

Supporting Information for

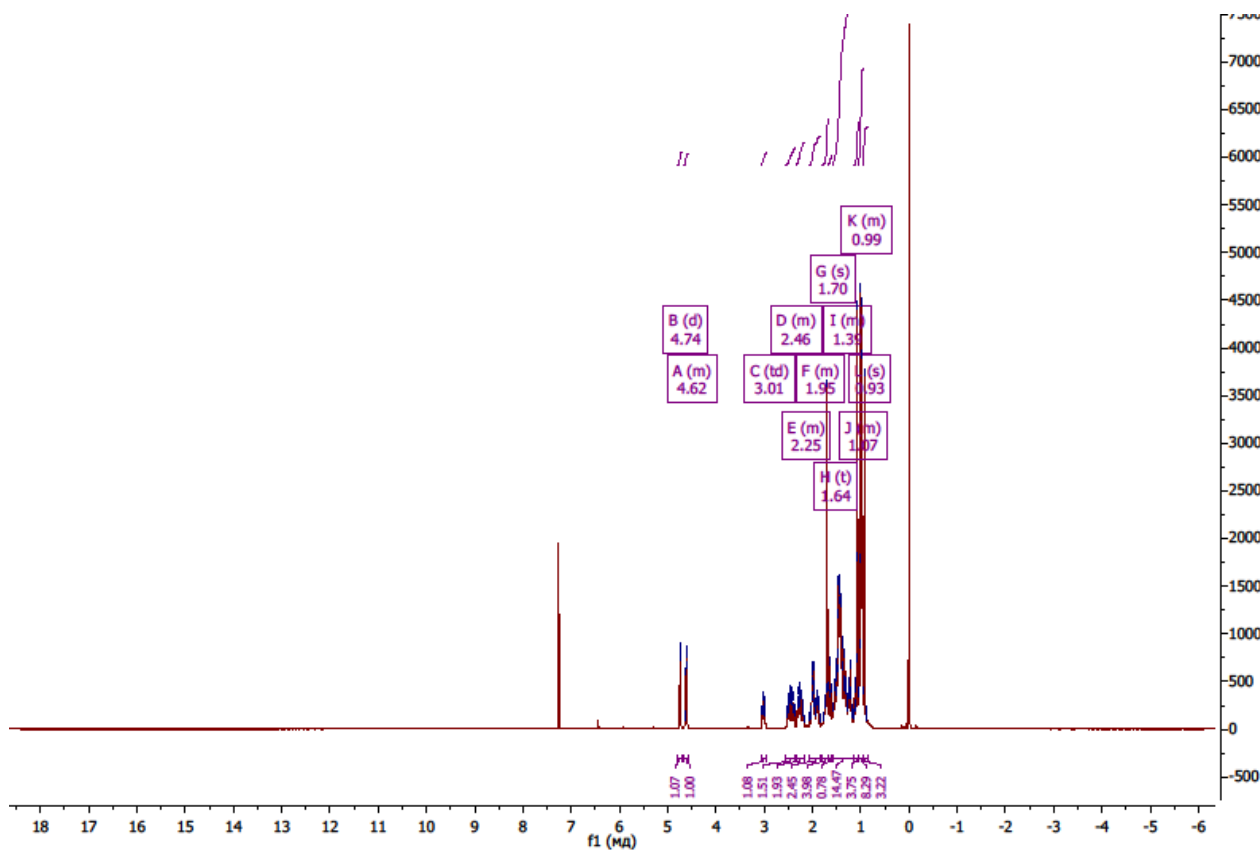
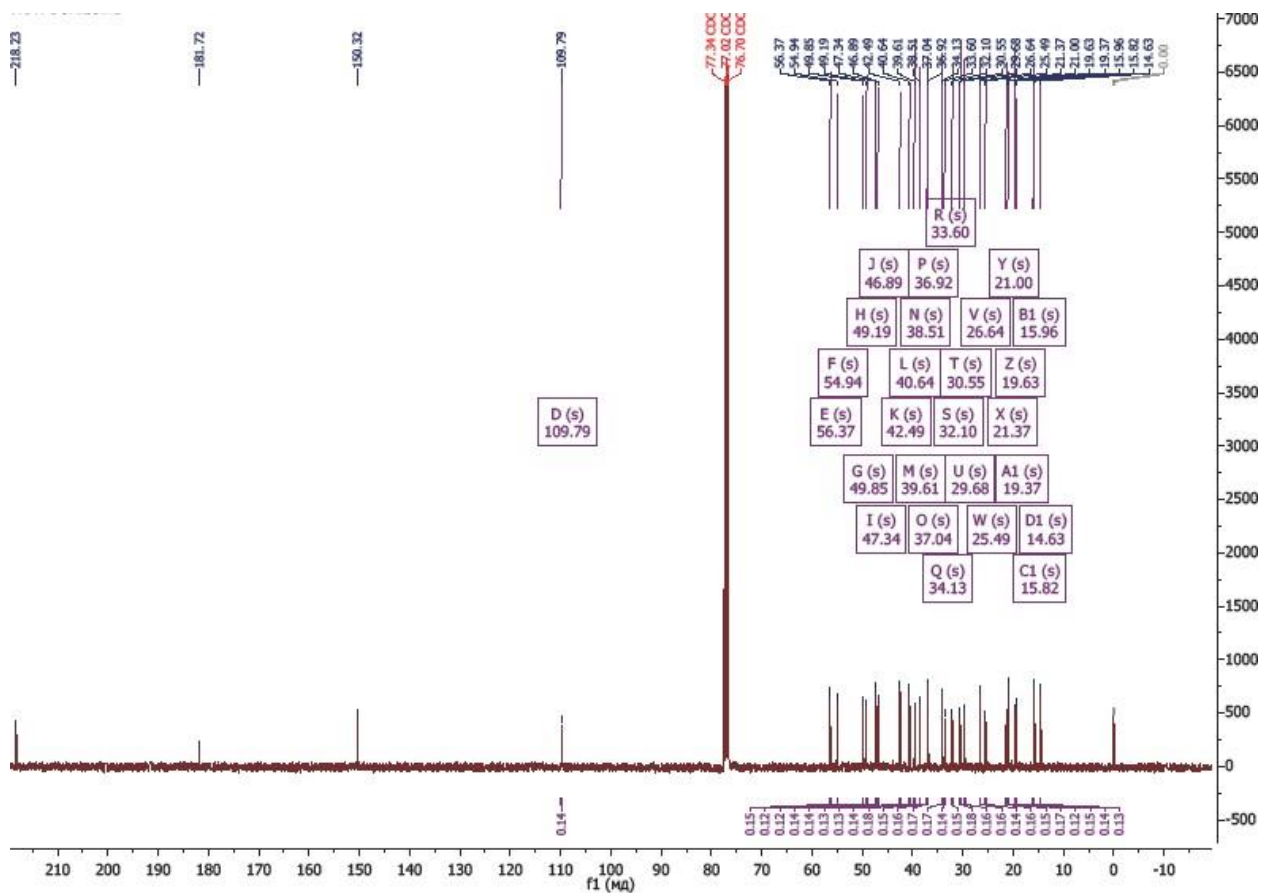
Synthesis and Investigation of Biological Activity of New Betulonic Acid Derivatives Containing 1,2,3-Triazole Fragments

List of Contents

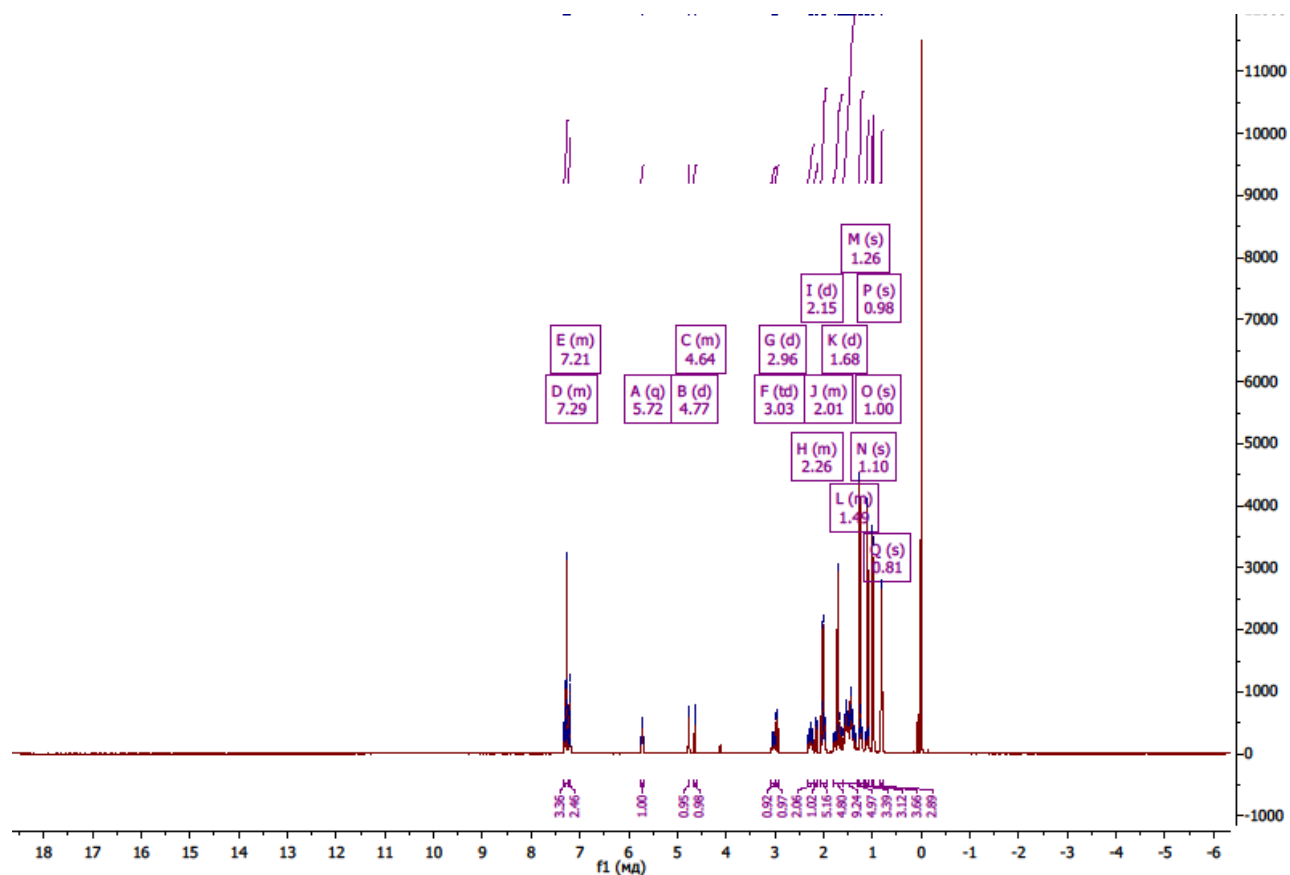
^1H , ^{13}C NMR and Mass-Spectra

Compounds 2–22

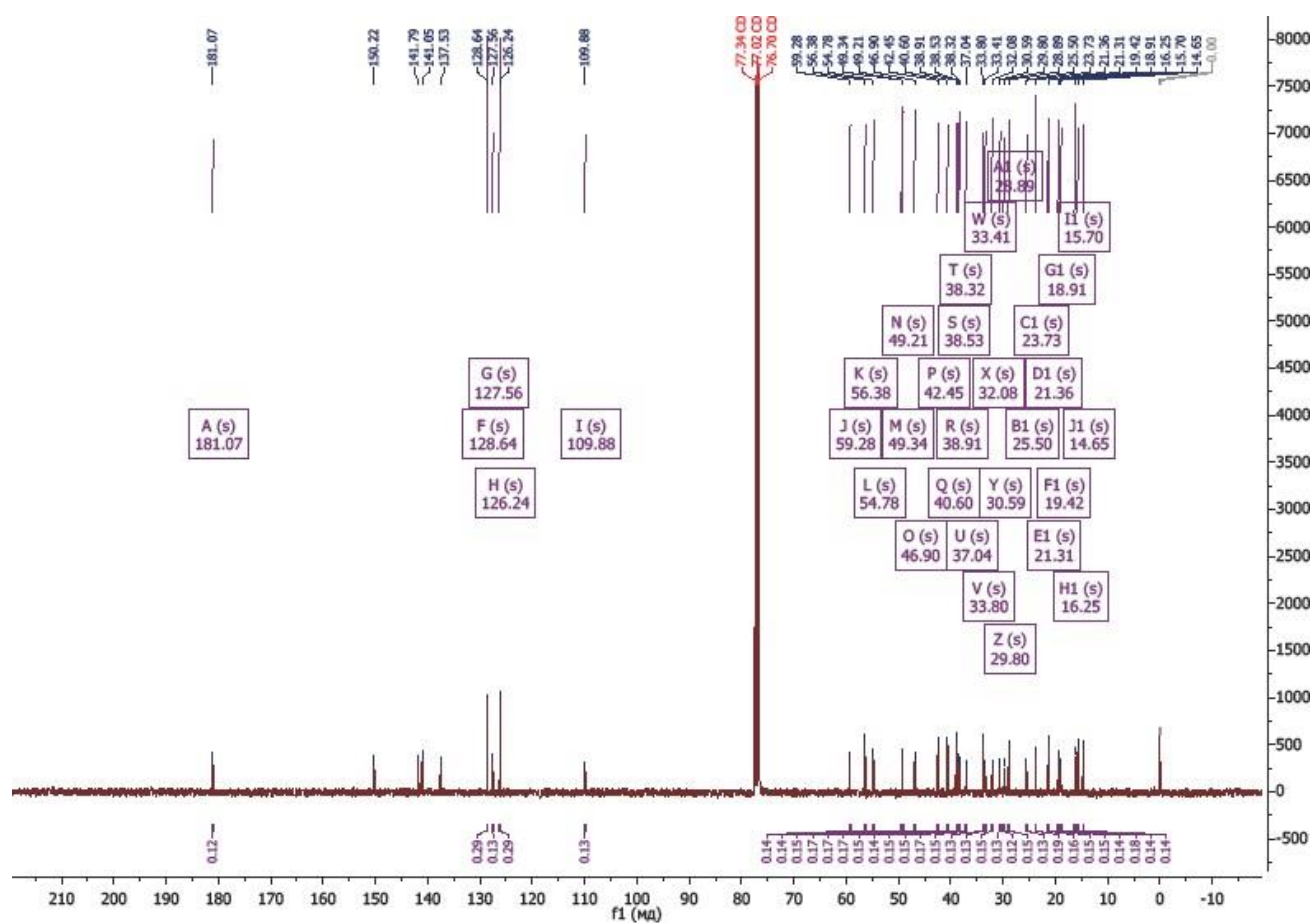
Compound **2**, ¹H NMR (400 MHz, CDCl₃)

 ^{13}C NMR (101 MHz, CDCl_3)

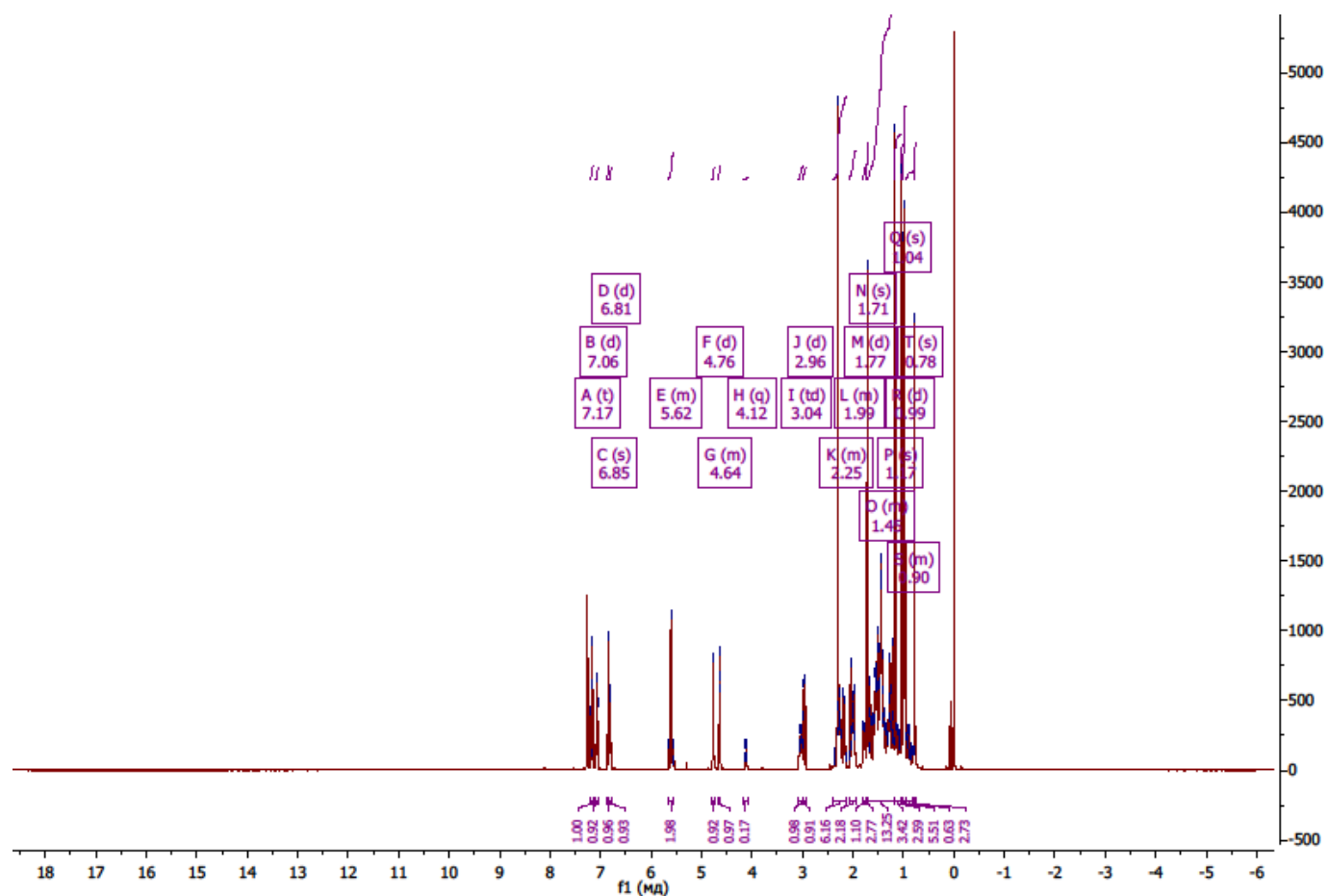
Compound **3**, ^1H NMR (400 MHz, CDCl_3)



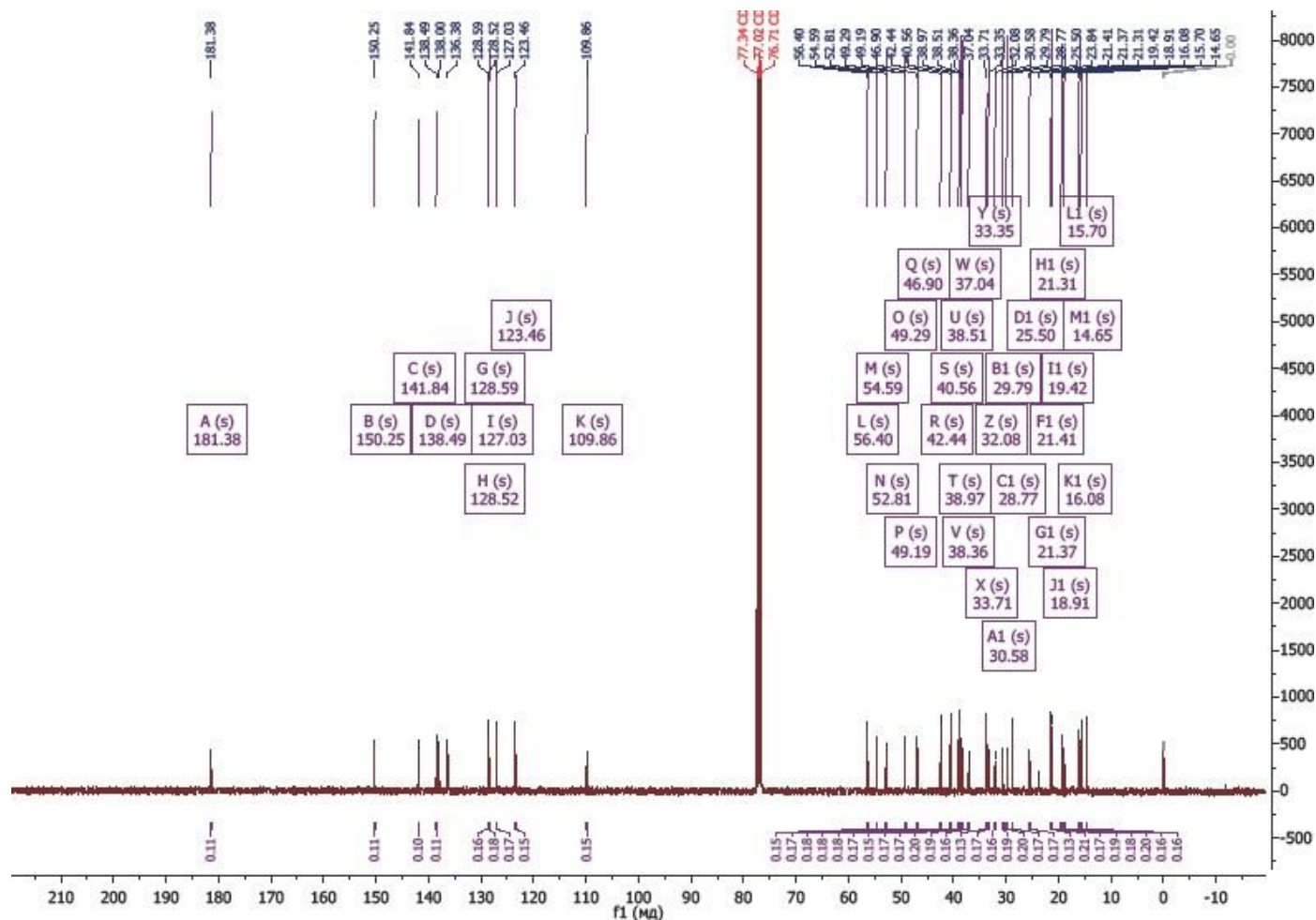
^{13}C NMR (101 MHz, CDCl_3)



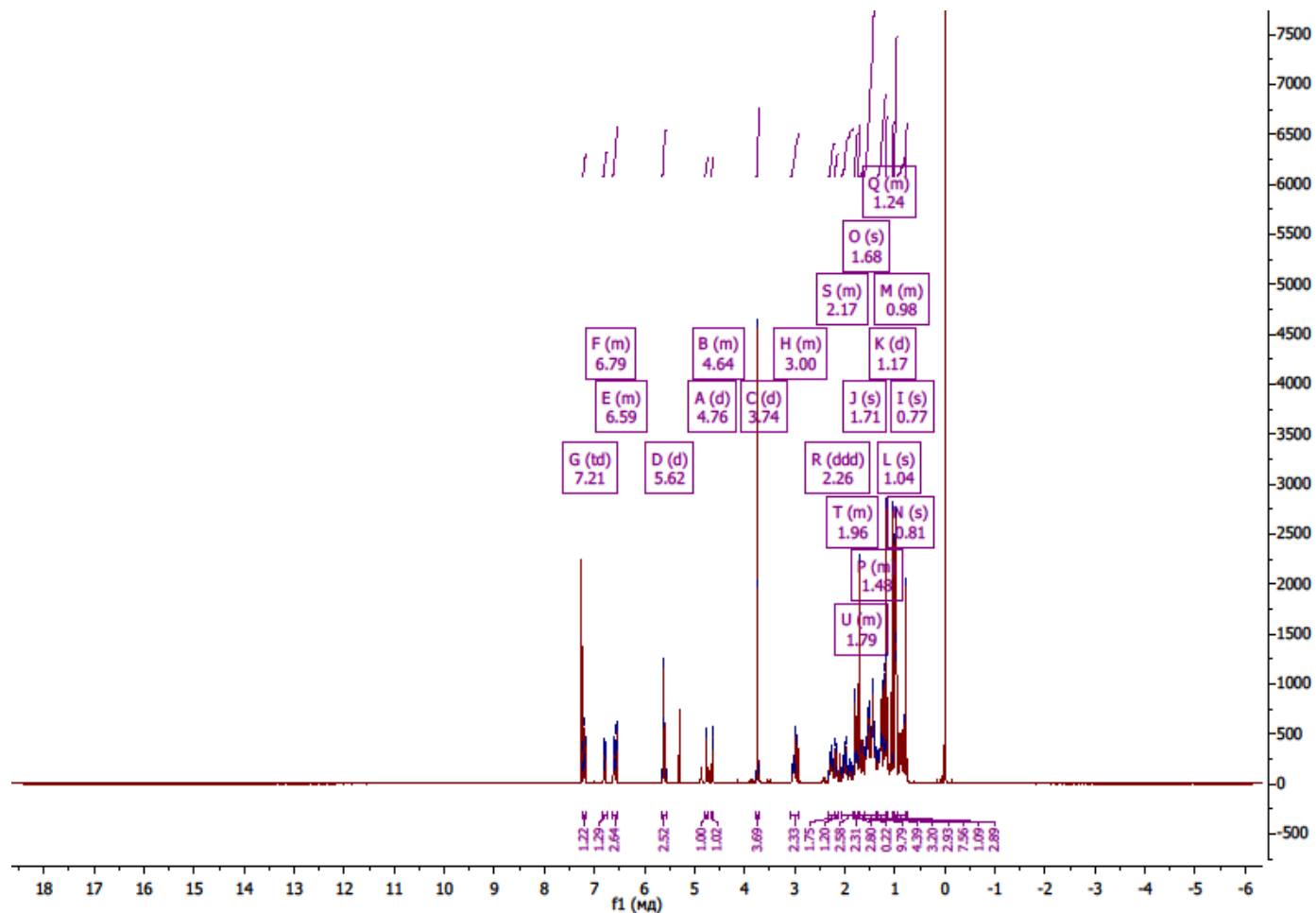
Compound **4**, ^1H NMR (400 MHz, CDCl_3)



