Synthesis

Reviews and Full Papers in Chemical Synthesis

Supporting Information

for DOI: 10.1055/s-0040-1700389

Georg Thieme Verlag KG, Rüdigerstraße 14, 70469 Stuttgart, Germany

Thieme

SUPPORTING INFORMATION.

A Facile Synthesis of 2-Aminopropane-1,2,3-tricarboxylic Acid and its Symmetrical Dimethyl Ester.

Alexey V. Nizovtsev*, Nicolai V. Bovin

Laboratory of Carbohydrates, Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow, Russian Federation

e-mail: alexey.nizovtsev@gmail.com

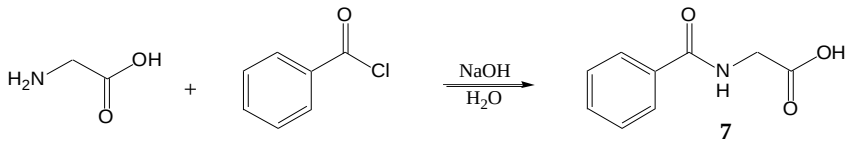
Table of Contents.

I. General Information

All reagents were obtained from commercial suppliers and were used without further purification unless stated. Organic solutions were dried over anhydrous sodium sulfate and, unless stated, were evaporated at 8 mbar. Yields quoted are for the purified compounds unless stated and any ratios given are calculated by comparing integrals in the ^{1}H NMR spectrum. All new compounds were homogeneous by TLC. TLC was performed using ALUGRAM SIL G/UV$_{254}$ (MACHEREY-NAGEL). Compounds were visualized either by examination under an ultraviolet source or by contact with phosphomolybdic acid hydrate (2% solution in ethanol) followed by heating to 200°C. Column chromatography was conducted with Matrex silica 60 gel under atmosphere pressure. Melting points are uncorrected. NMR spectra were recorded at 303K on a Bruker Avance III 700 spectrometer (Bruker BioSpin MRI GmbH) at 700 MHz for protons and 176.1 MHz for carbon and in the latter case were broad-band decoupled. Residual solvent signals were used as internal standards. [1] High-resolution mass spectra were obtained using a Bruker micrOTOF II spectrometer using electrospray ionisation (ESI). All previously described compounds were characterized by ^{1}H and ^{13}C NMR and gave data identical to those in the literature.

II. Experimental Information

*II-1. Synthesis of hippuric acid **7**.*



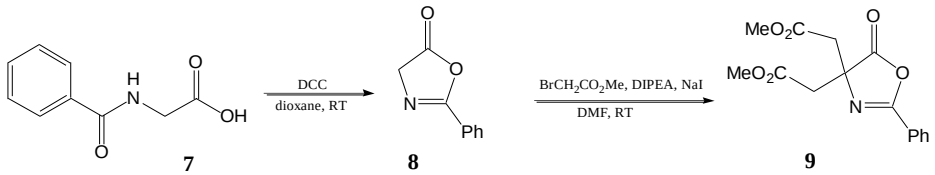
7

Benzoyl chloride (42.17 g, 300 mmol) was added in one portion to the solution of glycine (24.77 g, 330 mmol, 1.1 mol.eq.) and NaOH (25.2 g, 630 mmol, 2.1 mol. equiv.) in distilled water (240 ml) at +5°C. The reaction mixture was intensively stirred at +4 - +8°C for an hour and then at r.t. for additional 2 h, filtered, diluted with distilled water to 400 ml and acidified with concd HCl to pH2. The precipitate was filtered off, washed with water 3x150 ml and dried in oven at 50°C to give hippuric acid **7** (49.325 g, 275 mmol, 92%) as a white crystals with spectral data identical to those described in the literature. [2]

^{1}H NMR (700 MHz, DMSO-d_6): δ = 12.56 (br.s, 1 H), 8.81 (t, *J* = 5.9 Hz, 1 H), 7.89-7.87 (m, 2 H), 7.56-7.53 (m, 1 H), 7.49-7.47 (m, 2 H), 3.93 (d, *J* = 5.9 Hz, 2 H).

[1] Fulmer, G.R.; Miller, A.J.M.; Sherden, N.H.; Gottlieb, H.E.; Nudelman, A.; Stoltz, B.M.; Bercaw, J.E.; Goldberg, K.I. *Organometallics* **2010**, 29, 2176.
[2] Schulz, J.M.; Lanovoi, H.T.; Ames, A.M.; McKegg, P.C.; Patrone, J.D. *J. Nat. Prod.* **2019**, 82, 1045.

*II-2. The procedure for the screening of 2-phenyl-4,4-dimethoxycarbonylmethyl-5(4H)-oxazolone **9** isolation conditions.*



Solution of DCC (5.313 g, 25.75 mmol, 1.03 mol. equiv.) in dry dioxane (15 ml) was added to a suspension of hippuric acid **7** (4.479 g, 25 mmol) in dry dioxane (25 ml) and the reaction mixture was stirred at r.t. for 19 hours. The white precipitate was filtered off and washed with dry dioxane (5x10 ml). The combined deep yellow mother solutions were evaporated *in vacuo* to give 2-phenyl-5(4H)-oxazolone **8** (5.306 g) as a yellow solid which was used in the next step without additional purification; R_f = 0.62 (EtOAc/hexane 1:2). Analytically pure sample by obtained by crystallization of crude material (500 mg) from hot *t*-BuOH (1.5 ml), followed by dilution with hexane (5 ml).

^{1}H NMR (700 MHz, $CDCl_3$): δ = 7.99 (d, *J* = 7.6 Hz, 2 H), 7.58 (t, *J* = 7.6 Hz, 1 H), 7.49 (t, *J* = 7.6 Hz, 2 H), 4.42 (s, 2 H).

DIPEA (1.62 g, 2.2 ml, 12.5 mmol, 2.5 mol. equiv.) was added to a solution of 2-phenyl-5(4)-oxazolone **8** (1.061 g, estimated as 5.0 mmol), methylbromoacetate (1.912 g, 12.5 mmol, 2.5 mol. equiv.) and NaI (85 mg, 0.5 mmol) in dry DMF (10 ml). A strong exothermic effect during the addition was observed and the reaction mixture turned red. The obtained mixture was stirred 5 h at r.t. and evaporated *in vacuo*. The residue was dissolved in EtOAc (30 ml) and water (20 ml), shaked up, water layer was separated, organic layer was washed with sat. $NaHCO_3$ water solution (2x10 ml), dried over Na_2SO_4, filtered and evaporated *in vacuo* to give a yellow solid (1.462 g). Part of the solid (303 mg) was purified by column chromatography (Silica 40 g, hexane/EtOAc 10:1 - 2:1) to give 2-phenyl-4,4-dimethoxycarbonylmethyl-5(4H)-oxazolone **9** (136 mg, 43.0% after two steps) as a goldish yellowish solid; R_f = 0.23 (EtOAc/hexane 1:2).

The rest of the yellow solid was screened in purification be recrystallisation according to the following procedure: the compound (100 mg) was dissolved in alcoholic solvent (1 ml) at reflux to give a clear solution, which was cooled to r.t. and the formed precipitate was filtered off, washed with cold (+10°C) solvent used for the crystallisation (3x1 ml) and dried in air to give 2-phenyl-4,4-dimethoxycarbonylmethyl-5(4H)-oxazolone **9** as slightly yellowish crystals; mp 164.5-165.5°C.

^{1}H NMR (700 MHz, $CDCl_3$): δ = 8.02 (d, *J* = 7.6 Hz, 2 H), 7.56 (t, *J* = 7.6 Hz, 1 H), 7.47 (t, *J* = 7.6 Hz, 2 H), 3.60 (s, 6 H), 3.02 (d, *J* = 16.6 Hz, 2 H), 2.99 (d, *J* = 16.6 Hz, 2 H).

^{13}C NMR (176.1 MHz, $CDCl_3$): δ = 178.9, 168.9, 163.8, 133.1, 128.9, 128.4, 125.9, 67.3, 52.3, 41.5.

HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{15}H_{16}NO_6$: 306.0978; found: 306.0972.

Table 1. Screening of solvents for oxazolone **9** purification.

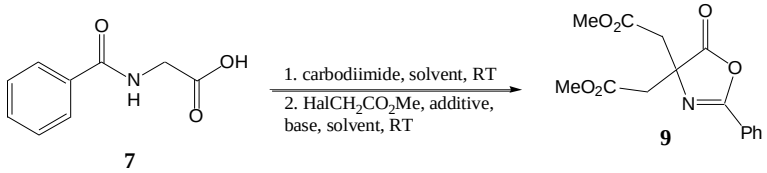
Entry	Solvent, purity	Yield of **9**, %[a]
1	MeOH, 99%	24
2	EtOH, 95%	34[b]
3	*i*-PrOH, 99%	39
4	*t*-BuOH, 99%	32
5	-[c]	43

[a] Isolated yield after two steps;

[b] The compound **9** was significantly contaminated by products derived from DCC or DCU;

[c] Isolated by preparative column chromatography on Silica

*II-3. General procedure for the screening of the conditions of 2-phenyl-4,4-dimethoxycarbonylmethyl-5(4H)-oxazolone **9** synthesis.*



7 **9**

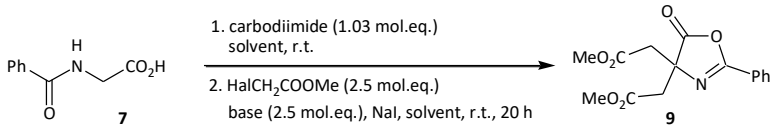
Hippuric acid **7** (1.792 g, 10 mmol) was added to the solution of carbodiimide (10.3 mmol, 1.03 mol. equiv.) in dry solvent (15 ml) and the resulted mixture was stirred at r.t. Methyl halogenoacetate (25 mmol, 2.5 mol. equiv.) was added followed with the additive and the mixture was cooled to +7°C. The base was added keeping the temperature of the reaction mixture below +25°C. The reaction mixture was stirred overnight, the precipitate was filtered off, washed with dry solvent used for the reaction (3x10 ml) and discarded. The combined mother solutions were evaporated *in vacuo*. The residue was dissolved in EtOAc (50 ml) and water (20 ml), shaken up, water layer was separated, organic layer was washed with sat. $NaHCO_3$ water solution (2x10 ml), brine (10 ml), dried over Na_2SO_4, filtered and evaporated *in vacuo*. The resulted product was recrystallized from hot *i*-PrOH (30 ml). The formed at r.t. material was filtered off, washed with cooled (+10°C) *i*-PrOH (3x10 ml) and dried in air to give 2-phenyl-4,4-dimethoxycarbonylmethyl-5(4H)-oxazolone **9** as slightly yellowish crystals; mp 164.5-165.5°C.

