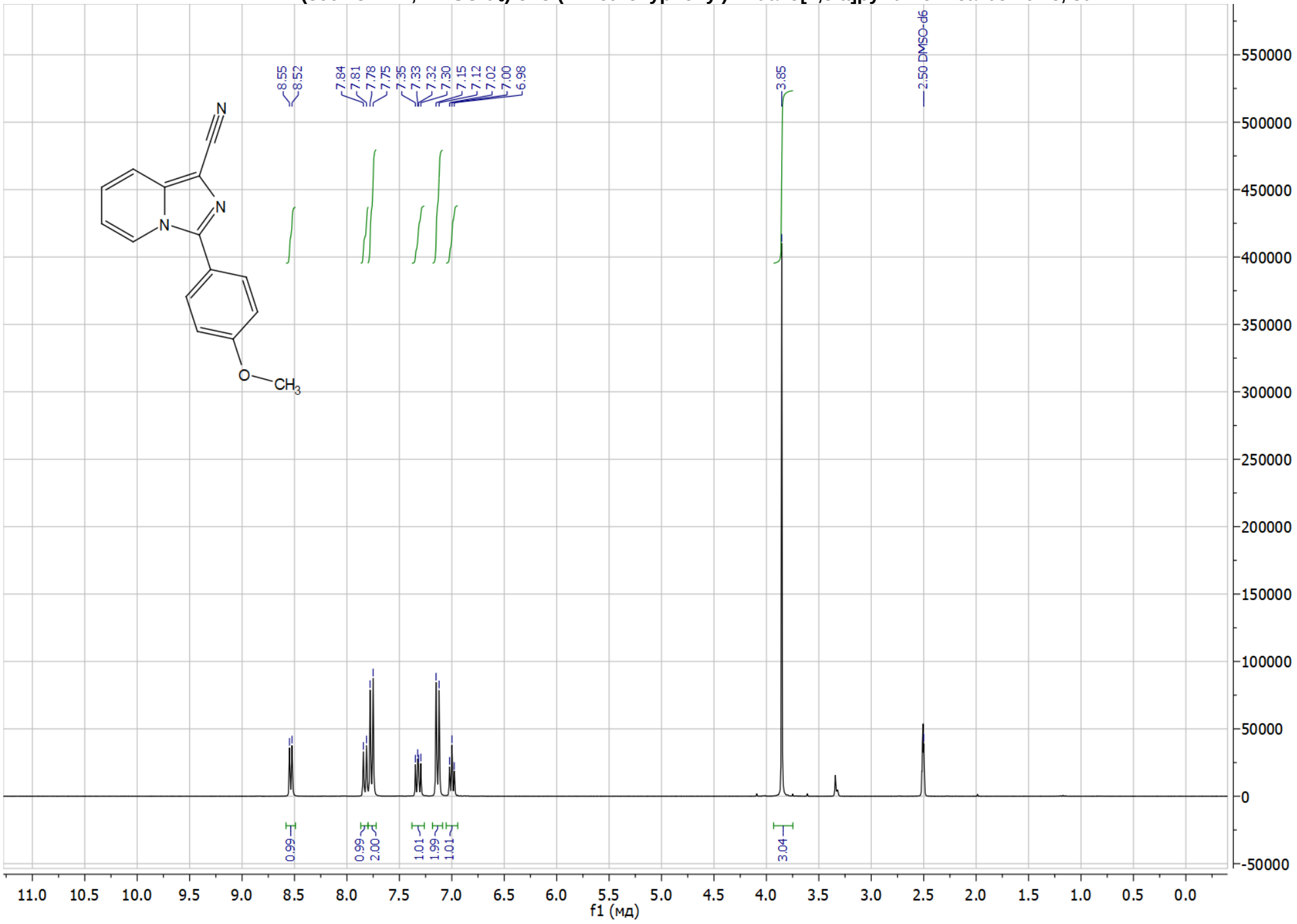
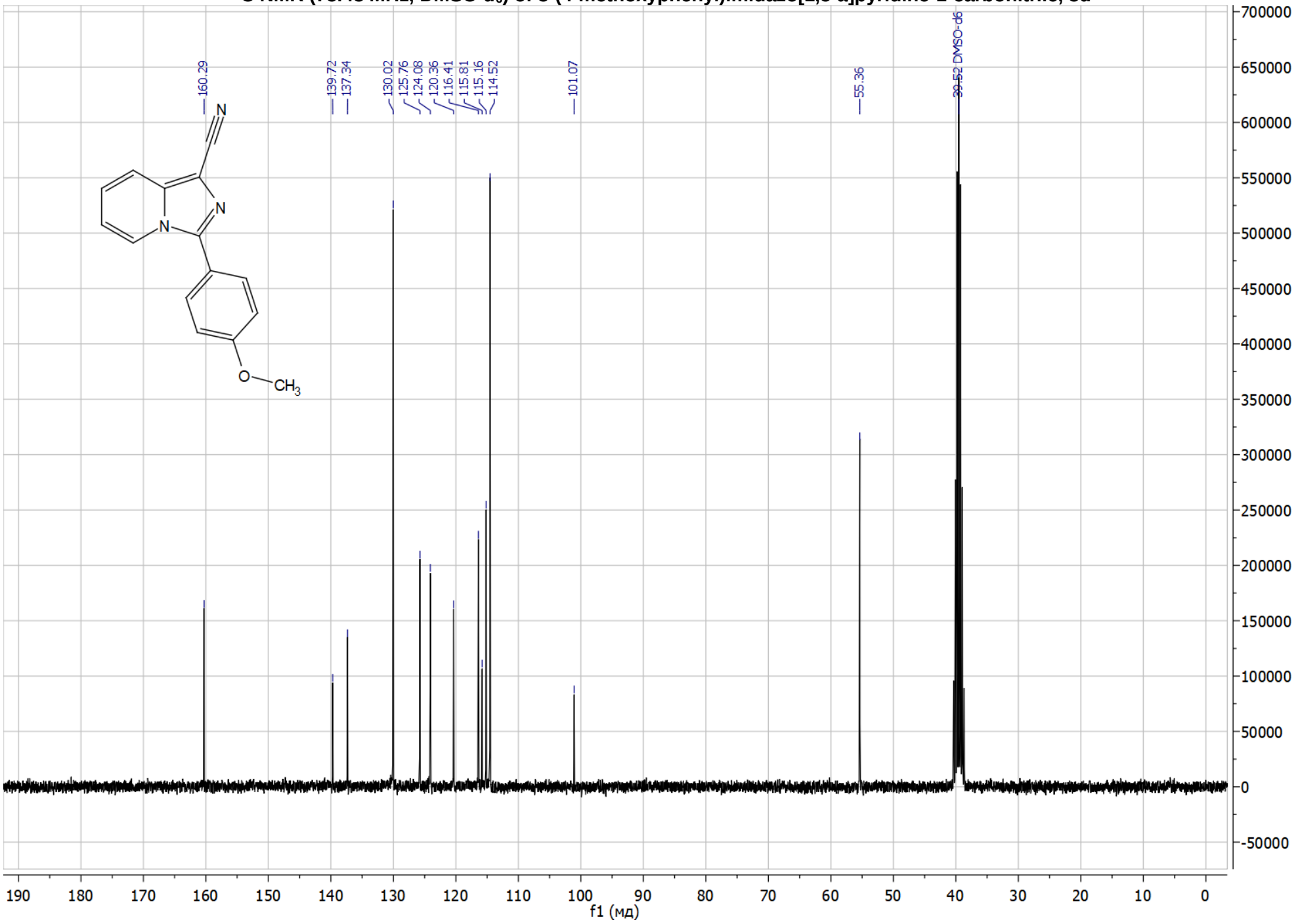


^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3d



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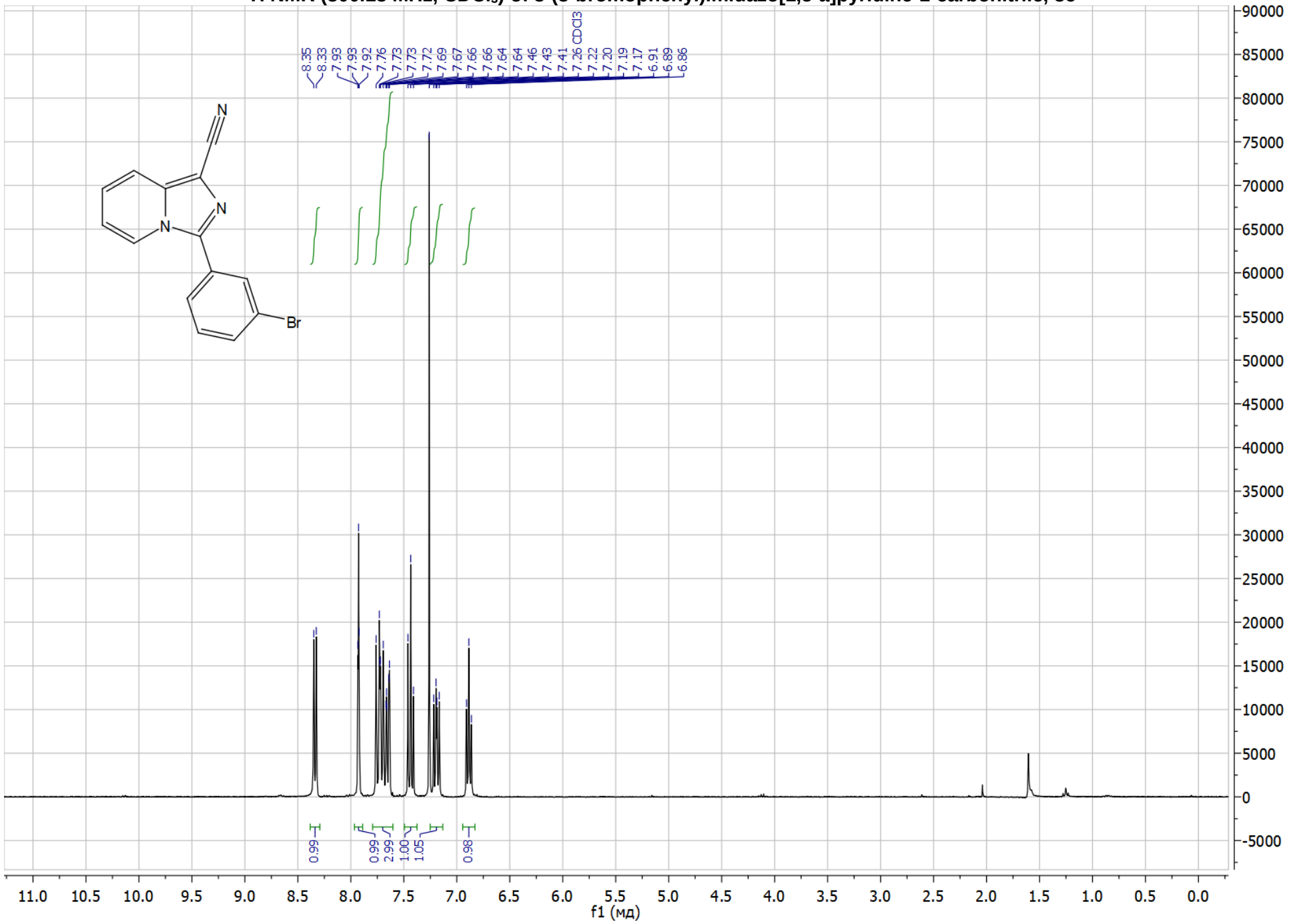
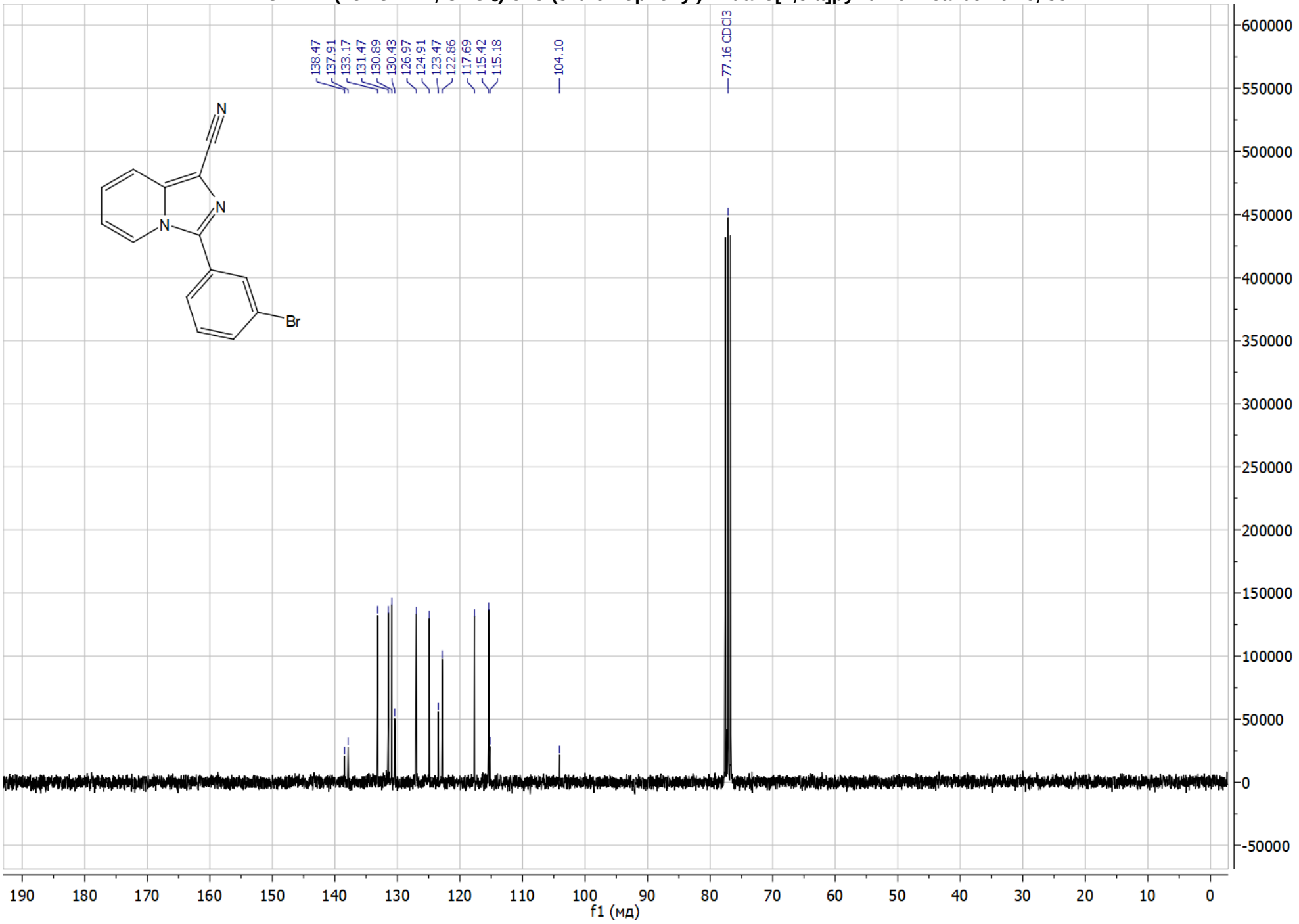
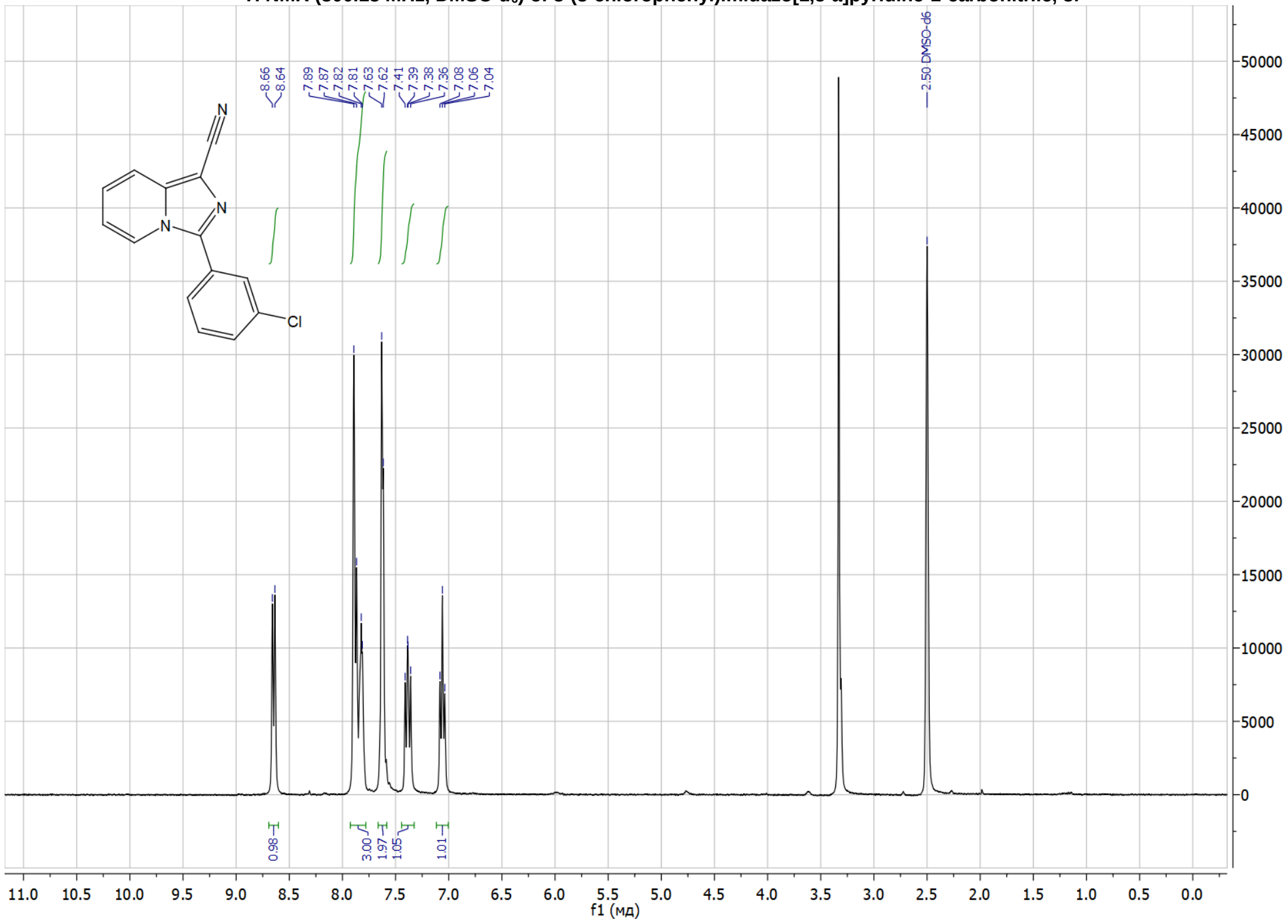


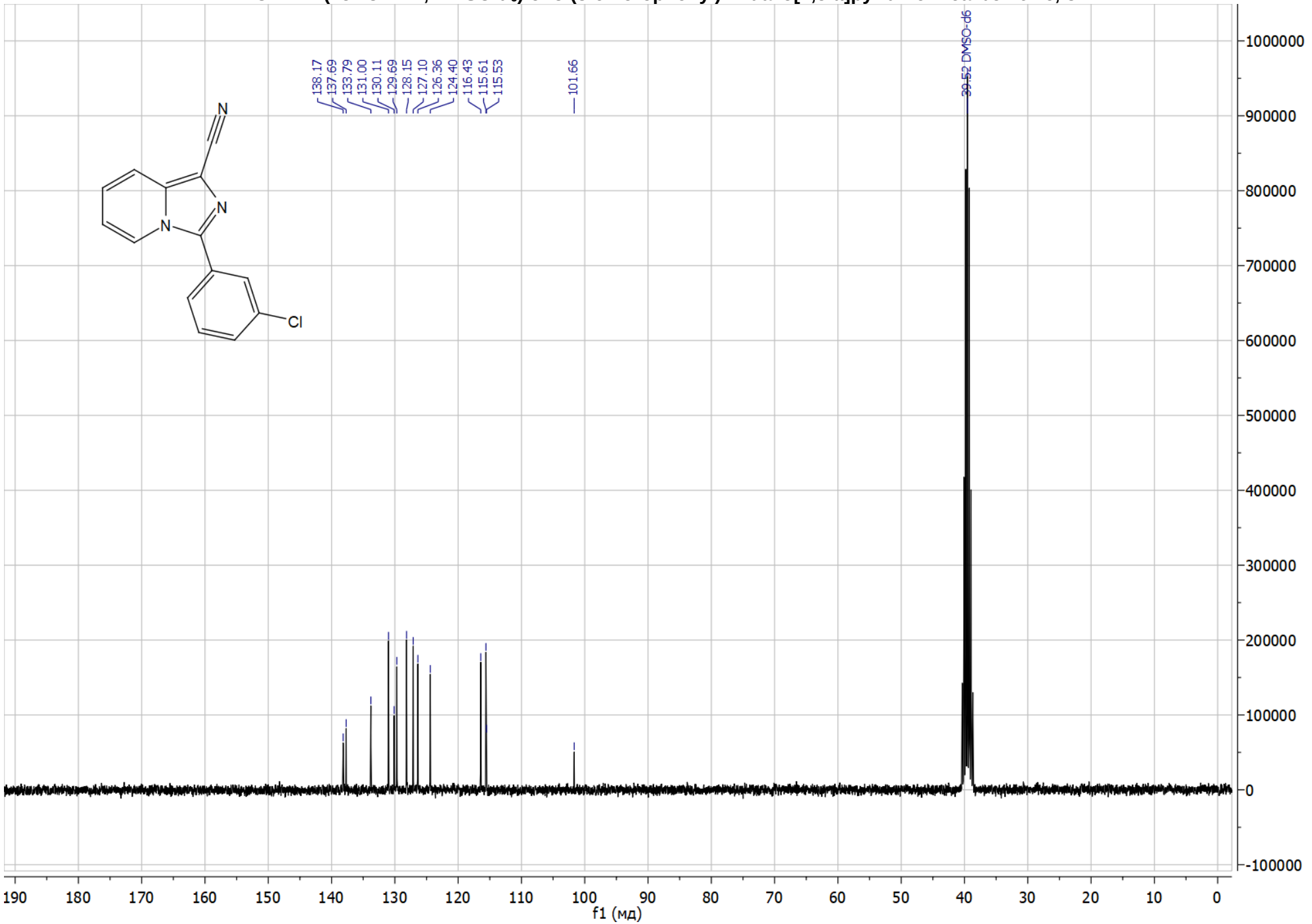
^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-(3-bromophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3e



^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(3-chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3f



^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(3-chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3f



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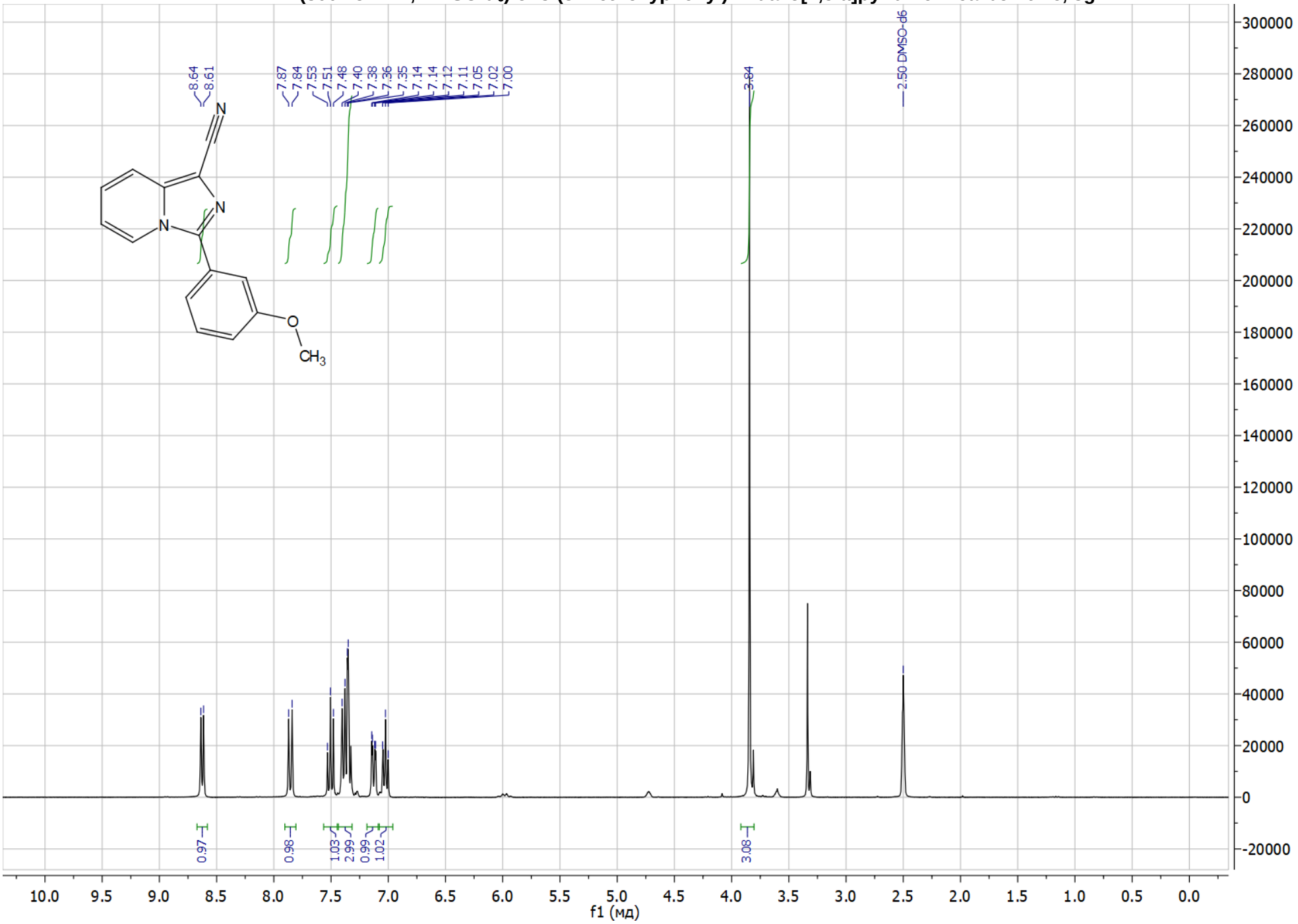
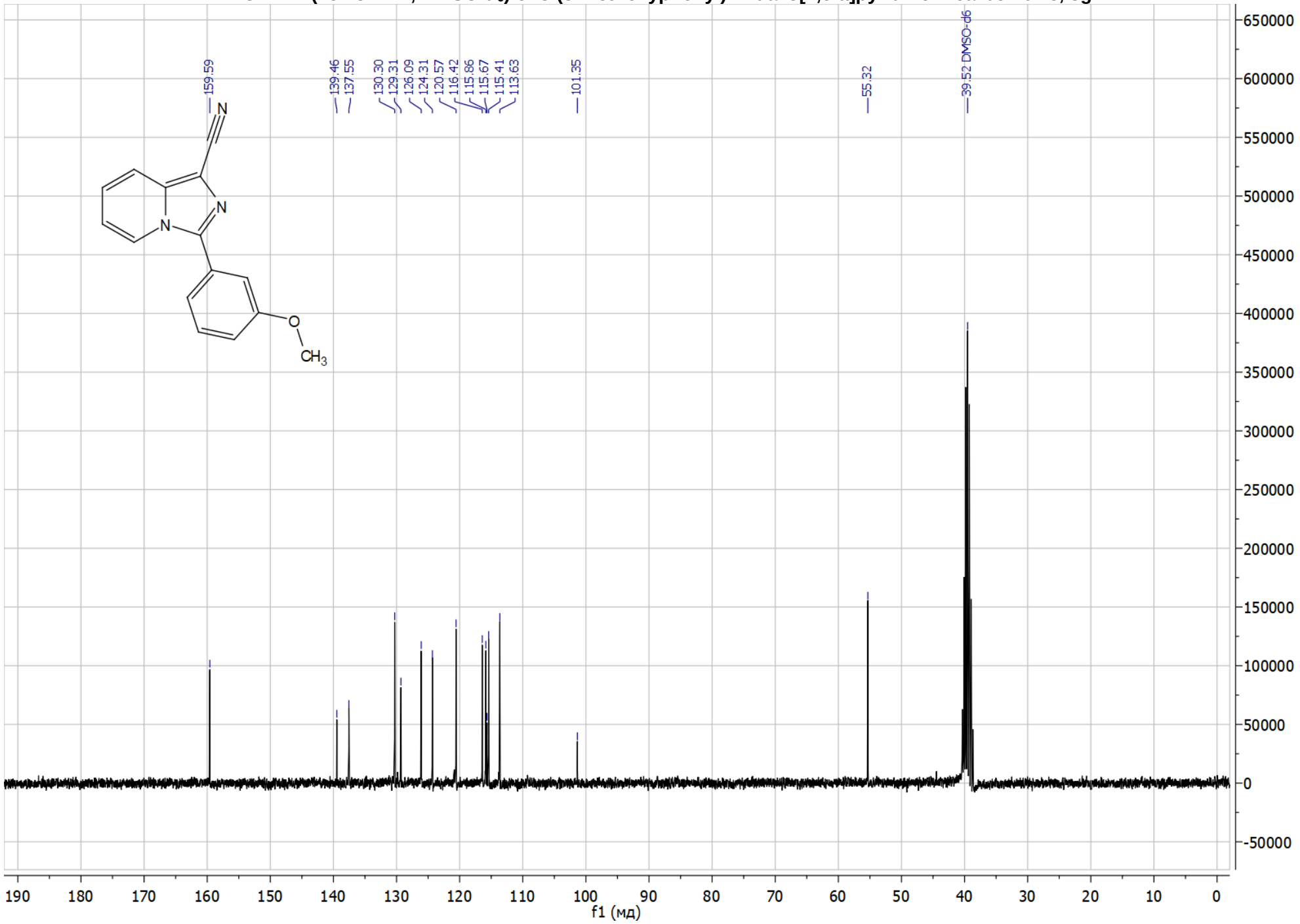