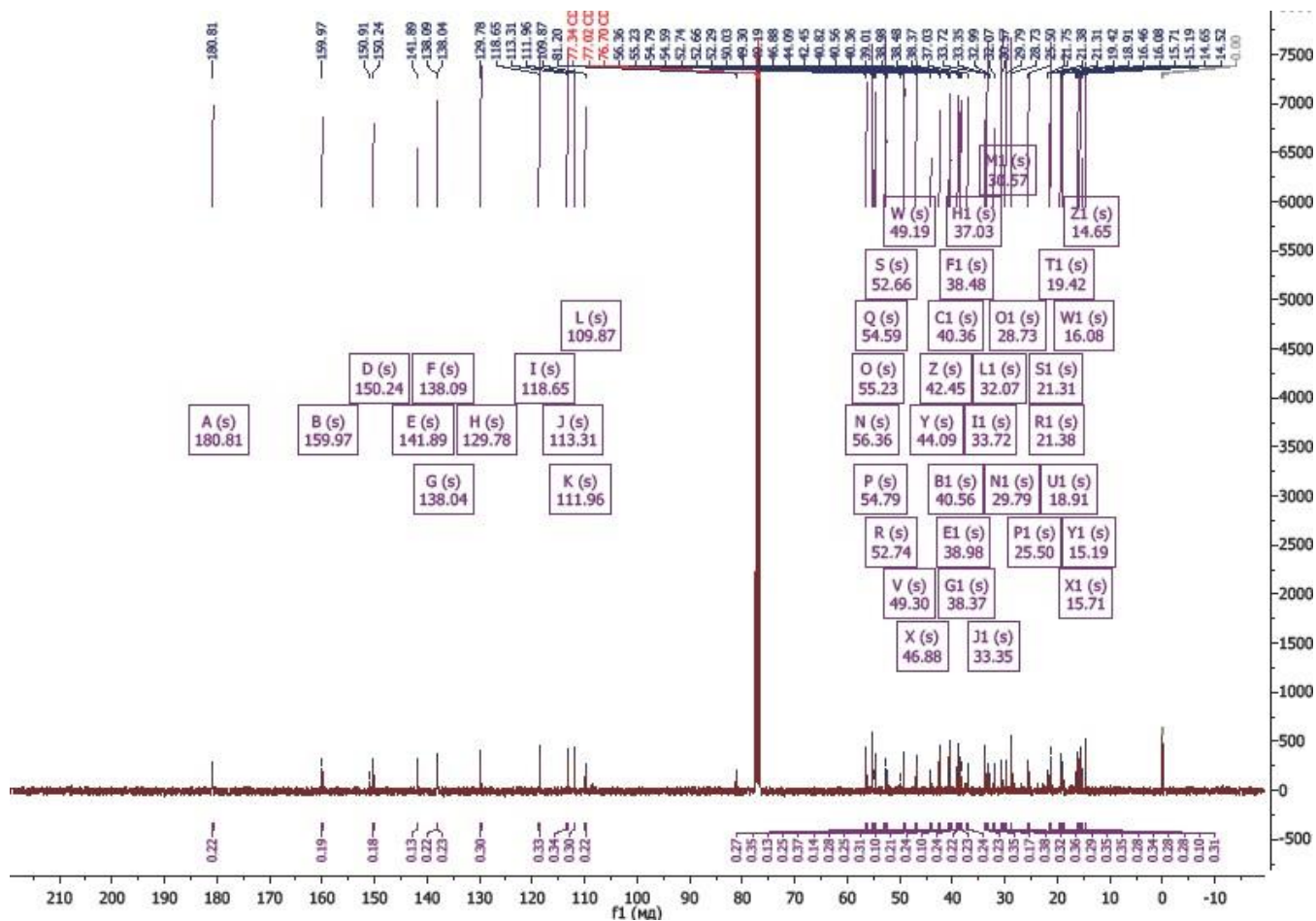
^{13}C NMR (101 MHz, CDCl_3)



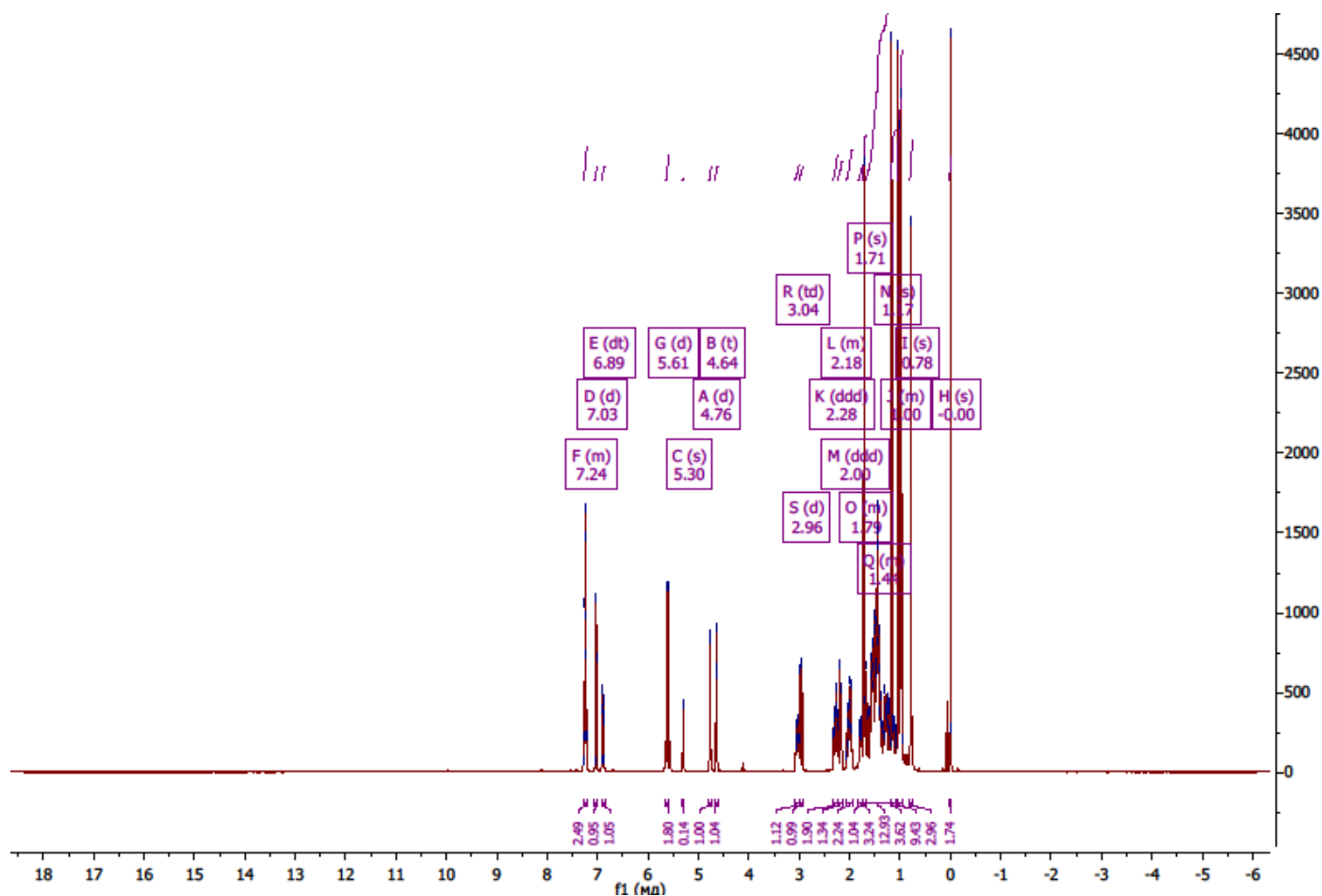
Compound 5, ^1H NMR (400 MHz, CDCl_3)



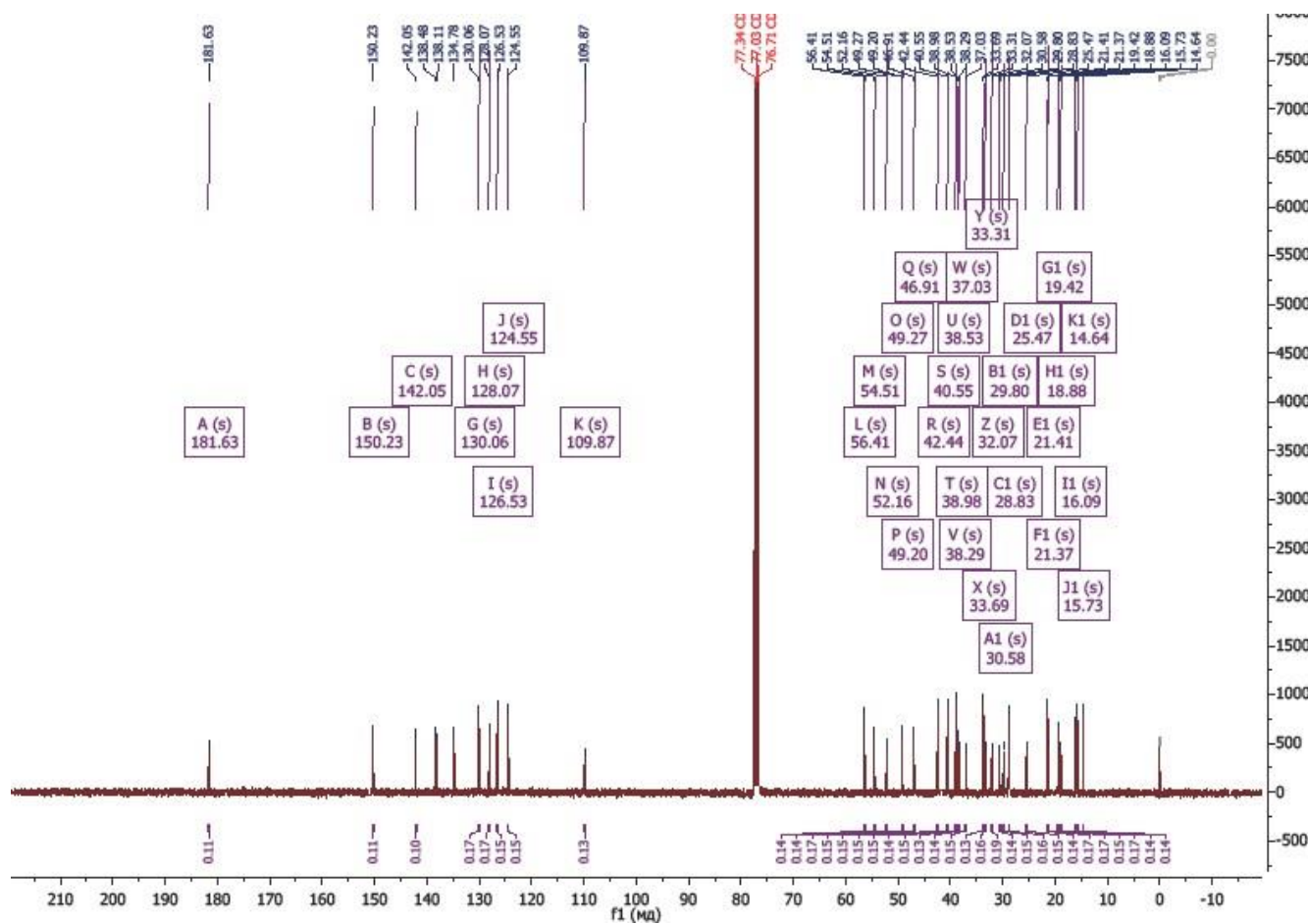
^{13}C NMR (101 MHz, CDCl_3)



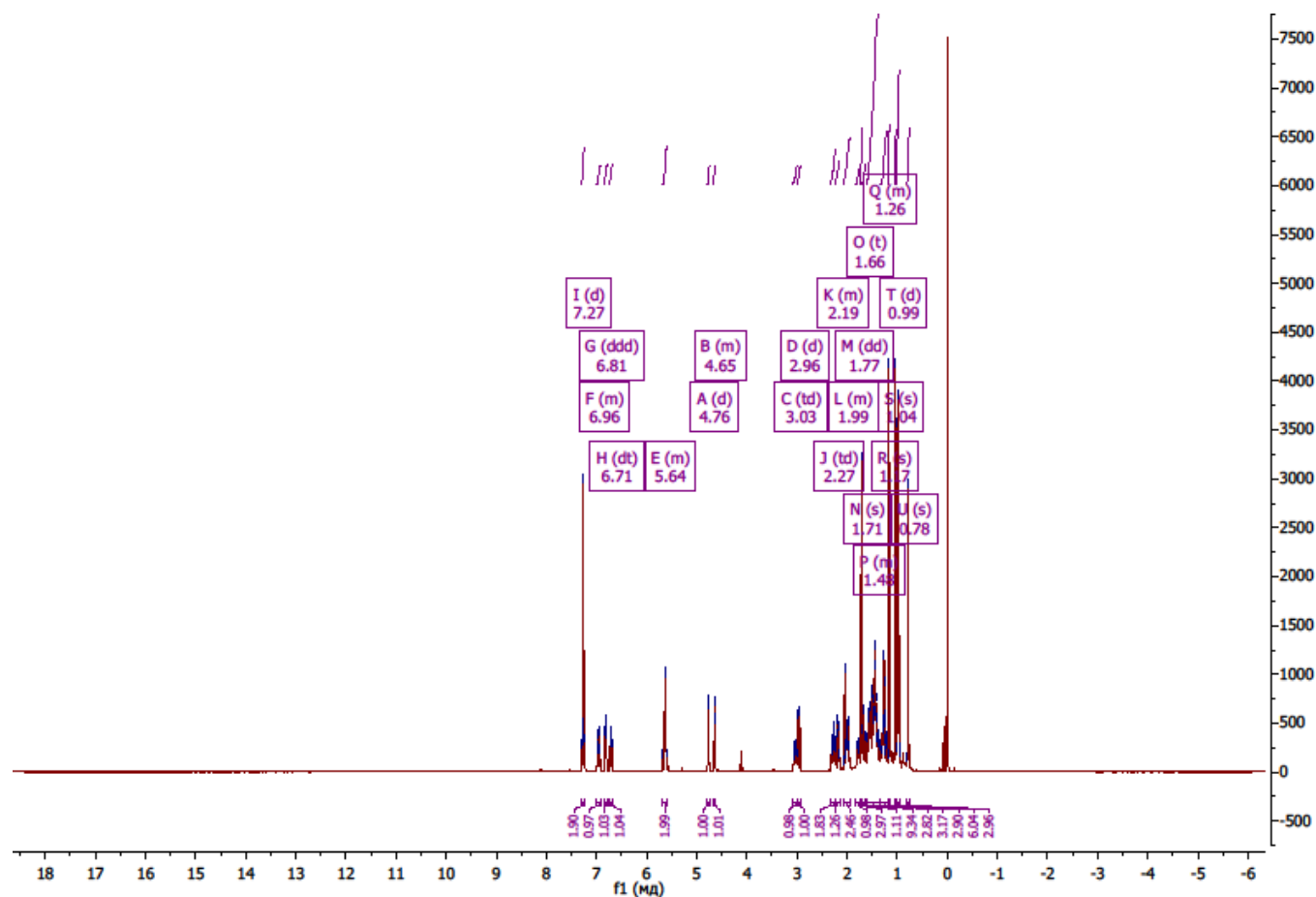
Compound **6**, ^1H NMR (400 MHz, CDCl_3)



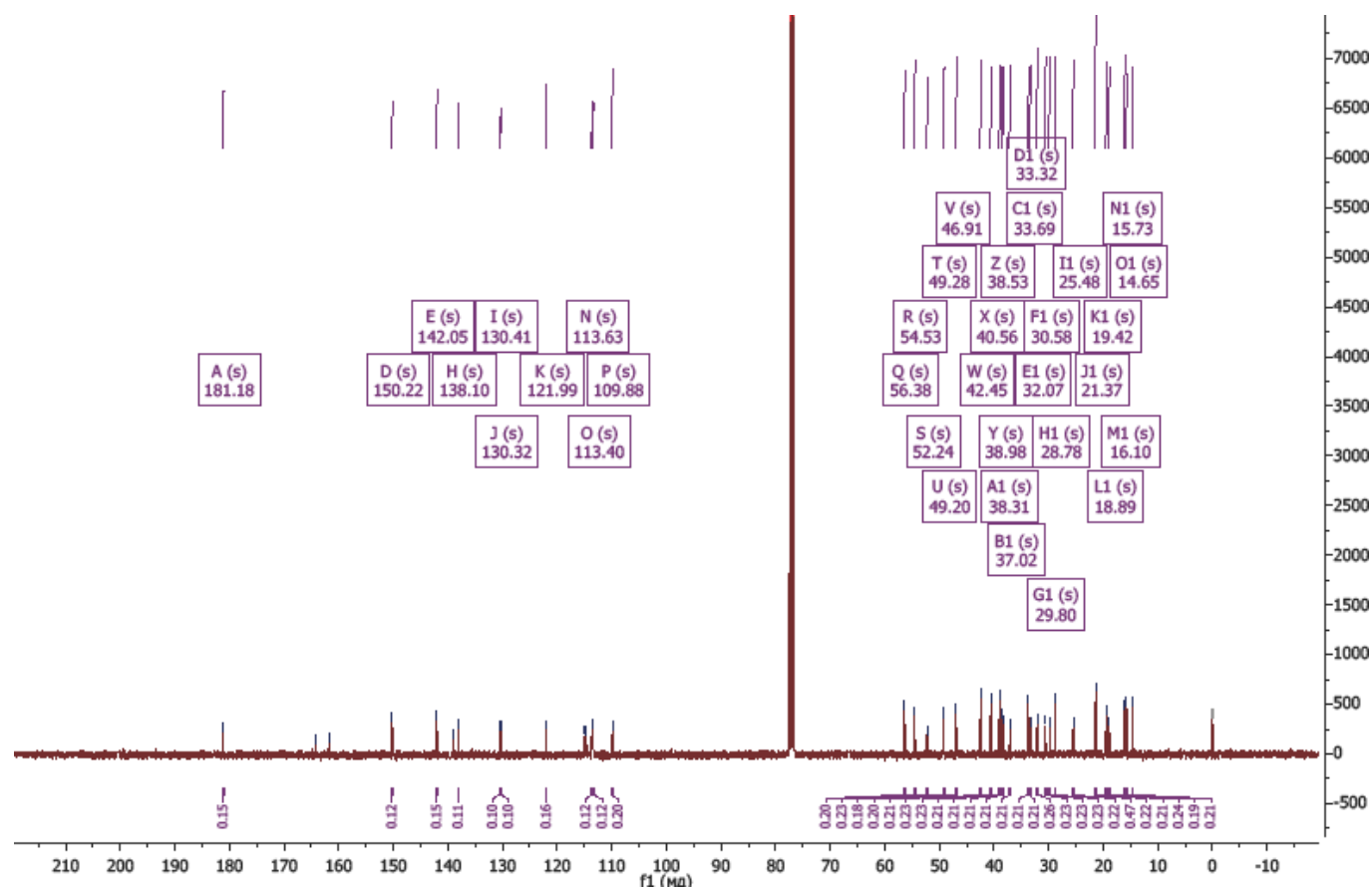
^{13}C NMR (101 MHz, CDCl_3)



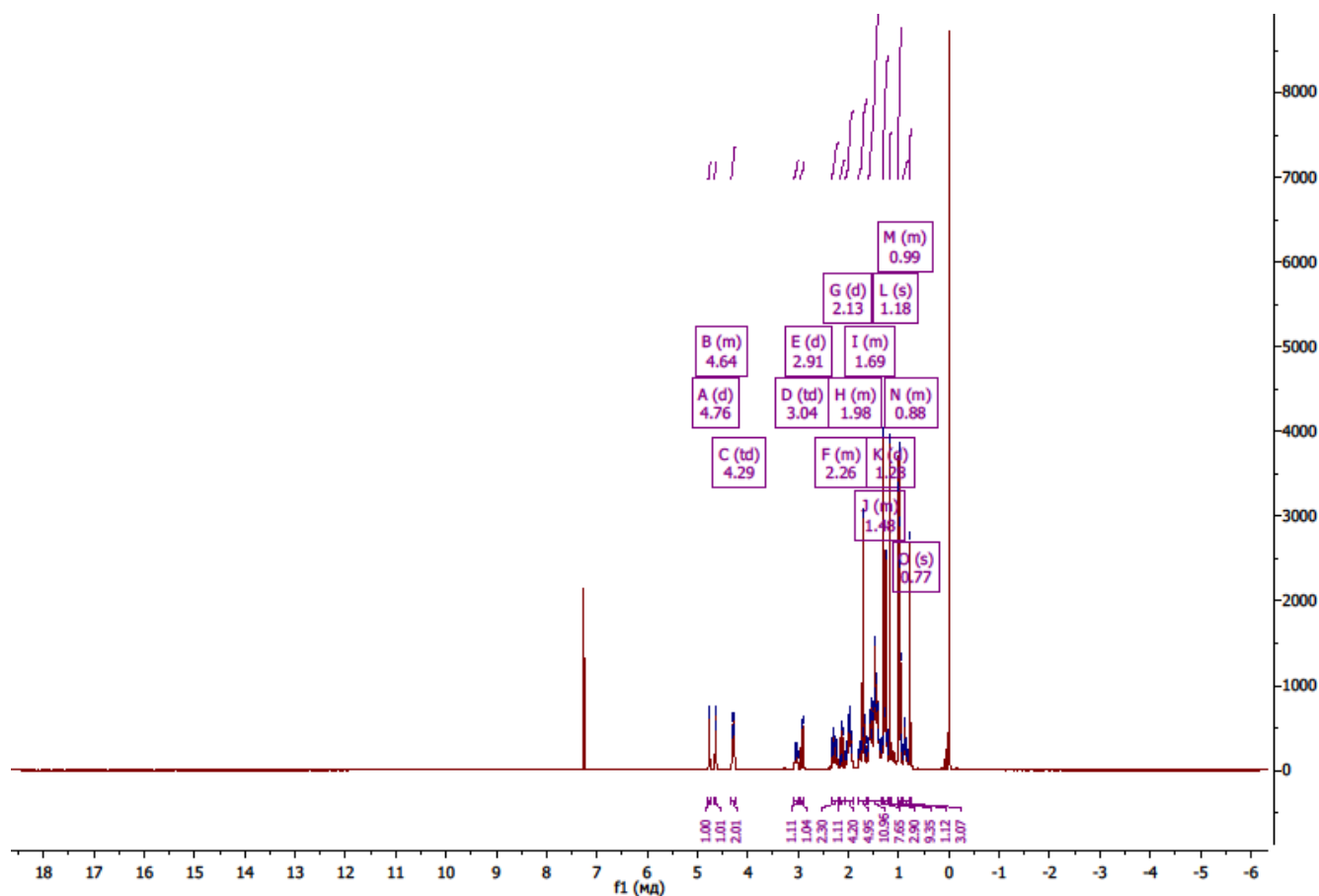
Compound **7**, ^1H NMR (400 MHz, CDCl_3)



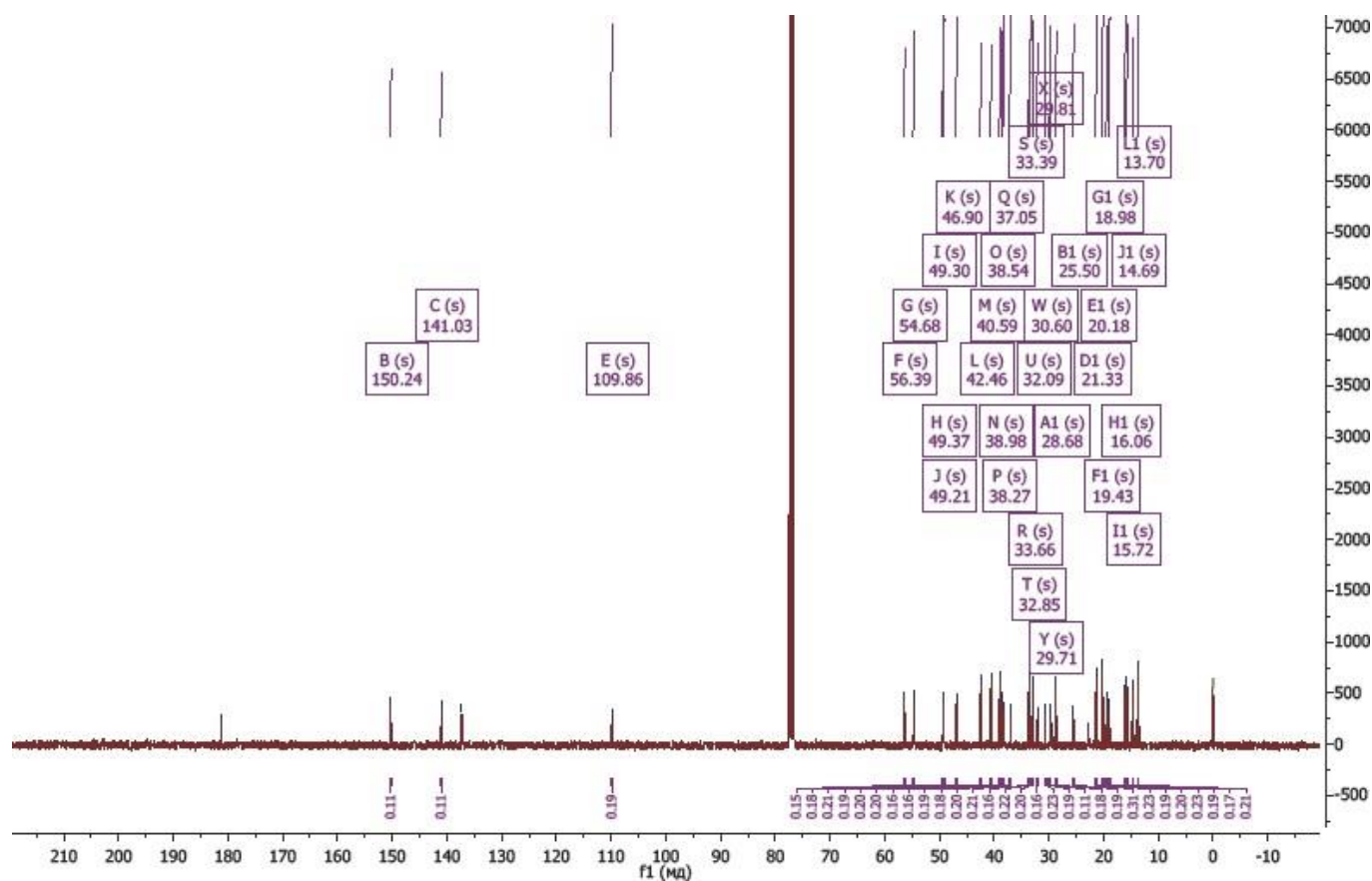
^{13}C NMR (101 MHz, CDCl_3)