^{1}H NMR (700 MHz, $CDCl_3$): δ = 8.02 (d, *J* = 7.6 Hz, 2 H), 7.56 (t, *J* = 7.6 Hz, 1 H), 7.47 (t, *J* = 7.6 Hz, 2 H), 3.60 (s, 6 H), 3.02 (d, *J* = 16.6 Hz, 2 H), 2.99 (d, *J* = 16.6 Hz, 2 H).

^{13}C NMR (176.1 MHz, $CDCl_3$): δ = 178.9, 168.9, 163.8, 133.1, 128.9, 128.4, 125.9, 67.3, 52.3, 41.5.

HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{15}H_{16}NO_6$: 306.0978; found: 306.0972.

Table 2. Optimization of the reaction conditions for the oxazolone **9** synthesis.

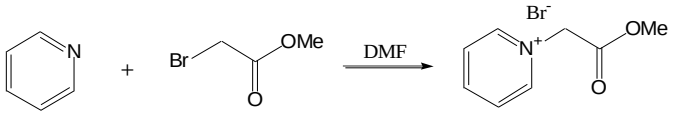


Entry	Reaction time of **7** with carbodiimide, h	Carbodiimide	Hal	NaI, mol. equiv.	Base	Solvent	Yield of **9**, %[a]
1	19	DCC	Br	0.1	DIPEA	DMF	48
2	3	DCC	Br	0.1	DIPEA	DMF	55
3	1	DCC	Br	0.1	DIPEA	DMF	55
4[b]	3	DCC	Br	-	DIPEA	DMF	55
5	3	DCC	Cl	-	DIPEA	DMF	-[c]
6	3	DCC	Cl	0.1	DIPEA	DMF	4
7	2[d]	DCC	Cl	2.75	DIPEA	DMF	50
8	3	DIC	Br	0.1	DIPEA	DMF	57
9	19	DCC	Br	0.1	DIPEA	Dioxane	-[e]
10	19	DCC	Br	0.1	DIPEA	THF	-[e]
11	19	DCC	Br	0.1	DIPEA	EtOAc	-[e]
12	19	DCC	Br	0.1	DIPEA	CH_2Cl_2	5[f]
13	19	DCC	Br	0.1	DIPEA	MeCN	25
14	3	DCC	Br	-	Et_3N	DMF	55
15	3	DCC	Br	0.1	py	DMF	-[g]
16	3	DCC	Br	-	py	DMF	-[g]
17	3	DCC	Br	0.1	2,6-Lutidine	DMF	-[e,h]
18	3	DCC	Br	0.1	Cs_2CO_3	DMF	34
19[i]	3	DCC	Br	0.1	K_2CO_3	DMF	45
20[j]	3	DCC	Br	0.1	K_2CO_3	DMF	49
21	3	DCC	Br	0.1	Na_2CO_3	DMF	36
22	3	DCC	Br	0.1	Li_2CO_3	DMF	33
23	3	DCC	Br	0.1	-	DMF	-[g]

[a] Isolated by recrystallization of the reaction mixture yield after two steps.
[b] When 1.2 mol.eq. of DCC were used in the reaction the obtained yield of **9** was 54%; in another experiment with 1.03 mol.eq. of DCC, 3 mol.eq. of methyl bromoacetate and 3 mol.eq. of DIPEA the obtained yield of **9** was 56%.
[c] According to ^{1}H NMR data the reaction mixture did not contain the product **9**.
[d] The reaction mixture was stirred for an additional hour after the addition of NaI.
[e] Despite the fact of the product was presented in the reaction mixture in trace amounts it was not isolable from the reaction mixture by recrystallization from *i*-PrOH.
[f] Isolated by two recrystallizations from *i*-PrOH.
[g] According to ^{1}H NMR data the reaction mixture contained only oxazolone **8** together with some amount of unidentified impurities. We found that pyridine reacts rapidly with methyl bromoacetate in DMF forming the quaternary pyridinium salt and thus both reagents leave the reaction medium shortly after the mixing.
[h] According to ^{1}H NMR data the reaction mixture contained about 40% of oxazolone **8** and 15% of the intermediate mono alkylated oxazolone among all the identified products derived from **7**. The mono alkylated product was identified by comparison with the literature data. [3]
[i] The reaction is highly exothermic and the temperature of the mixture raised up to 45°C, when it was kept below 25°C by the yield of the compound **9** was dropped to 41%.
[j] 1.5 Mol.eq. of the base were used in the reaction.

[3] Mandai, H.; Hongo, K.; Fujiwara, T.; Fujii, K.; Mitsudo, K.; Suga, S. *Org. Lett.* **2018**, 20, 4811.

II-4. Synthesis of 1-(2-methoxy-2-oxoethyl)pyridin-1-ium bromide.



Dry pyridine (396 mg, 0.4 ml, 5 mmol) was added to a solution of methylbromoacetate (765 mg, 5 mmol) in dry DMF (5 ml) and white precipitate was formed within a few min of stirring at r.t. The precipitate was filtered off, washed with dry DMF (3x2 ml) and dried *in vacuo* to give 1-(2-methoxy-2-oxoethyl)pyridin-1-ium bromide (840 mg, 3.6 mmol, 72%) with spectral data identical to those described in literature. [4]

^{1}H NMR (700 MHz, DMSO-d_6): δ = 9.08 (dd, *J* = 8.2, 1.3 Hz, 2 H), 8.73 (tt, *J* = 7.9, 1.3 Hz, 1 H), 8.26 (dd, *J* = 8.2, 7.8 Hz, 2 H), 5.72 (s, 2 H), 3.78 (s, 3 H).

*II-5. Isolation of the additional crop of **10**.*

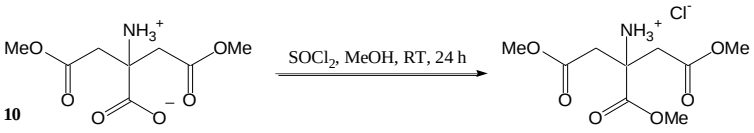
Mother solution from the synthesis of **10** (see the Main text) was evaporated *in vacuo* at 50°C to give yellow oil (9.760 g) with alcoholic smell. The oil was refluxed in a mixture of distilled water (50 ml) and concd HCl (50 ml) for 24 h to give dark yellow solution with drops of brownish light oil. The mixture was extracted with CH_2Cl_2 (5x10 ml) and evaporated *in vacuo*. The obtained solid was dissolved in distilled water (200 ml), decolorized with charcoal, filtered and again evaporated *in vacuo* to give colorless powder (7.375 g). According to ^{1}H NMR data this powder contained some unidentified derivatives from propylene oxide.

The powder was dissolved in MeOH (120 ml), cooled to -20°C and thionyl chloride (10 ml) was added to the solution over 10 min keeping the temperature of the reaction mixture below -5°C. The resulted clear solution was stirred at r.t. for 24 h and evaporated *in vacuo*. The obtained solid was triturated with Et_2O (3x40 ml) and dried *in vacuo* at 40°C to give white powder (8.24 g).

A solution of the obtained powder in a mixture of MeOH (50 ml) and propylene oxide (17 ml) was refluxed for 3 h, cooled to r.t. and Et_2O (90 ml) was added. The formed precipitate was filtered off, washed with a mixture Et_2O/MeOH = 4/1 (3x20 ml) and dried in air to give additional crop of **10** (2.762 g, 12.6 mmol, 14% from **9**) as a white solid.

[4] Brioche, J.; Meyer, C.; Cossy, J. *Org. Lett.* **2015**, 17, 2800.

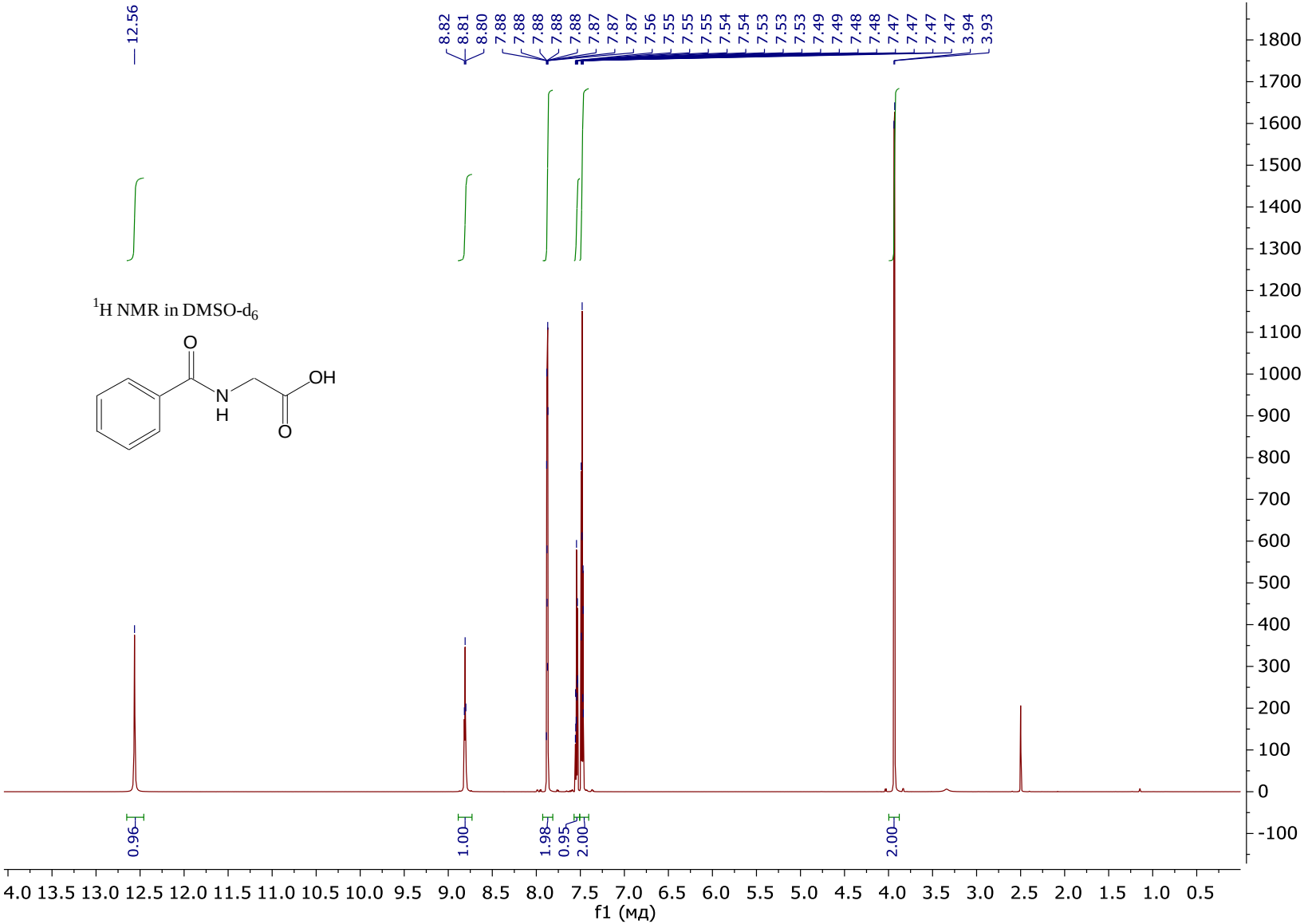
*II-6. Reaction of **10** with thionyl chloride in MeOH.*