^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3g



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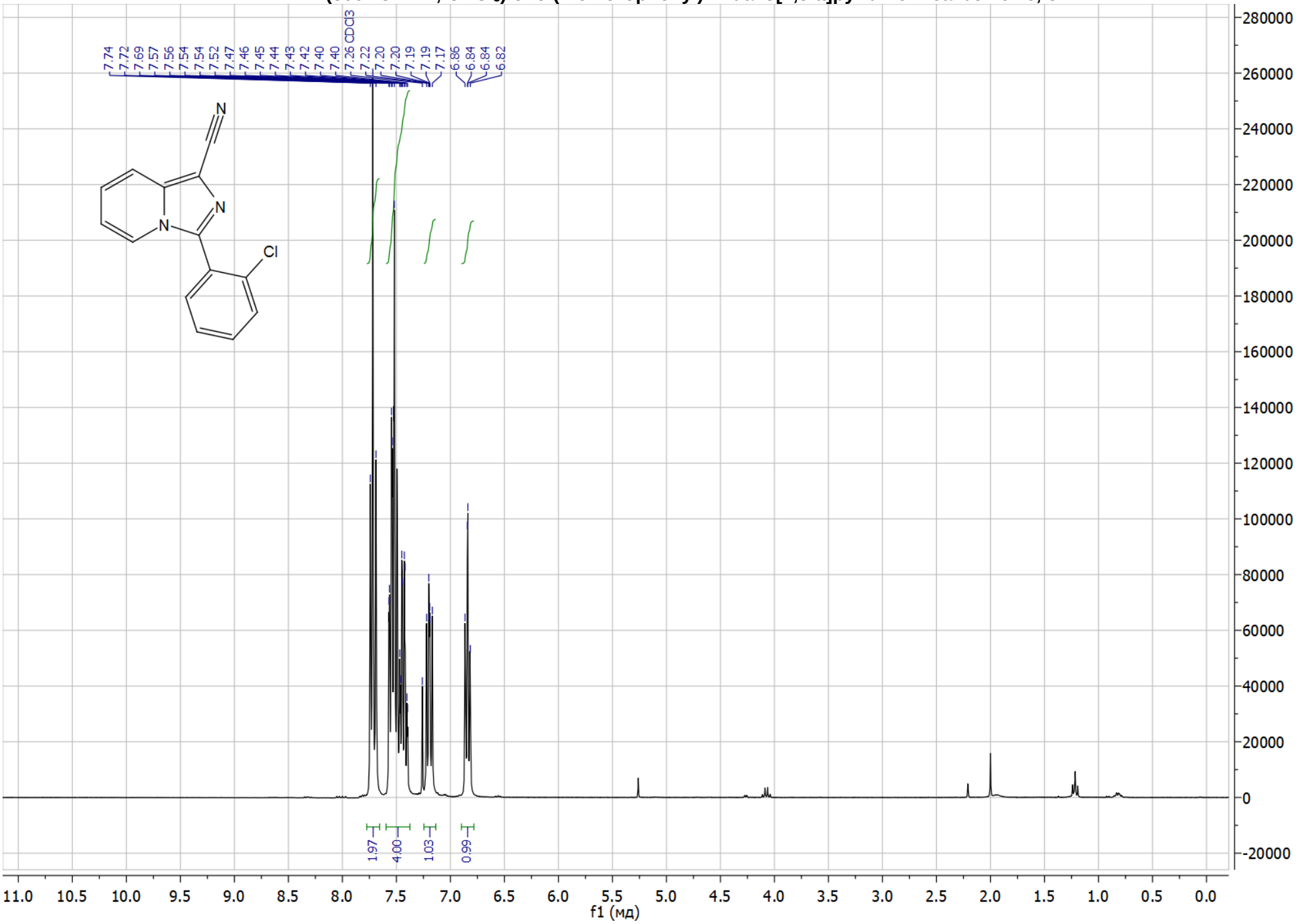
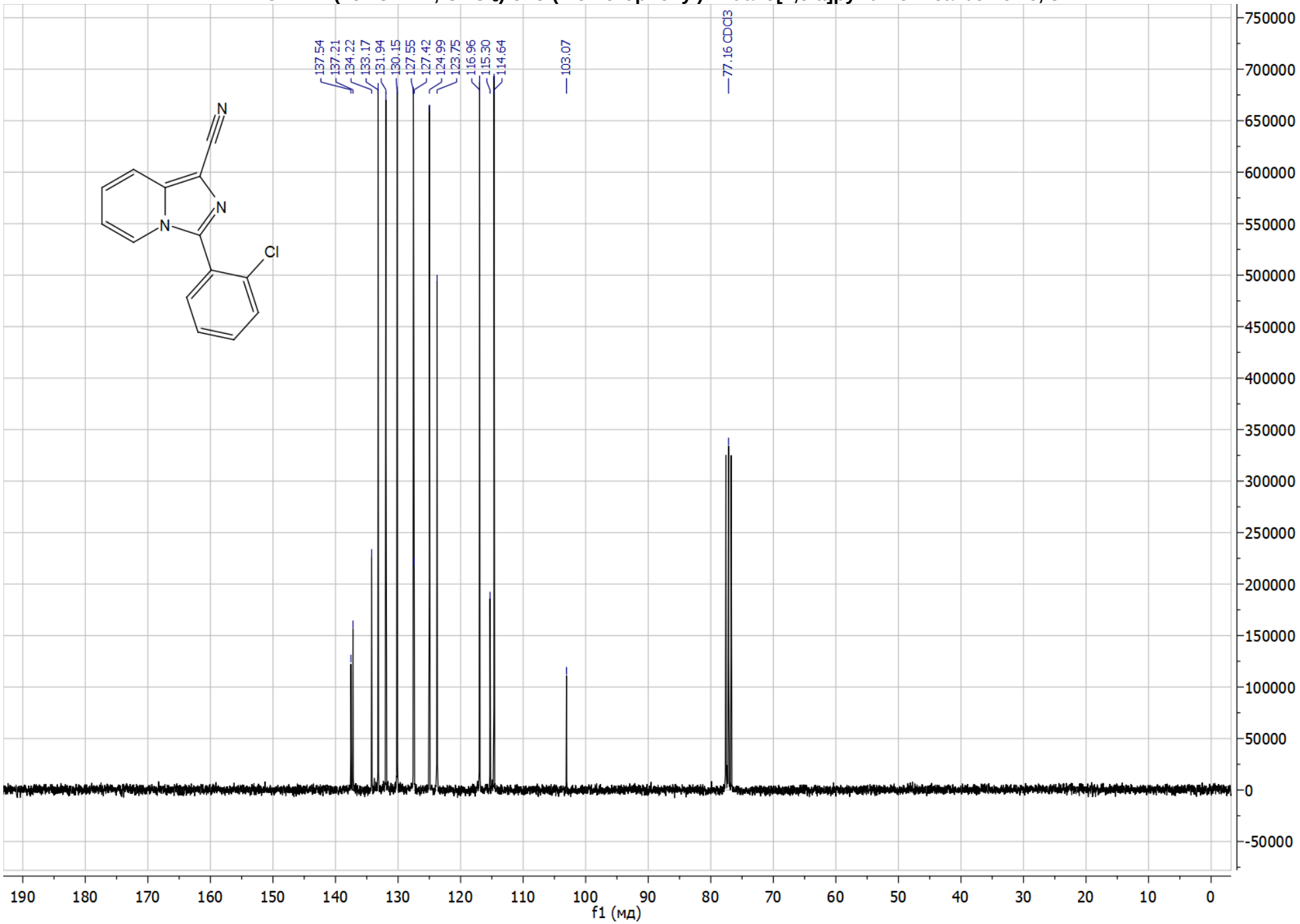
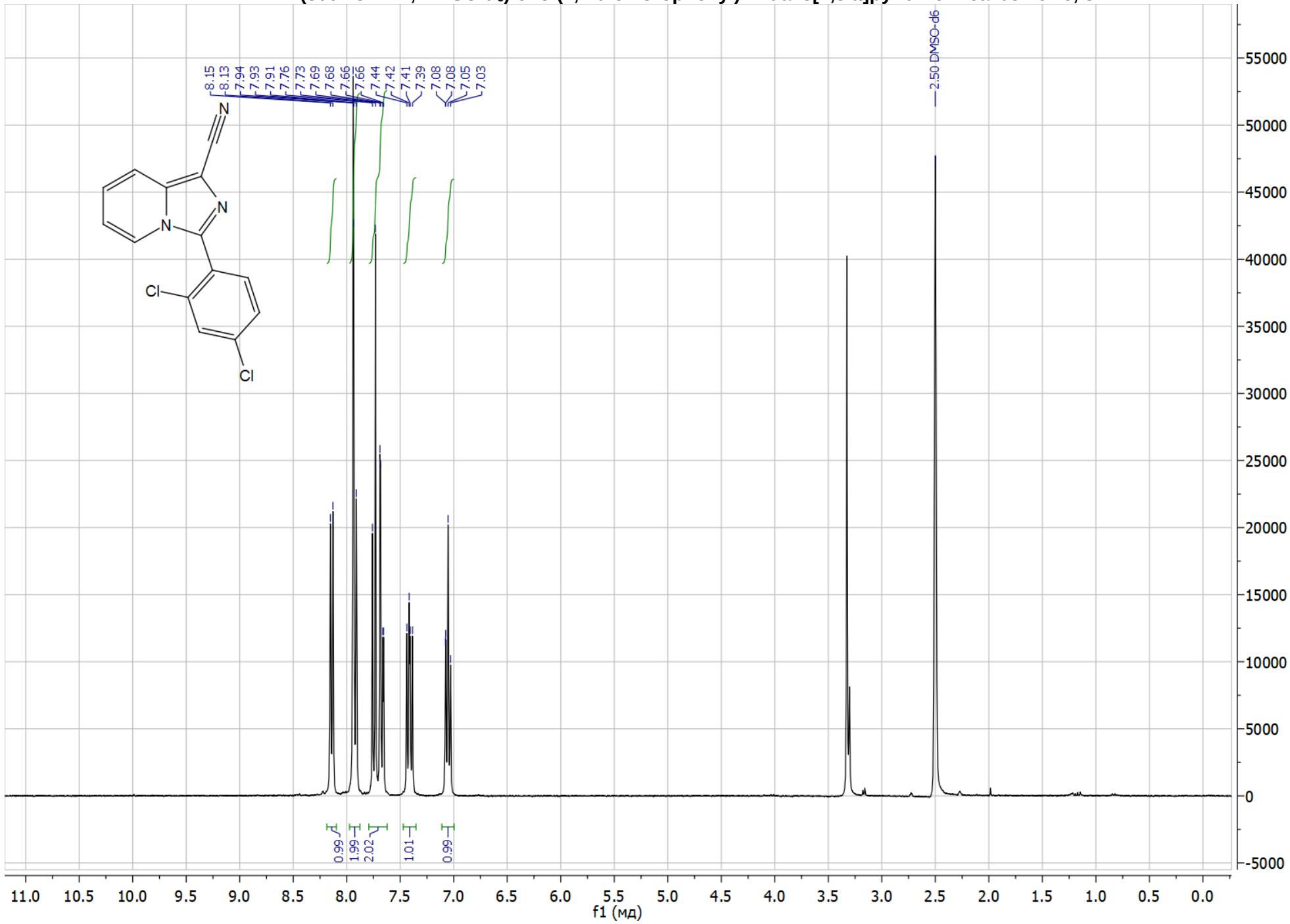


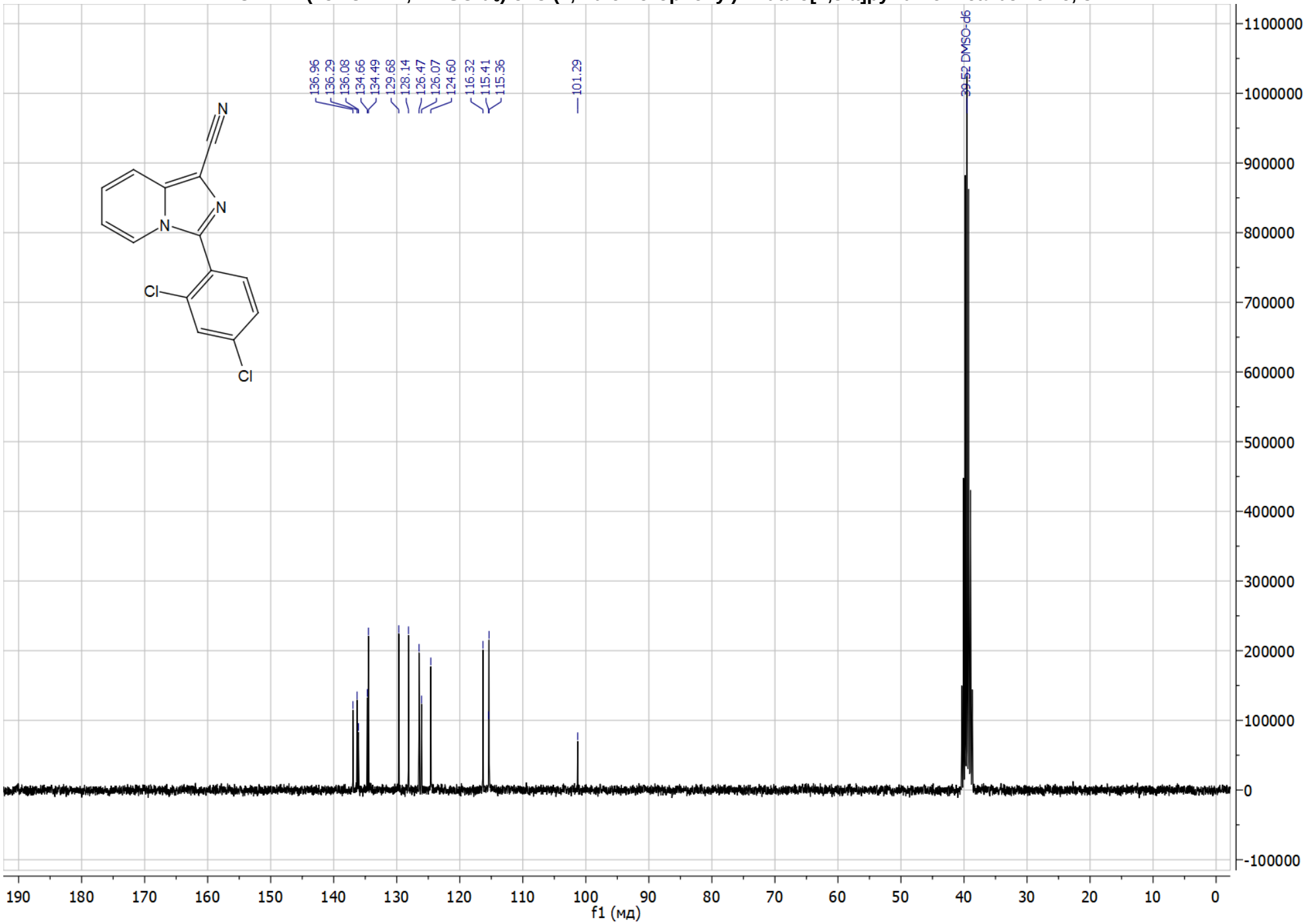
^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-(2-chlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3h



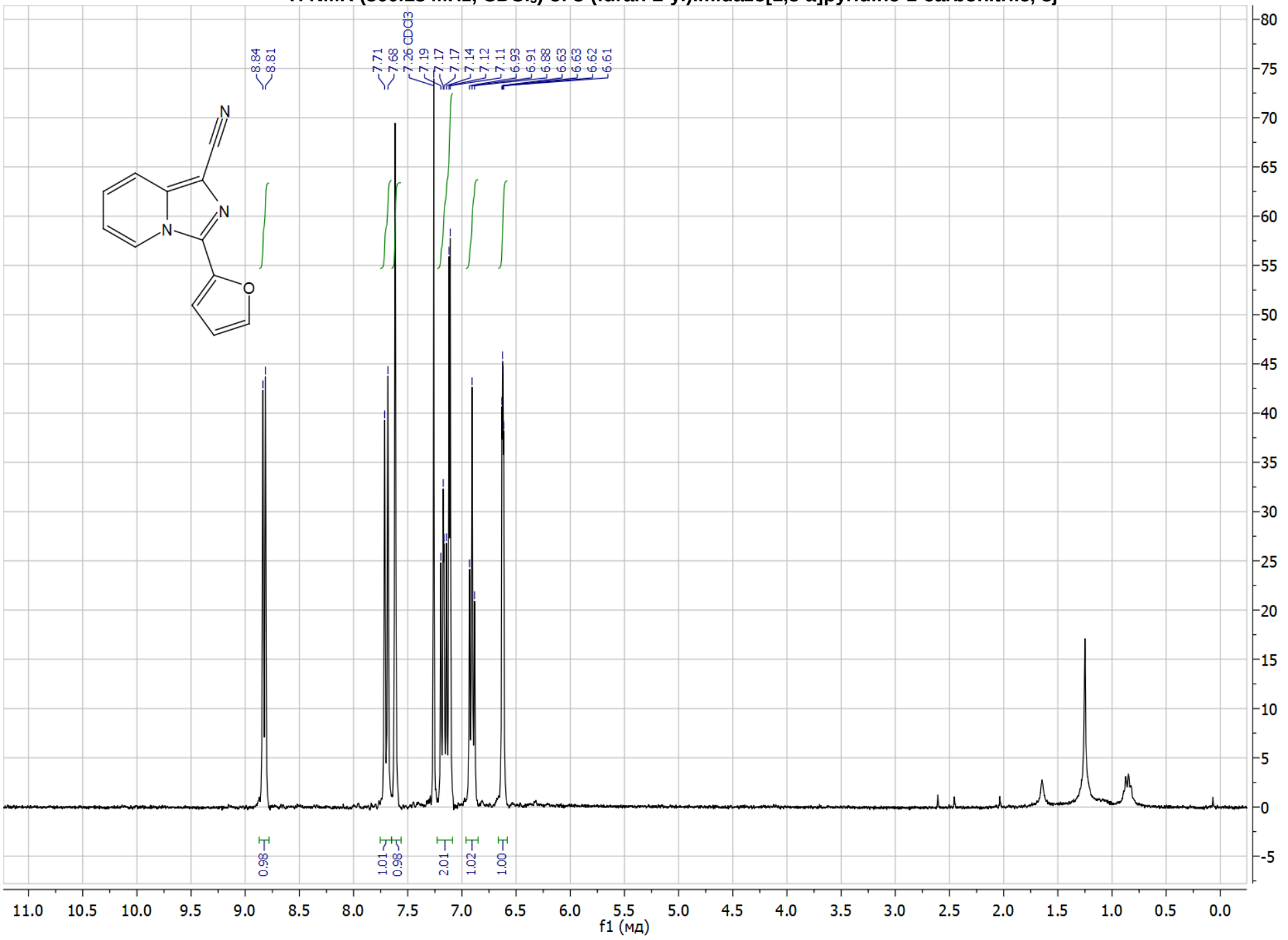
^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(2,4-dichlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3i



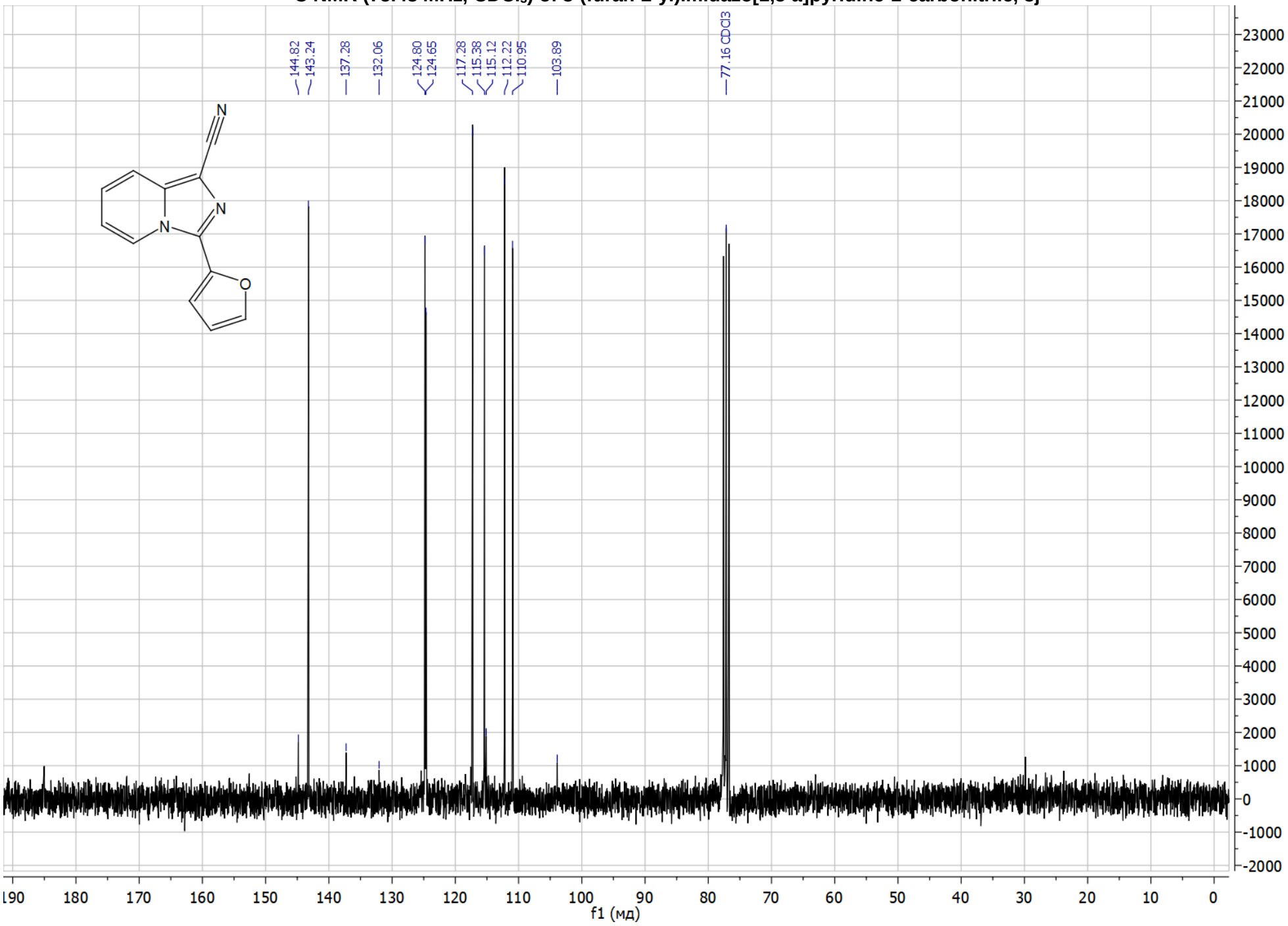
^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(2,4-dichlorophenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3i



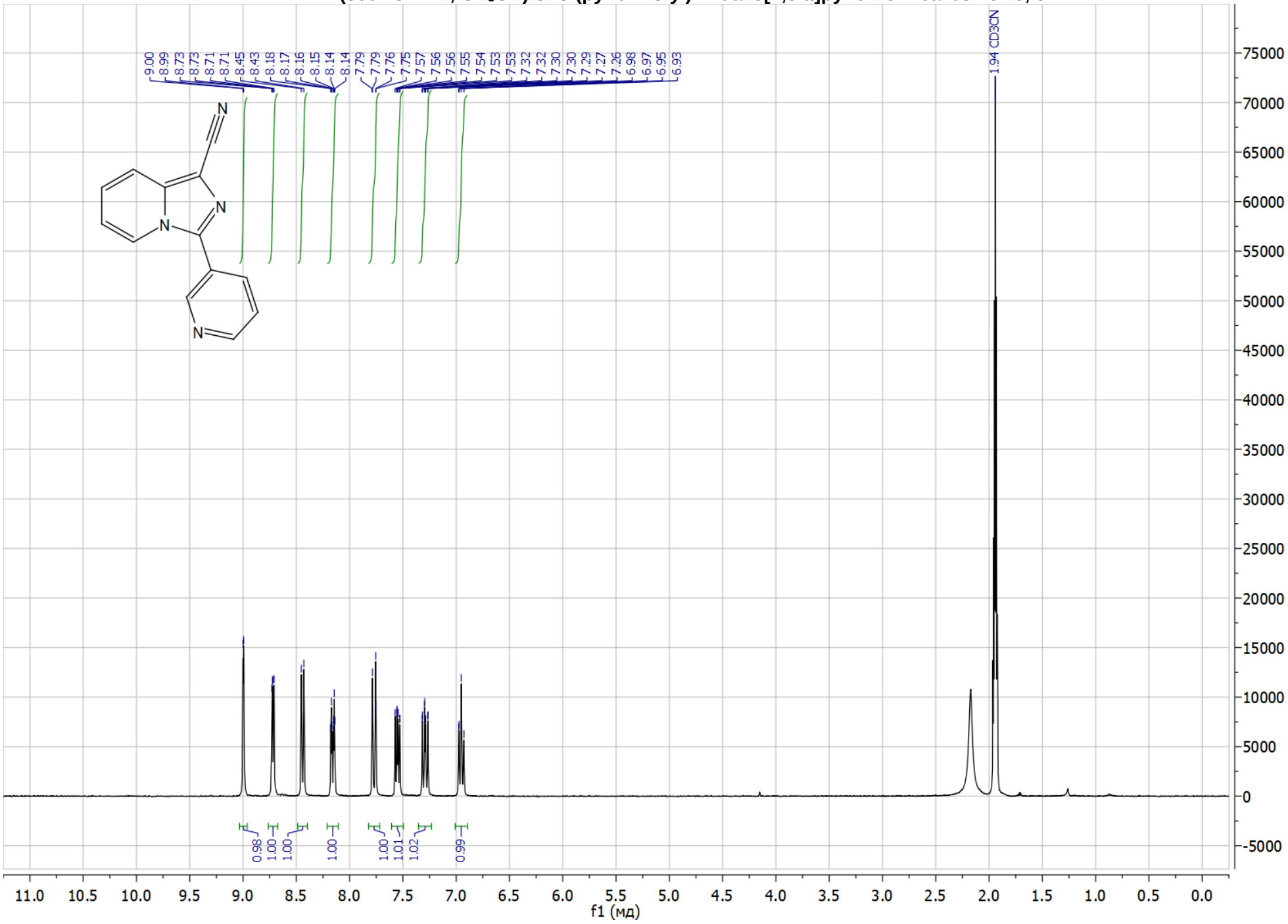
^{1}H NMR (300.13 MHz, $CDCl_3$) of 3-(furan-2-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3j



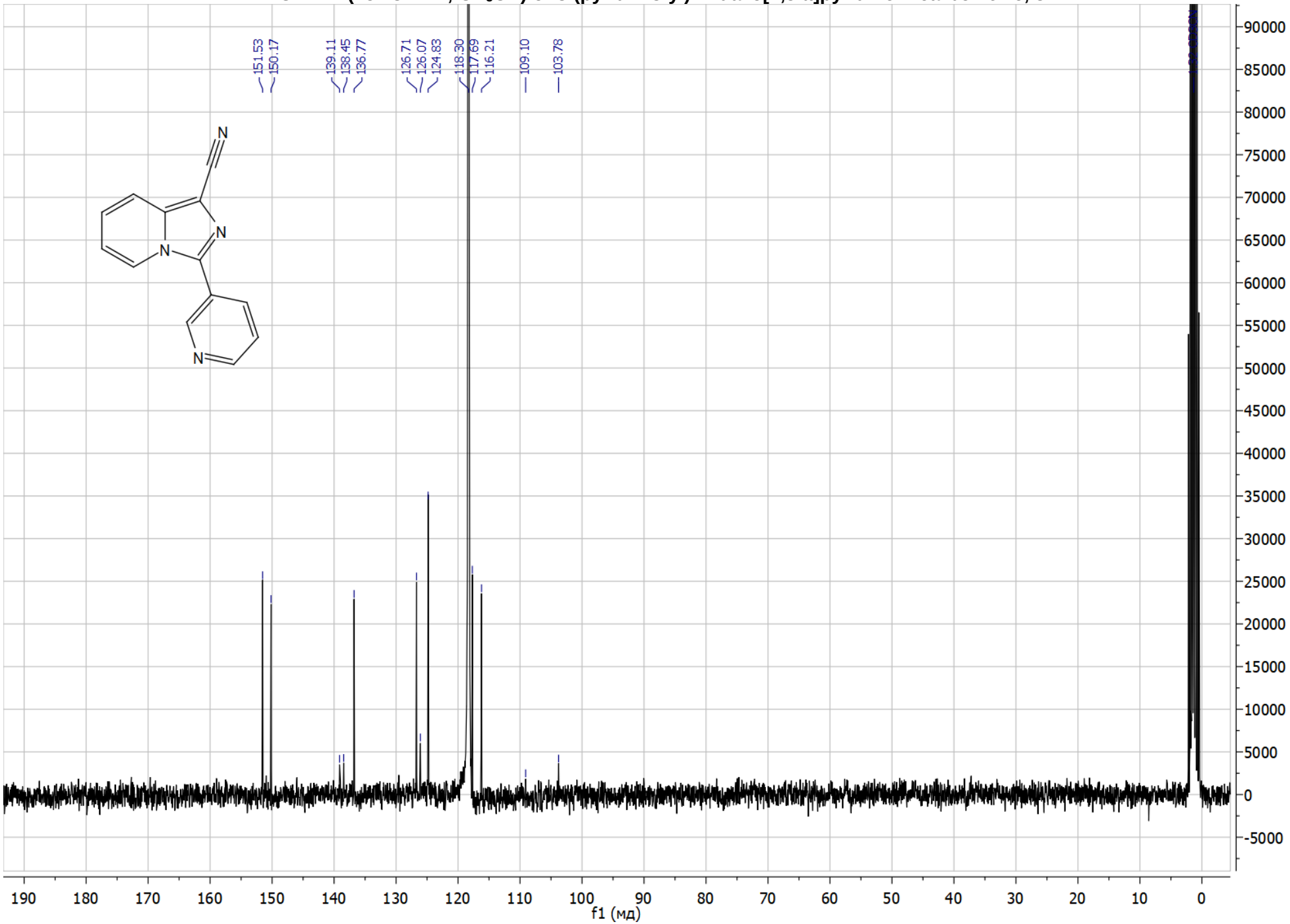
^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-(furan-2-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3j



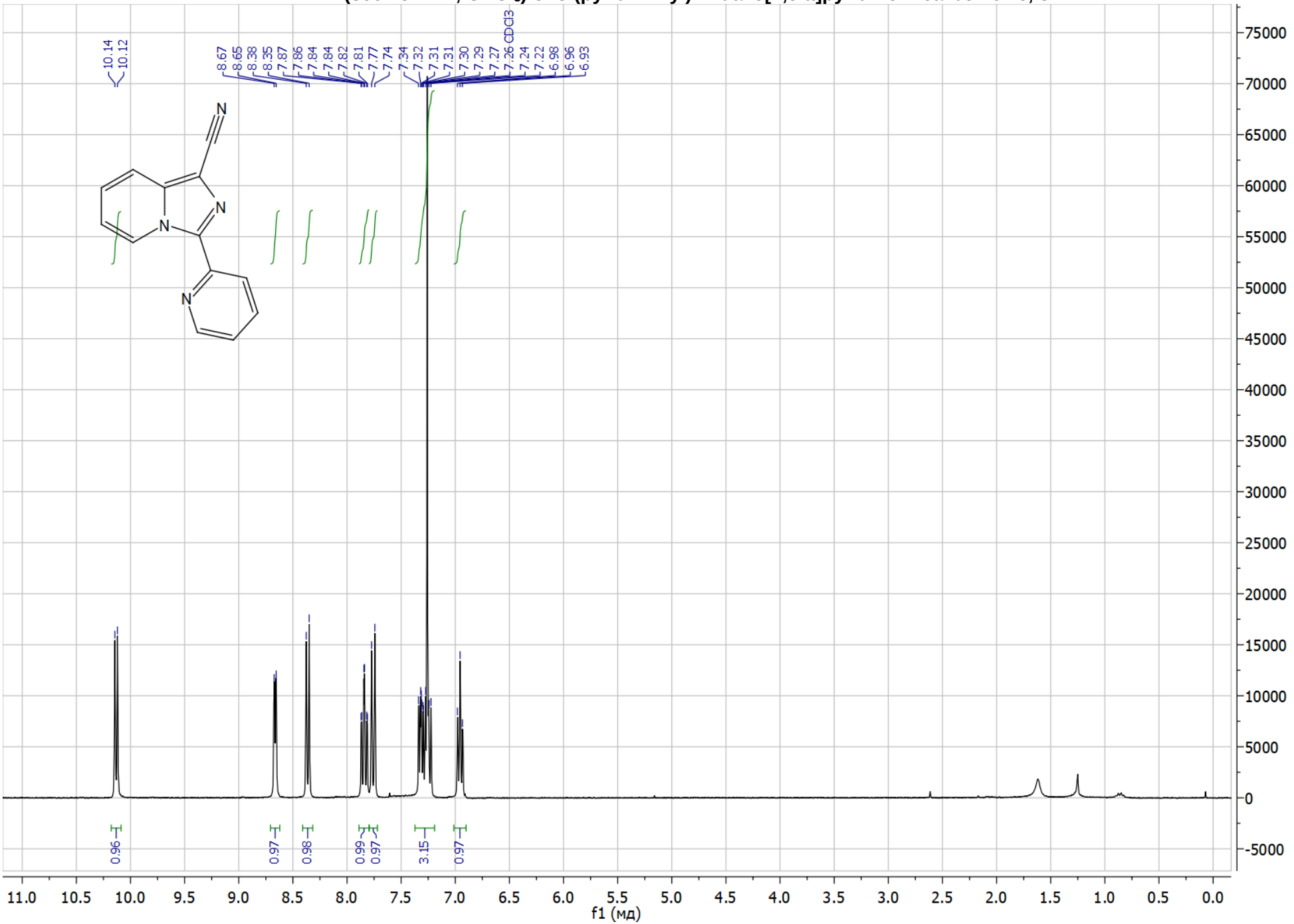
^{1}H NMR (300.13 MHz, CD_3CN) of 3-(pyridin-3-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3k