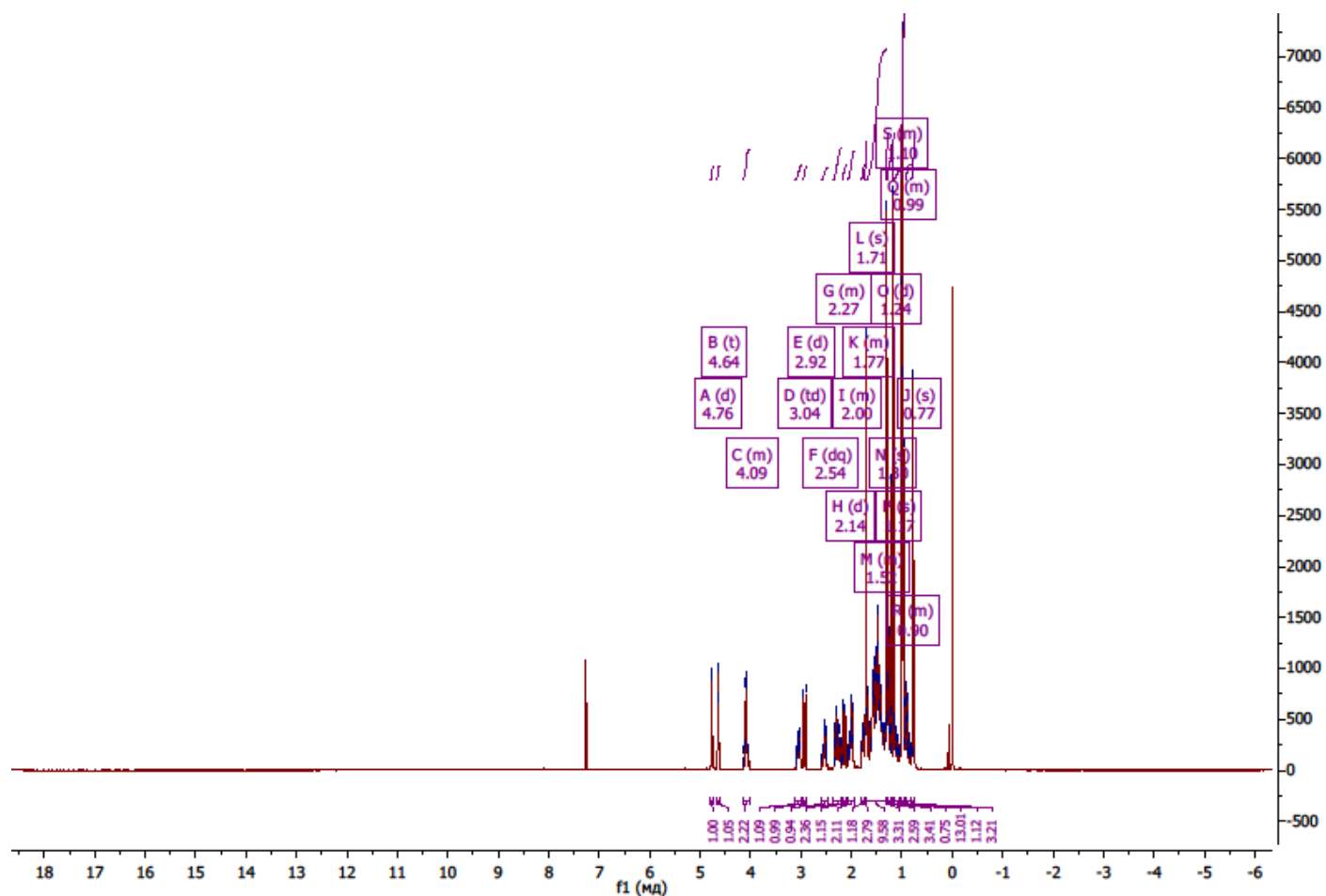
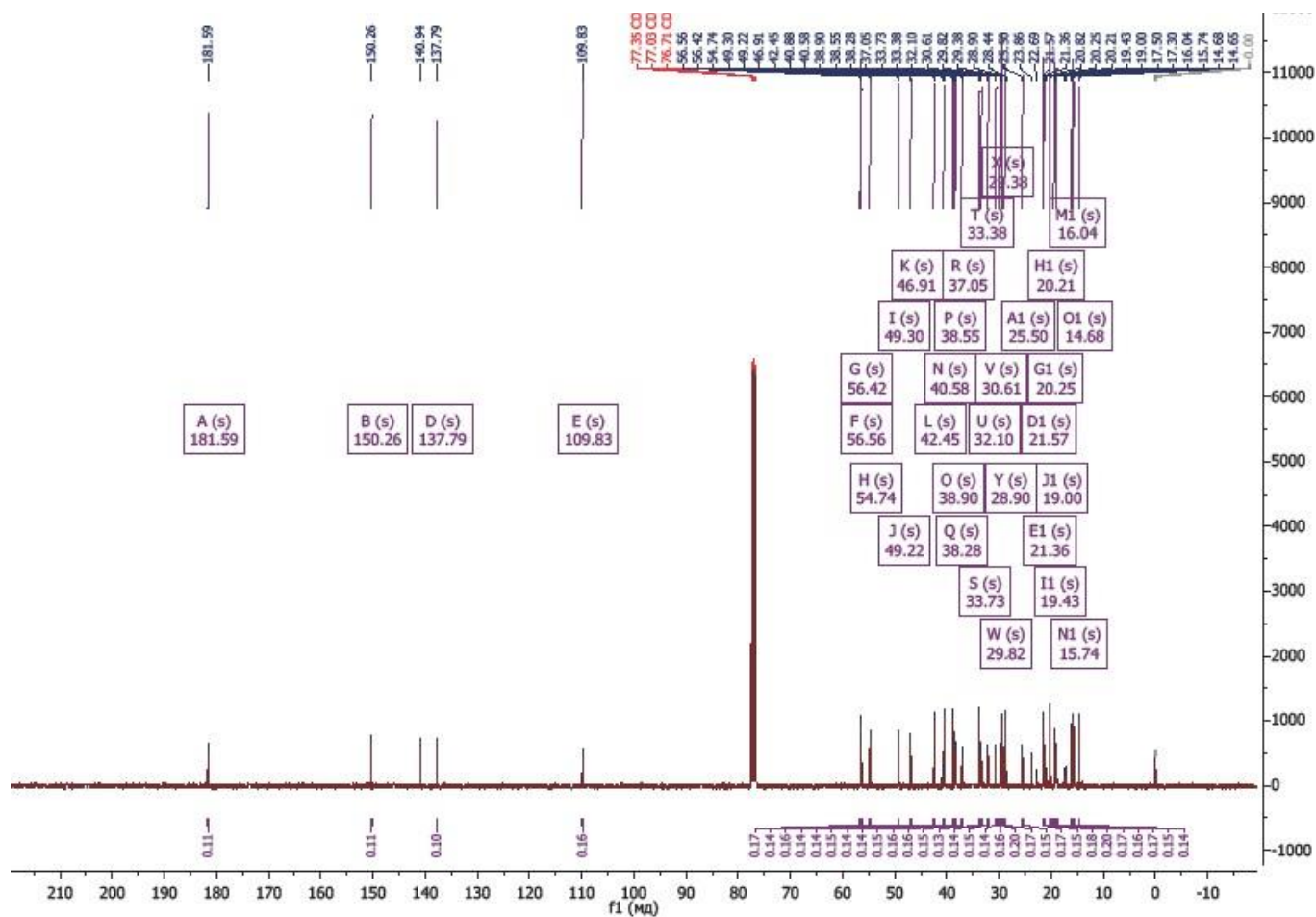
Compound **8**, ^1H NMR (400 MHz, CDCl_3)



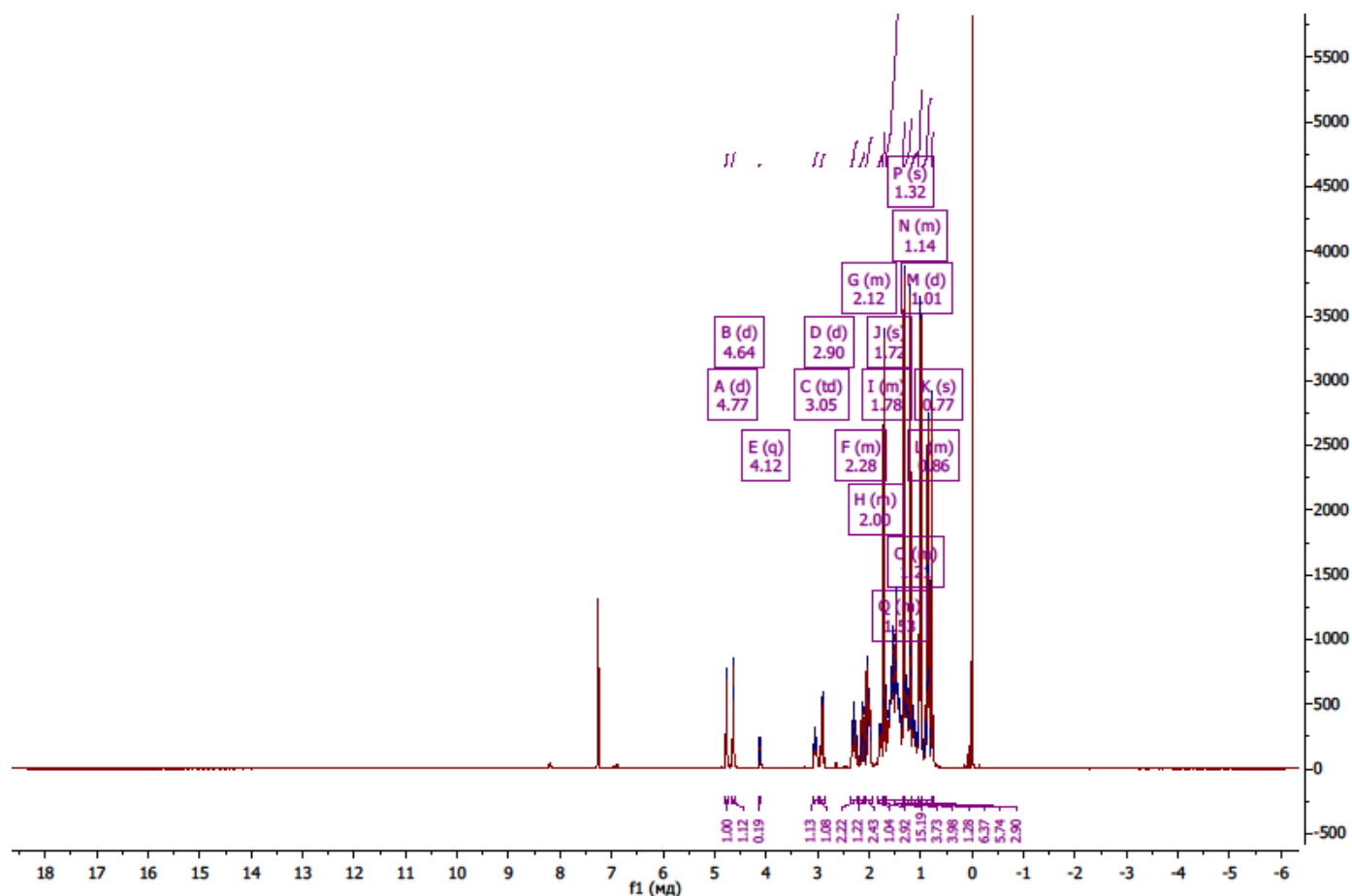
^{13}C NMR (101 MHz, CDCl_3)



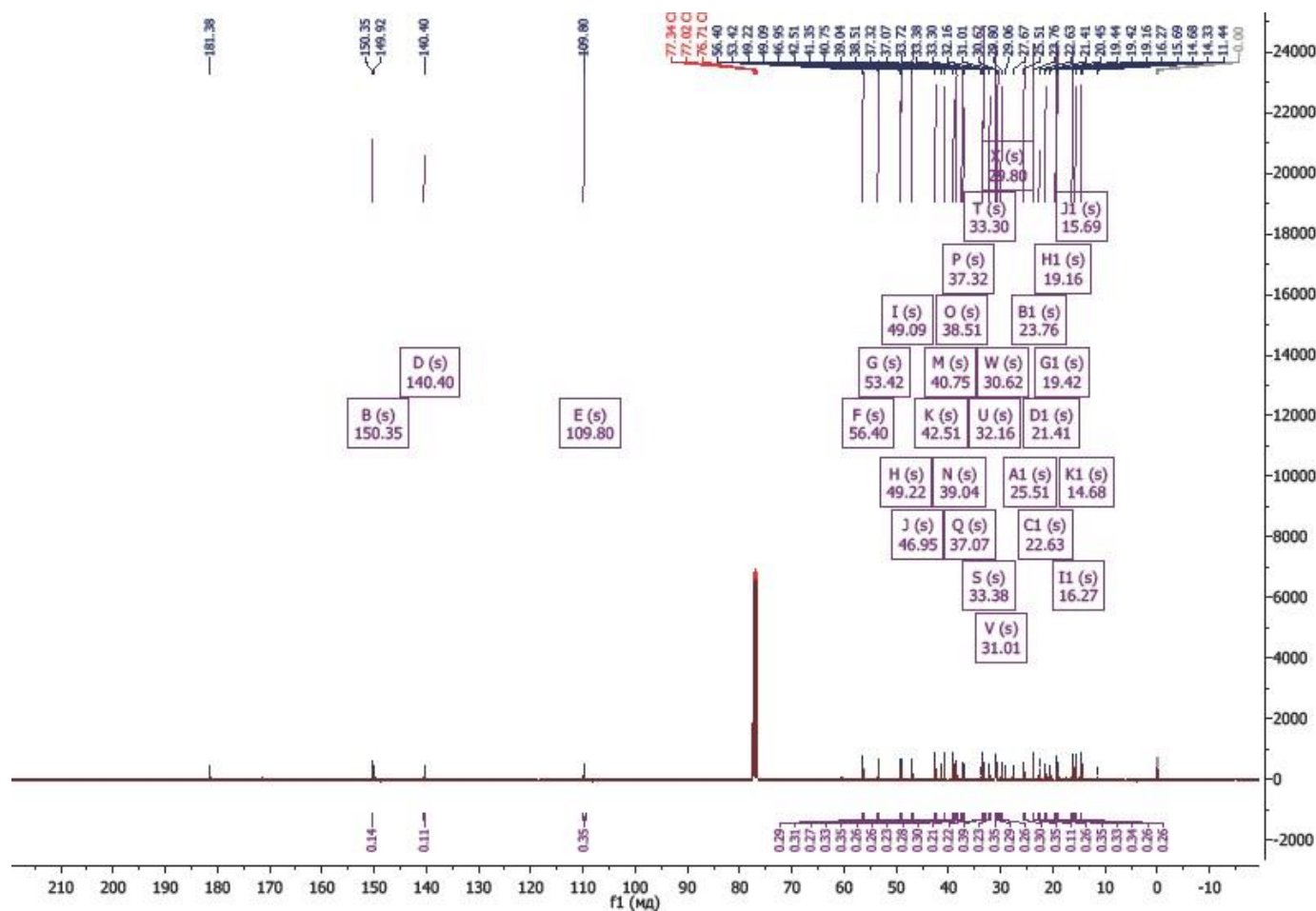
Compound **9**, ¹H NMR (400 MHz, CDCl₃)

 ^{13}C NMR (101 MHz, CDCl_3)

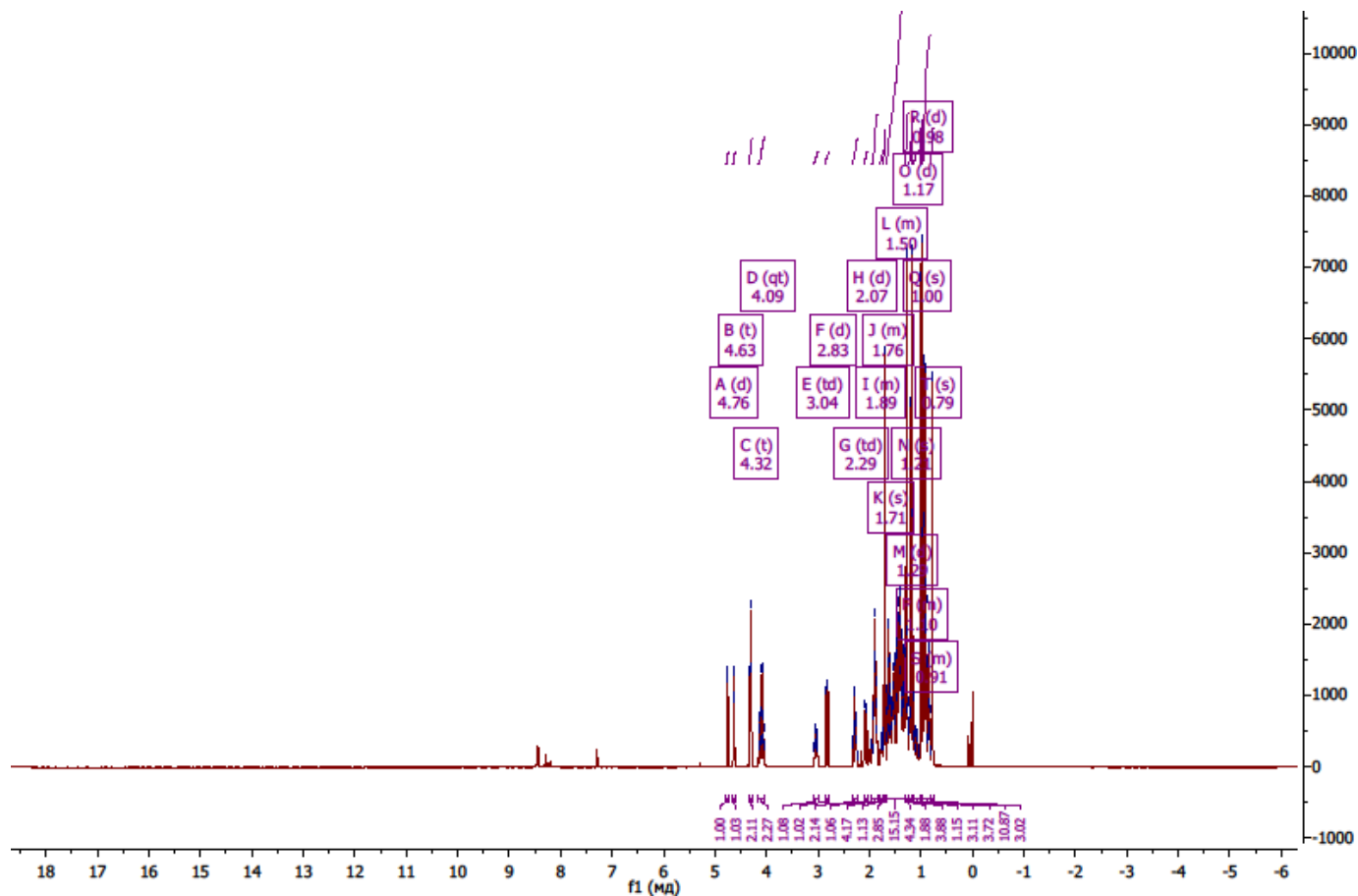
Compound **10**, ^1H NMR (400 MHz, CDCl_3)



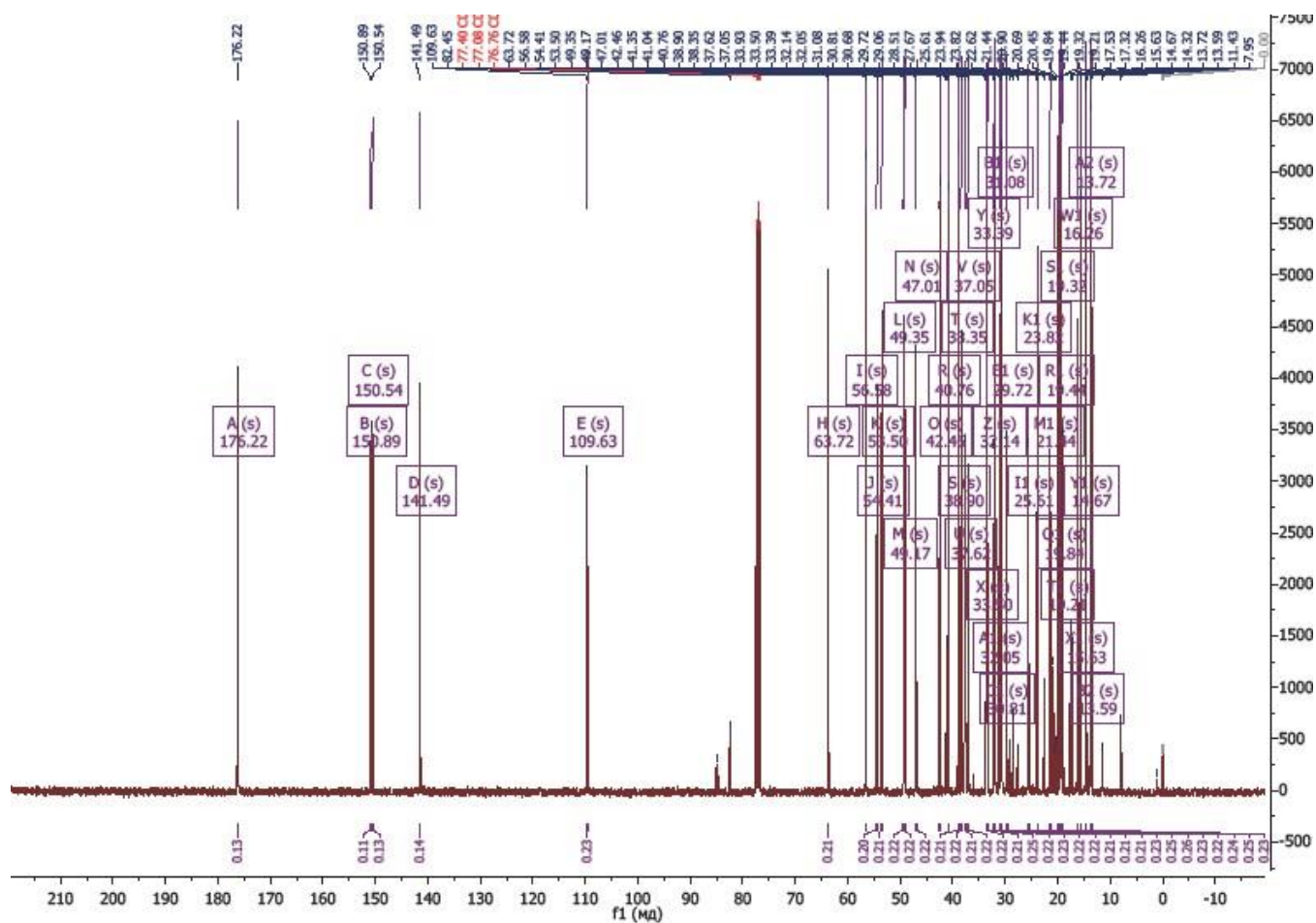
^{13}C NMR (101 MHz, CDCl_3)



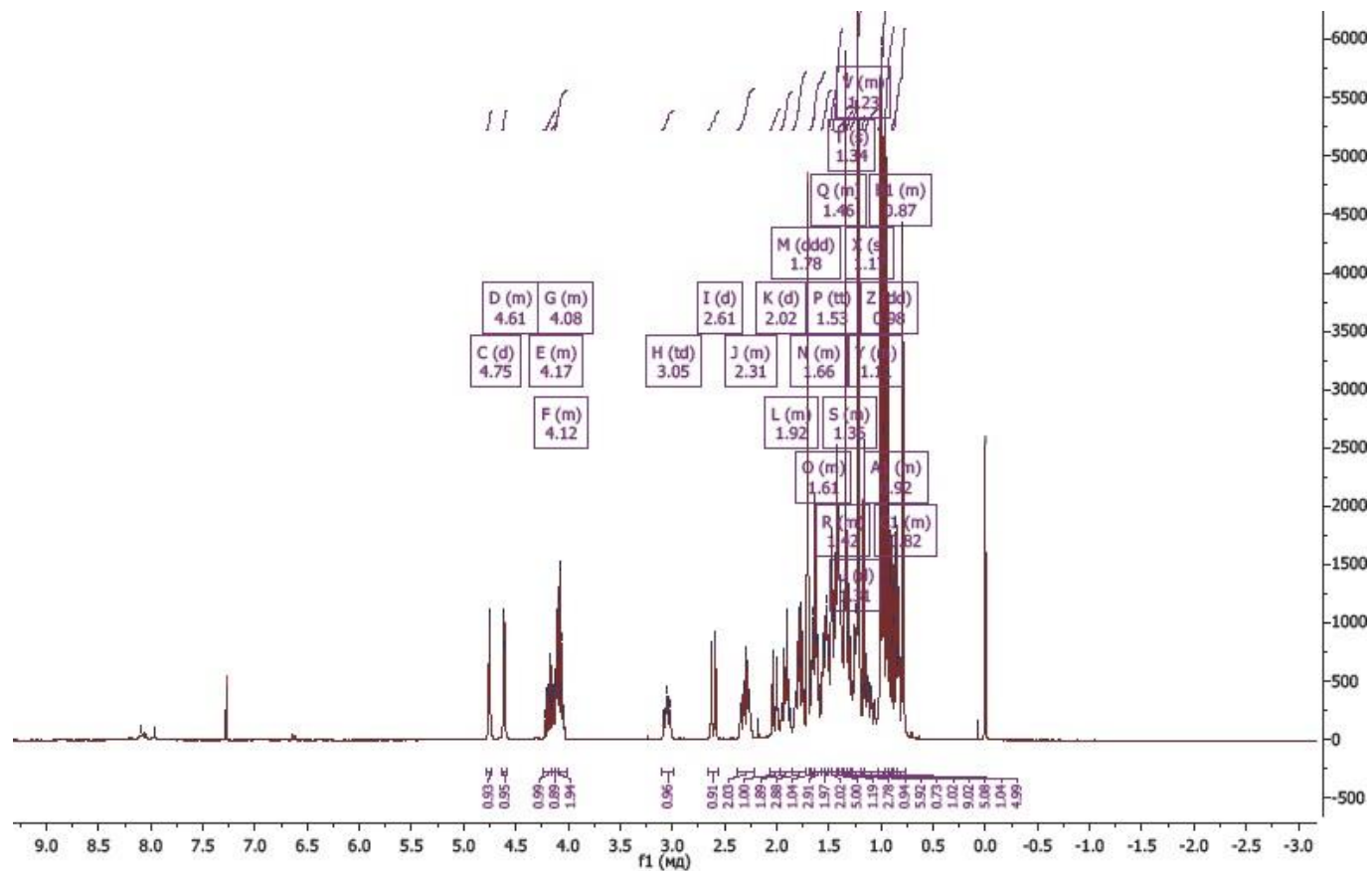
Compound **11**, ^1H NMR (400 MHz, CDCl_3)



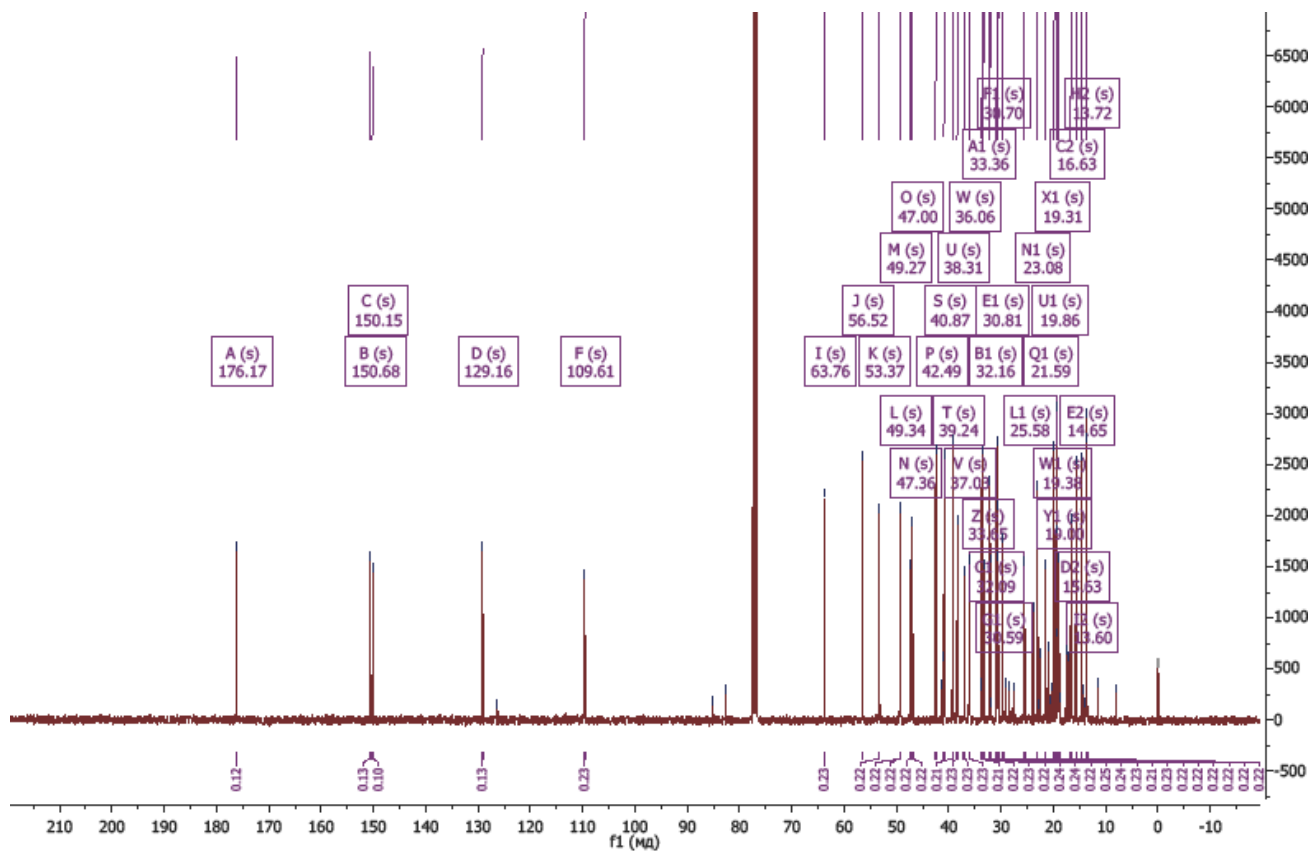
^{13}C NMR (101 MHz, CDCl_3)