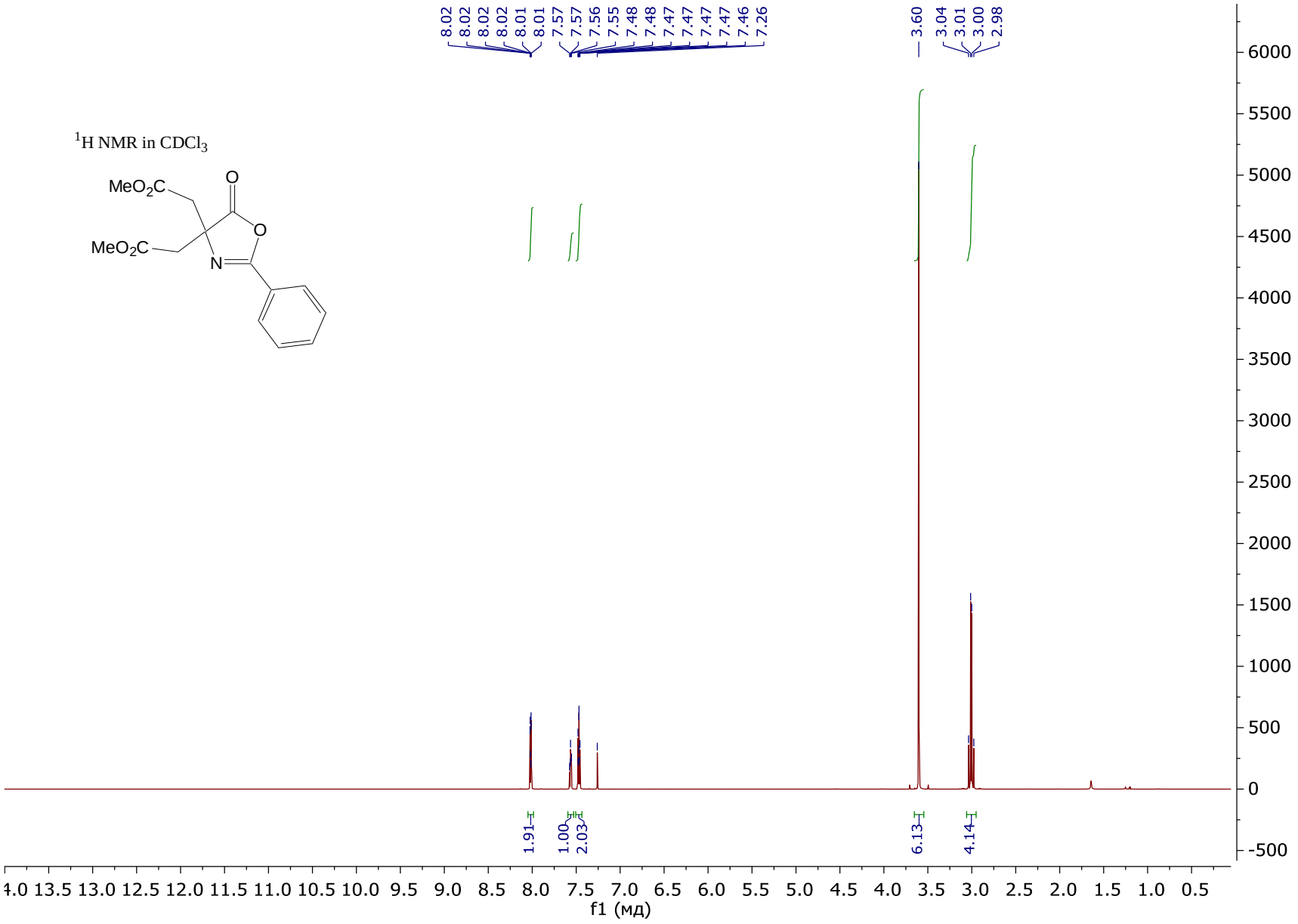


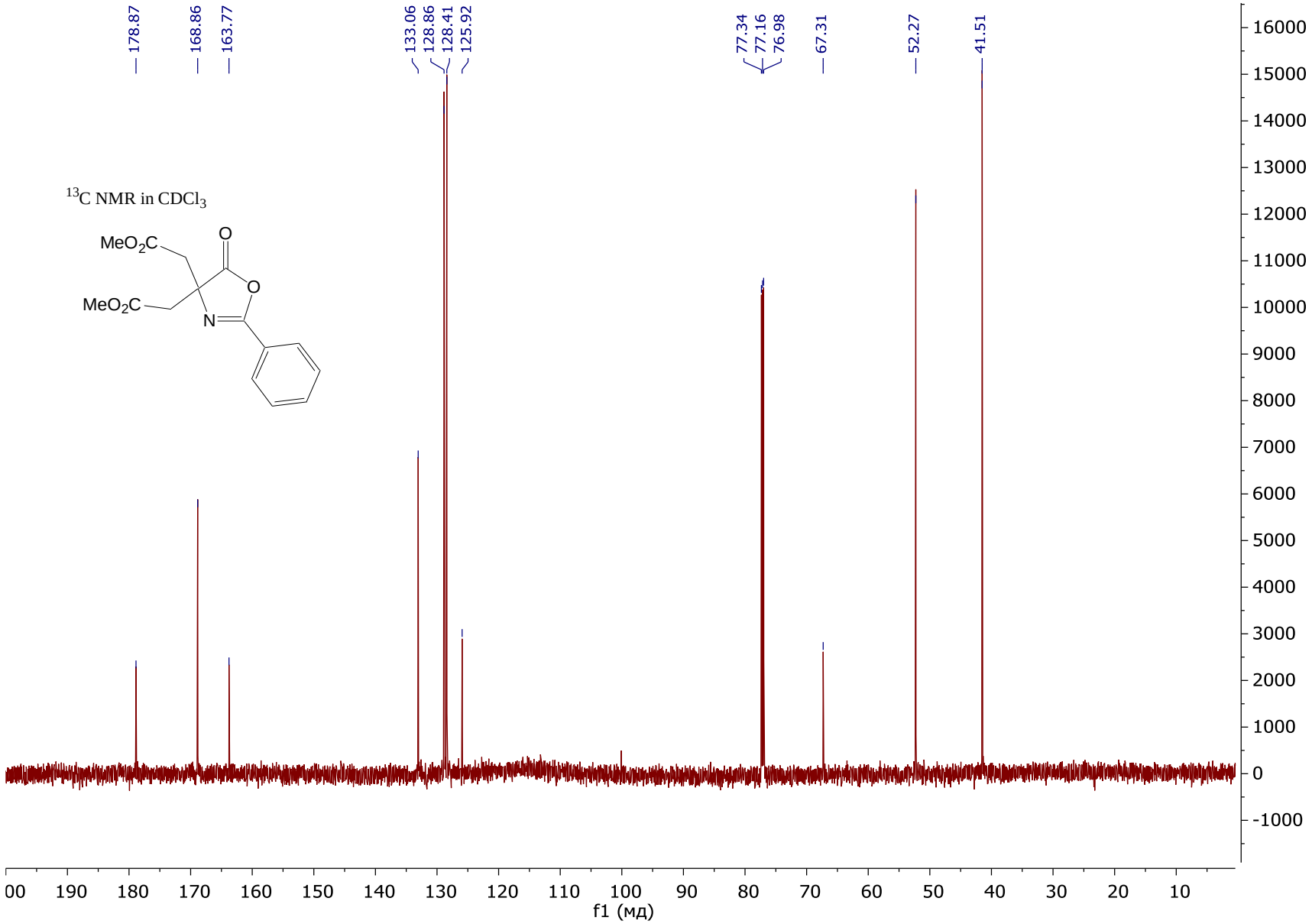
10

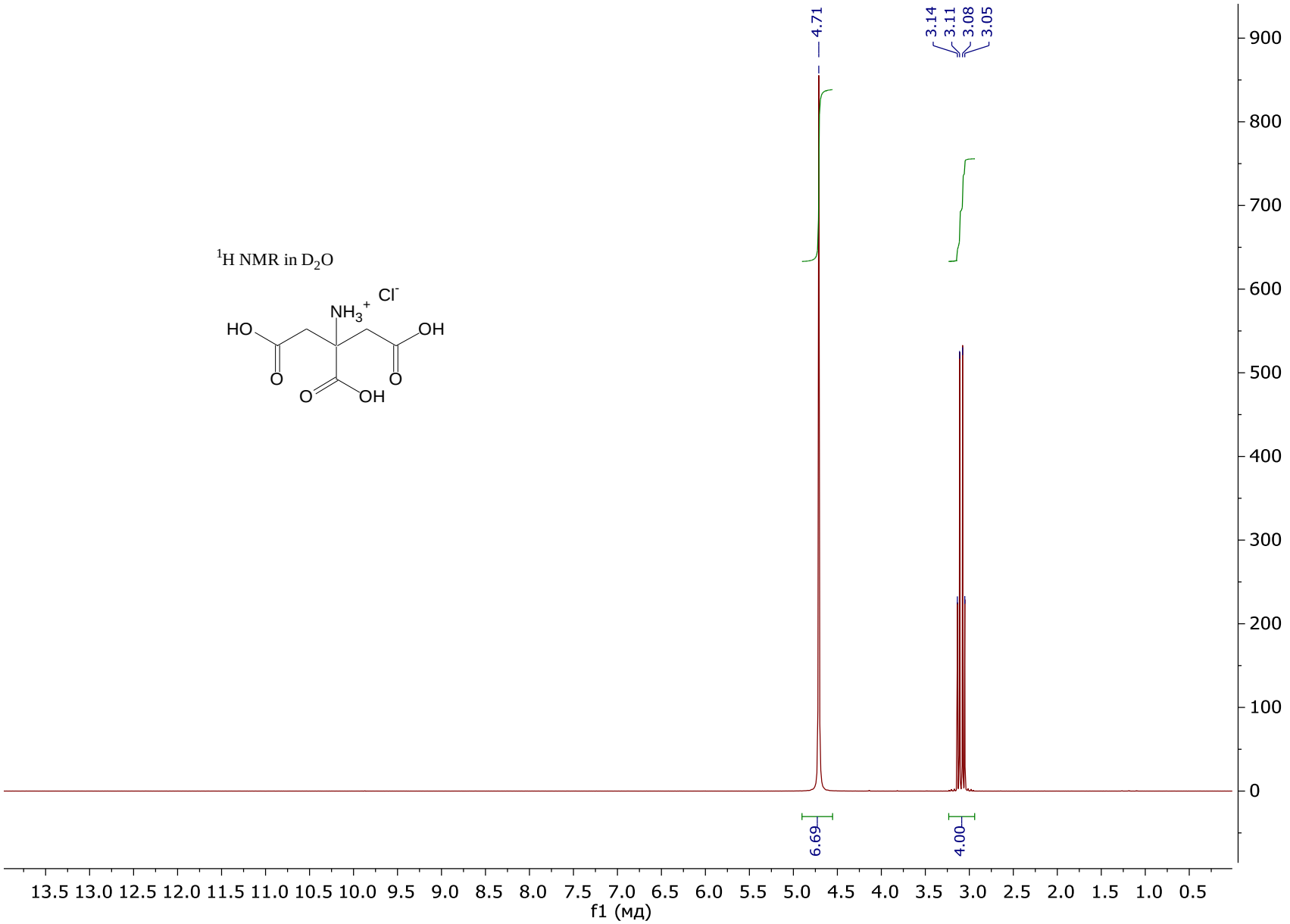
Thionyl chloride (1.78 g, 15 mmol, 30 mol. equiv.) was added to a solution of **10** (109.6 mg, 0.5 mmol) in MeOH (7 ml) at -20°C over 3 min keeping the temperature of the reaction mixture below -5°C. The resulted clear solution was stirred at r.t. for 24 h and evaporated *in vacuo*. The obtained colorless viscous oil was triturated with Et_2O (3x4 ml) and dried *in vacuo* at 40°C to give a white solid (128.4 mg) which according to ^1H NMR data consisted from 1,3-dimethyl-2-aminopropane-2-carboxyl-1,3-dicarboxylate hydrochloride **10 (HCl)** and 1,2,3-trimethyl-2-aminopropane-1,2,3-tricarboxylate hydrochloride (approximately 90/10). The compounds were identified only by ^1H NMR of the reaction mixture without isolation.