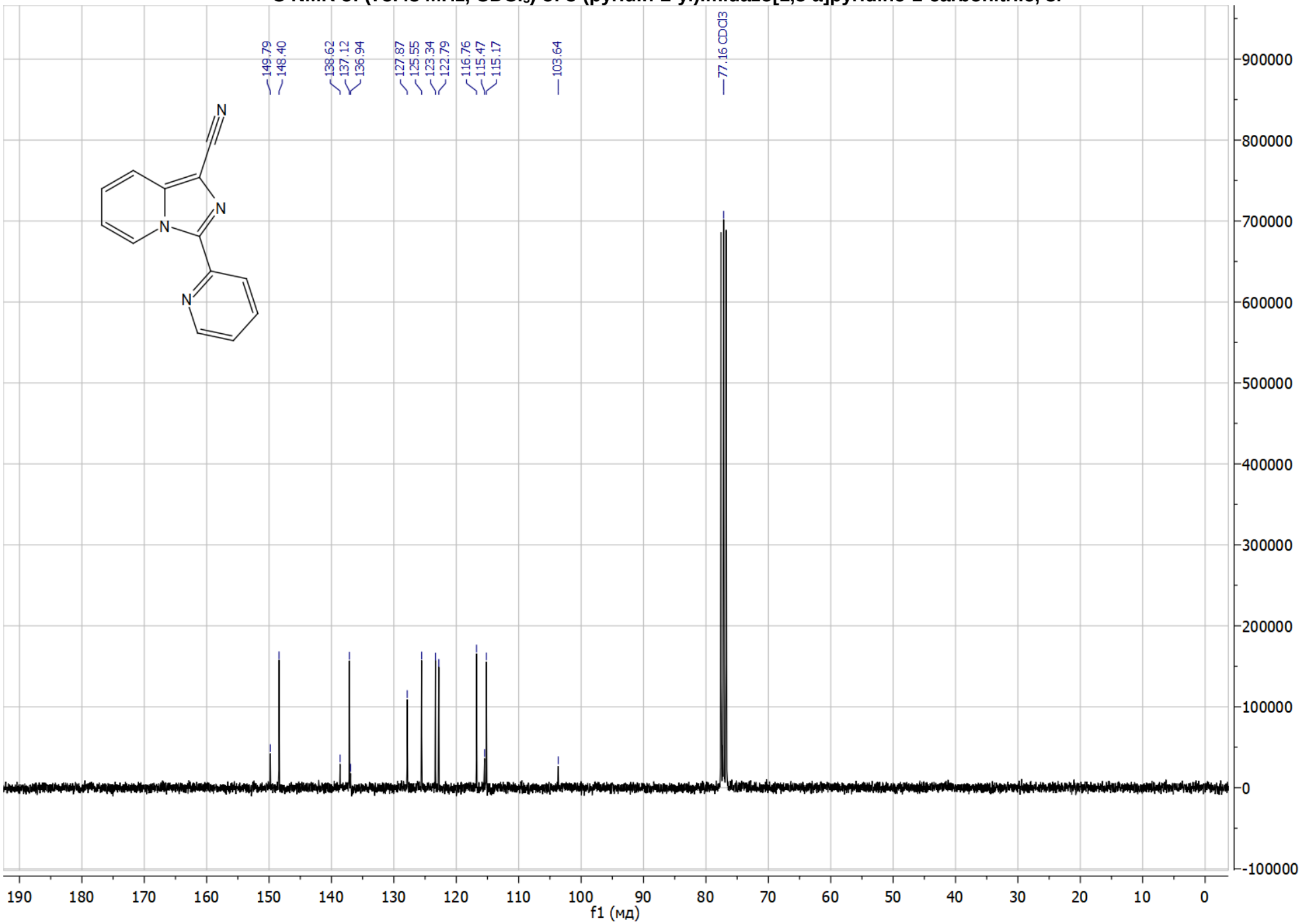
^{13}C NMR (75.48 MHz, CD_3CN) of 3-(pyridin-3-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3k



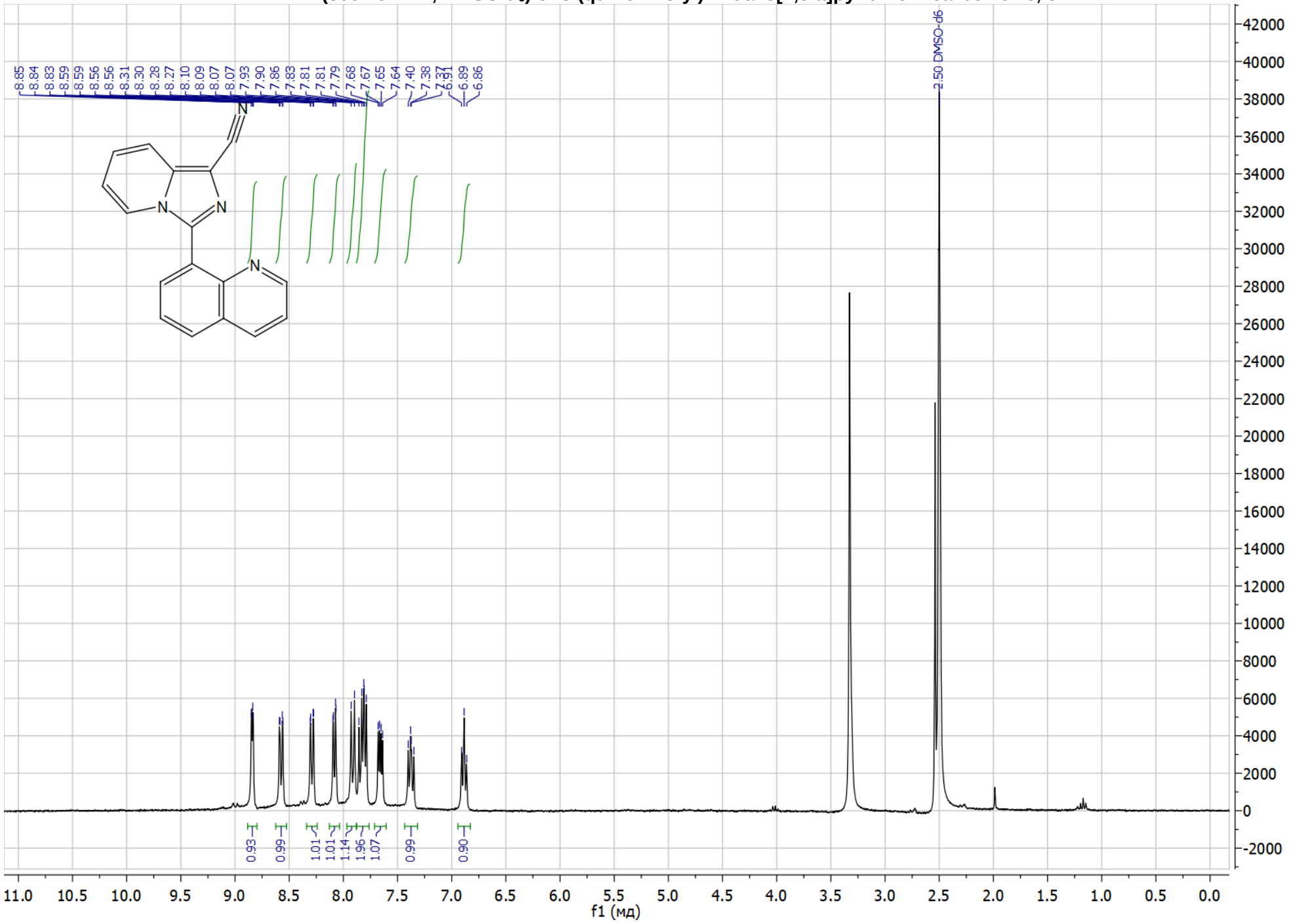
^{1}H NMR (300.13 MHz, $CDCl_3$) of 3-(pyridin-2-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3l



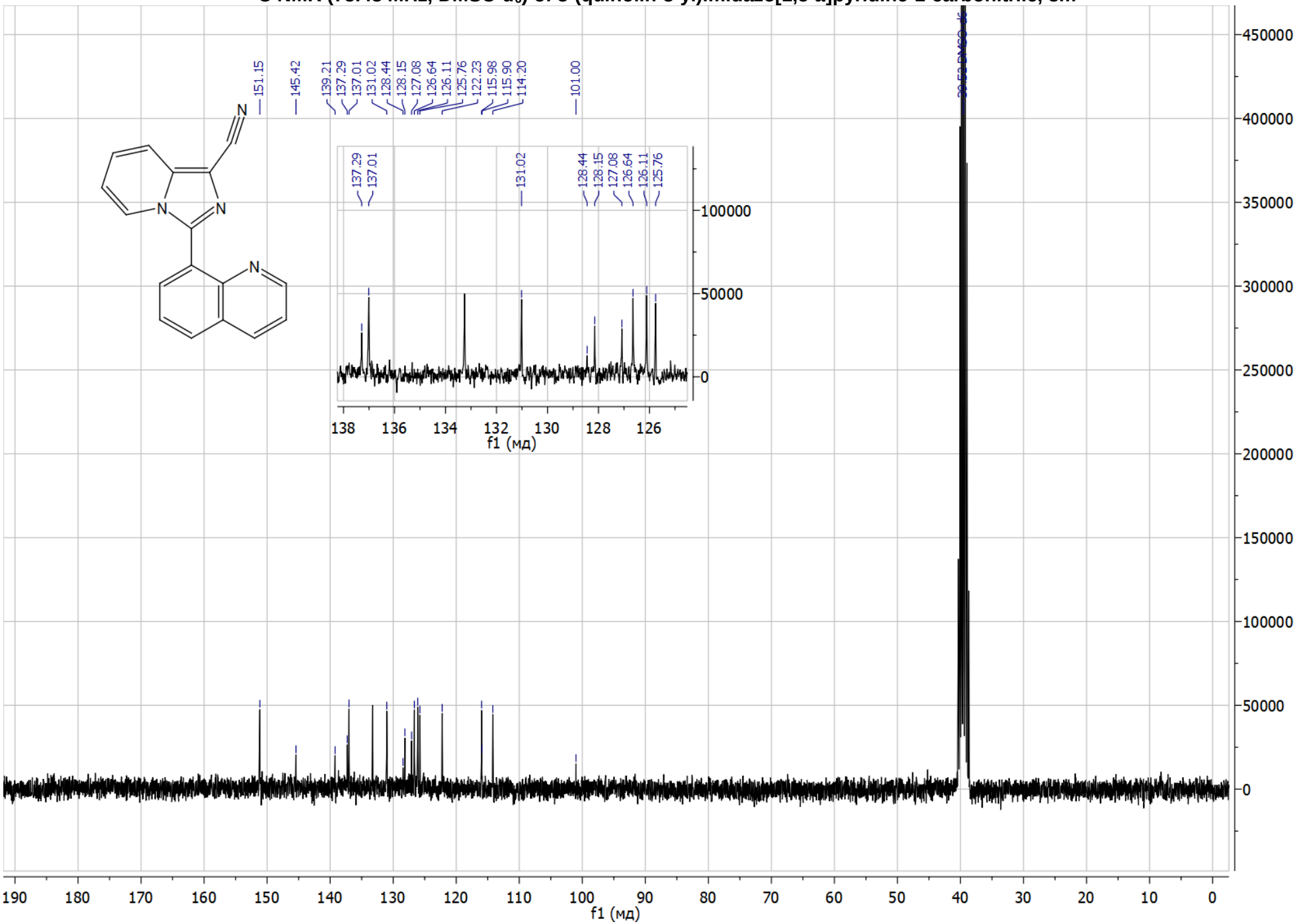
^{13}C NMR of (75.48 MHz, $CDCl_3$) of 3-(pyridin-2-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3l



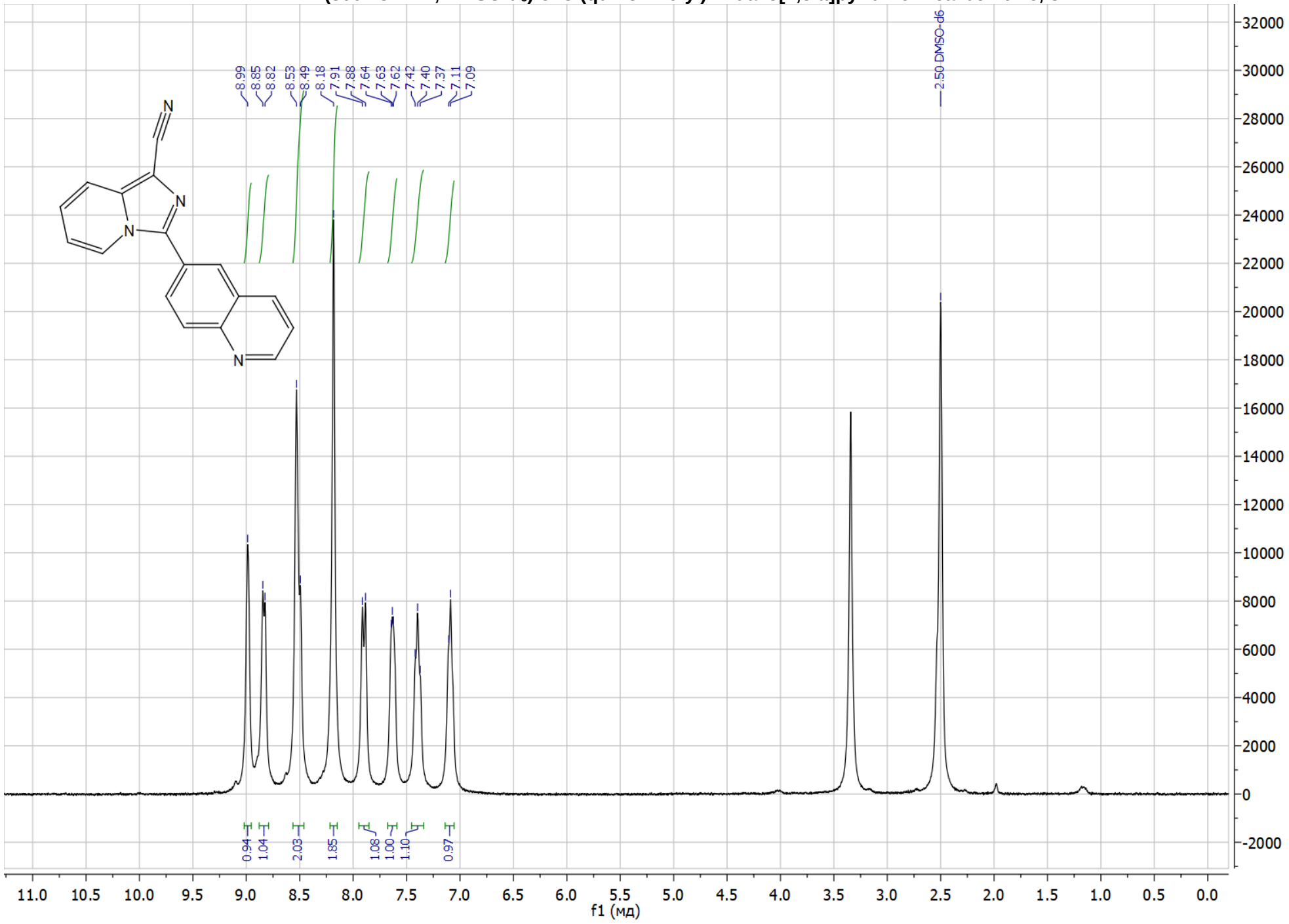
^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(quinolin-8-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3m



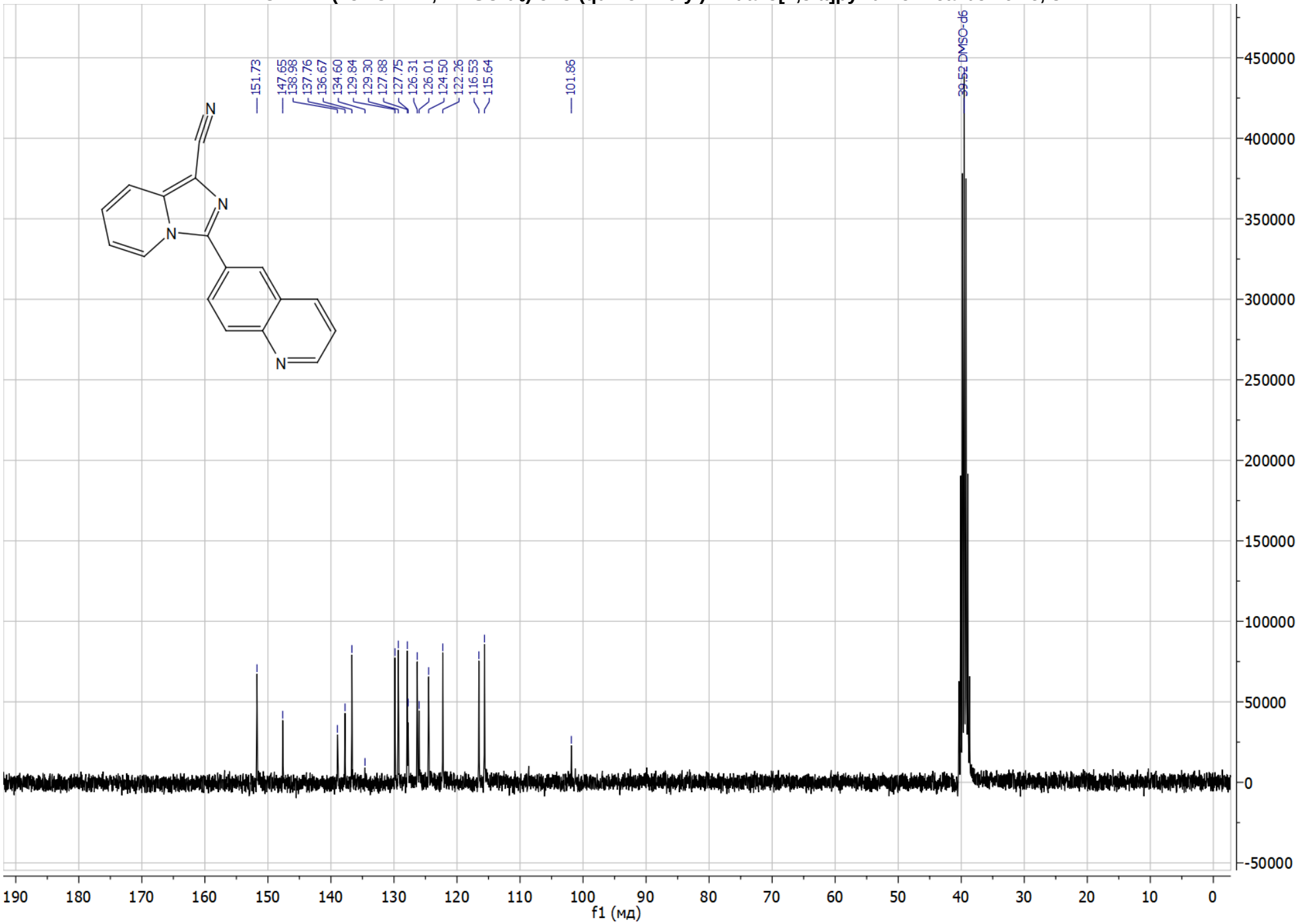
^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(quinolin-8-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3m



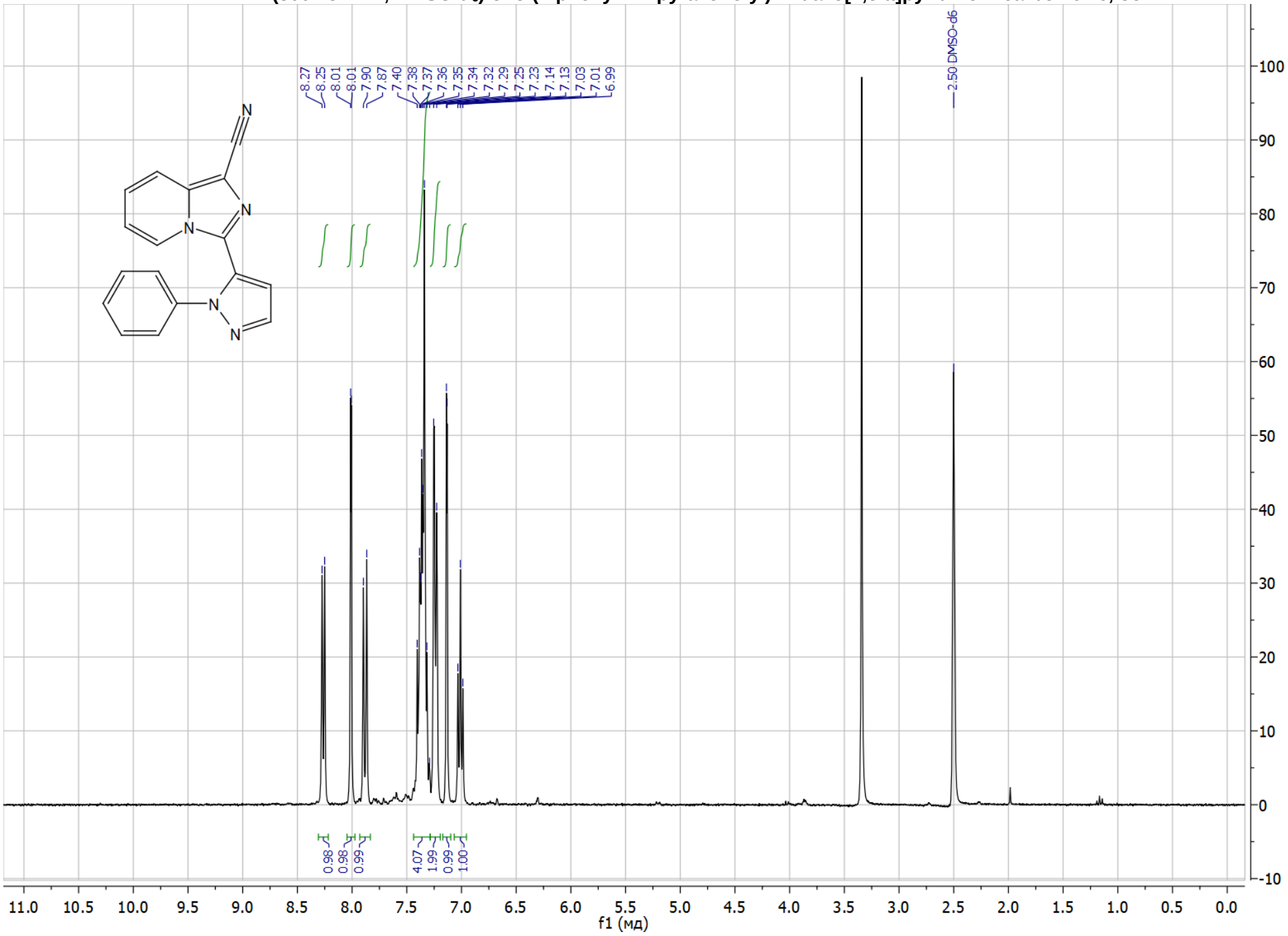
^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(quinolin-6-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3n



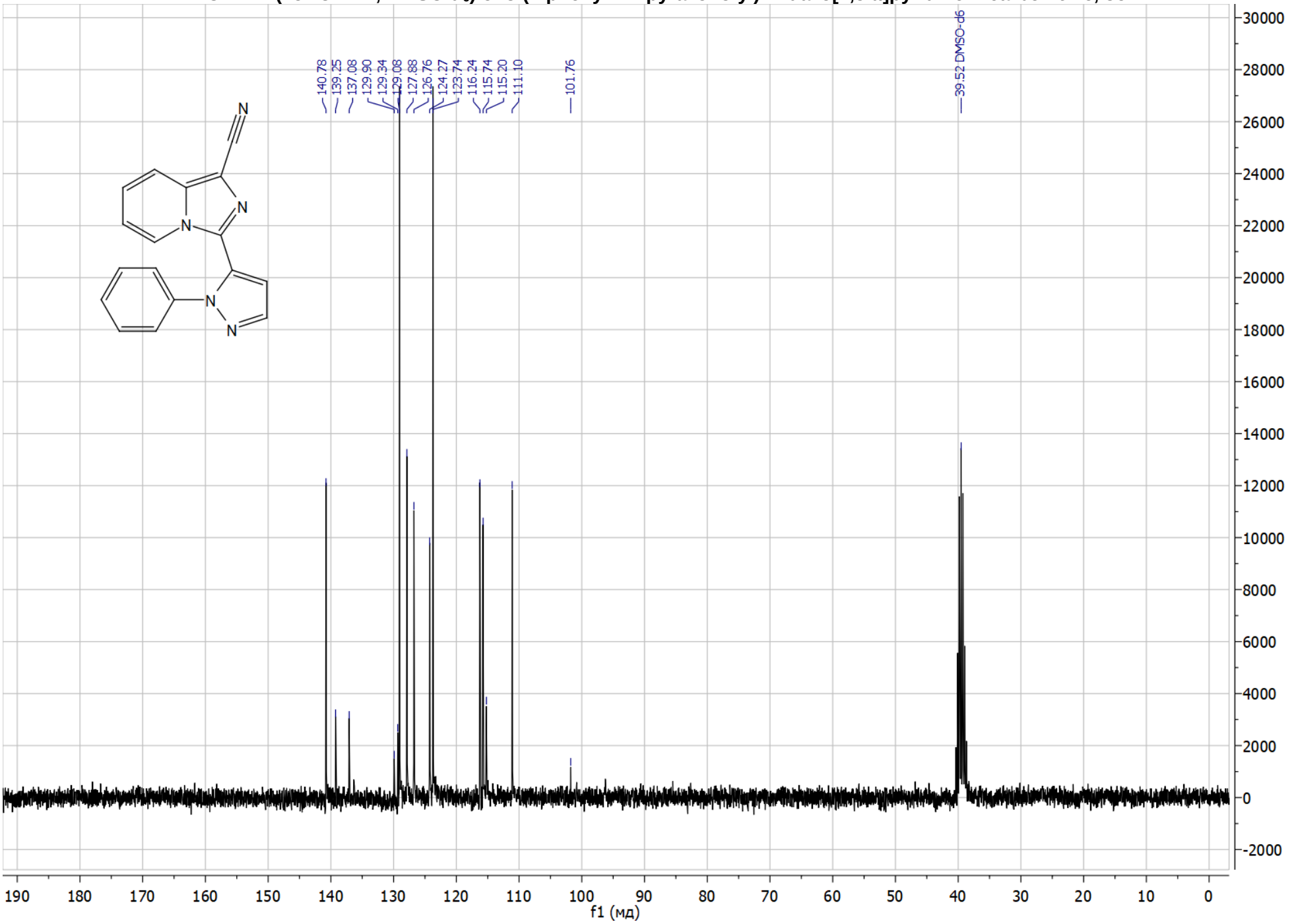
^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(quinolin-6-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3n



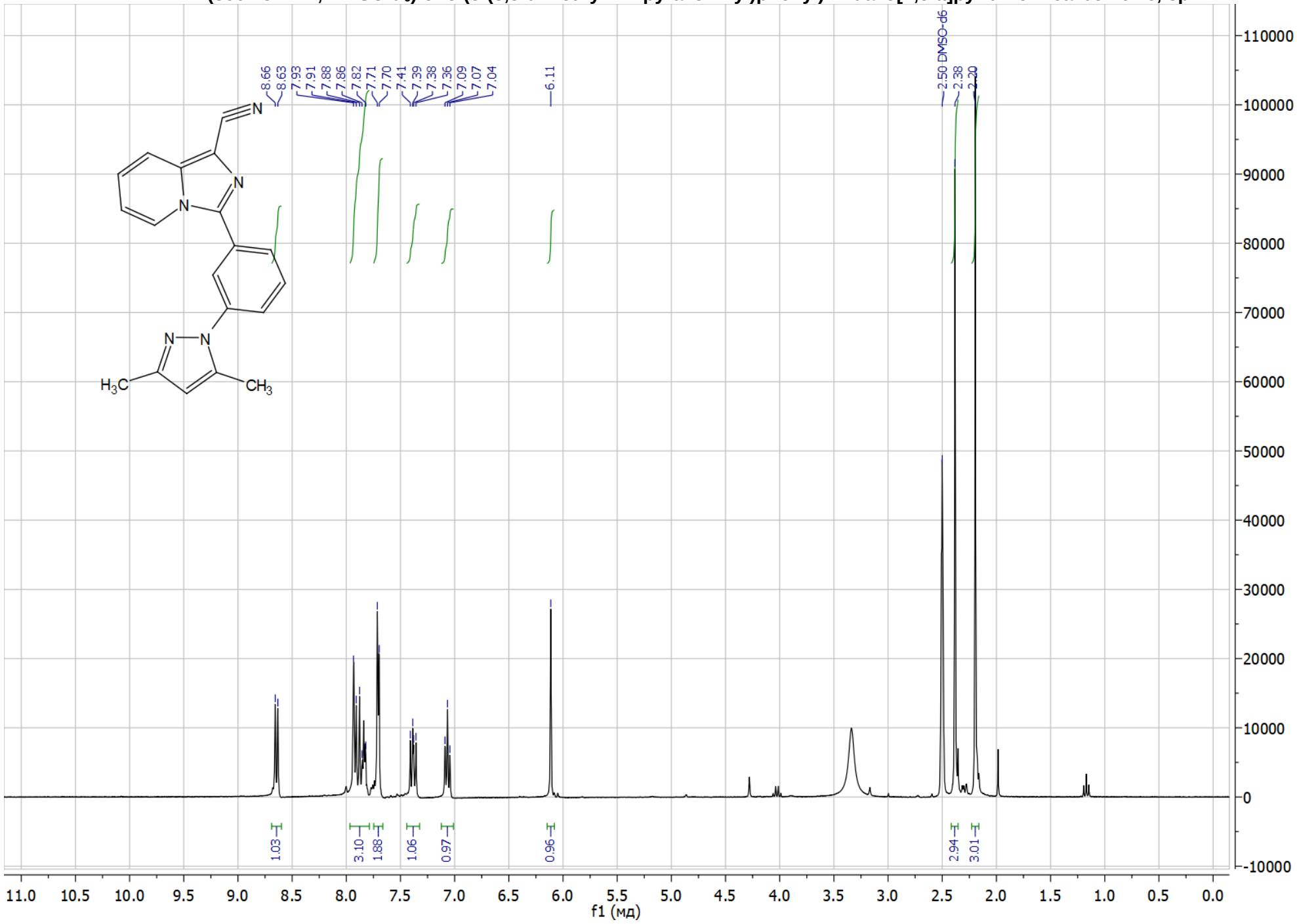
^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(1-phenyl-1H-pyrazol-5-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3o



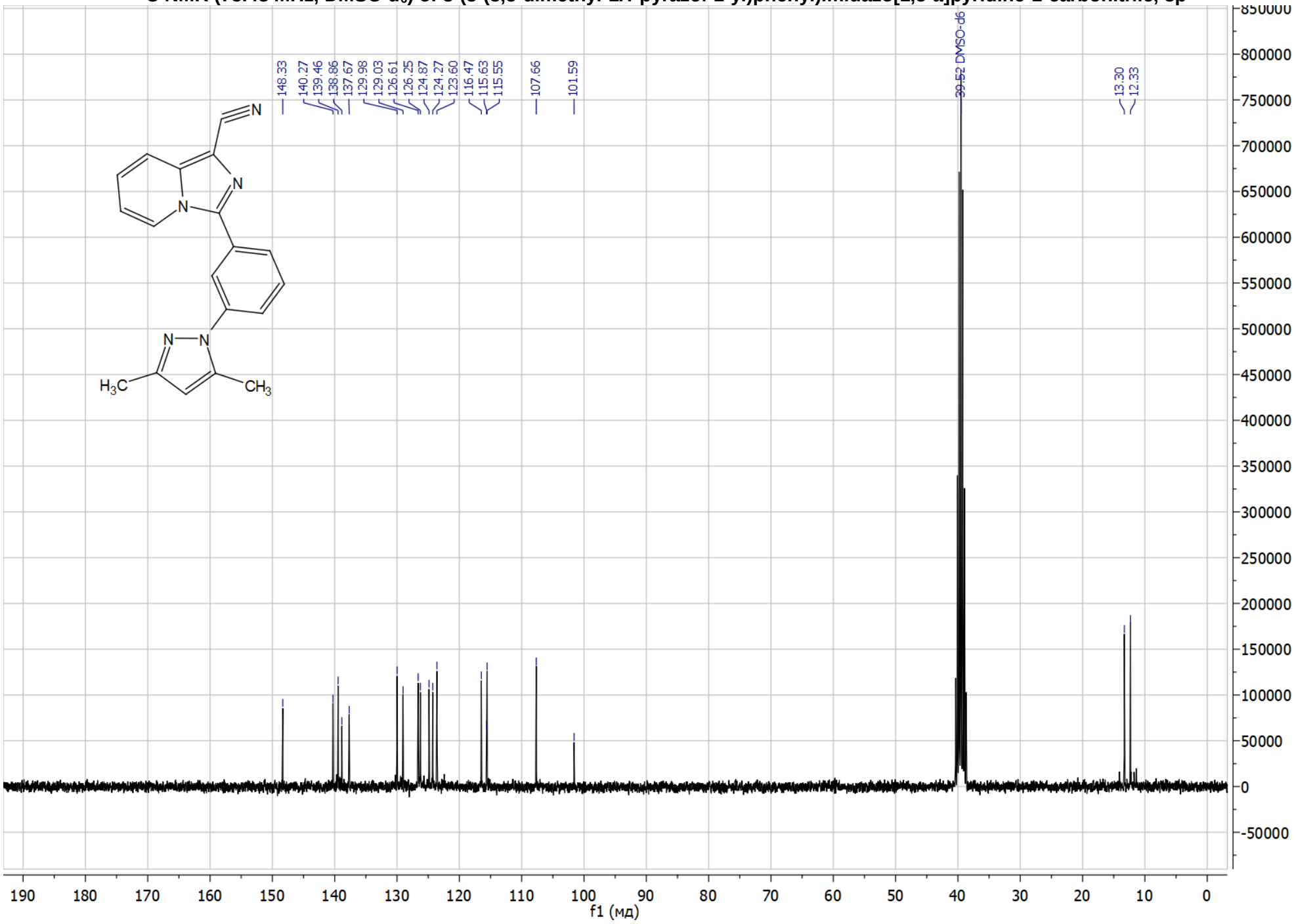
^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(1-phenyl-1H-pyrazol-5-yl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3o