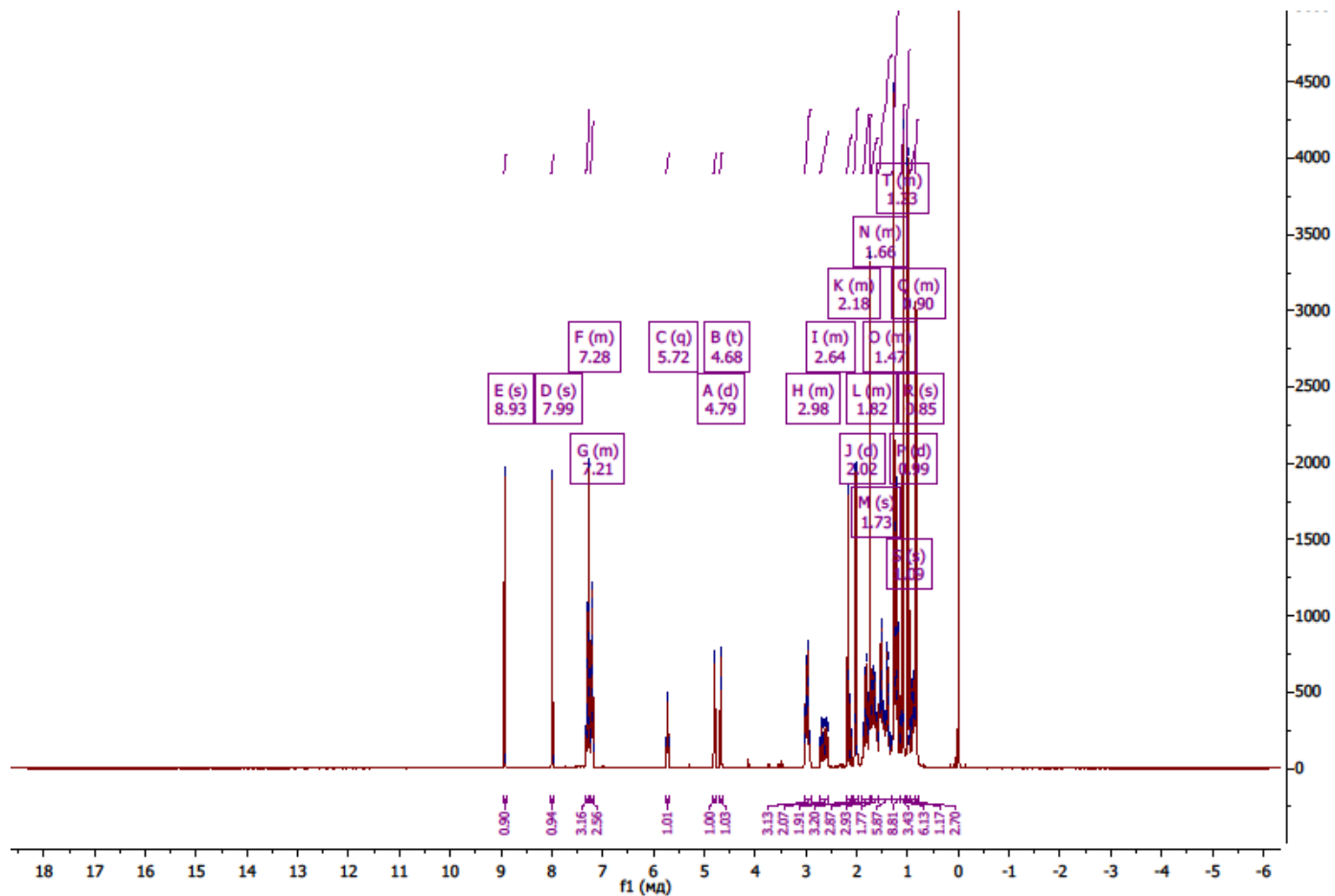
Compound **12**, ^1H NMR (400 MHz, CDCl_3)



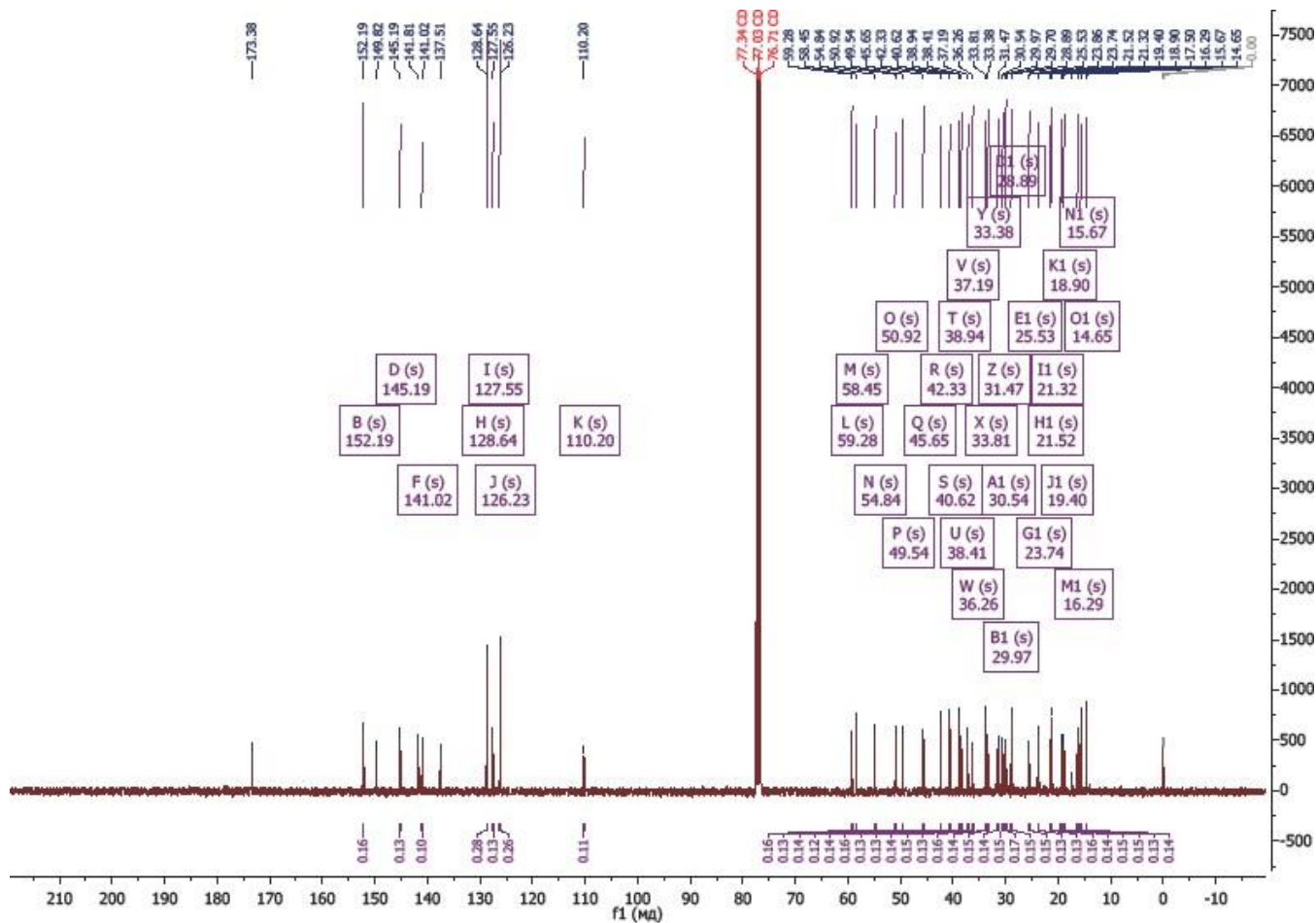
^{13}C NMR (101 MHz, CDCl_3)



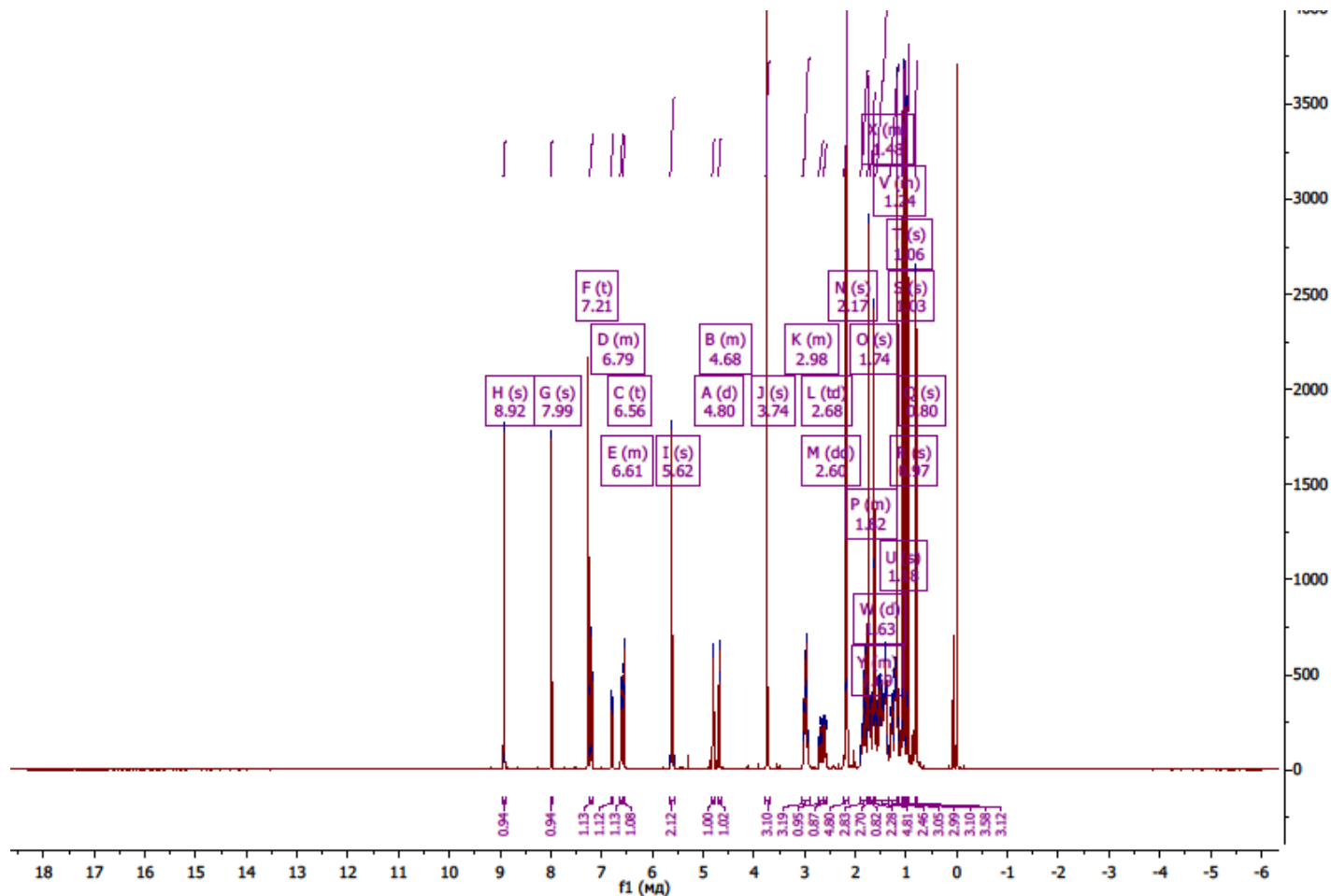
Compound **13**, ^1H NMR (400 MHz, CDCl_3)



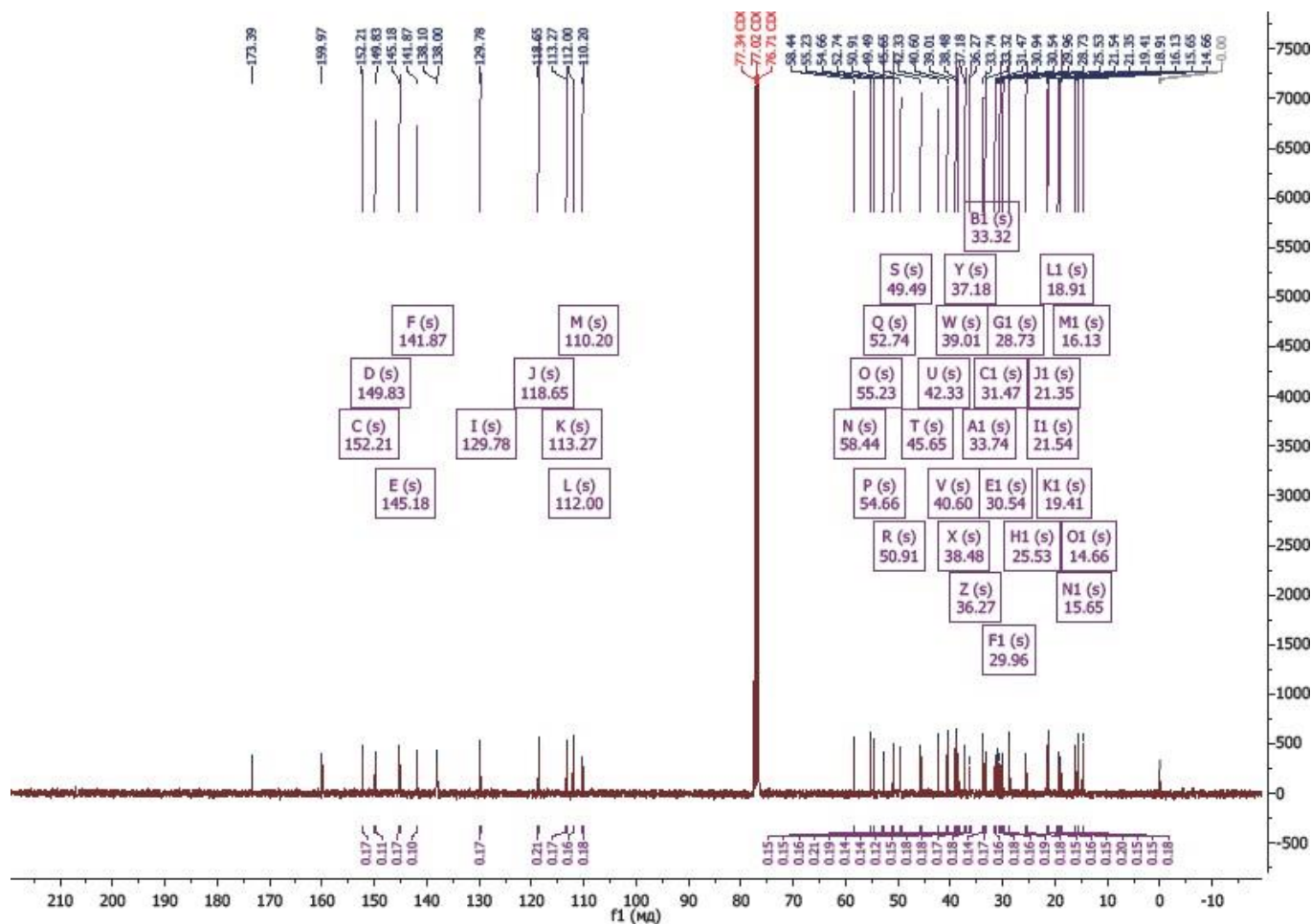
^{13}C NMR (101 MHz, CDCl_3)



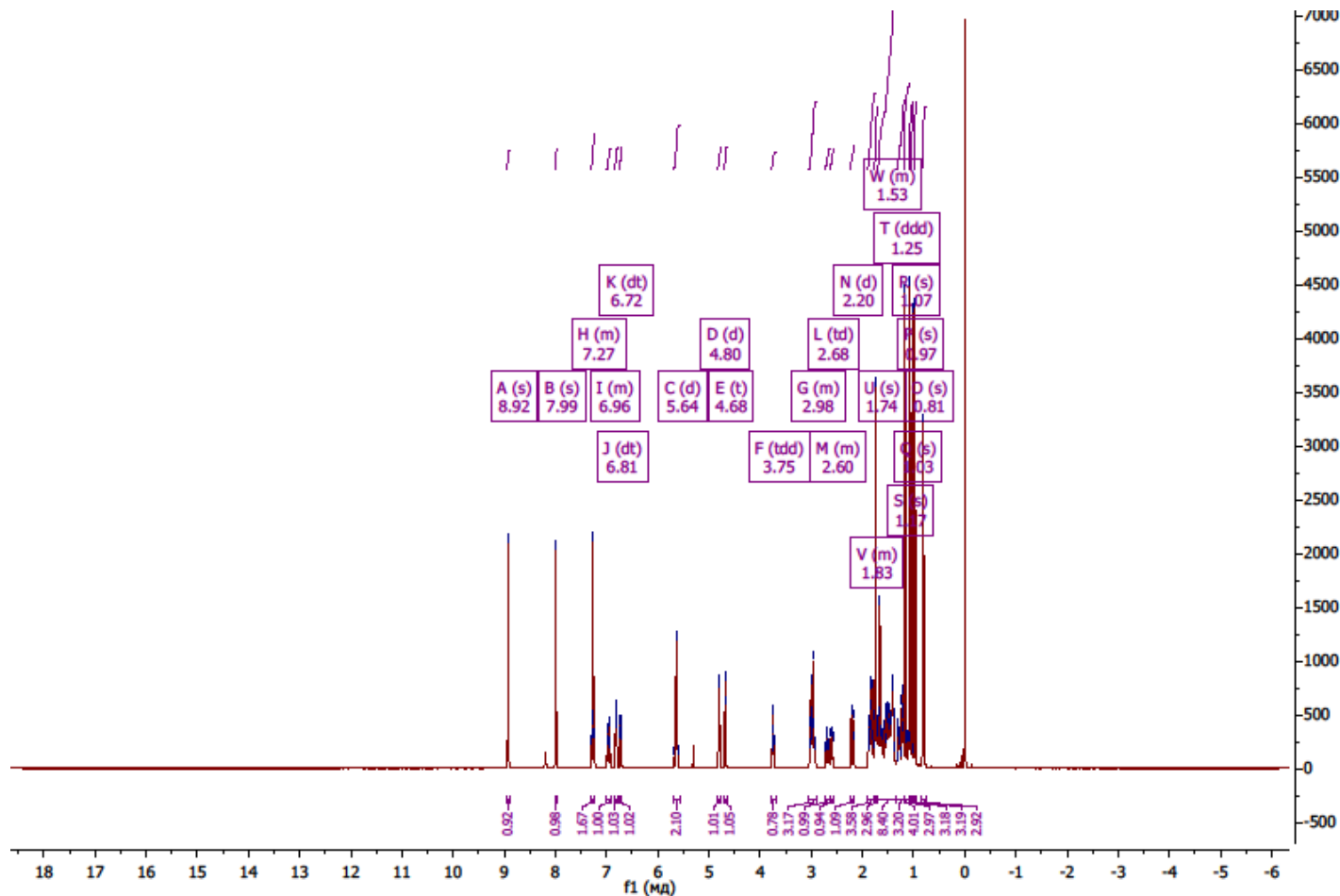
Compound **14**, ^1H NMR (400 MHz, CDCl_3)



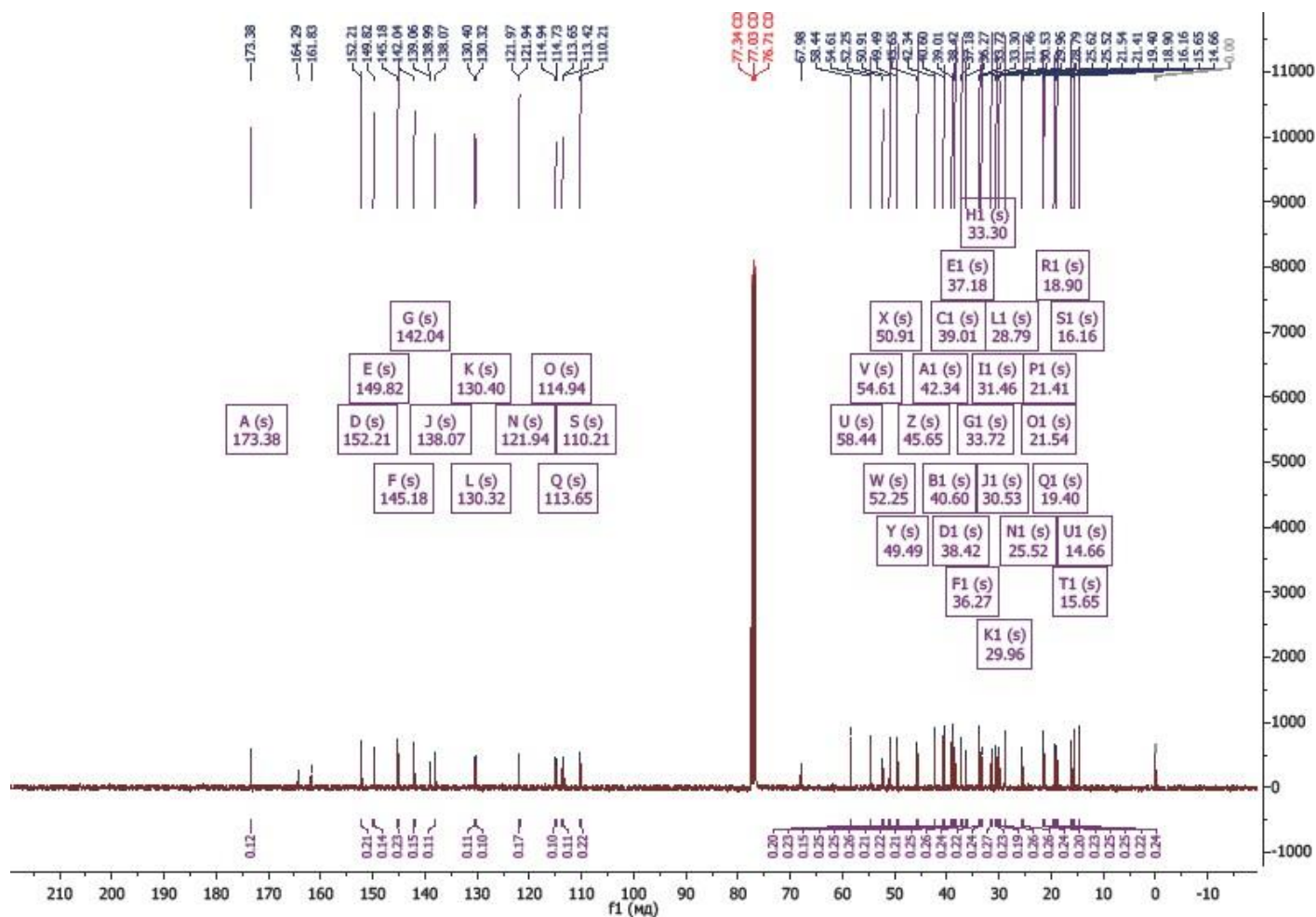
^{13}C NMR (101 MHz, CDCl_3)



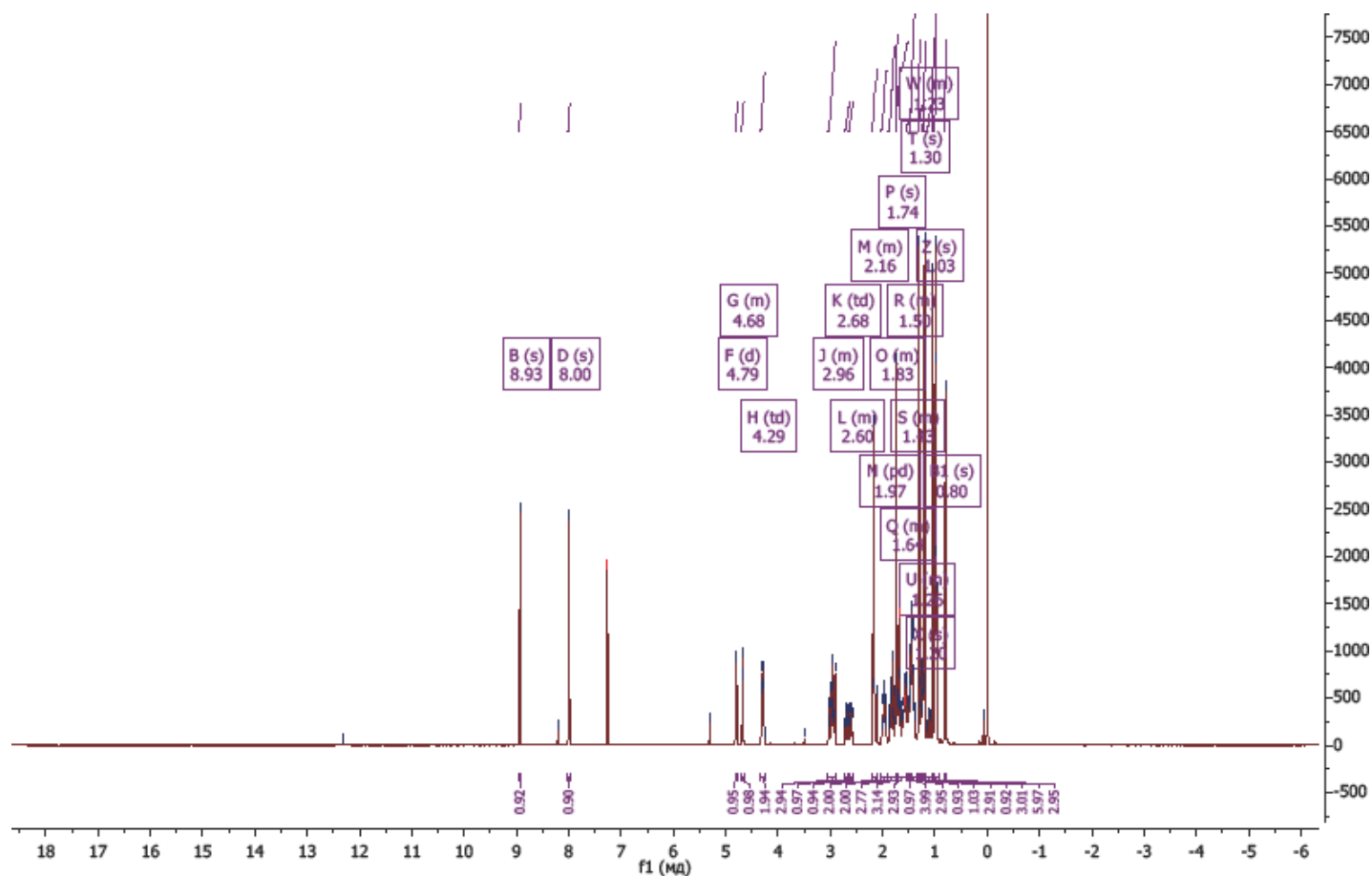
Compound **15**, ^1H NMR (400 MHz, CDCl_3)