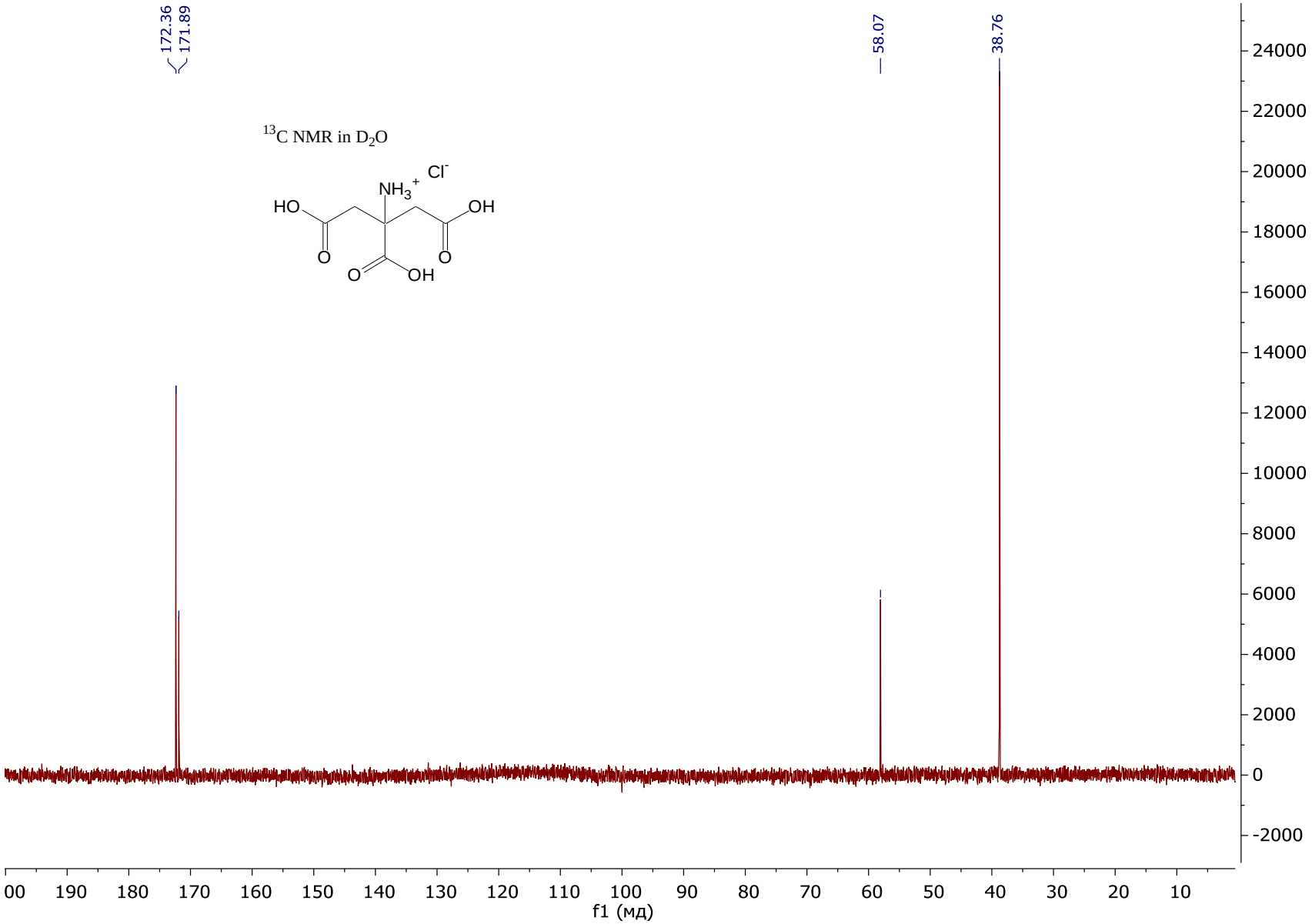
III. Copies of ^{1}H and ^{13}C NMR spectra.