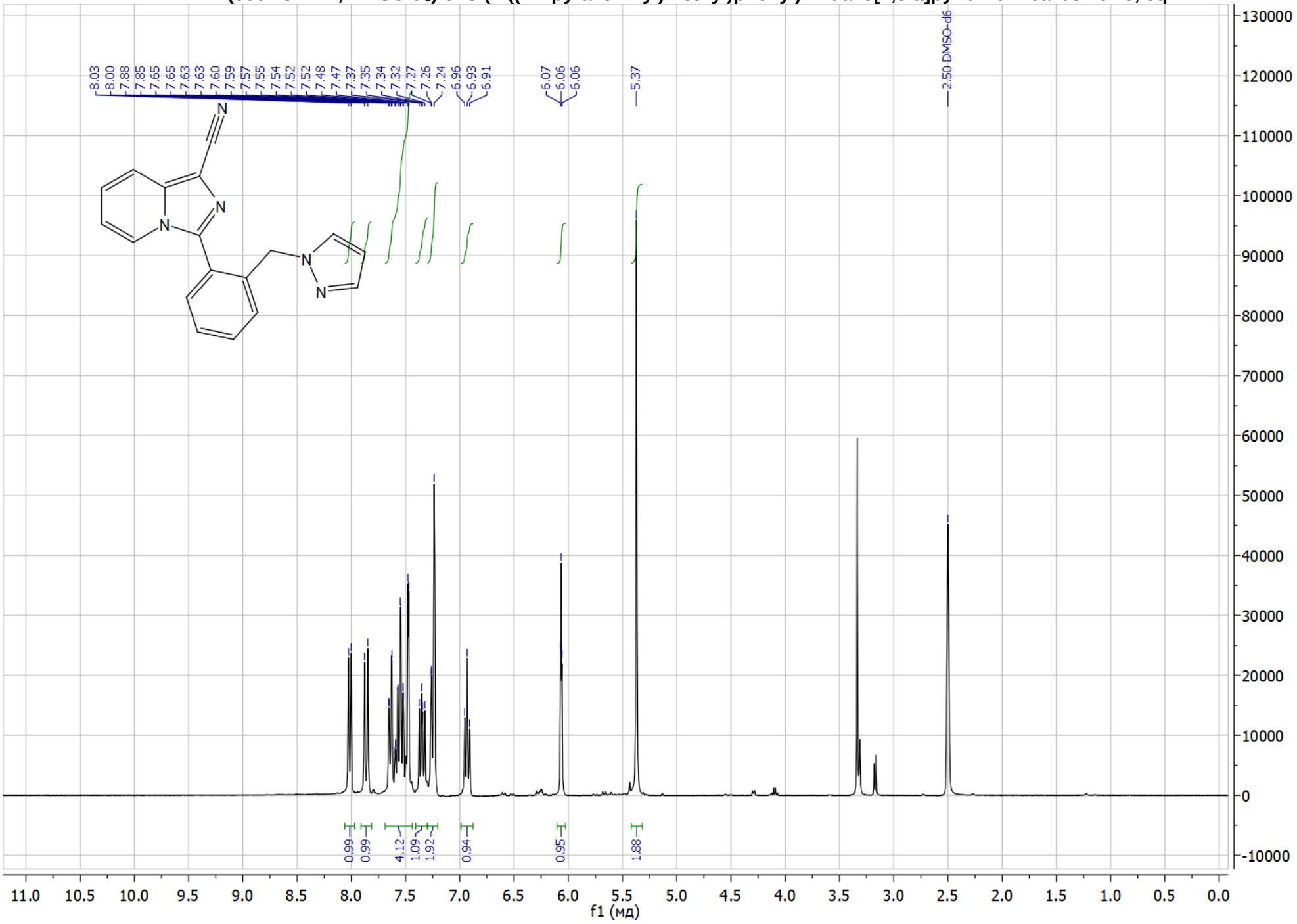
^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(3-(3,5-dimethyl-1*H*-pyrazol-1-yl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3p



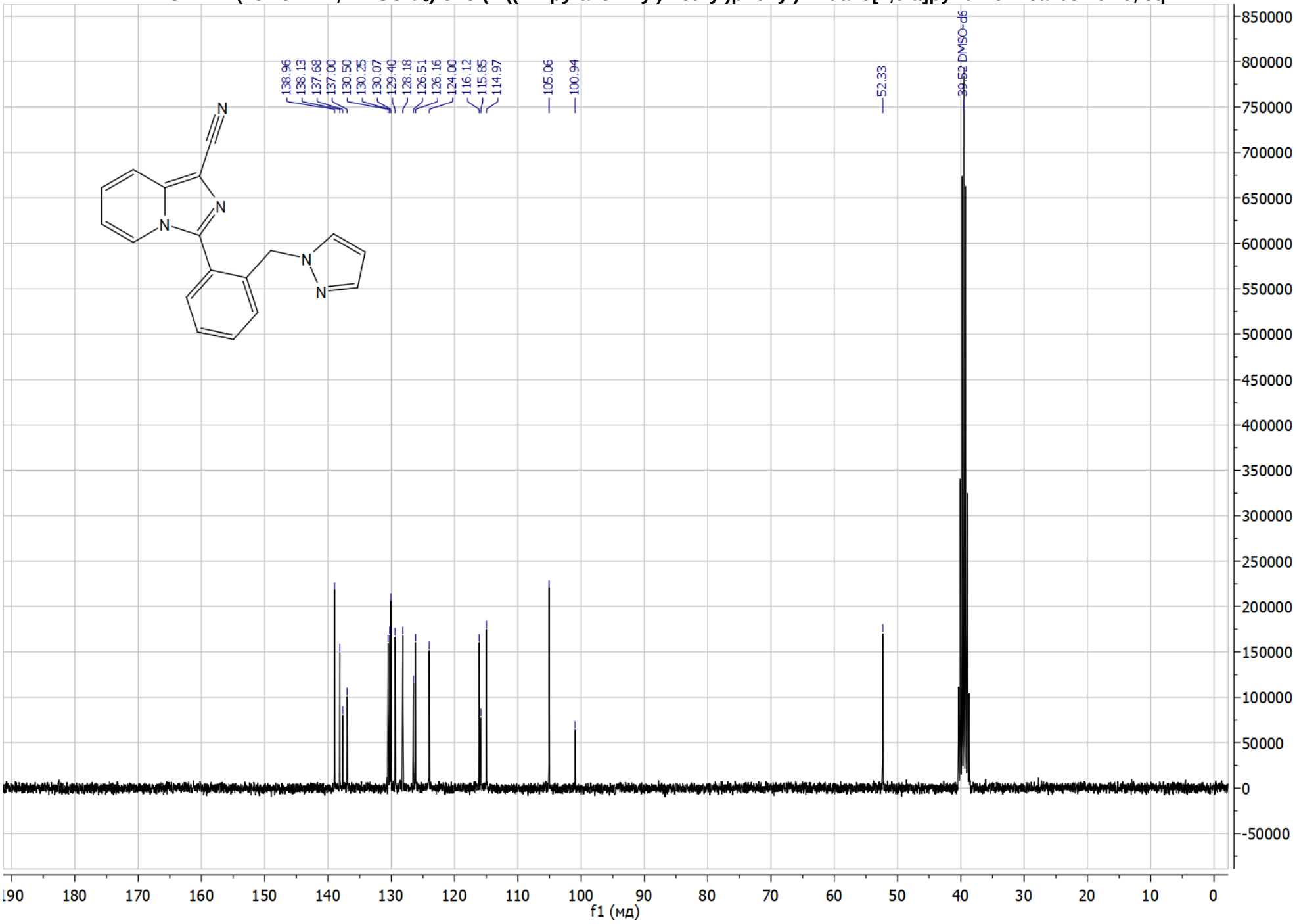
^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(3-(3,5-dimethyl-1*H*-pyrazol-1-yl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3p



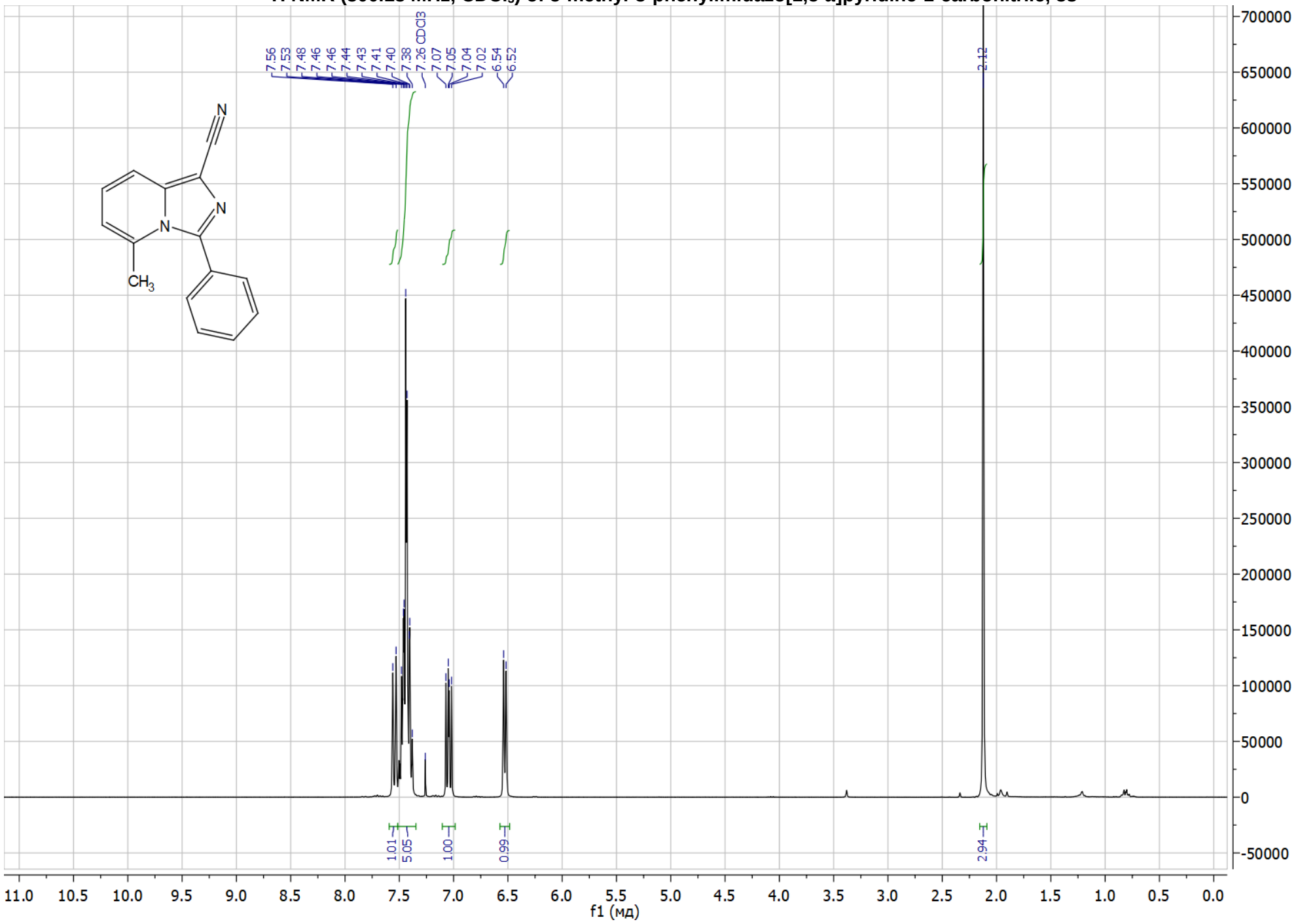
^{1}H NMR (300.13 MHz, DMSO-d_6) of 3-(2-((1*H*-pyrazol-1-yl)methyl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3q



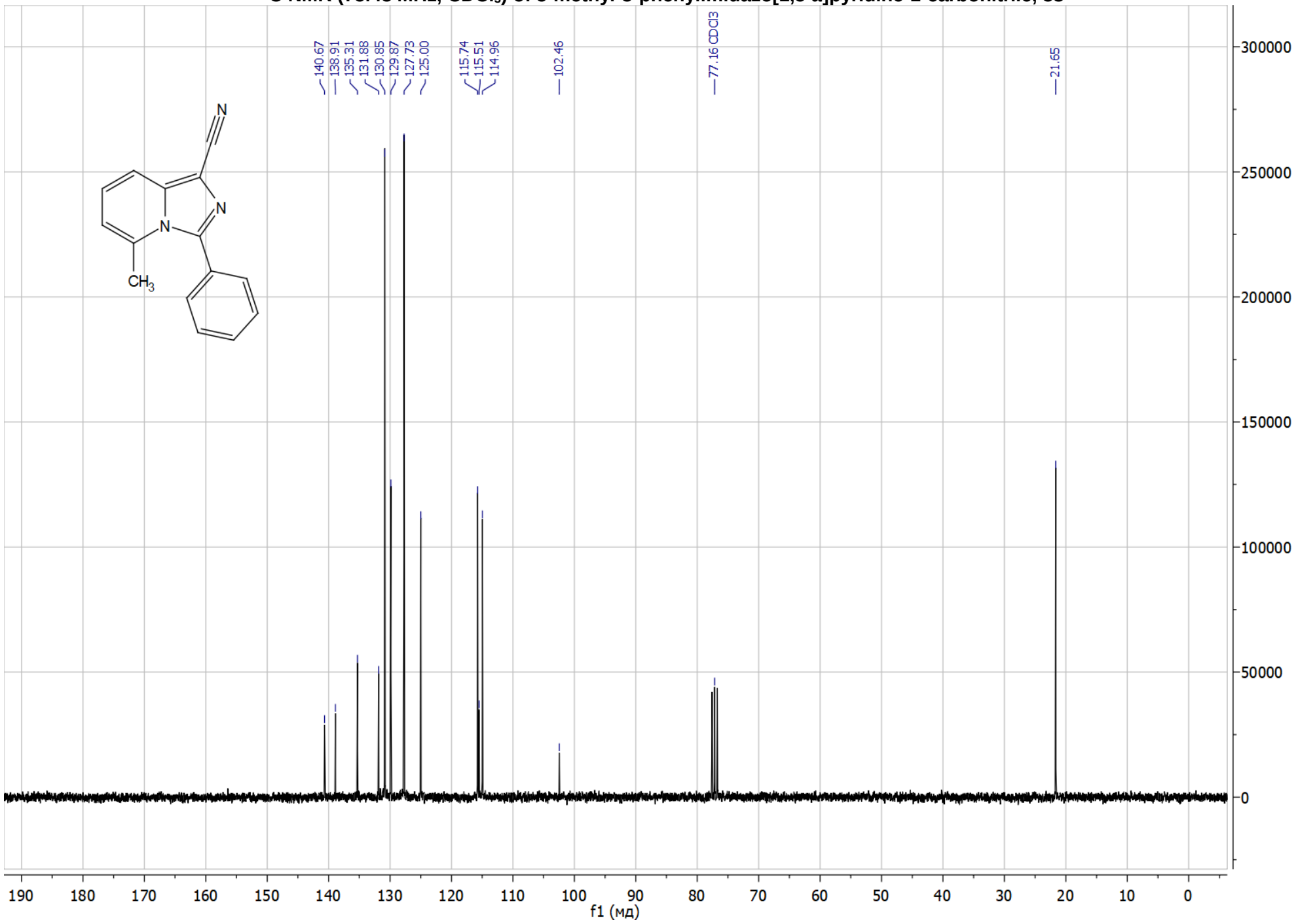
^{13}C NMR (75.48 MHz, DMSO-d_6) of 3-(2-((1*H*-pyrazol-1-yl)methyl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3q



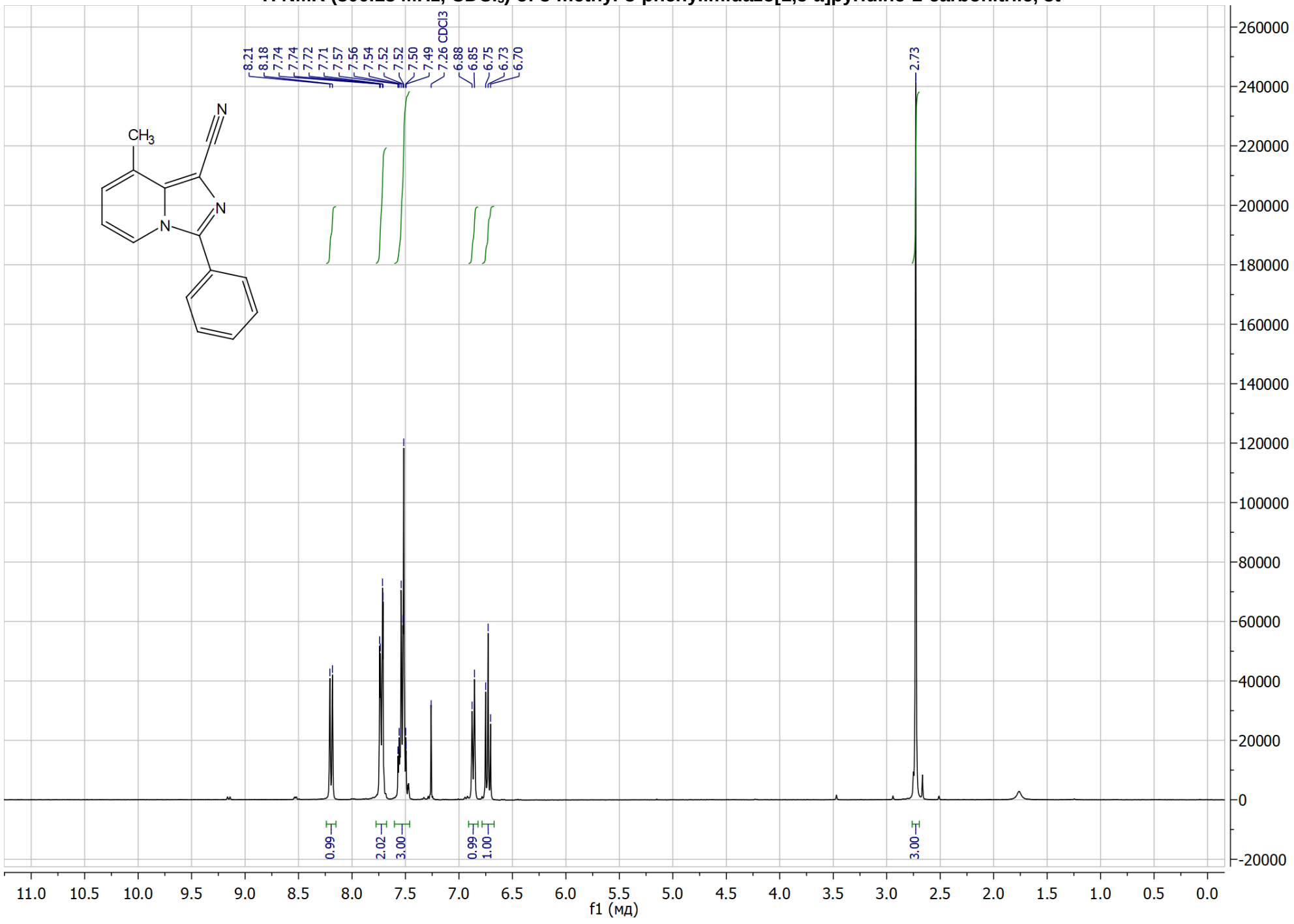
^{1}H NMR (300.13 MHz, $CDCl_3$) of 5-methyl-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3s



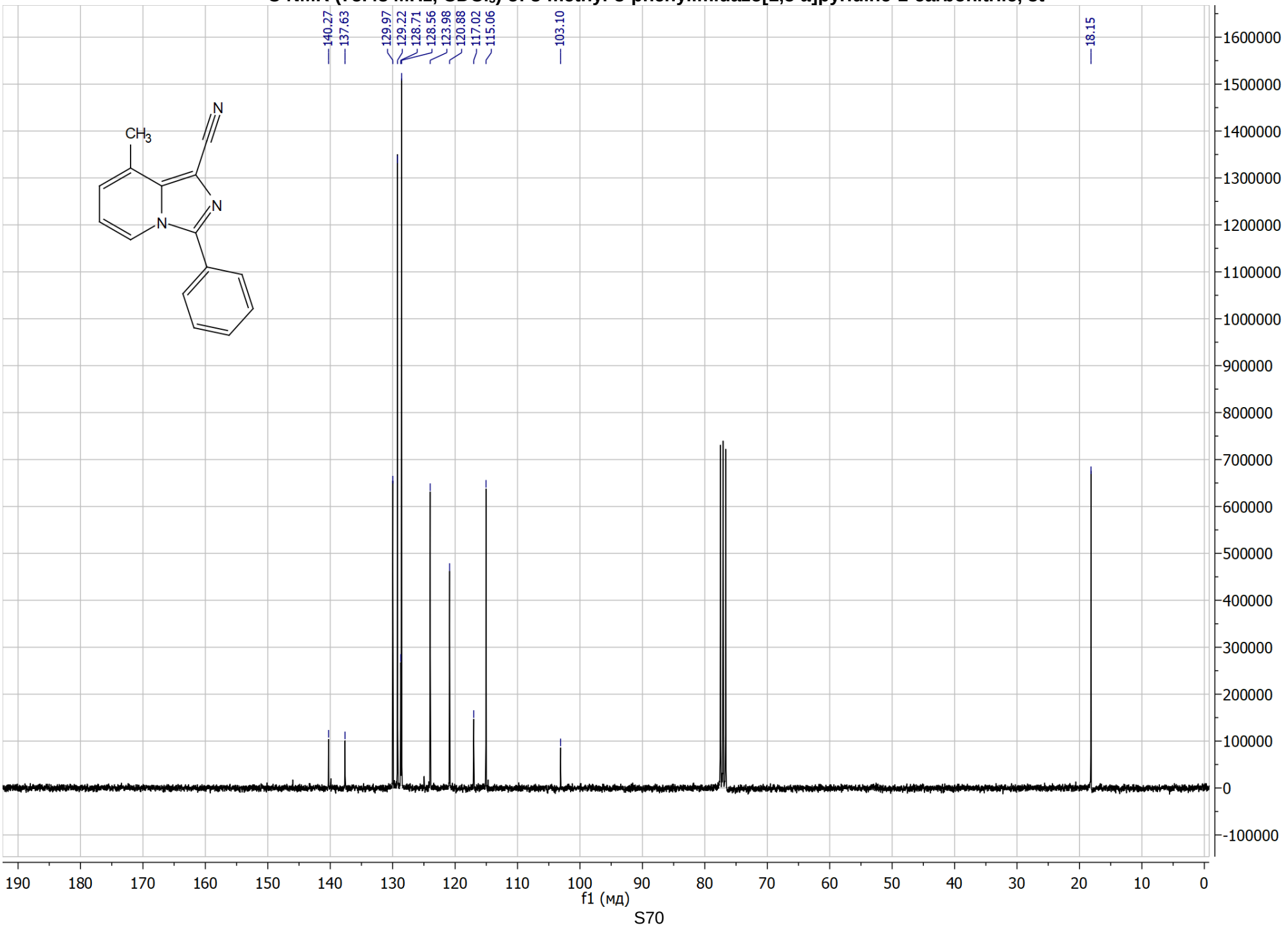
^{13}C NMR (75.48 MHz, $CDCl_3$) of 5-methyl-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3s



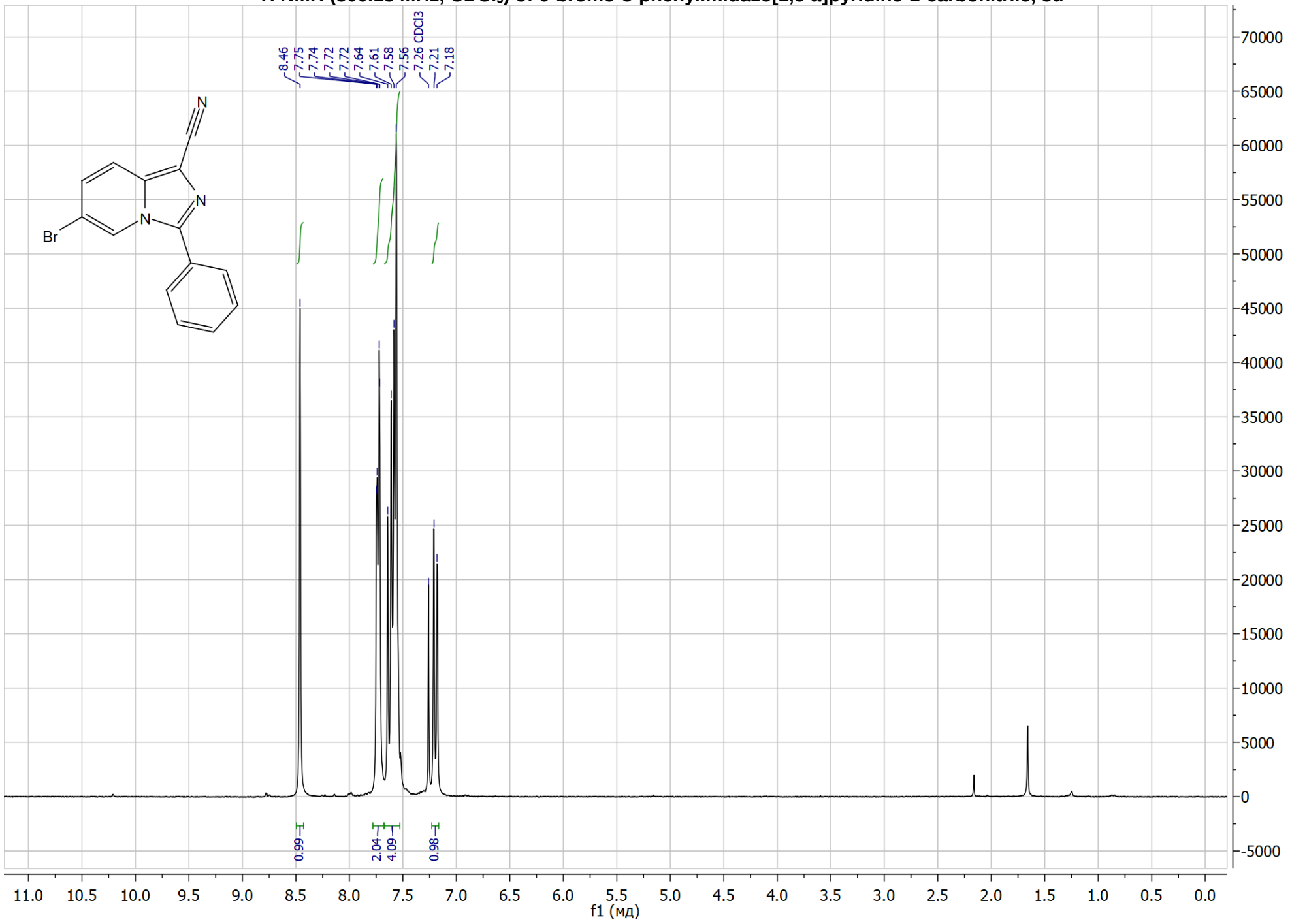
^{1}H NMR (300.13 MHz, $CDCl_3$) of 8-methyl-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3t



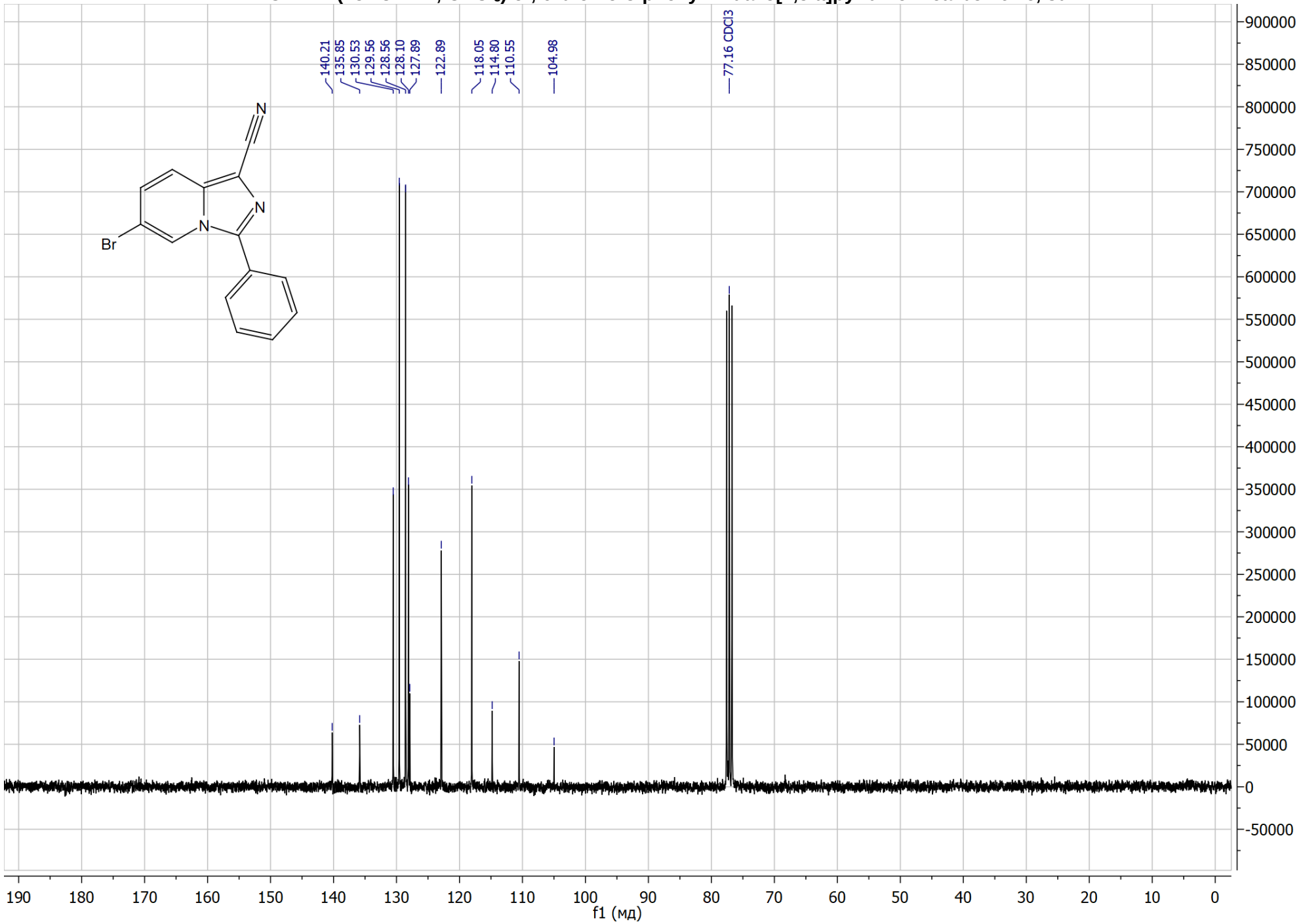
^{13}C NMR (75.48 MHz, $CDCl_3$) of 8-methyl-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3t