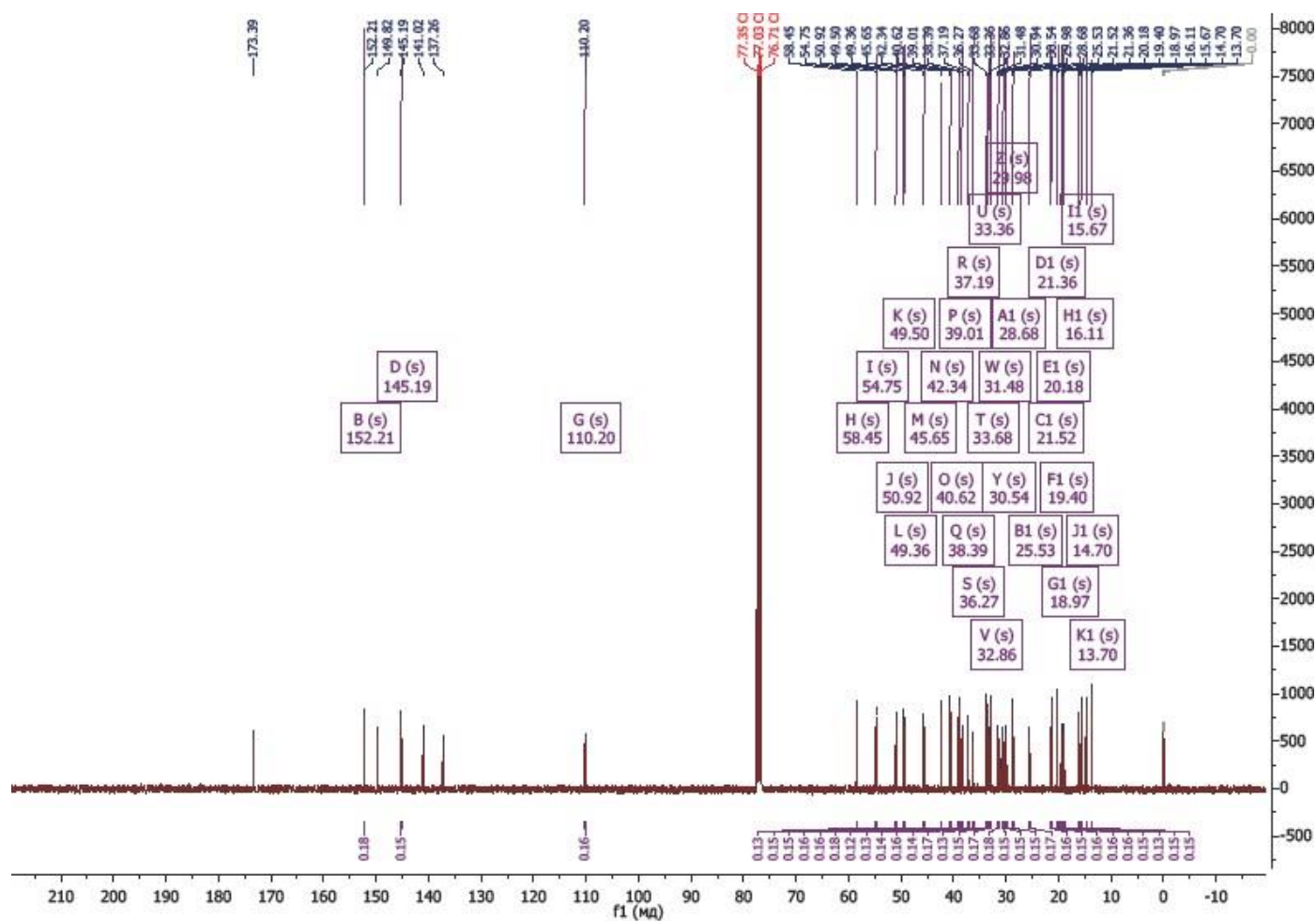
^{13}C NMR (101 MHz, CDCl_3)



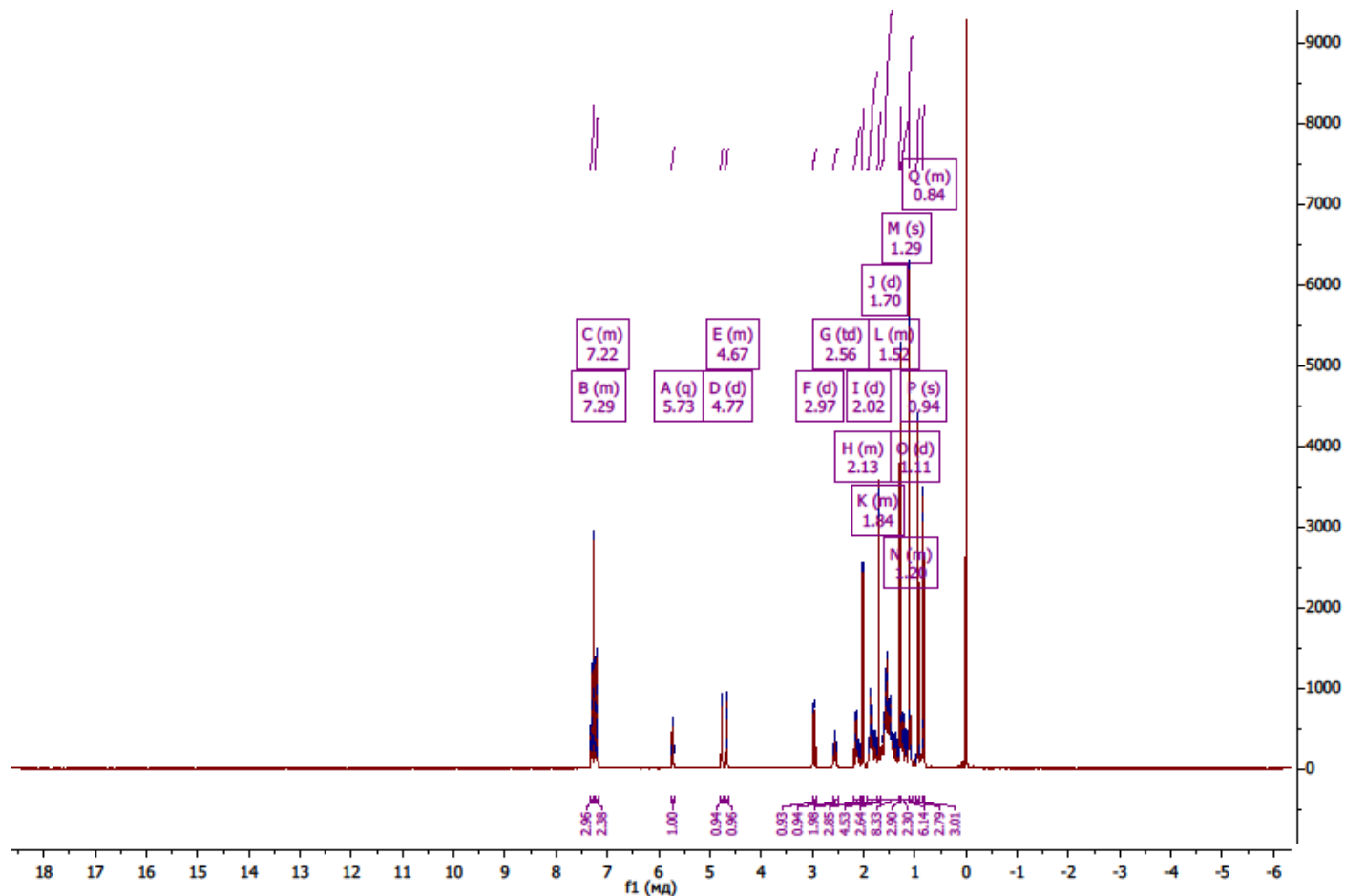
Compound **16**, ^1H NMR (400 MHz, CDCl_3)



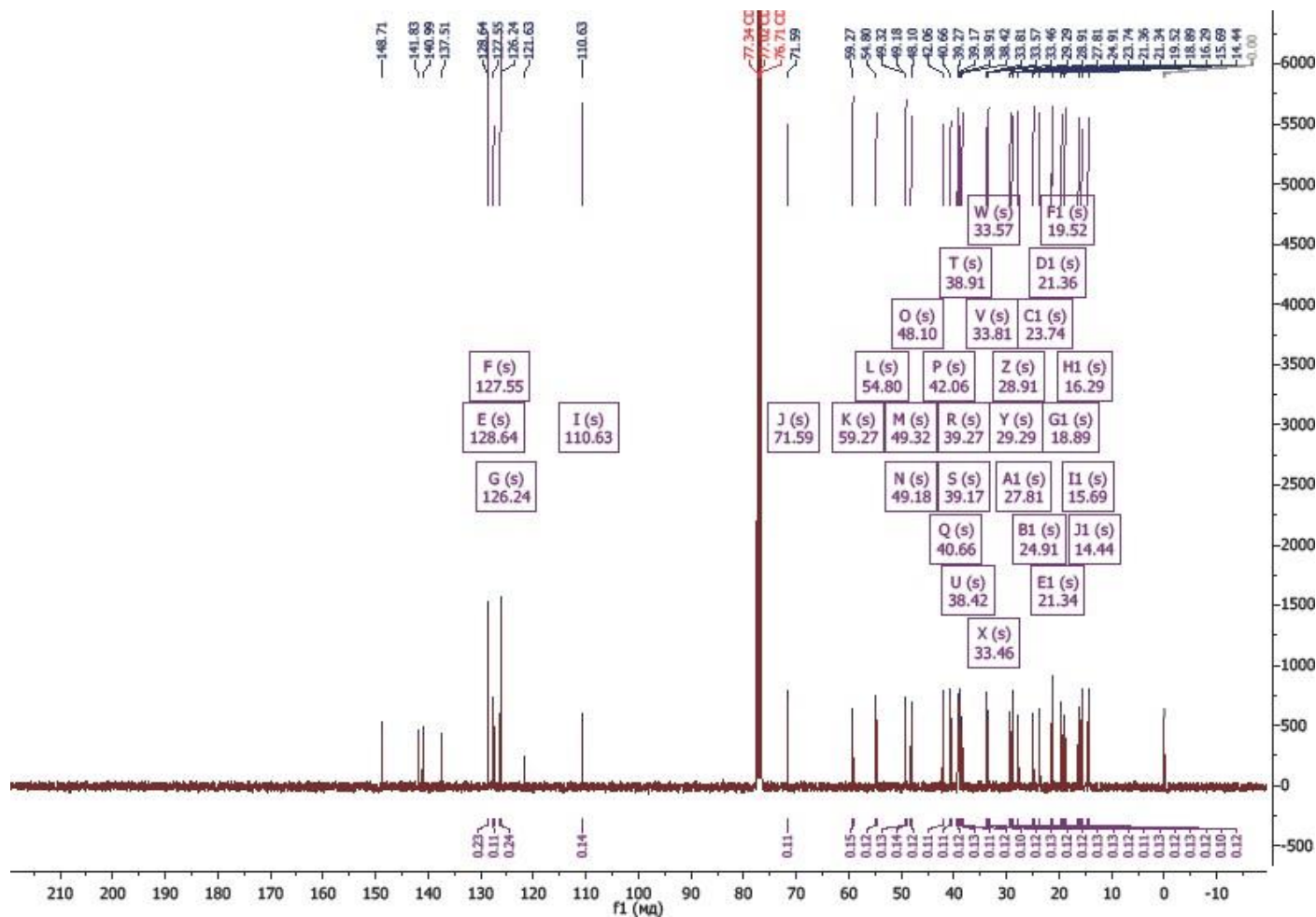
^{13}C NMR (101 MHz, CDCl_3)



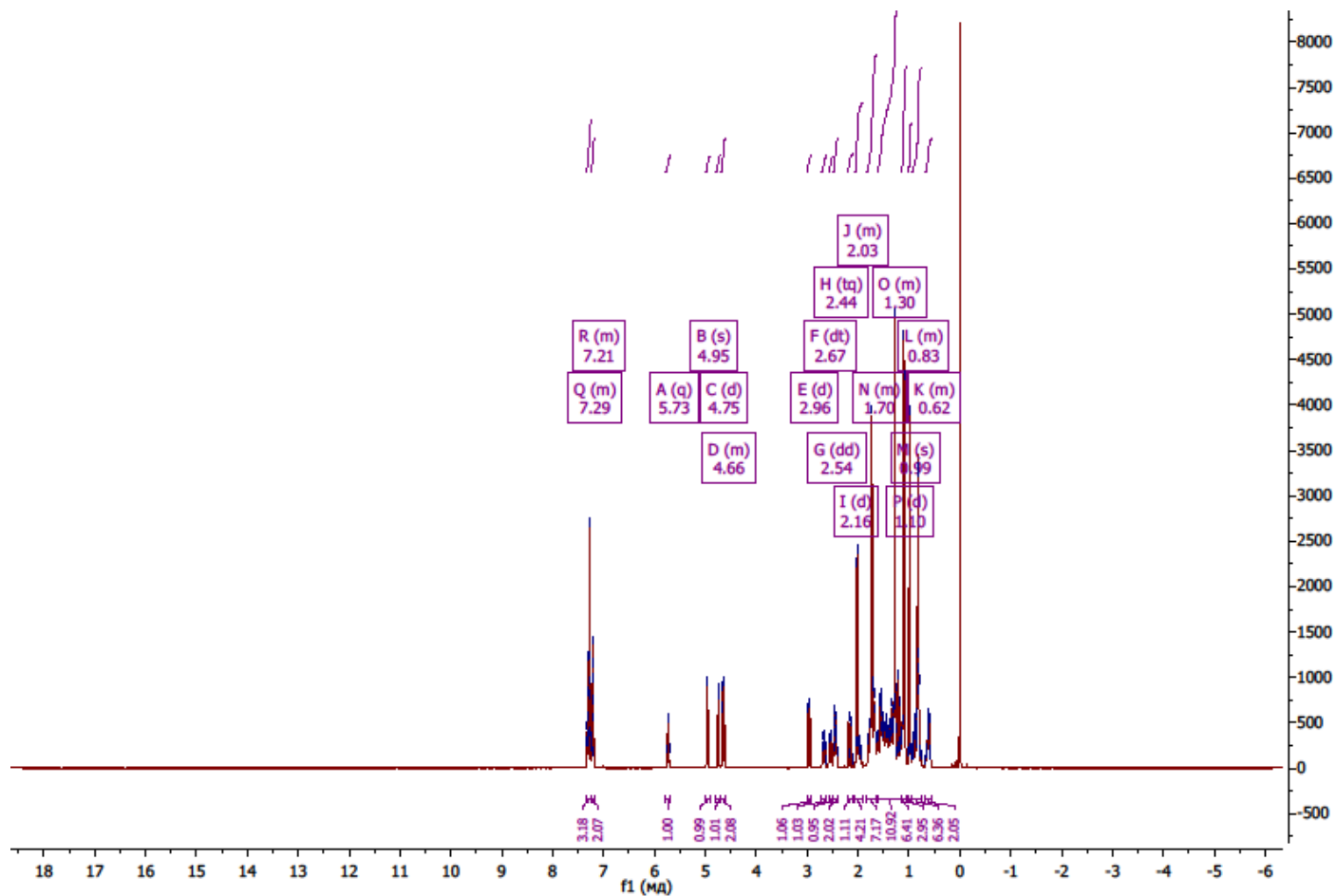
Compound **17**, ^1H NMR (400 MHz, CDCl_3)



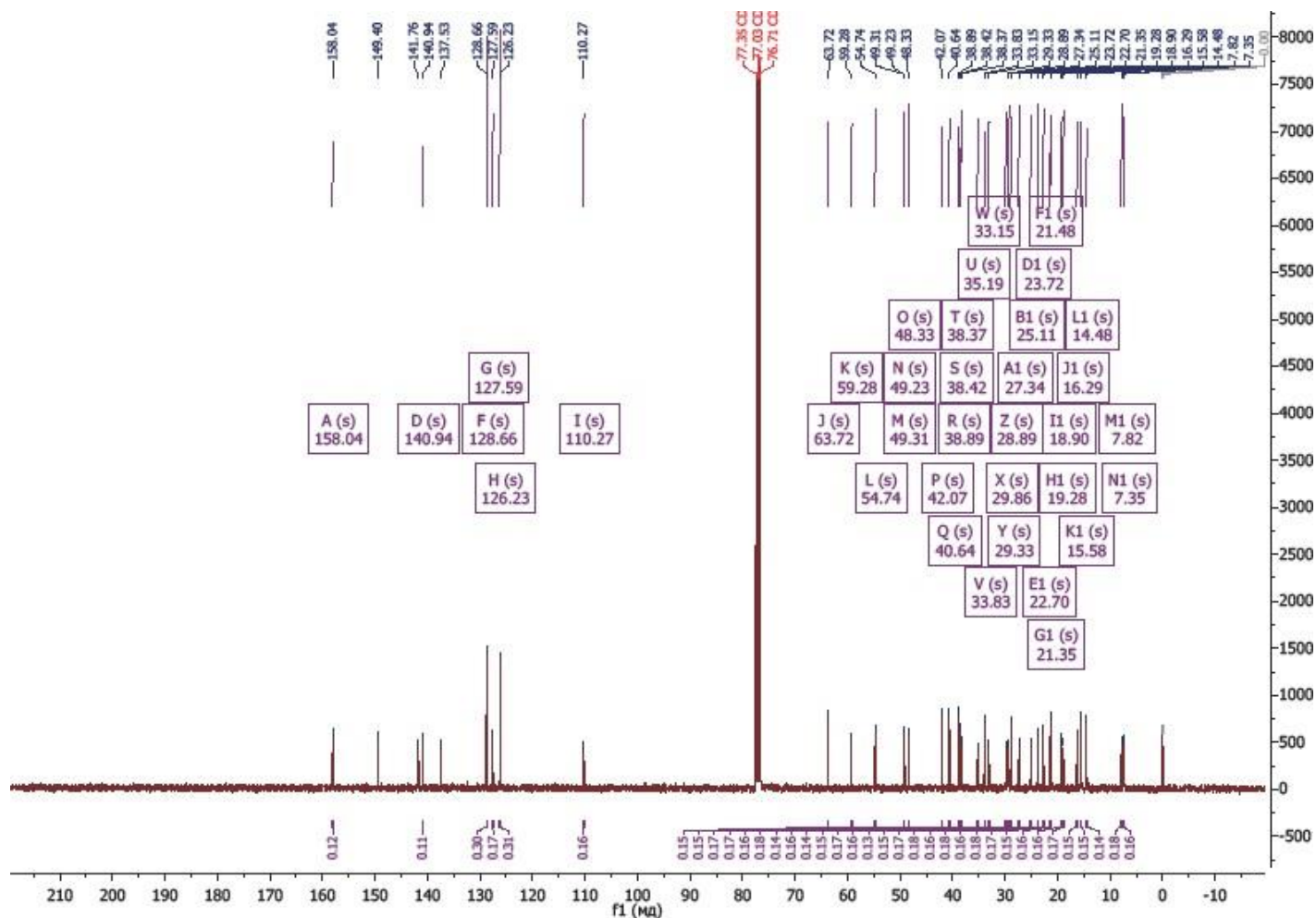
^{13}C NMR (101 MHz, CDCl_3)



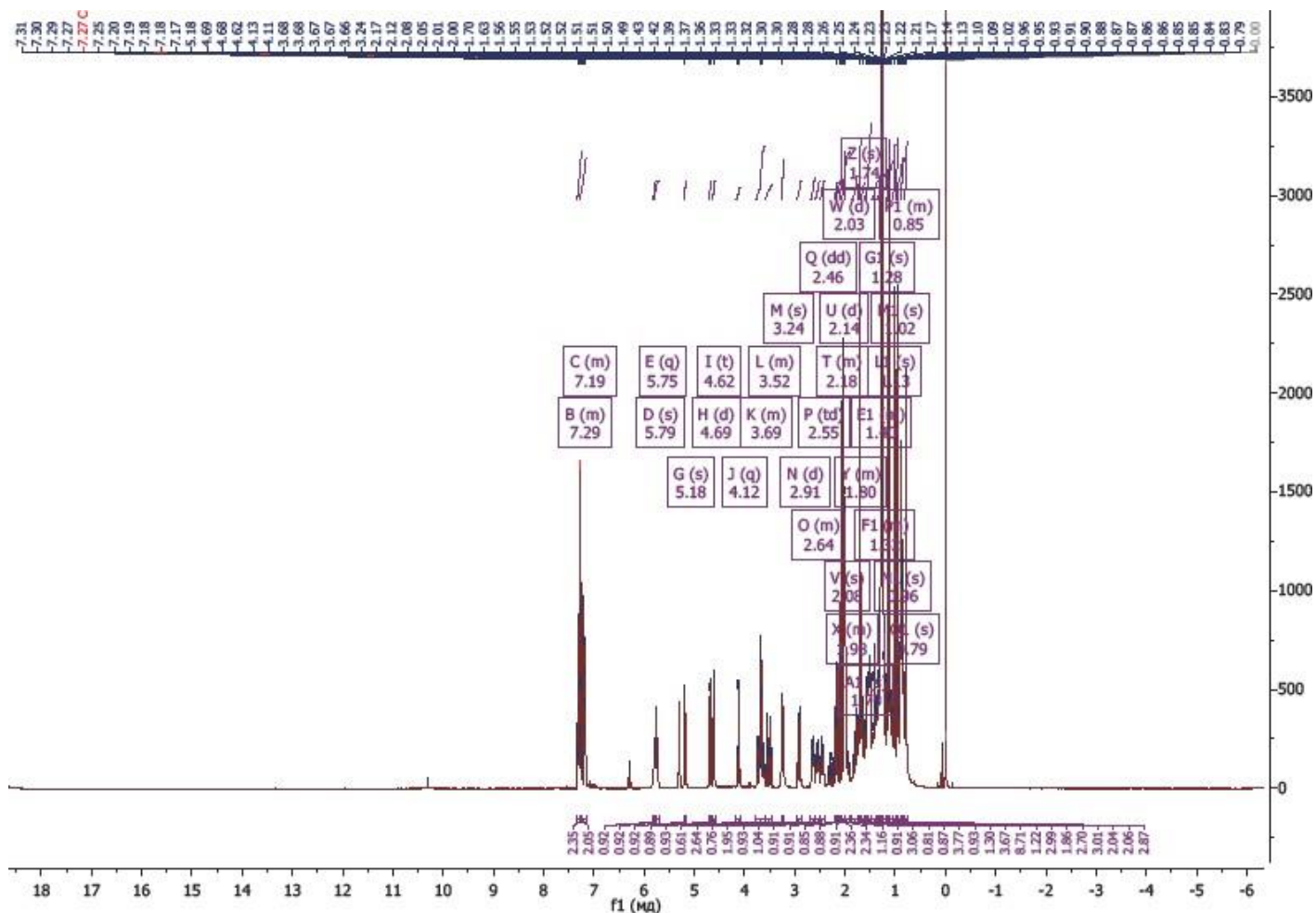
Compound **18**, ^1H NMR (400 MHz, CDCl_3)



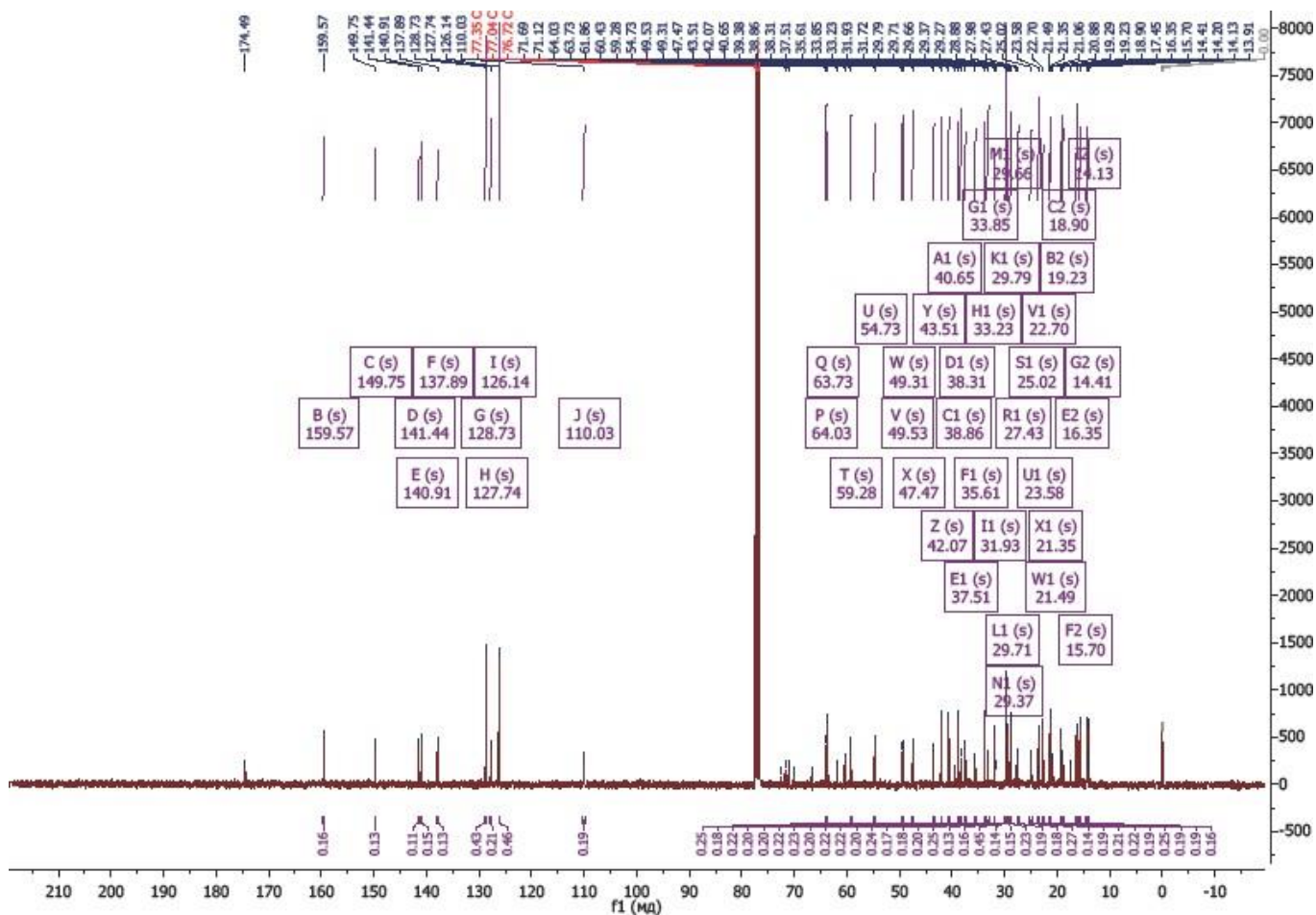
^{13}C NMR (101 MHz, CDCl_3)



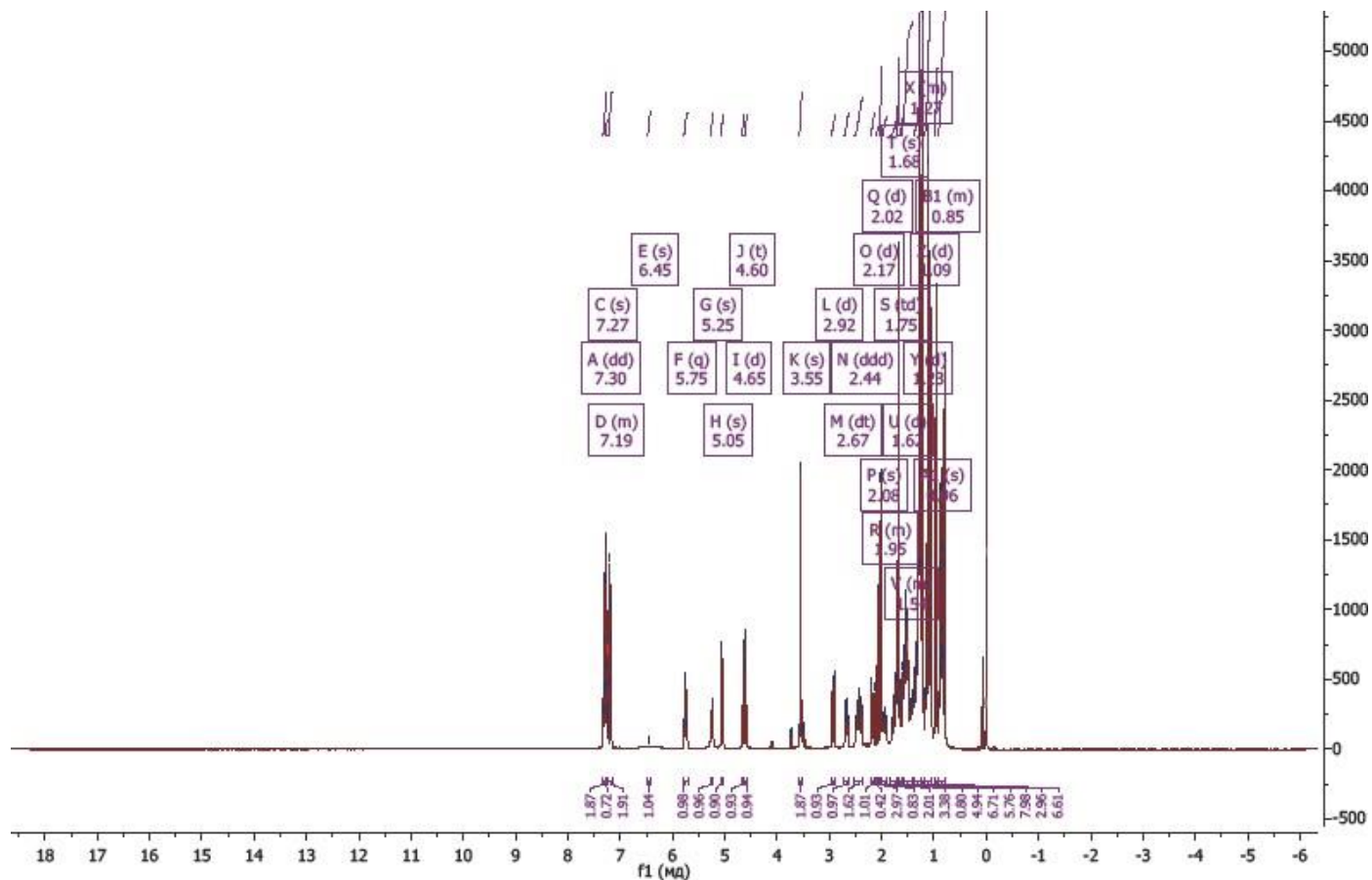
Compound **19**, ^1H NMR (400 MHz, CDCl_3)



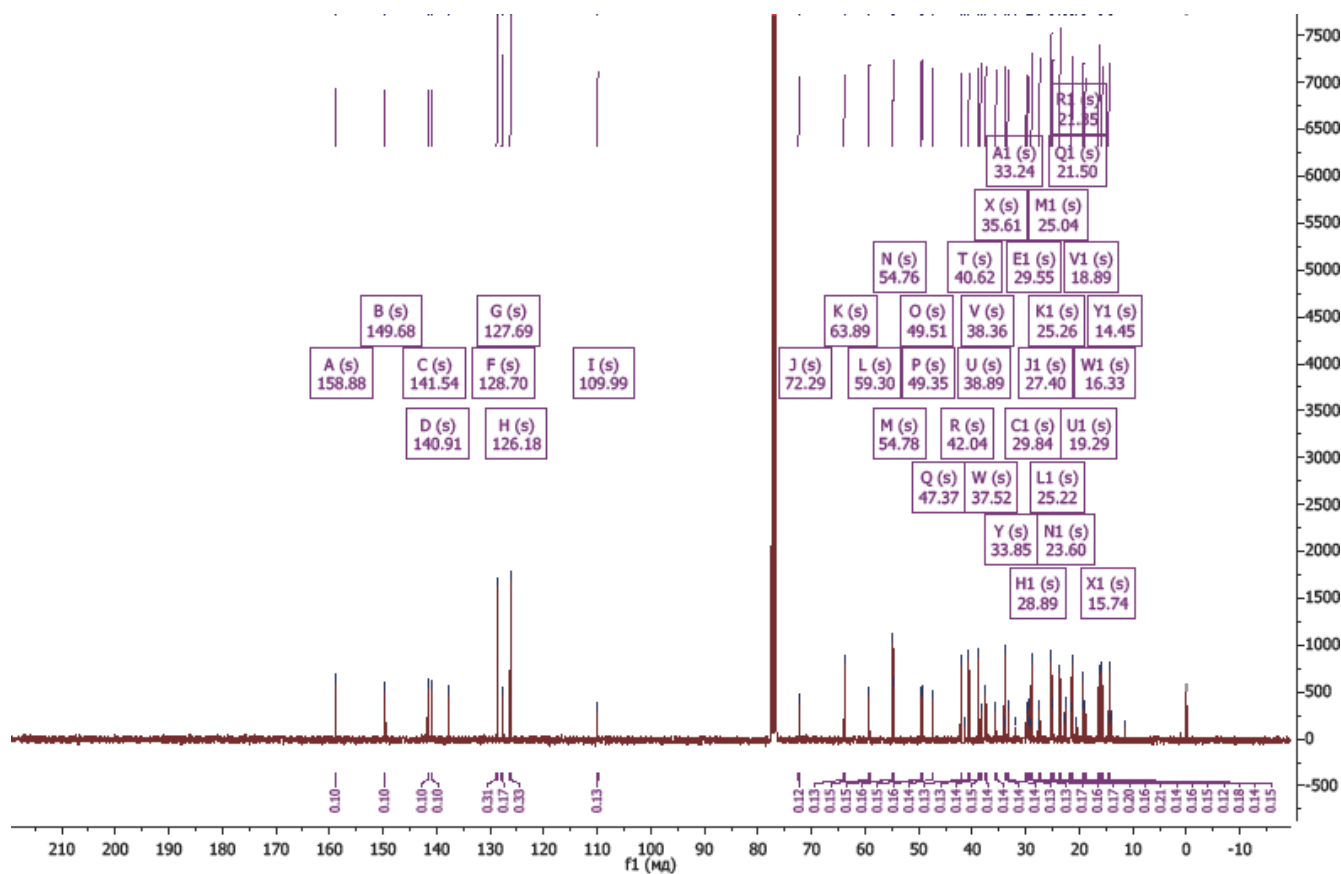
^{13}C NMR (101 MHz, CDCl_3)



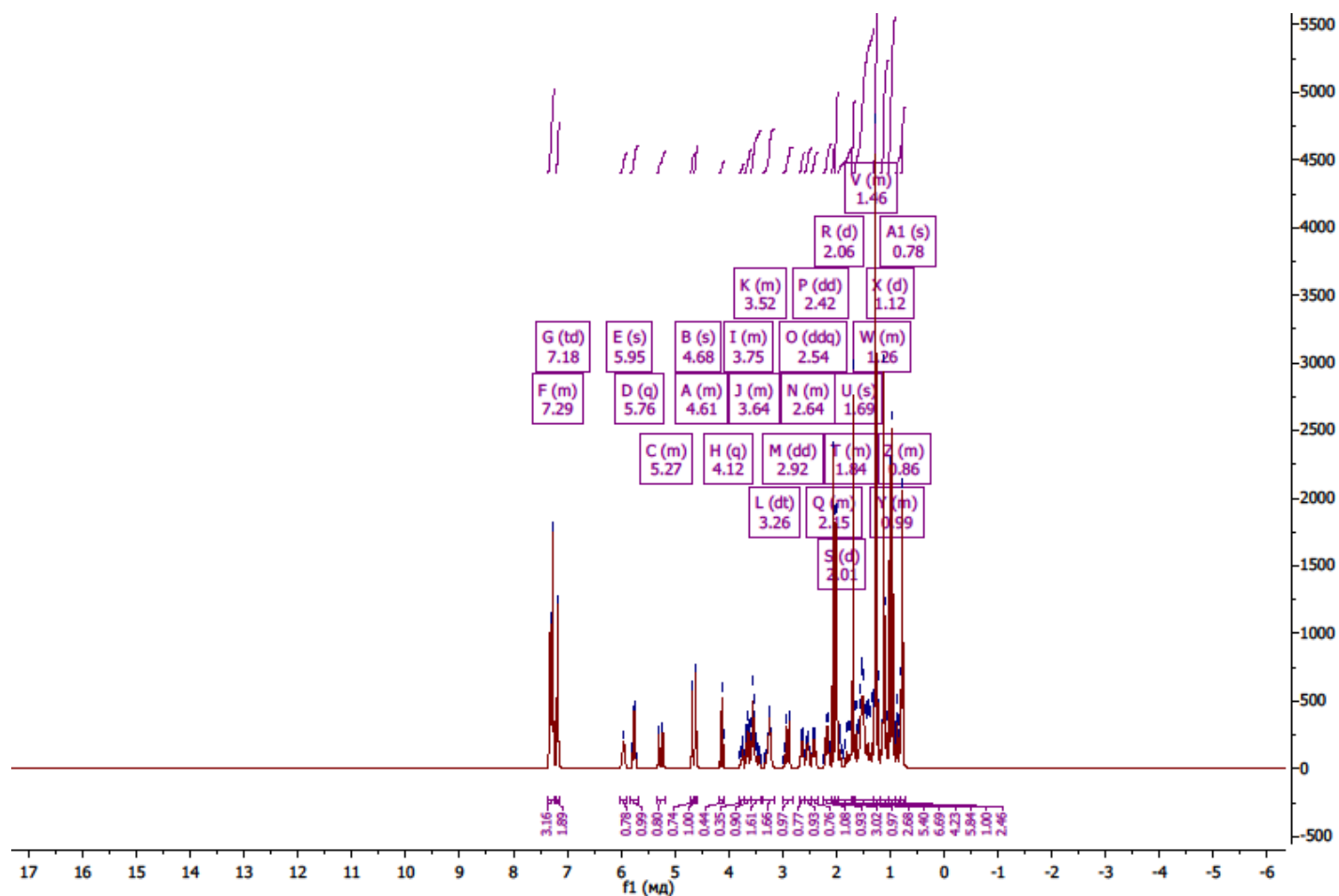
Compound **20**, ^1H NMR (400 MHz, CDCl_3)



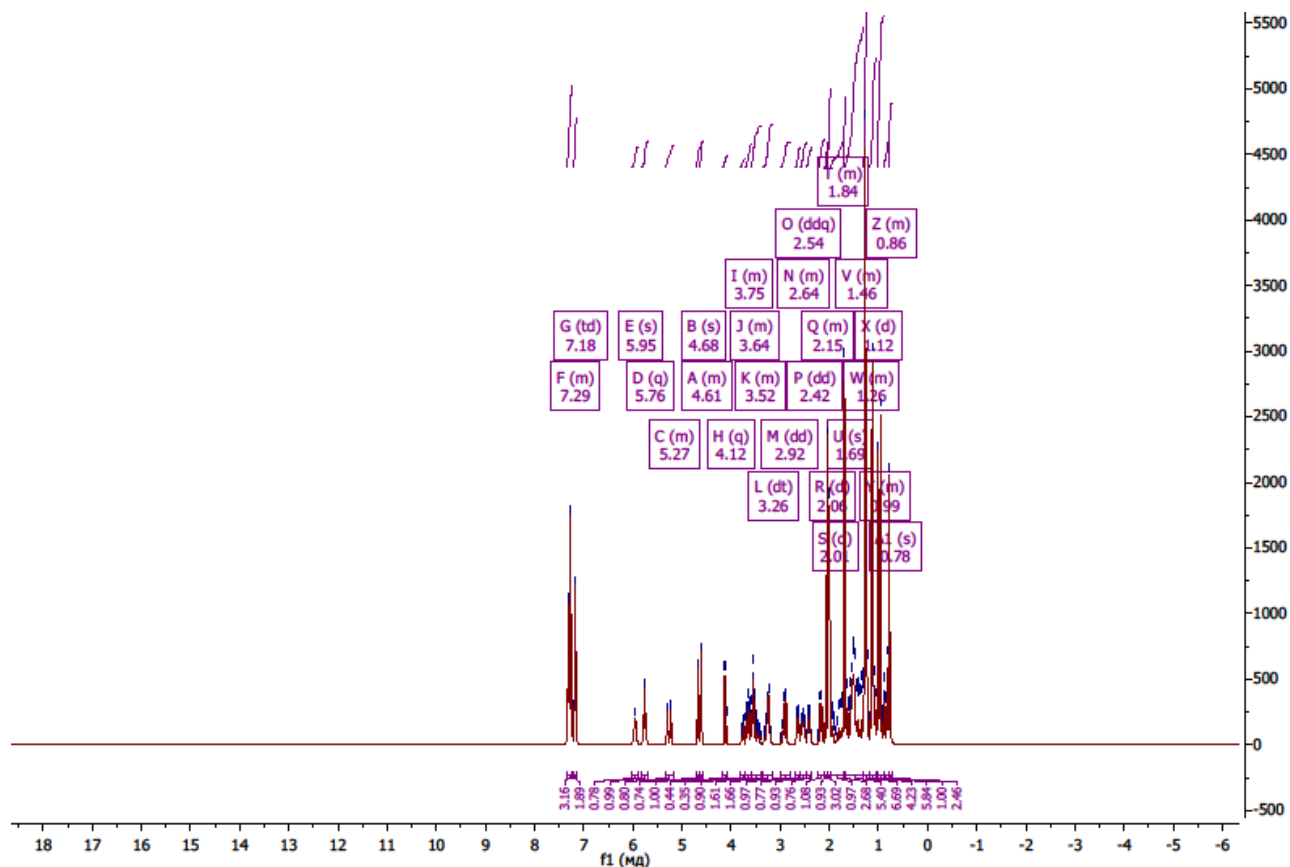
^{13}C NMR (101 MHz, CDCl_3)



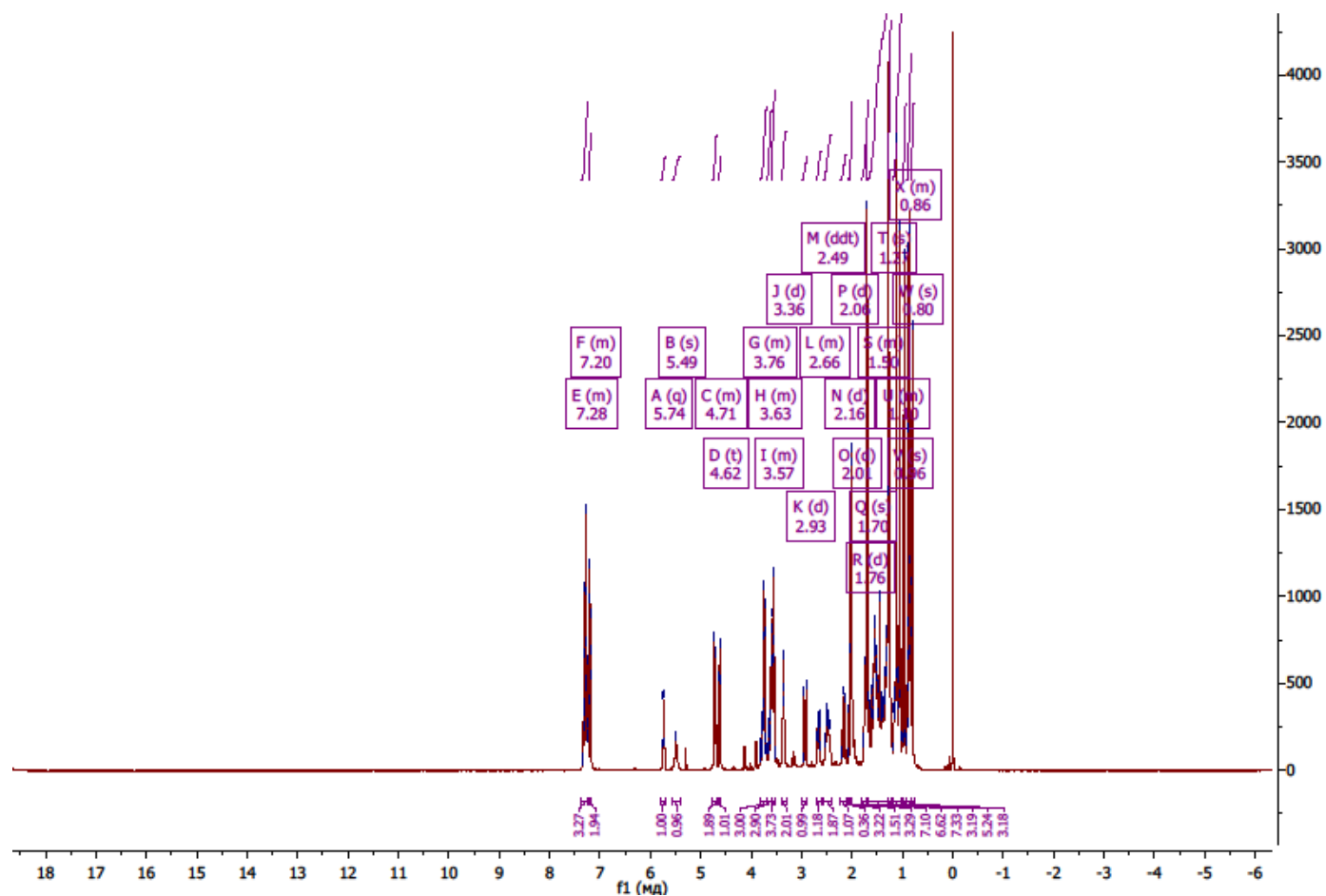
Compound **21**, ^1H NMR (400 MHz, CDCl_3)



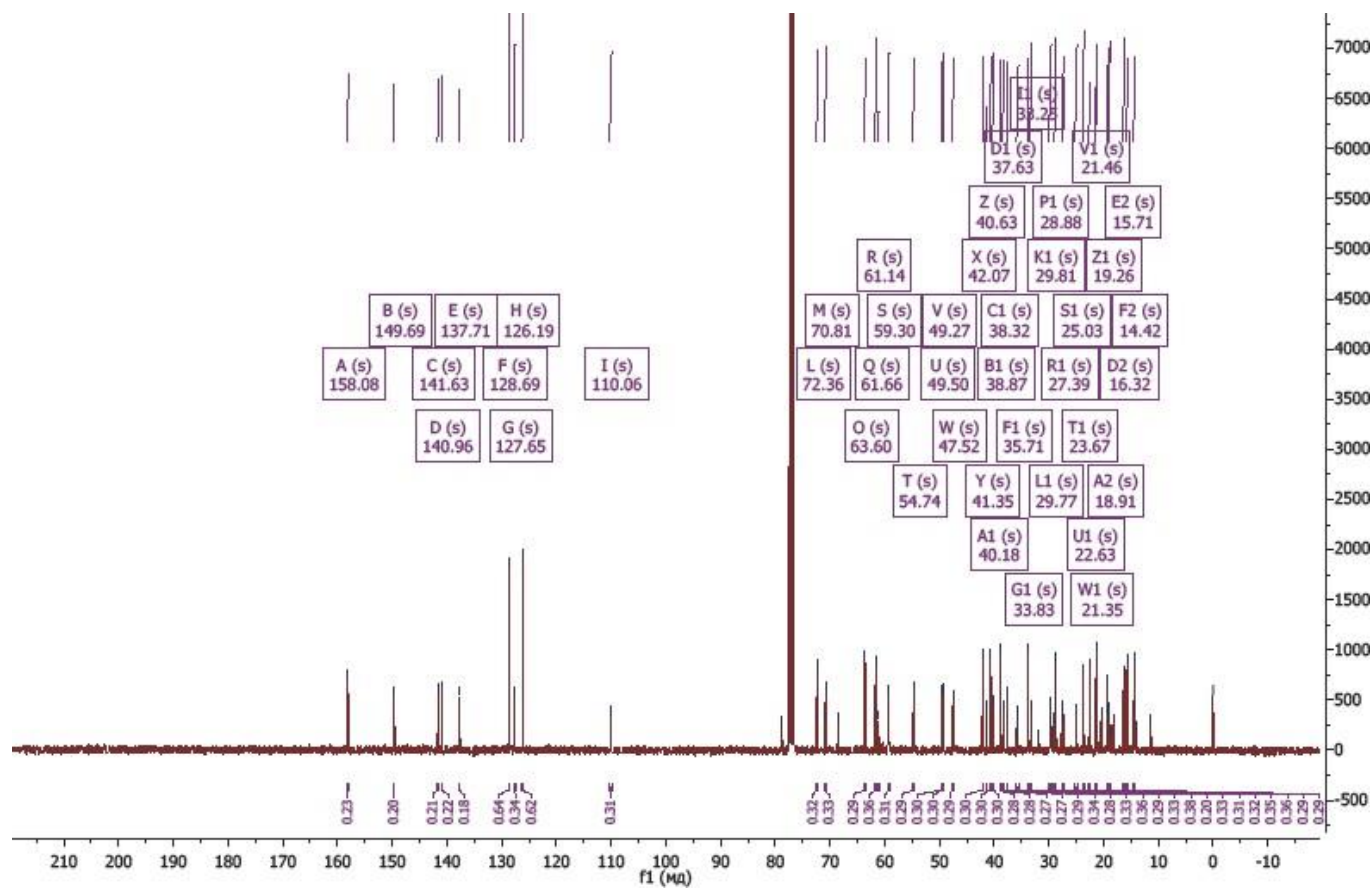
^{13}C NMR (101 MHz, CDCl_3)



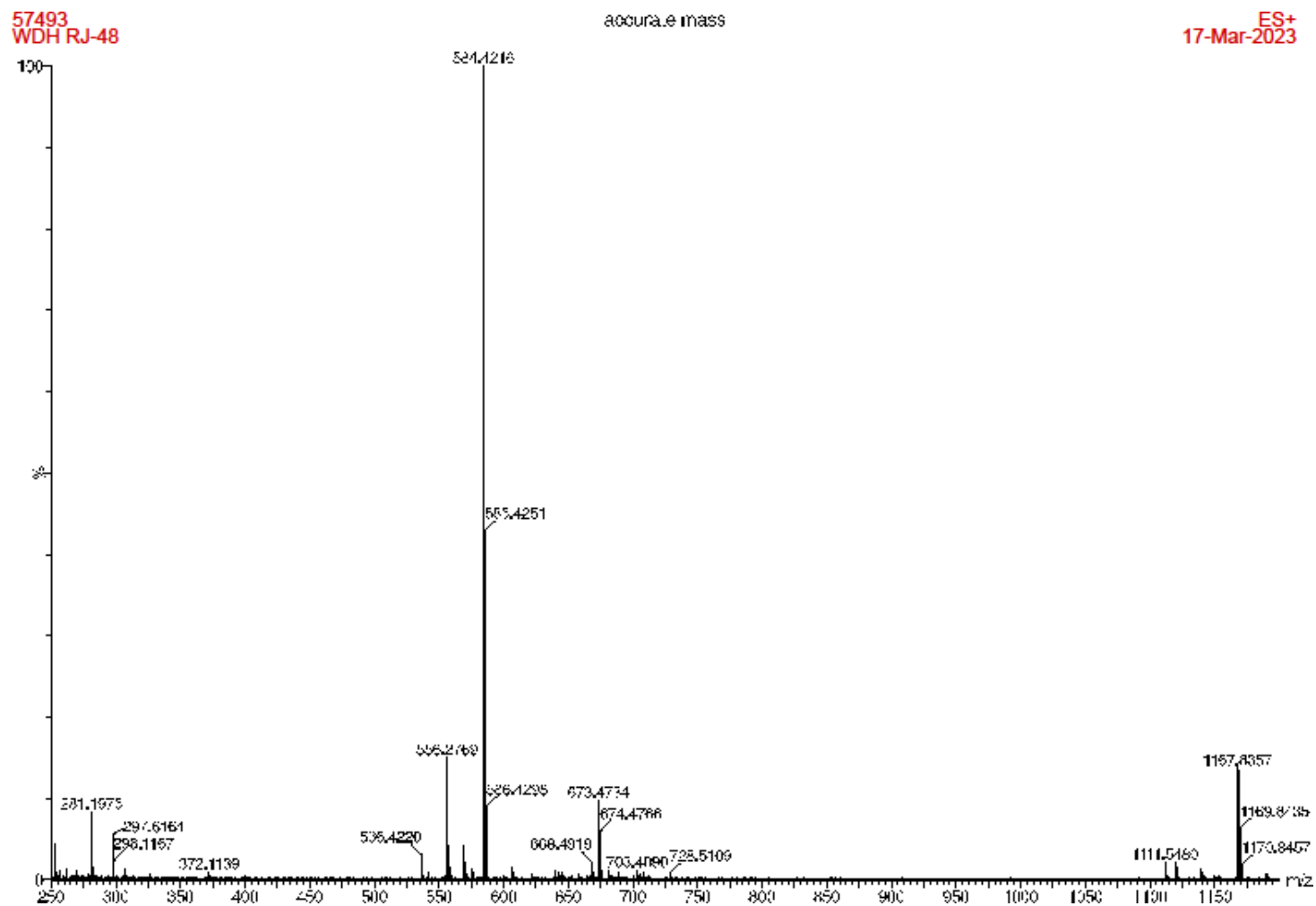
Compound **22**, ^1H NMR (400 MHz, CDCl_3)



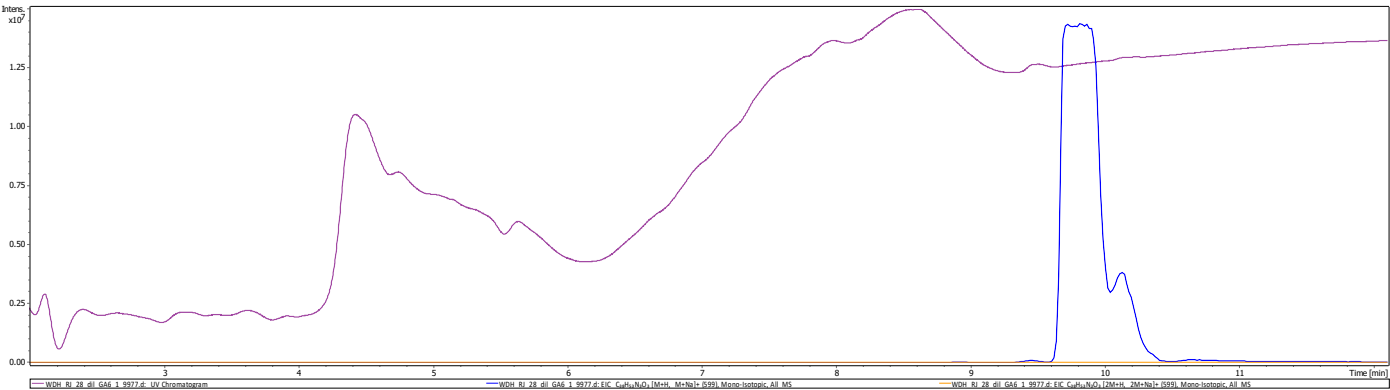
^{13}C NMR (101 MHz, CDCl_3)



Compound 4 (MS)



Compound 5 (MS)



Lower

Generate

Upper

Help

C 30-n, H 53-n, N 3-n, O 3-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos.

M+H

Collect adducts

Adducts, neg.

M-H

Measured

600.4194

Tolerance

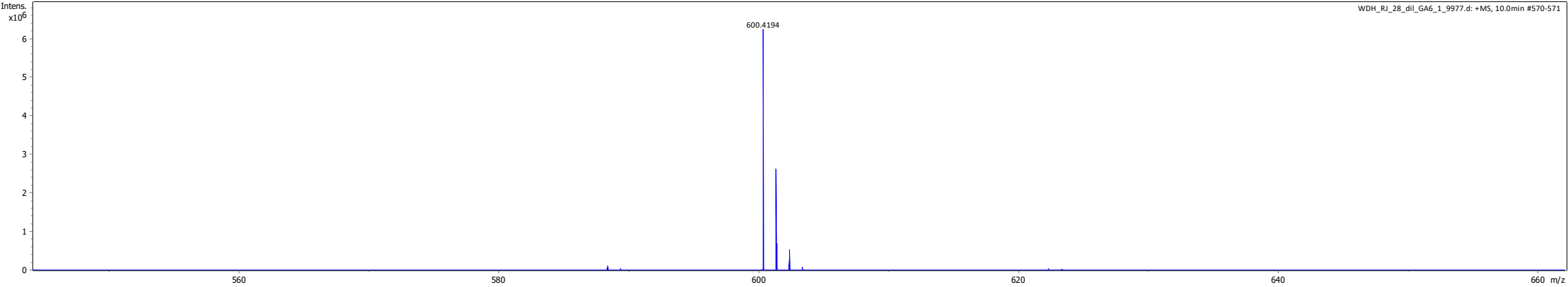
5

mDa

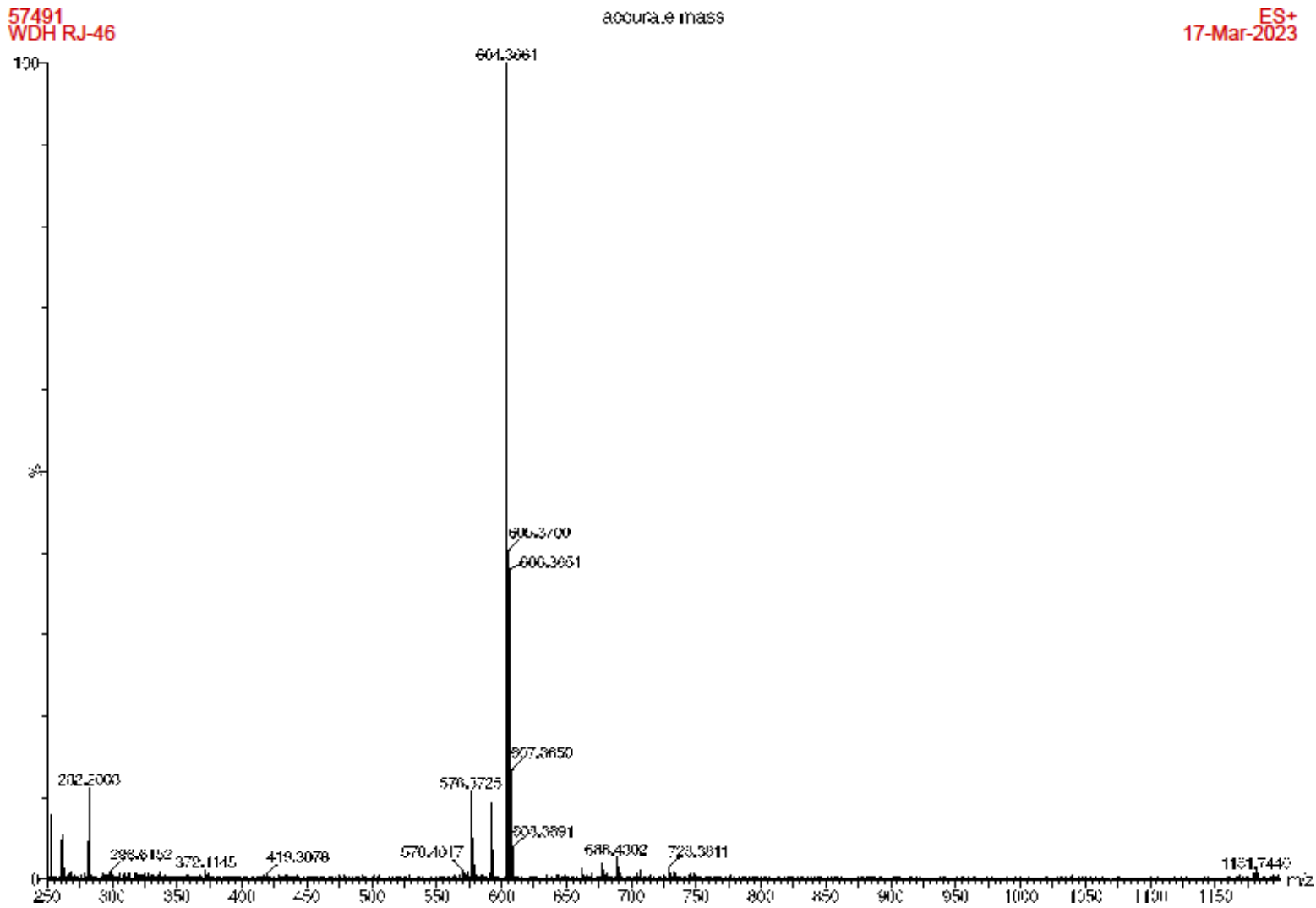
Charge:

1

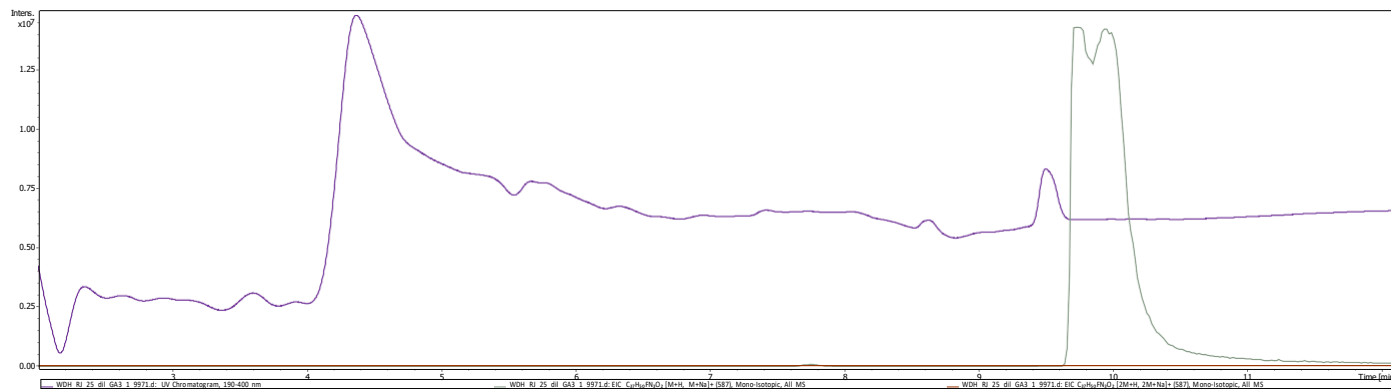
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
600.4194	1	C ₃₈ H ₅₄ N ₃ O ₃	600.4160	-5.8	7.1	1	61.18	14.



Compound 6 (MS)



Compound 7 (MS)



Lower

Upper

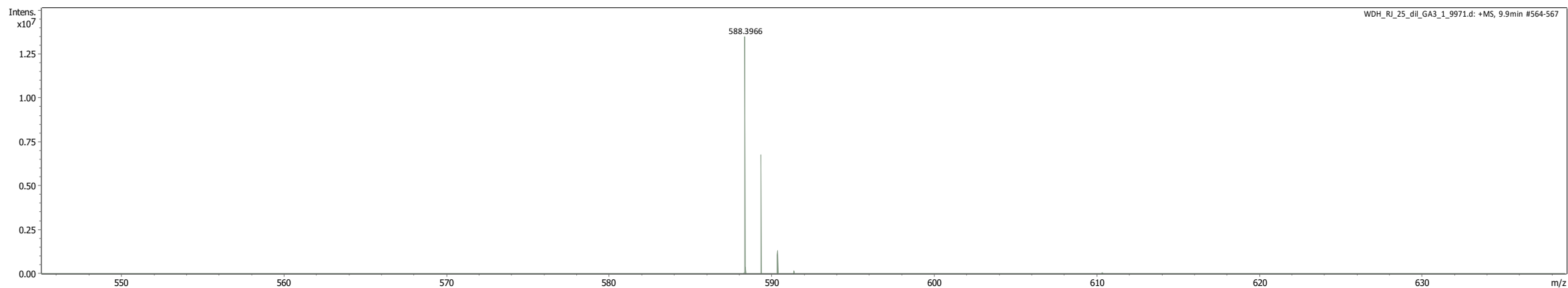
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

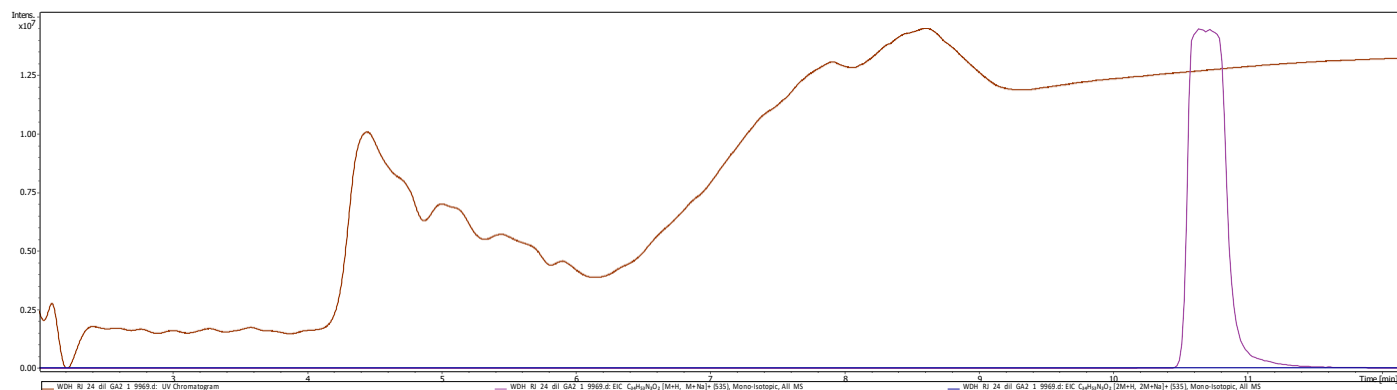
Adducts, neg.

Measured Tolerance mDa Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	r
588.3966	1	C ₃₇ H ₅₁ FN ₃ O ₂	588.3960	-1.1	41.9	1	100.00	14



Compound 8 (MS)



Lower

Upper

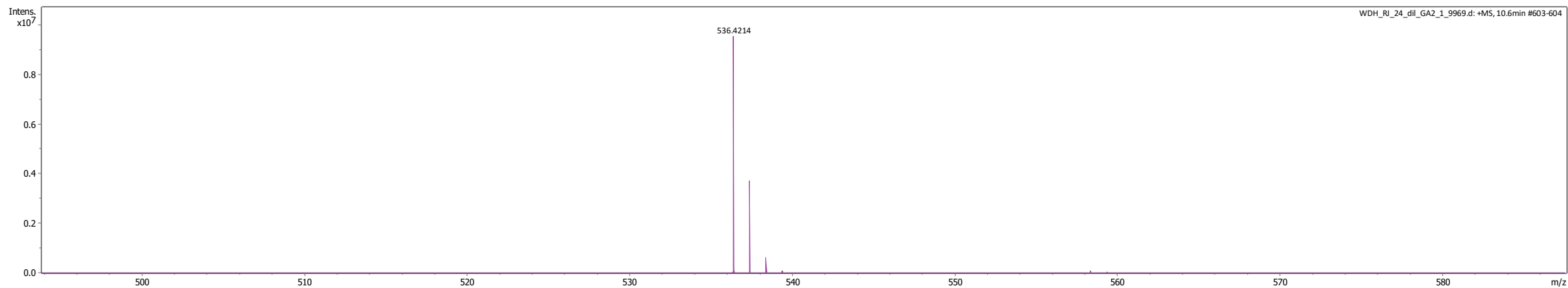
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

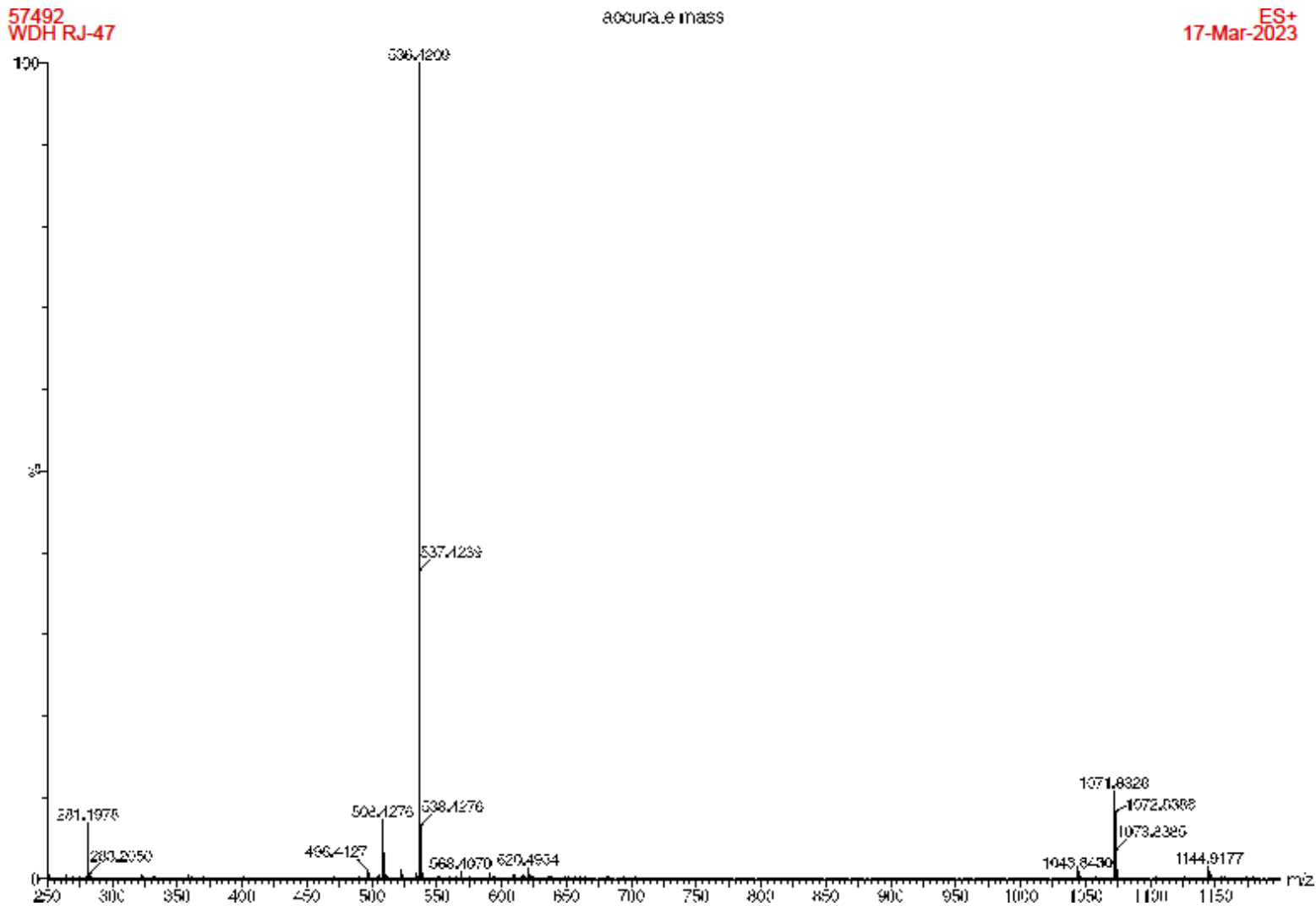
Adducts, neg.

Measured Tolerance mDa Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
536.4214	1	C ₃₄ H ₅₄ N ₃ O ₂	536.4211	-0.6	5.2	1	100.00	10.



Compound 9 (MS)

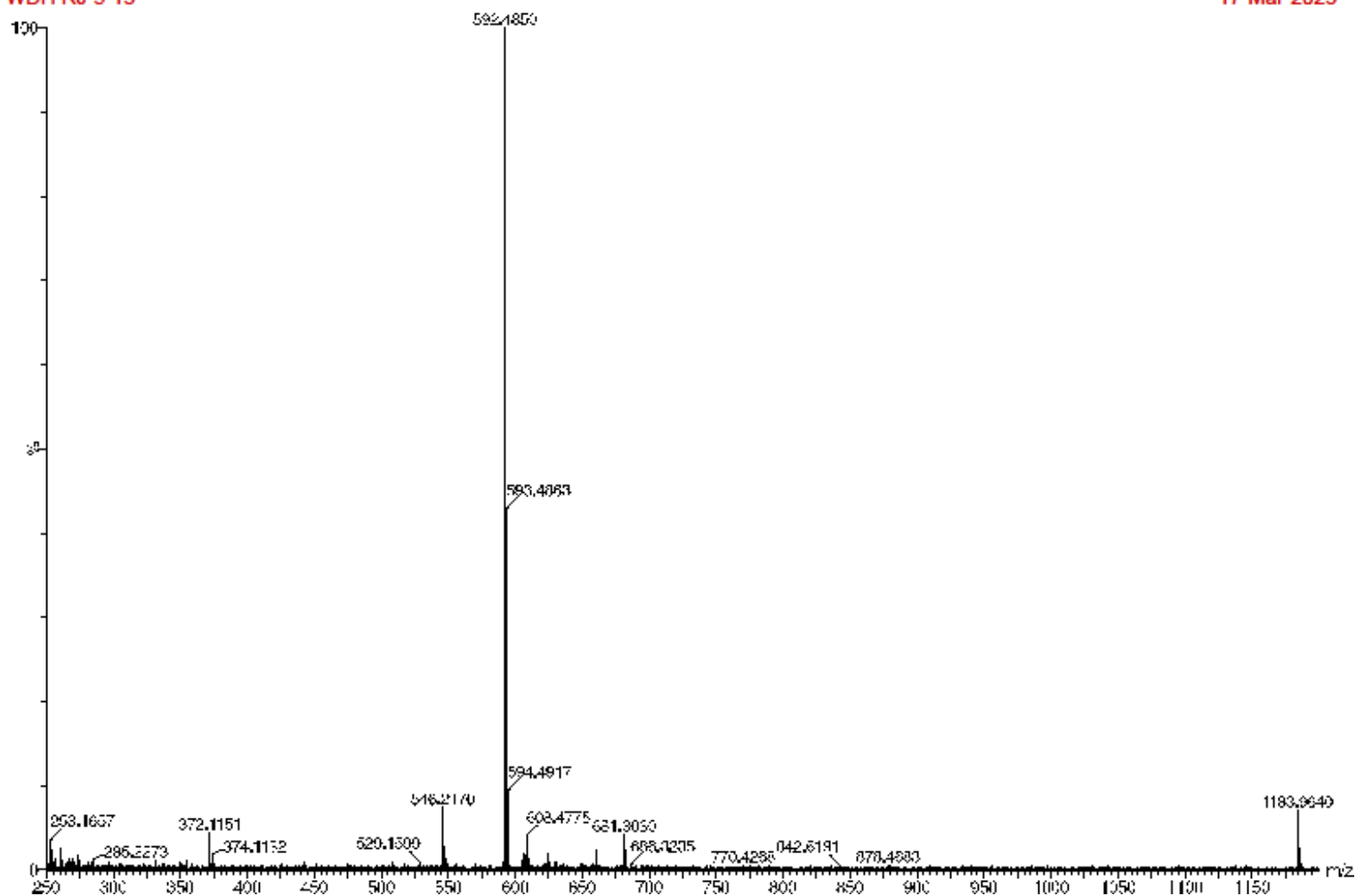


Compound **11** (MS)

57489
WDH RJ-5-13

accurate mass

ES+
17-Mar-2023

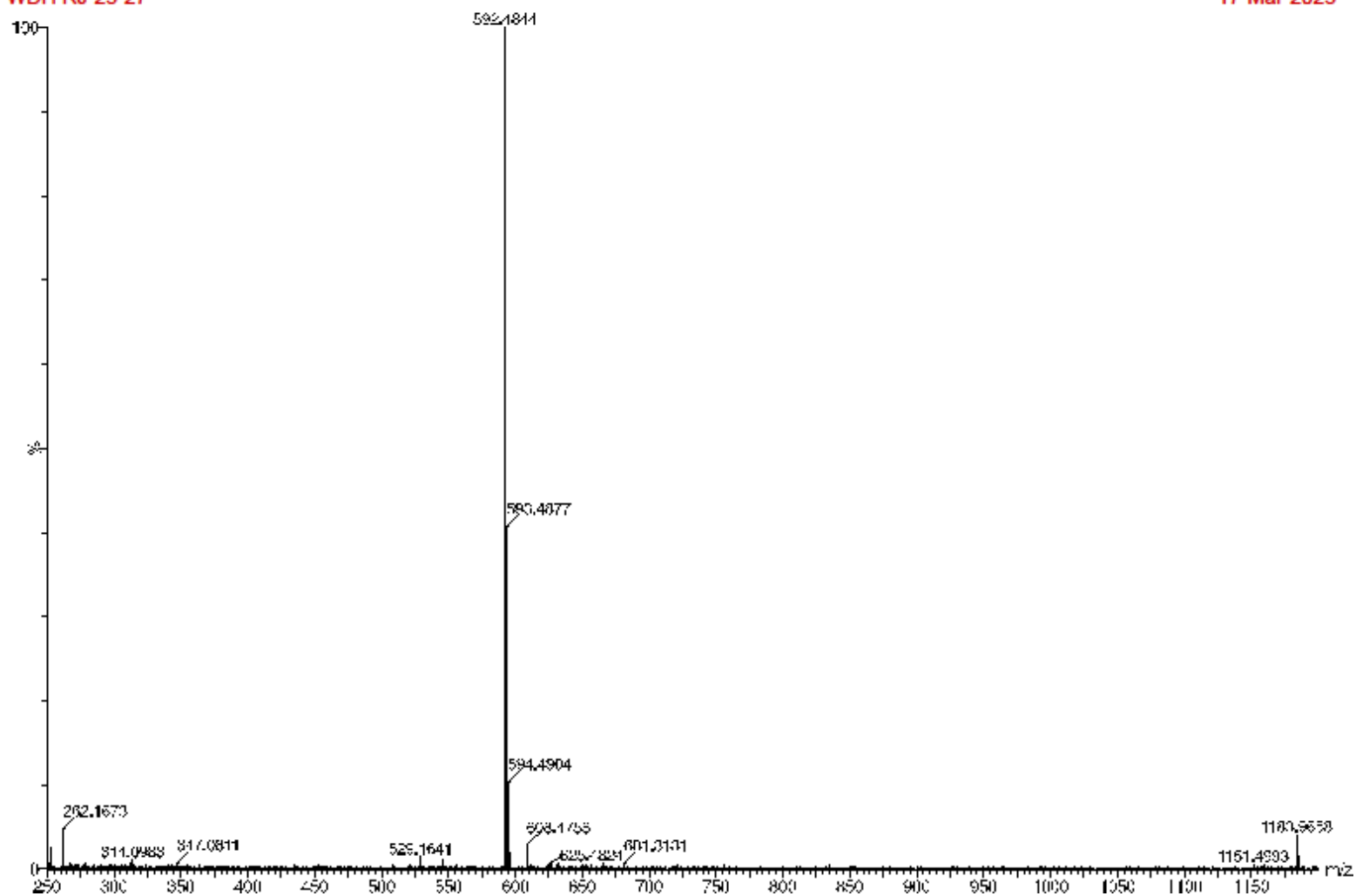


Compound **12** (MS)

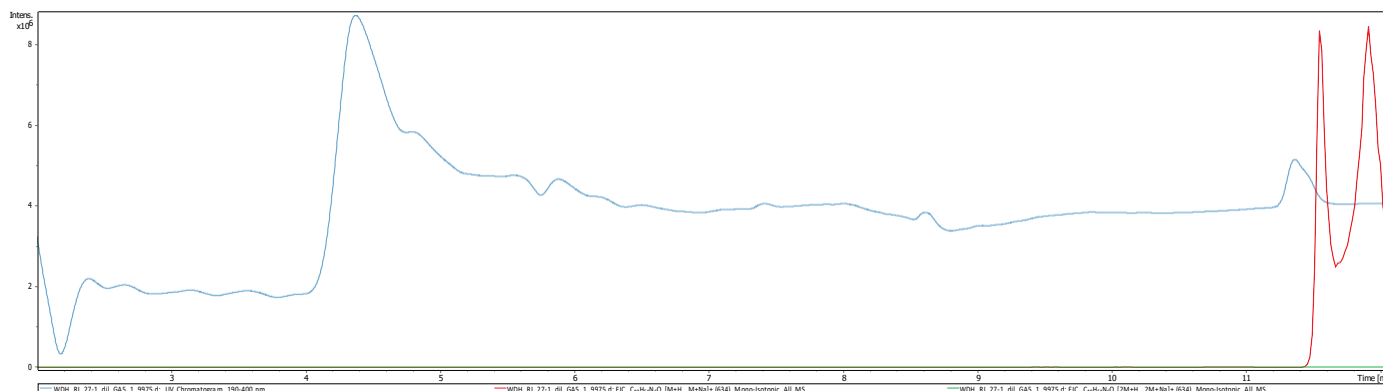
57490
WDH RJ-23-27

accurate mass

ES+
17-Mar-2023



Compound **13** (MS)



Lower

Upper

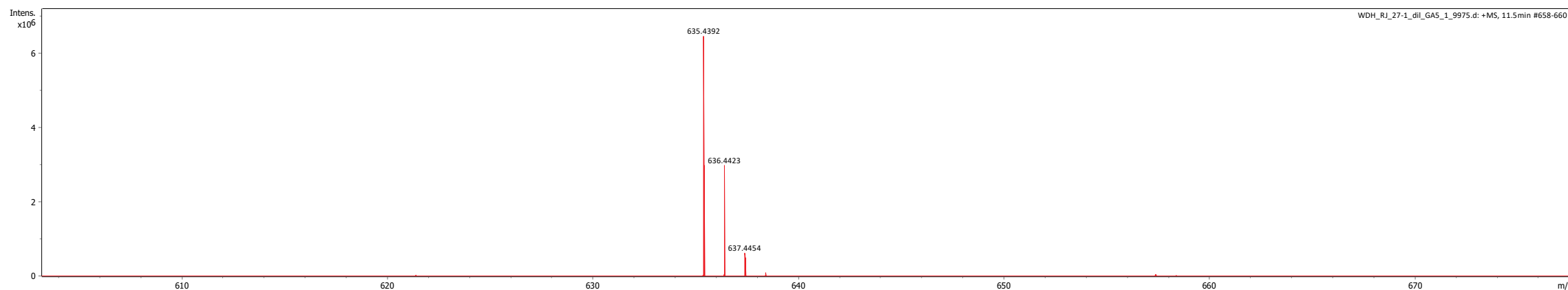
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

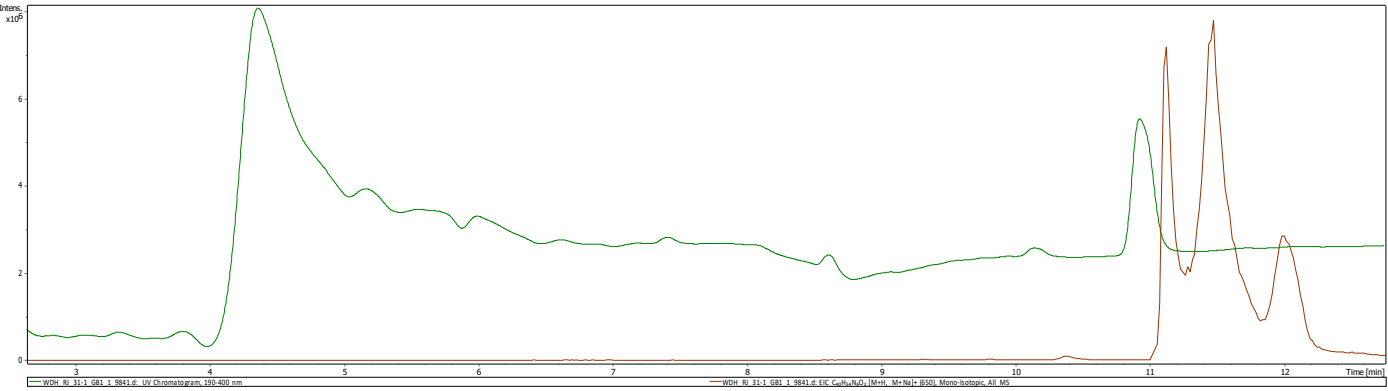
Adducts, neg.

Measured Tolerance mDa Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
635.4393	1	C ₄₀ H ₅₅ N ₆ O	635.4432	6.2	5.0	1	7.60	17.



Compound **14** (MS)



Lower

C₃₂H₅₄N₆O₂

Generate

Upper

Help

C 32-n, H 54-n, N 6-n, O 2-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos.

M+H; M+Na

Collect adducts

Adducts, neg.

M-H

Measured

651.4378

Tolerance

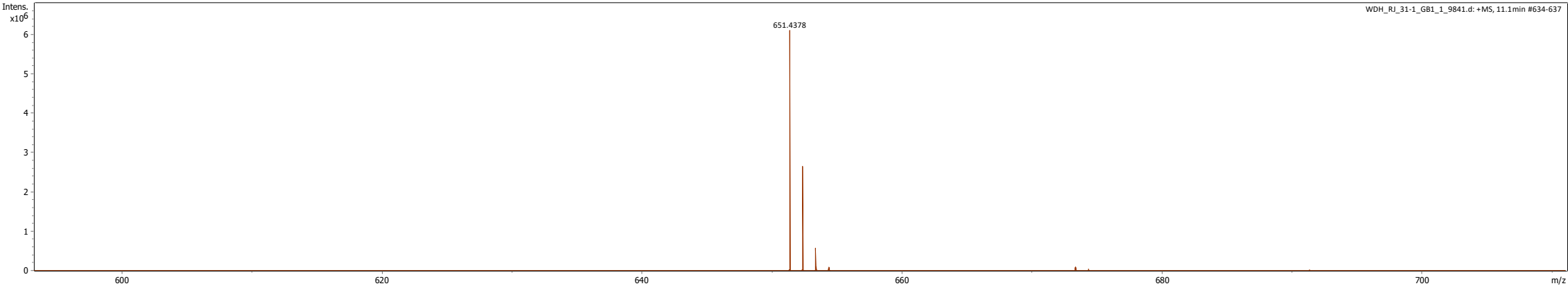
2

mDa

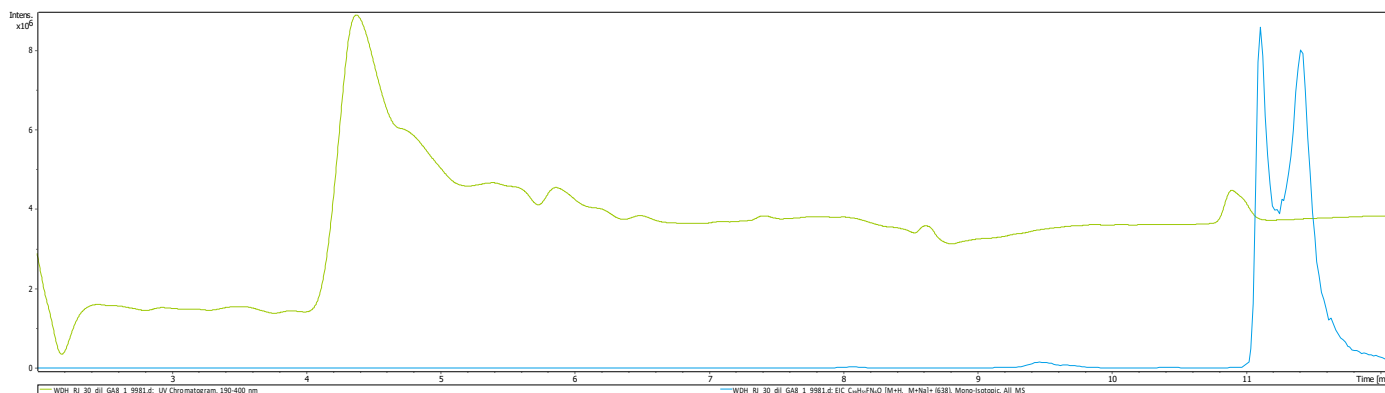
Charge:

1

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
651.4378	1	C ₄₀ H ₅₅ N ₆ O ₂	651.4381	0.5	14.9	1	100.00	17.



Compound **15** (MS)



Lower

Upper

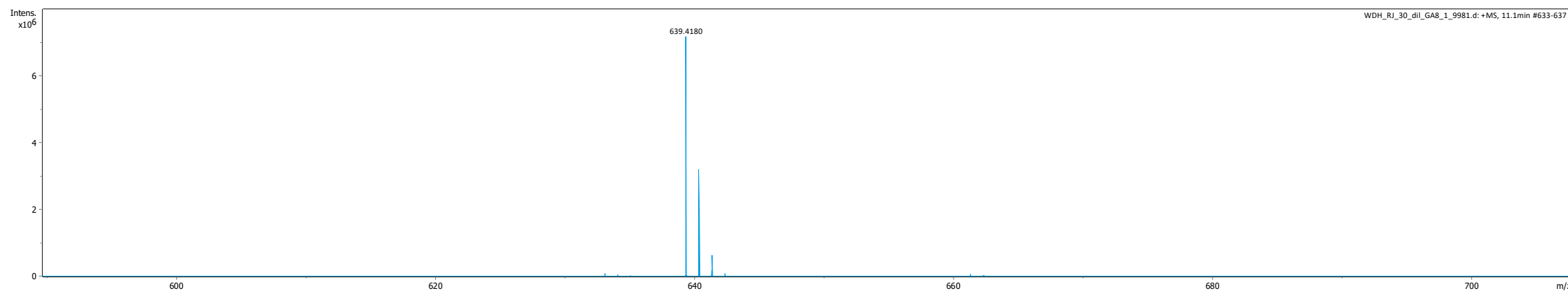
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

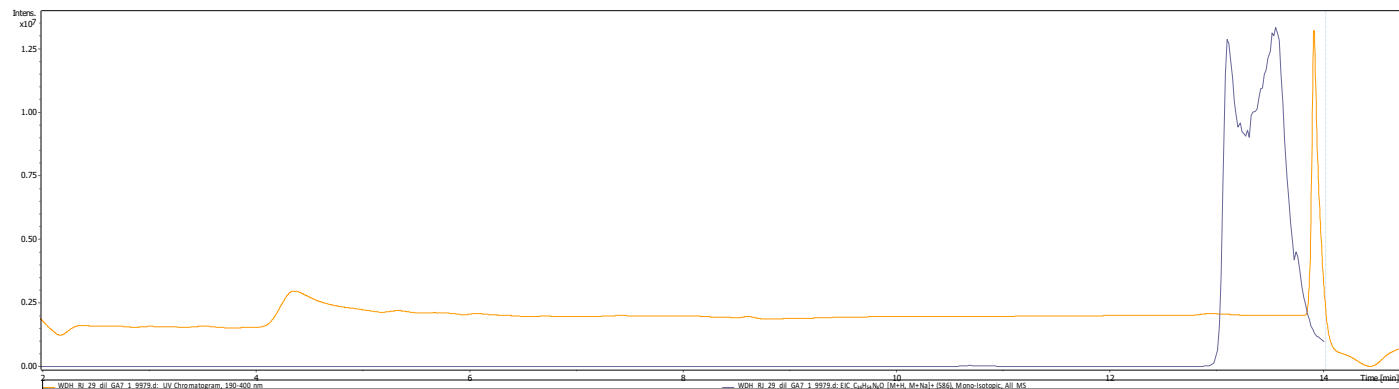
Adducts, neg.

Measured Tolerance mDa Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
639.4180	1	C ₃₉ H ₅₂ FN ₆ O	639.4181	0.1	6.6	1	100.00	17.



Compound **16** (MS)



Lower

Upper

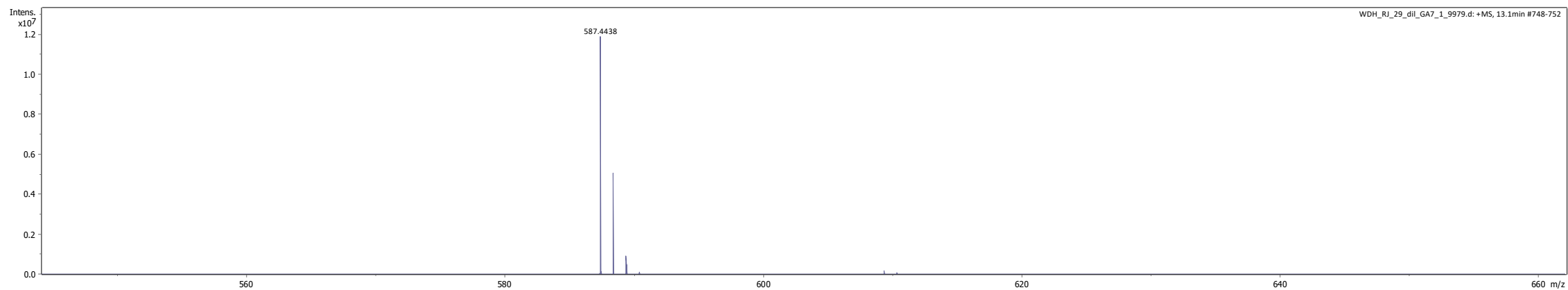
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

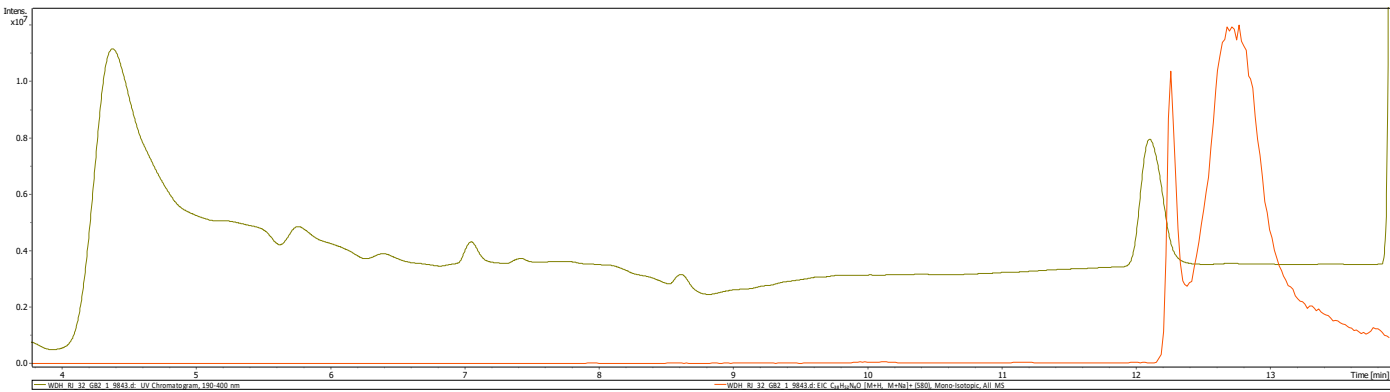
Adducts, neg.

Measured Tolerance mDa Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb
587.4438	1	C ₃₆ H ₅₅ N ₆ O	587.4432	-1.1	6.3	1	100.00	13.0



Compound 17 (MS)



Lower

C₃₀H₅₂N₄O₁

Generate

Upper

Help

C 30-n, H 52-n, N 4-n, O 1-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos.

M+H; M+Na

Collect adducts

Adducts, neg.

M-H

Measured

581.4218

Tolerance

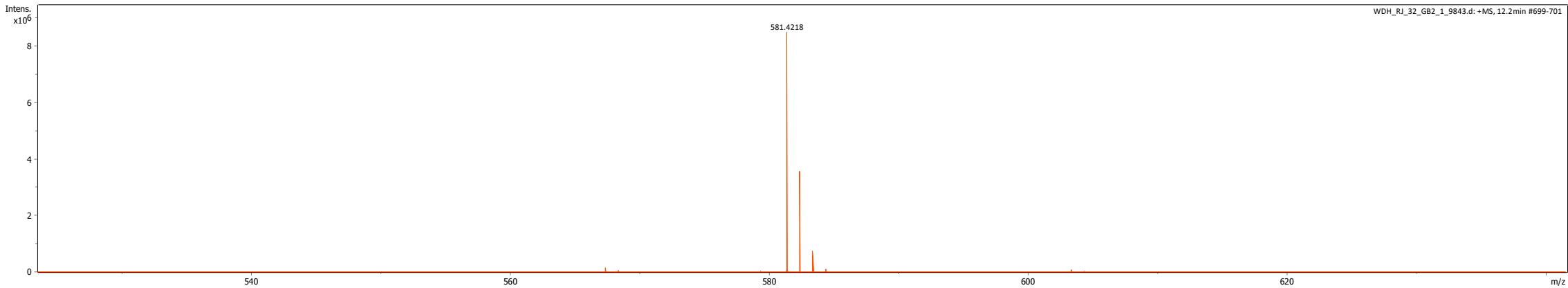
2

mDa

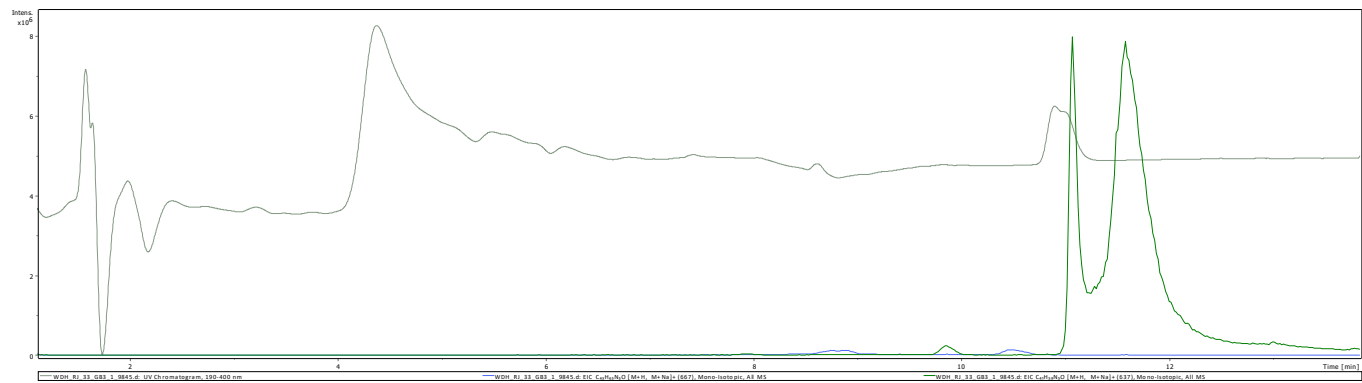
Charge:

1

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb
581.4218	1	C ₃₈ H ₅₃ N ₄ O	581.4214	-0.7	7.2	1	100.00	15.0



Compound 18 (MS)



Lower

C₄₁H₅₉N₅O₁

Generate

Upper

Help

C 41-n, H 59-n, N 5-n, O 1-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos.

M+H; M+Na

Collect adducts

Adducts, neg.

M-H

Measured

638.475

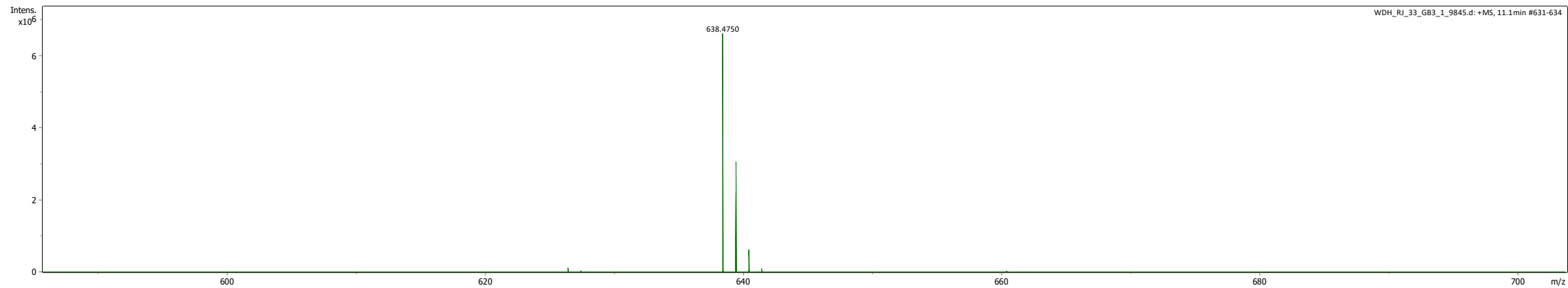
Tolerance

10

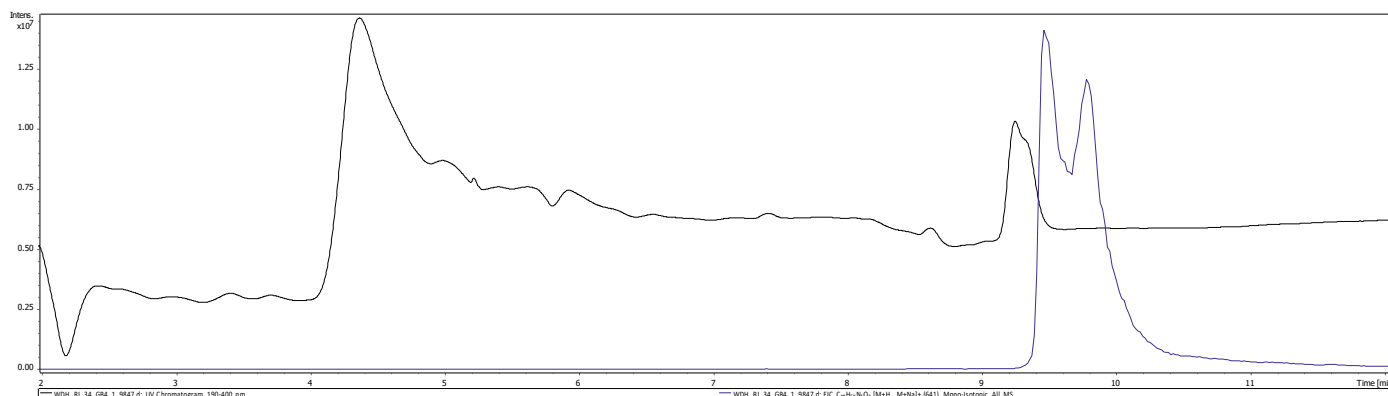
ppm

Charge: 1

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb
638.4750	1	C ₄₁ H ₆₀ N ₅ O	638.4792	6.6	8.0	1	100.00	15.0



Compound **19** (MS)



Lower

Upper

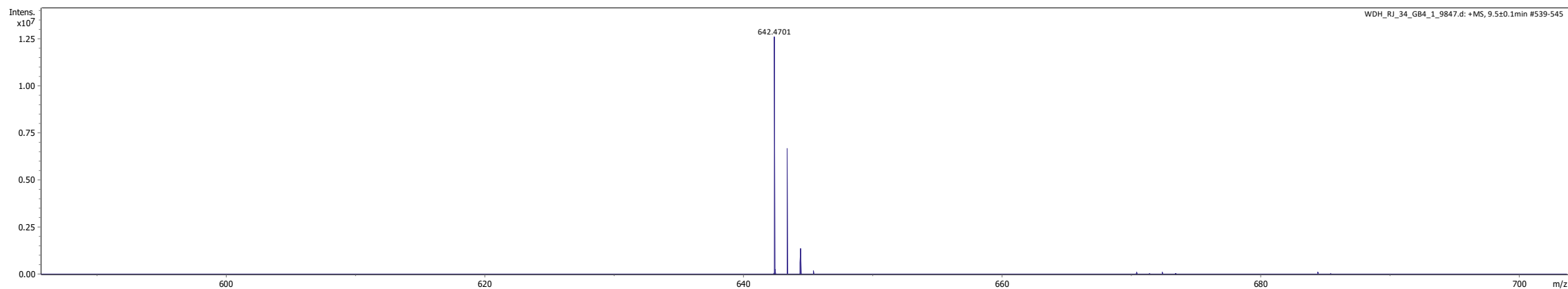
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

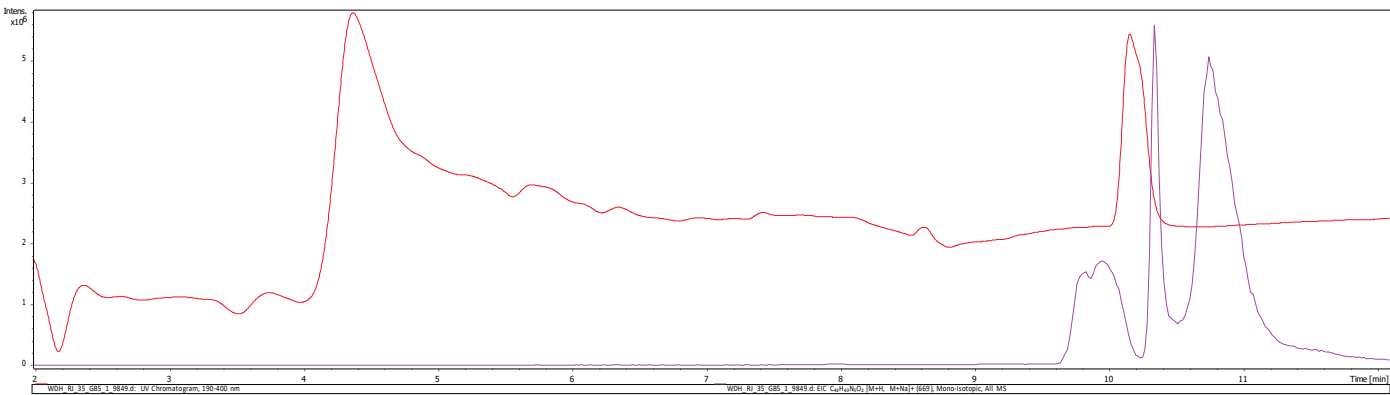
Adducts, neg.

Measured Tolerance ppm Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
642.4701	1	C ₄₀ H ₆₀ N ₅ O ₂	642.4742	6.4	36.1	1	100.00	14.



Compound **20** (MS)



Lower

Upper

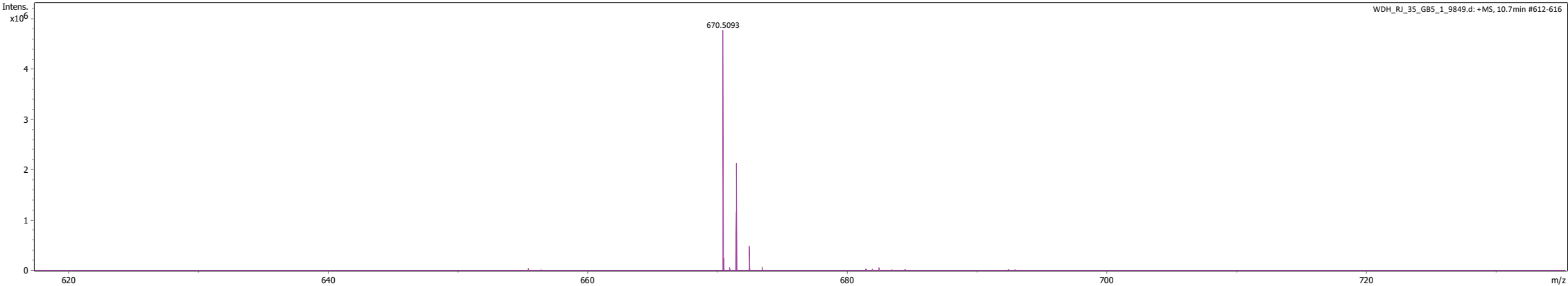
Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

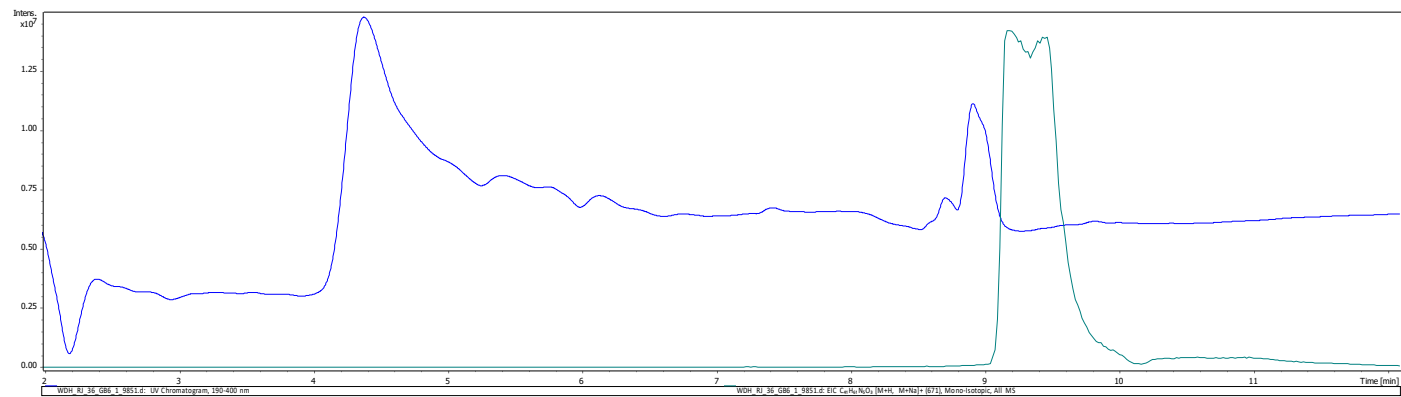
Adducts, neg.

Measured Tolerance ppm

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
670.5093	1	C ₄₂ H ₆₄ N ₅ O ₂	670.5055	-5.7	19.4	1	100.00	14.



Compound **21** (MS)



Lower

C₃₅H₆₁N₅O₃

Generate

Upper

Help

C 35-n, H 61-n, N 5-n, O 3-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos.

M+H⁺; M+Na⁺

☐ Collect adducts

Adducts, neg.

M-H⁻

Measured

672.4858

Tolerance

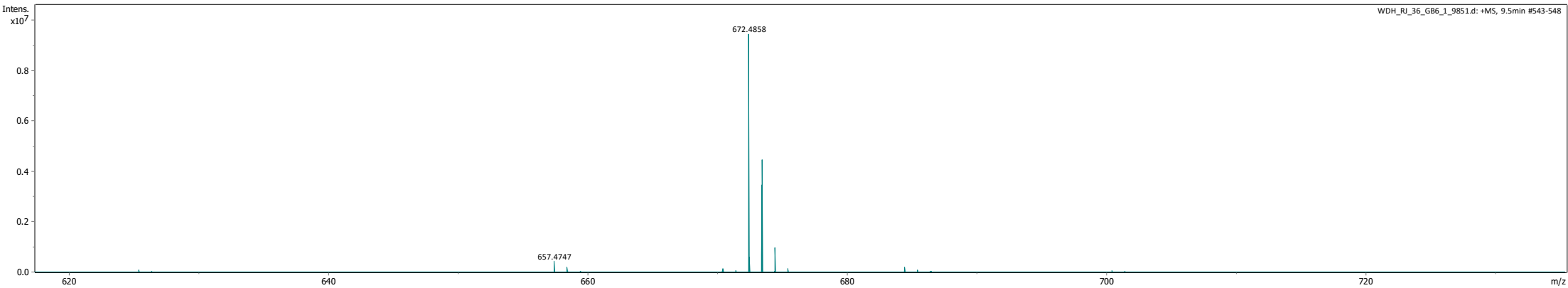
2

ppm

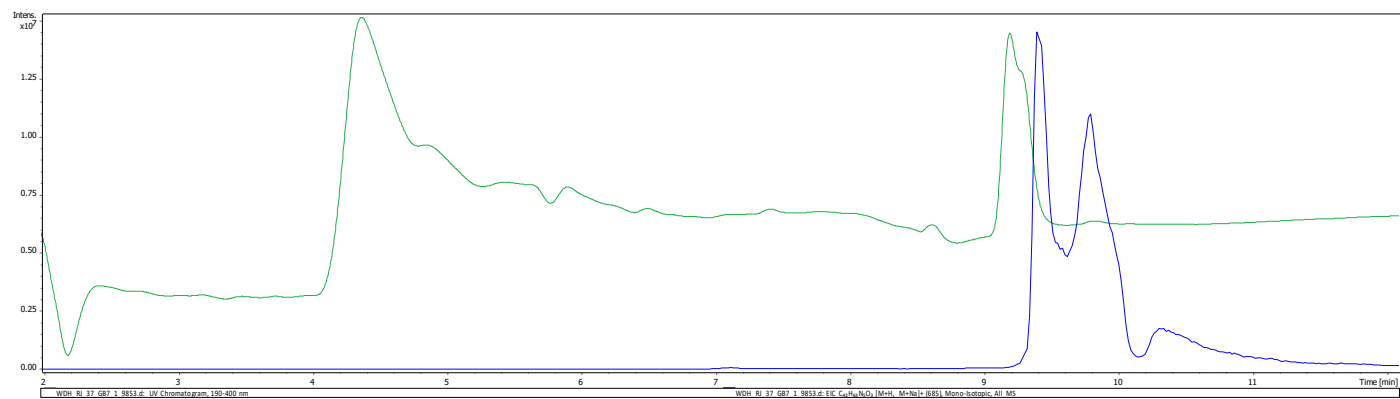
Charge:

1

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
672.4858	1	C ₄₁ H ₆₂ N ₅ O ₃	672.4847	-1.6	5.2	1	100.00	14.



Compound **22** (MS)



Lower

C₄₂H₆₃N₅O₃

Generate

Upper

Help

C 42-n, H 63-n, N 5-n, O 3-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos.

M+H; M+Na

Collect adducts

Adducts, neg.

M-H

Measured

686.4954

Tolerance

10

ppm

Charge:

1

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rd
686.4954	1	C ₄₂ H ₆₄ N ₅ O ₃	686.5004	7.3	8.9	1	100.00	14.