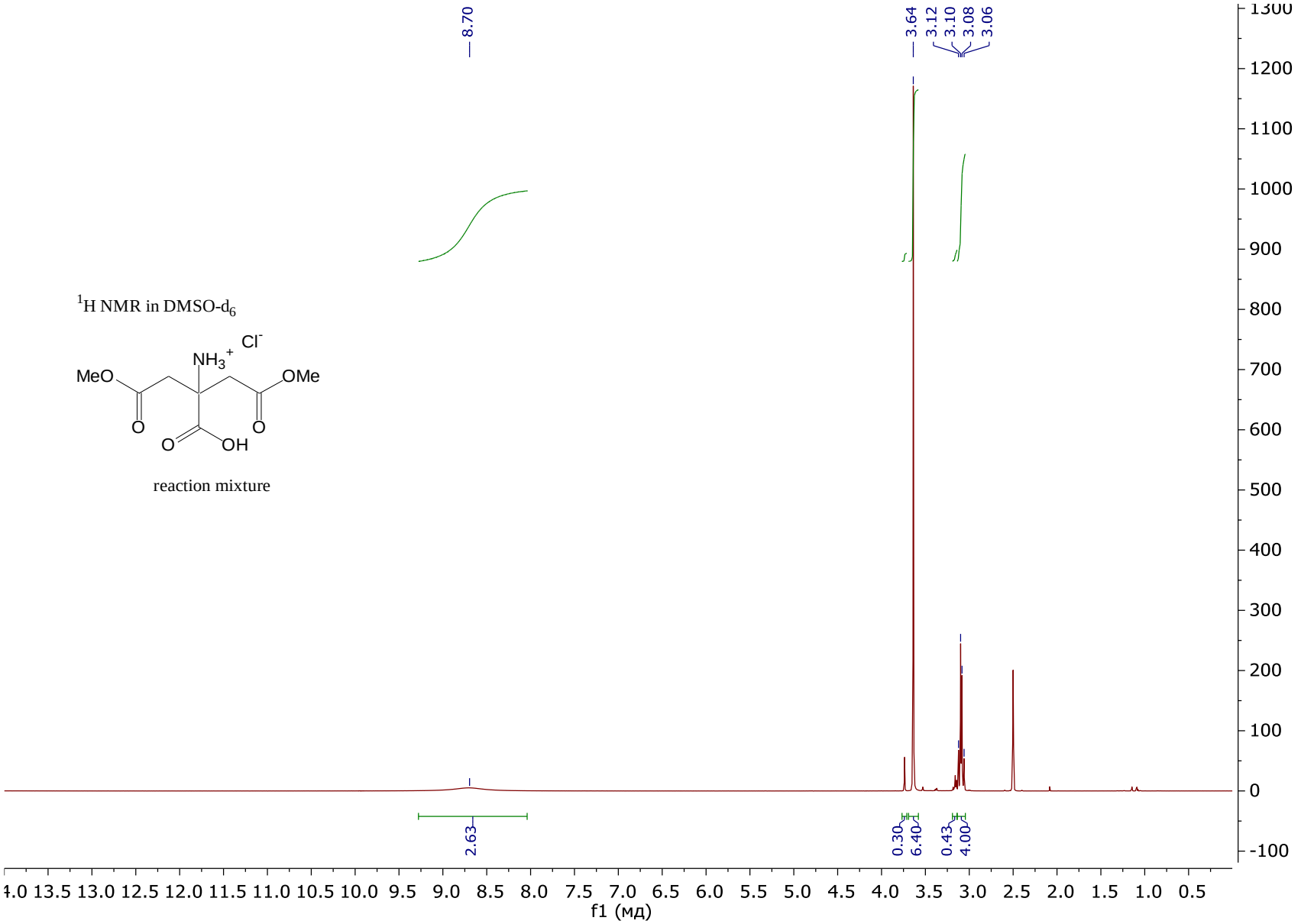


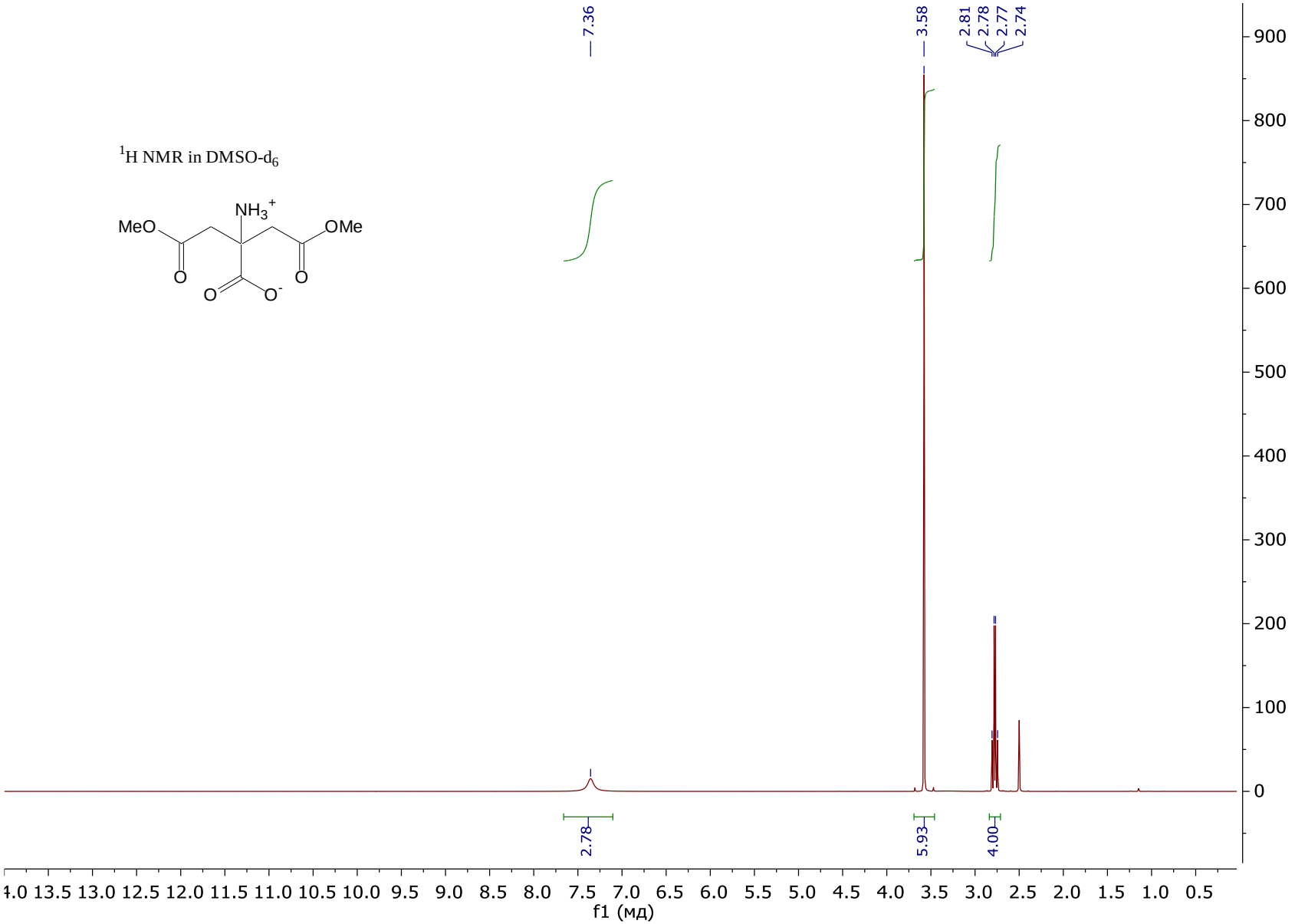

^{1}H NMR in $CDCl_3$
MeO_2C
MeO_2C
O
O
N
8.02
8.02
8.02
8.02
8.01
8.01
7.57
7.57
7.56
7.55
7.48
7.48
7.47
7.47
7.47
7.47
7.46
7.26
3.60
3.04
3.01
3.00
2.98
1.91
1.00
2.03
6.13
4.14
f1 (мд)

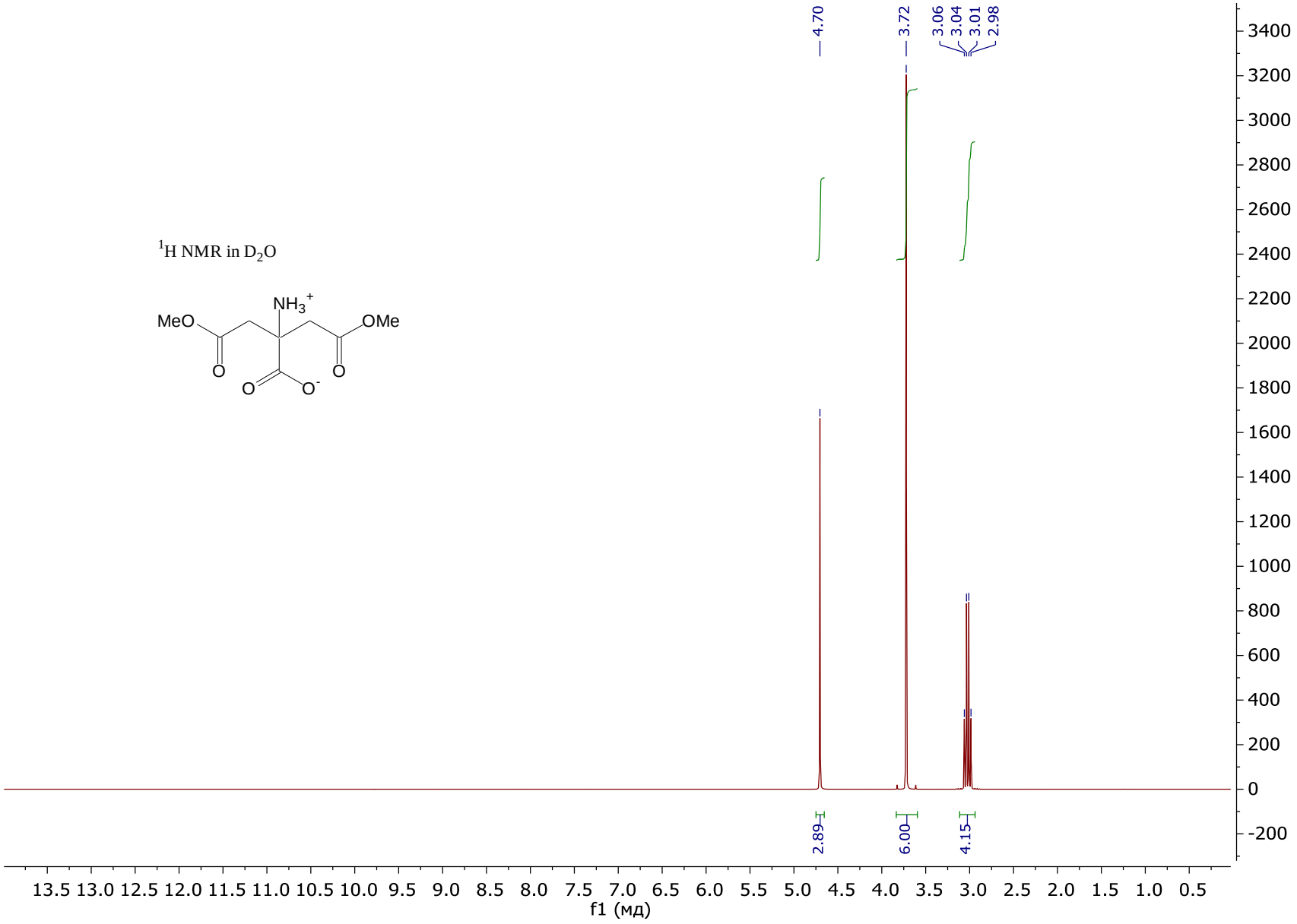

178.87
168.86
163.77
133.06
128.86
128.41
125.92
77.34
77.16
76.98
67.31
52.27
41.51
^{13}C NMR in CDCl$_3$
MeO$_2$C
MeO$_2$C
O
O
N
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

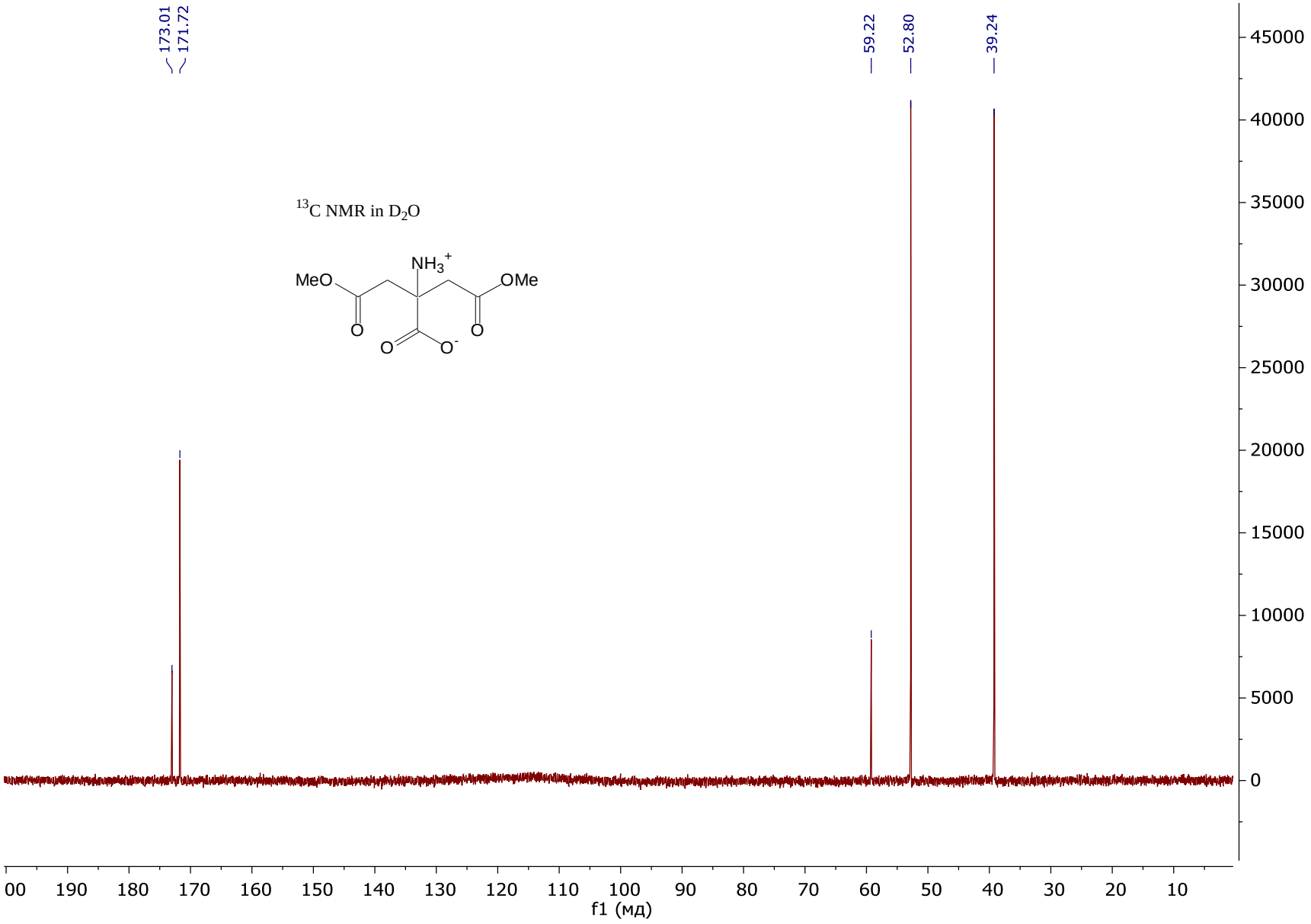

^{1}H NMR in D_2O
Cl$^-$
NH$_3^+$
HO
OH
O
O
O
OH
4.71
3.14
3.11
3.08
3.05
6.69
4.00
900
800
700
600
500
400
300
200
100
0
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (мд)