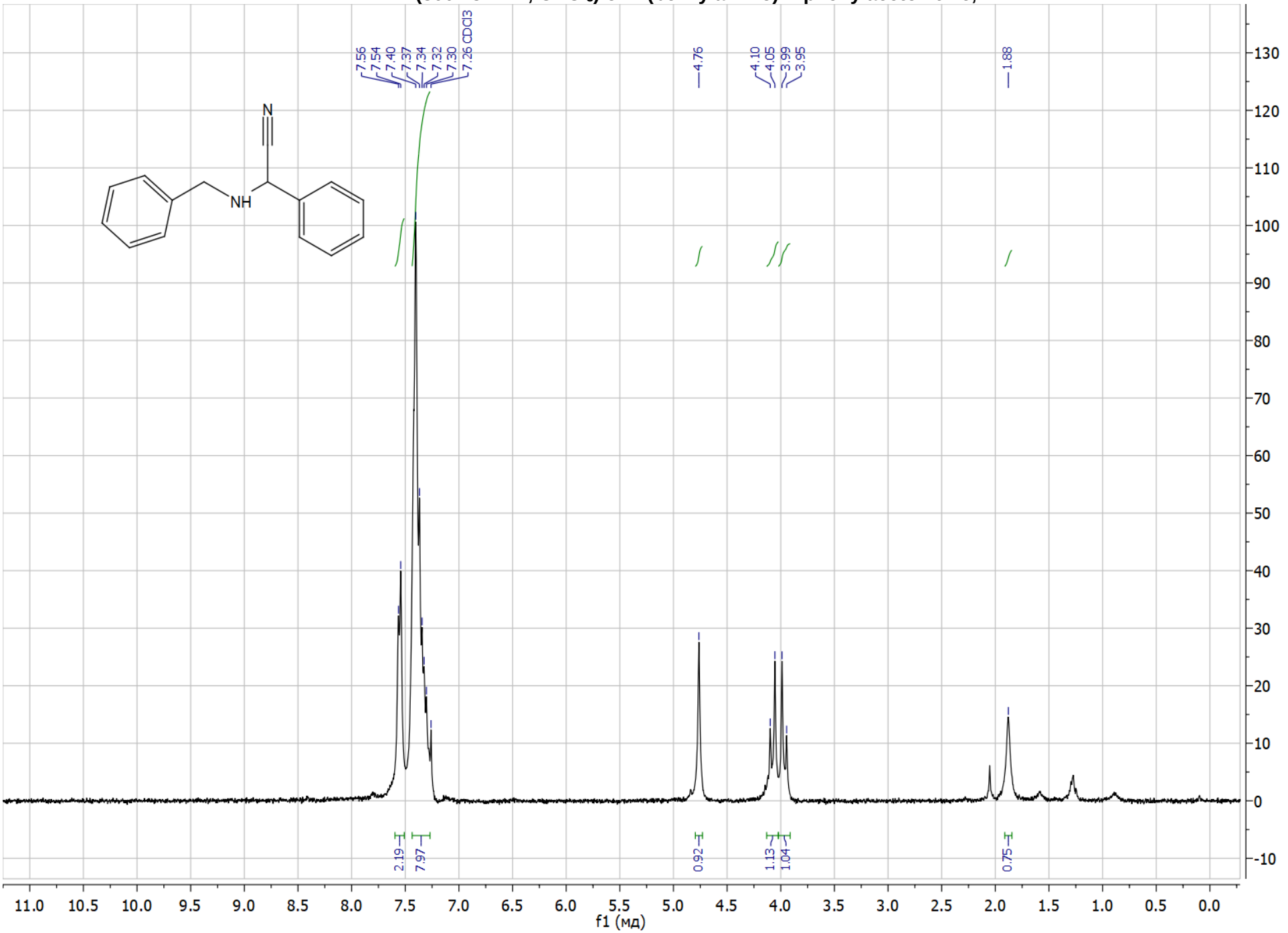
^{1}H NMR (300.13 MHz, $CDCl_3$) of 6-bromo-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3u



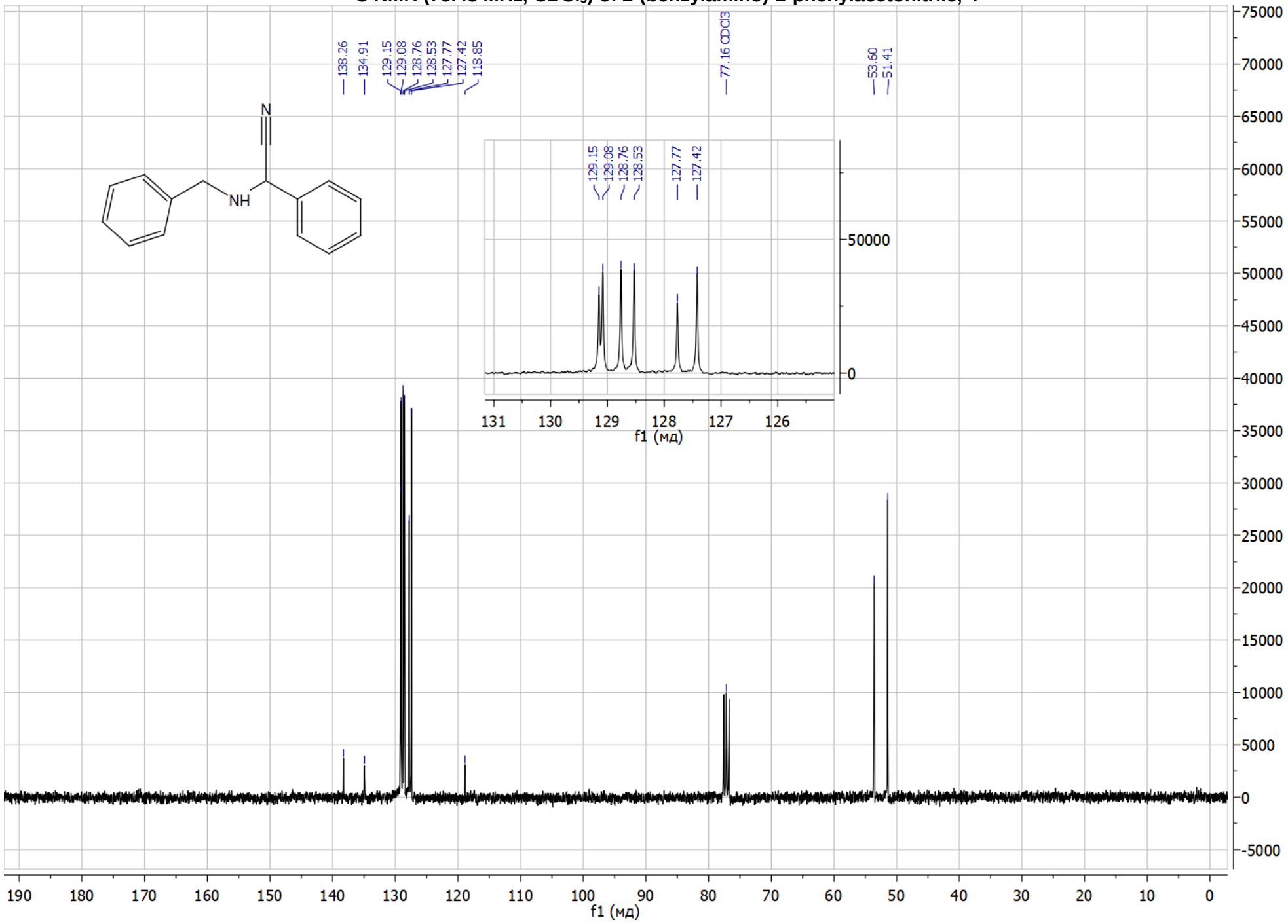
^{13}C NMR (75.48 MHz, $CDCl_3$) of, 6-bromo-3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3u



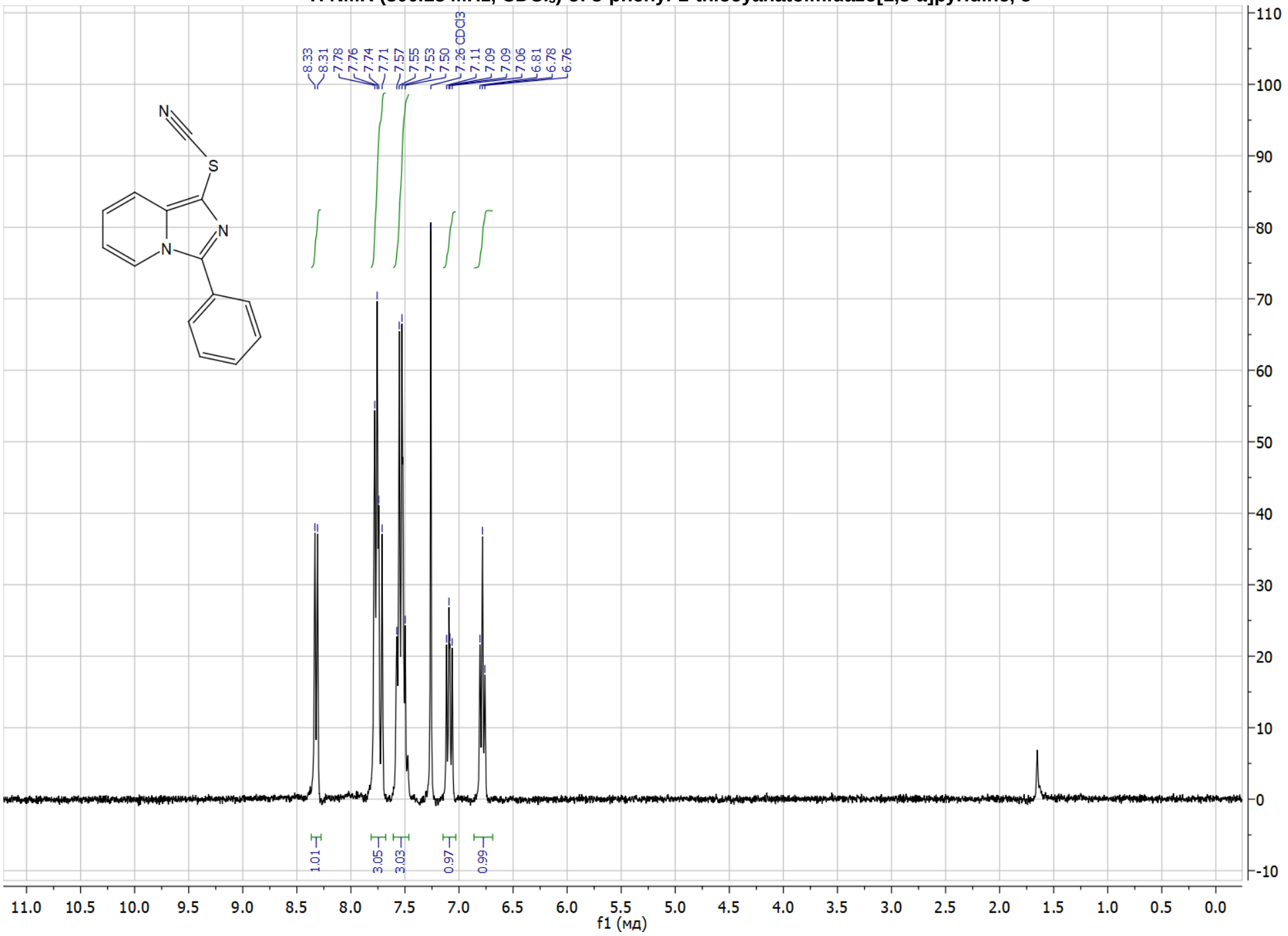
^{1}H NMR (300.13 MHz, $CDCl_3$) of 2-(benzylamino)-2-phenylacetonitrile, 4



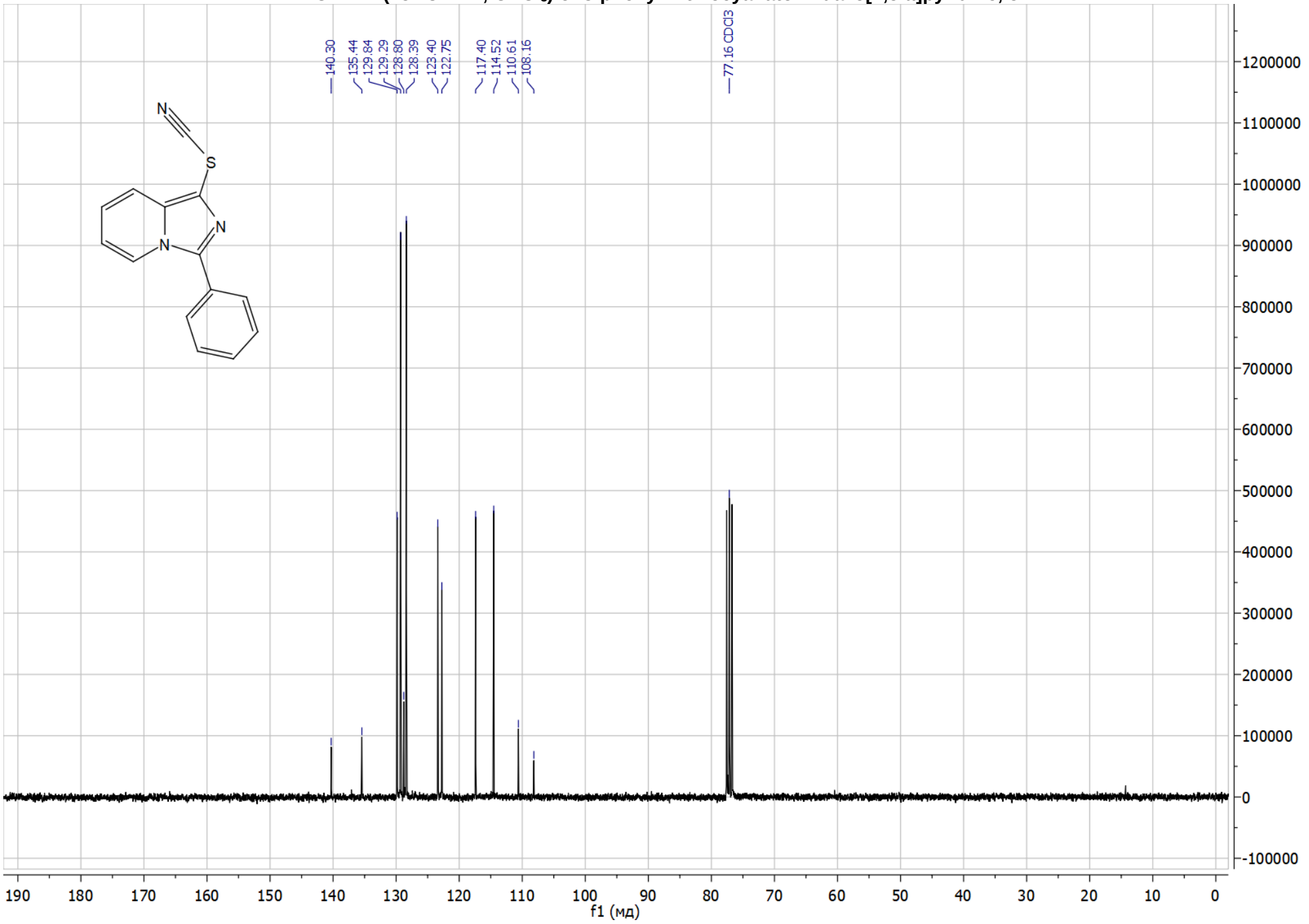
^{13}C NMR (75.48 MHz, $CDCl_3$) of 2-(benzylamino)-2-phenylacetonitrile, 4



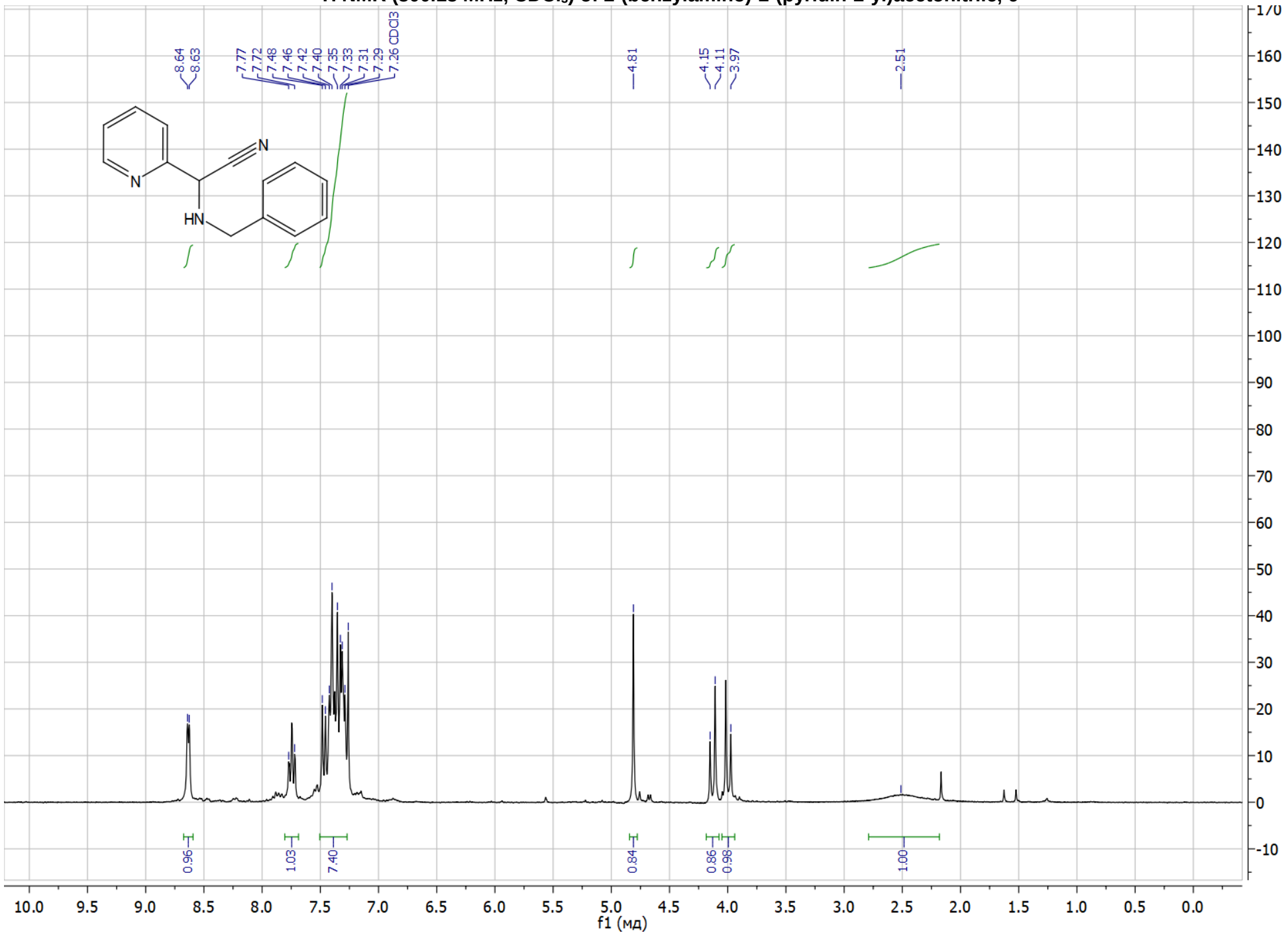
^{1}H NMR (300.13 MHz, $CDCl_3$) of 3-phenyl-1-thiocyanatoimidazo[1,5-*a*]pyridine, 5



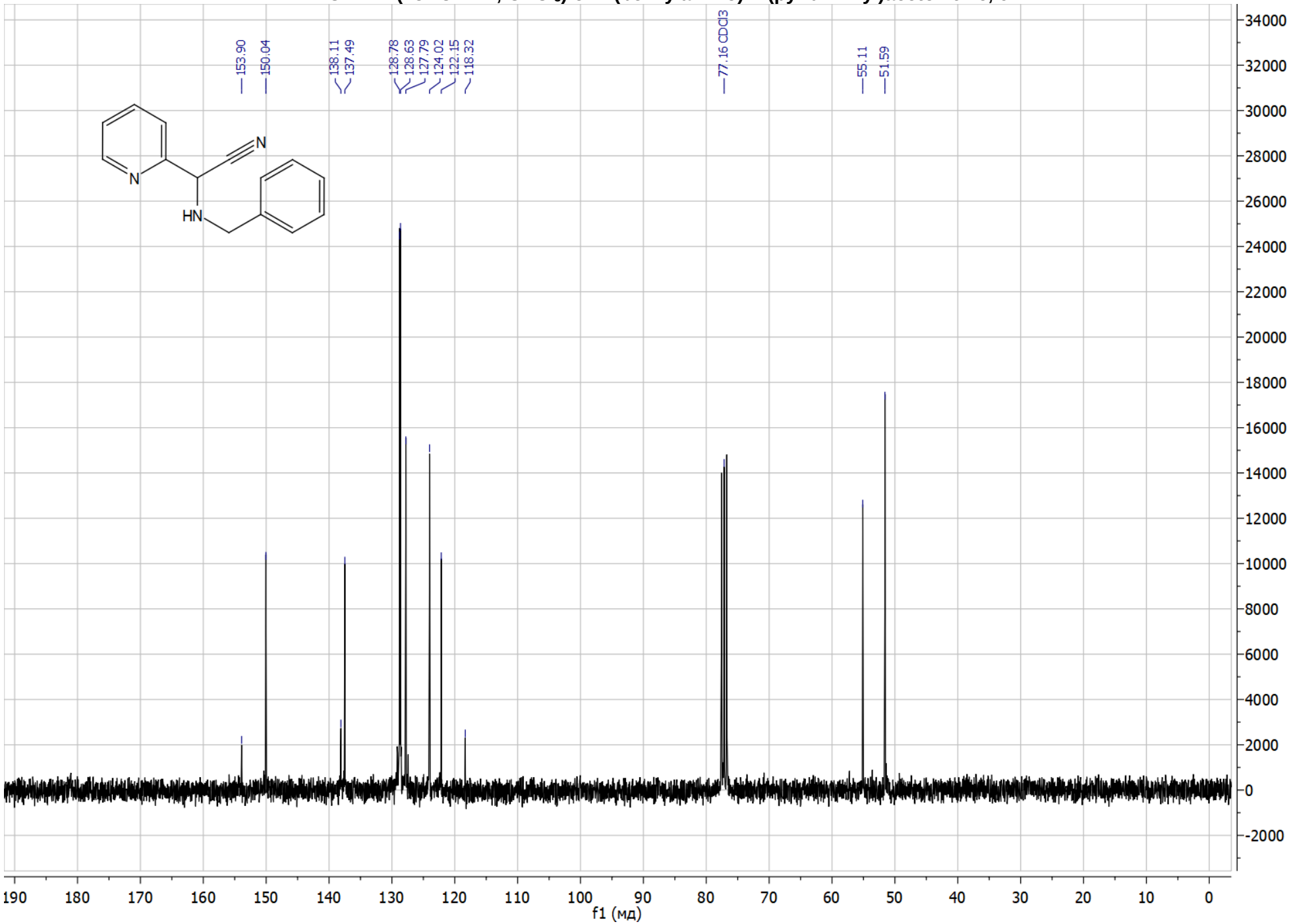
^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-phenyl-1-thiocyanatoimidazo[1,5-*a*]pyridine, 5



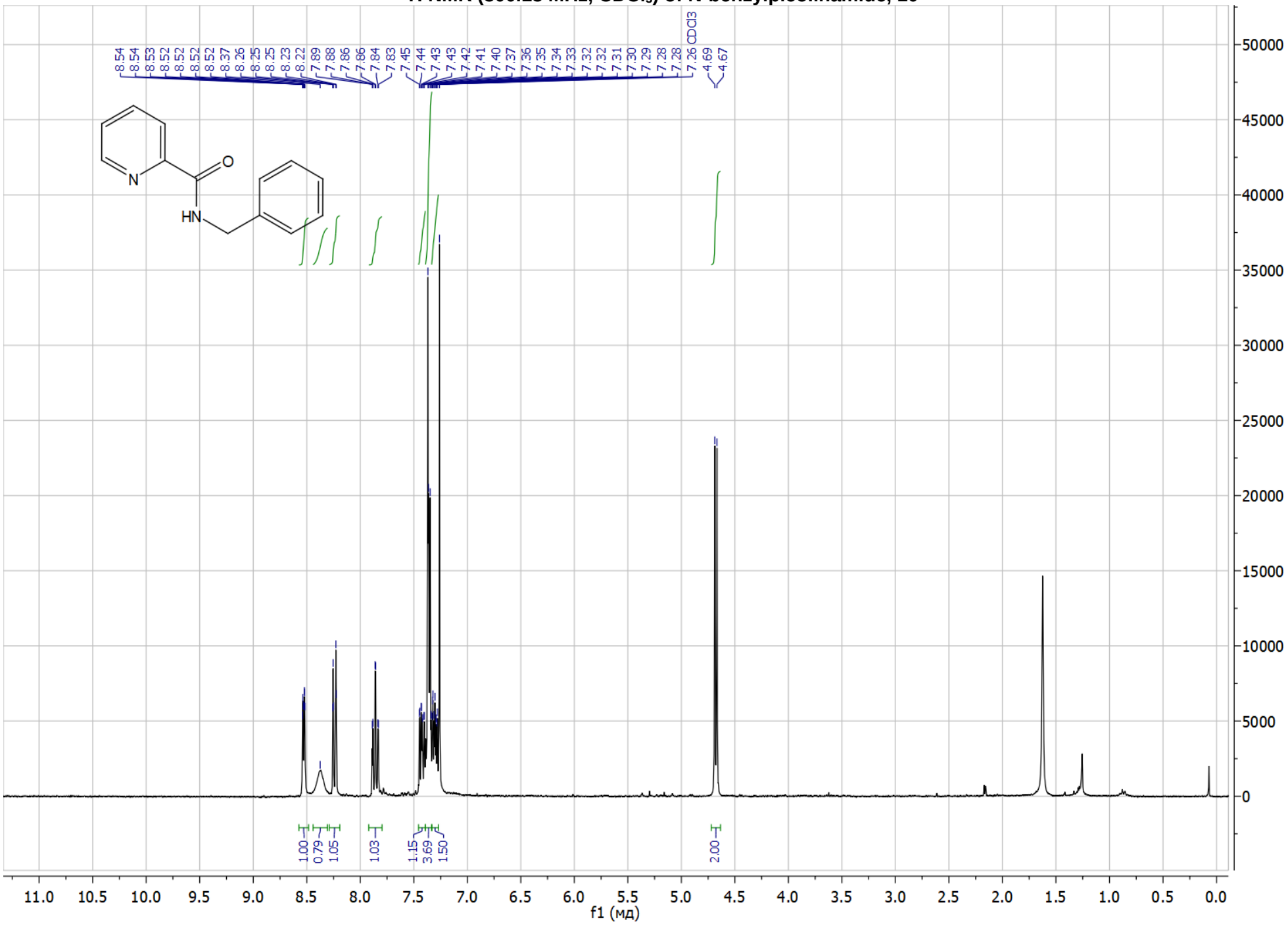
^{1}H NMR (300.13 MHz, $CDCl_3$) of 2-(benzylamino)-2-(pyridin-2-yl)acetonitrile, 9



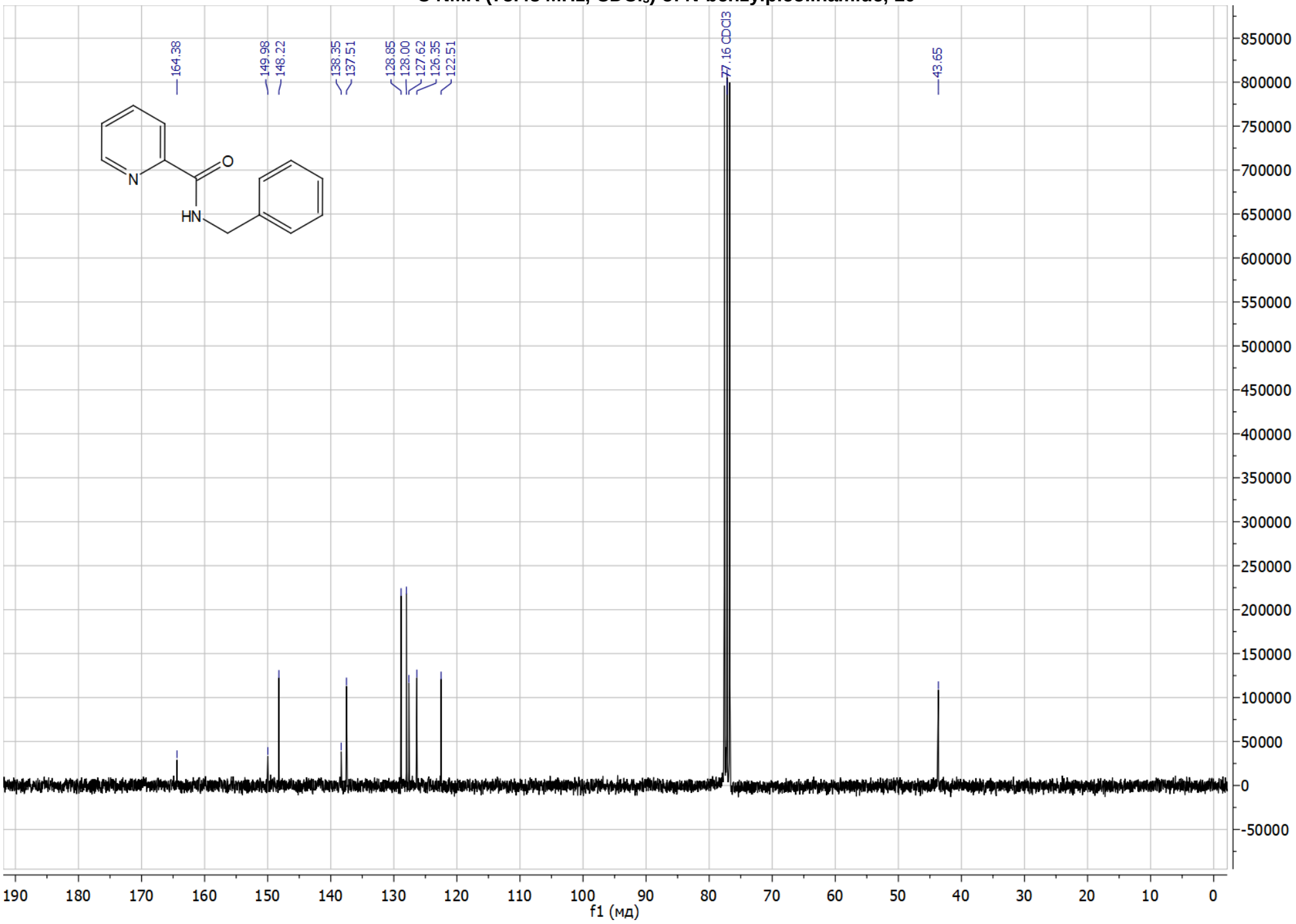
^{13}C NMR (75.48 MHz, $CDCl_3$) of 2-(benzylamino)-2-(pyridin-2-yl)acetonitrile, 9