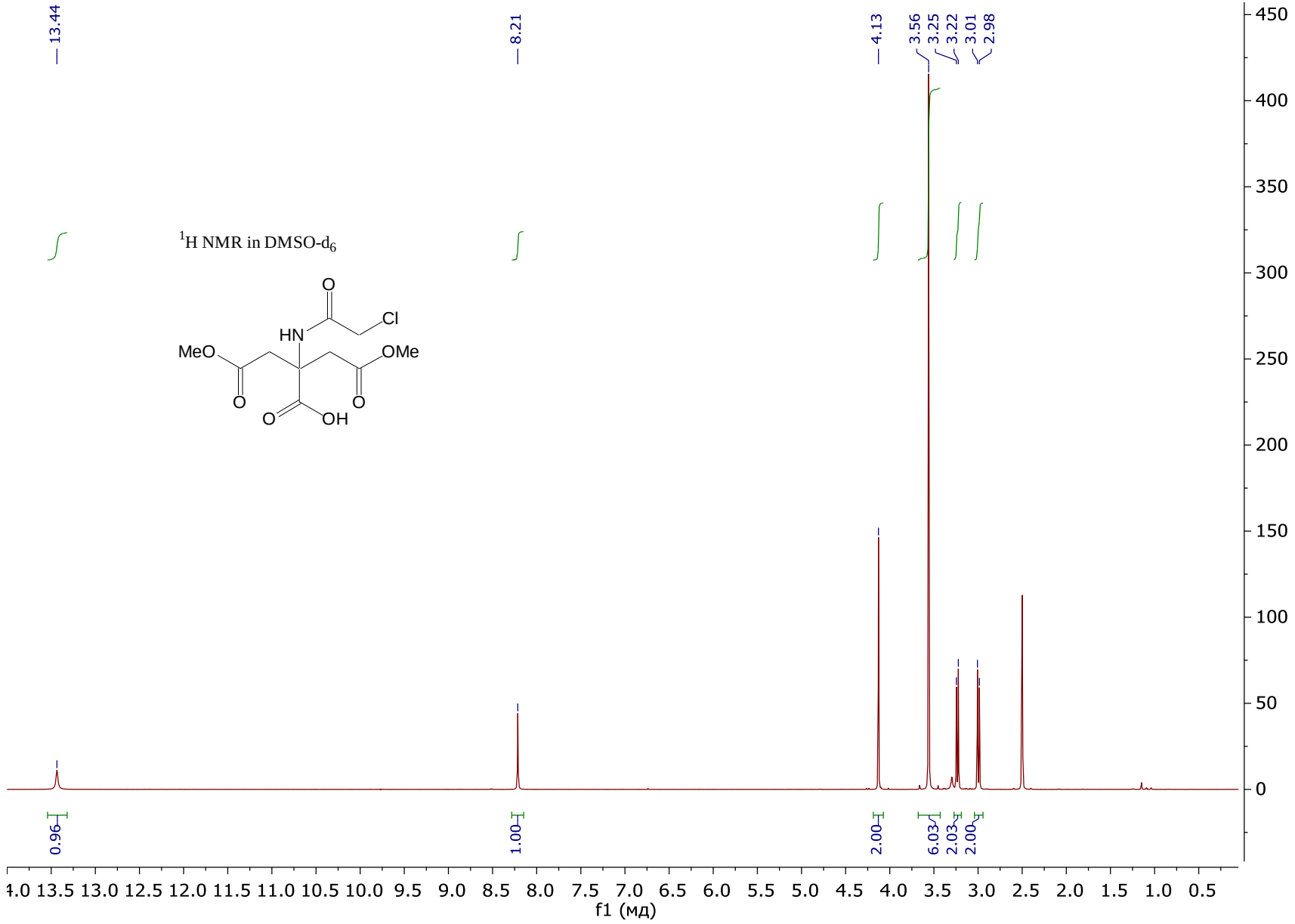

172.36
171.89
58.07
38.76
^{13}C NMR in D_2O
Cl^-
NH_3^+
HO
OH
O
O
O
OH
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)

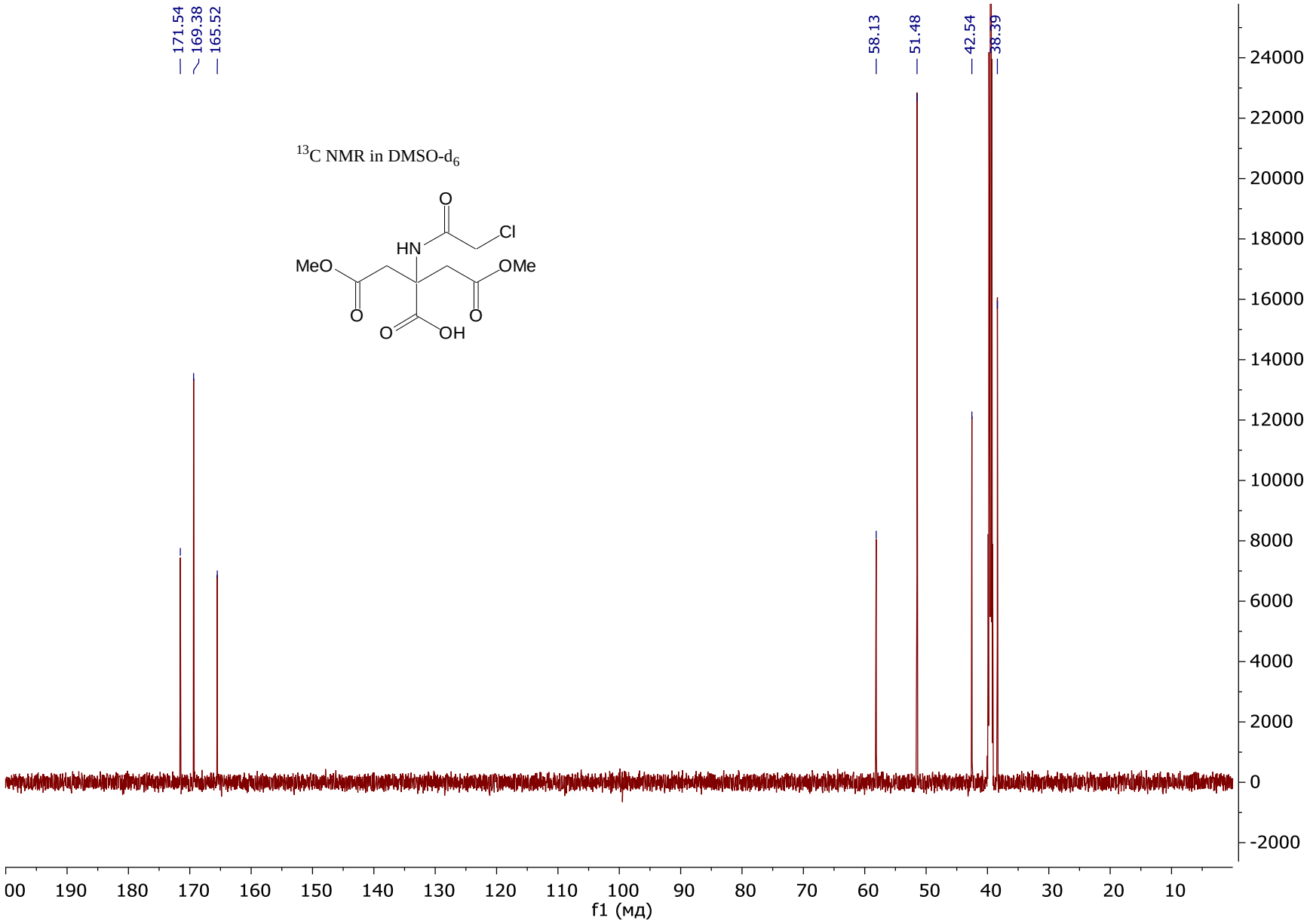

8.70
3.64
3.12
3.10
3.08
3.06
1H NMR in DMSO-d6
Cl-
NH3+
MeO
OMe
O
O
O
OH
reaction mixture
2.63
0.30
6.40
0.43
4.00
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (мд)