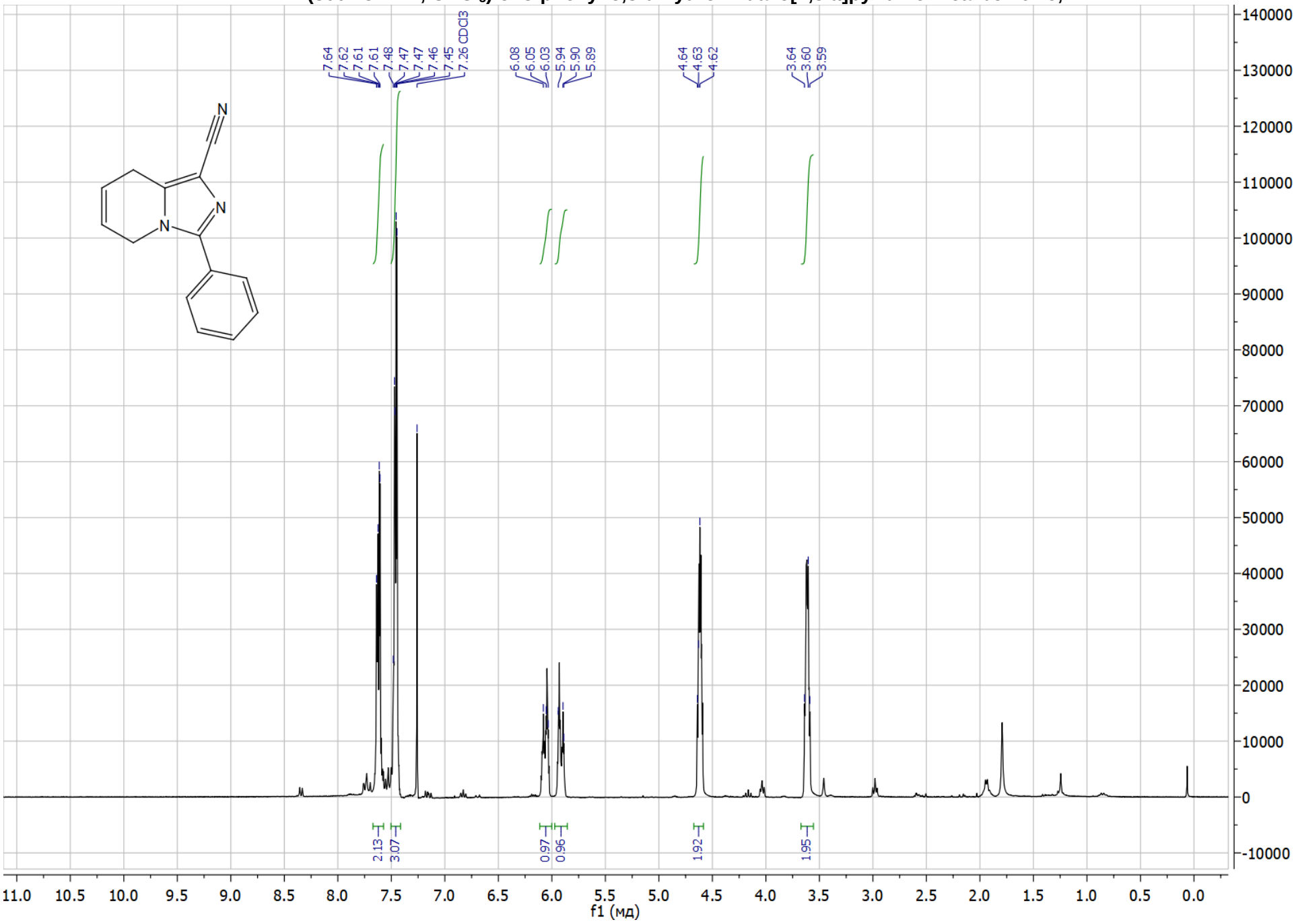
^{1}H NMR (300.13 MHz, $CDCl_3$) of N-benzylpicolinamide, 10



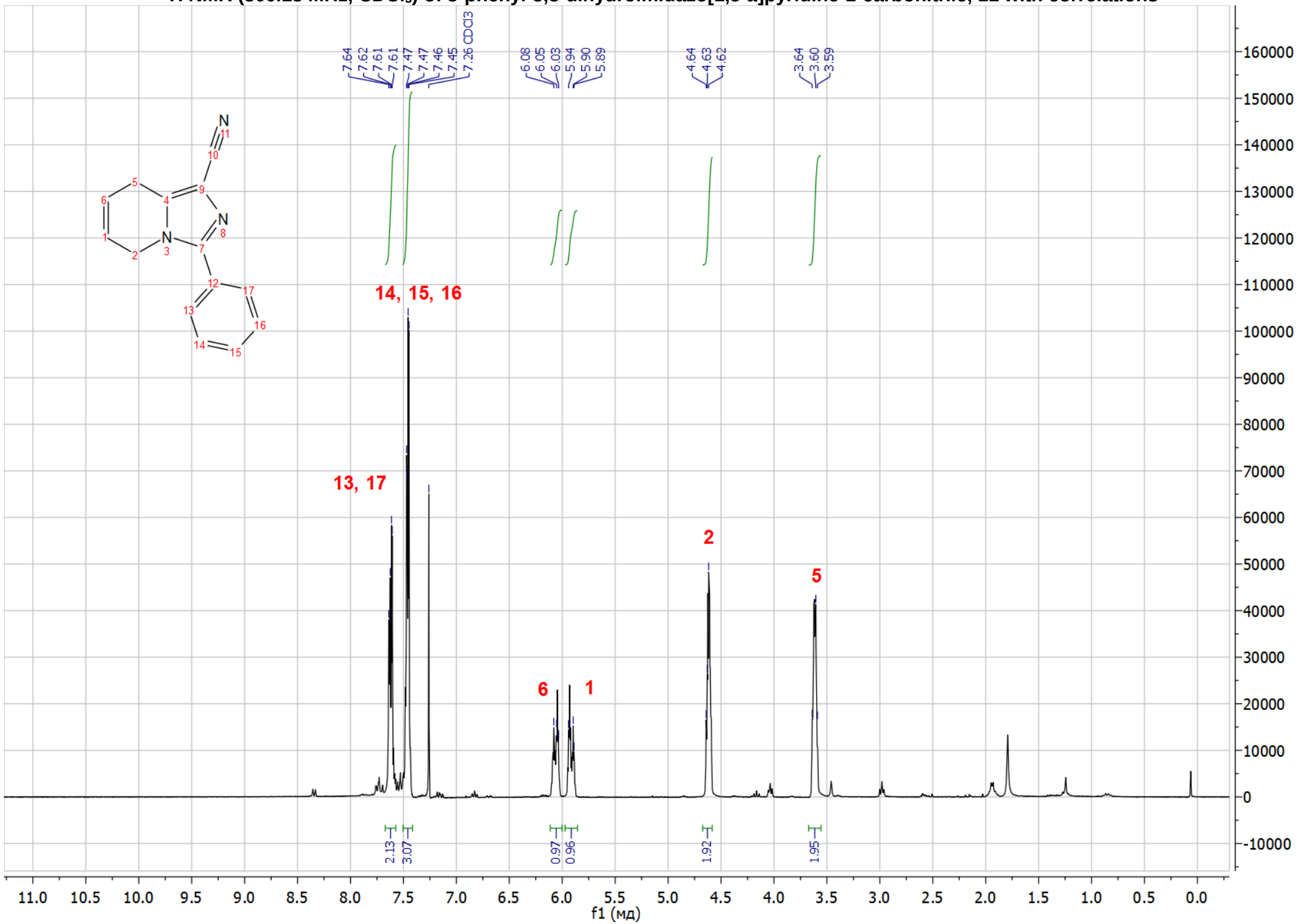
^{13}C NMR (75.48 MHz, $CDCl_3$) of N-benzylpicolinamide, 10



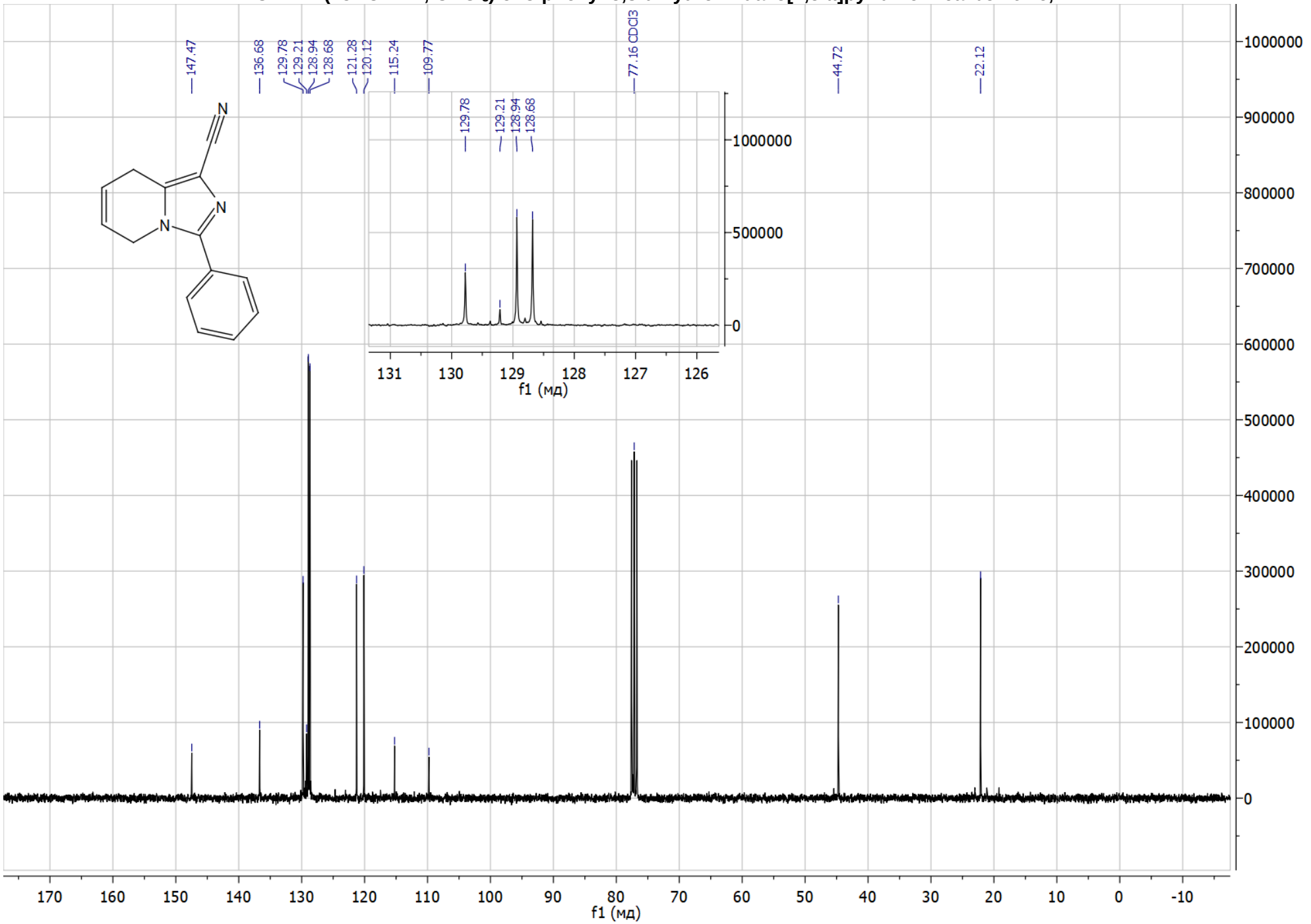
^{1}H NMR (300.13 MHz, $CDCl_3$) of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11



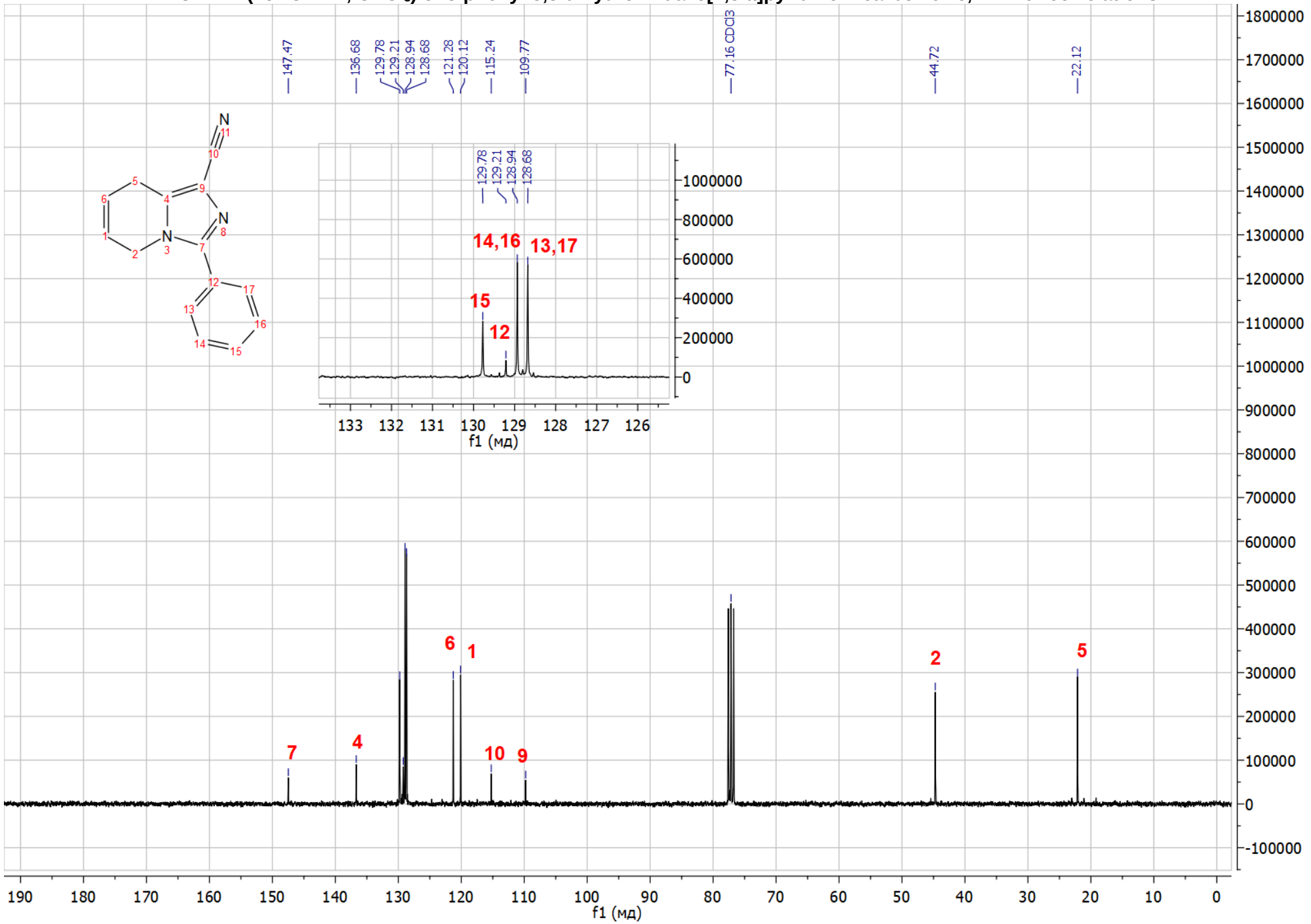
^{1}H NMR (300.13 MHz, $CDCl_3$) of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11 with correlations



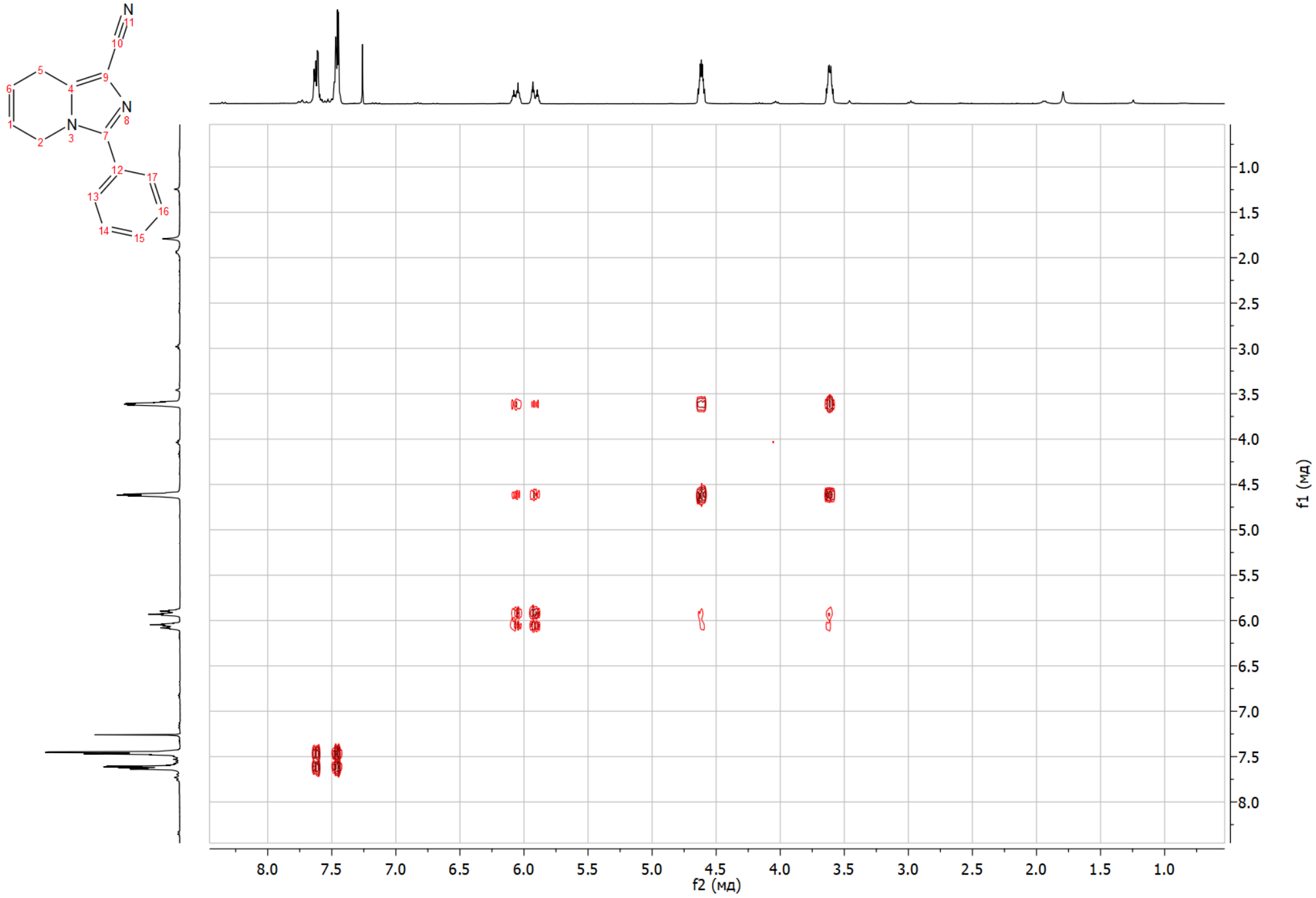
^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11



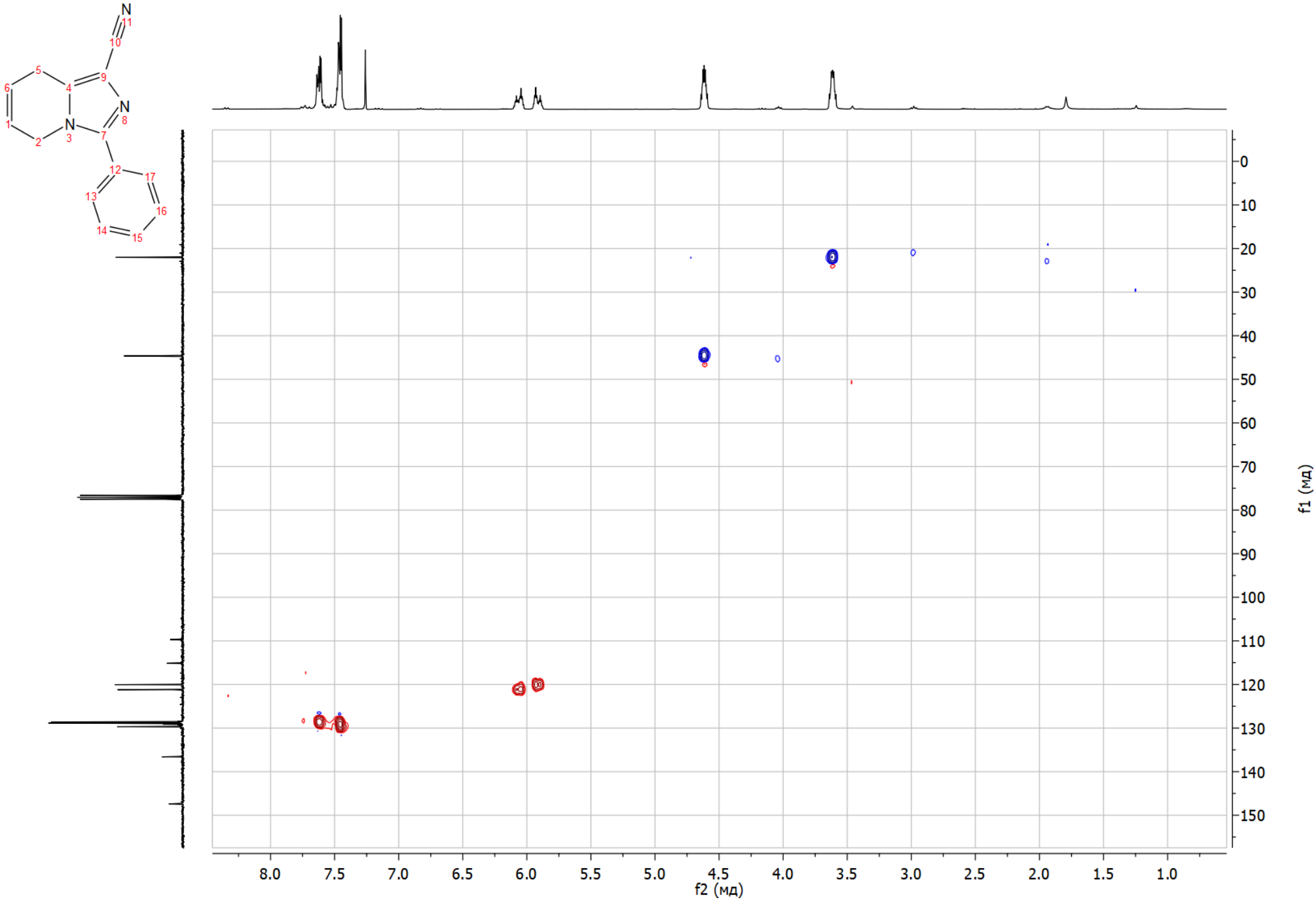
^{13}C NMR (75.48 MHz, $CDCl_3$) of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11 with correlations



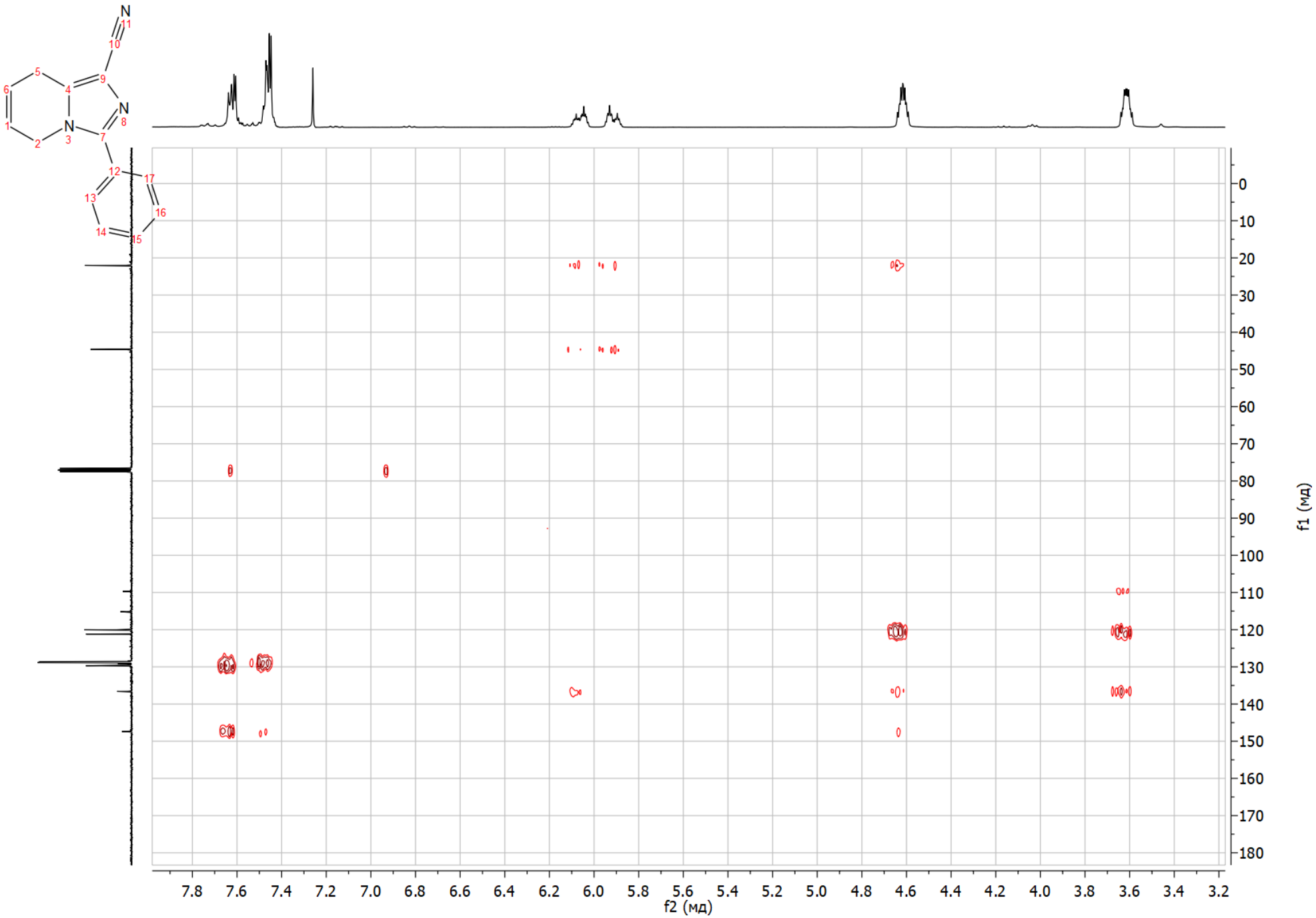
{^{1}H-^{1}H} COSY of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11



{^{1}H-^{13}C} HSQC of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11



{^{1}H-^{13}C} HMBC of 3-phenyl-5,8-dihydroimidazo[1,5-*a*]pyridine-1-carbonitrile, 11



HRMS spectra of the synthesized compounds

HRMS of 3-phenylimidazo[1,5-*a*]pyridine-1-carbonitrile, 3a

Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2022\Vil\0725007.d	Acquisition Date	25.07.2022 11:30:24
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-561	Instrument / Ser#	maXis 43
Comment	C14H9N3 mH 220.0869 clb added CH3CN		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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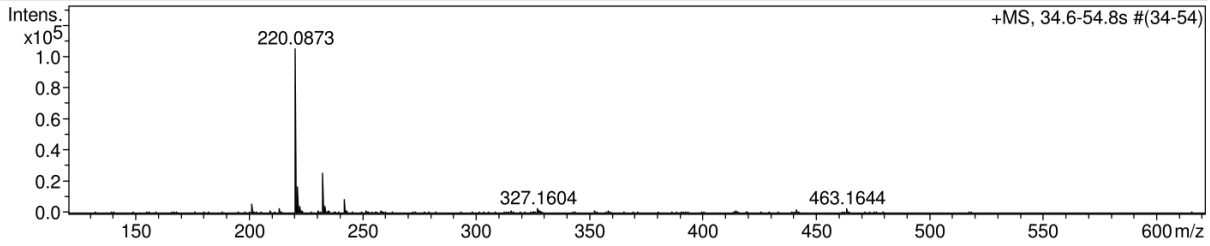
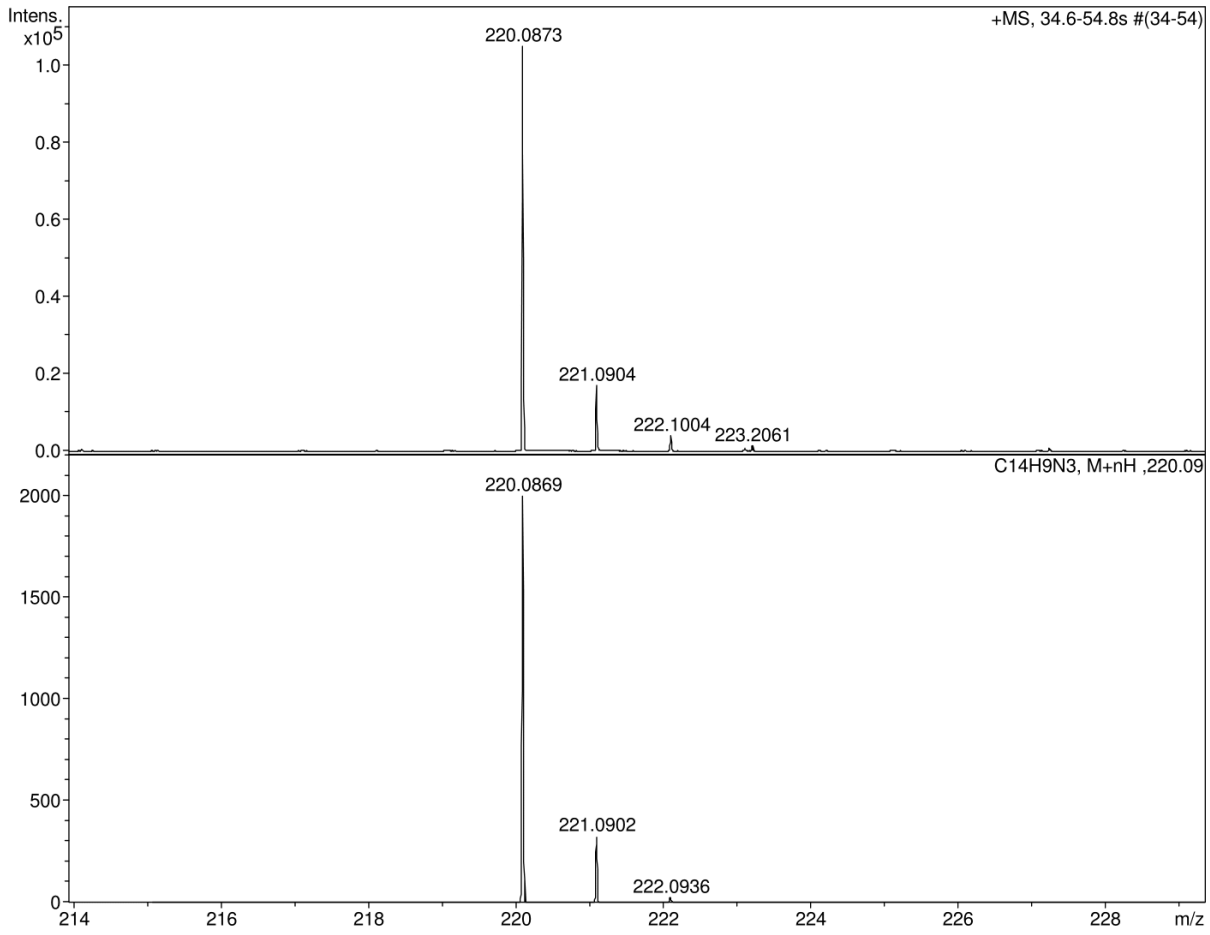
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source





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Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Wil\sg-647_&clblow.d	Acquisition Date	26.07.2023 13:35:51
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-647	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 1000, calibrant added		

Acquisition Parameter

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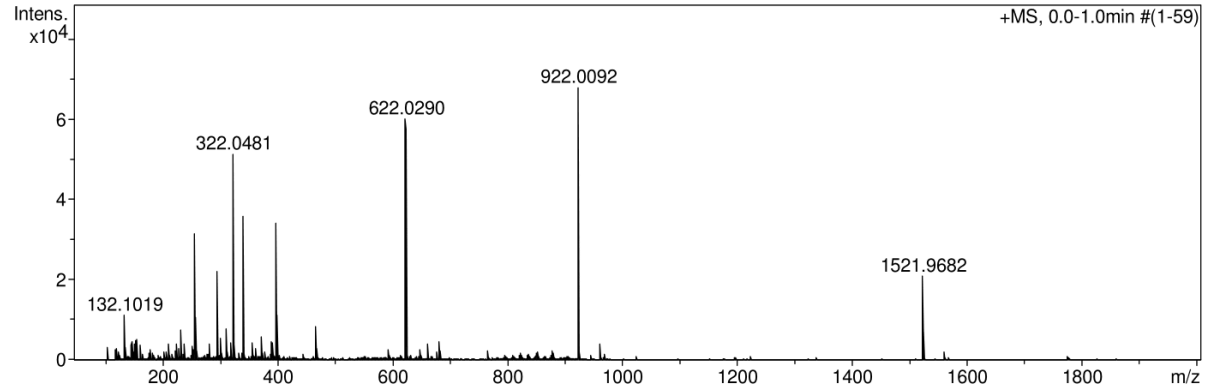