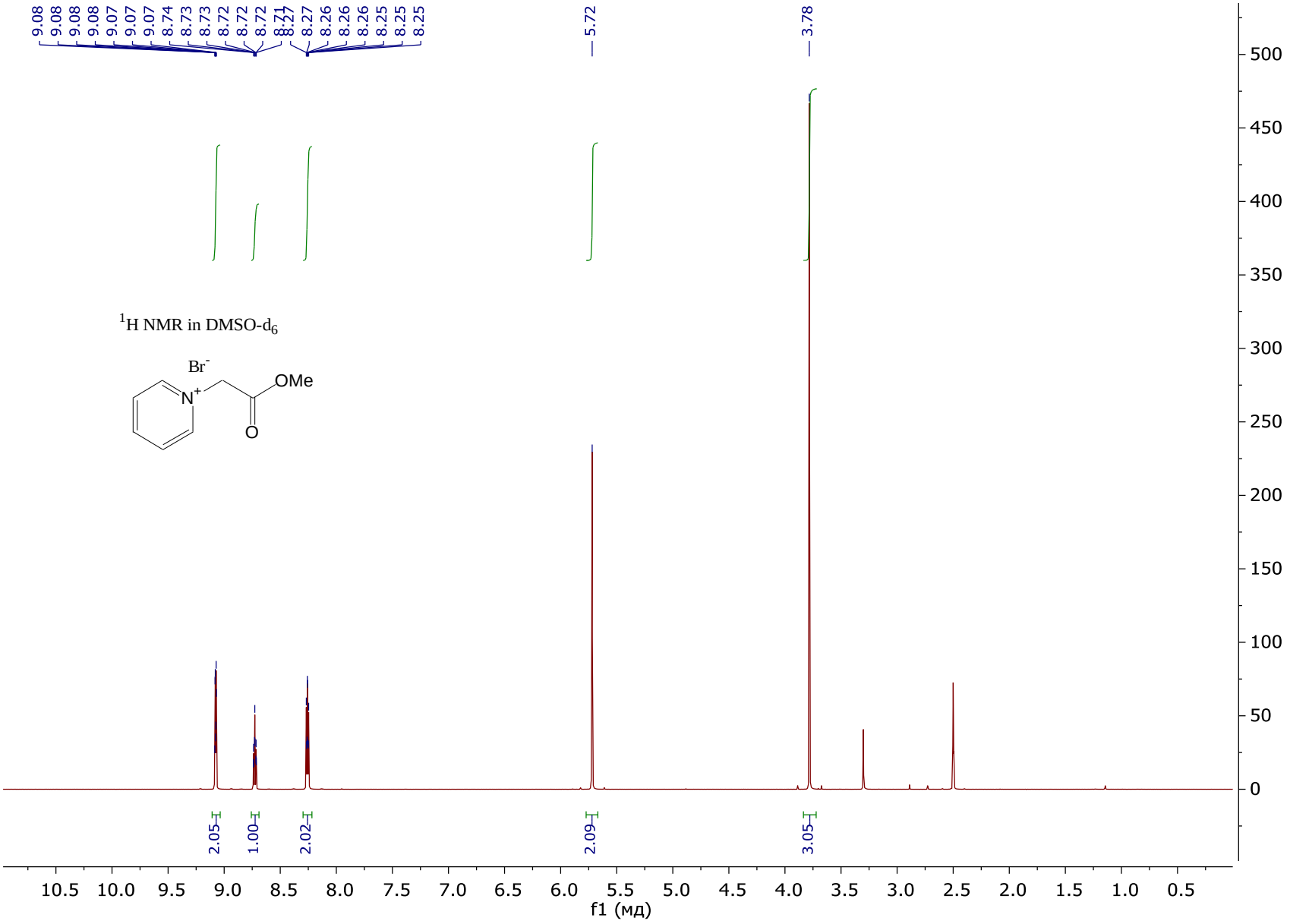

^{1}H NMR in DMSO-d$_6$
MeO
OMe
NH$_3^+$
O
O
O
O$^-$
7.36
3.58
2.81
2.78
2.77
2.74
2.78
5.93
4.00
f1 (мд)

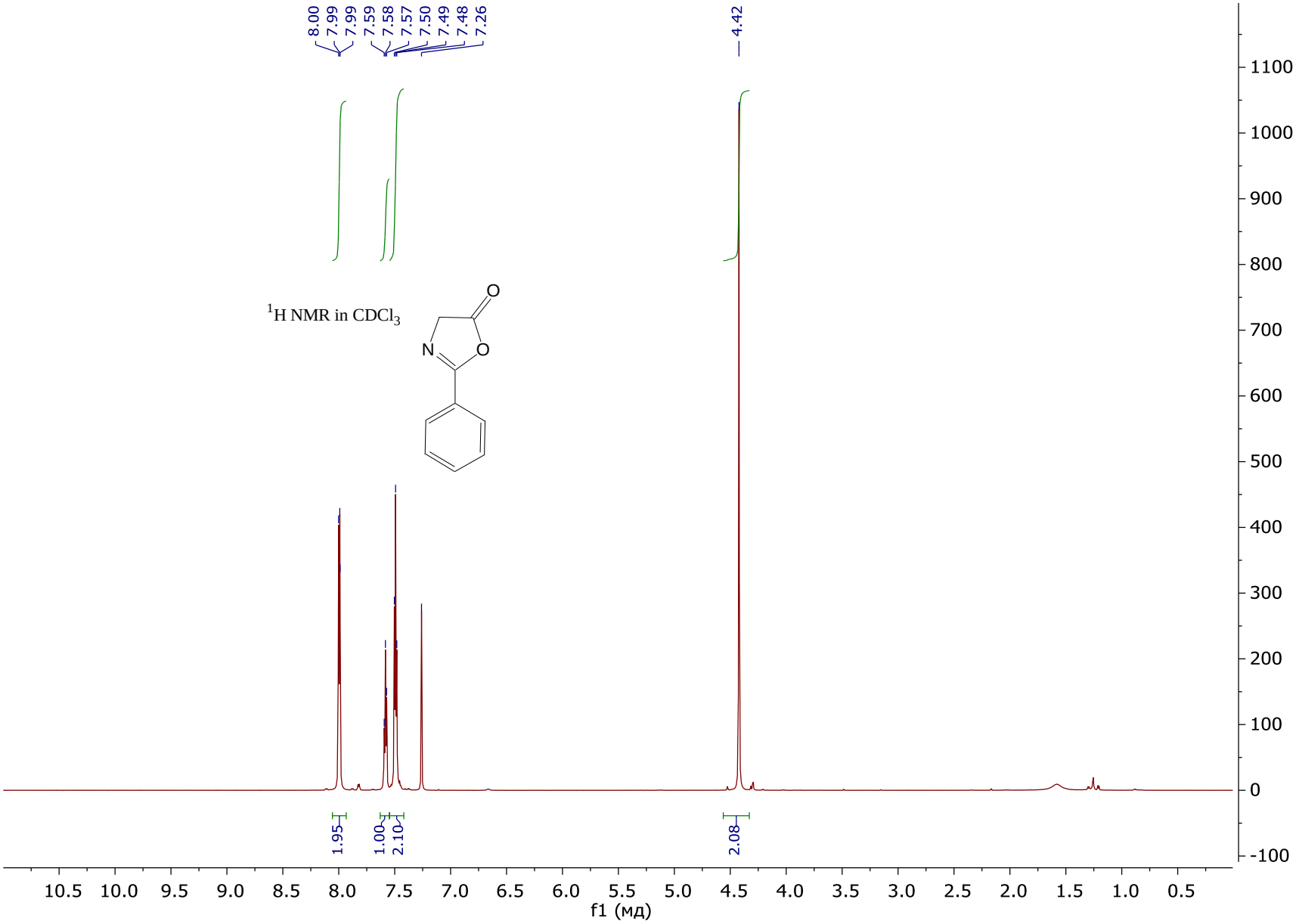

^{1}H NMR in D_2O
MeO
OMe
NH_3^+
O
O
O
O
O^-
4.70
3.72
3.06
3.04
3.01
2.98
2.89
6.00
4.15
f1 (мд)


173.01
171.72
59.22
52.80
39.24
^{13}C NMR in D_2O
MeO
NH_3^+
OMe
O
O
O
O$^-$
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (мд)

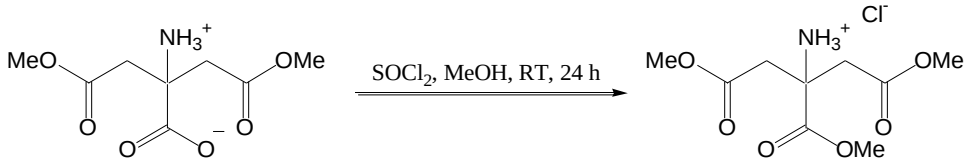

13.44
8.21
4.13
3.56
3.25
3.22
3.01
2.98
^{1}H NMR in DMSO-d$_6$
O
HN
Cl
MeO
OMe
O
O
O
O
OH
0.96
1.00
2.00
6.03
2.03
2.00
450
400
350
300
250
200
150
100
50
0
f1 (мд)


171.54
169.38
165.52
58.13
51.48
42.54
38.39
^{13}C NMR in DMSO-d$_6$
O
HN
Cl
MeO
OMe
O
O
O
OH
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (мд)


9.08
9.08
9.08
9.08
9.07
9.07
9.07
8.74
8.73
8.73
8.72
8.72
8.72
8.71
8.27
8.27
8.26
8.26
8.26
8.25
8.25
8.25
5.72
3.78
^{1}H NMR in DMSO-d$_6$
Br$^-$
N$^+$
OMe
O
2.05
1.00
2.02
2.09
3.05
500
450
400
350
300
250
200
150
100
50
0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (мд)


8.00
7.99
7.99
7.59
7.58
7.57
7.50
7.49
7.48
7.26
4.42
^{1}H NMR in $CDCl_3$
O
N
O
1.95
1.00
2.10
2.08
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (мд)

^{1}H NMR in DMSO-d_6 of the reaction mixture



IV. Copies of HRMS data.

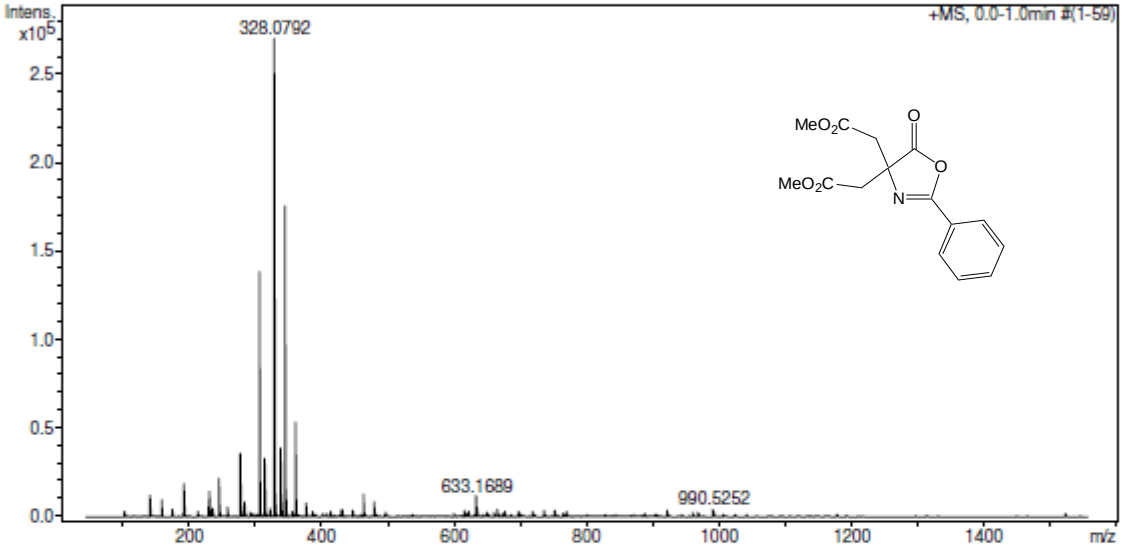
Display Report

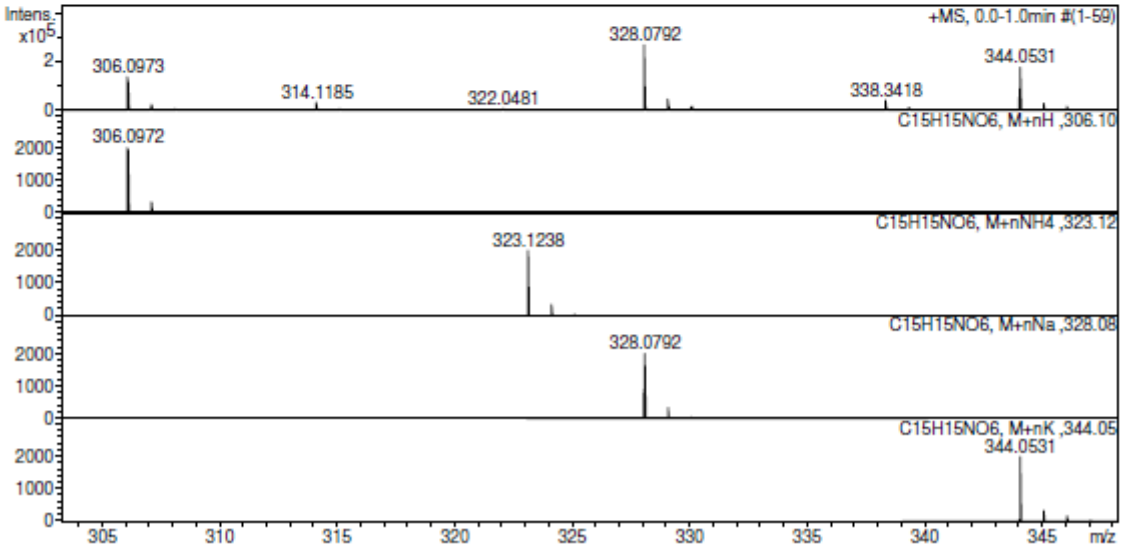
Analysis Info

Analysis Name	D:\Data\Chizhov\IBC\Bovin\Nizovtsev\an350_&clblow.d	Acquisition Date	18.06.2019 12:54:17
Method	tune_low_1550.m	Operator	BDAL@DE
Sample Name	/CHIZ AN350	Instrument	maXis 43
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source





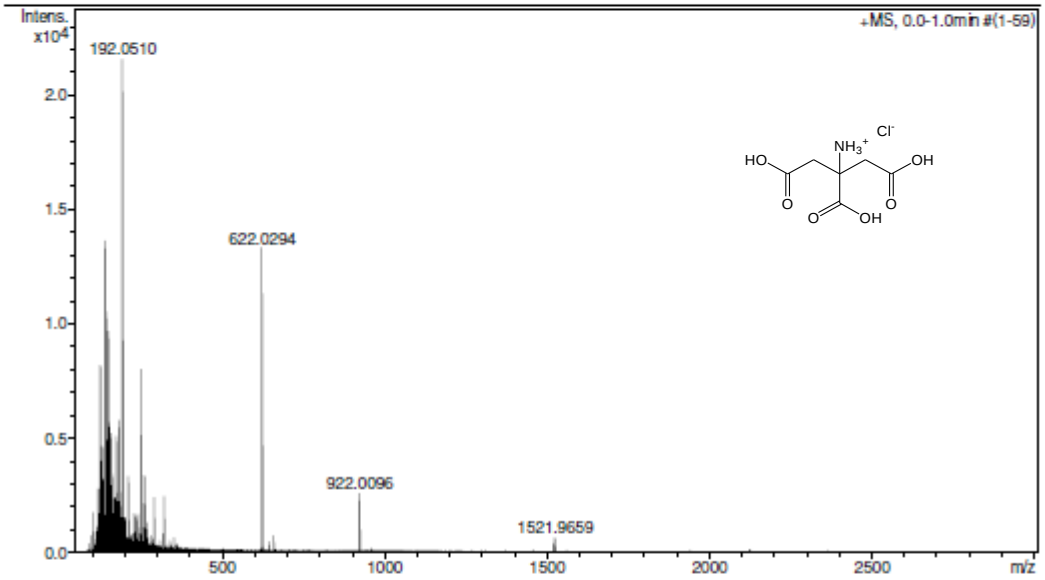
Display Report

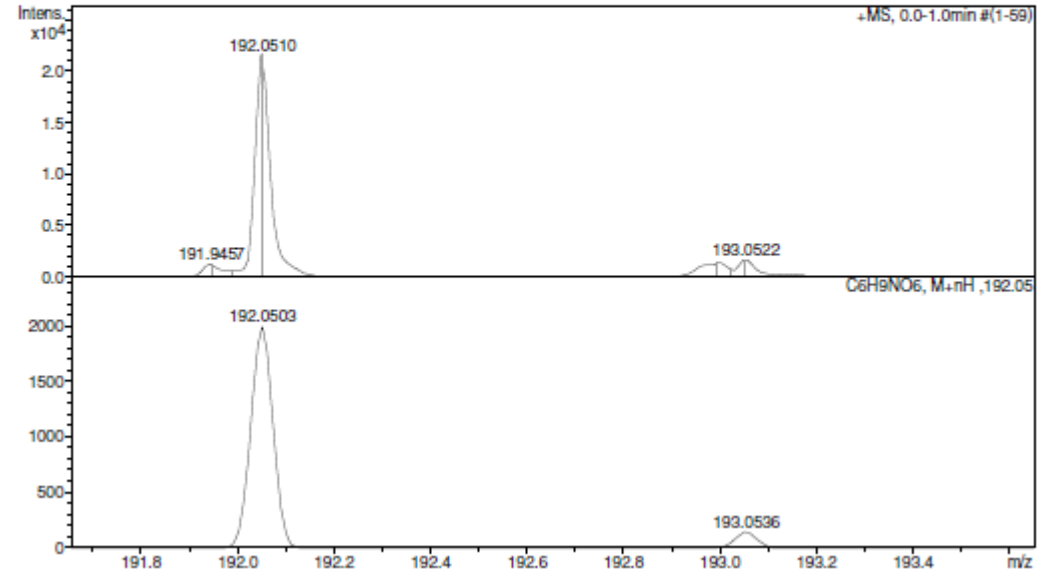
Analysis Info

Analysis Name	D:\Data\Chizhov\IBC\Bovin\Nizovtsev\an359_&clblow.d	Acquisition Date	23.08.2019 15:29:46
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/CHIZ AN359	Instrument / Ser#	micrOTOF 10248
Comment	H2O 100 %, dil. 200, calibtant added		

Acquisition Parameter

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





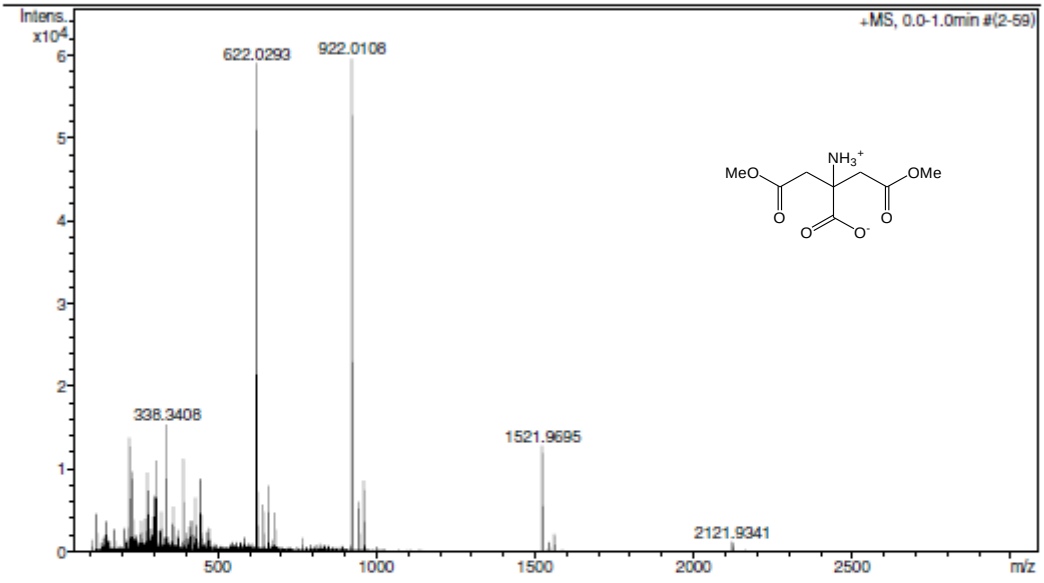
Display Report

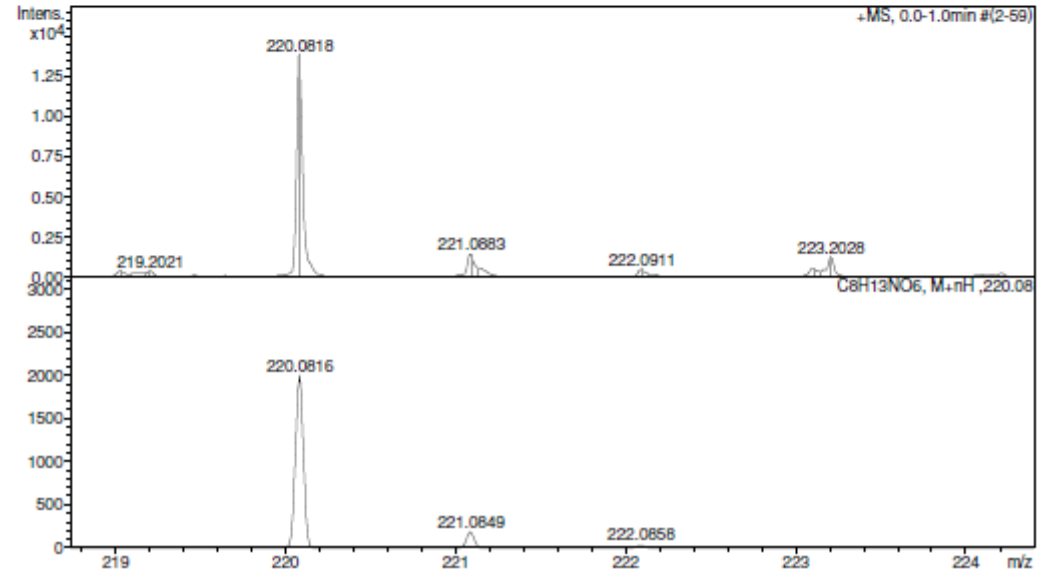
Analysis Info

Analysis Name	D:\Data\Chizhov\IBC\Bovin\Nizovtsev\an368_&clblow.d	Acquisition Date	23.08.2019 15:52:59
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/CHIZ AN368	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN : H2O 50/50 %, dil. 400, calibtant added		

Acquisition Parameter

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





Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\IBC\Bovin\Nizovtsev\an367_&clblow.d	Acquisition Date	23.08.2019 15:45:46
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/CHIZ AN367	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, calibtant added		

Acquisition Parameter

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