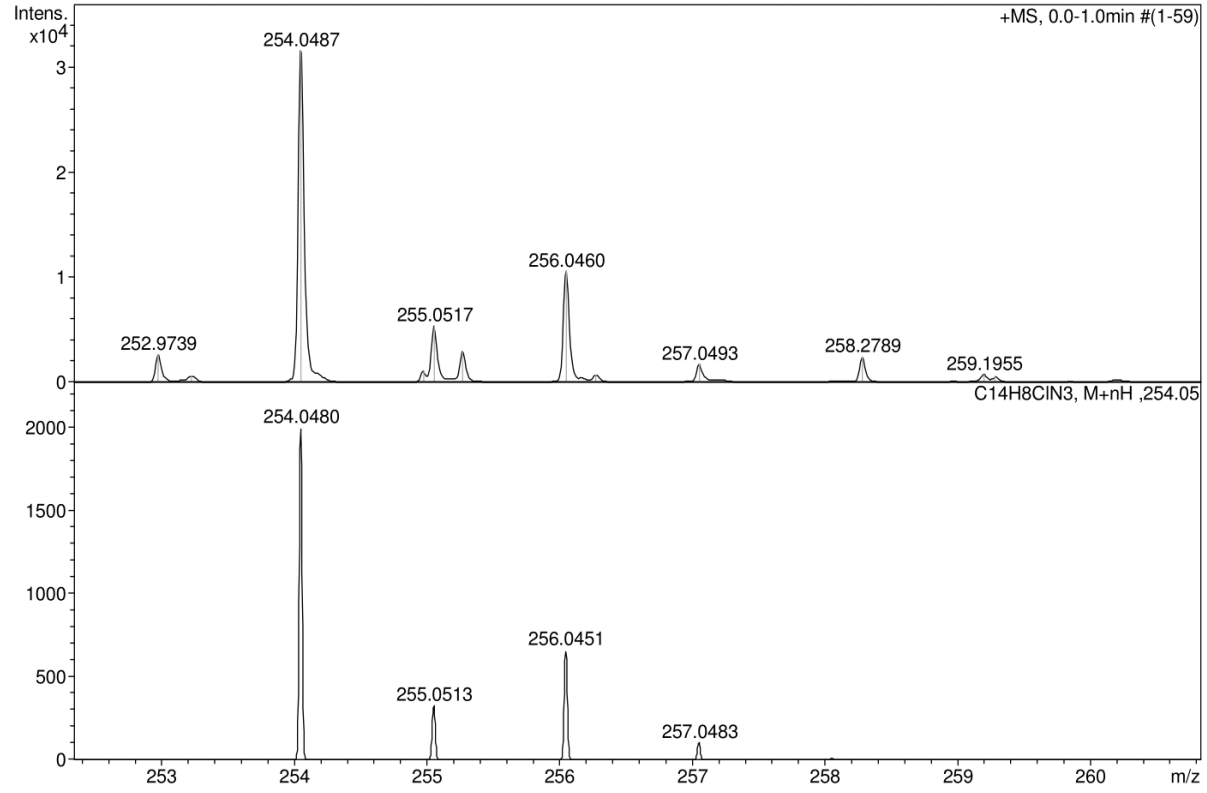

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Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Wil\sg-711_&clblow.d	Acquisition Date	26.07.2023 13:46:34
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-711	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 1000, calibrant added		

Acquisition Parameter

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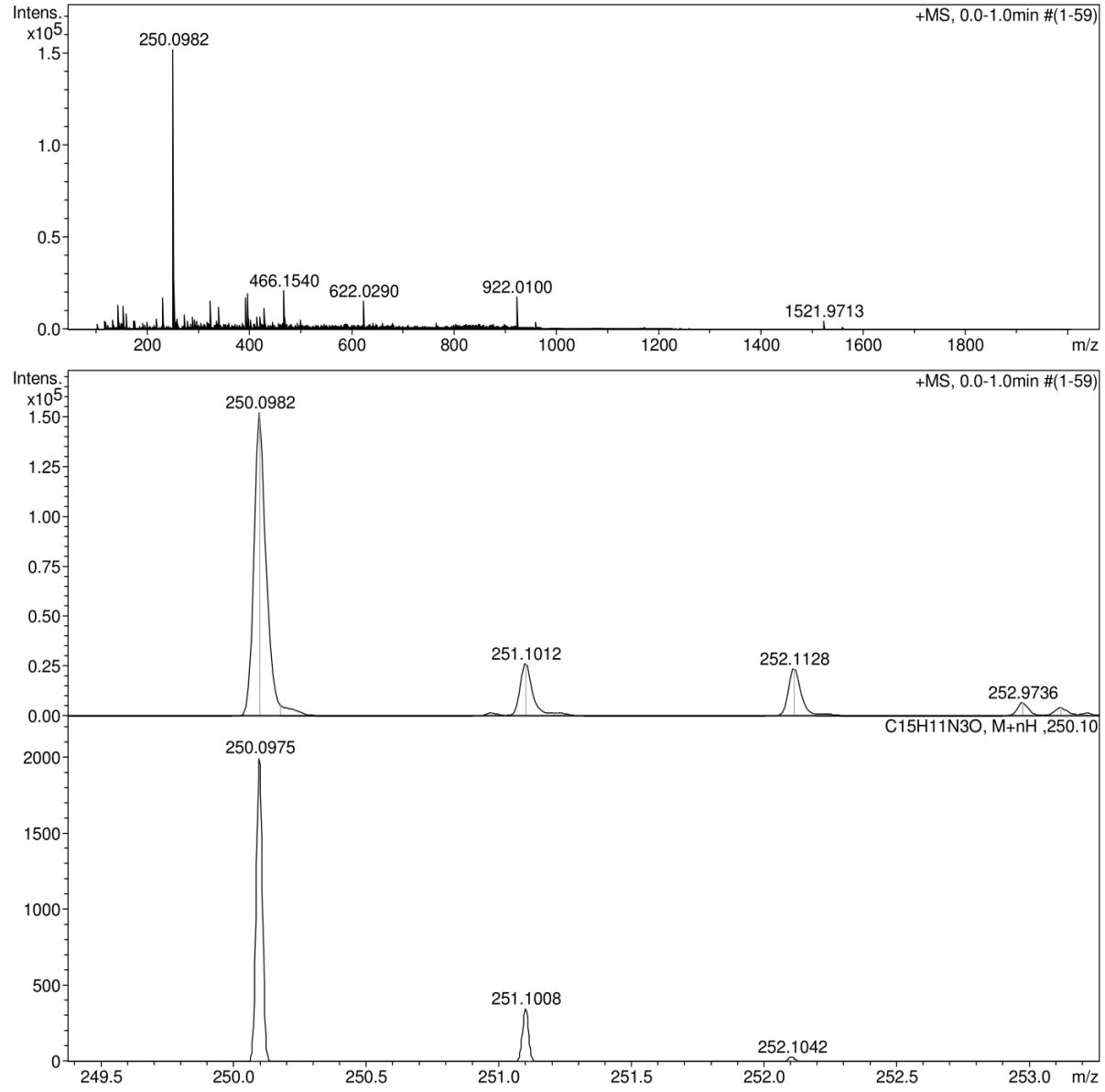
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



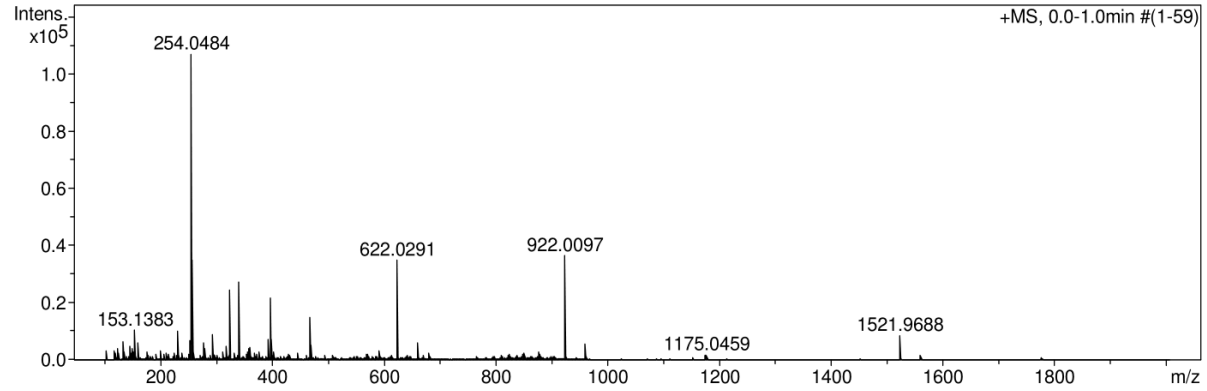
Display Report

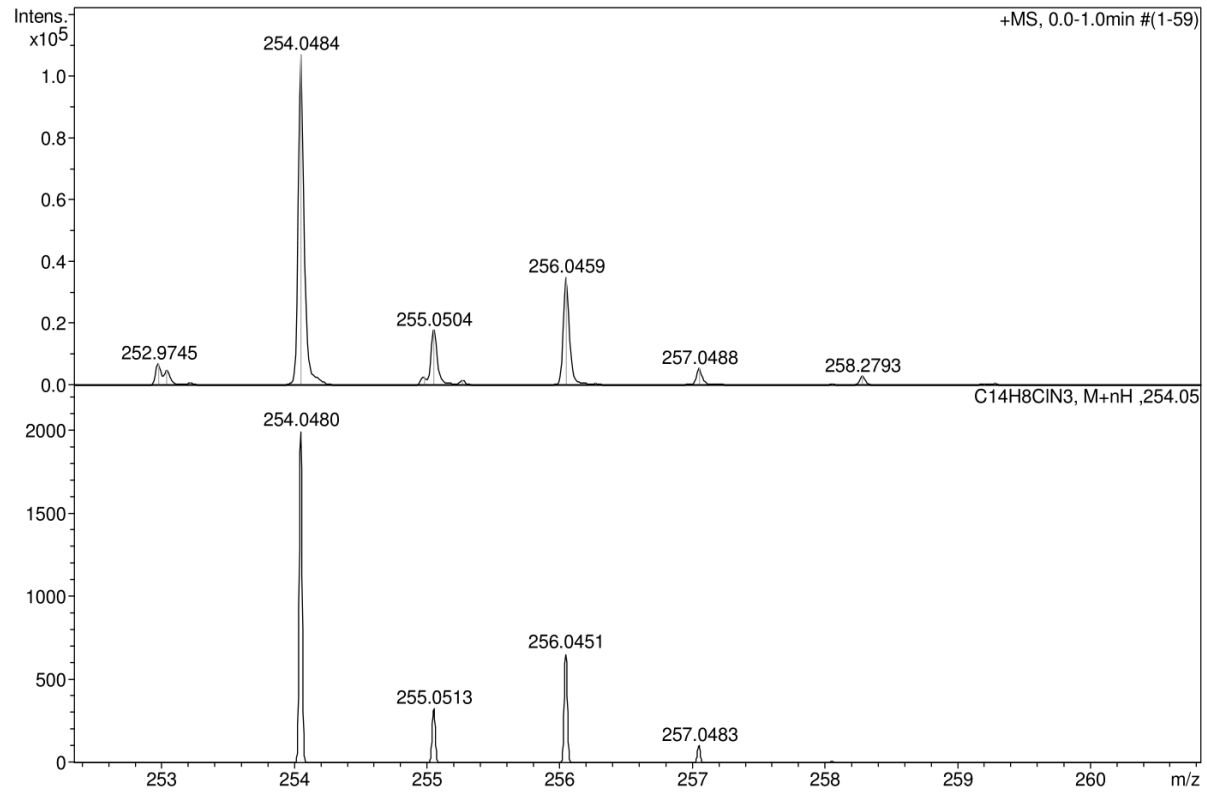
Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Wil\sg-648_&clblow.d	Acquisition Date	26.07.2023 13:42:21
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-648	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 10000, 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	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





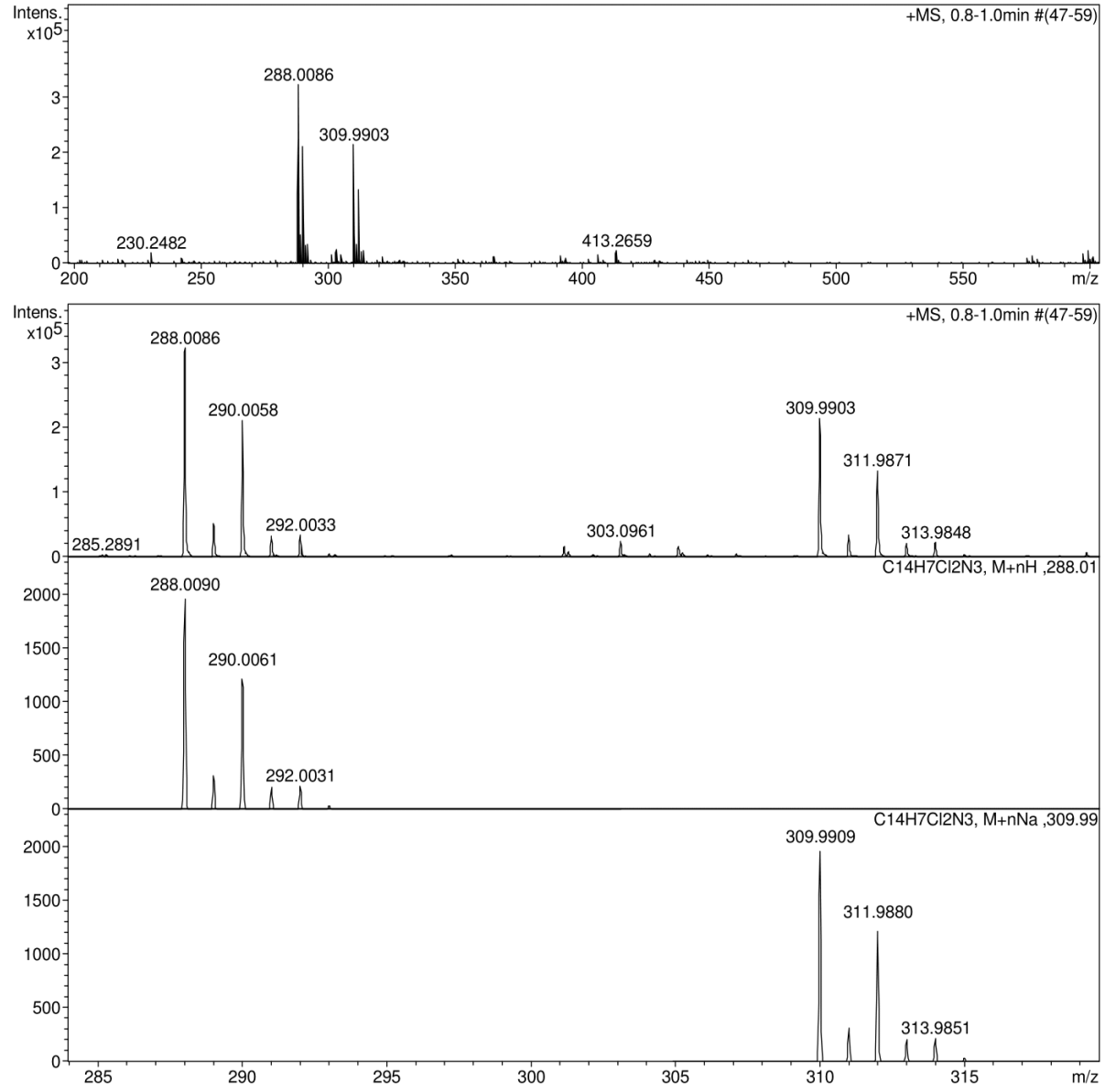
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Vil\0703005.d	Acquisition Date	03.07.2023 10:28:09
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG704	Instrument / Ser#	micrOTOF 10248
Comment	C14H7Cl2N3 mH288.0089 clb added CH3OH		

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	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



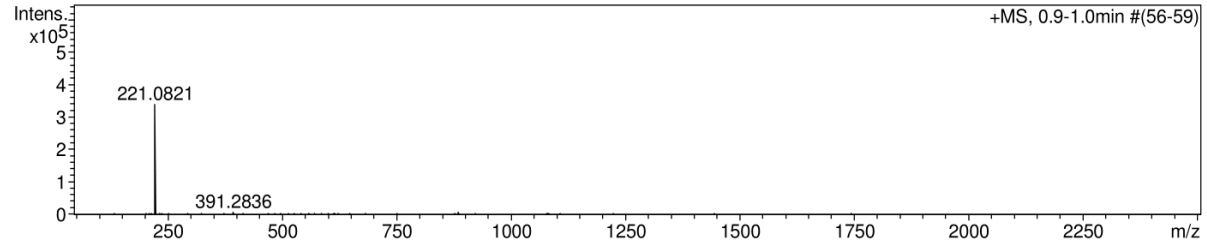
Display Report

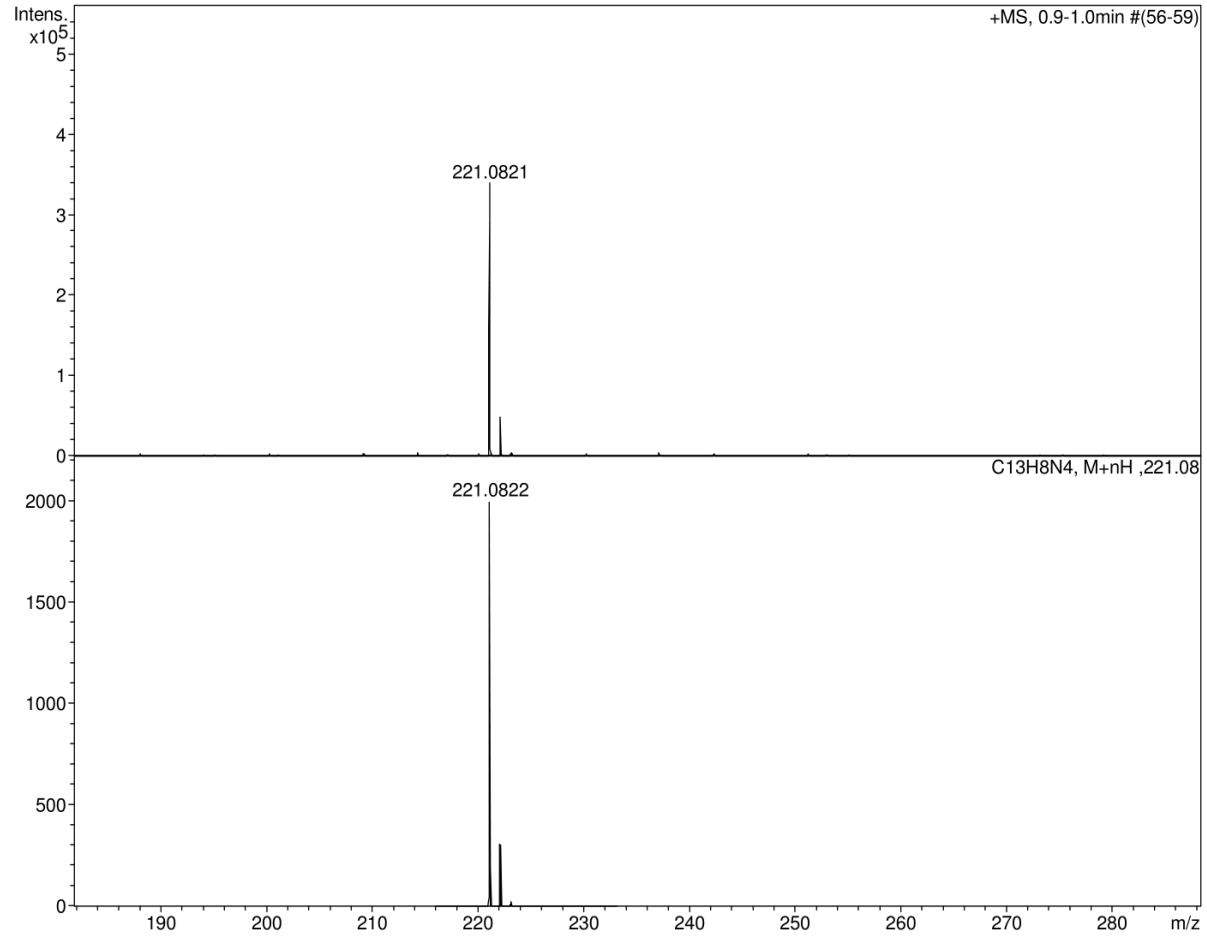
Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Vil\0220016.d	Acquisition Date	20.02.2023 15:25:31
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-651	Instrument / Ser#	micrOTOF 10248
Comment	C13H8N4 mH 221.0821 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





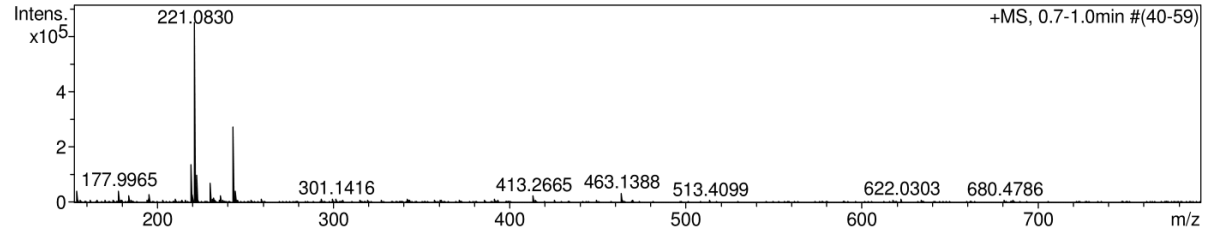
Display Report

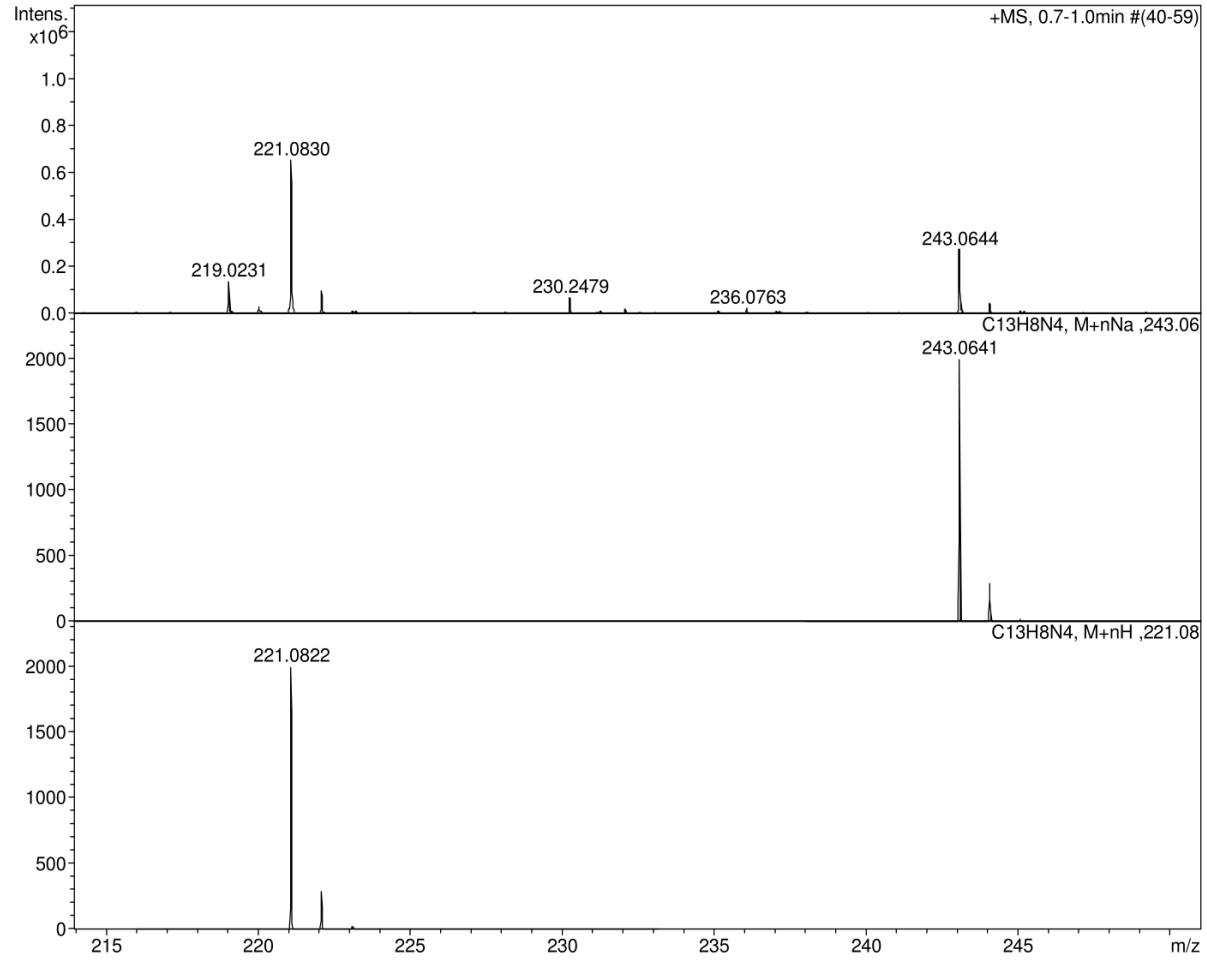
Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2022\Vil\1229011.d	Acquisition Date	29.12.2022 13:52:43
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-630	Instrument / Ser#	micrOTOF 10248
Comment	C15H8N4S2 mH 309.0263 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





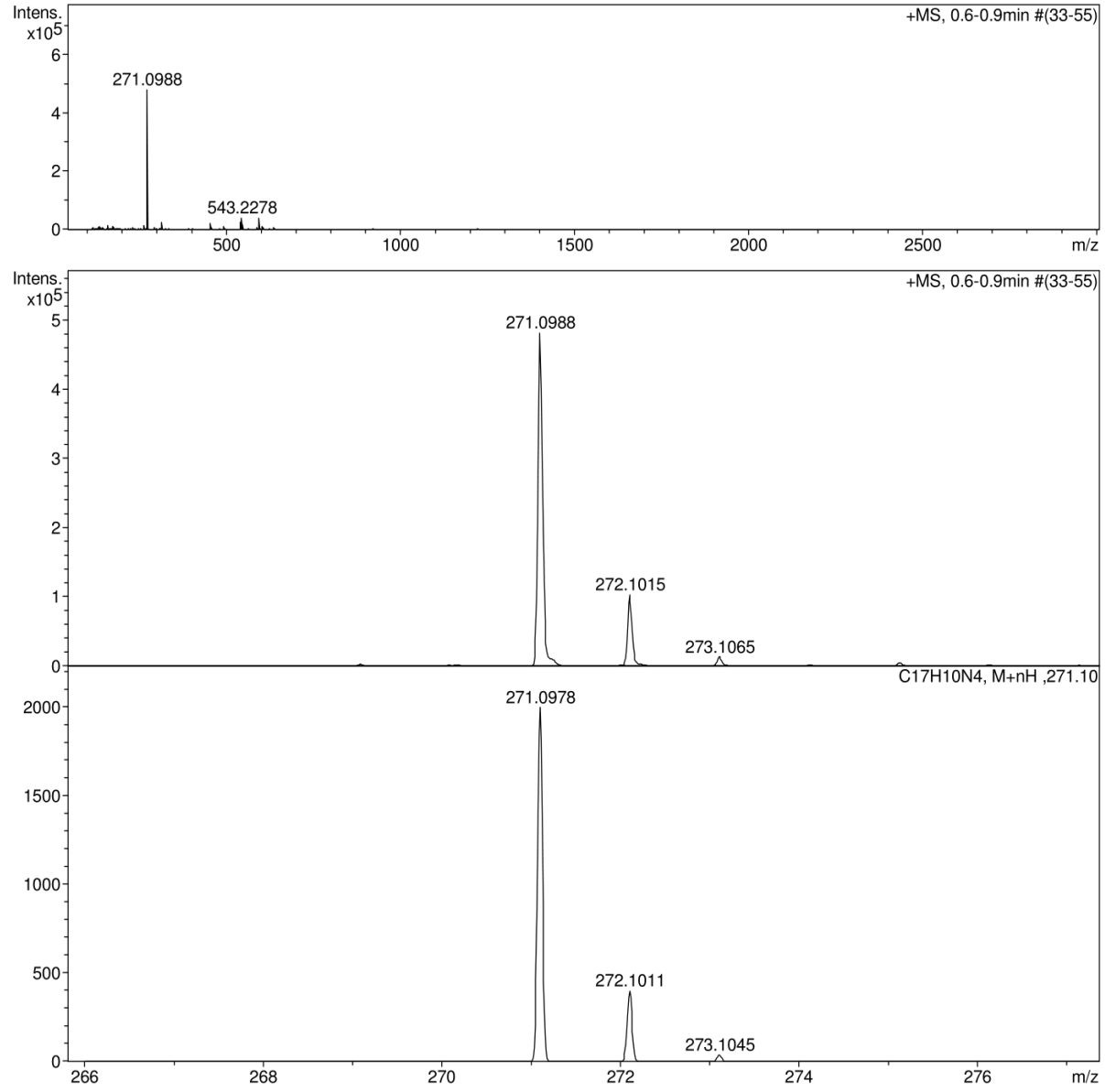
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Vil\0619041.d	Acquisition Date	19.06.2023 16:52:48
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-695	Instrument / Ser#	micrOTOF 10248
Comment	C17H10N4 mH 271.0978 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	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



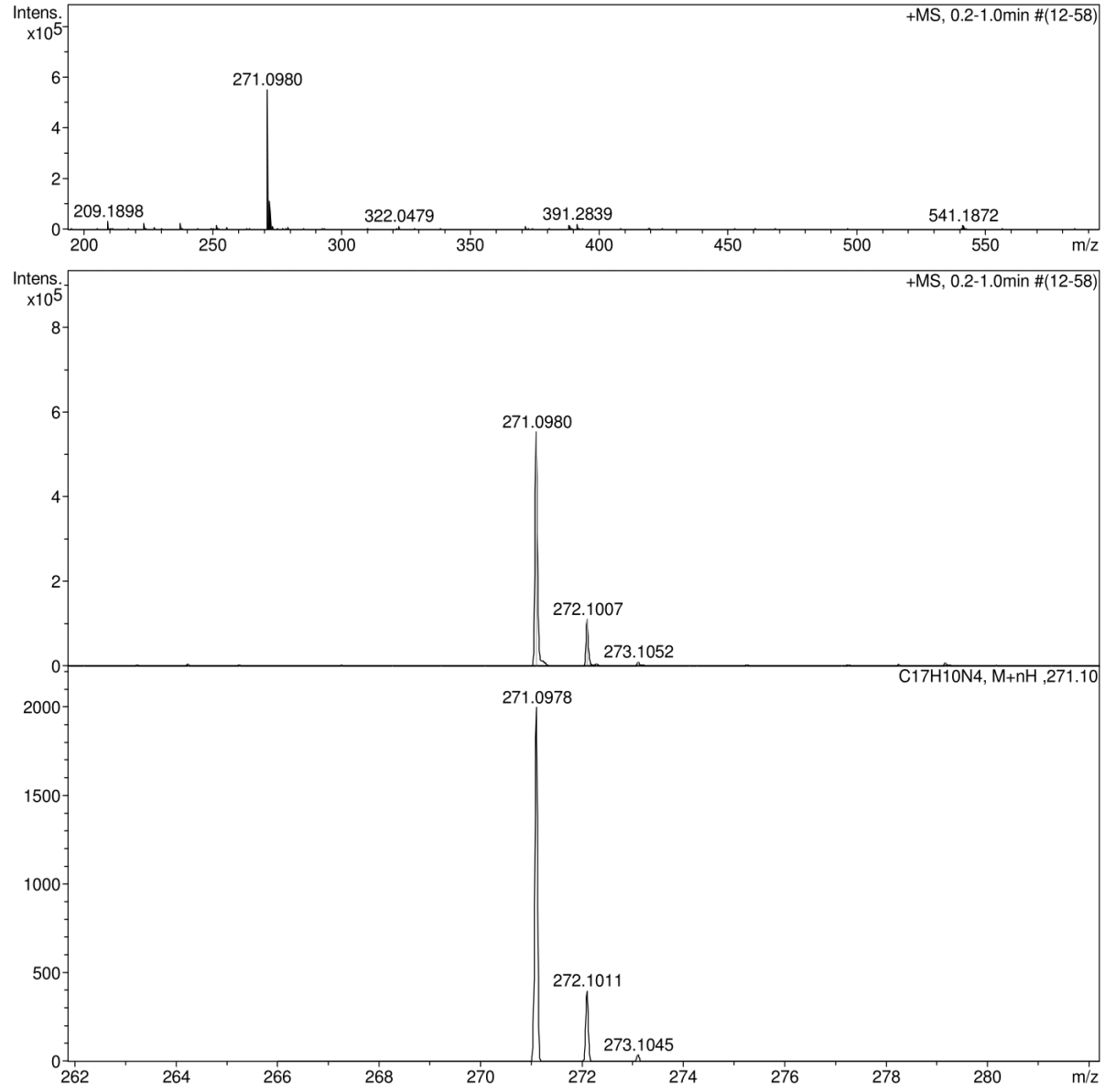
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Vil\0620022.d	Acquisition Date	20.06.2023 15:45:52
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-701	Instrument / Ser#	micrOTOF 10248
Comment	C17H10N4 mH 271.0978 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	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



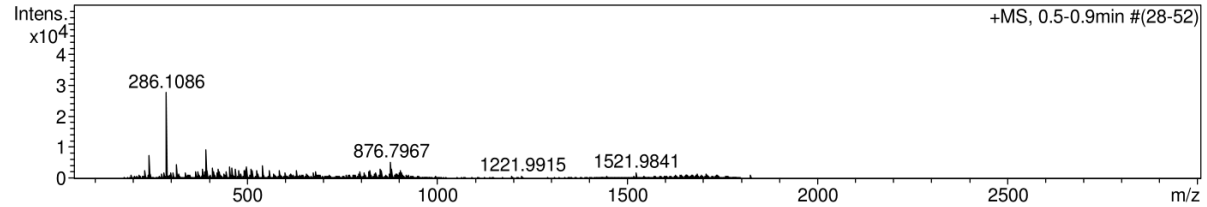
Display Report

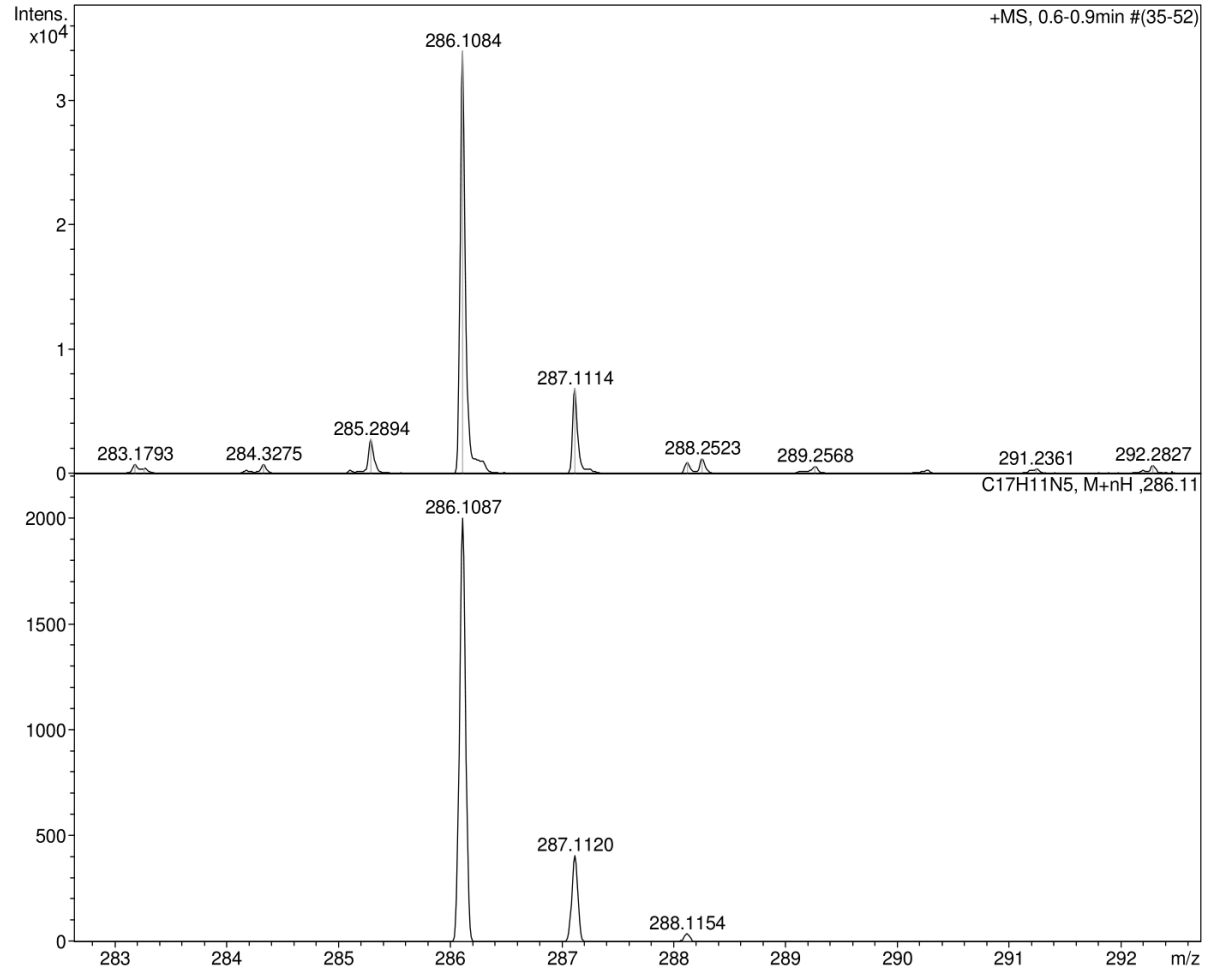
Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Vil\0606029.d	Acquisition Date	06.06.2023 15:49:55
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-691	Instrument / Ser#	micrOTOF 10248
Comment	C17H11N5 mH 286.1087 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	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





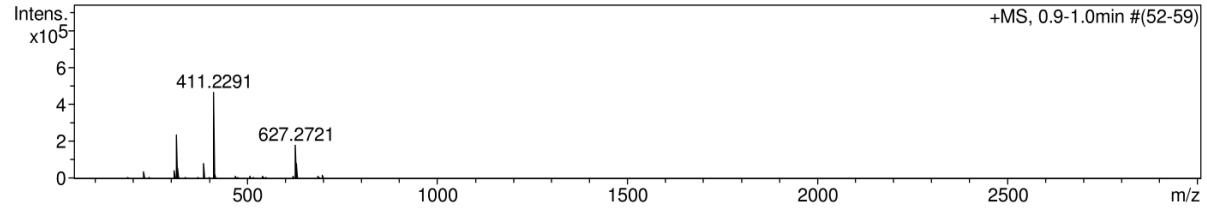
Display Report

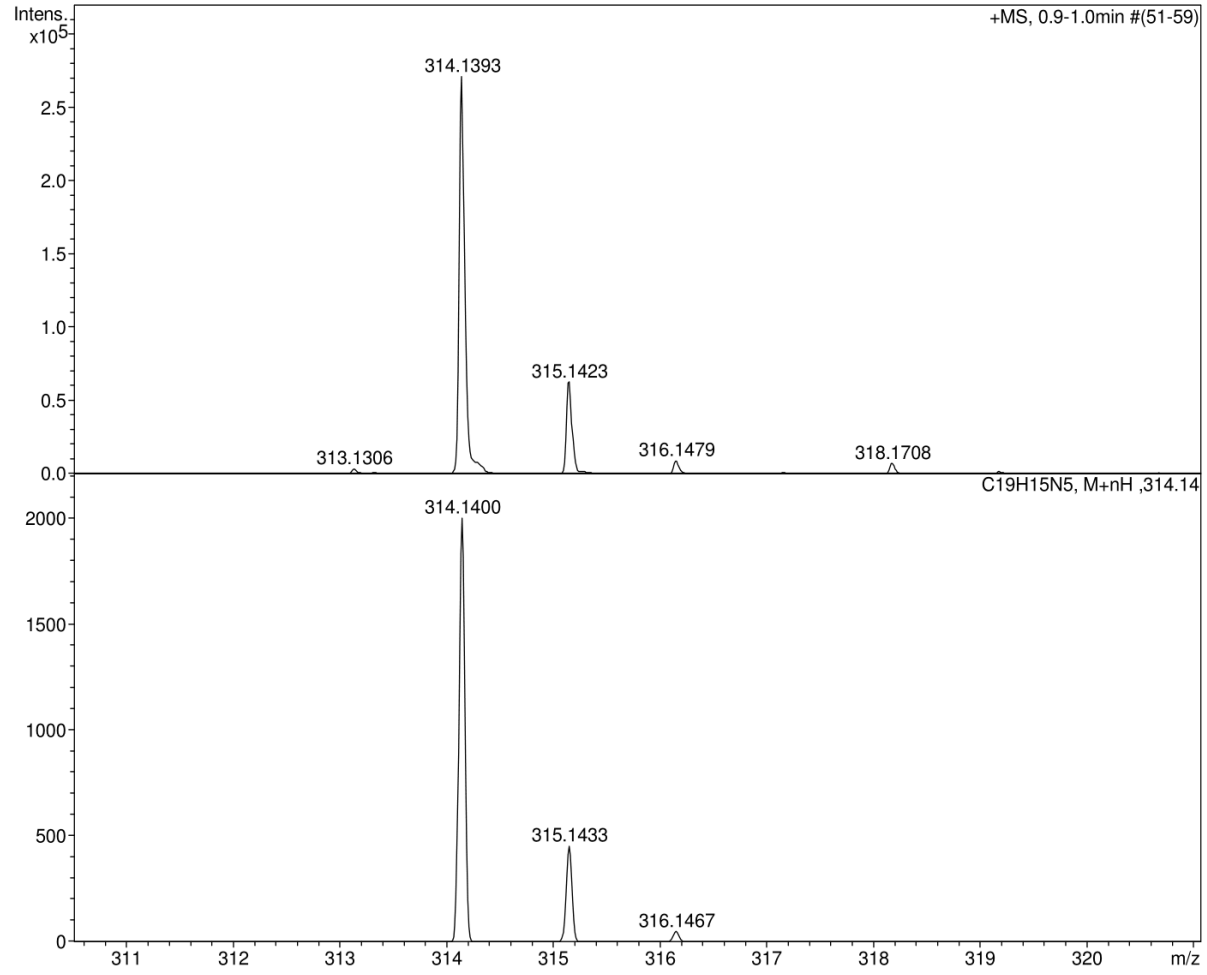
Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Vil\0606028.d	Acquisition Date	06.06.2023 15:43:56
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-692	Instrument / Ser#	micrOTOF 10248
Comment	C19H15N5 mH 314.1400 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	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





HRMS of 3-(2-((1H-pyrazol-1-yl)methyl)phenyl)imidazo[1,5-*a*]pyridine-1-carbonitrile, 3q

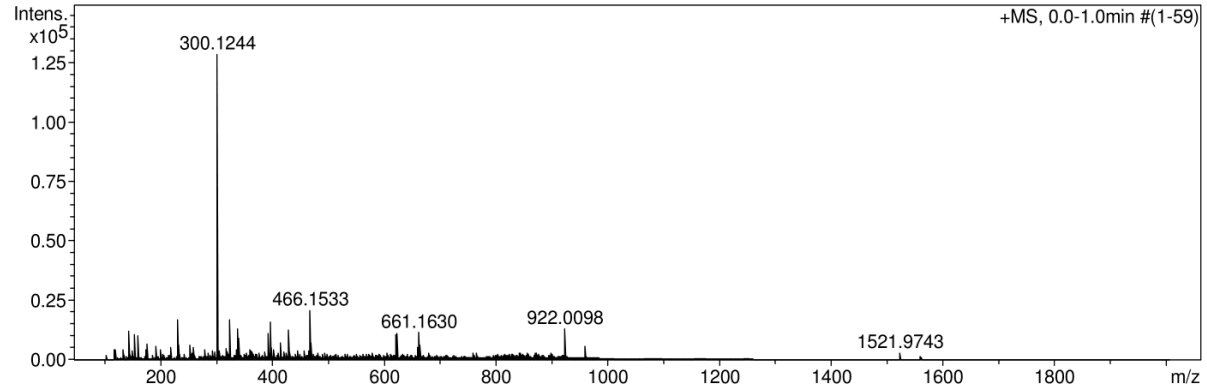
Display Report

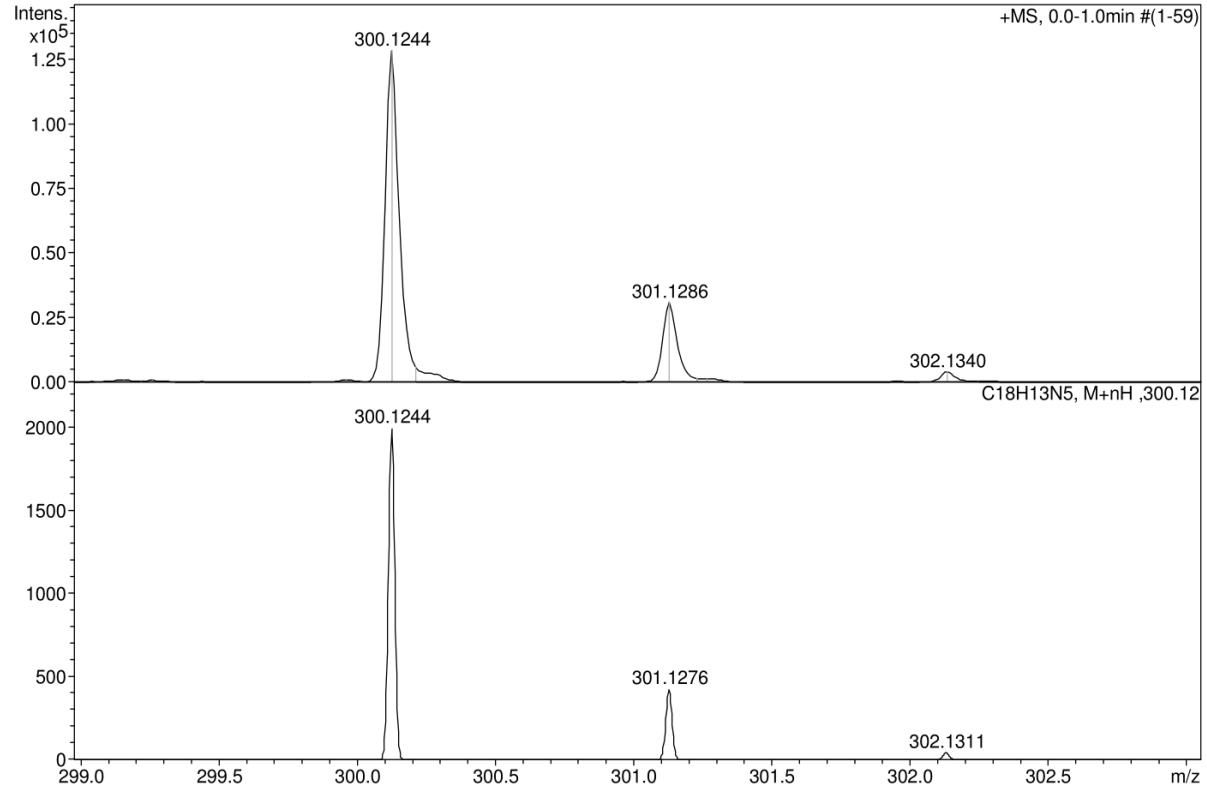
Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Wil\sg-708_&clblow.d	Acquisition Date	26.07.2023 13:50:21
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-708	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 1000, 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	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





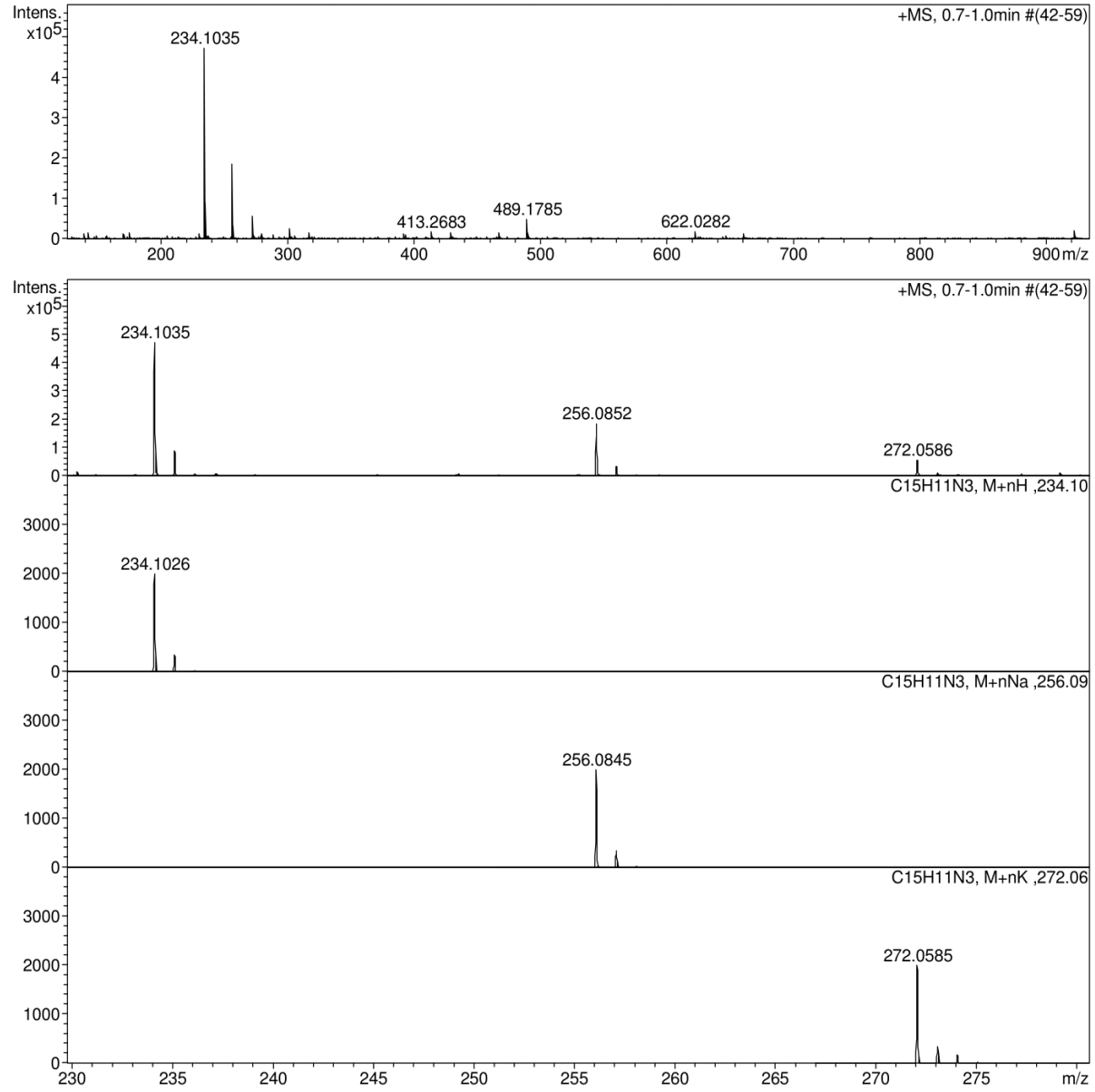
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Grishin\1109006.d	Acquisition Date	09.11.2023 12:49:52
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/VILV SG-767	Instrument / Ser#	micrOTOF 10248
Comment	C15H11N3 mH234.1025 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	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



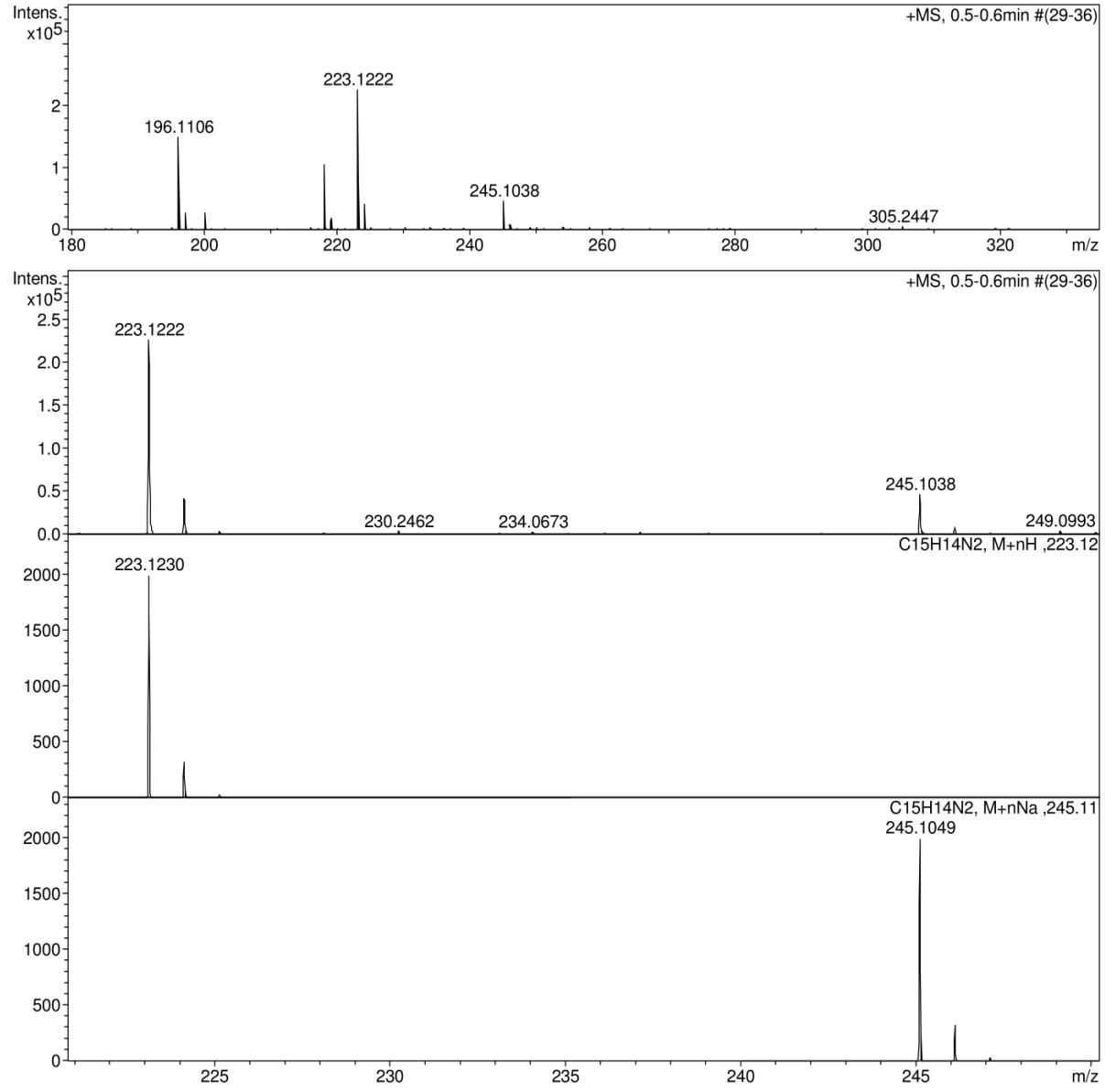
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2022\Vil\1222008.d	Acquisition Date	22.12.2022 13:29:36
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-626	Instrument / Ser#	micrOTOF 10248
Comment	C15H14N2 mH 223.1229calibrant added CH3OH		

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



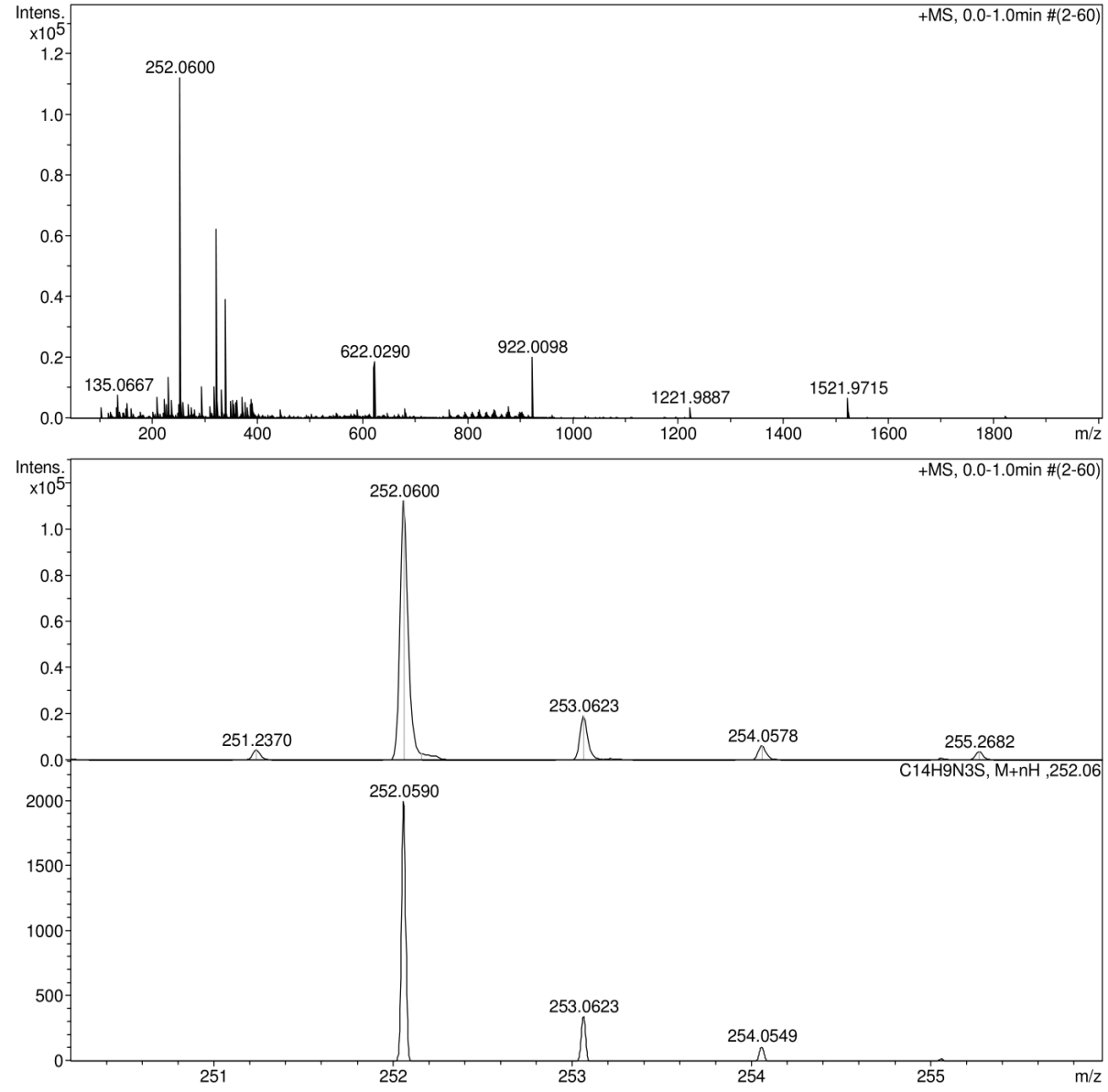
Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Wil\sg-717_&clb_low.d	Acquisition Date	17.07.2023 15:09:29
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-717	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, 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	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



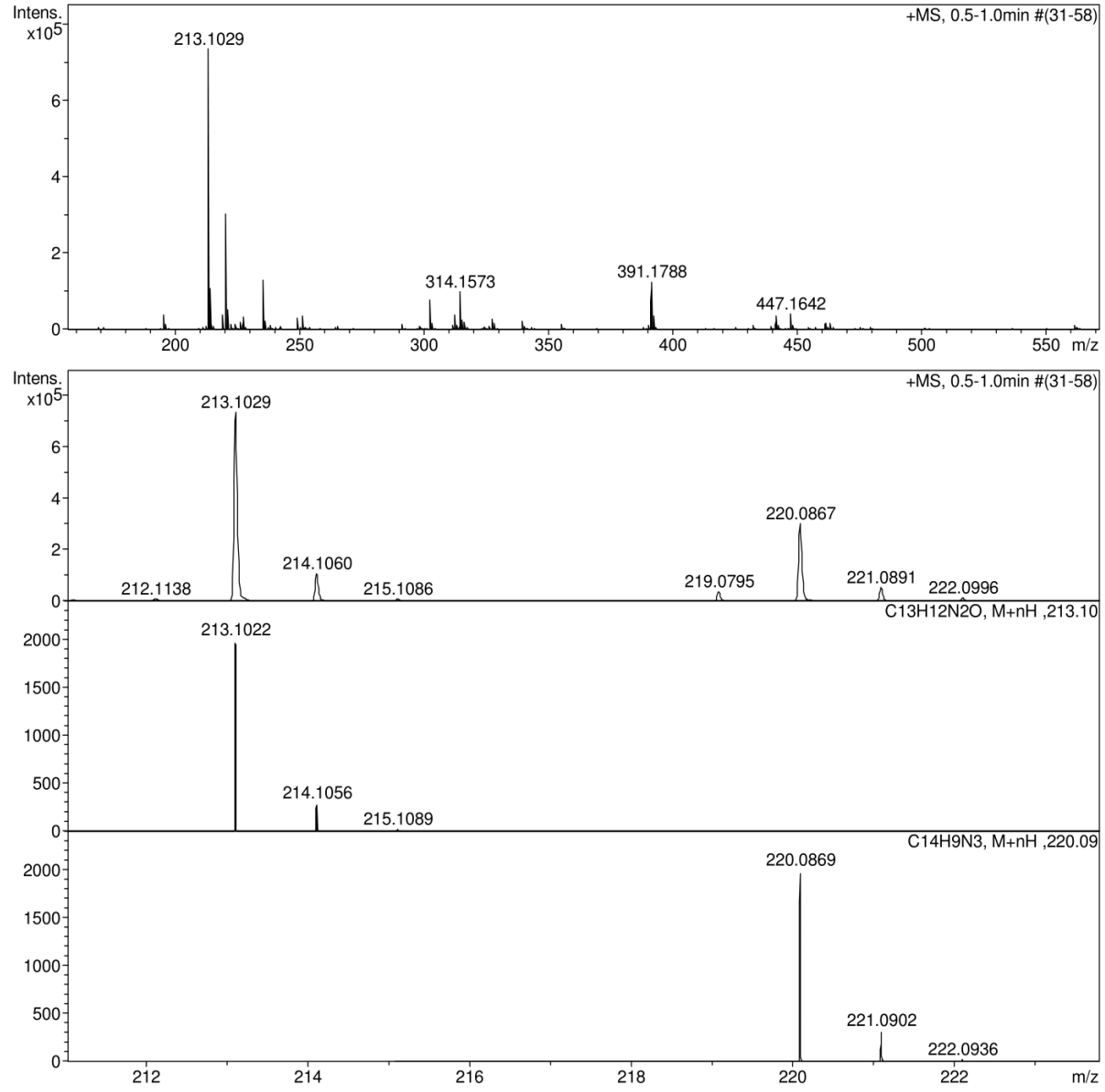
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2023\Grishin\0920002.d	Acquisition Date	20.09.2023 10:36:14
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SG-729-1	Instrument / Ser#	micrOTOF 10248
Comment	C14H9N3 mH 220.0869 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	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Wil\sb-715_&clblow.d	Acquisition Date	14.07.2023 16:38:05
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN Sb-715	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, 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	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste