Supporting Information (SI)

The use of aryl-substituted homophthalic anhydrides in the Castagnoli-Cushman reaction provides access to novel tetrahydroisoquinolone carboxylic acid bearing an all-carbon quaternary stereogenic center

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1. X-ray crystallographic data

X-ray Single Crystal analysis was performed on Rigaku XtaLAB Synergy-S diffractometer with monochromated CuKα radiation. Crystal growth was performed by slow evaporation of solution in methanol/acetone mixture (1:1) at 5 °C. The crystal was kept at 100 K during data collection. Using Olex2[1], the structures were solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the SHELXL[3] refinement package using Least Squares minimization. CCDC 2211662 **(9a)** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/.

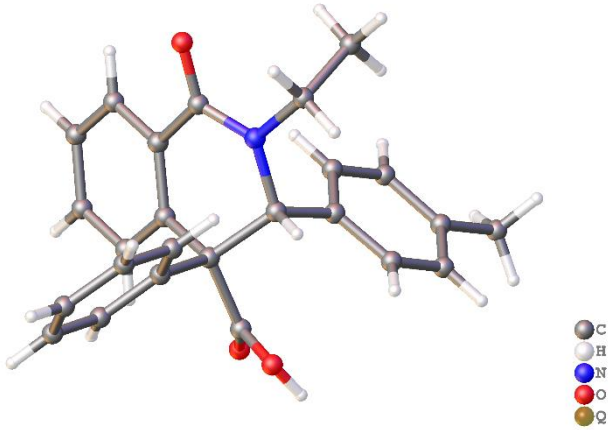

Figure S1. Crystal structure of compound 9a (ORTEP plot at 50% probability level)

Table S1 Crystal data and structure refinement for compound 9a.	
Identification code	9a
Empirical formula	$C_{28.57}H_{26.29}N_{1.14}O_{3.43}$
Formula weight	440.51
Temperature/K	100.15
Crystal system	orthorhombic
Space group	Pbca
a/Å	15.8652(2)
b/Å	14.6469(2)
c/Å	16.7176(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3884.77(9)
Z	7
ρ_{calc}g/cm^3	1.318
μ/mm^{-1}	0.689
F(000)	1632.0
Crystal size/mm^3	0.28 × 0.24 × 0.16
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.774 to 152.44
Index ranges	-19 ≤ h ≤ 19, -18 ≤ k ≤ 18, -21 ≤ l ≤ 20

Reflections collected	41022
Independent reflections	4053 [R_{int} = 0.0439, R_{sigma} = 0.0168]
Data/restraints/parameters	4053/0/265
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1069
Final R indexes [all data]	R_1 = 0.0437, wR_2 = 0.1105
Largest diff. peak/hole / e $Å^{-3}$	0.39/-0.22

2. References

1. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: a complete structure solution, refinement and analysis program. *Journal of Applied Crystallography* **2009,** 42, (2), 339-341, 10.1107/s0021889808042726.

2. Sheldrick, G. M., SHELXT - integrated space-group and crystal-structure determination. *Acta Crystallogr A Found Adv* **2015,** 71, (Pt 1), 3-8, 10.1107/S2053273314026370.

3. Sheldrick, G. M., Crystal structure refinement with SHELXL. *Acta Crystallogr C Struct Chem* **2015,** 71, (Pt 1), 3-8, 10.1107/S2053229614024218.

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Datablock: 1ver0-20683_usa-041

Bond precision: C-C = 0.0017 A Wavelength=1.54184
Cell: a=15.8652(2) b=14.6469(2) c=16.7176(2)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3884.77(9)	3884.77(9)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C25 H23 N O3	1.143(C25 H23 N O3)
Sum formula	C25 H23 N O3	C28.57 H26.29 N1.14 O3.43
Mr	385.44	440.51
Dx,g cm-3	1.318	1.318
Z	8	7
Mu (mm-1)	0.689	0.689
F000	1632.0	1632.0
F000'	1636.83	
h,k,lmax	19,18,21	19,18,21
Nref	4062	4053
Tmin,Tmax	0.825,0.896	
Tmin'	0.825	

Correction method= Not given
Data completeness= 0.998 Theta(max)= 76.220
R(reflections)= 0.0408(3728) wR2(reflections)= 0.1105(4053)
S = 1.029 Npar= 265

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 7
From the CIF: _chemical_formula_sum C28.57 H26.29 N1.14 O3.43
TEST: Compare cell contents of formula and atom_site data

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H	184.03	184.00	0.03
N	7.98	8.00	-0.02
O	24.01	24.00	0.01

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PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 1.143 Check
PLAT793_ALERT_4_G Model has Chirality at C4 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C5 (Centro SPGR) S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 22 Info

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
8 ALERT level G = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor

alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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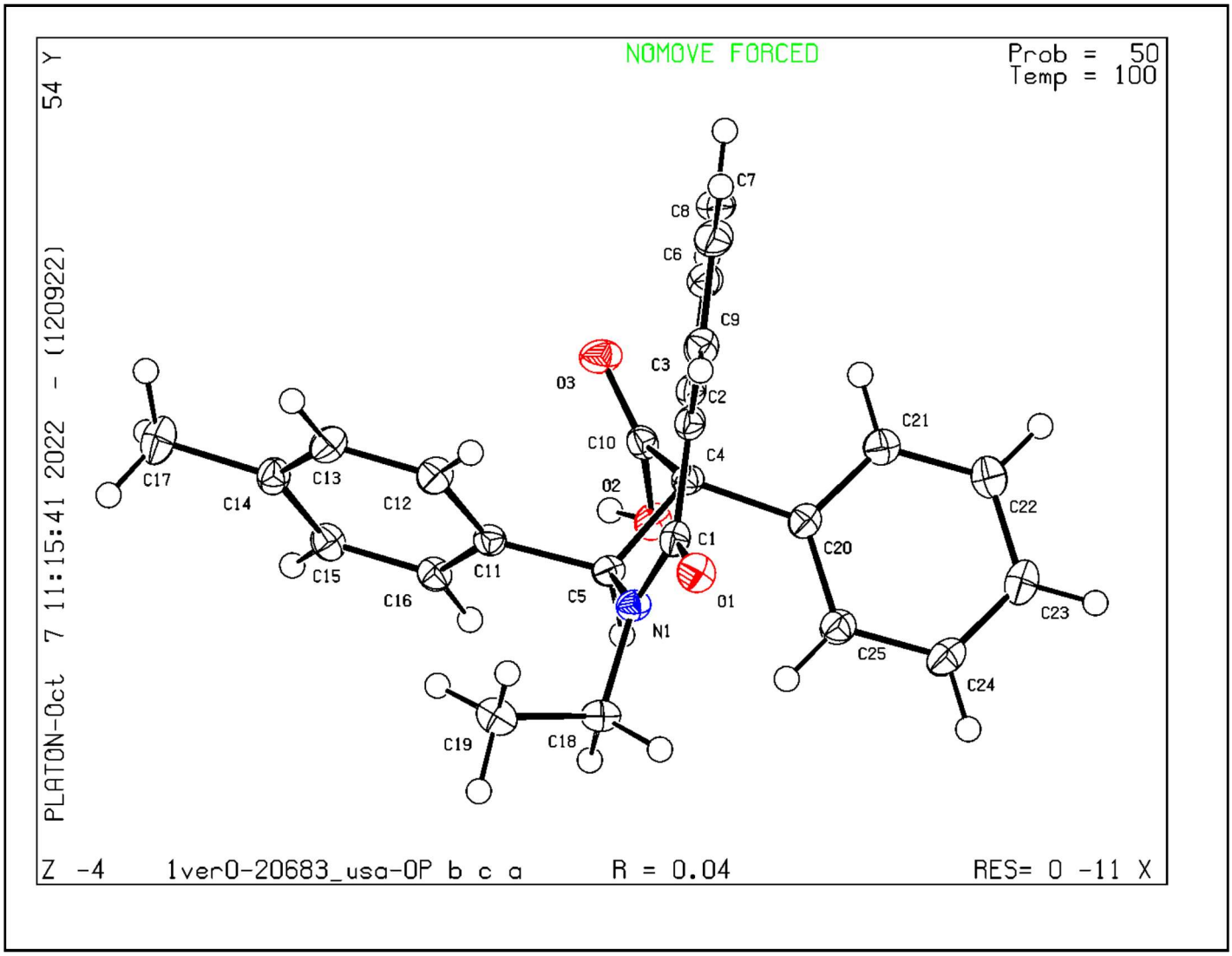

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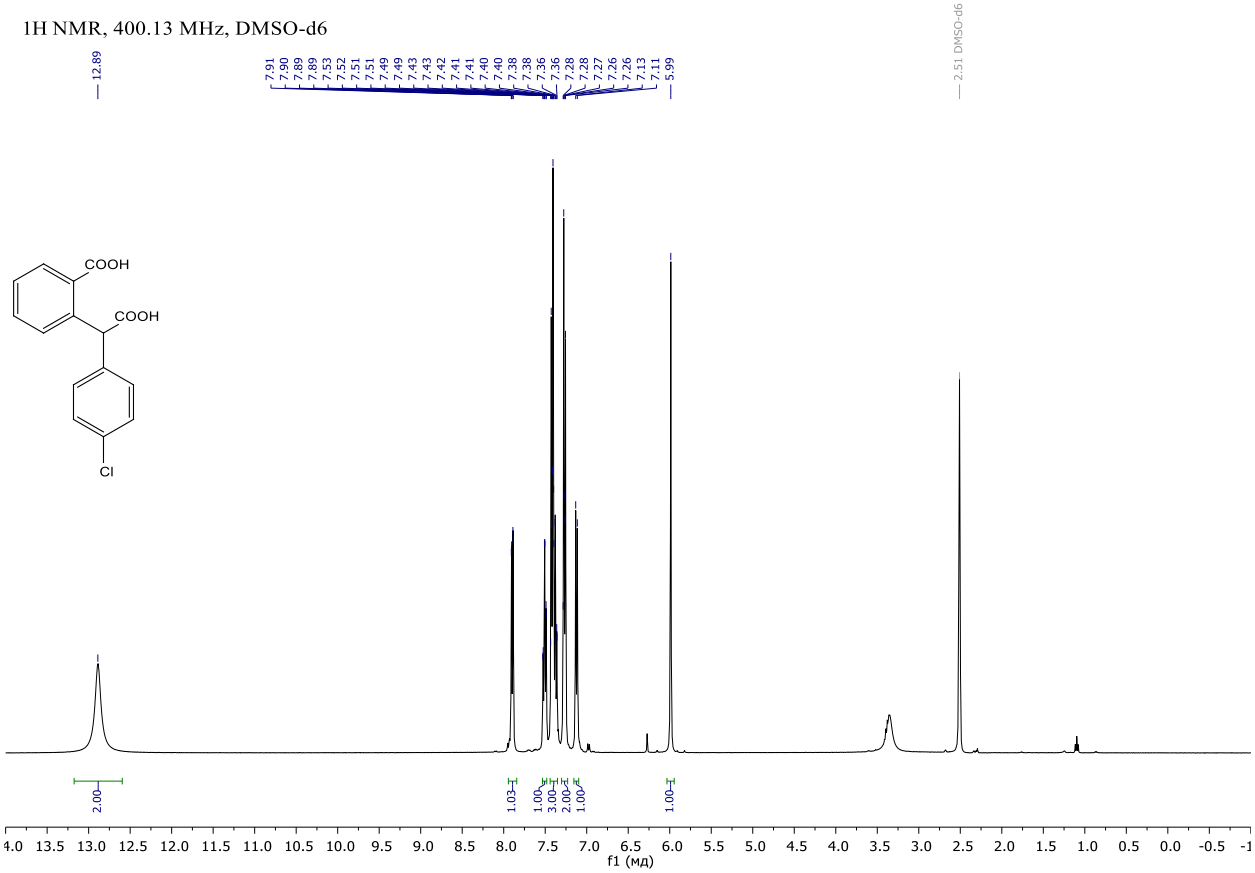
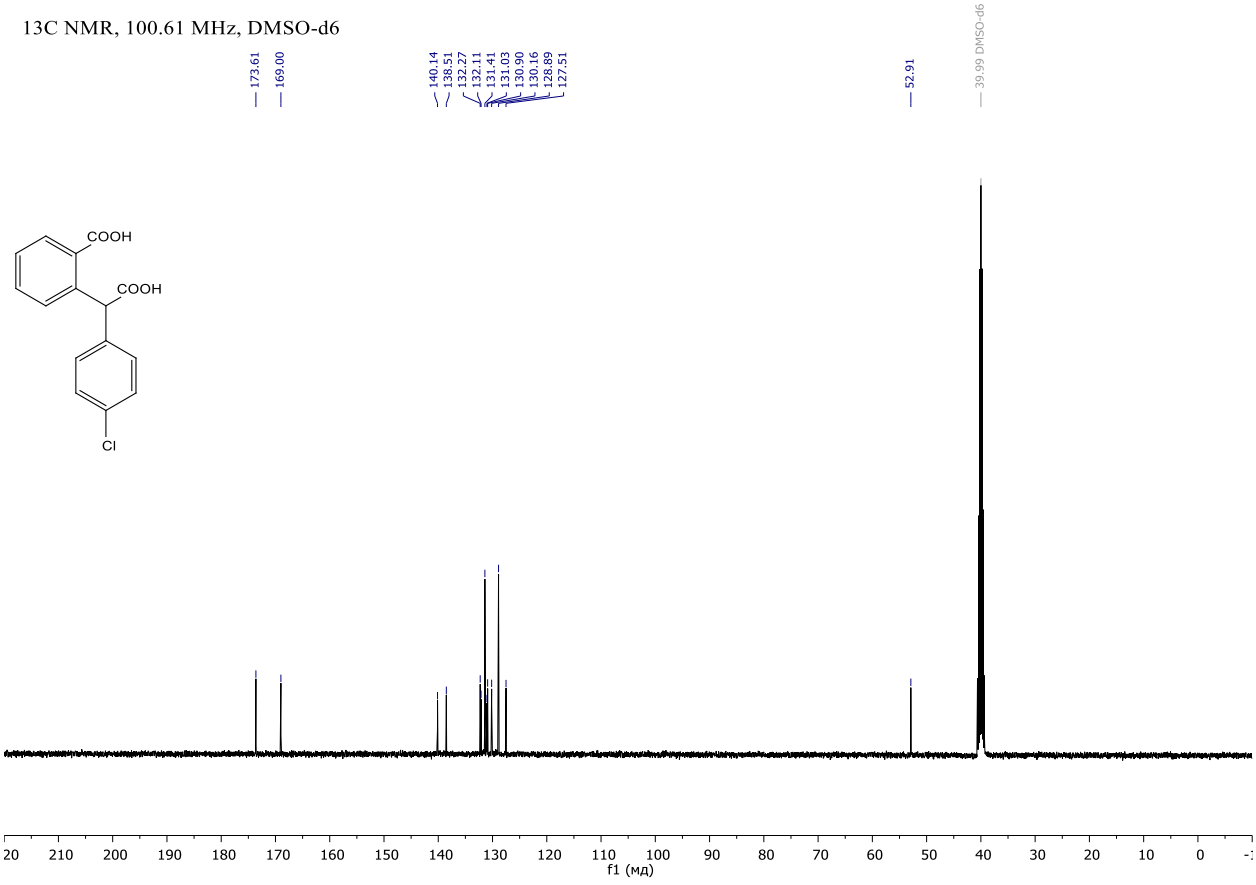
3. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra

^{1}H and ^{13}C NMR spectra of compound **10a**





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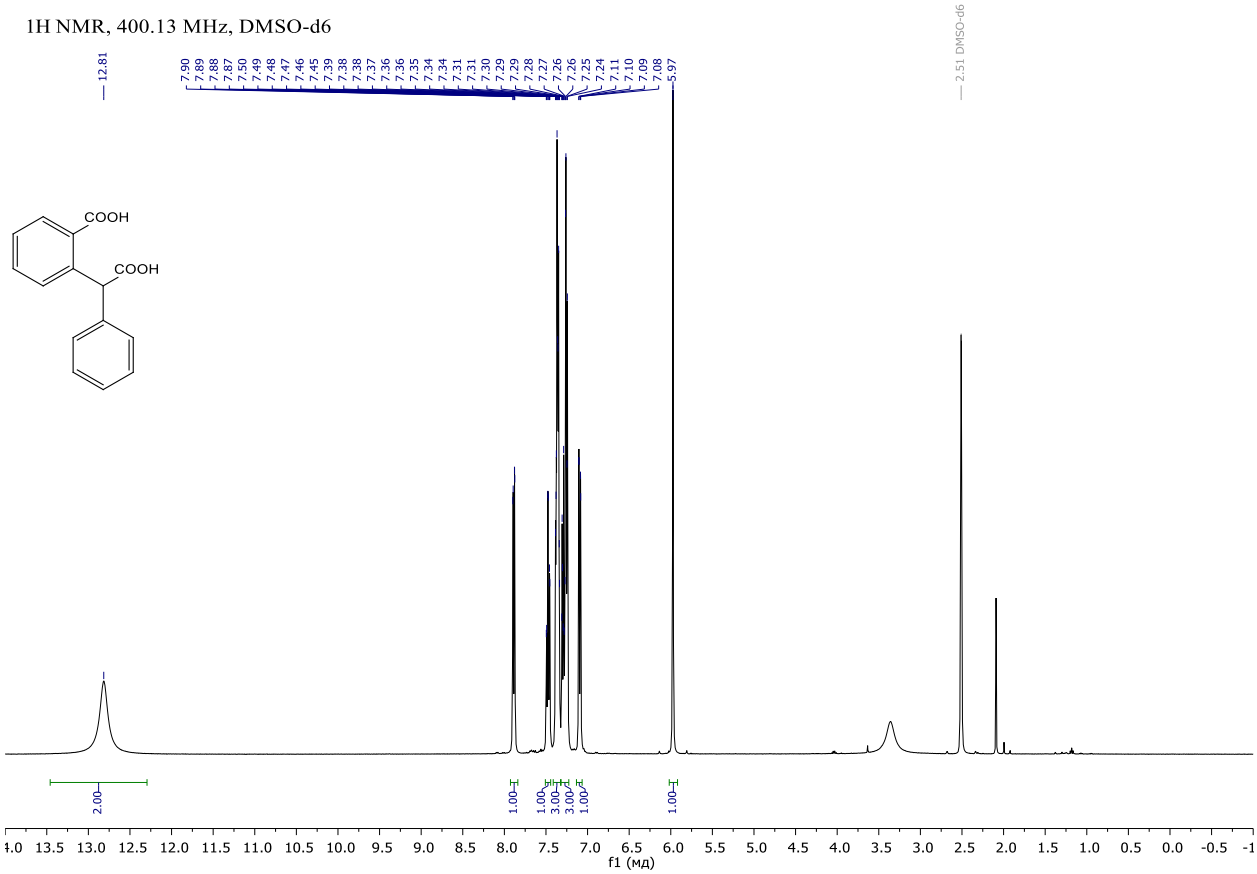
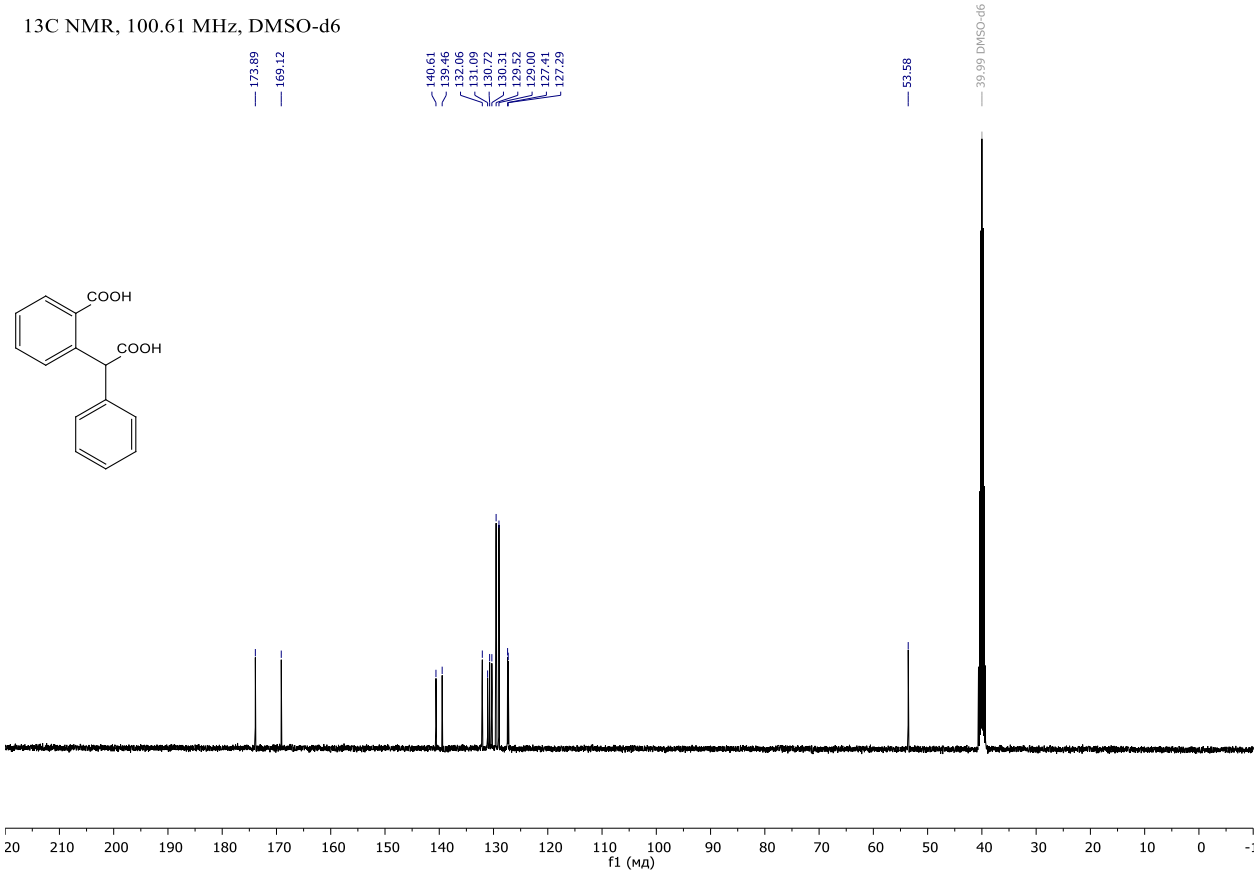
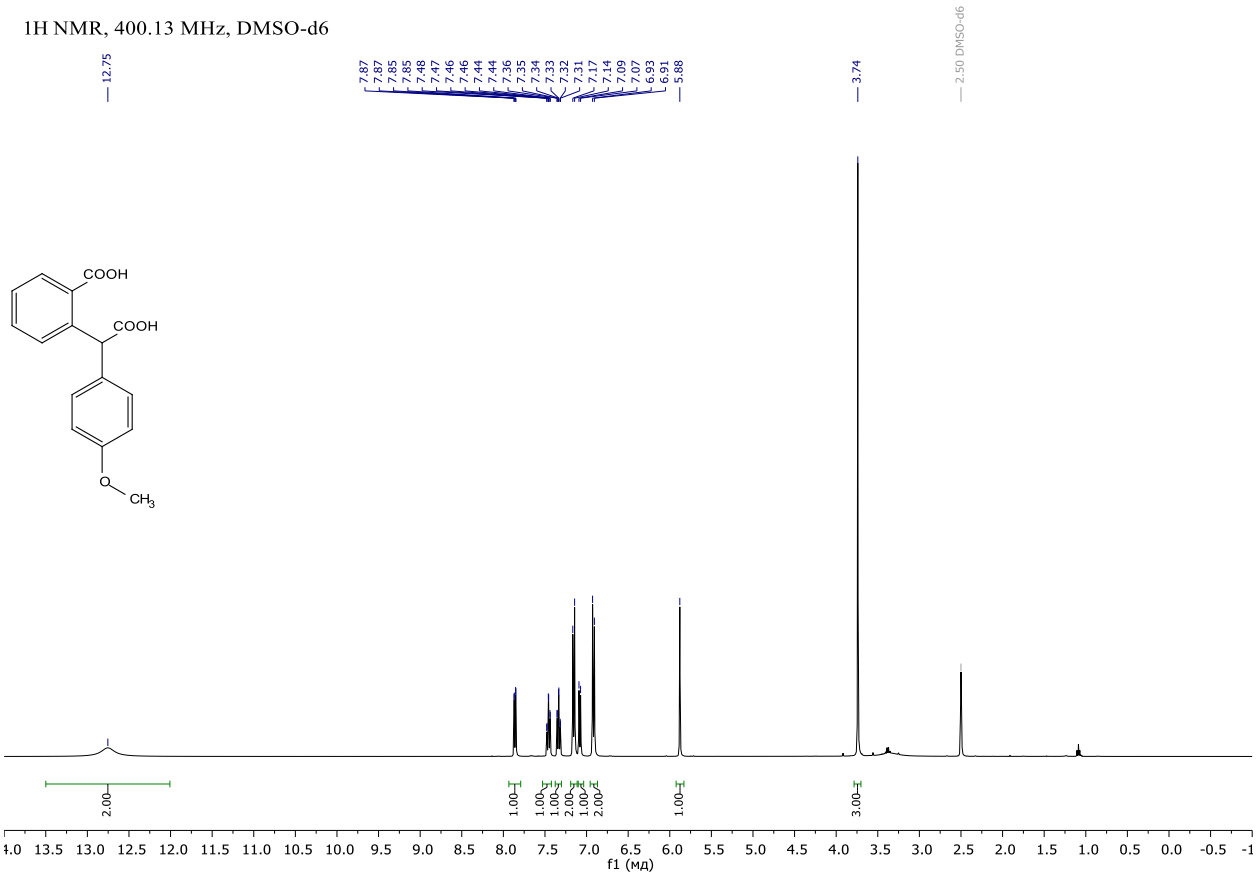
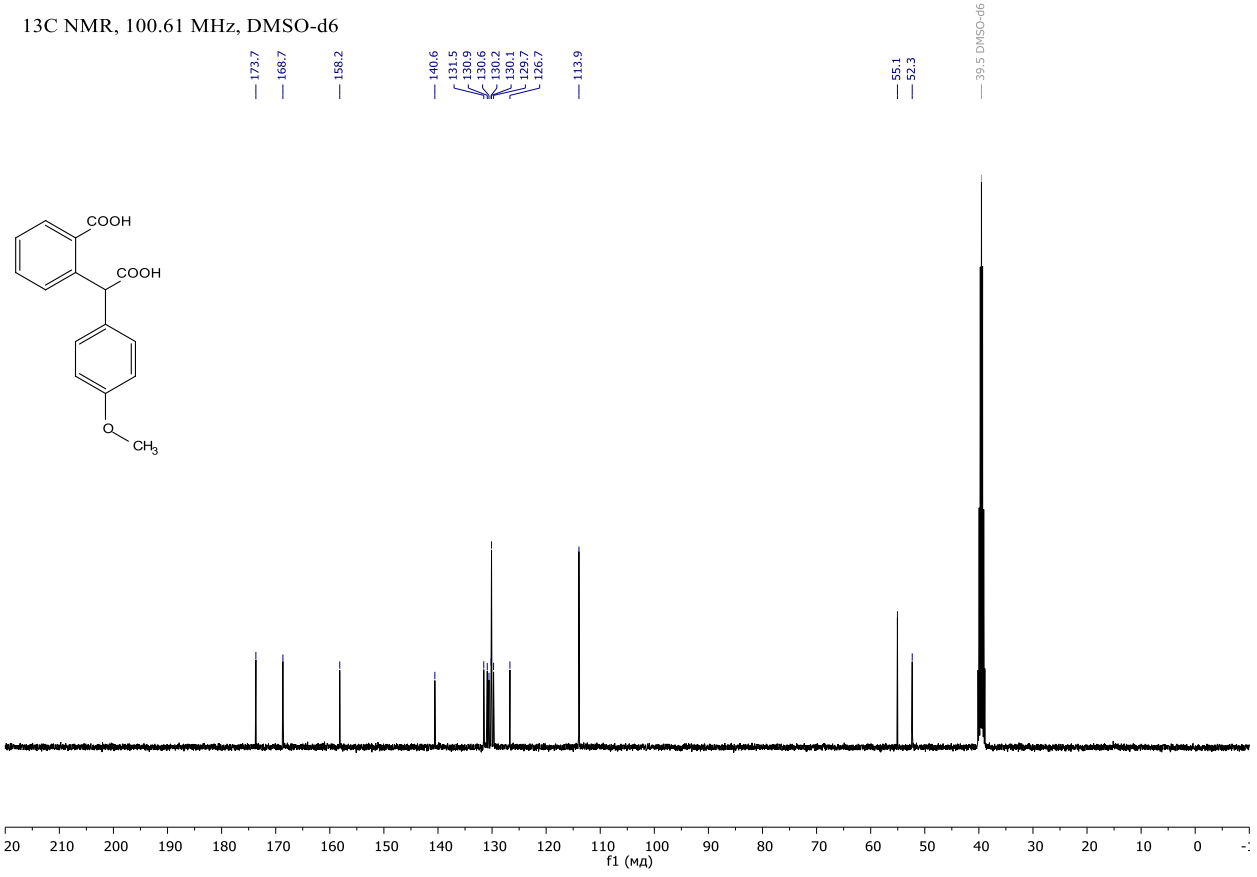




^{1}H and ^{13}C NMR spectra of compound **10c**





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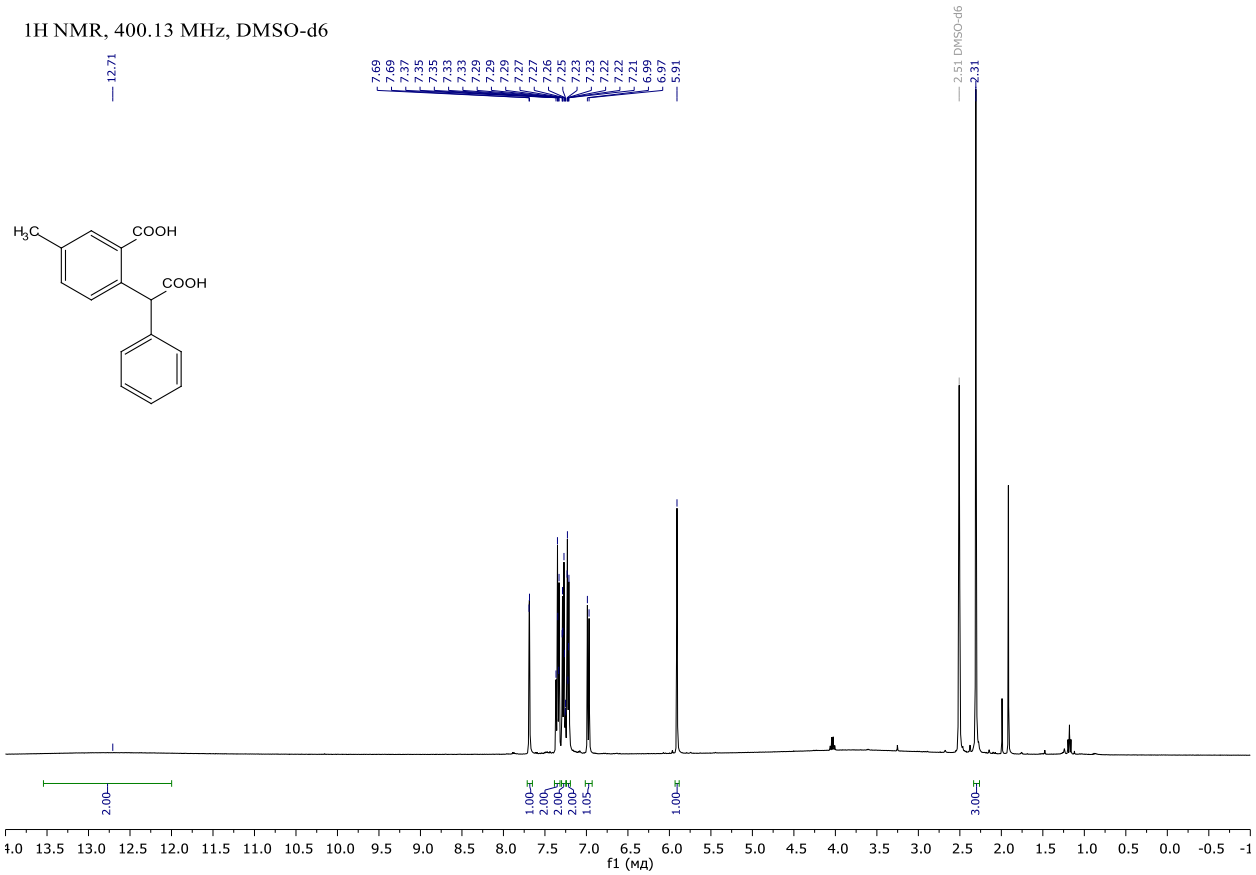
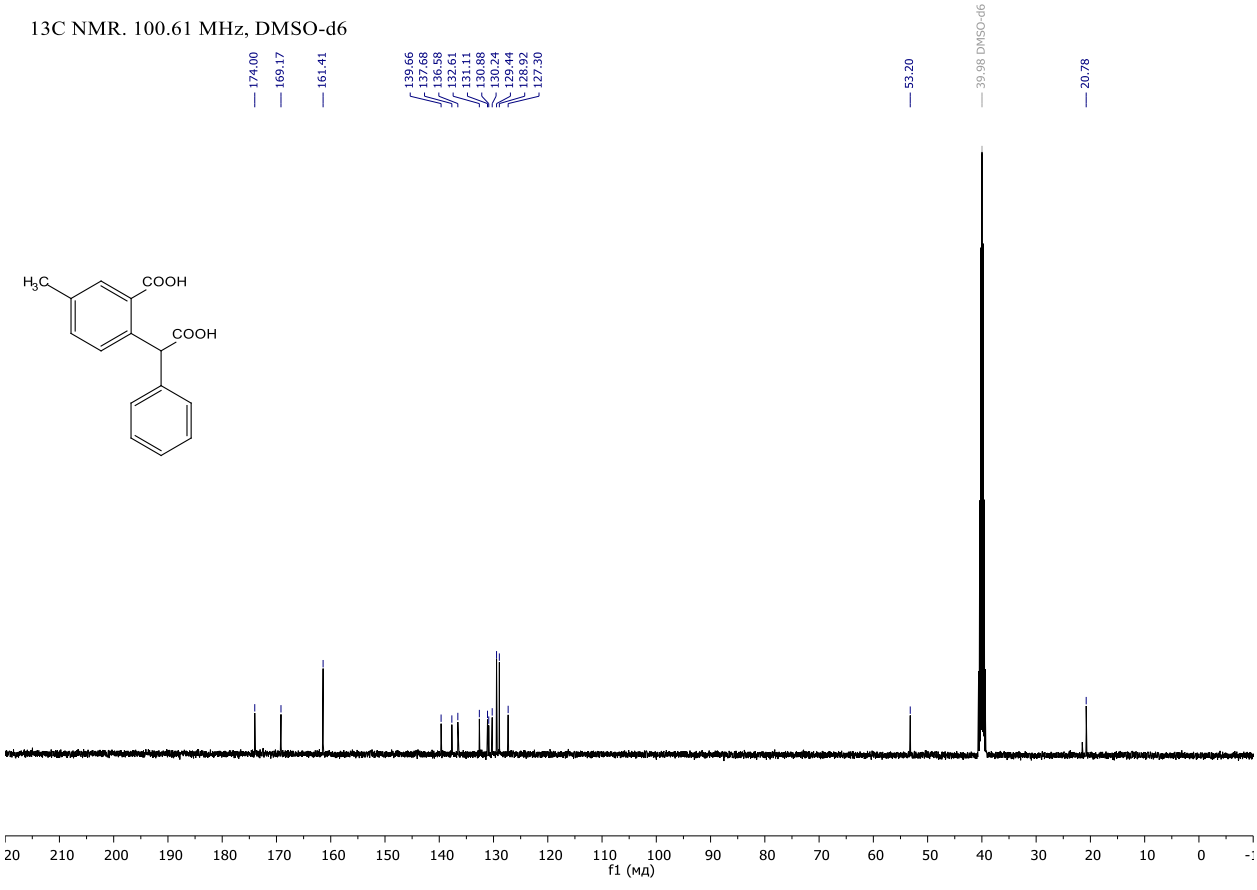
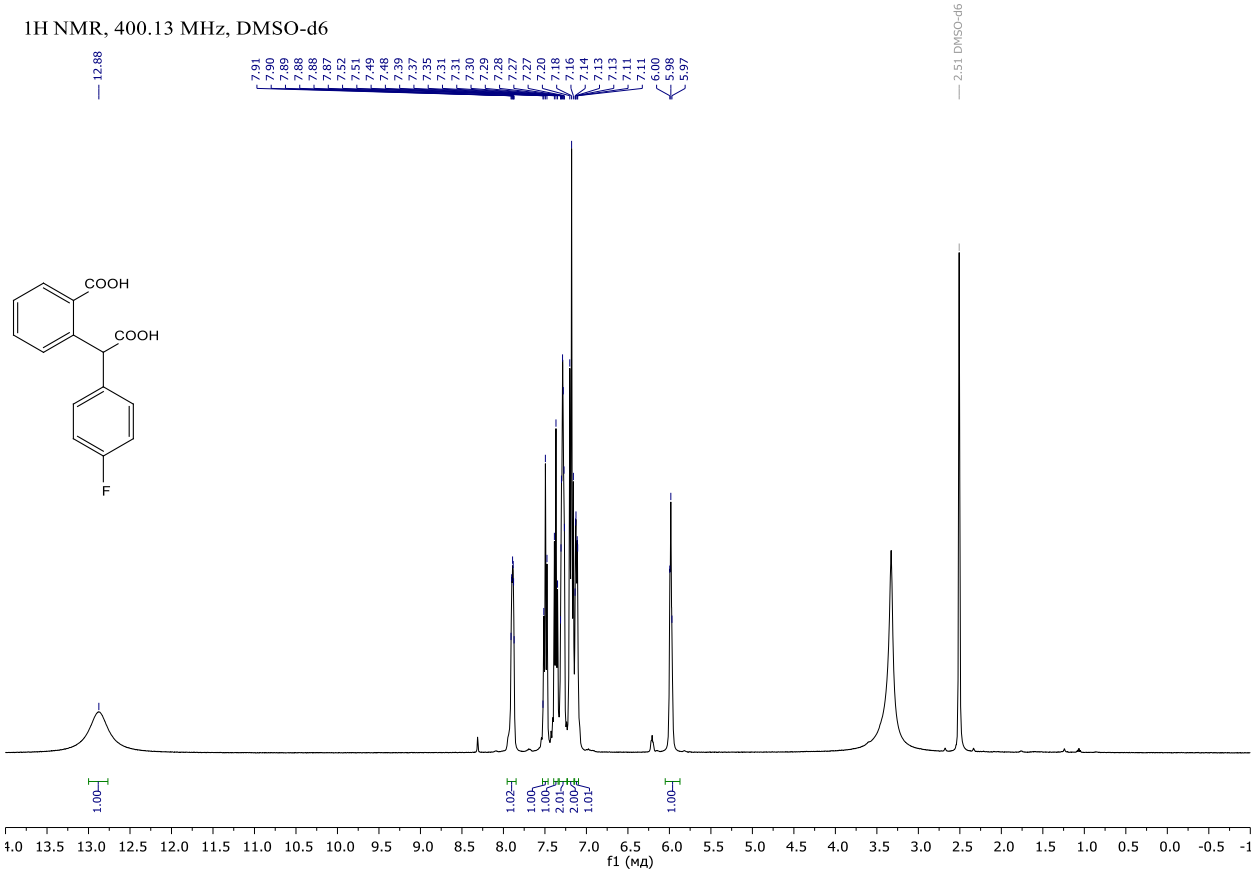
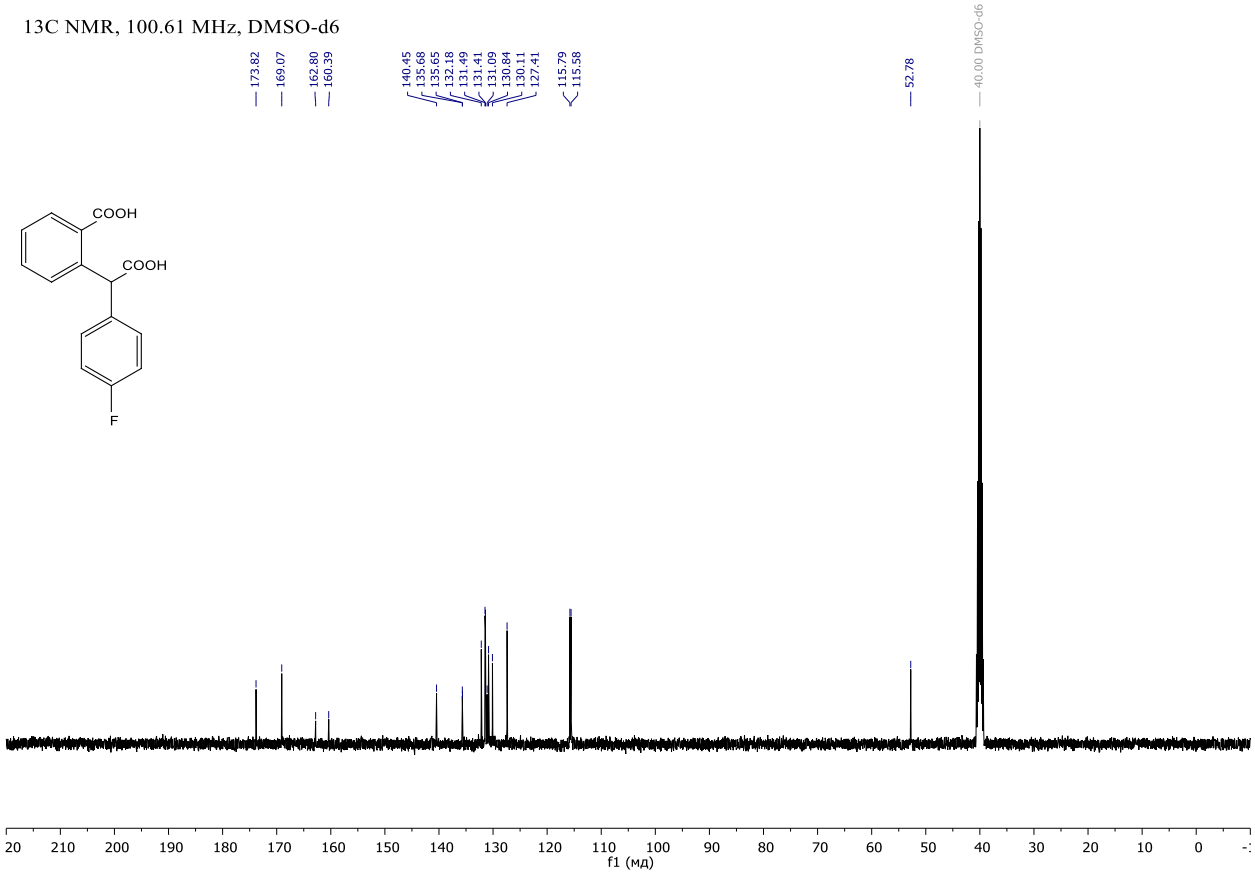


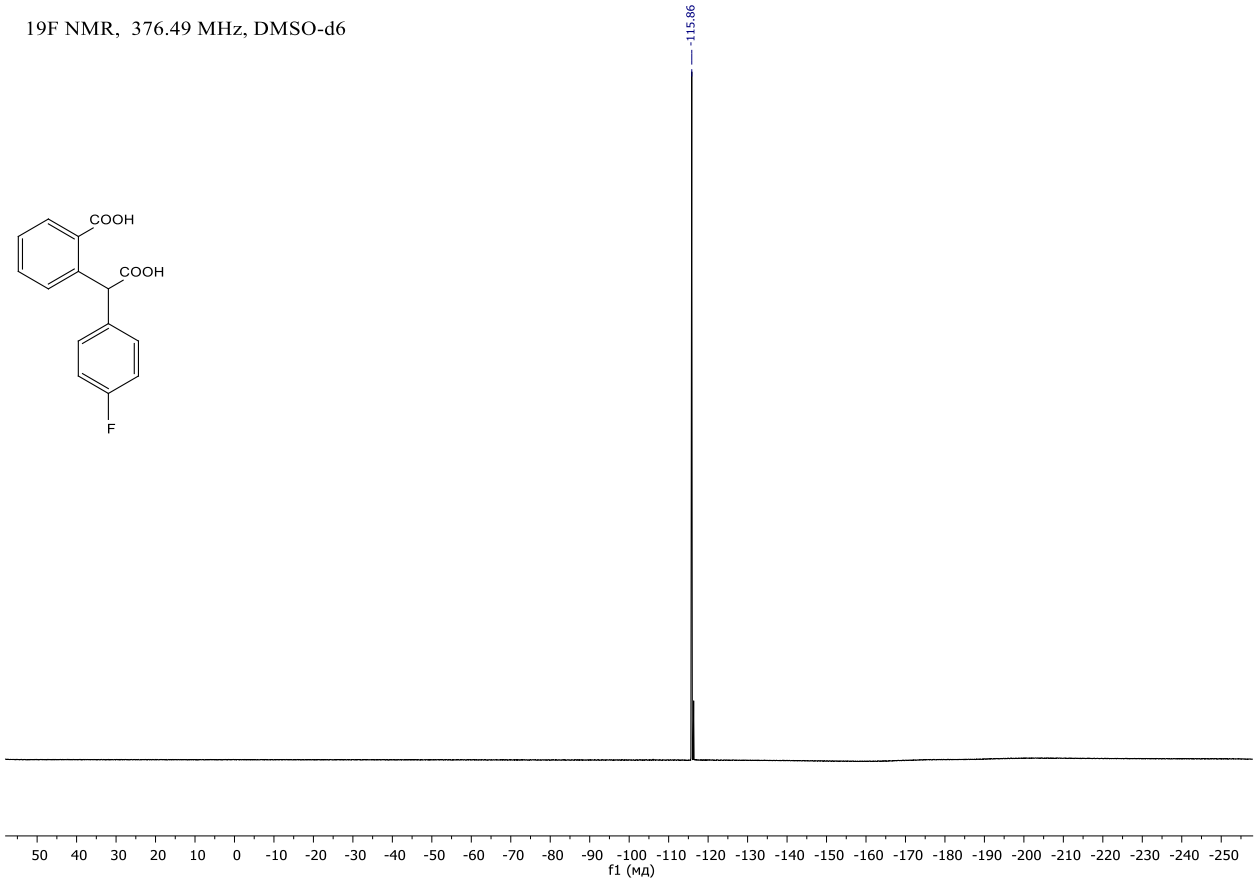


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **10e**





19F NMR, 376.49 MHz, DMSO-d6



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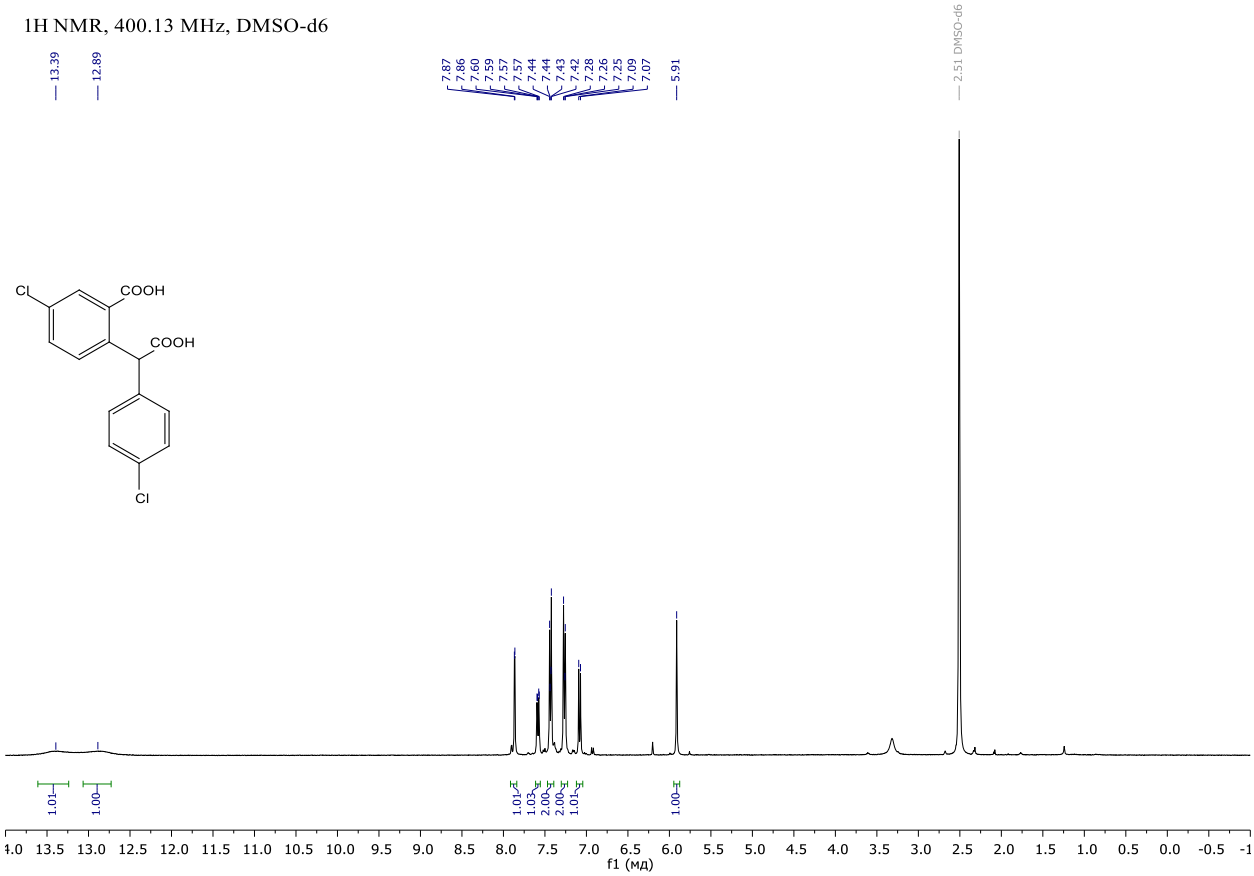
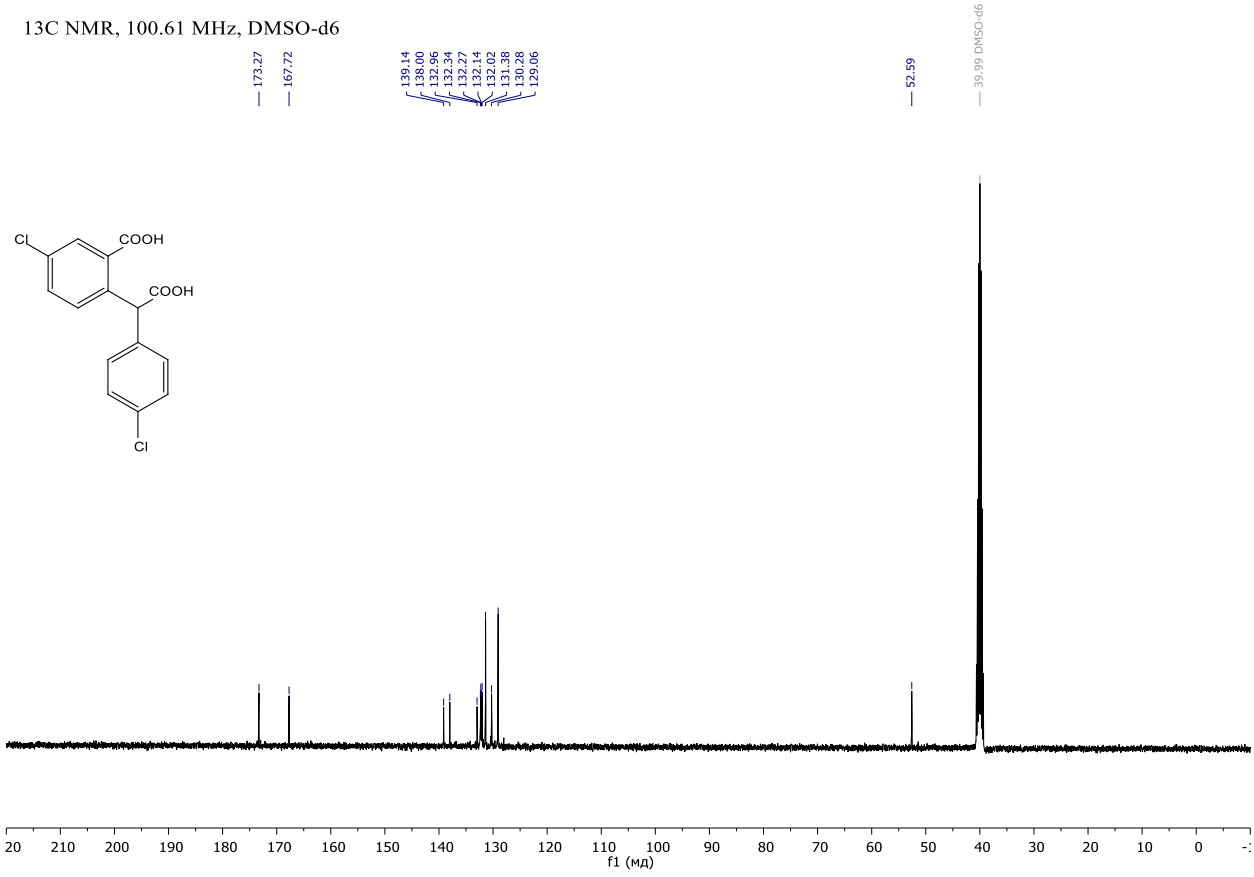
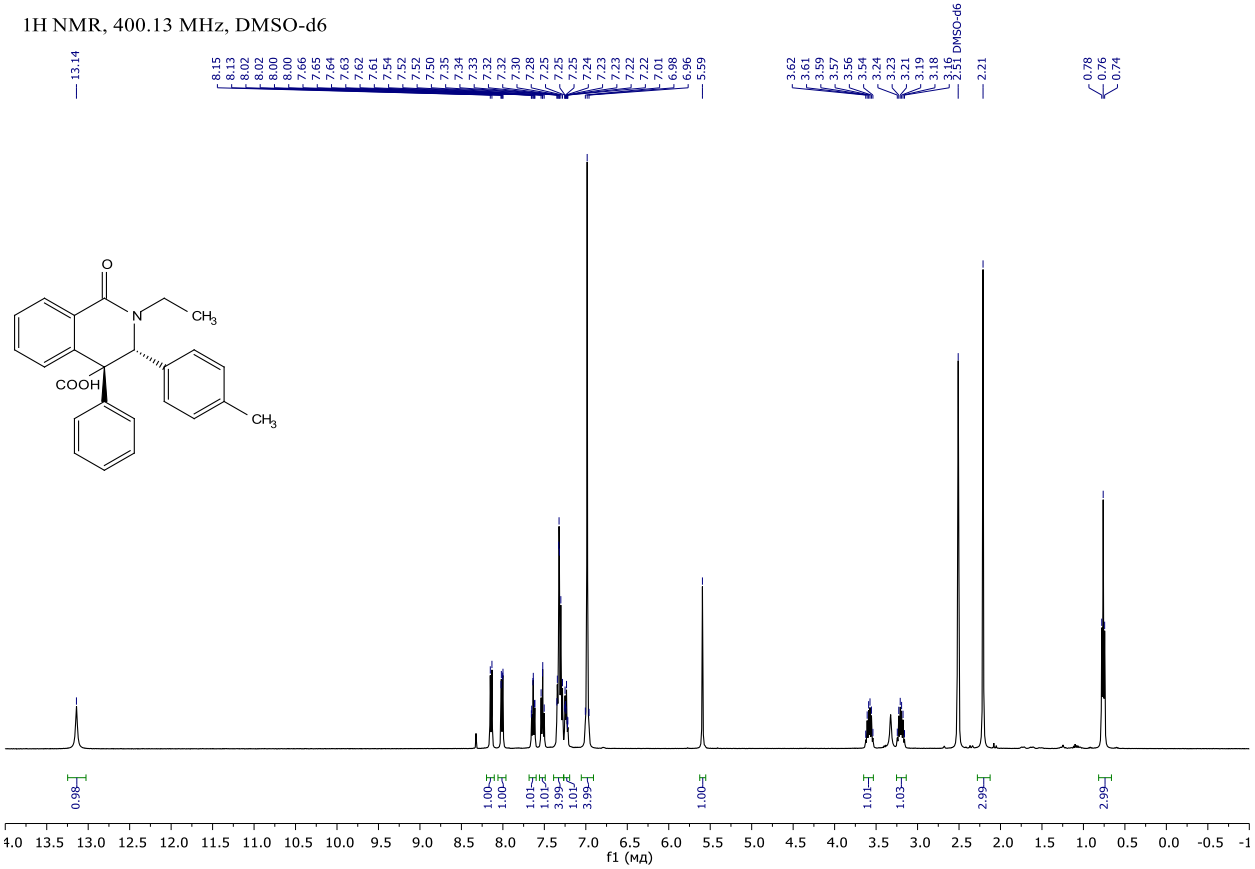
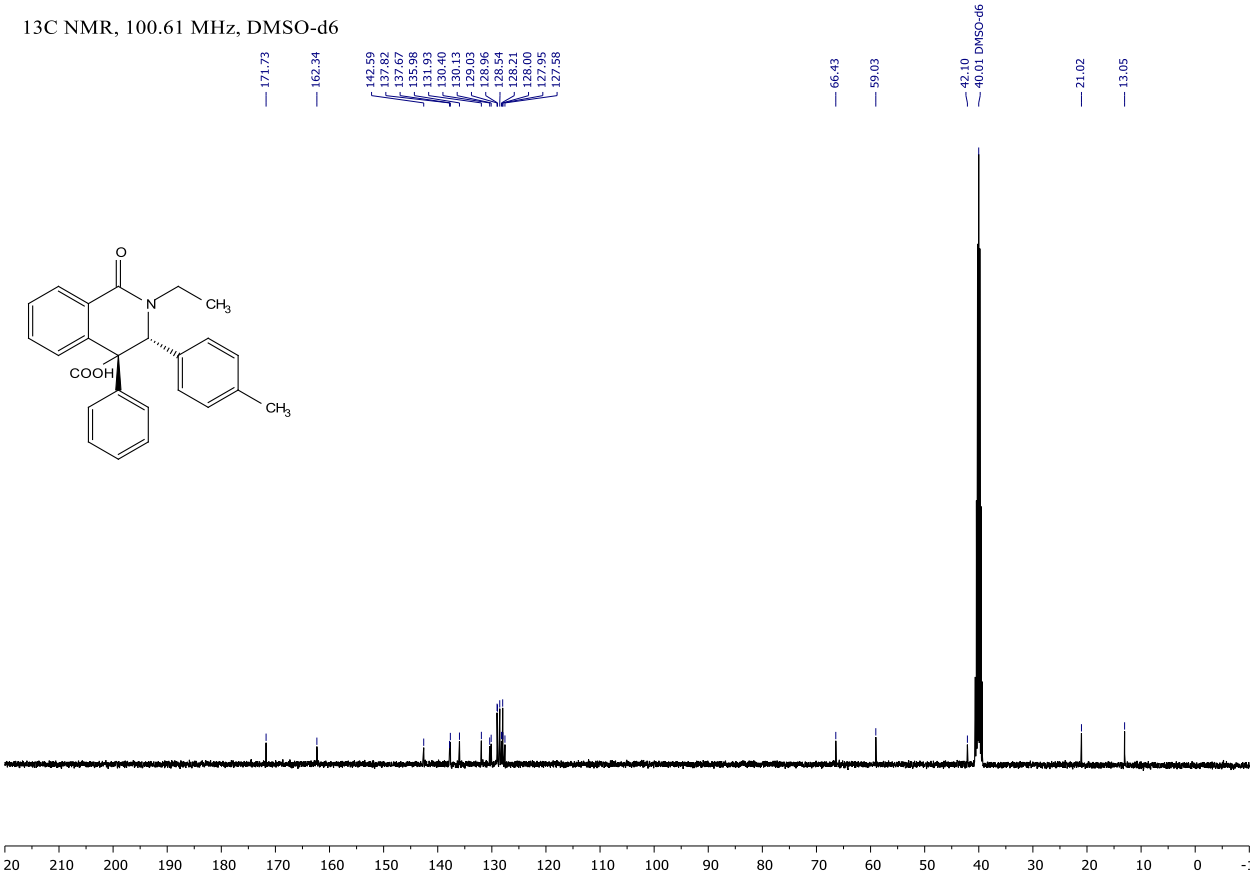




^{1}H and ^{13}C NMR spectra of compound **9a**





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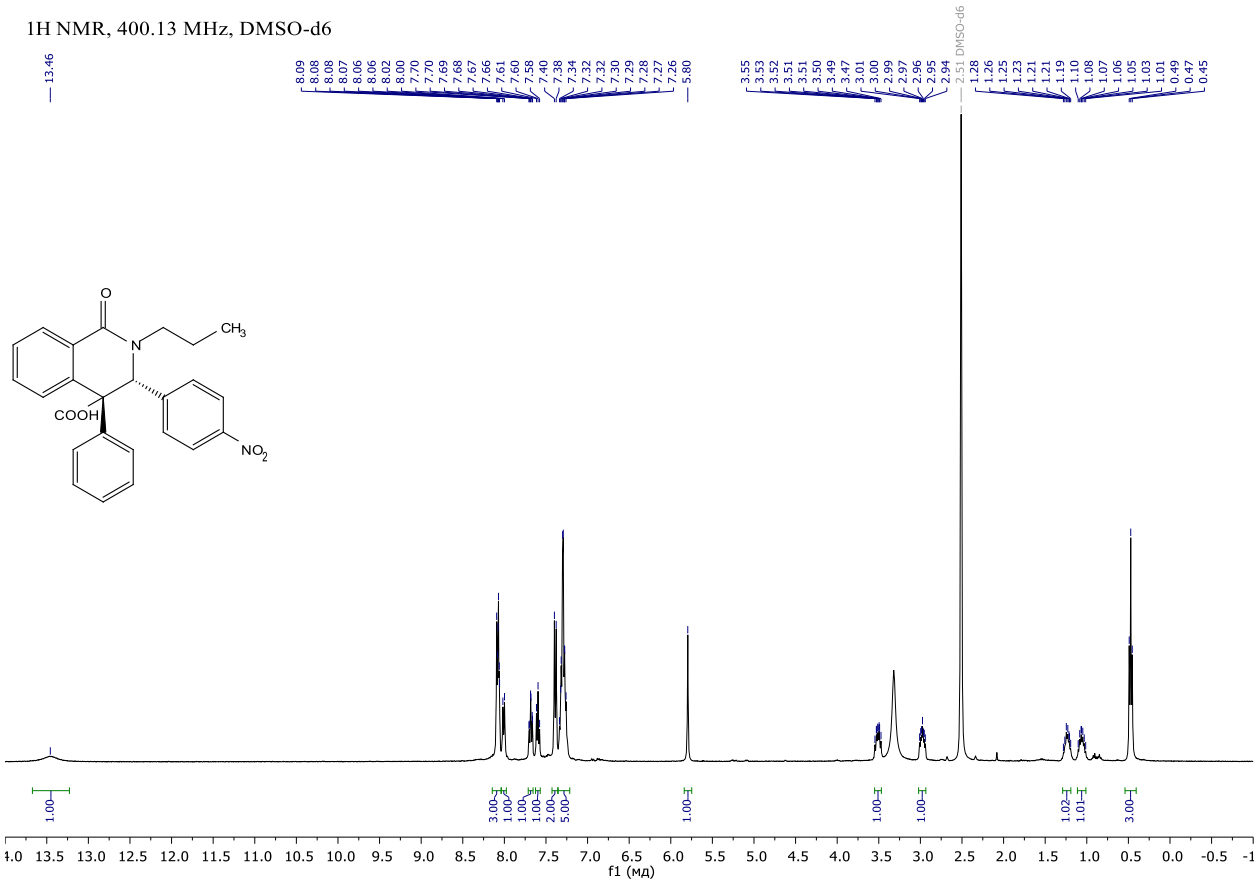

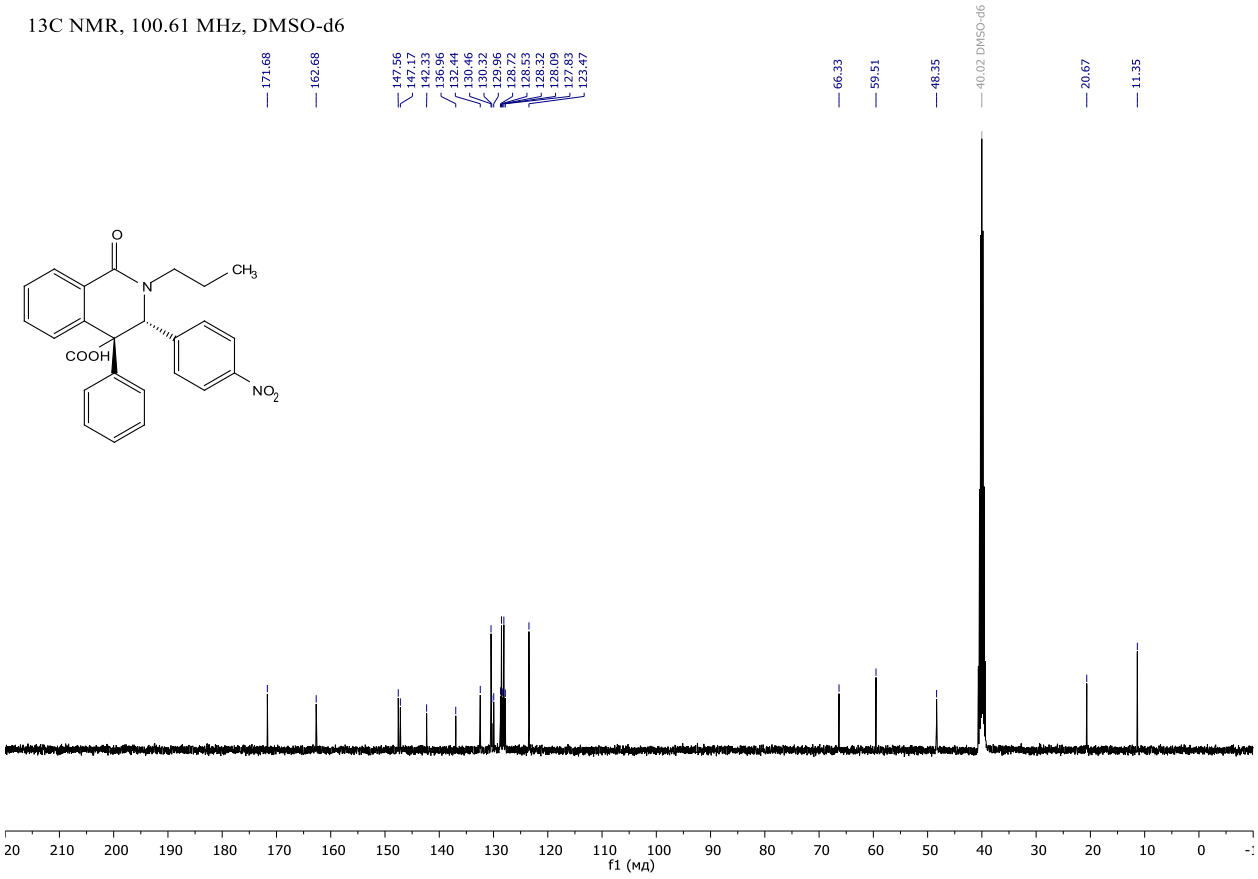

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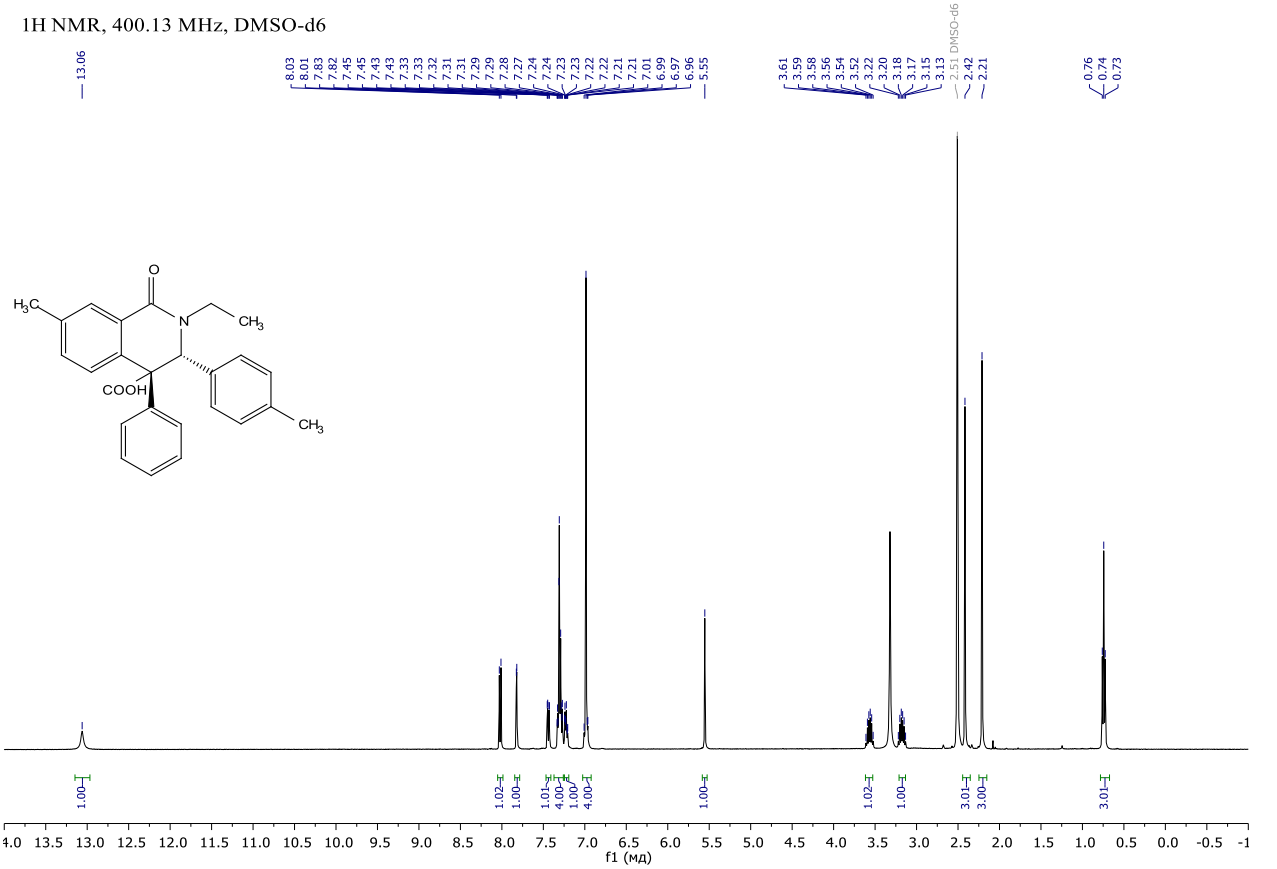

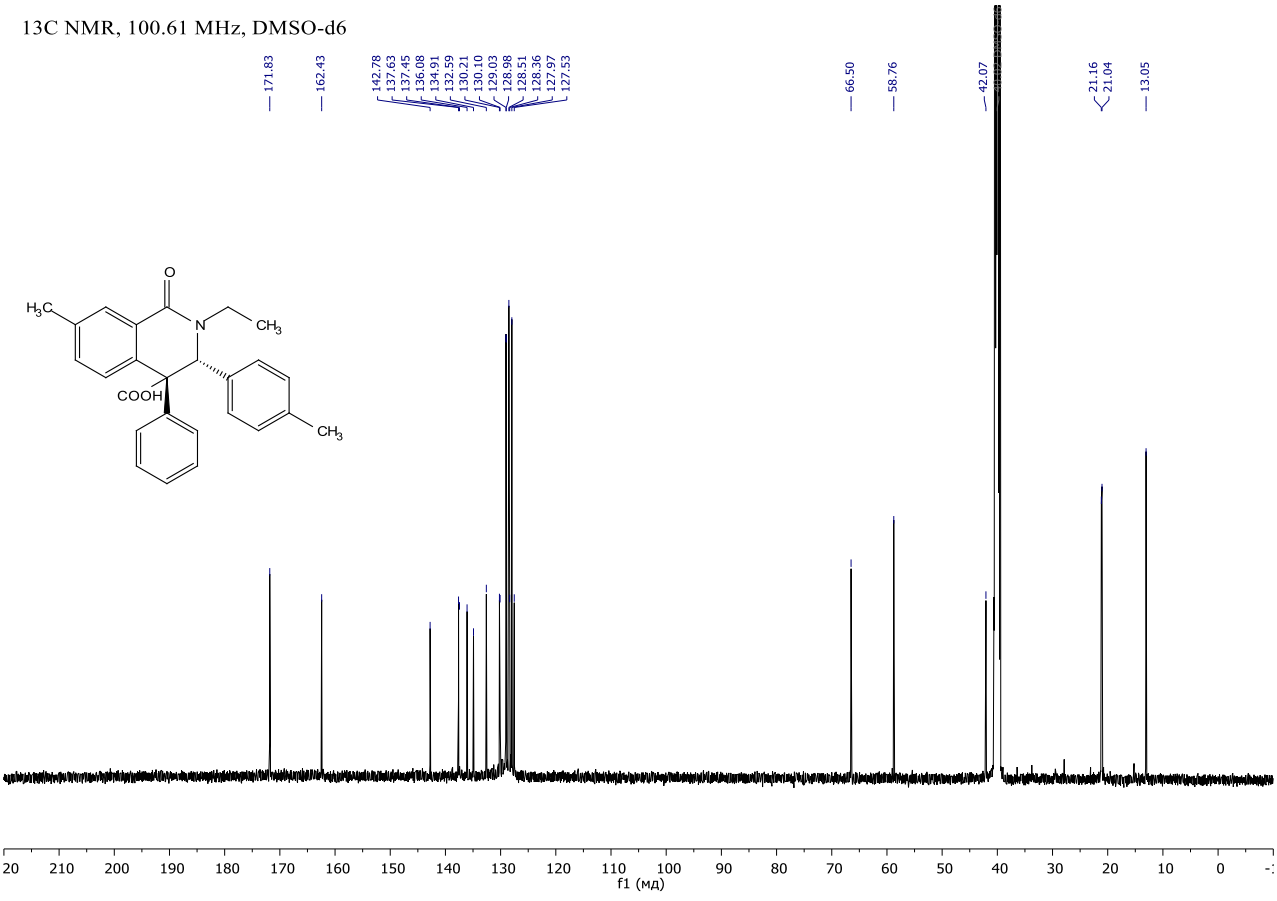

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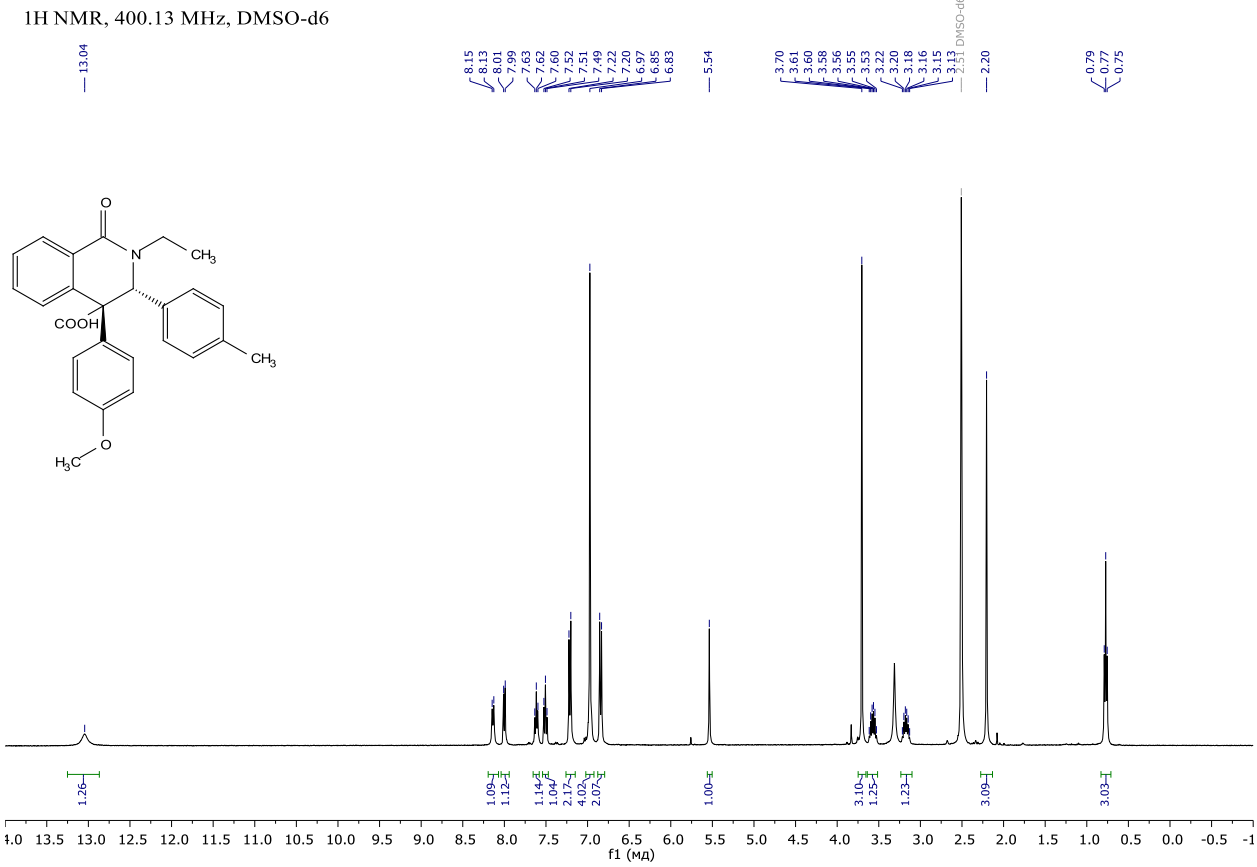

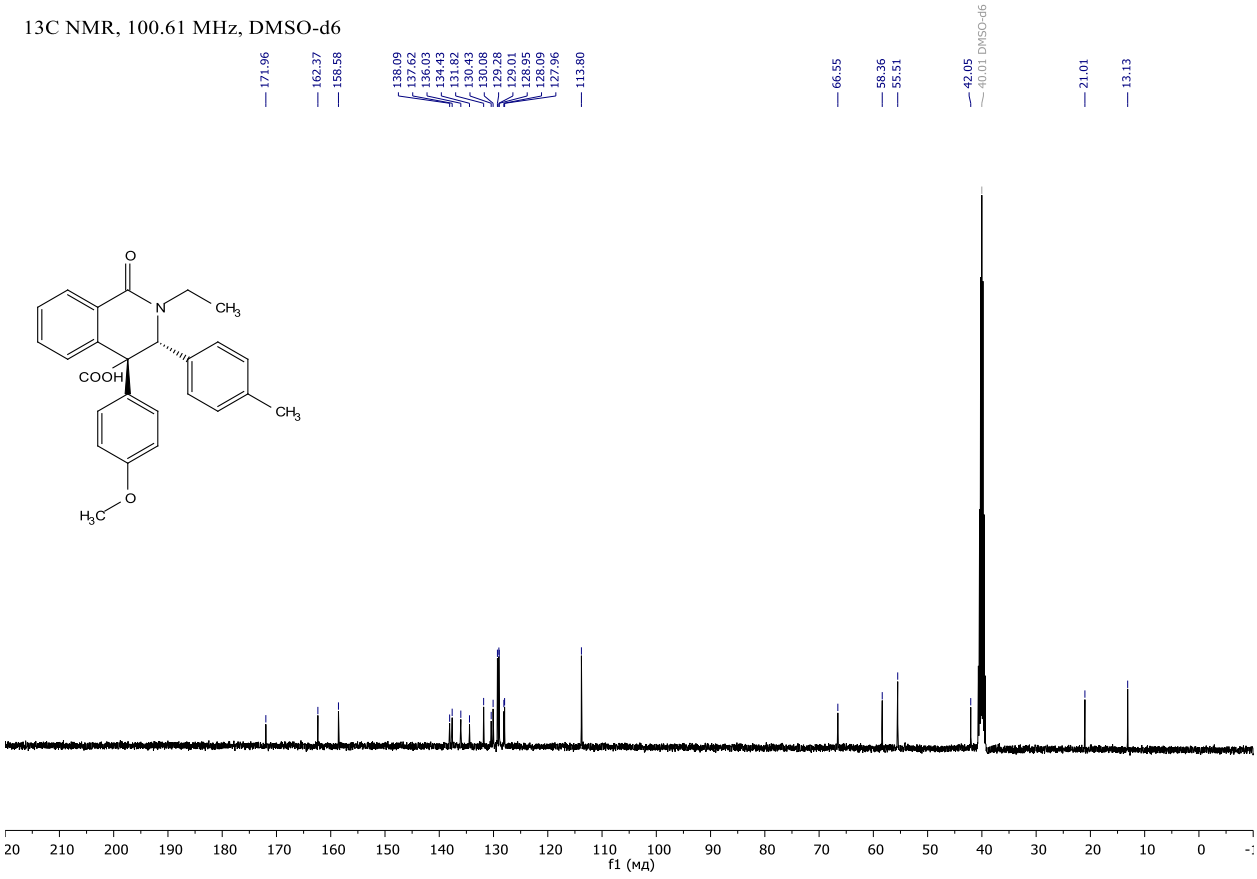

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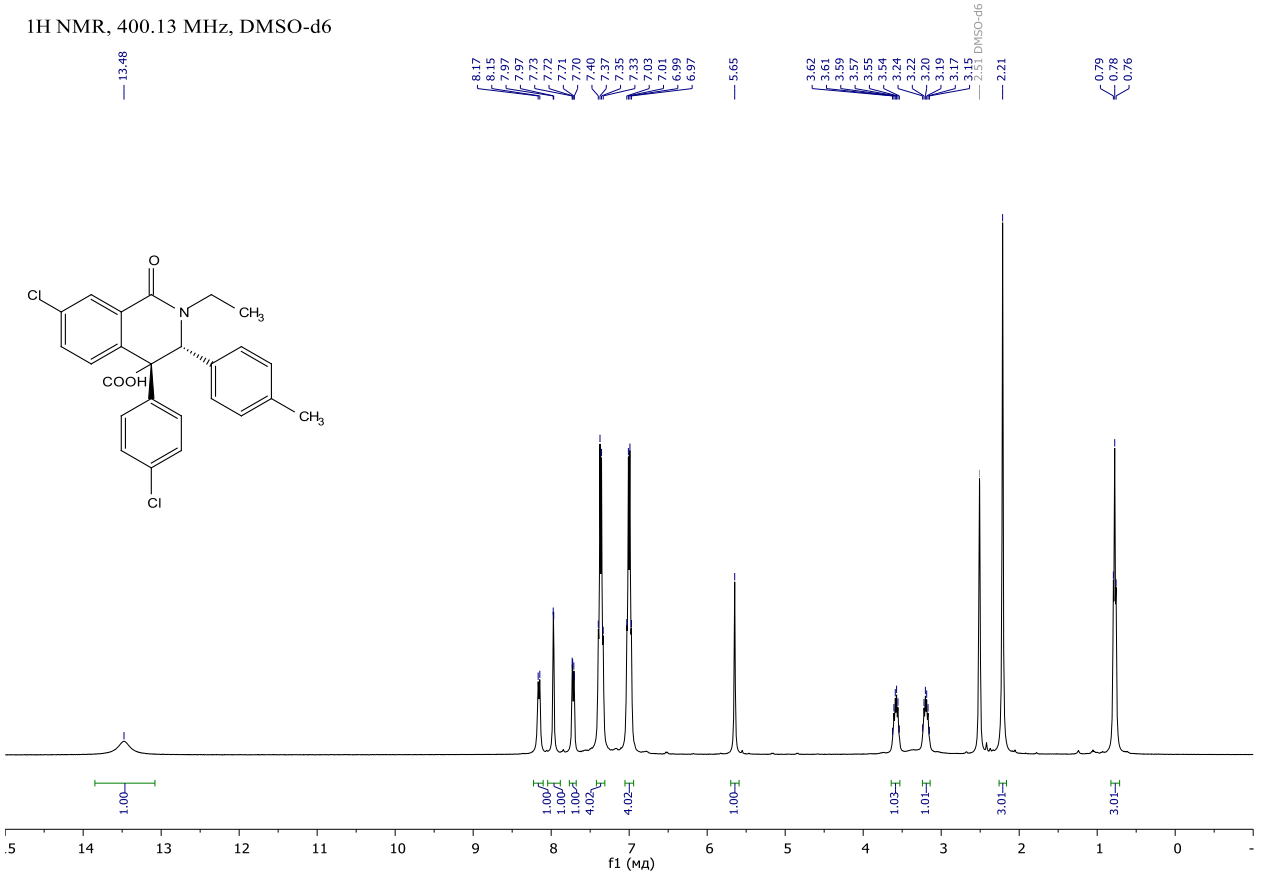
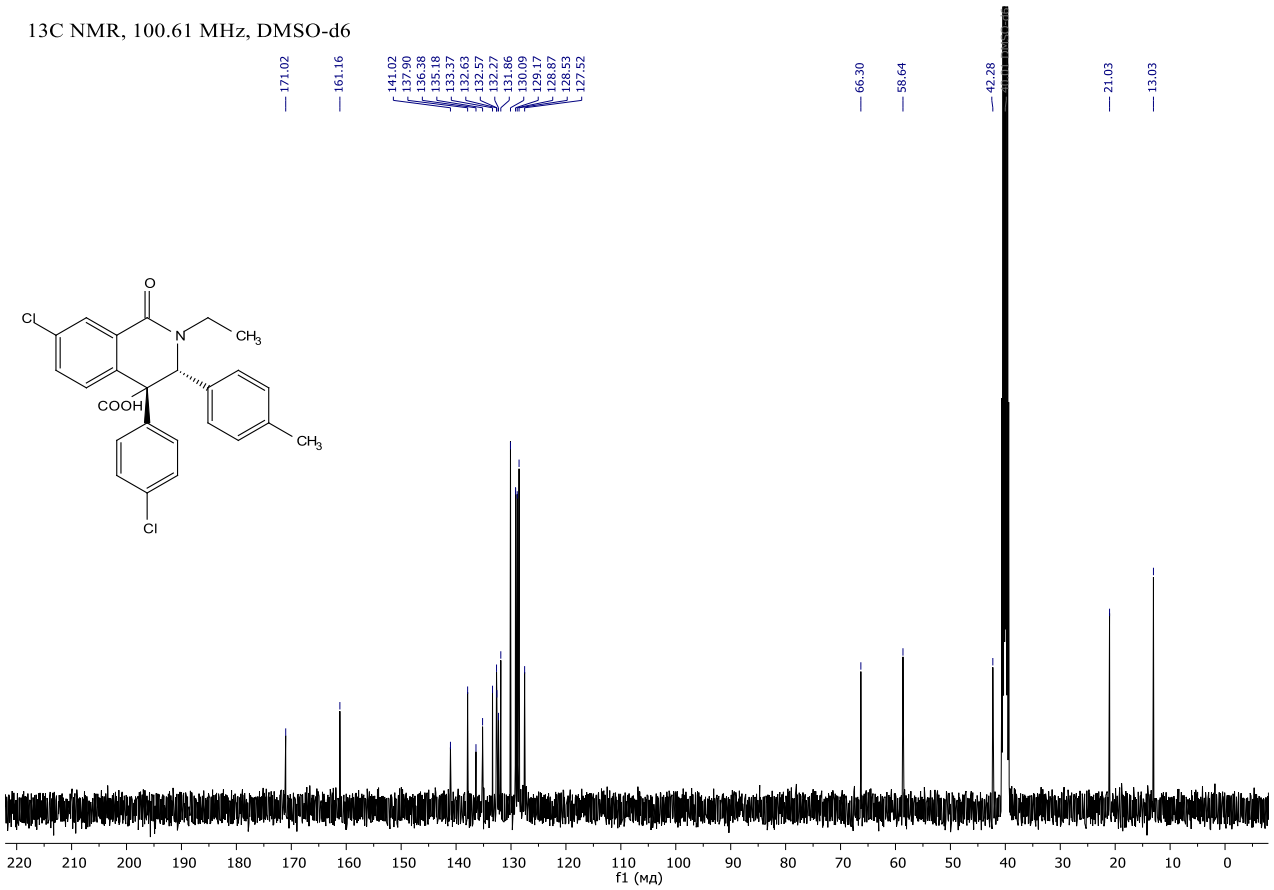
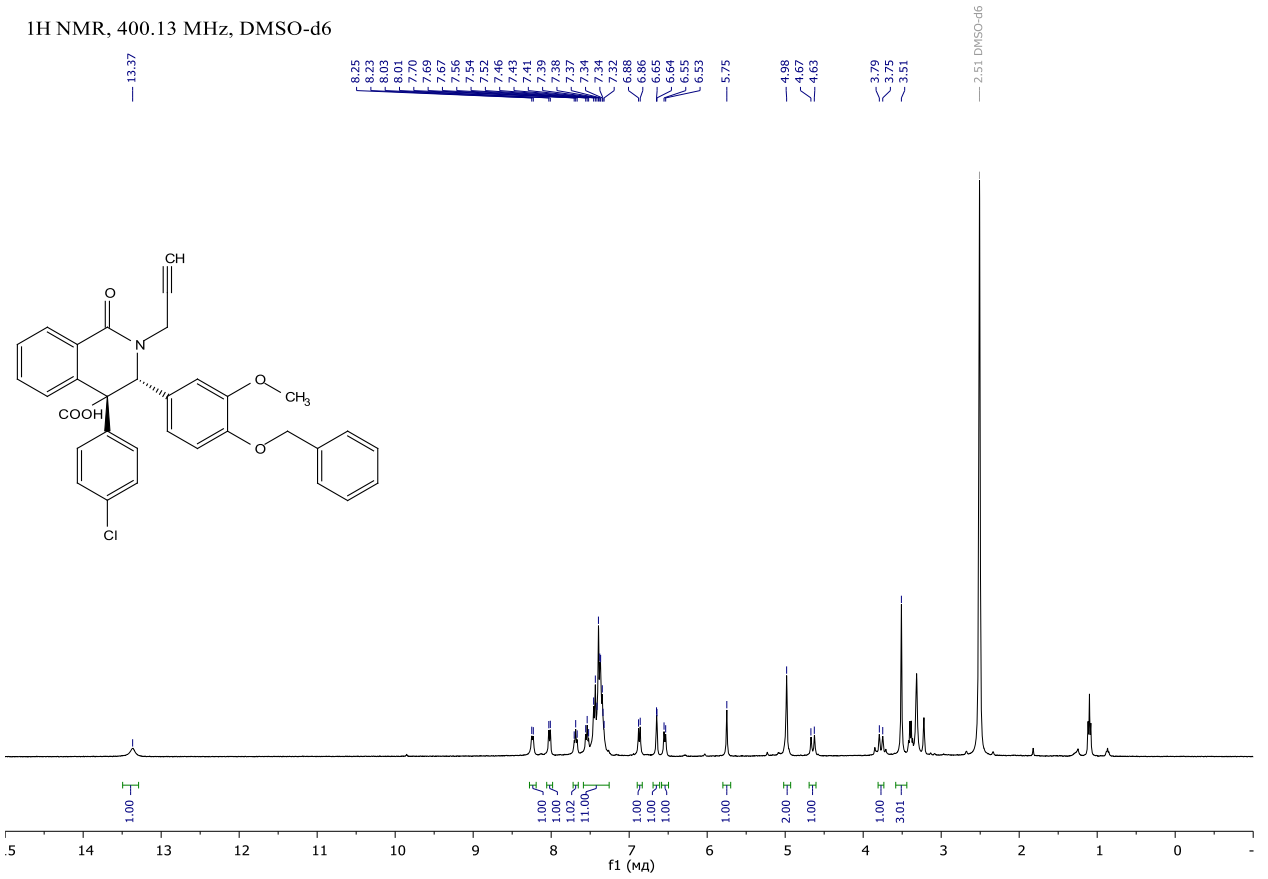
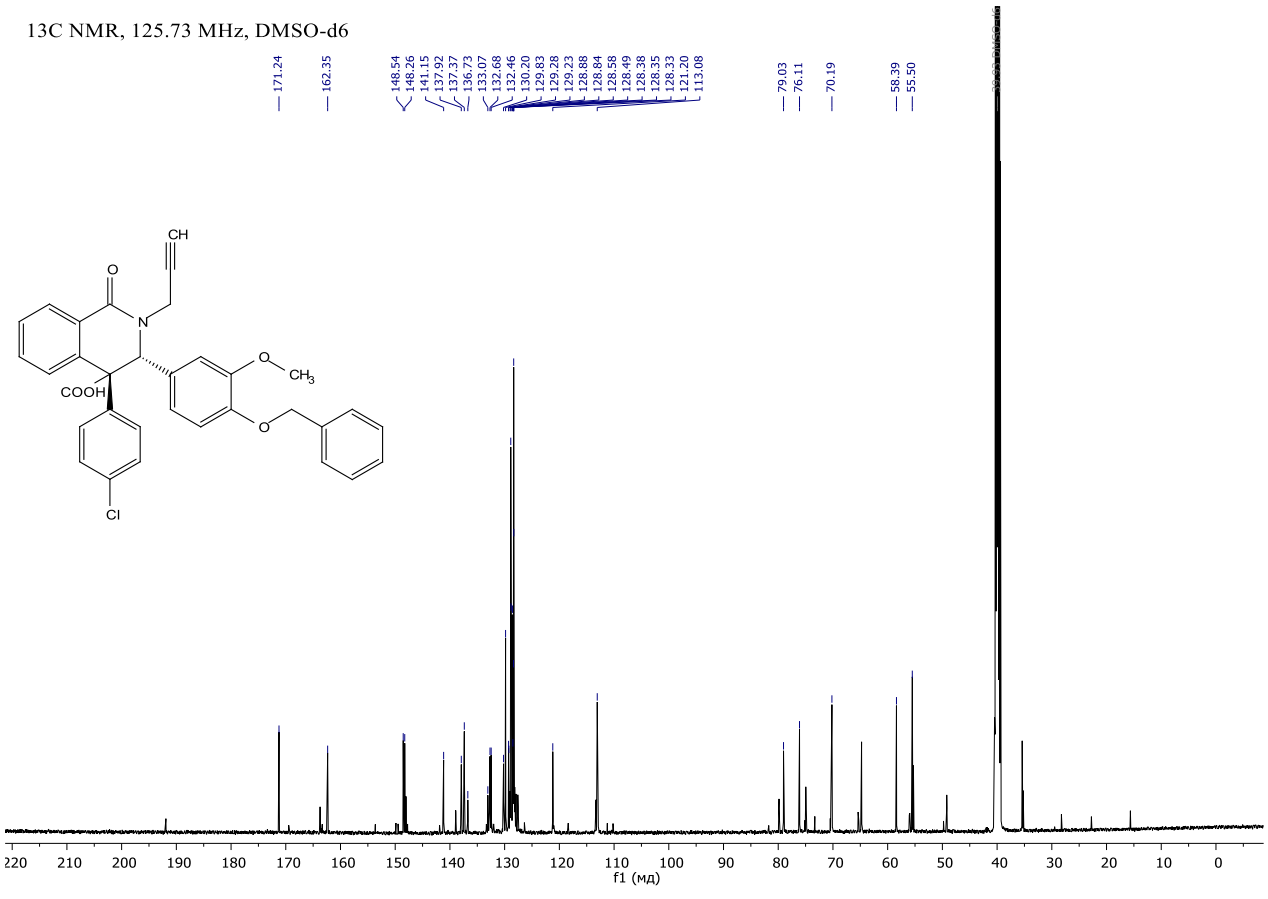


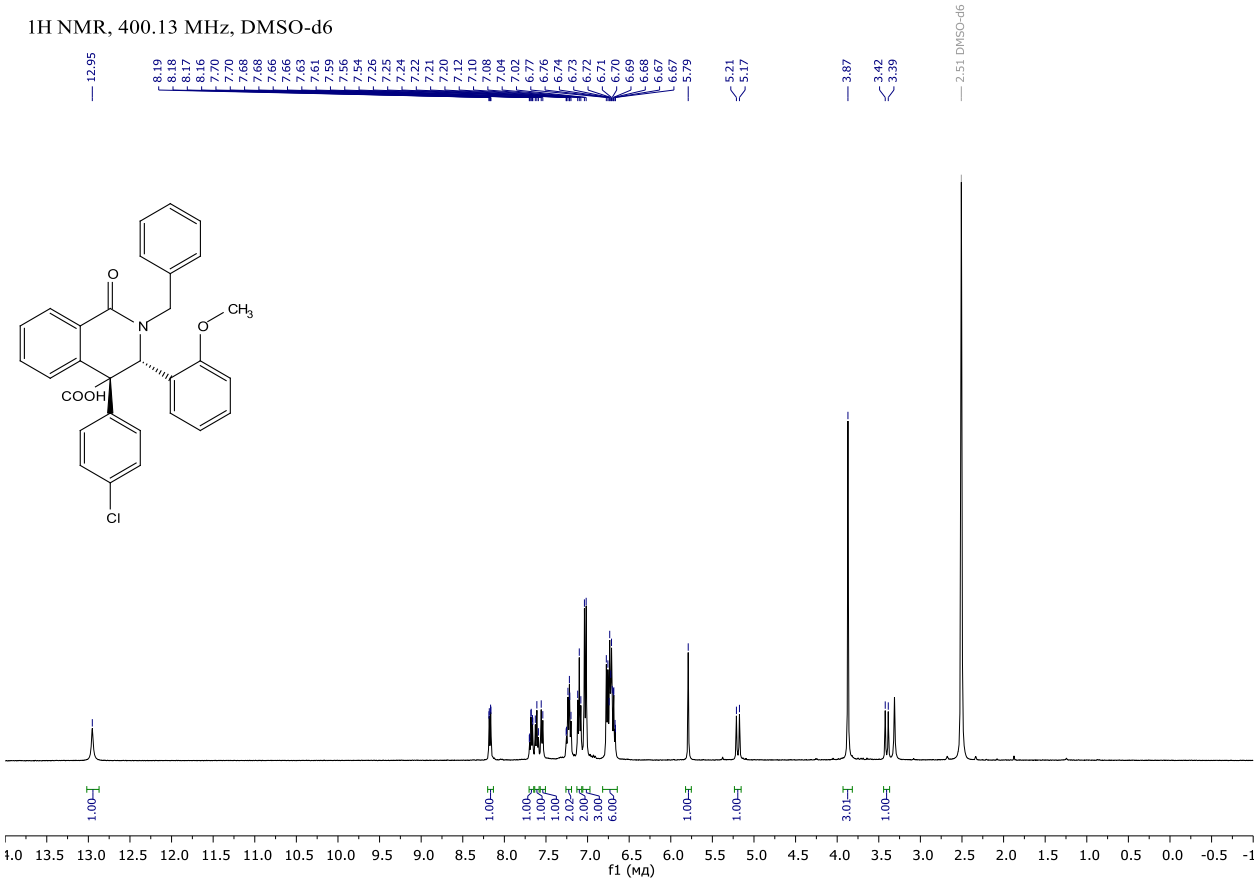


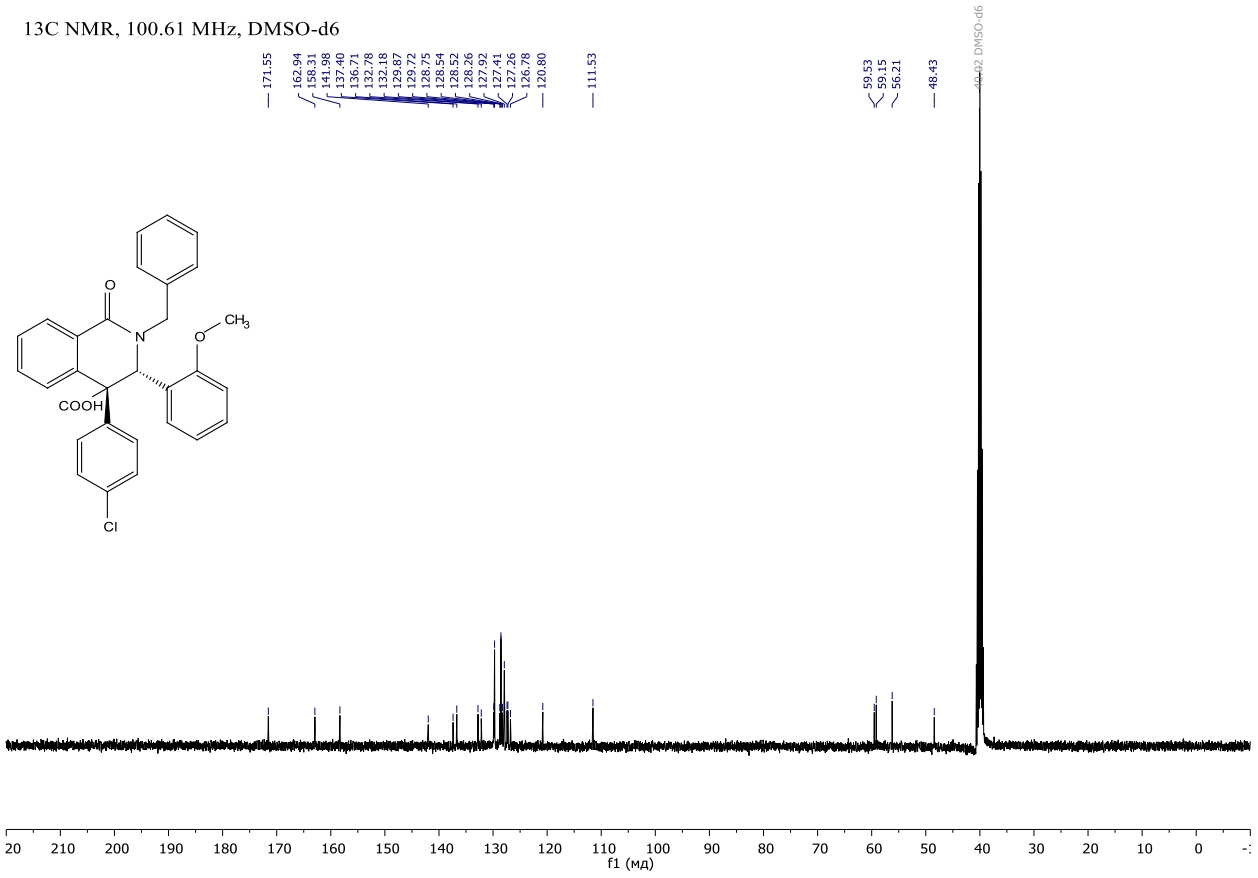
^{1}H and ^{13}C NMR spectra of compound **9f**



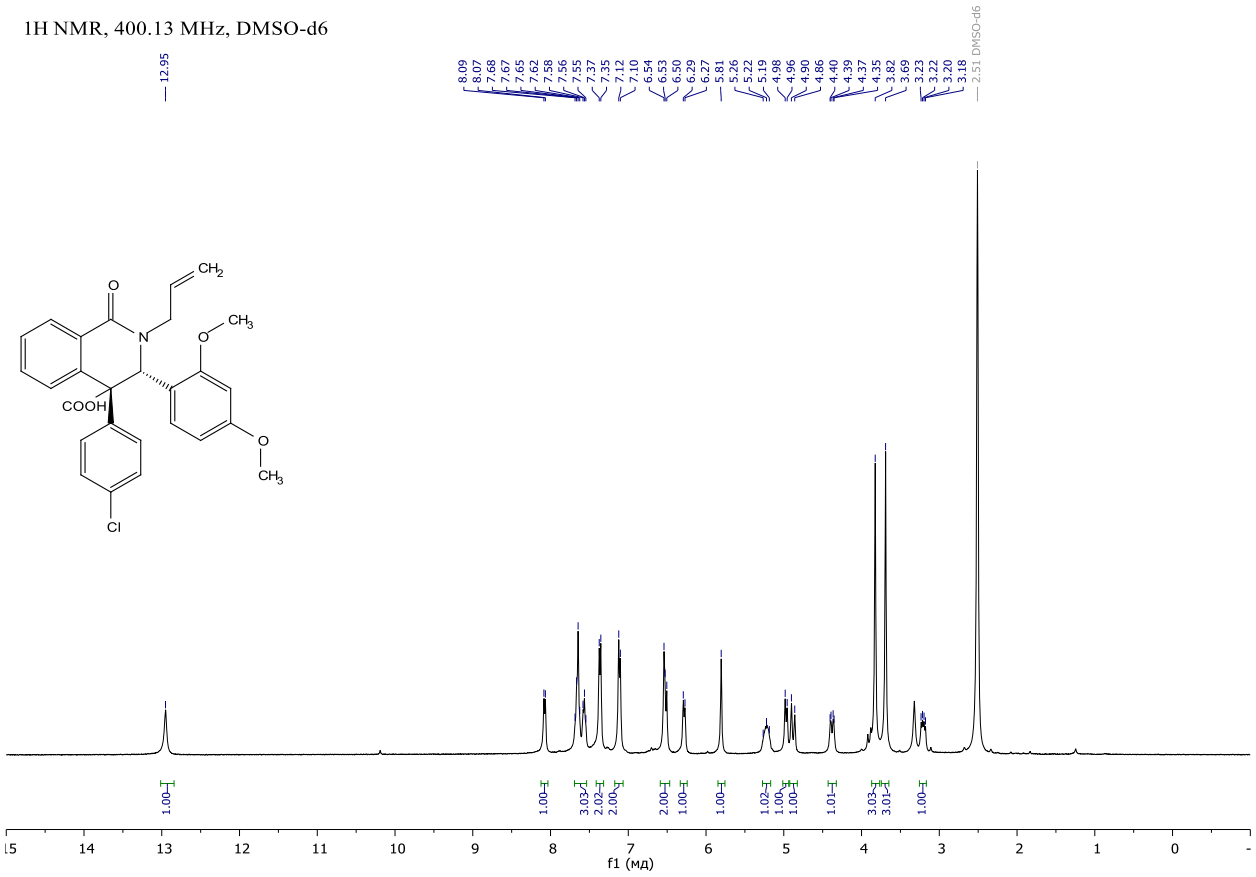


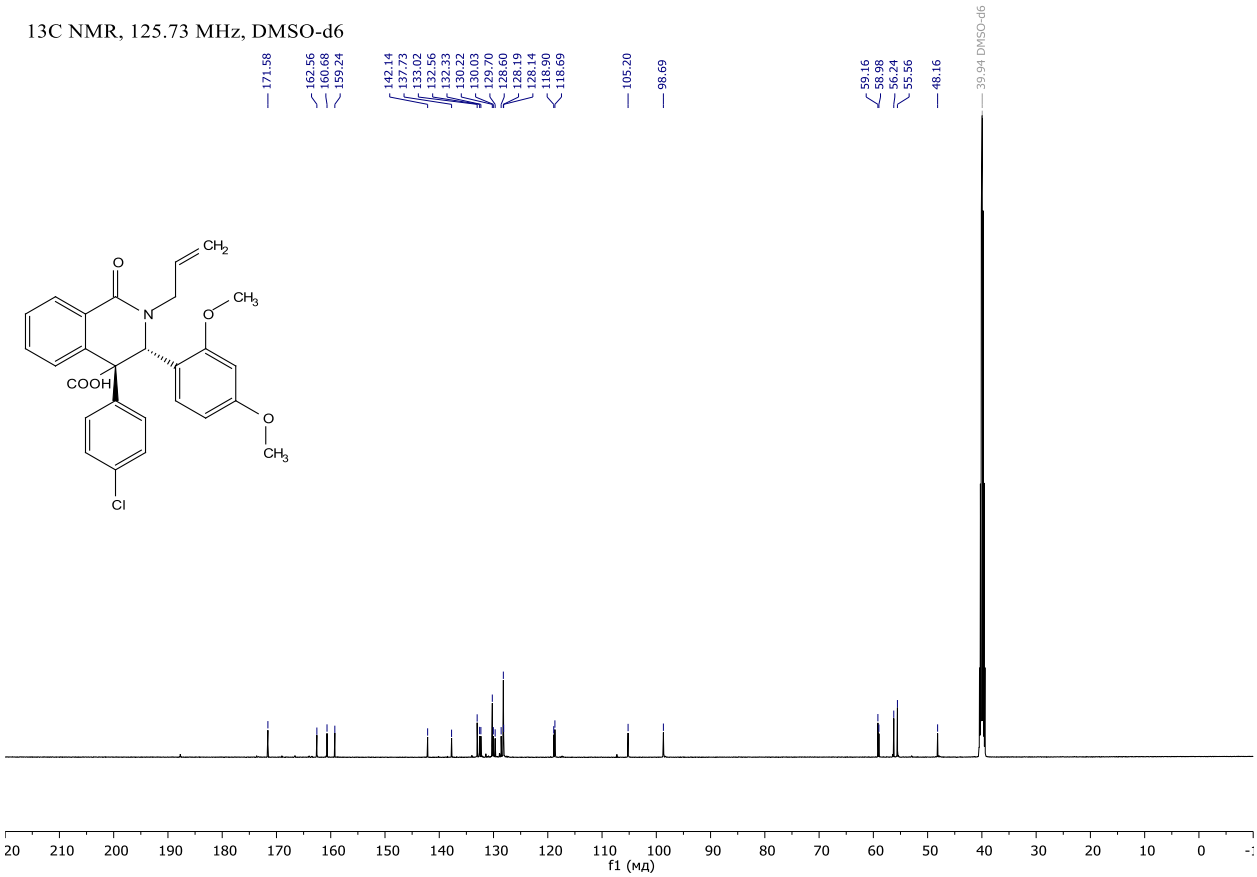
^{1}H and ^{13}C NMR spectra of compound **9g**



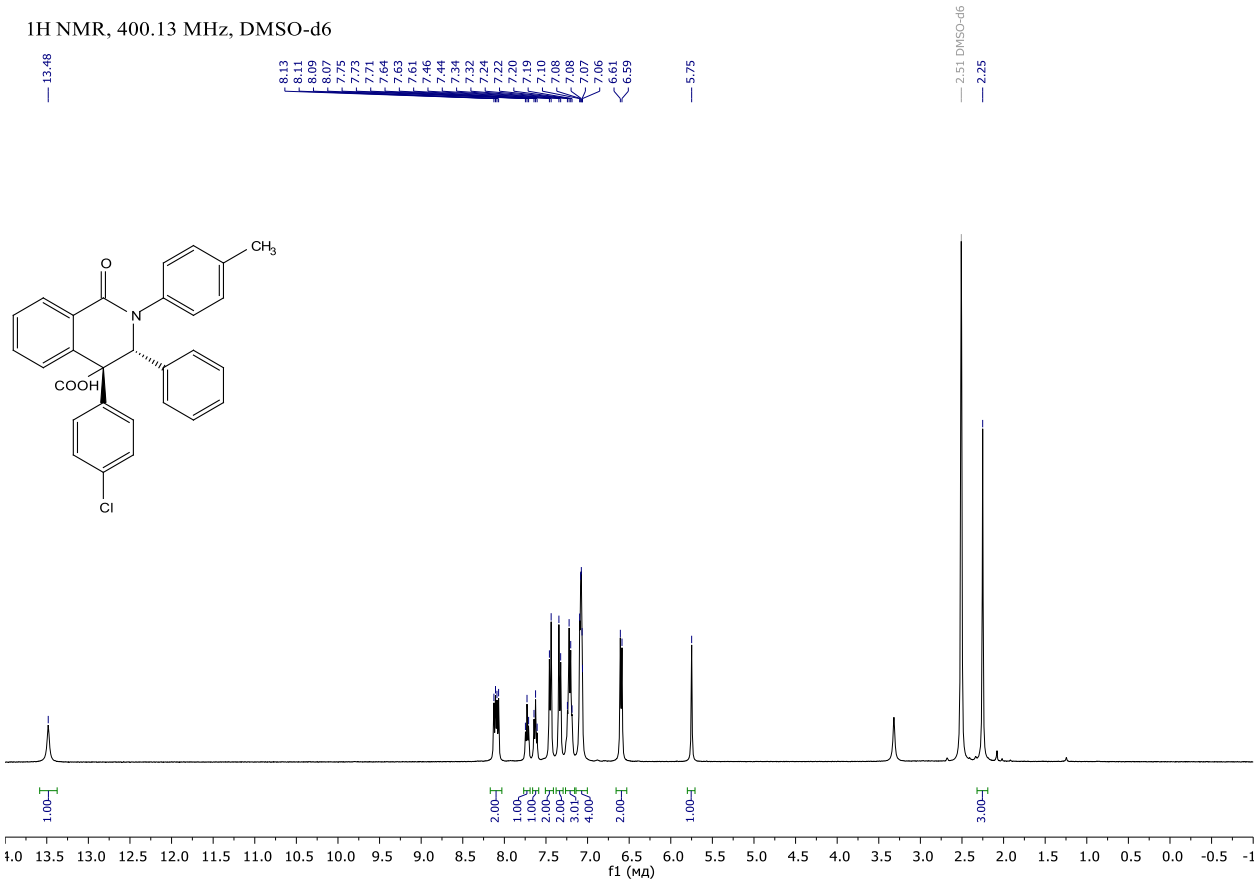


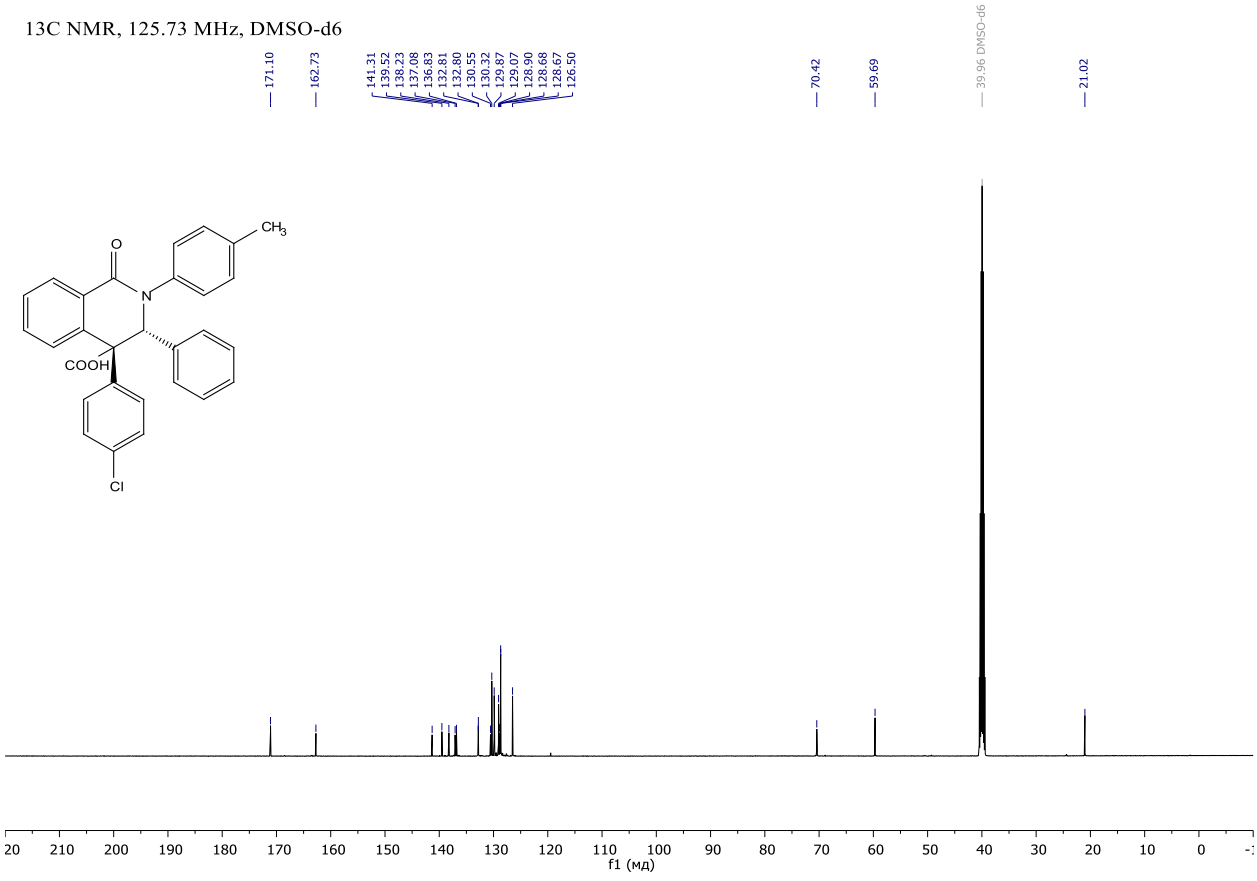
^{1}H and ^{13}C NMR spectra of compound **9h**



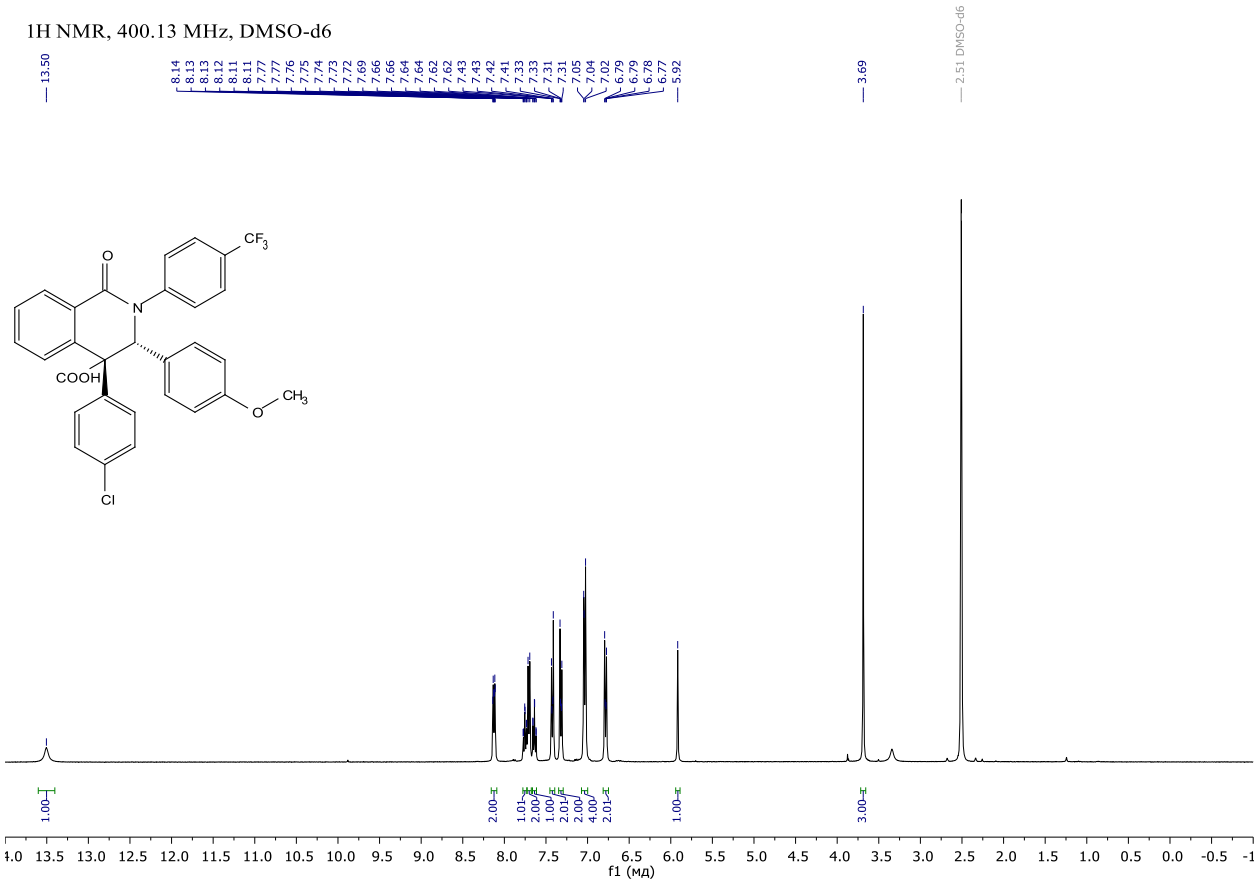


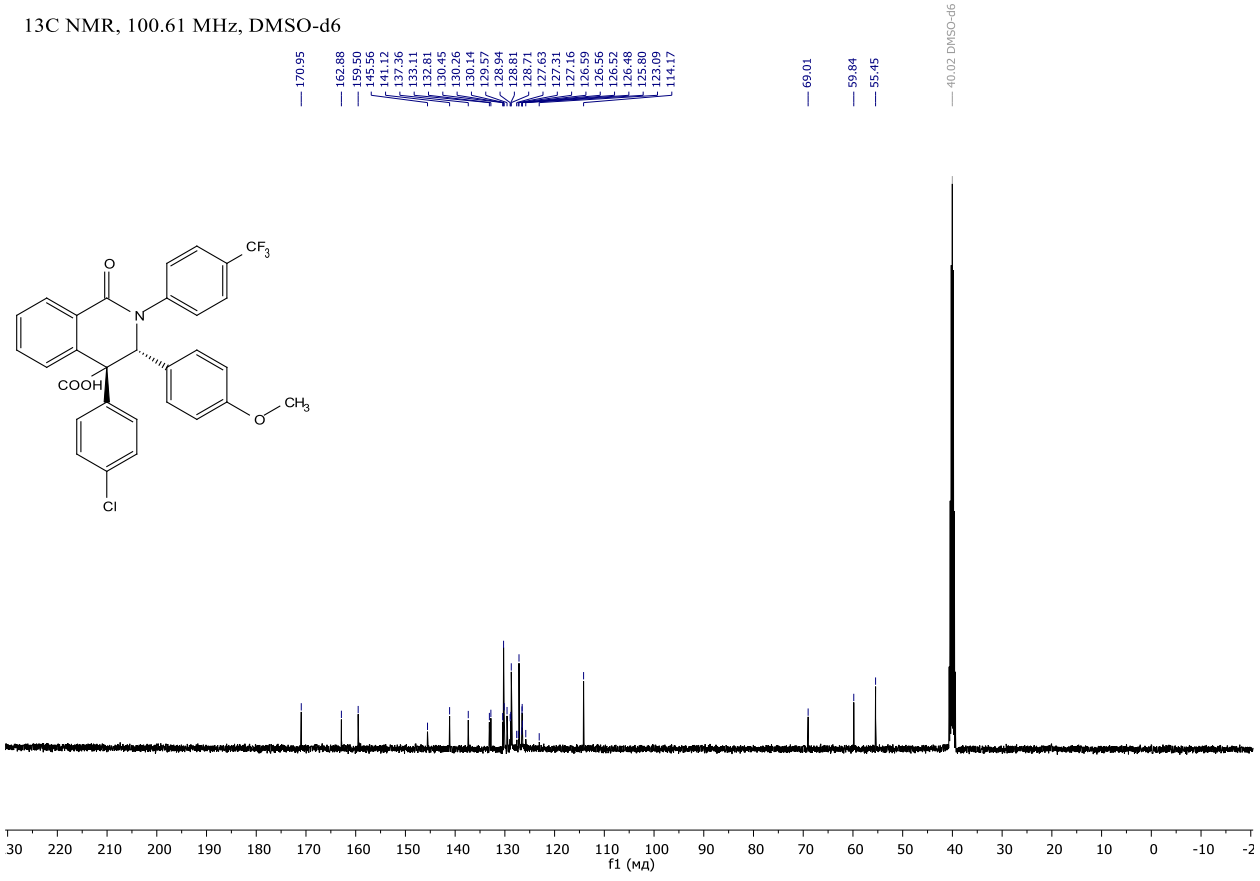
^{1}H and ^{13}C NMR spectra of compound **9i**



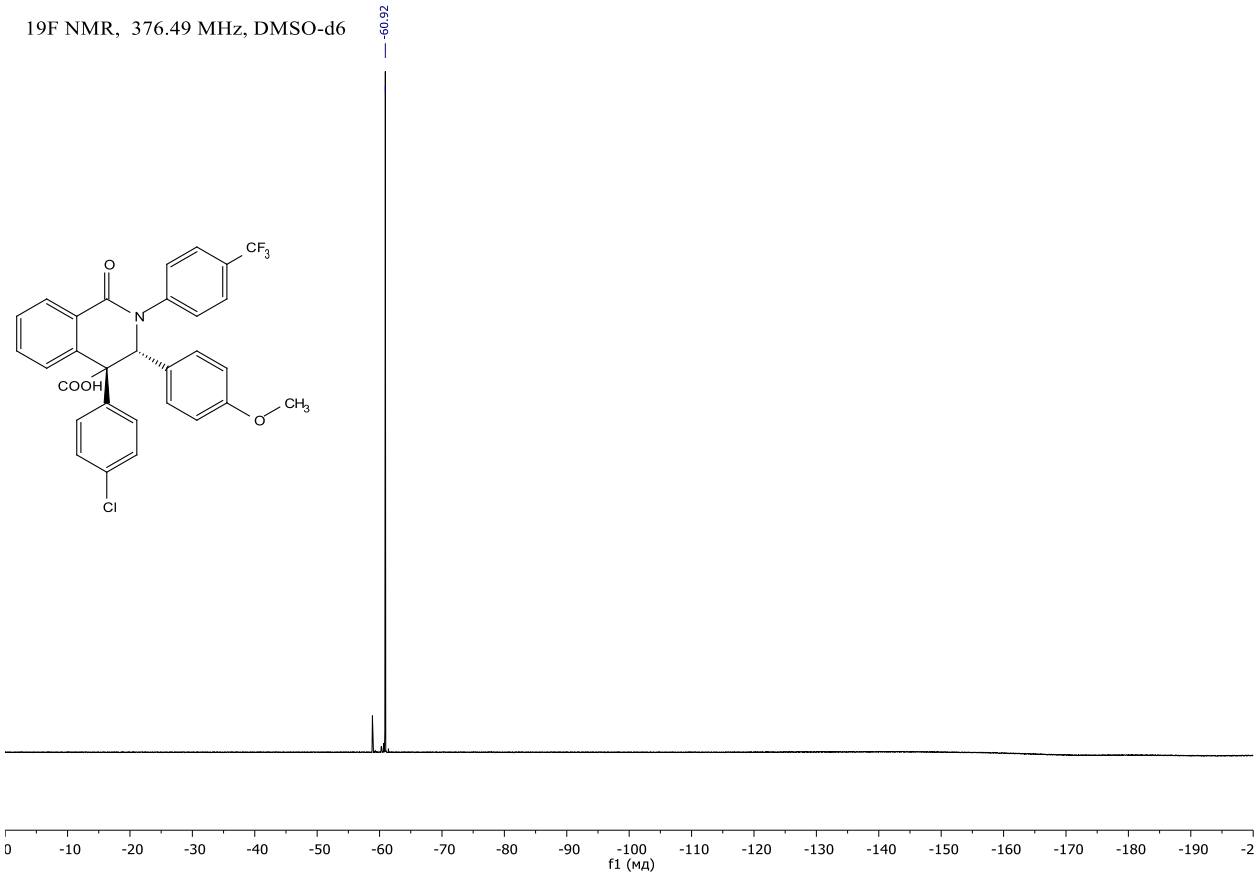


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9j**

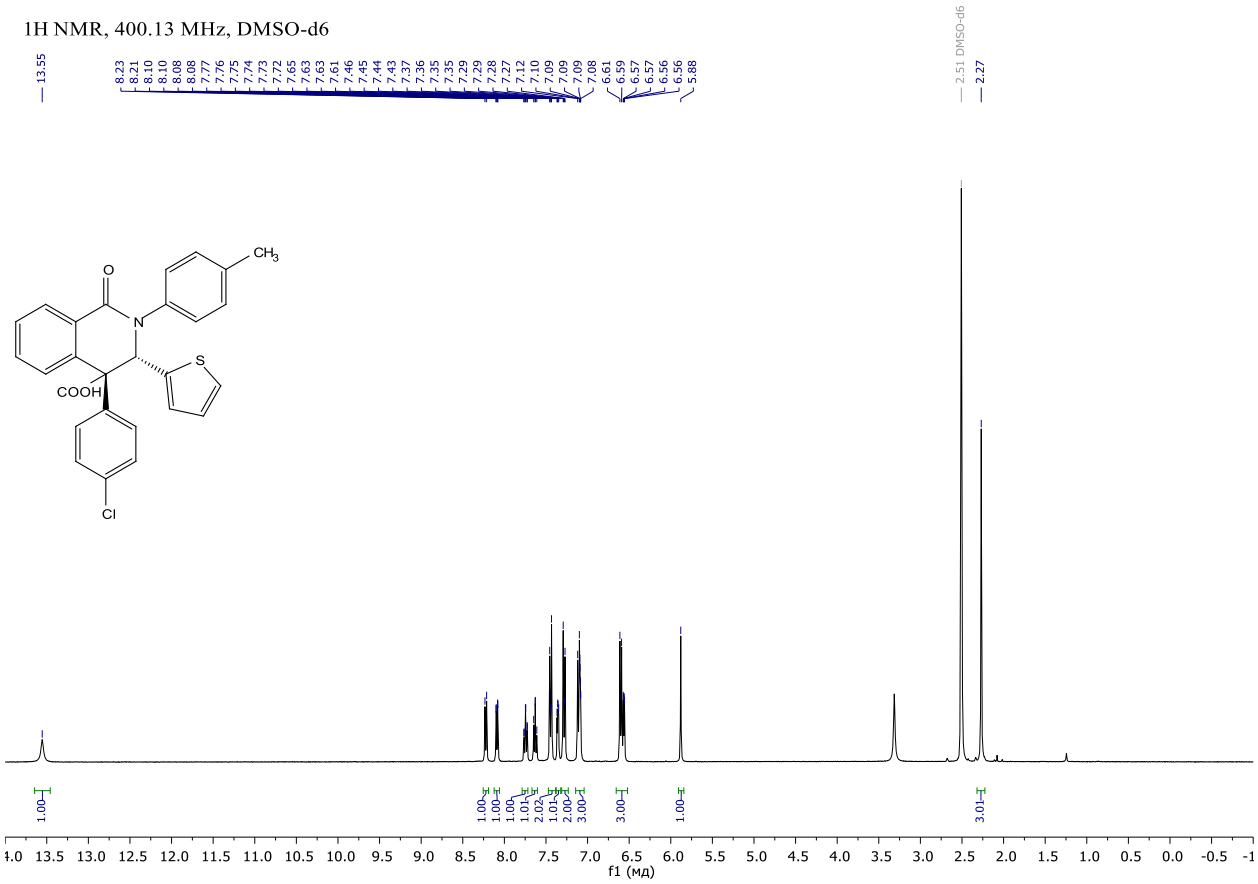


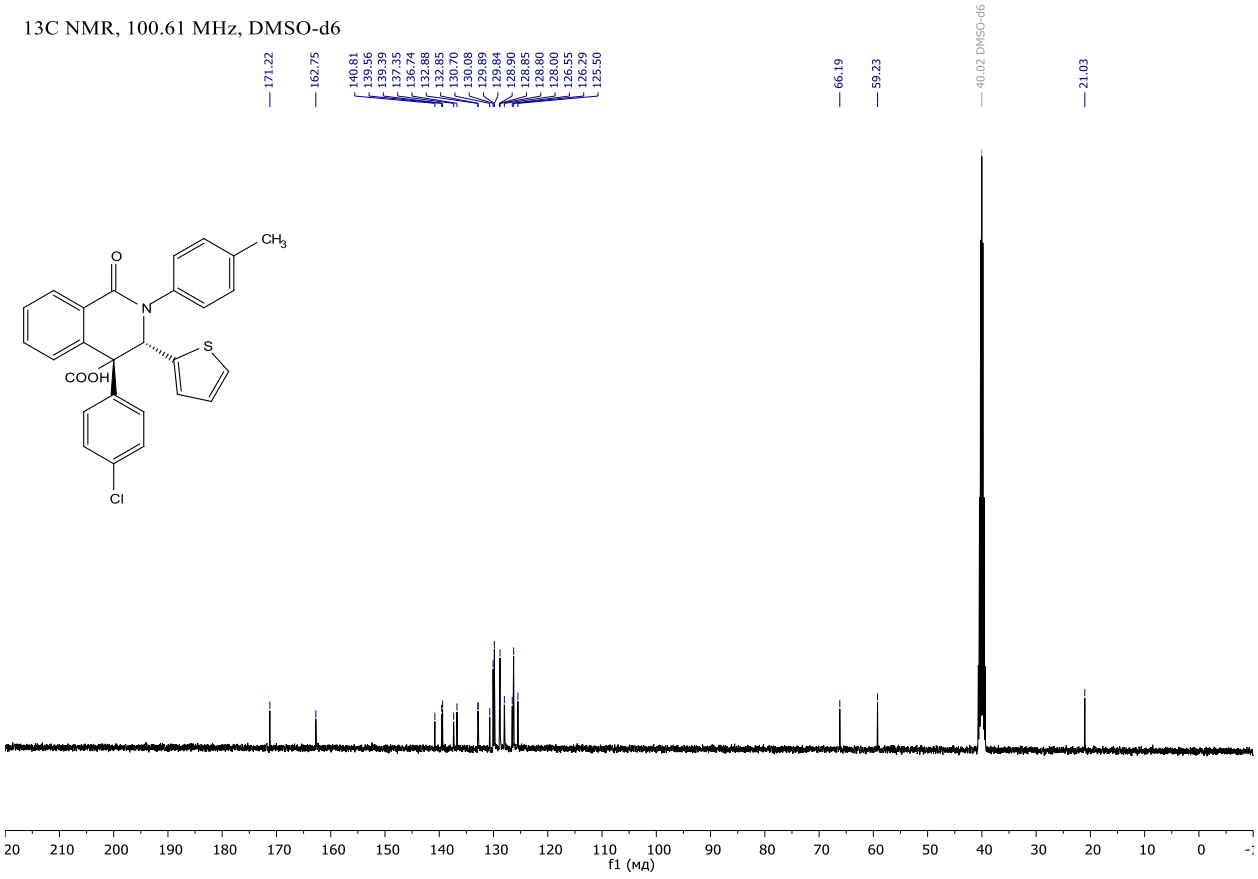


19F NMR, 376.49 MHz, DMSO-d6



^{1}H and ^{13}C NMR spectra of compound **9k**





^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9l**

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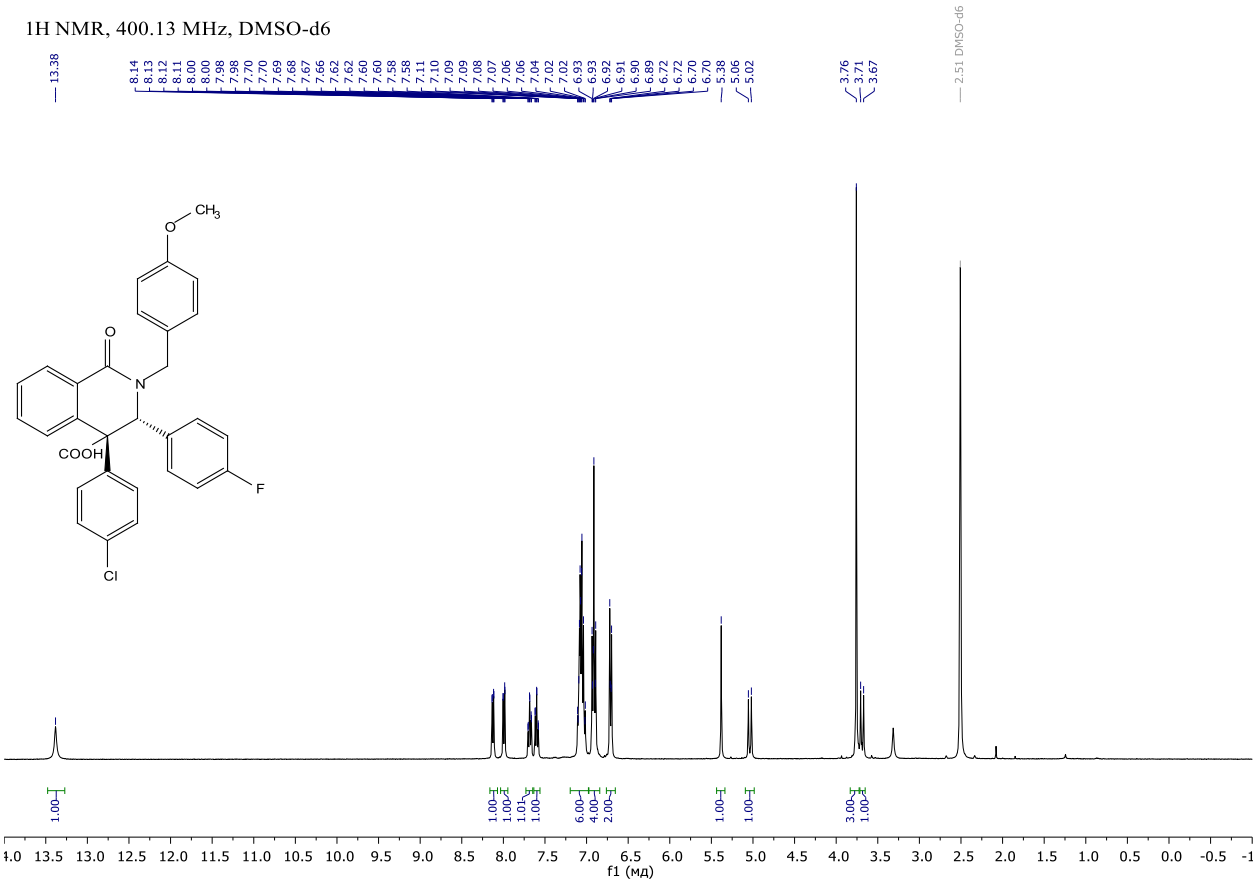
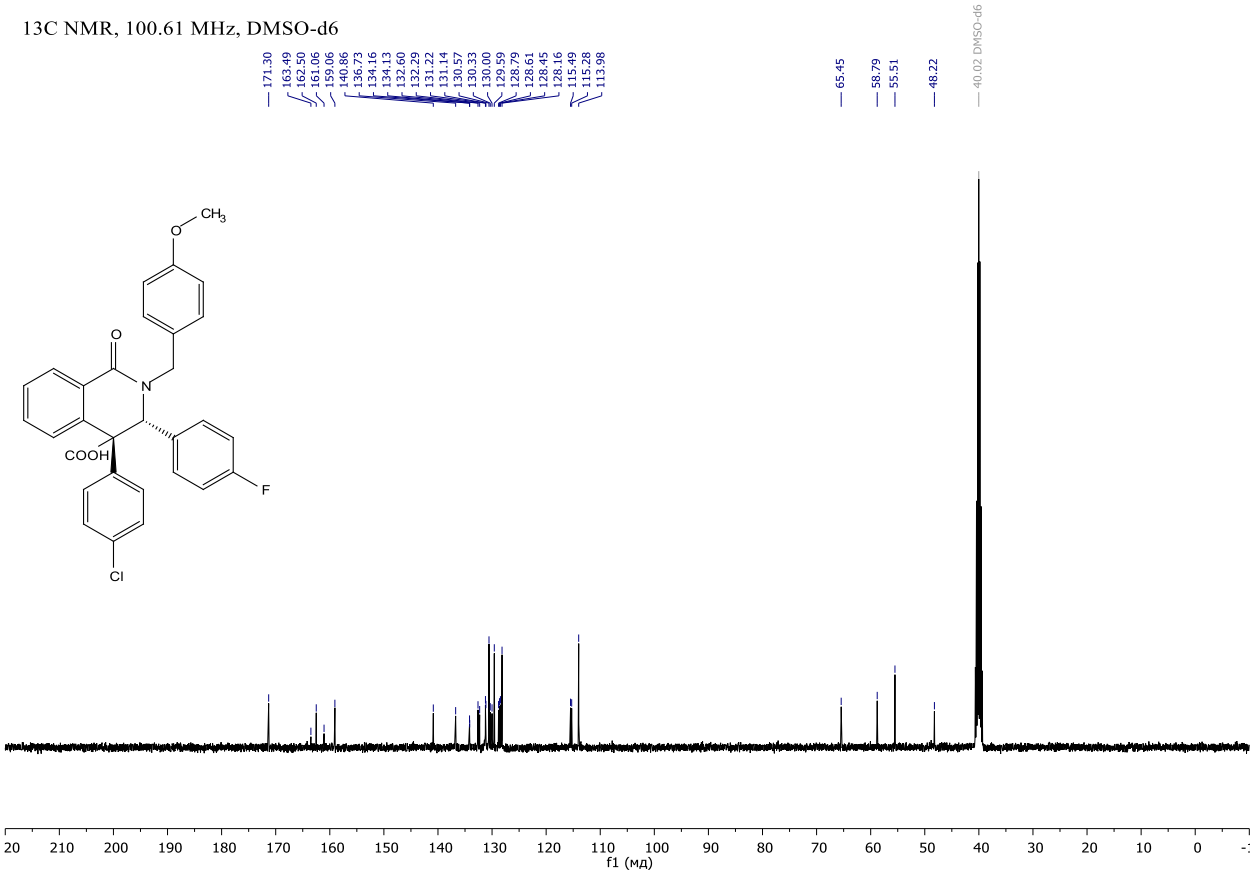
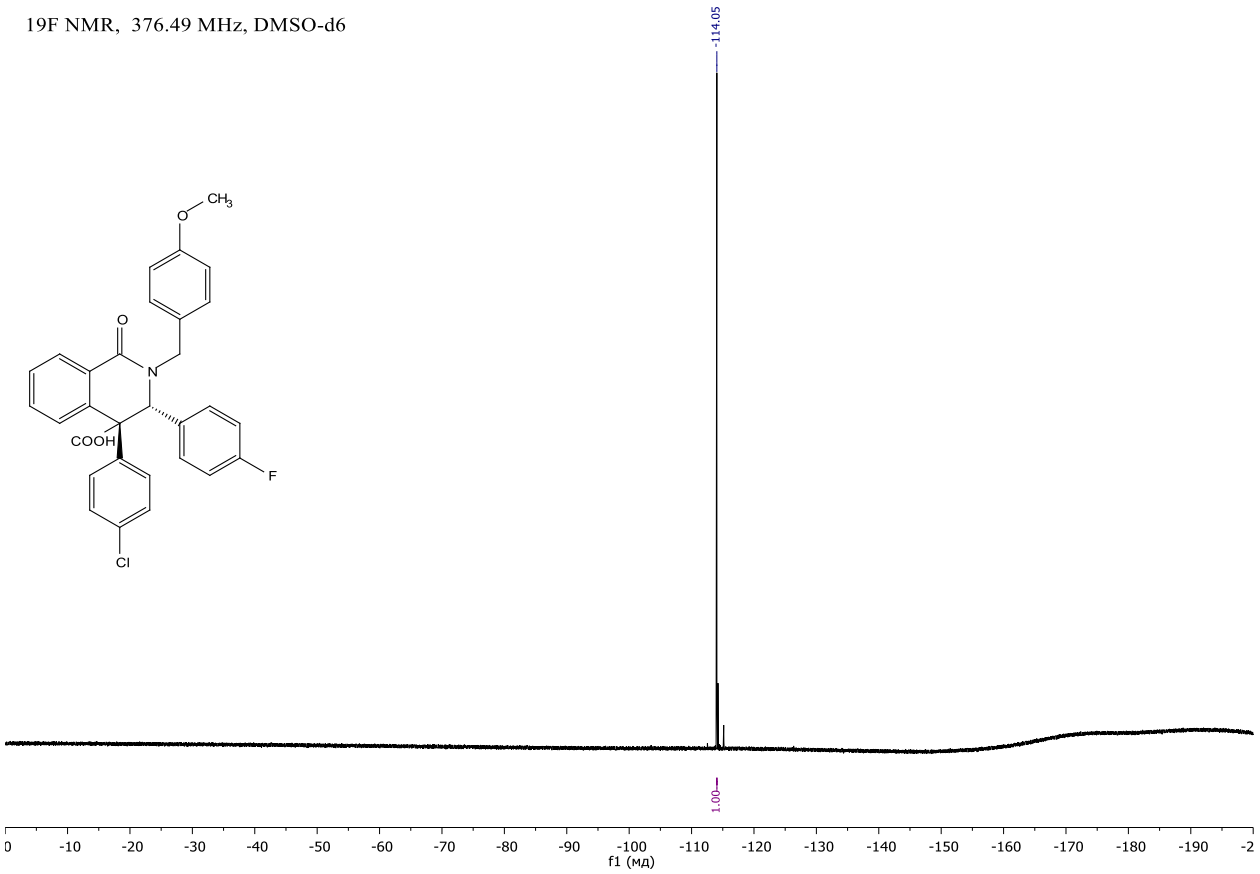


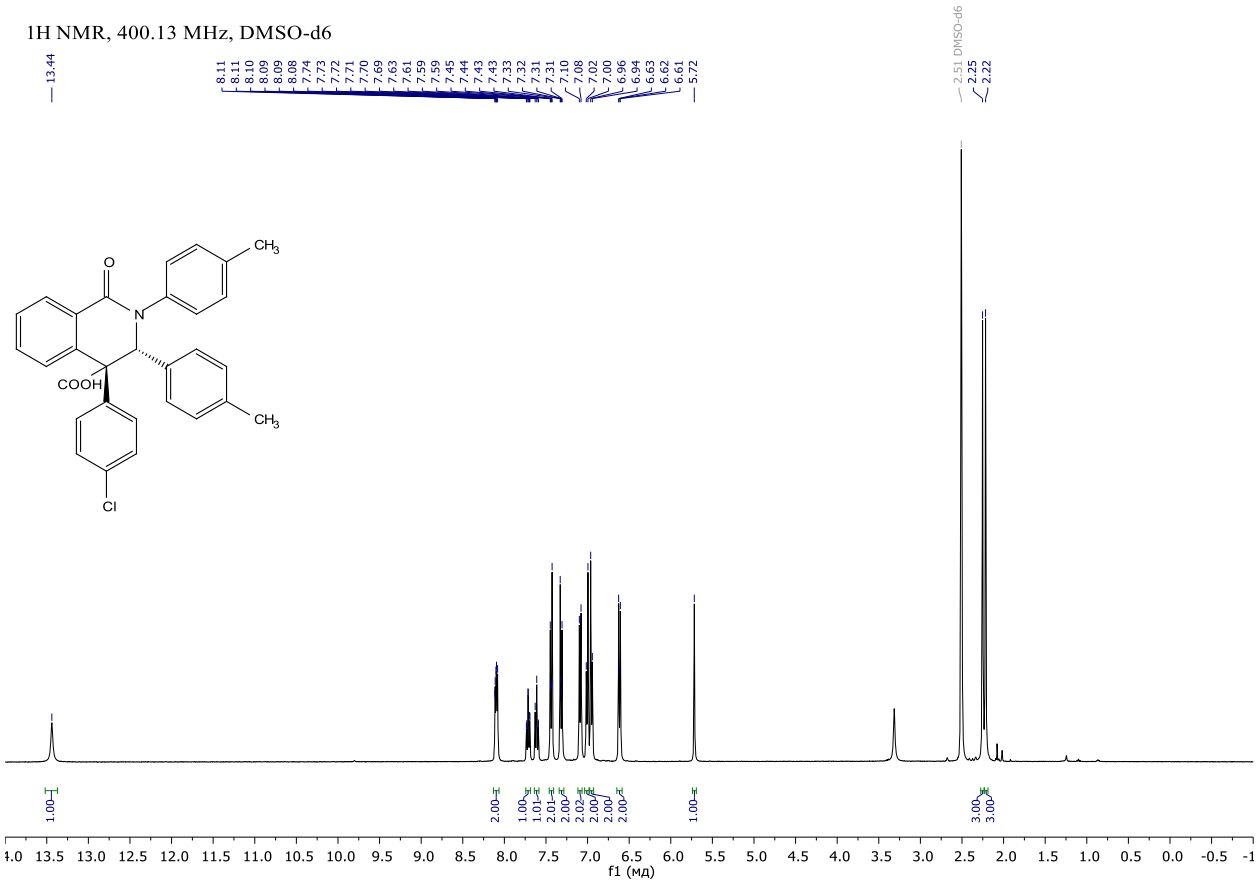
13C NMR, 100.61 MHz, DMSO-d6

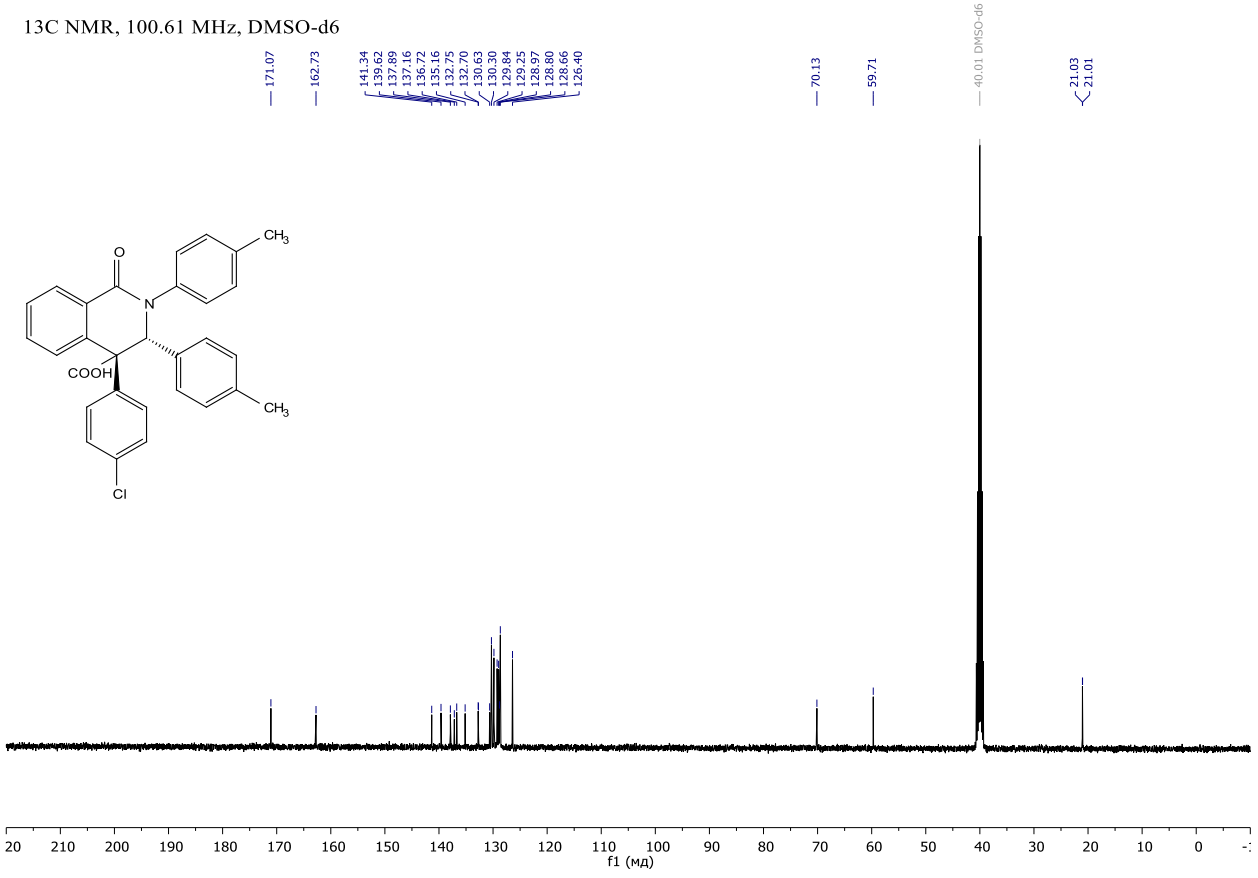


19F NMR, 376.49 MHz, DMSO-d6

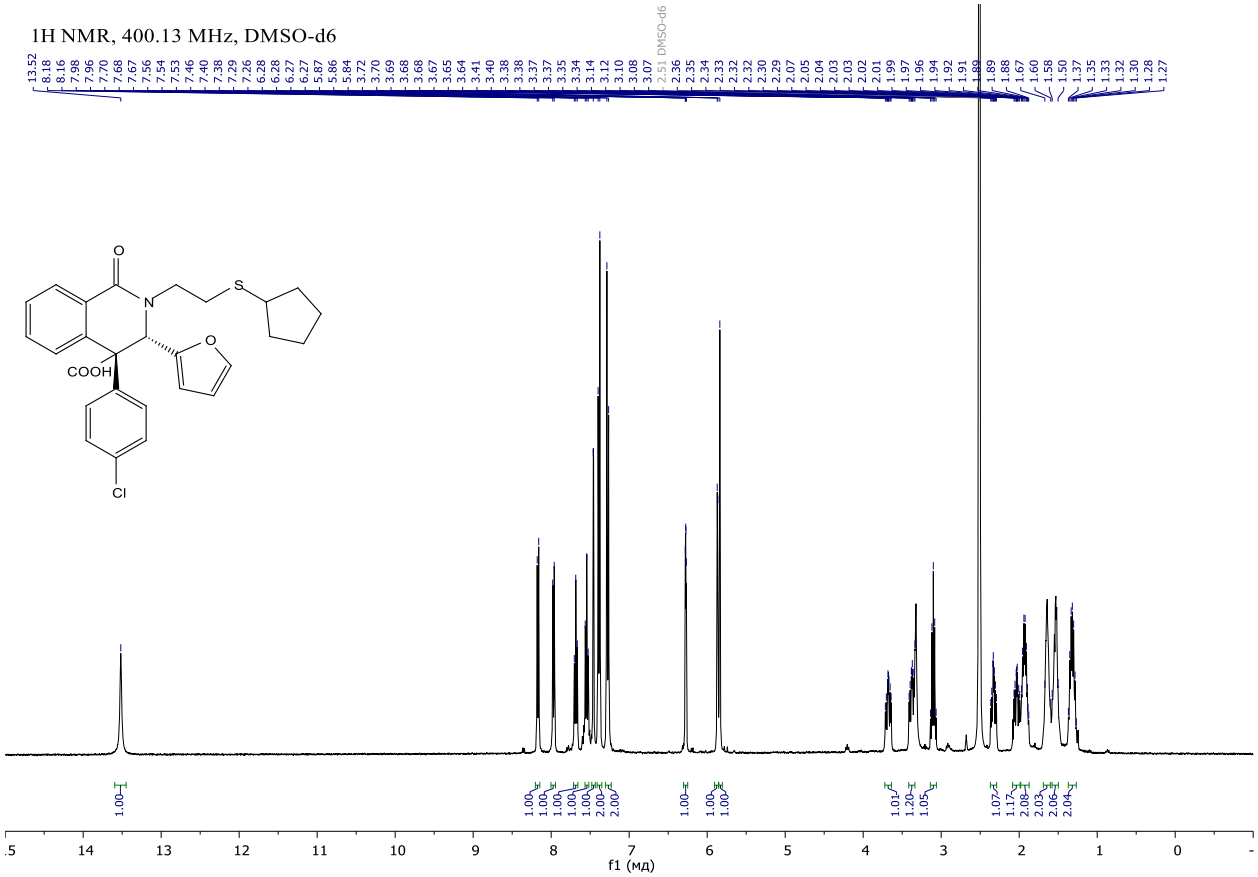


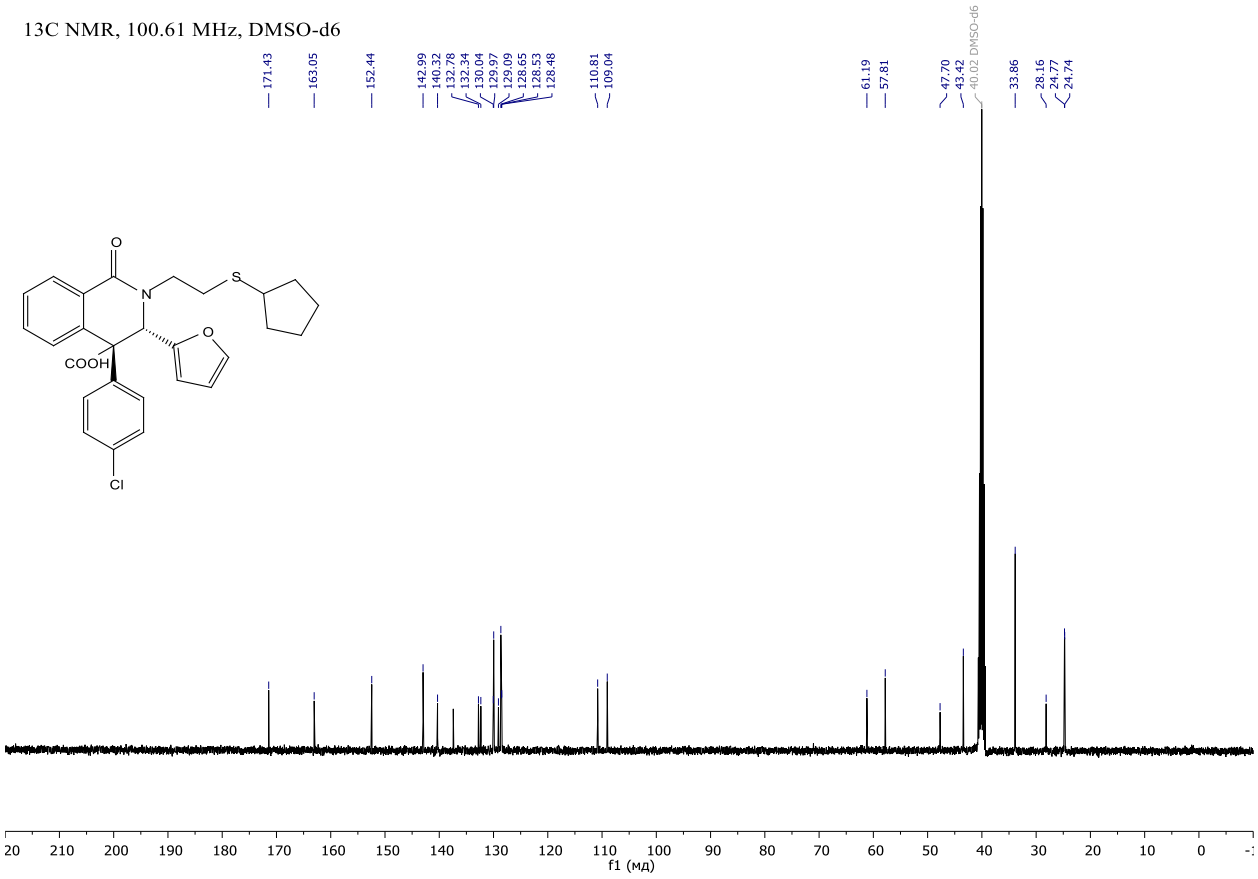
^{1}H and ^{13}C NMR spectra of compound **9m**



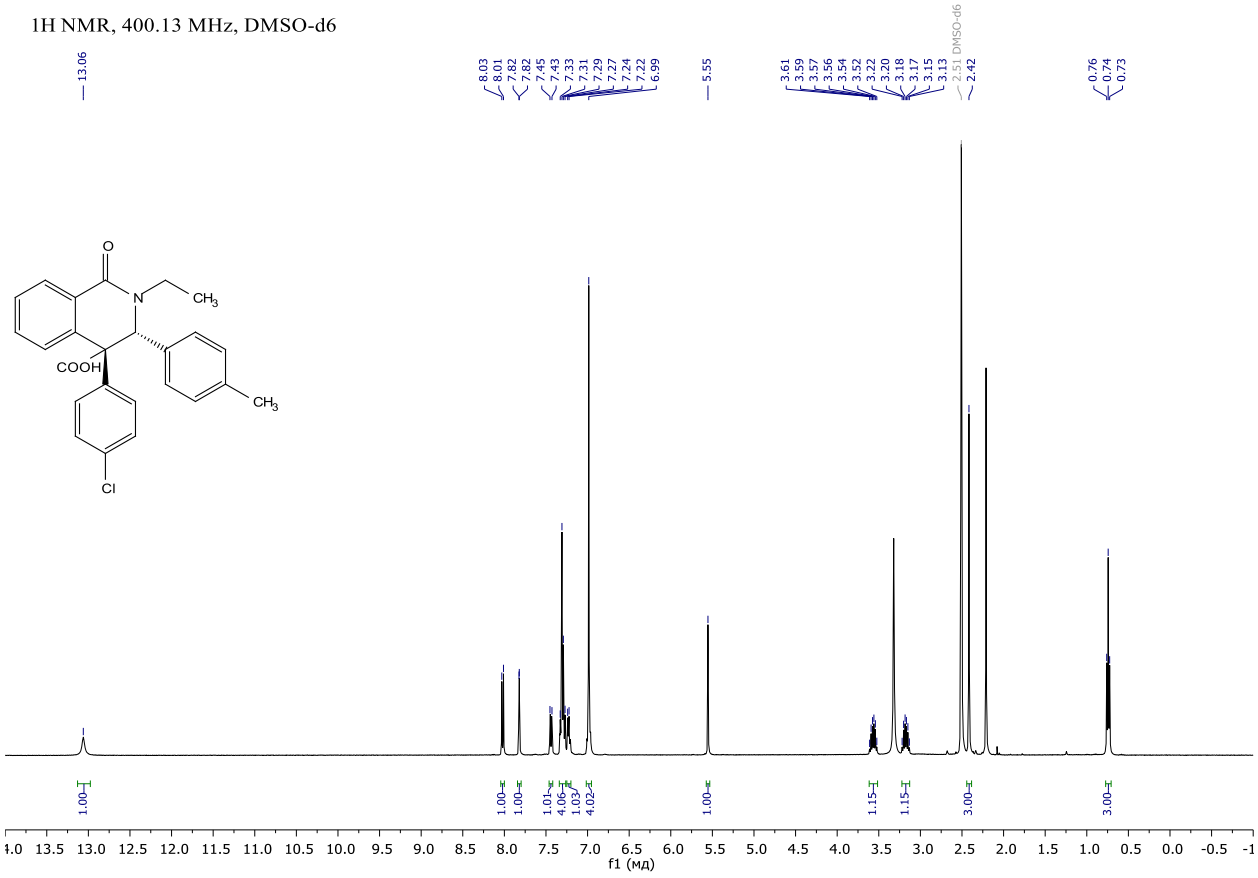


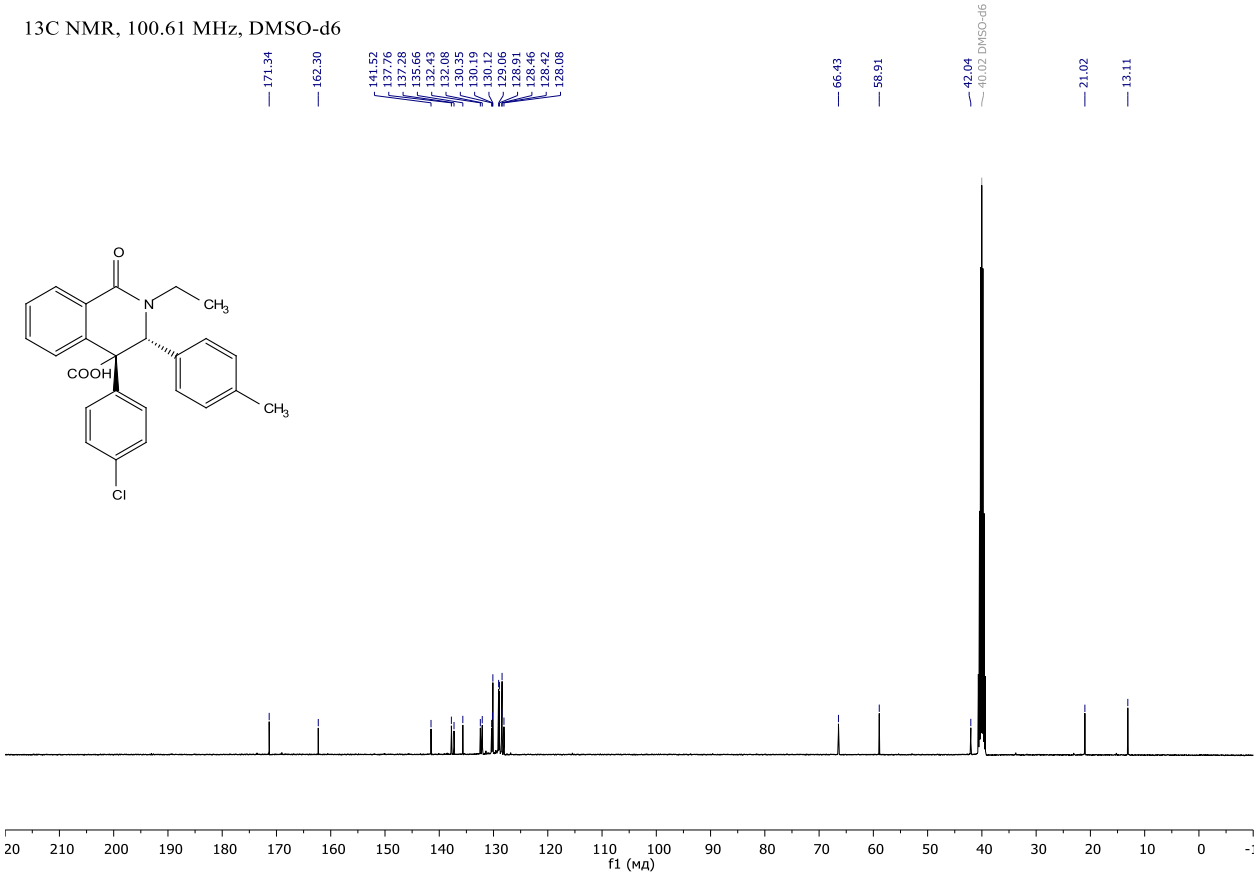
^{1}H and ^{13}C NMR spectra of compound **9n**





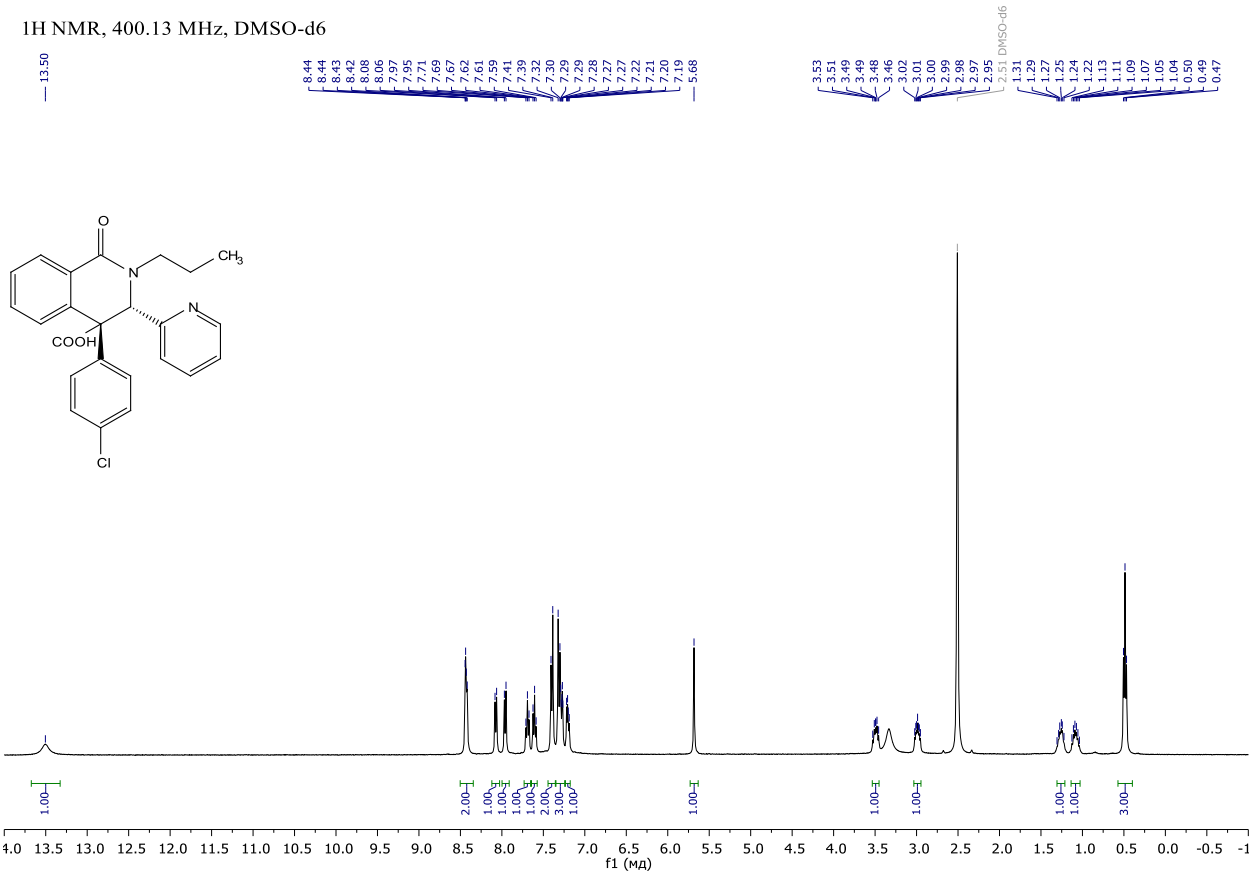
^{1}H and ^{13}C NMR spectra of compound **9o**



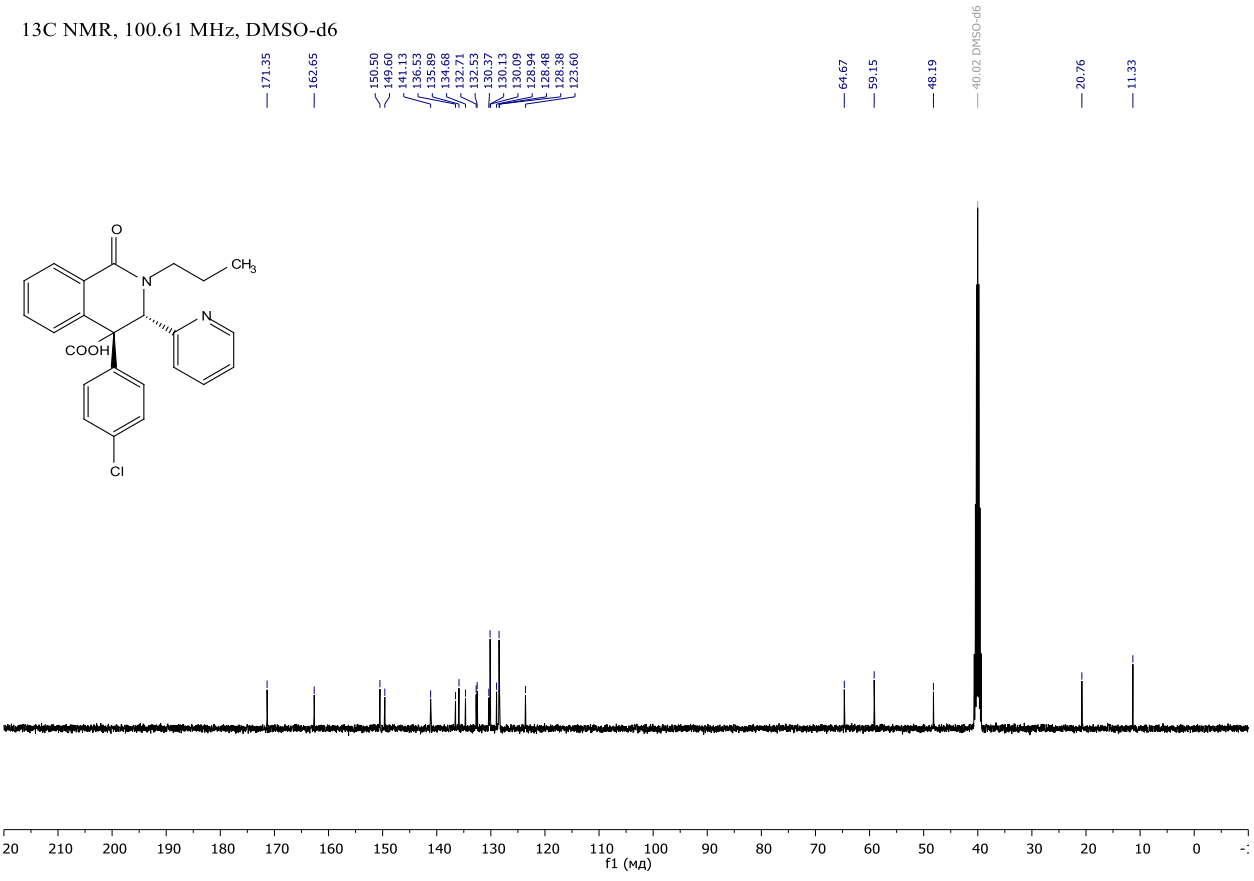


^{1}H and ^{13}C NMR spectra of compound **9p**

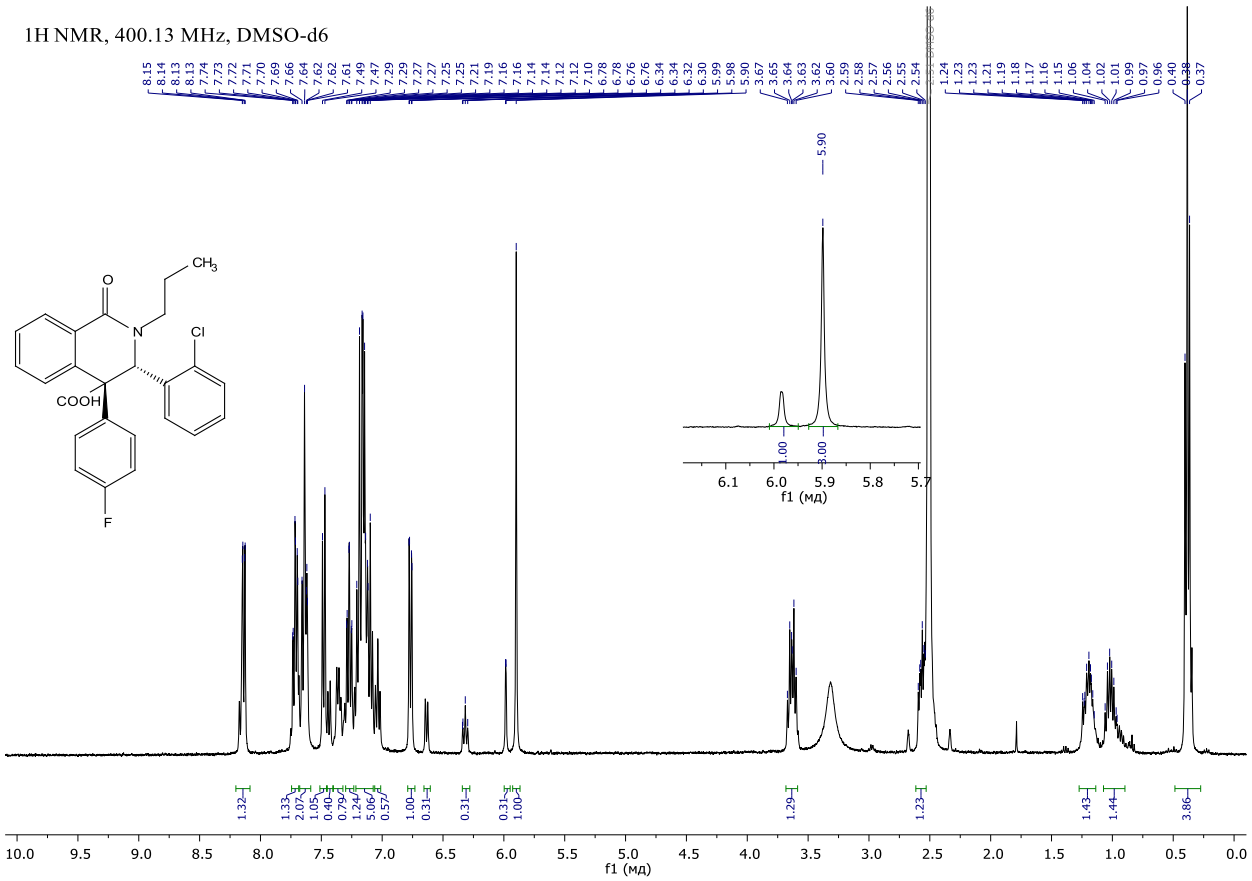
1H NMR, 400.13 MHz, DMSO-d6

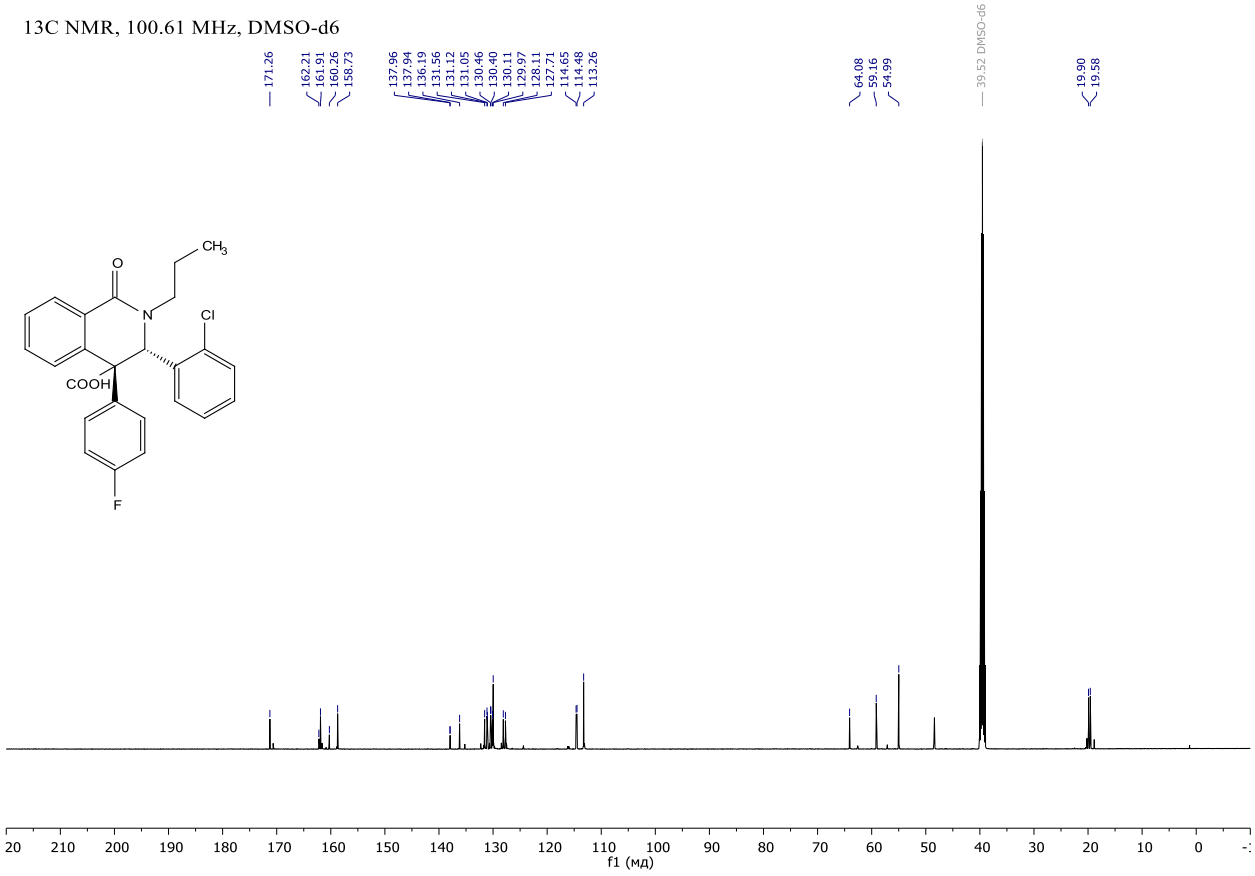


13C NMR, 100.61 MHz, DMSO-d6

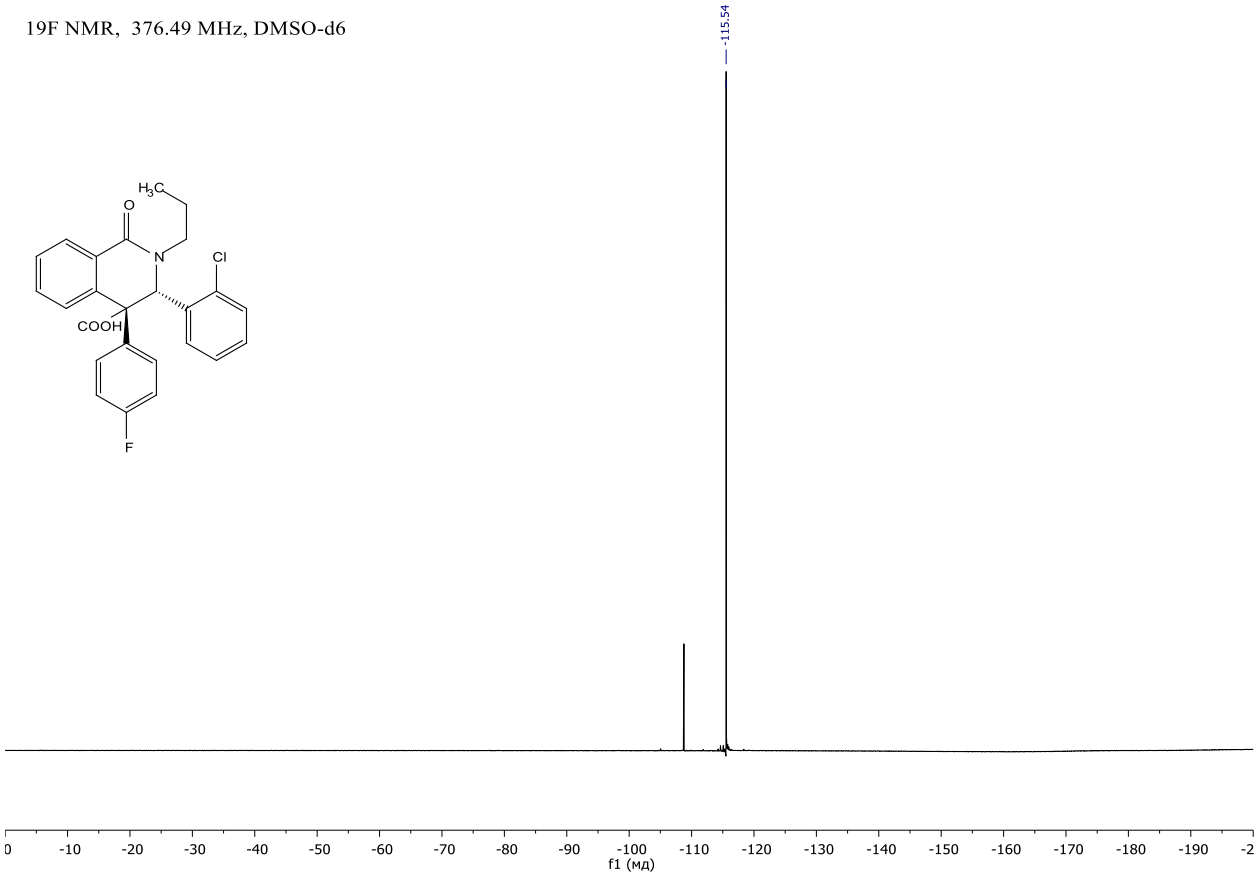


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9q**



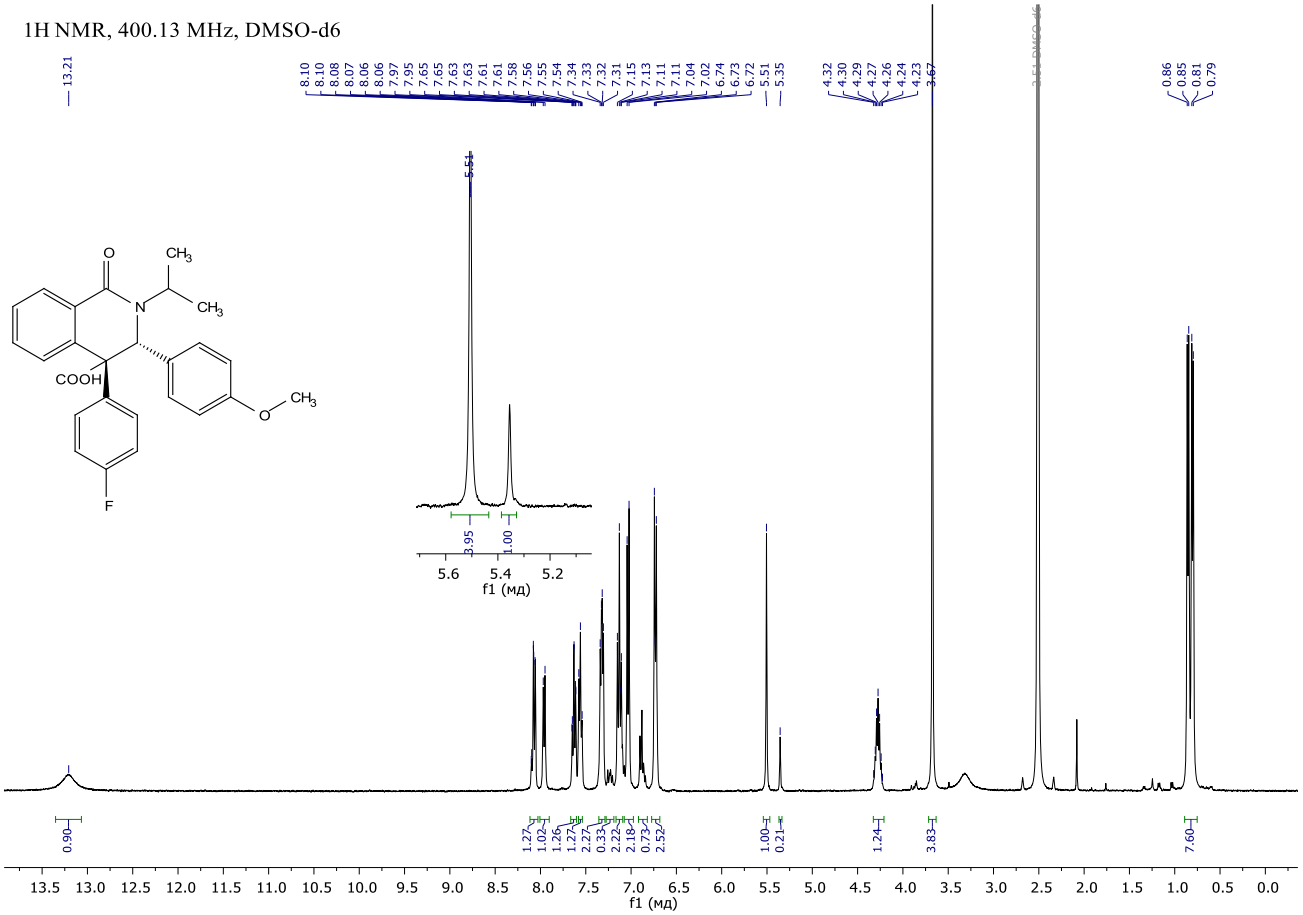


19F NMR, 376.49 MHz, DMSO-d6

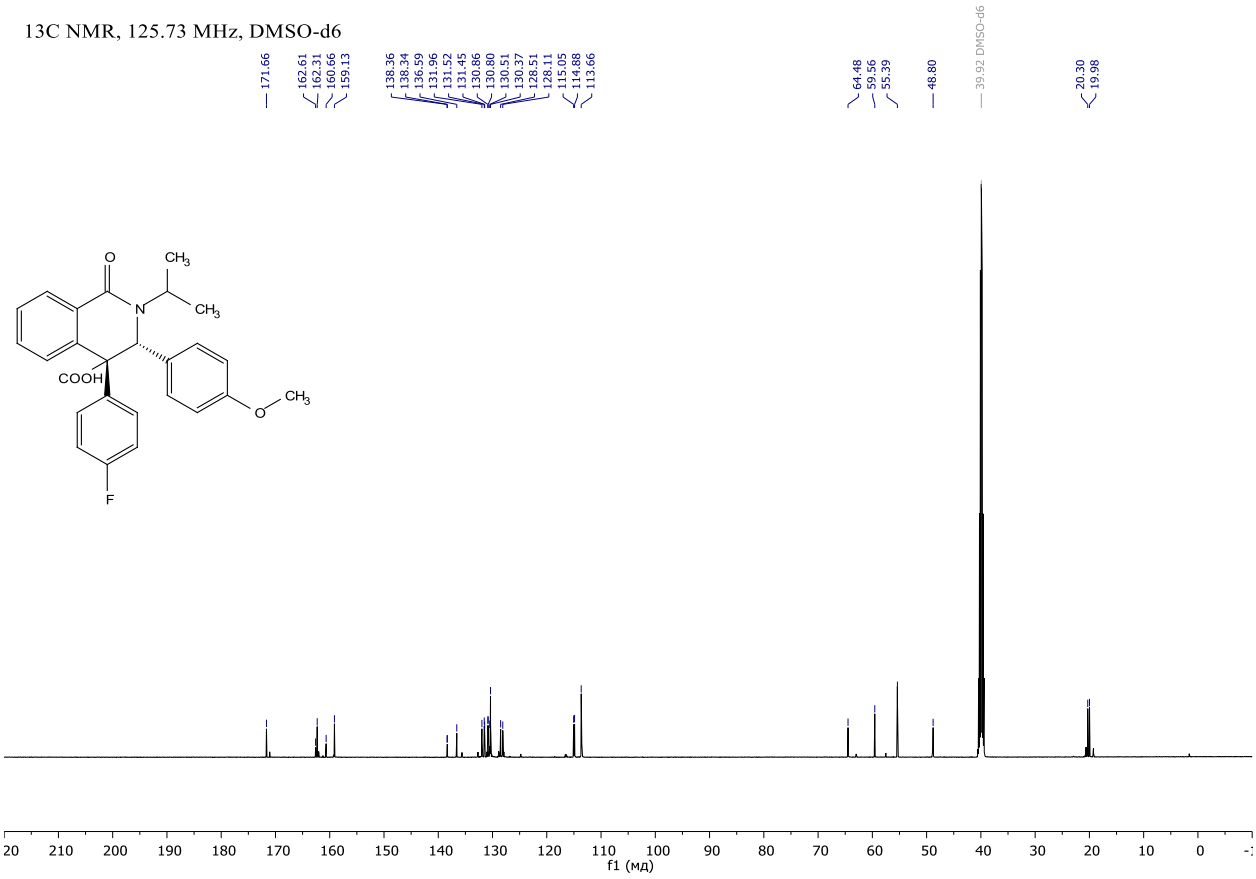


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9r**

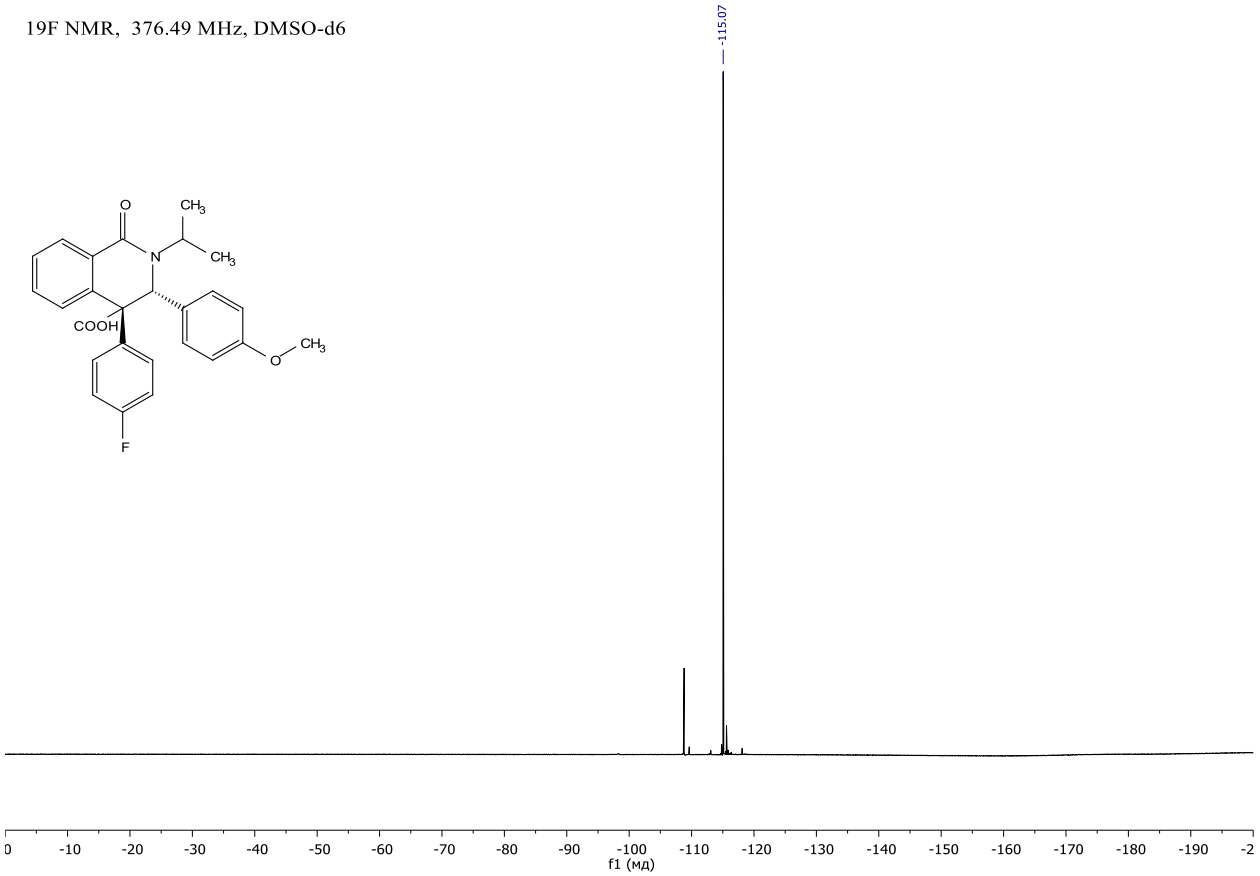
1H NMR, 400.13 MHz, DMSO-d6



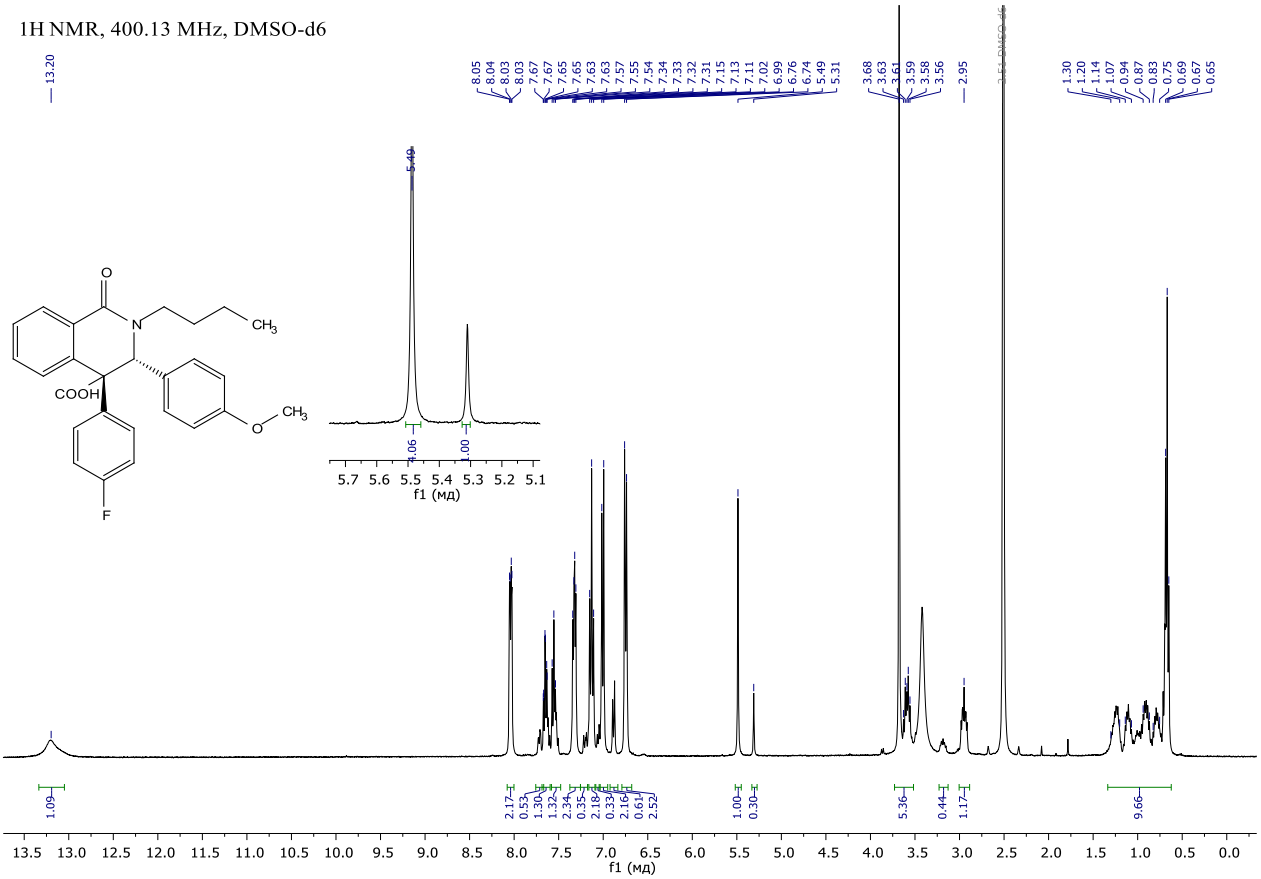
13C NMR, 125.73 MHz, DMSO-d6

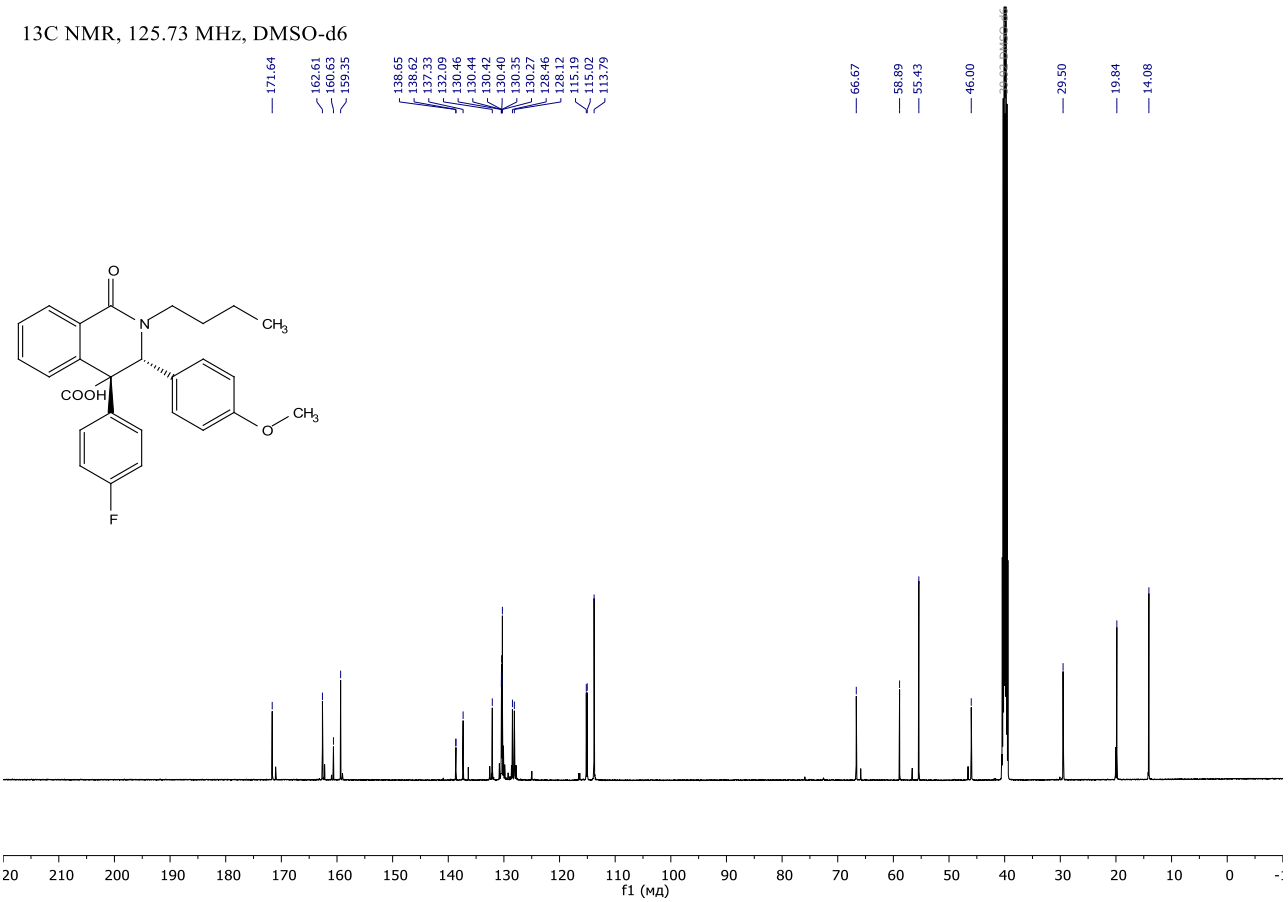


19F NMR, 376.49 MHz, DMSO-d6

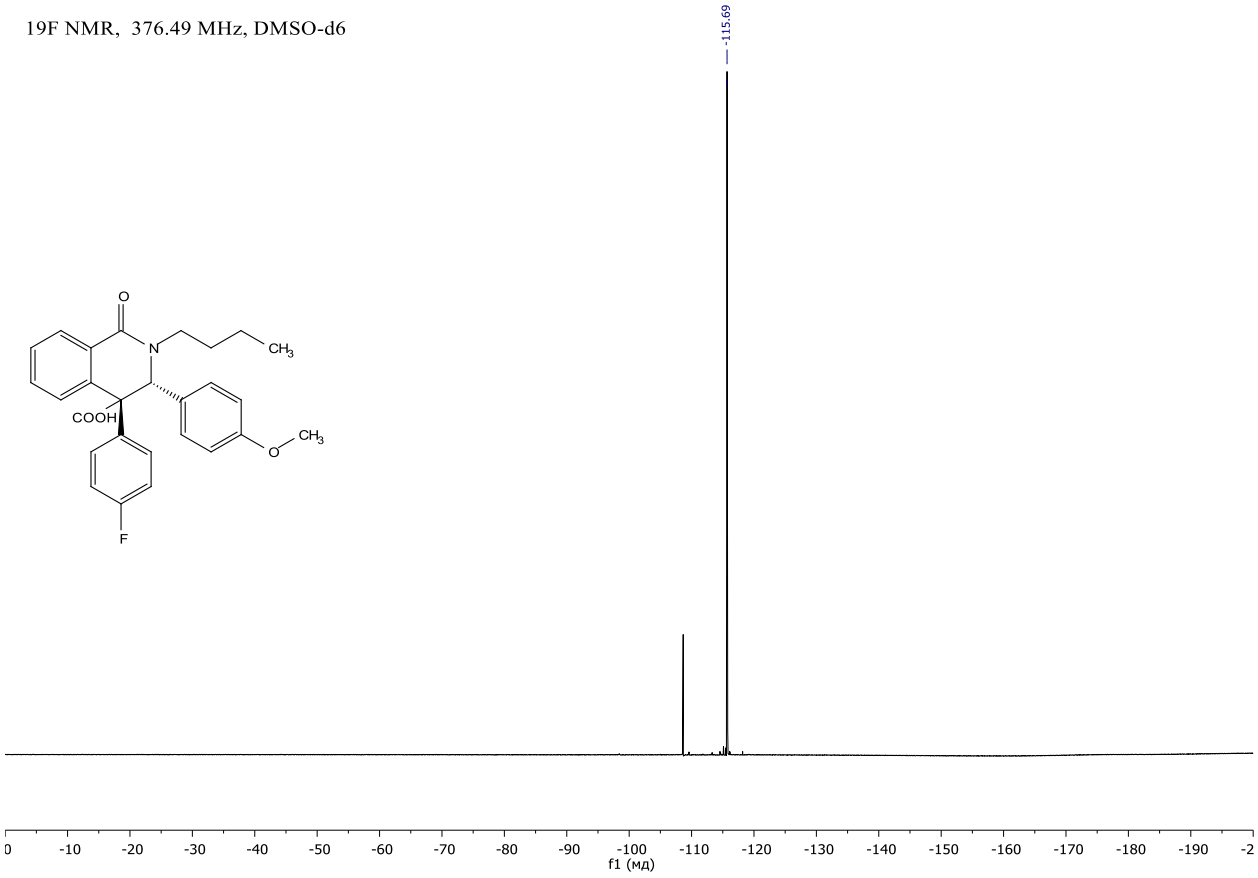


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9s**



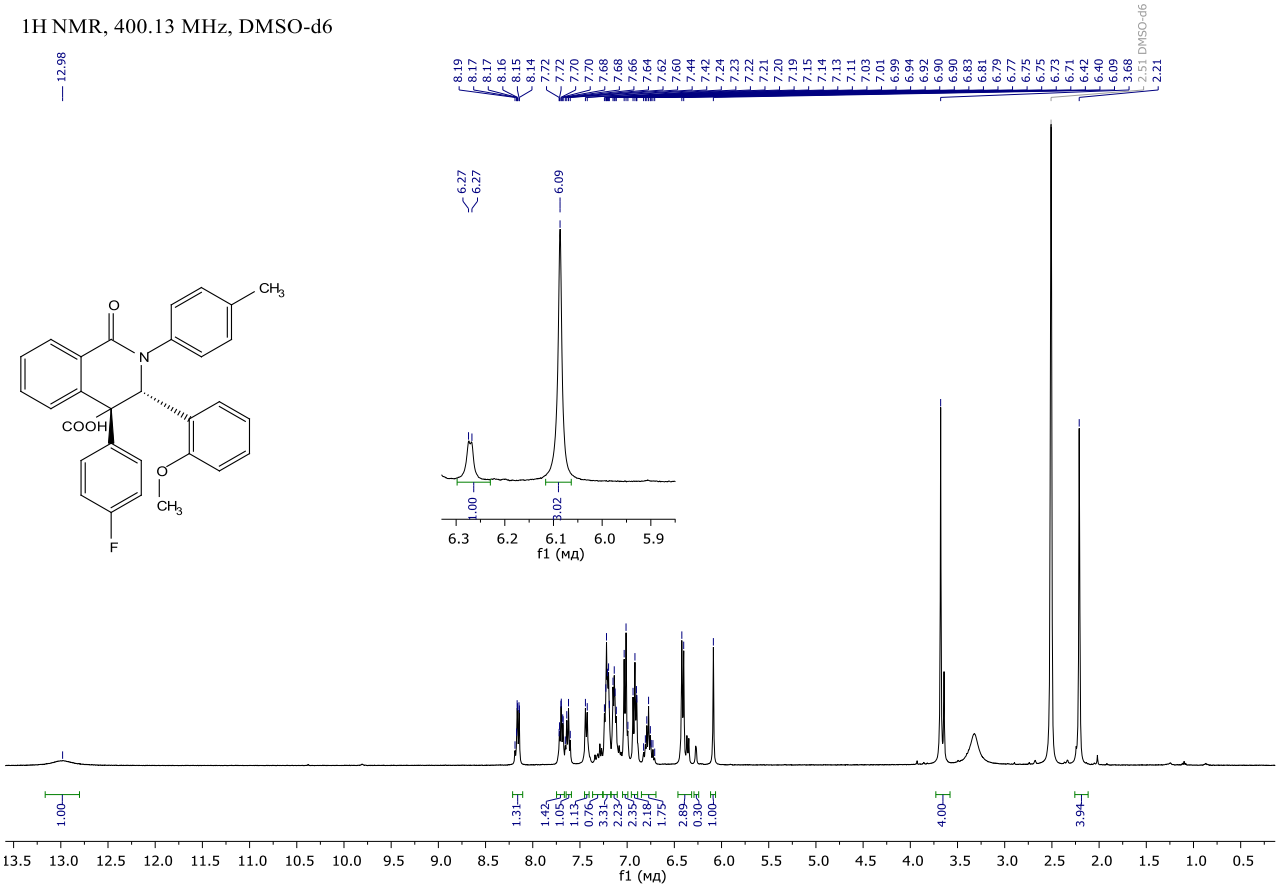


19F NMR, 376.49 MHz, DMSO-d6

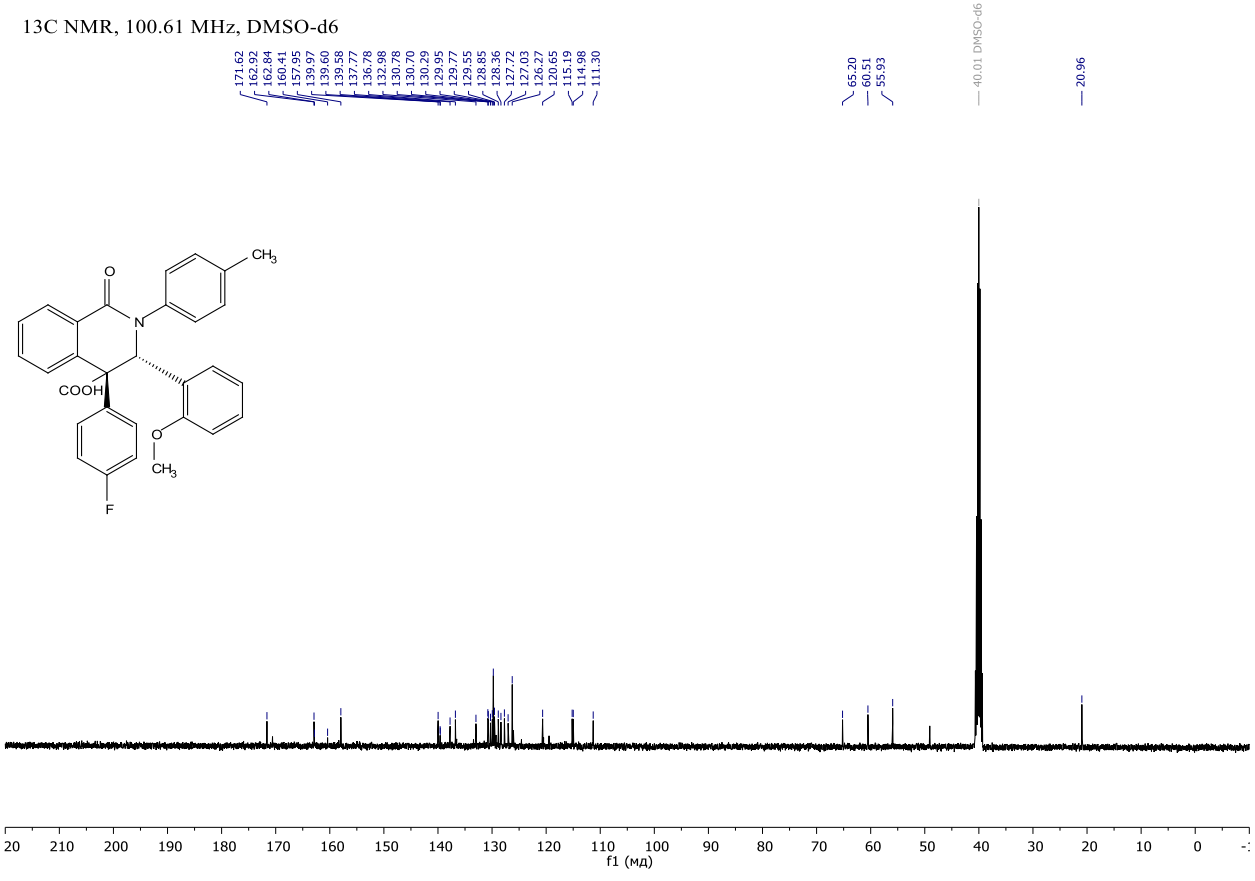


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9t**

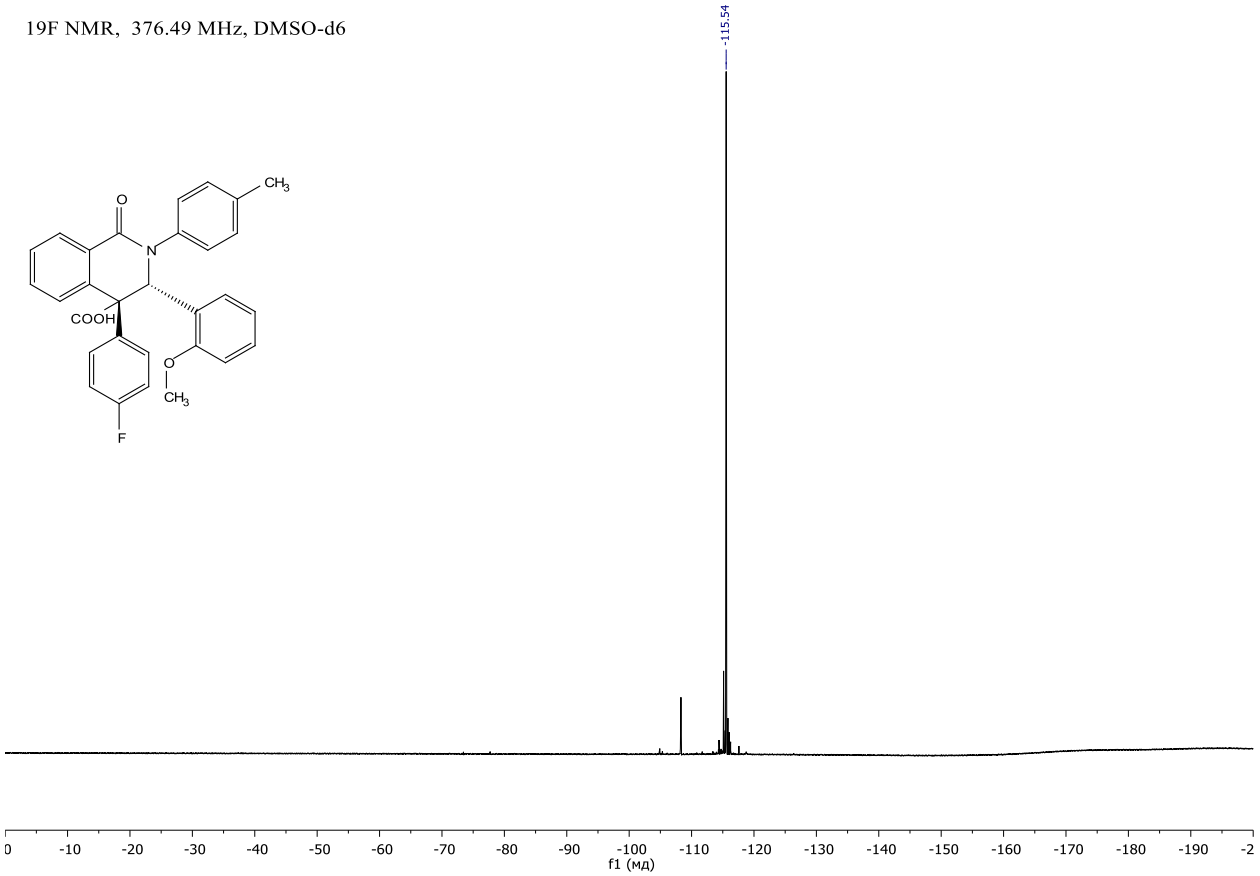
1H NMR, 400.13 MHz, DMSO-d6



13C NMR, 100.61 MHz, DMSO-d6

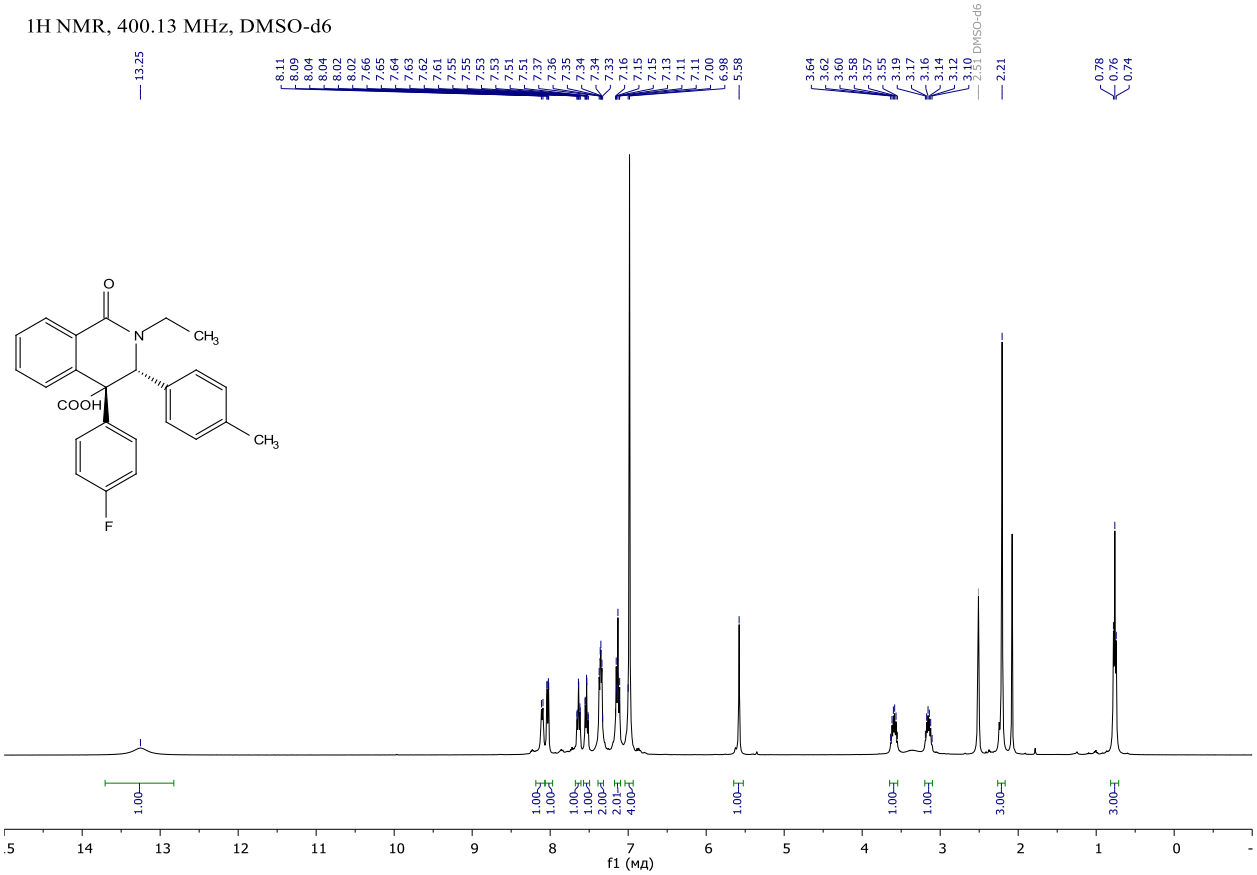


19F NMR, 376.49 MHz, DMSO-d6

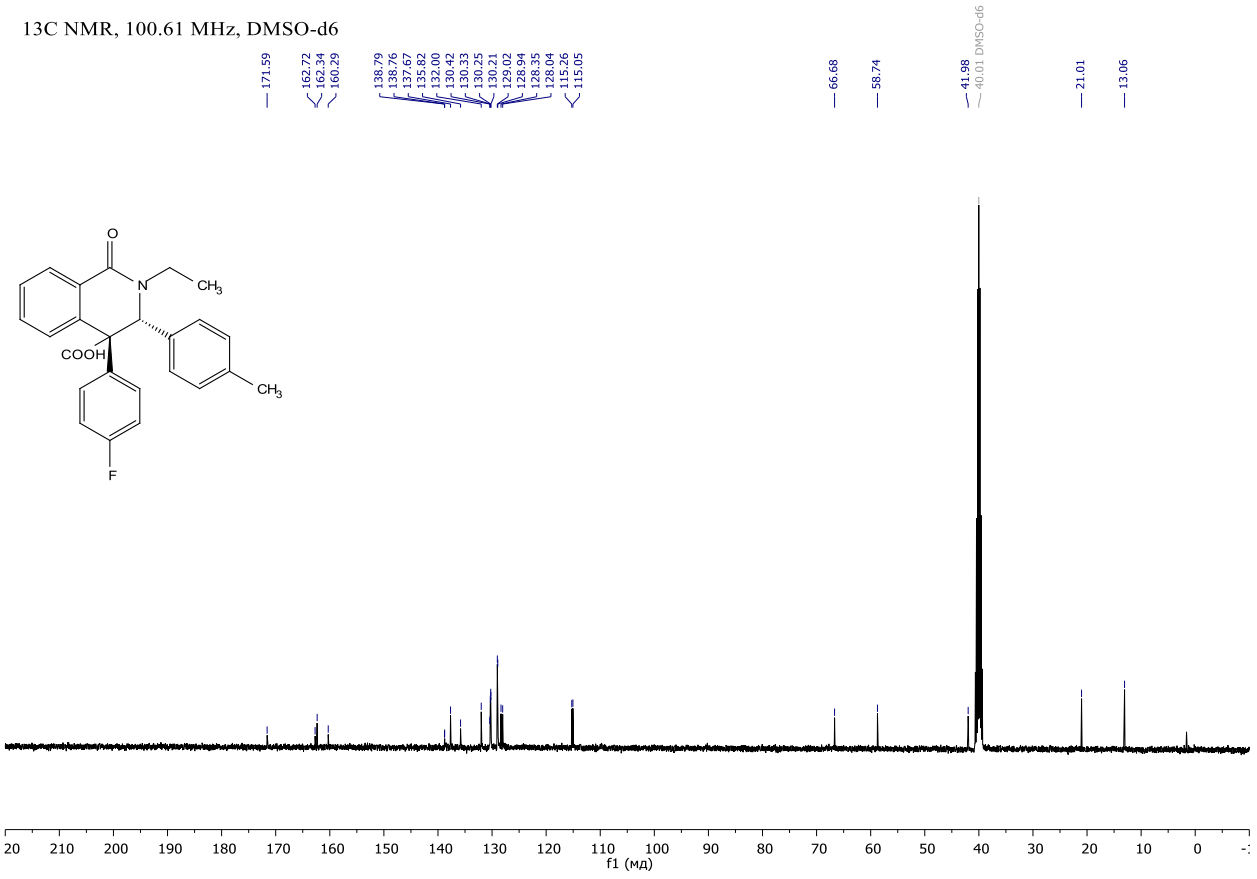


^{1}H, ^{13}C and ^{19}F NMR spectra of compound **9u**

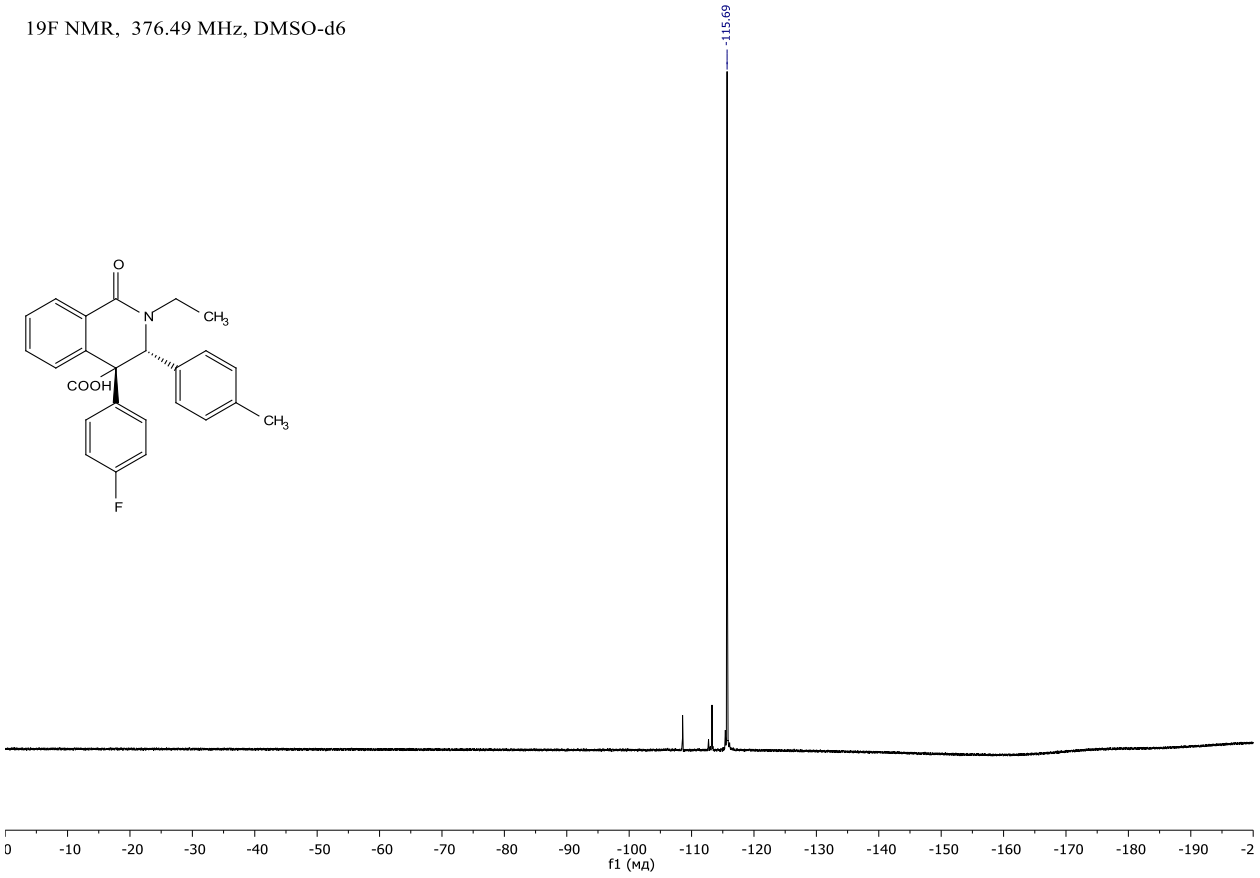
1H NMR, 400.13 MHz, DMSO-d6



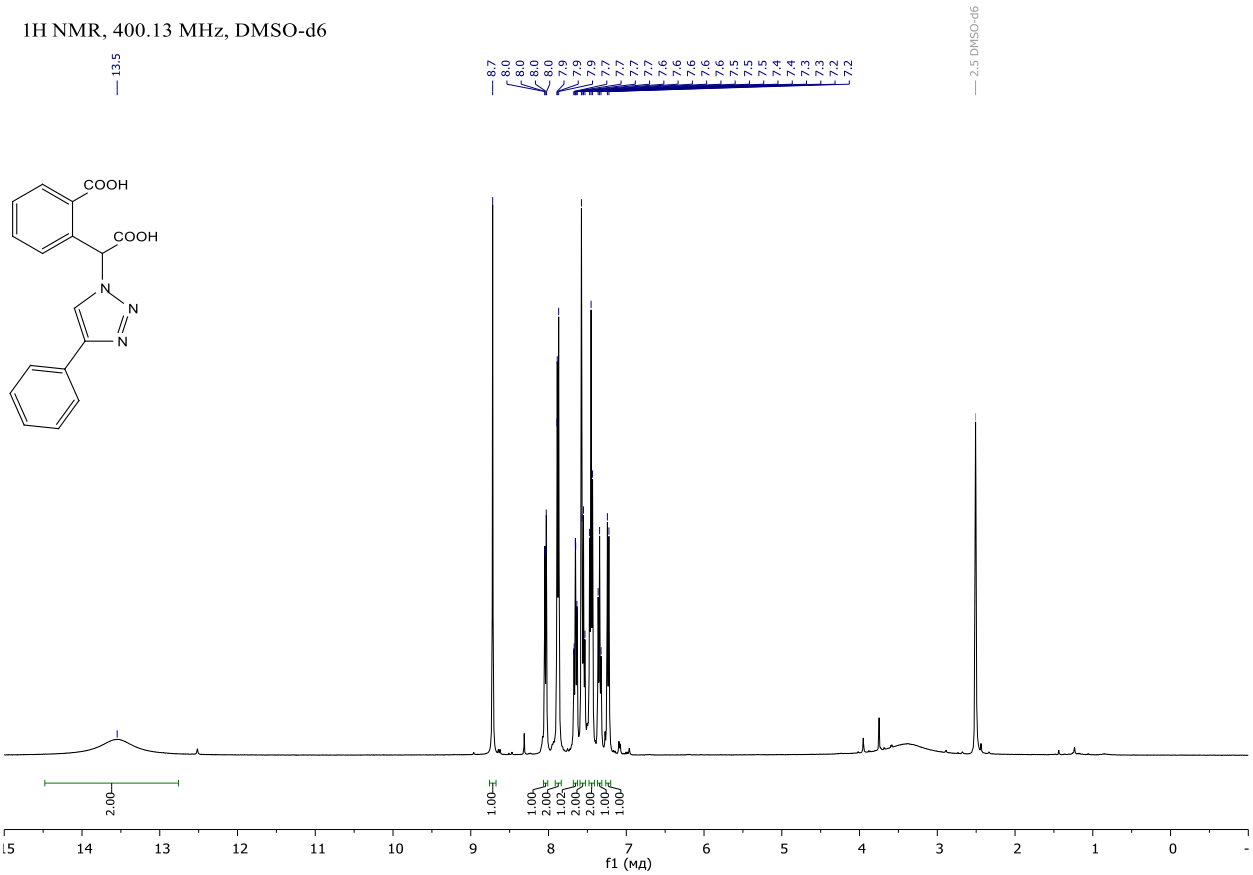
13C NMR, 100.61 MHz, DMSO-d6

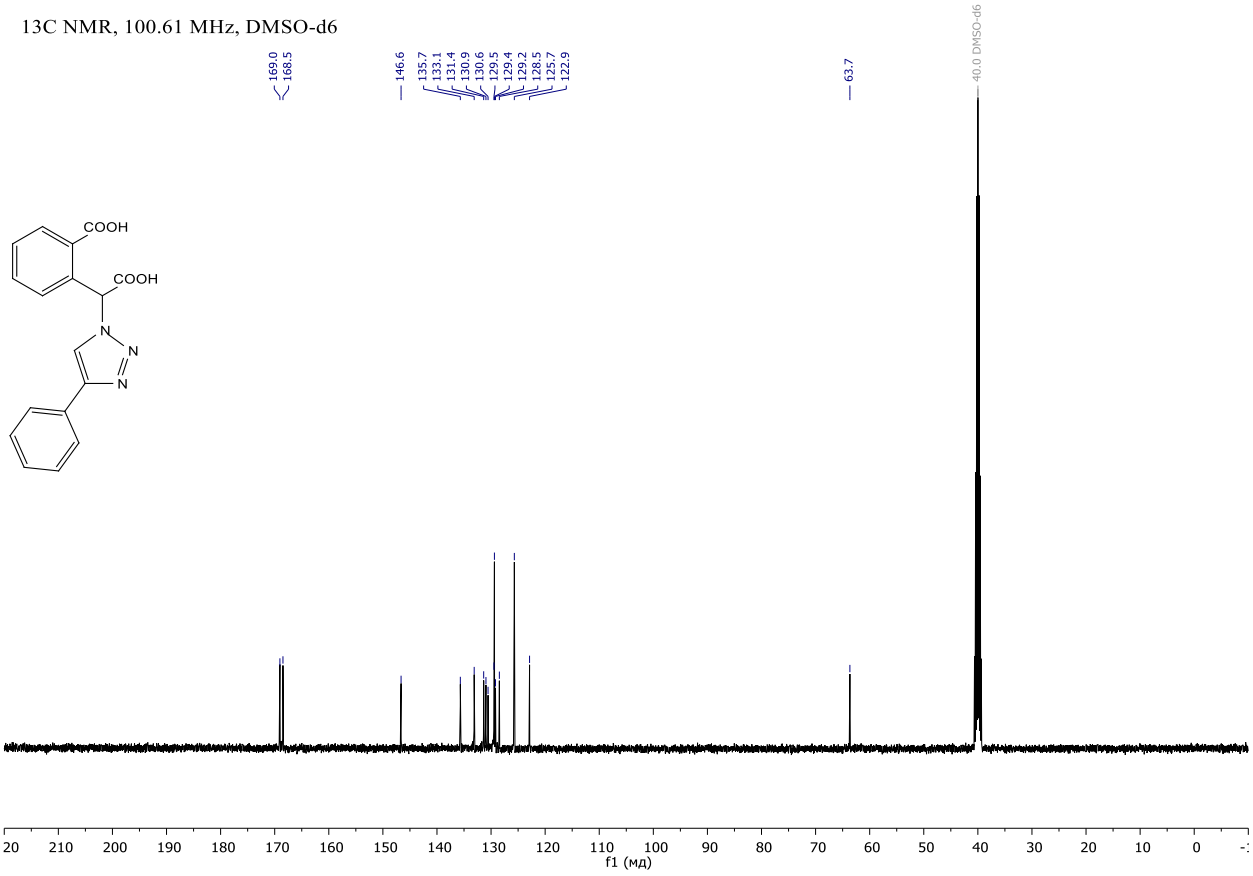


19F NMR, 376.49 MHz, DMSO-d6

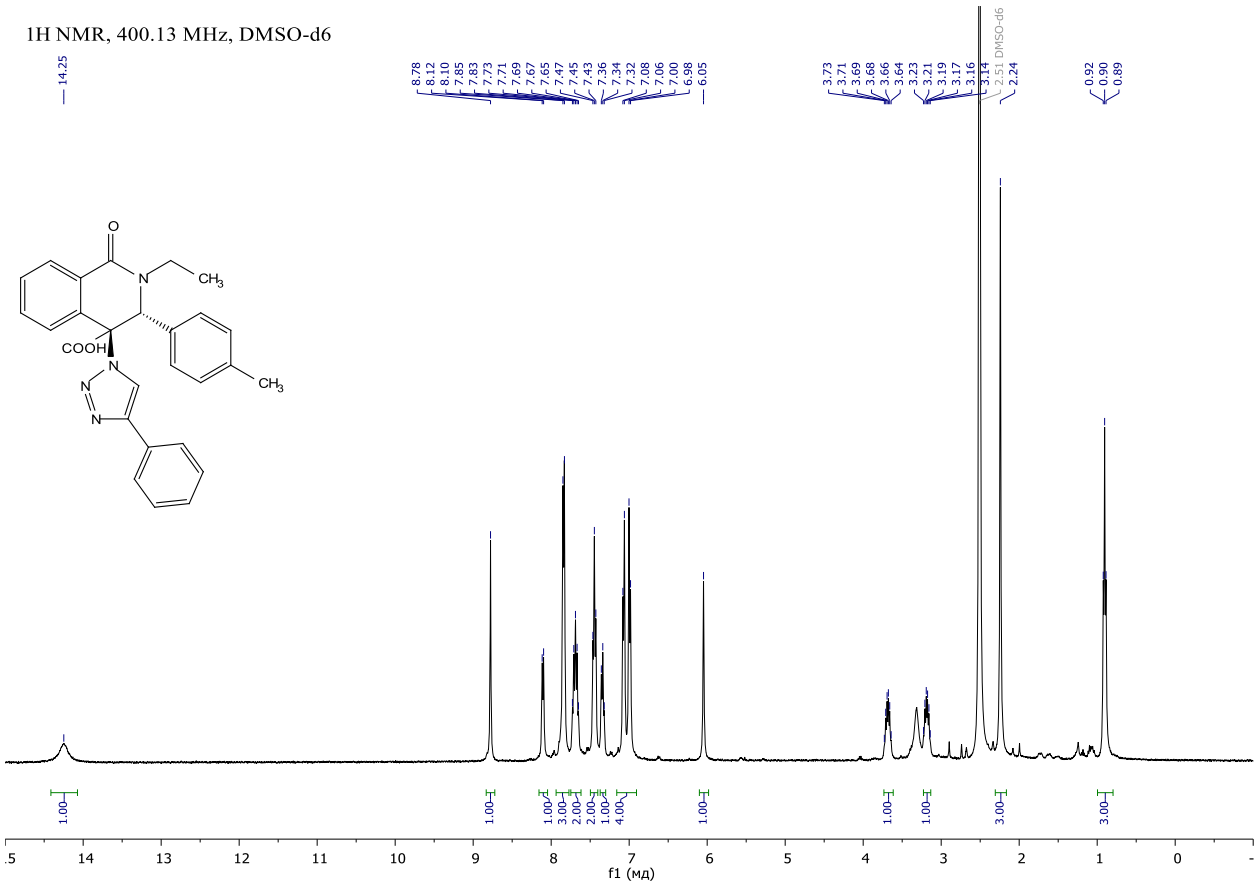


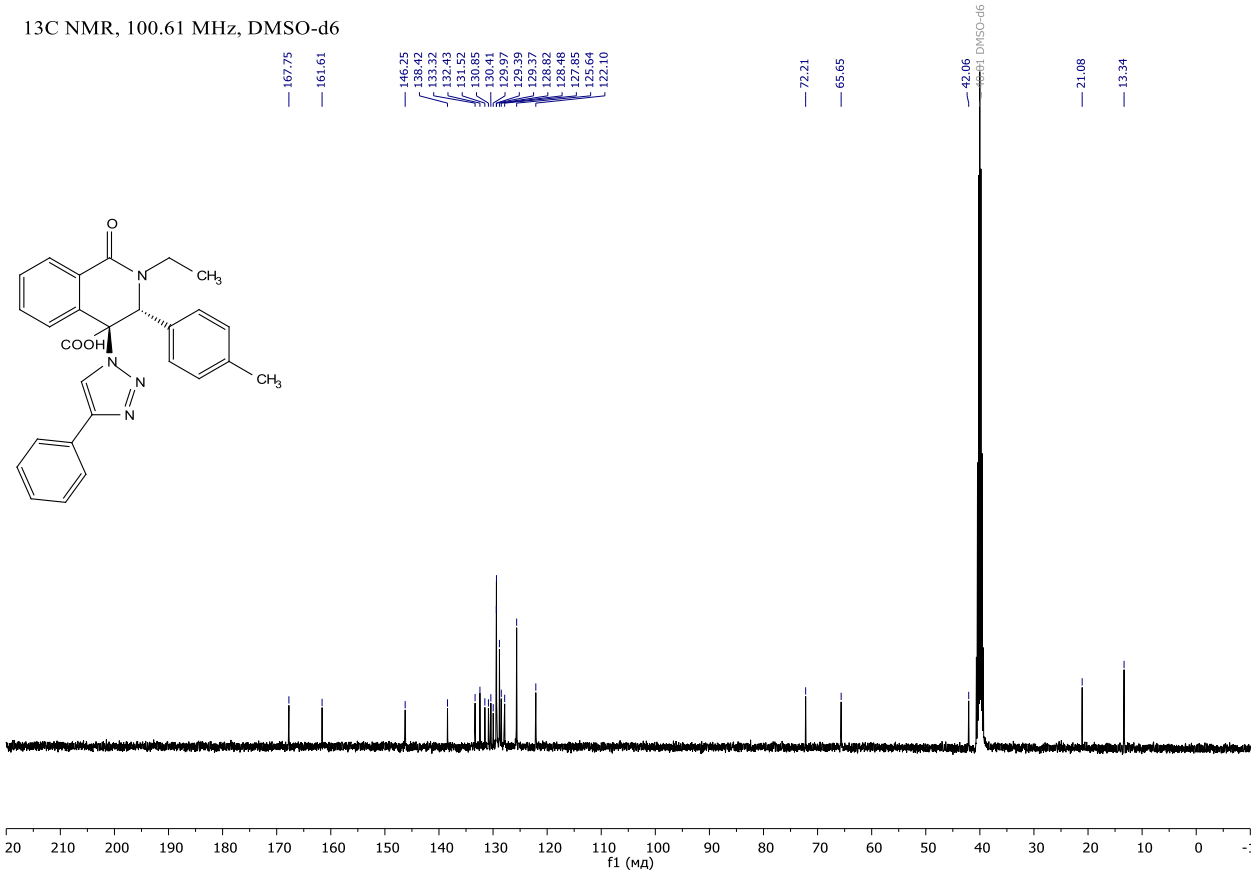
^{1}H and ^{13}C NMR spectra of compound **15**

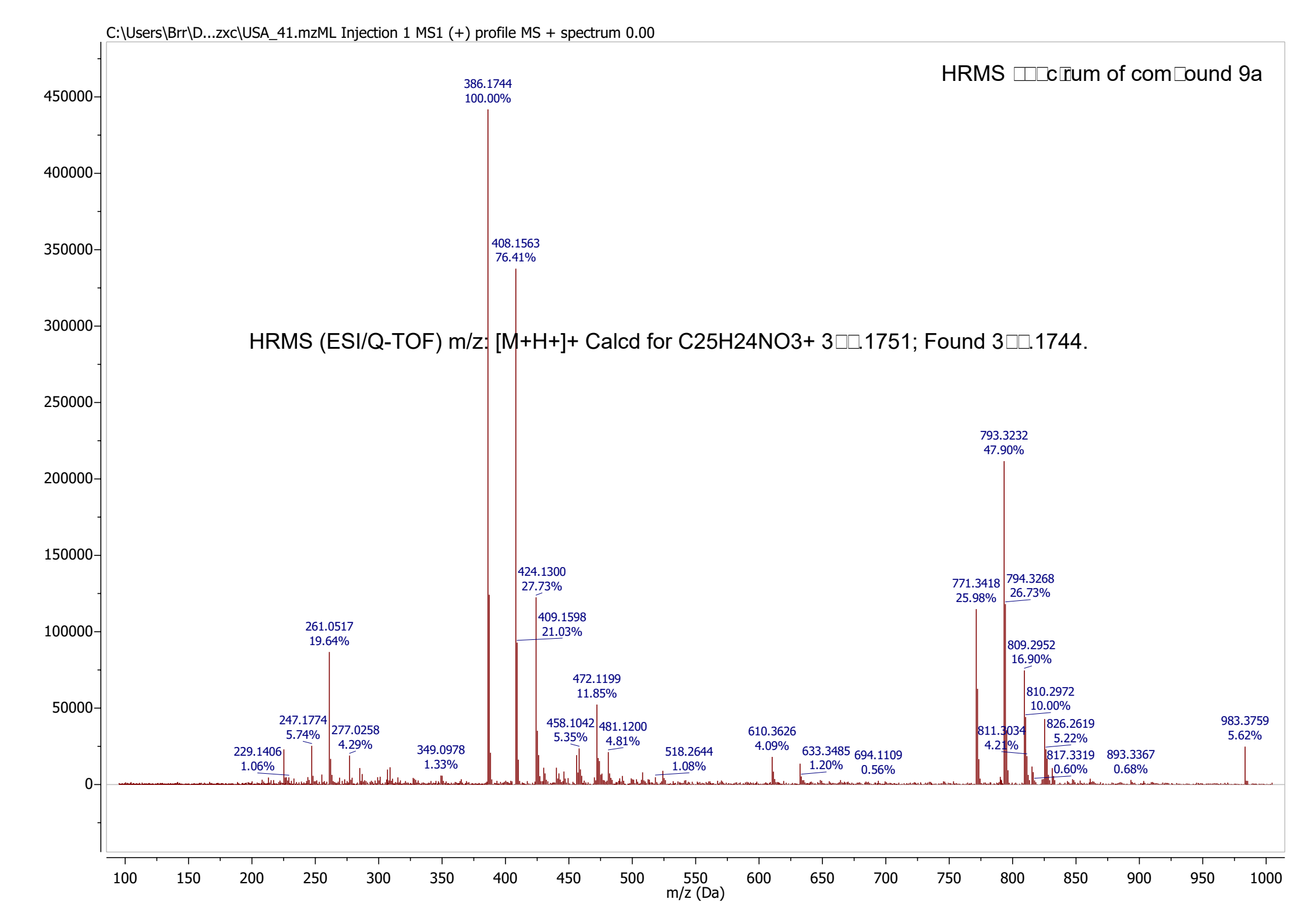


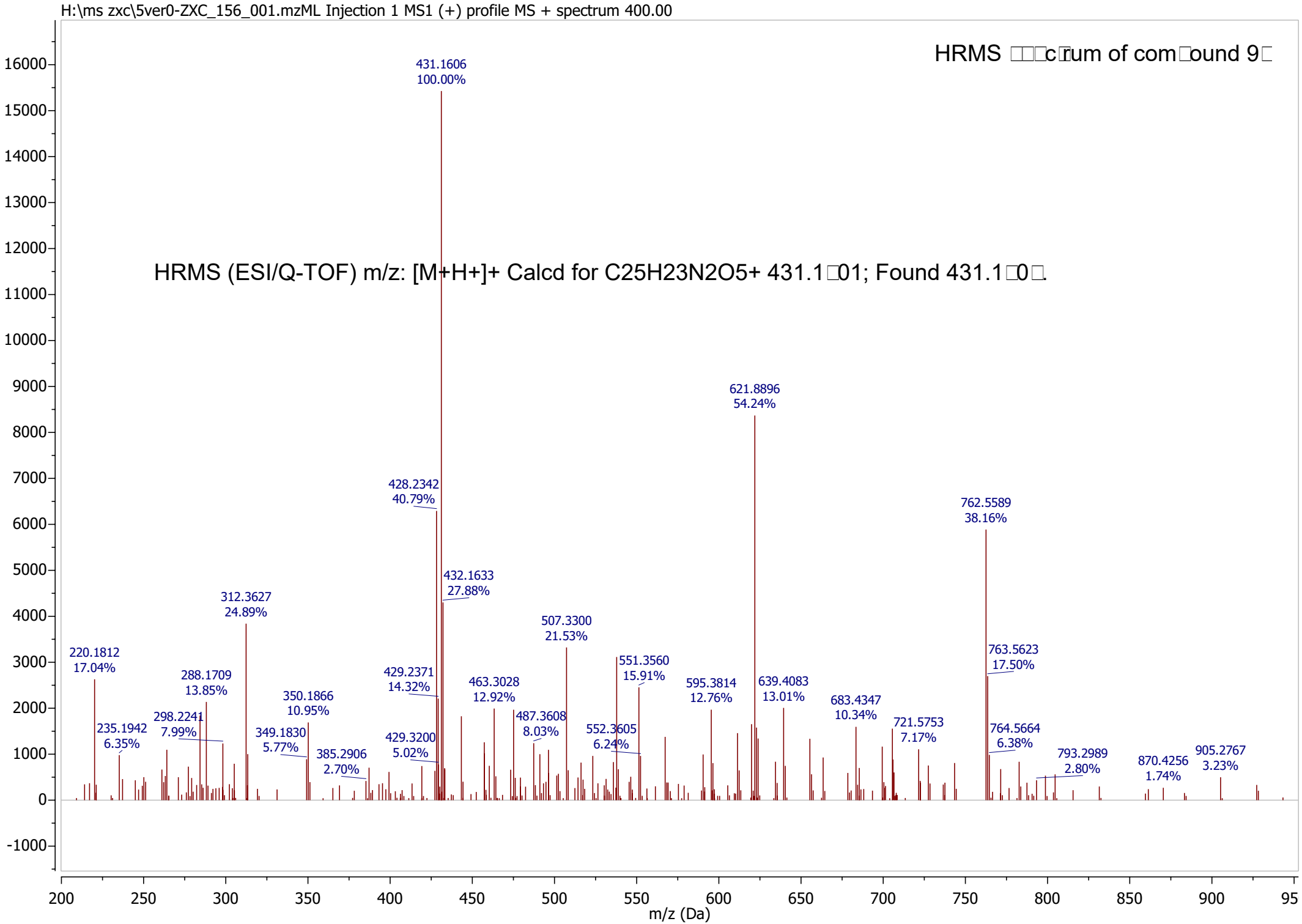


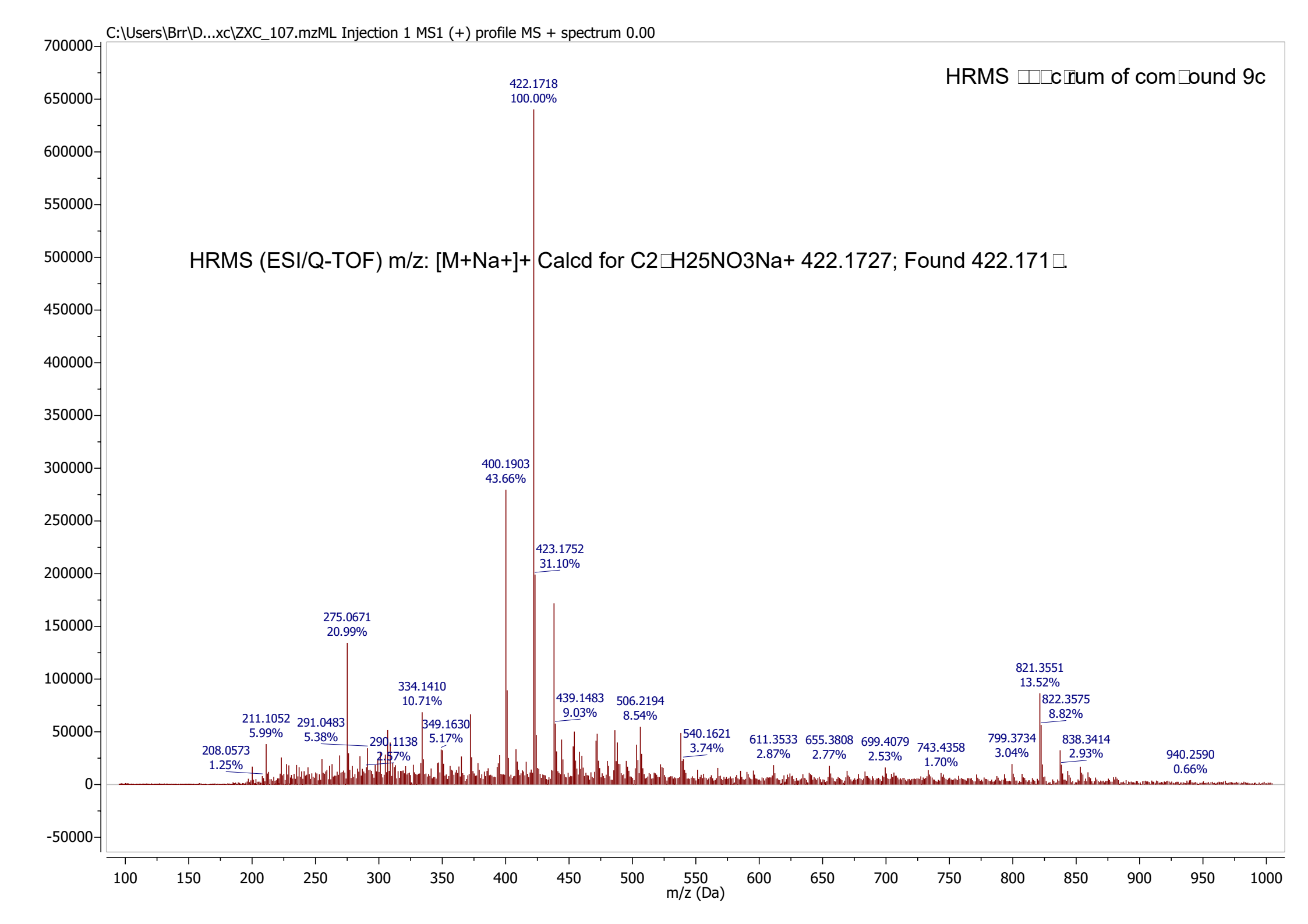
^{1}H and ^{13}C NMR spectra of compound **18**

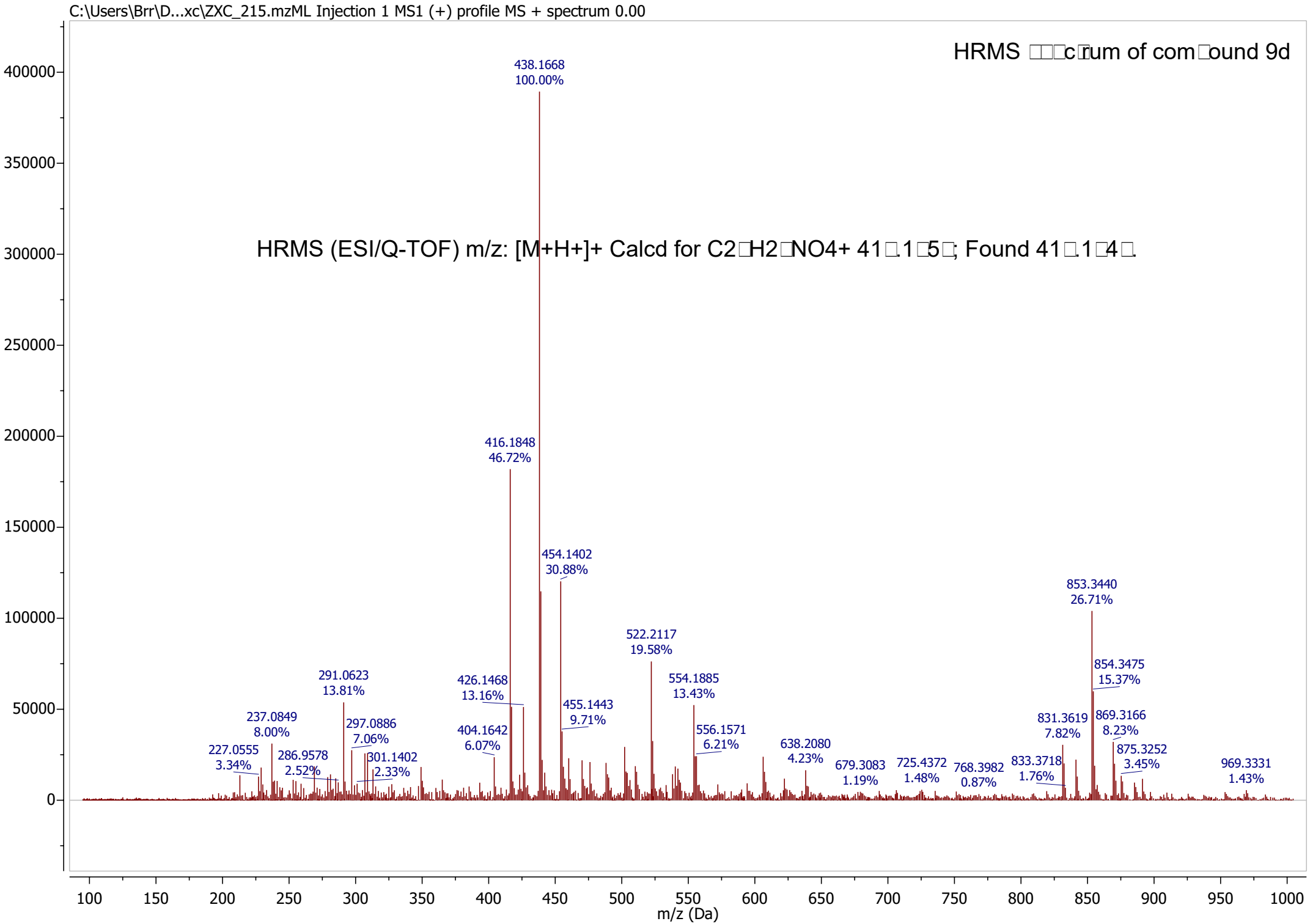


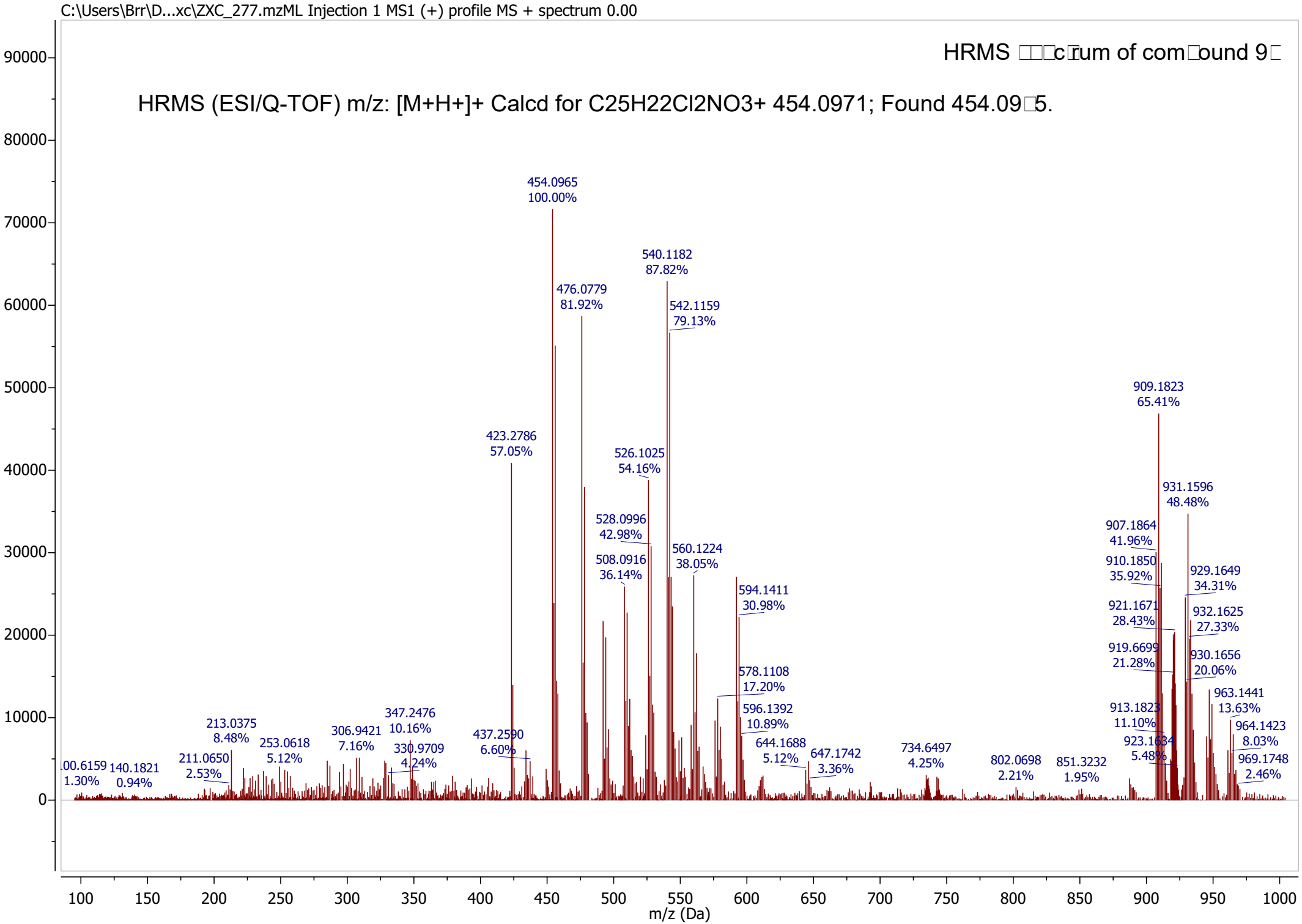


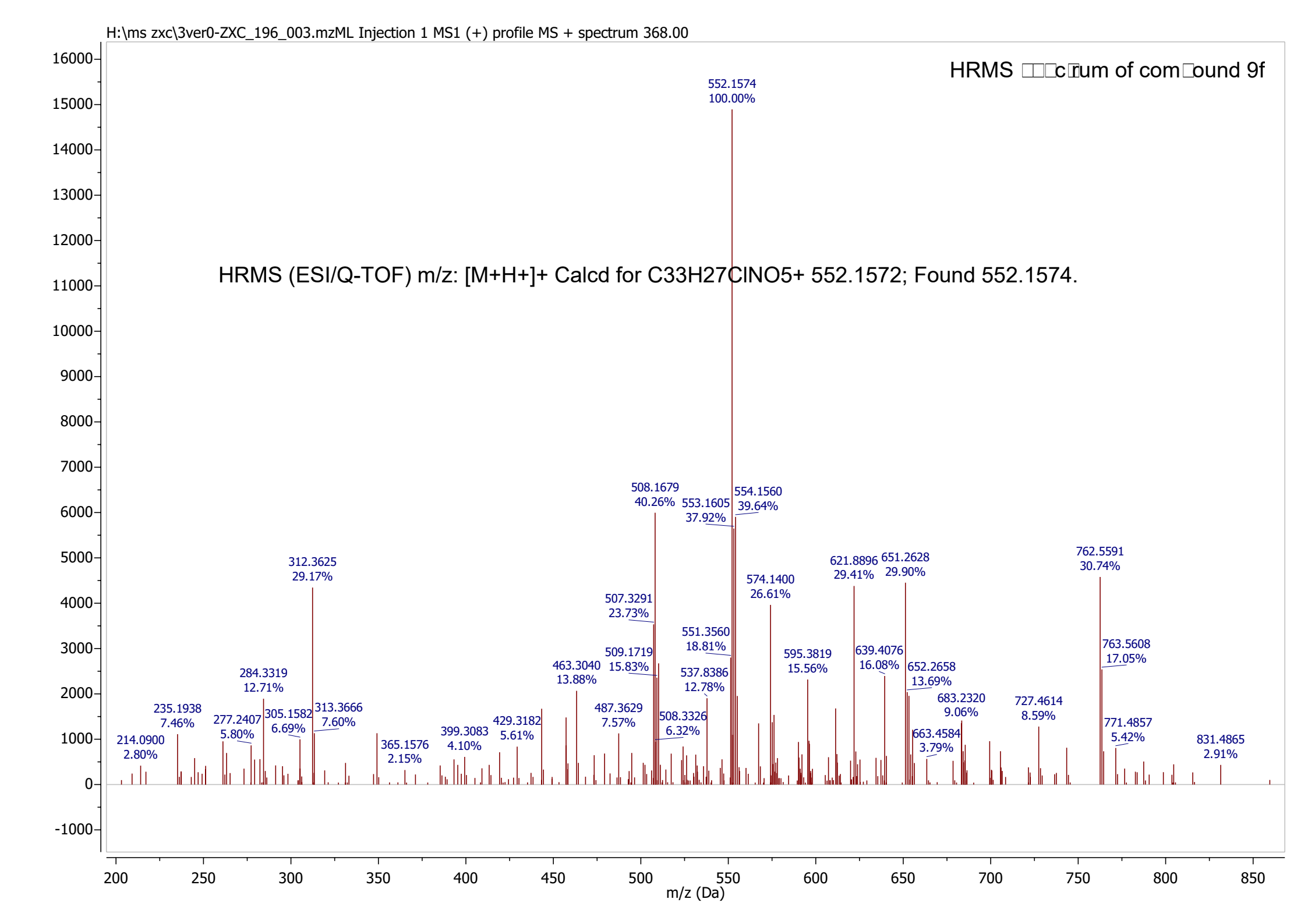

C:\Users\Brr\D...zxc\USA_41.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□um of com□ound 9a
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C25H24NO3+ 3□□.1751; Found 3□□.1744.
386.1744
100.00%
408.1563
76.41%
424.1300
27.73%
409.1598
21.03%
261.0517
19.64%
472.1199
11.85%
247.1774
5.74%
277.0258
4.29%
458.1042
5.35%
481.1200
4.81%
229.1406
1.06%
349.0978
1.33%
518.2644
1.08%
610.3626
4.09%
633.3485
1.20%
694.1109
0.56%
793.3232
47.90%
771.3418
25.98%
794.3268
26.73%
809.2952
16.90%
810.2972
10.00%
826.2619
5.22%
811.3034
4.21%
817.3319
0.60%
893.3367
0.68%
983.3759
5.62%
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z (Da)

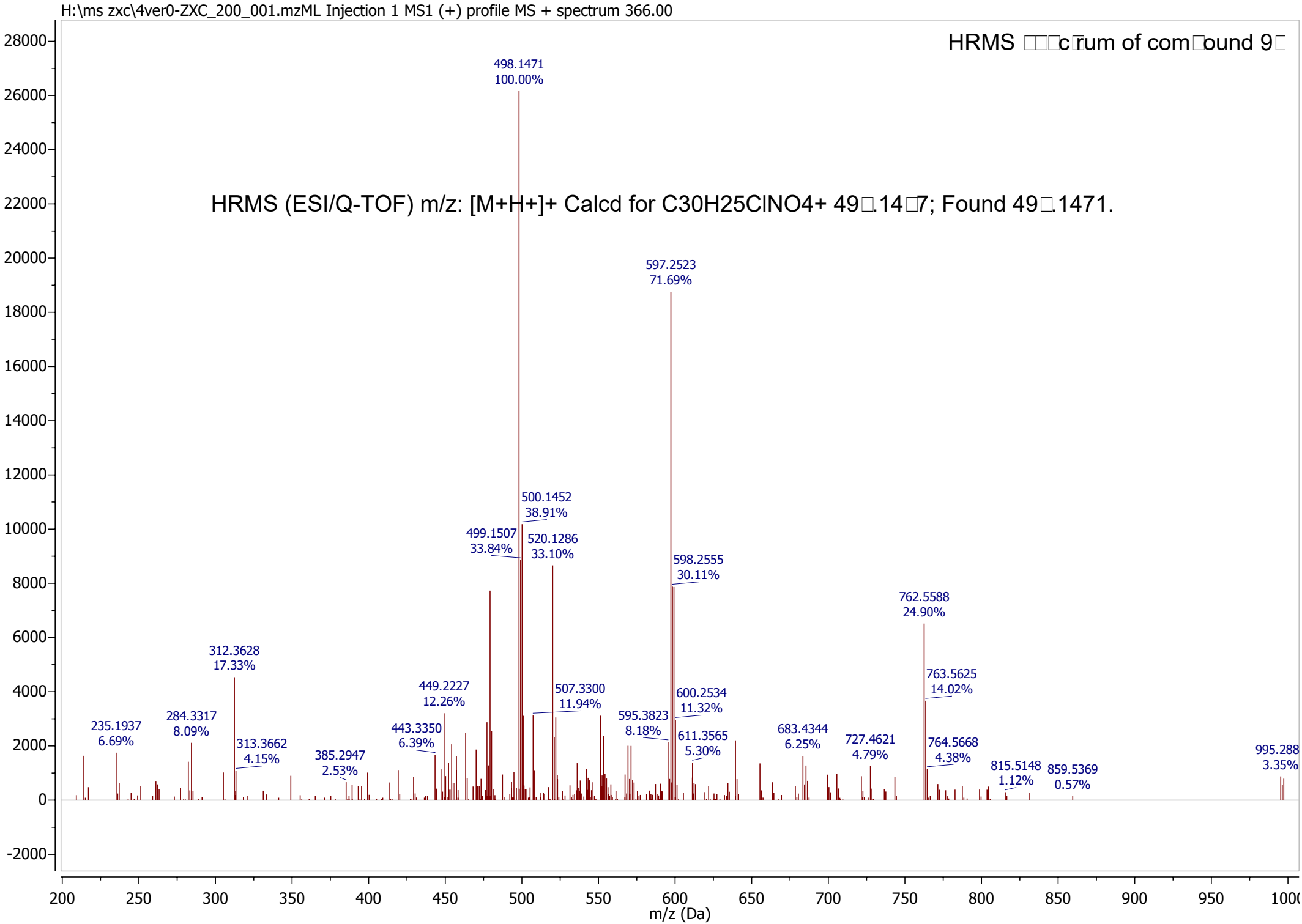

H:\ms zxc\5ver0-ZXC_156_001.mzML Injection 1 MS1 (+) profile MS + spectrum 400.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C25H23N2O5+ 431.1□01; Found 431.1□0□.
431.1606
100.00%
621.8896
54.24%
428.2342
40.79%
762.5589
38.16%
432.1633
27.88%
312.3627
24.89%
507.3300
21.53%
220.1812
17.04%
763.5623
17.50%
551.3560
15.91%
288.1709
13.85%
429.2371
14.32%
463.3028
12.92%
595.3814
12.76%
639.4083
13.01%
683.4347
10.34%
350.1866
10.95%
487.3608
8.03%
721.5753
7.17%
298.2241
7.99%
552.3605
6.24%
764.5664
6.38%
235.1942
6.35%
349.1830
5.77%
429.3200
5.02%
793.2989
2.80%
870.4256
1.74%
905.2767
3.23%
385.2906
2.70%
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
95
m/z (Da)

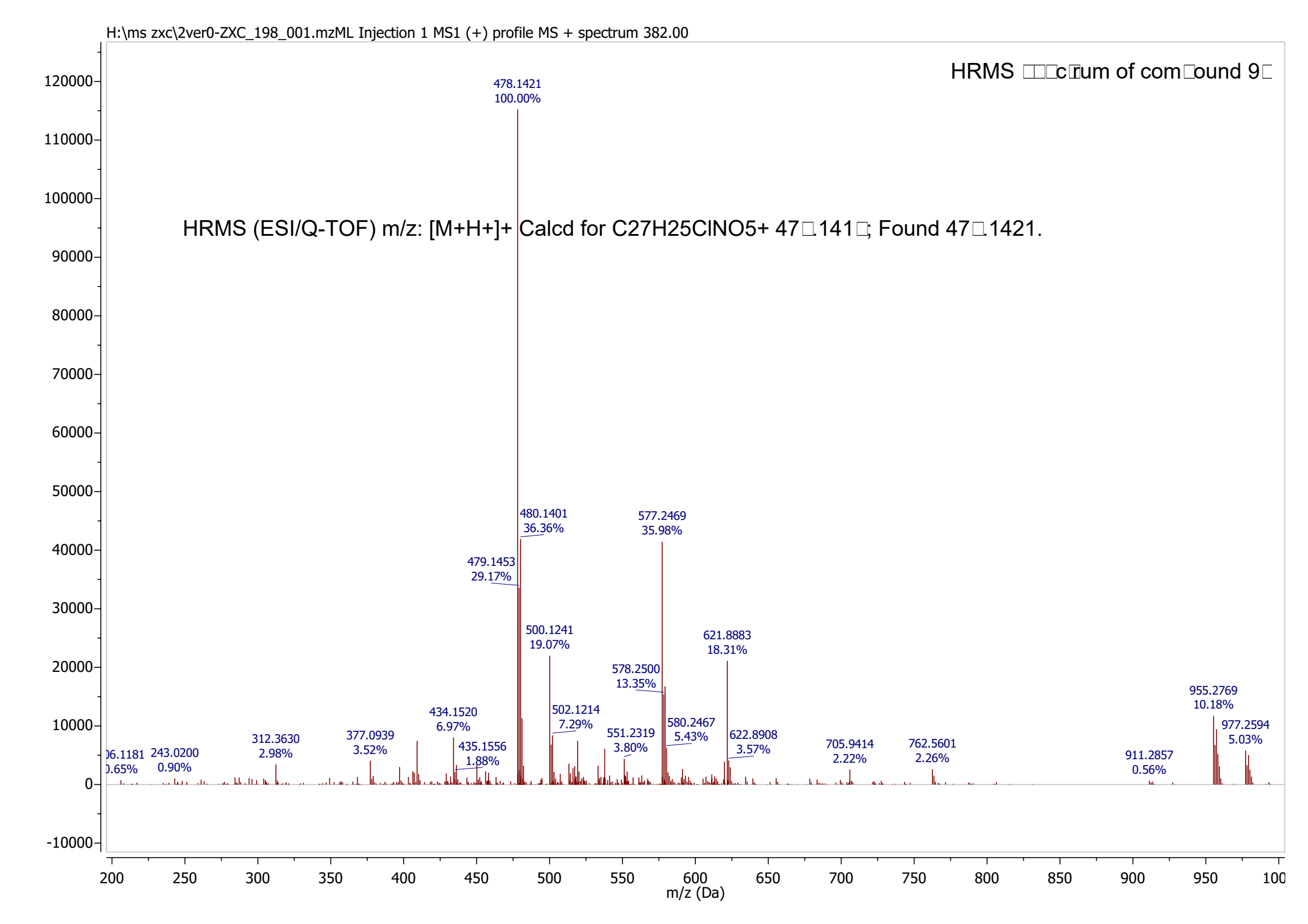

C:\Users\Brr\D...xc\ZXC_107.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□rum of com□ound 9c
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C2□H25NO3Na+ 422.1727; Found 422.171□.
422.1718
100.00%
400.1903
43.66%
423.1752
31.10%
275.0671
20.99%
334.1410
10.71%
211.1052
5.99%
291.0483
5.38%
349.1630
5.17%
208.0573
1.25%
290.1138
2.57%
439.1483
9.03%
506.2194
8.54%
540.1621
3.74%
611.3533
2.87%
655.3808
2.77%
699.4079
2.53%
743.4358
1.70%
821.3551
13.52%
822.3575
8.82%
799.3734
3.04%
838.3414
2.93%
940.2590
0.66%
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z (Da)

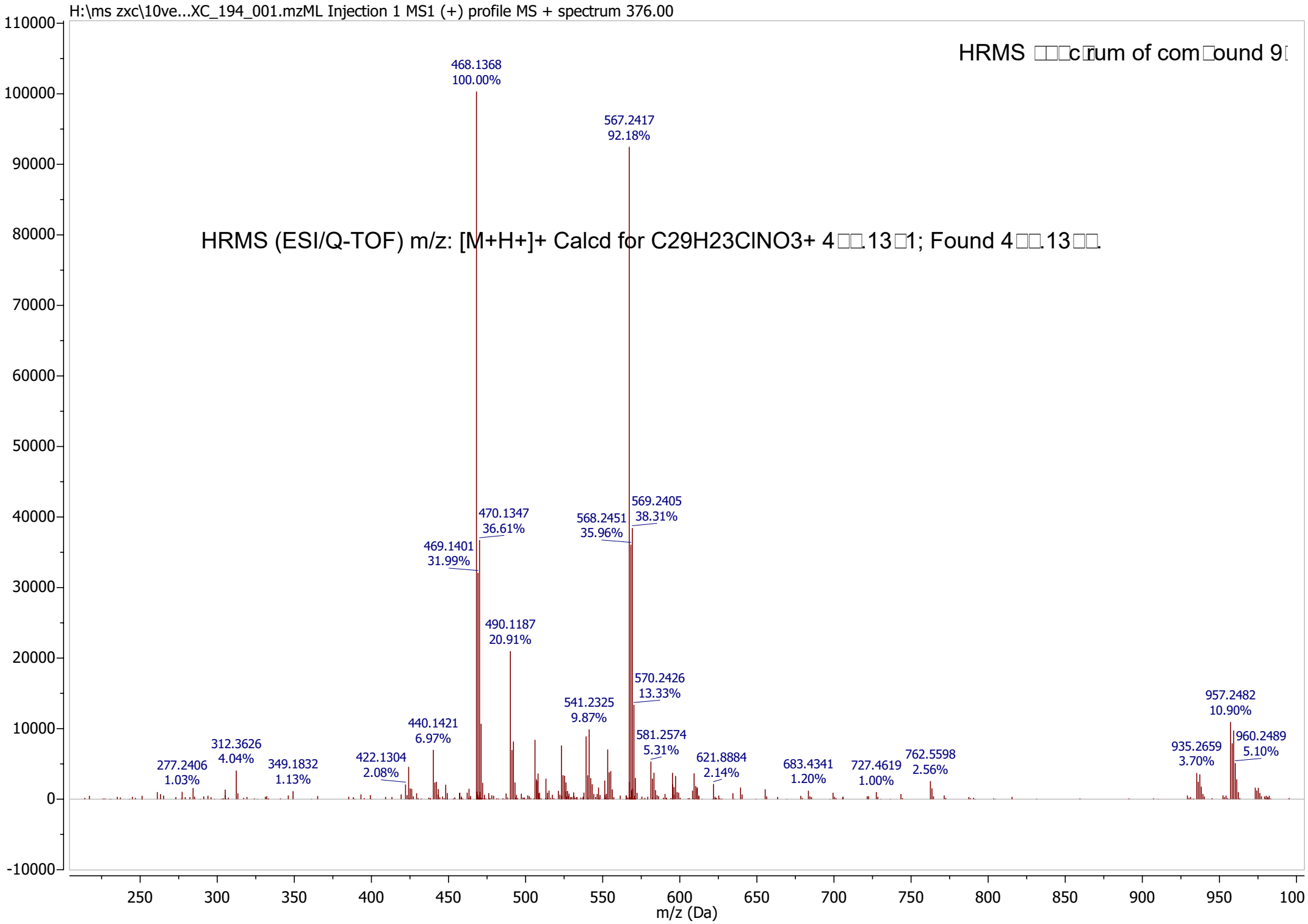

C:\Users\Brr\D...xc\ZXC_215.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□um of com□ound 9d
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C2□H2□NO4+ 41□.1□5□; Found 41□.1□4□.
438.1668
100.00%
416.1848
46.72%
454.1402
30.88%
853.3440
26.71%
522.2117
19.58%
854.3475
15.37%
554.1885
13.43%
291.0623
13.81%
426.1468
13.16%
455.1443
9.71%
237.0849
8.00%
297.0886
7.06%
404.1642
6.07%
831.3619
7.82%
869.3166
8.23%
556.1571
6.21%
227.0555
3.34%
286.9578
2.52%
301.1402
2.33%
638.2080
4.23%
875.3252
3.45%
679.3083
1.19%
725.4372
1.48%
768.3982
0.87%
833.3718
1.76%
969.3331
1.43%
400000
350000
300000
250000
200000
150000
100000
50000
0
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z (Da)

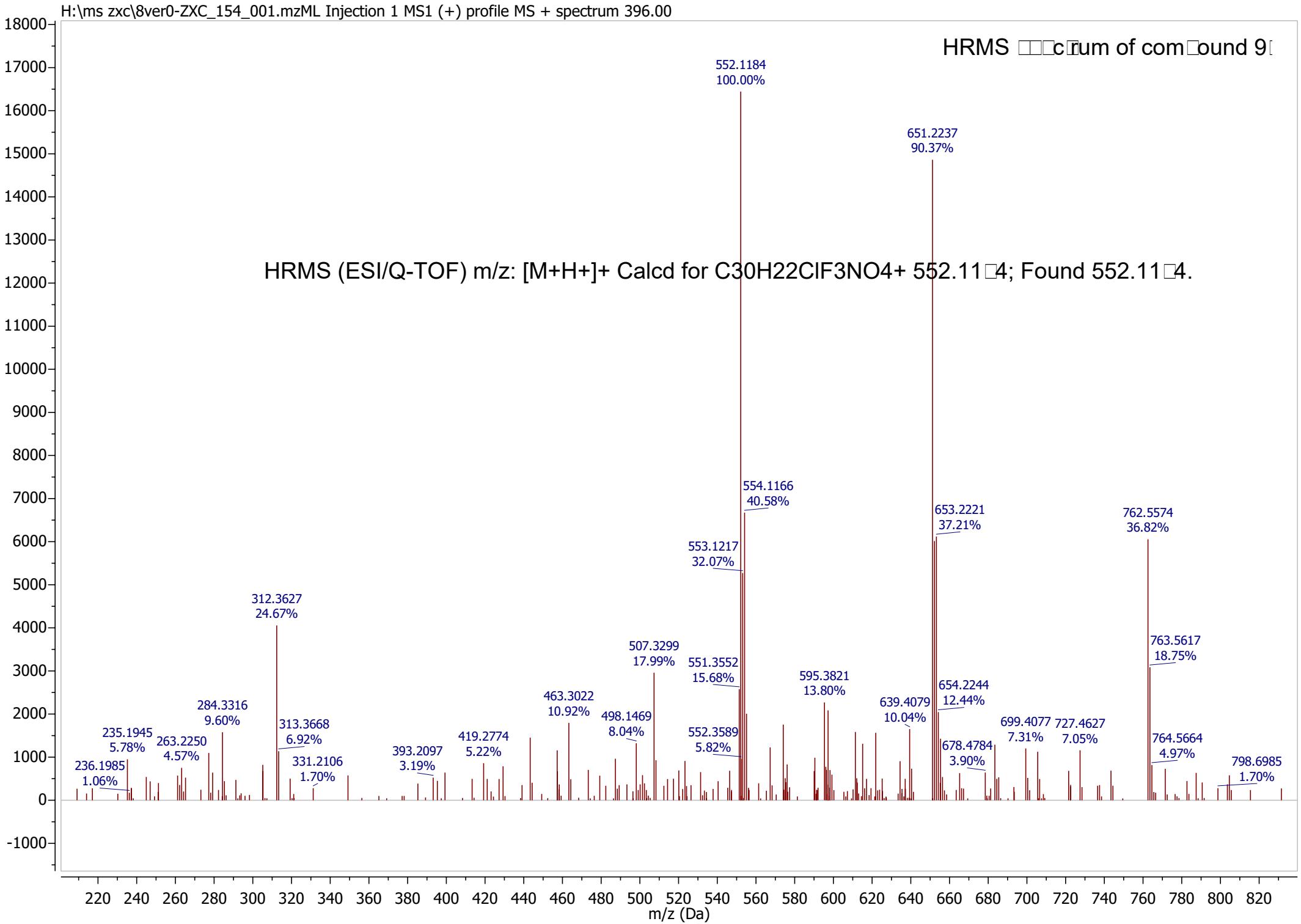

C:\Users\Brr\D...xc\ZXC_277.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C25H22Cl2NO3+ 454.0971; Found 454.09□5.
454.0965 100.00%
540.1182 87.82%
476.0779 81.92%
542.1159 79.13%
909.1823 65.41%
423.2786 57.05%
526.1025 54.16%
931.1596 48.48%
528.0996 42.98%
907.1864 41.96%
560.1224 38.05%
508.0916 36.14%
910.1850 35.92%
929.1649 34.31%
594.1411 30.98%
921.1671 28.43%
932.1625 27.33%
919.6699 21.28%
930.1656 20.06%
578.1108 17.20%
963.1441 13.63%
596.1392 10.89%
913.1823 11.10%
964.1423 8.03%
347.2476 10.16%
213.0375 8.48%
306.9421 7.16%
253.0618 5.12%
437.2590 6.60%
330.9709 4.24%
644.1688 5.12%
923.1634 5.48%
969.1748 2.46%
647.1742 3.36%
734.6497 4.25%
802.0698 2.21%
851.3232 1.95%
211.0650 2.53%
140.1821 0.94%
00.6159 1.30%
m/z (Da)

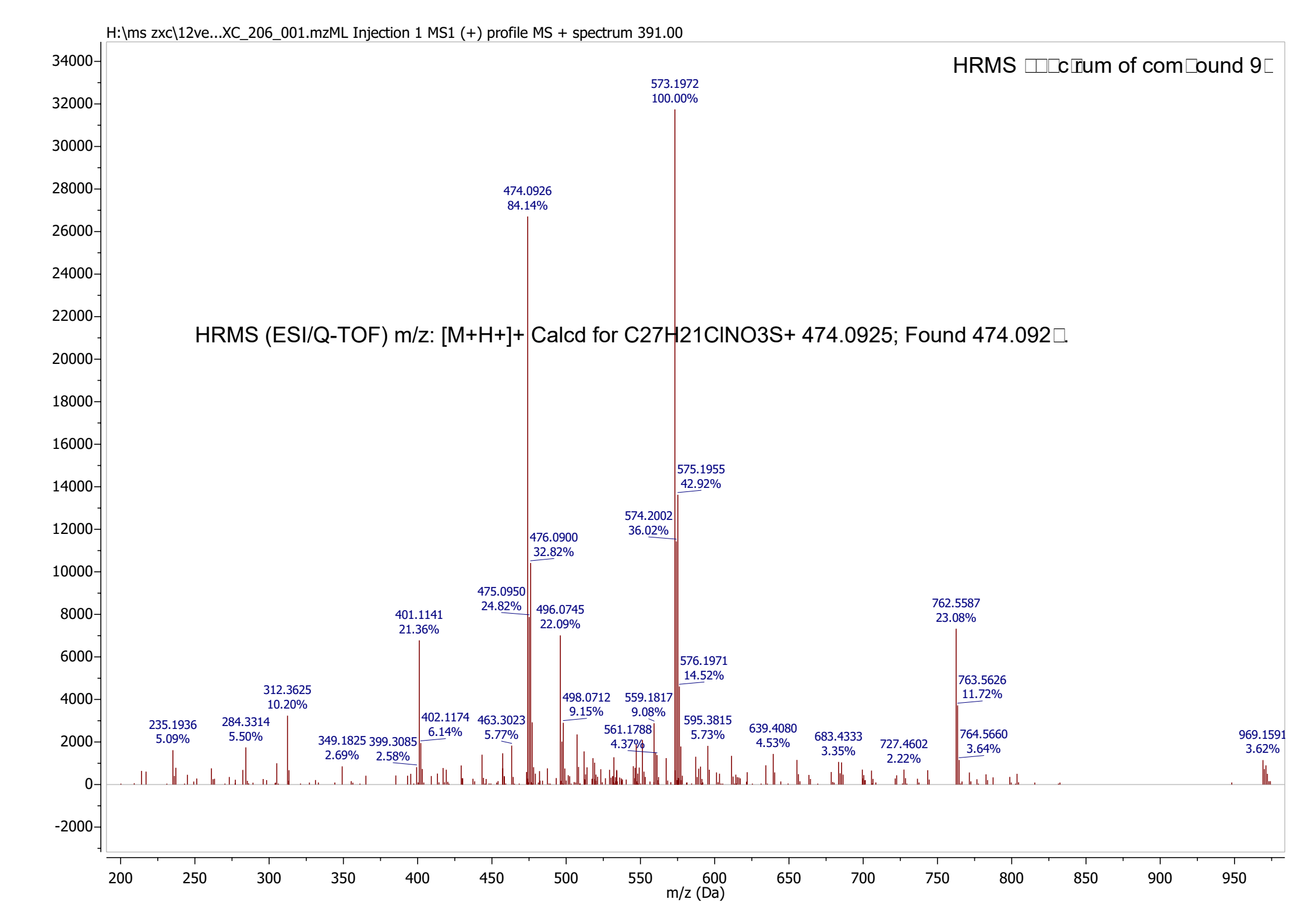

H:\ms zxc\3ver0-ZXC_196_003.mzML Injection 1 MS1 (+) profile MS + spectrum 368.00
HRMS □□□c□um of com□ound 9f
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C33H27ClNO5+ 552.1572; Found 552.1574.
552.1574 100.00%
508.1679 40.26%
553.1605 37.92%
554.1560 39.64%
312.3625 29.17%
621.8896 29.41%
651.2628 29.90%
762.5591 30.74%
574.1400 26.61%
507.3291 23.73%
551.3560 18.81%
595.3819 15.56%
639.4076 16.08%
763.5608 17.05%
509.1719 15.83%
463.3040 13.88%
537.8386 12.78%
652.2658 13.69%
284.3319 12.71%
683.2320 9.06%
727.4614 8.59%
235.1938 7.46%
305.1582 6.69%
313.3666 7.60%
277.2407 5.80%
487.3629 7.57%
508.3326 6.32%
429.3182 5.61%
399.3083 4.10%
663.4584 3.79%
771.4857 5.42%
214.0900 2.80%
365.1576 2.15%
831.4865 2.91%
m/z (Da)

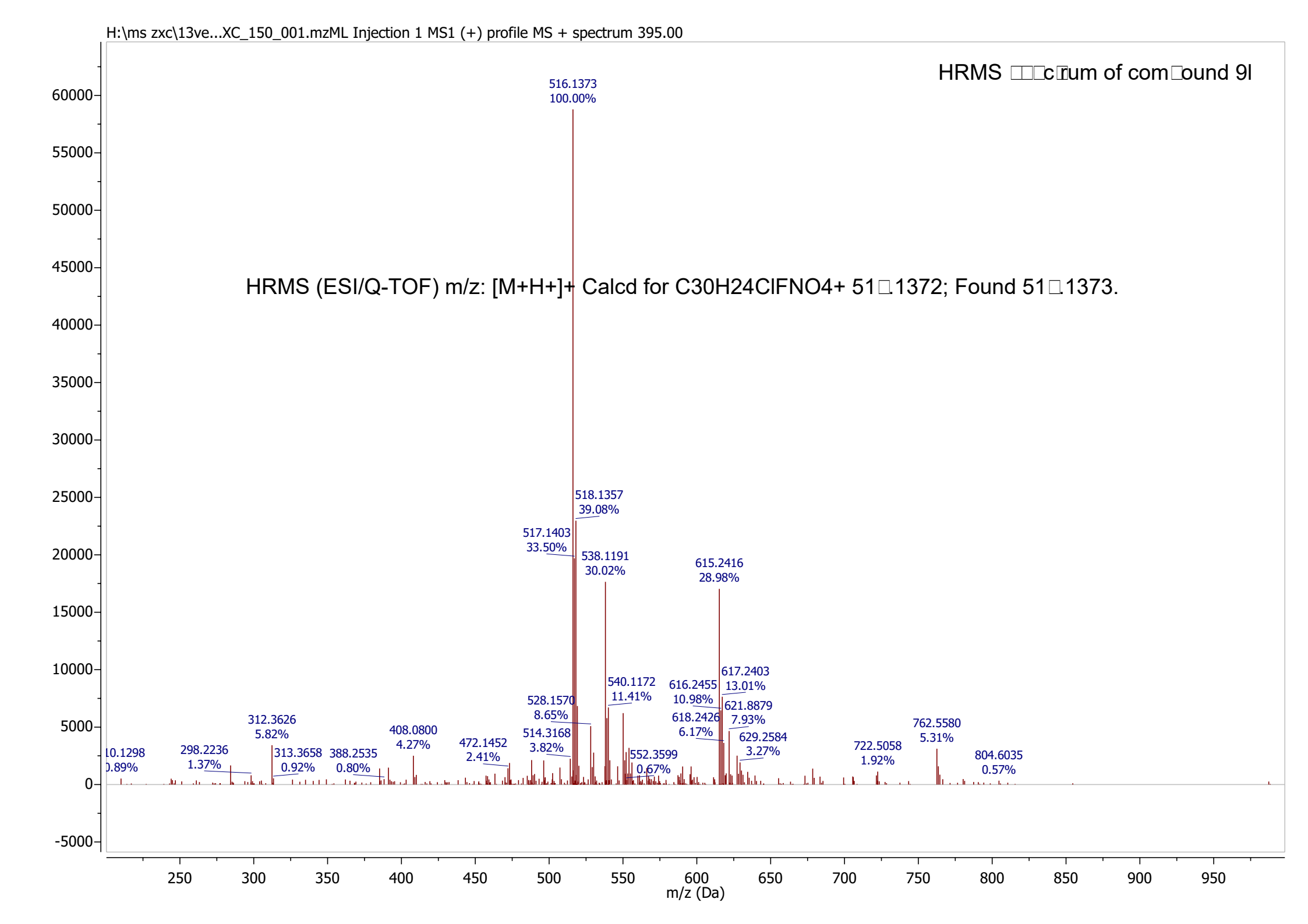

H:\ms zxc\4ver0-ZXC_200_001.mzML Injection 1 MS1 (+) profile MS + spectrum 366.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C30H25ClNO4+ 49□.14□7; Found 49□.1471.
498.1471
100.00%
597.2523
71.69%
500.1452
38.91%
499.1507
33.84%
520.1286
33.10%
598.2555
30.11%
762.5588
24.90%
312.3628
17.33%
763.5625
14.02%
449.2227
12.26%
507.3300
11.94%
600.2534
11.32%
595.3823
8.18%
611.3565
5.30%
683.4344
6.25%
727.4621
4.79%
764.5668
4.38%
235.1937
6.69%
284.3317
8.09%
313.3662
4.15%
385.2947
2.53%
443.3350
6.39%
815.5148
1.12%
859.5369
0.57%
995.288
3.35%
m/z (Da)

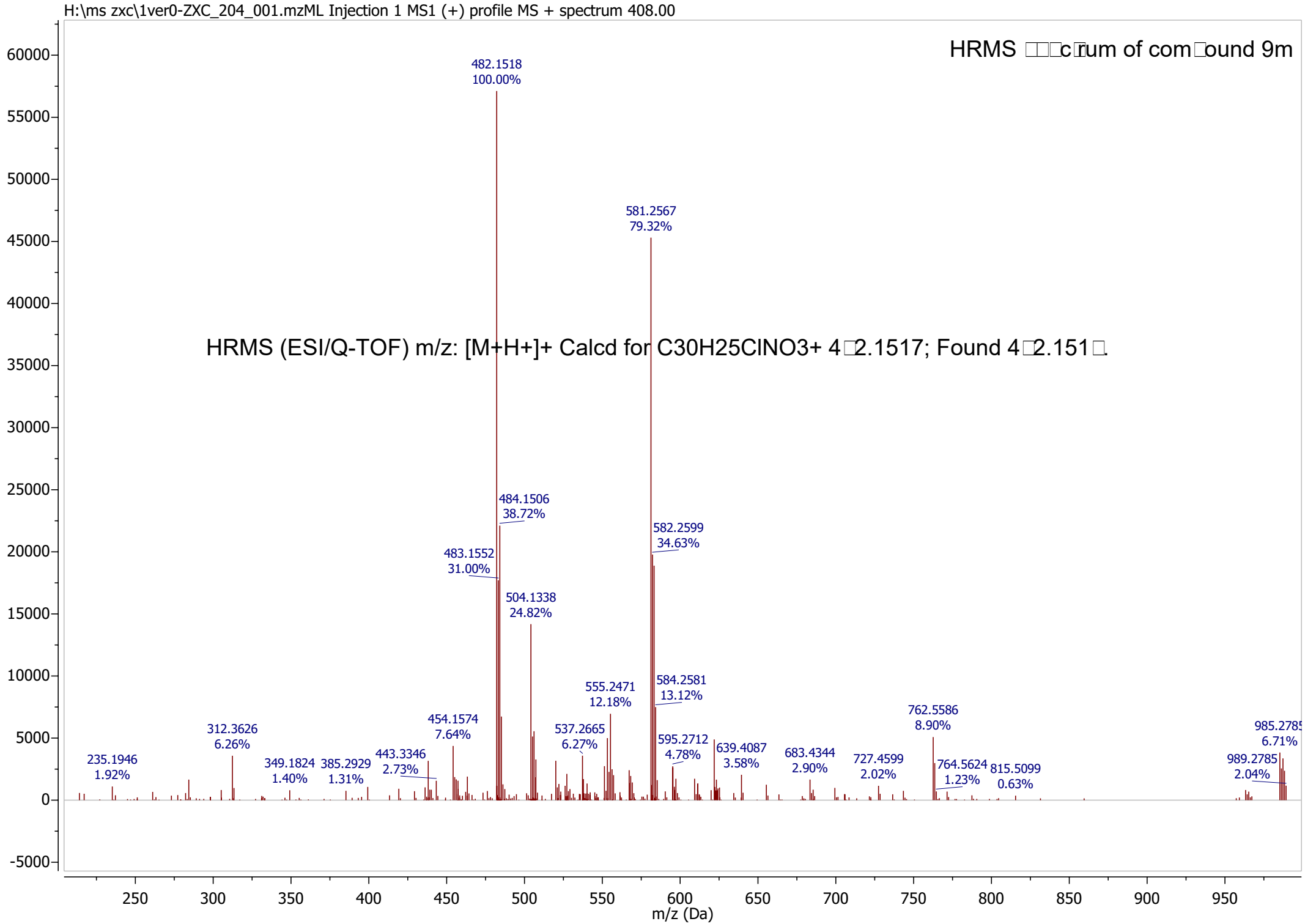

H:\ms zxc\2ver0-ZXC_198_001.mzML Injection 1 MS1 (+) profile MS + spectrum 382.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C27H25ClNO5+ 47□.141□; Found 47□.1421.
478.1421
100.00%
480.1401
36.36%
577.2469
35.98%
479.1453
29.17%
500.1241
19.07%
621.8883
18.31%
578.2500
13.35%
955.2769
10.18%
434.1520
6.97%
502.1214
7.29%
580.2467
5.43%
977.2594
5.03%
551.2319
3.80%
622.8908
3.57%
312.3630
2.98%
377.0939
3.52%
435.1556
1.88%
705.9414
2.22%
762.5601
2.26%
243.0200
0.90%
911.2857
0.56%
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
m/z (Da)

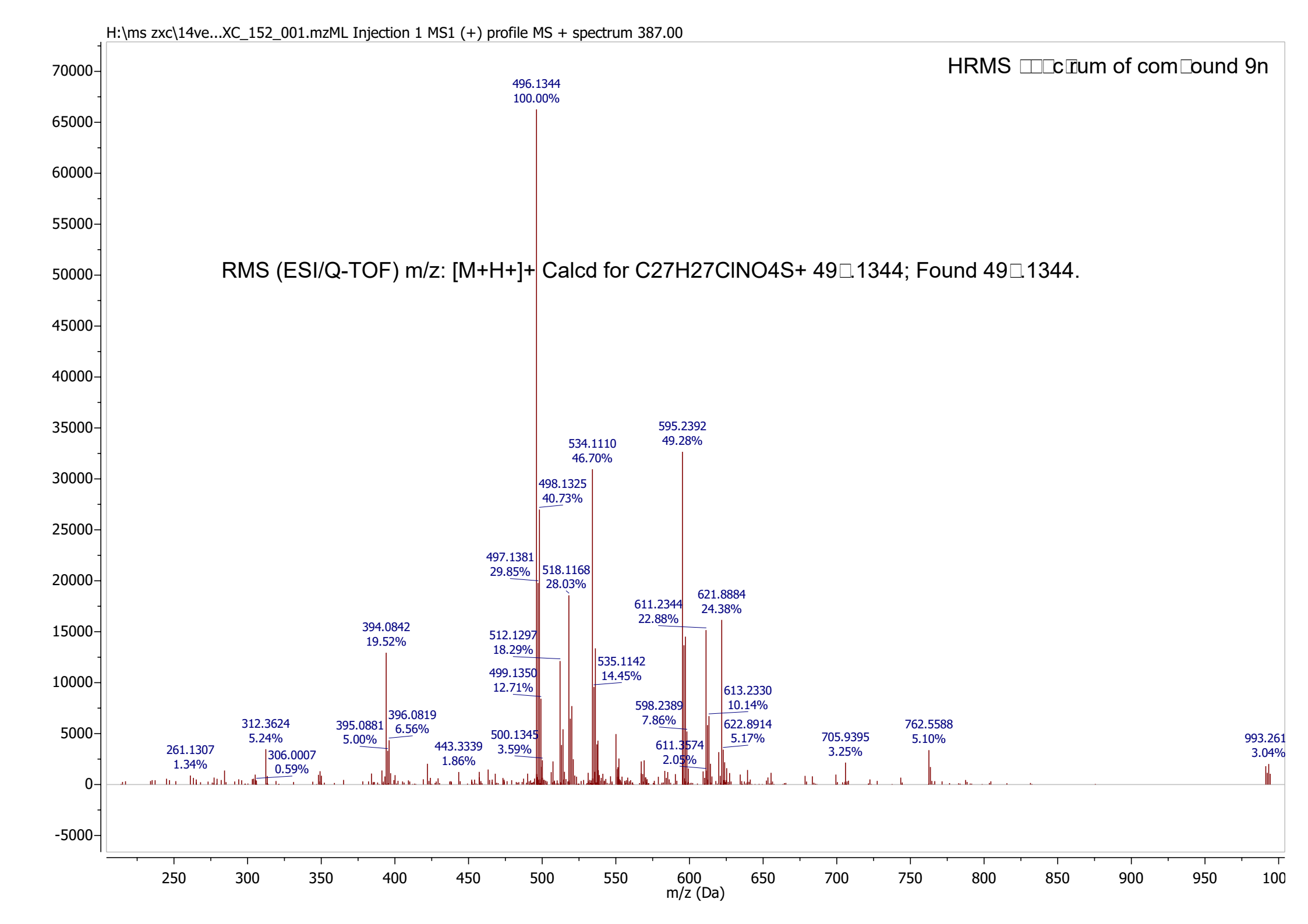

H:\ms zxc\10ve...XC_194_001.mzML Injection 1 MS1 (+) profile MS + spectrum 376.00
HRMS □□□c□rum of com□ound 9[
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C29H23ClNO3+ 4□□.13□1; Found 4□□.13□□.
468.1368
100.00%
567.2417
92.18%
470.1347
36.61%
569.2405
38.31%
568.2451
35.96%
469.1401
31.99%
490.1187
20.91%
570.2426
13.33%
541.2325
9.87%
440.1421
6.97%
581.2574
5.31%
957.2482
10.90%
960.2489
5.10%
312.3626
4.04%
277.2406
1.03%
349.1832
1.13%
422.1304
2.08%
621.8884
2.14%
683.4341
1.20%
727.4619
1.00%
762.5598
2.56%
935.2659
3.70%
m/z (Da)

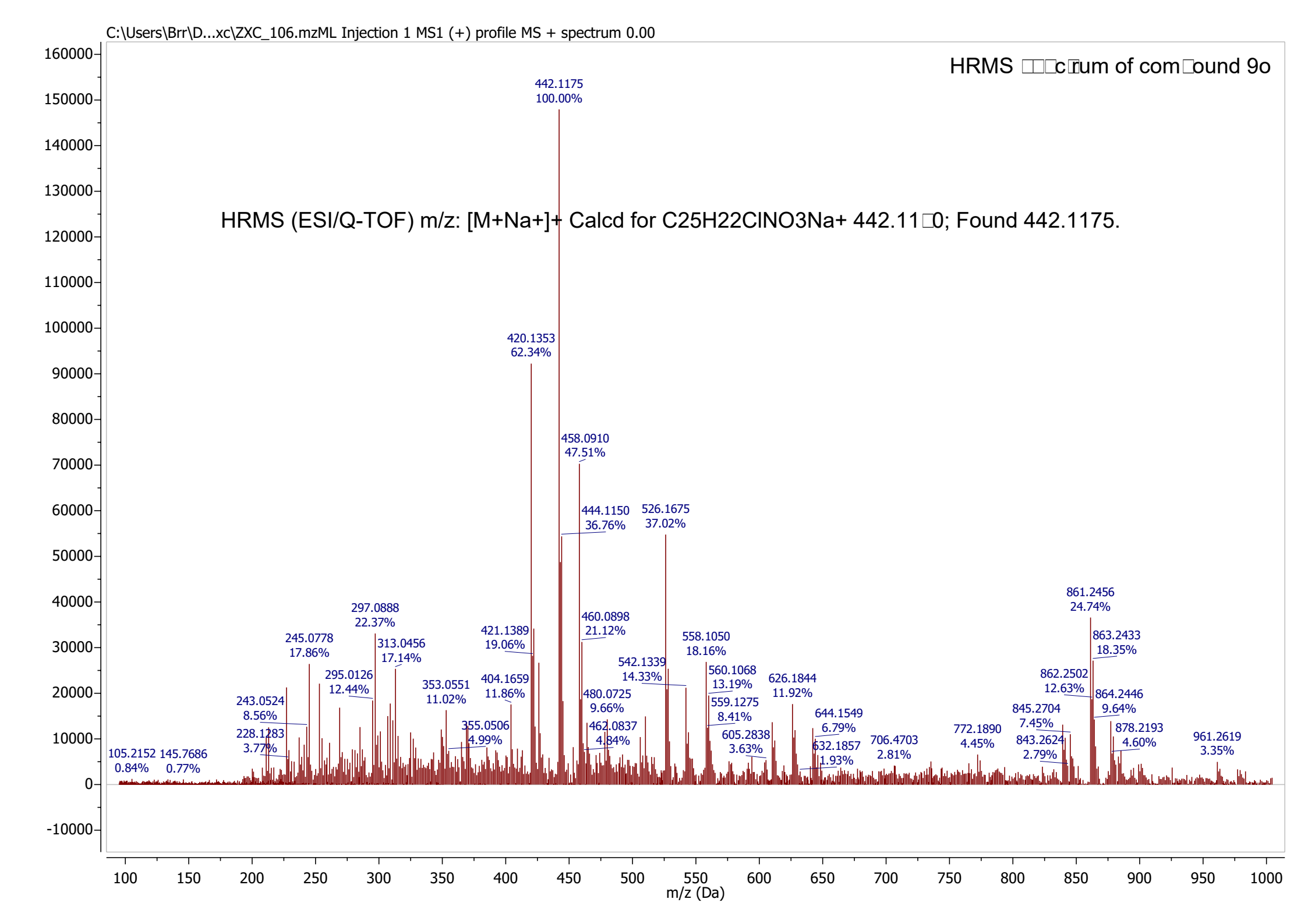

H:\ms zxc\8ver0-ZXC_154_001.mzML Injection 1 MS1 (+) profile MS + spectrum 396.00
HRMS □□□c□um of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C30H22ClF3NO4+ 552.11□4; Found 552.11□4.
552.1184
100.00%
651.2237
90.37%
554.1166
40.58%
653.2221
37.21%
762.5574
36.82%
553.1217
32.07%
312.3627
24.67%
507.3299
17.99%
763.5617
18.75%
551.3552
15.68%
595.3821
13.80%
654.2244
12.44%
639.4079
10.04%
463.3022
10.92%
498.1469
8.04%
284.3316
9.60%
313.3668
6.92%
699.4077
7.31%
727.4627
7.05%
235.1945
5.78%
263.2250
4.57%
419.2774
5.22%
552.3589
5.82%
764.5664
4.97%
678.4784
3.90%
393.2097
3.19%
331.2106
1.70%
798.6985
1.70%
236.1985
1.06%
m/z (Da)

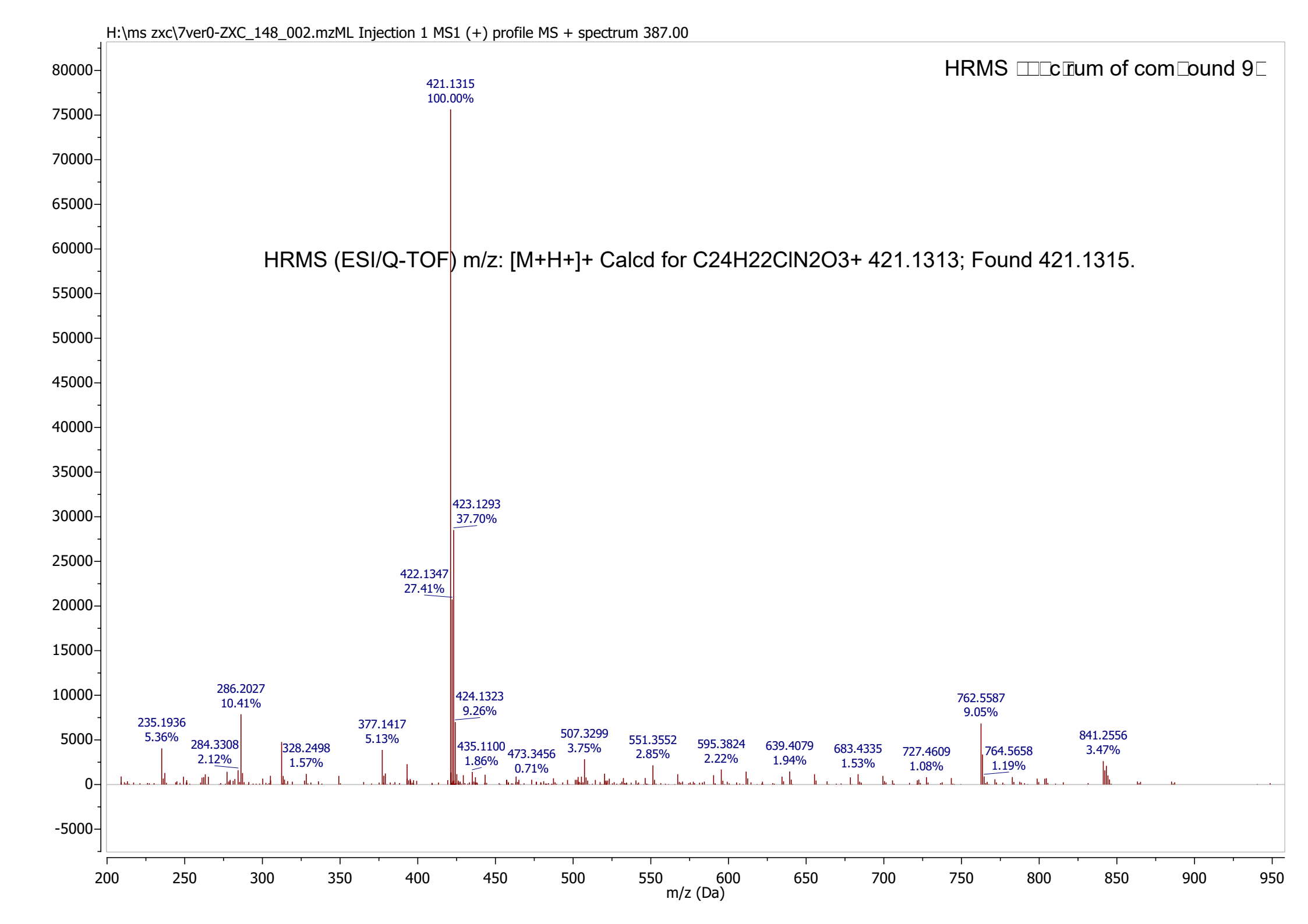

H:\ms zxc\12ve...XC_206_001.mzML Injection 1 MS1 (+) profile MS + spectrum 391.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C27H21ClNO3S+ 474.0925; Found 474.092□.
573.1972
100.00%
474.0926
84.14%
575.1955
42.92%
574.2002
36.02%
476.0900
32.82%
475.0950
24.82%
496.0745
22.09%
401.1141
21.36%
762.5587
23.08%
576.1971
14.52%
763.5626
11.72%
312.3625
10.20%
498.0712
9.15%
559.1817
9.08%
235.1936
5.09%
284.3314
5.50%
402.1174
6.14%
463.3023
5.77%
595.3815
5.73%
639.4080
4.53%
561.1788
4.37%
683.4333
3.35%
727.4602
2.22%
764.5660
3.64%
969.1591
3.62%
349.1825
2.69%
399.3085
2.58%
m/z (Da)

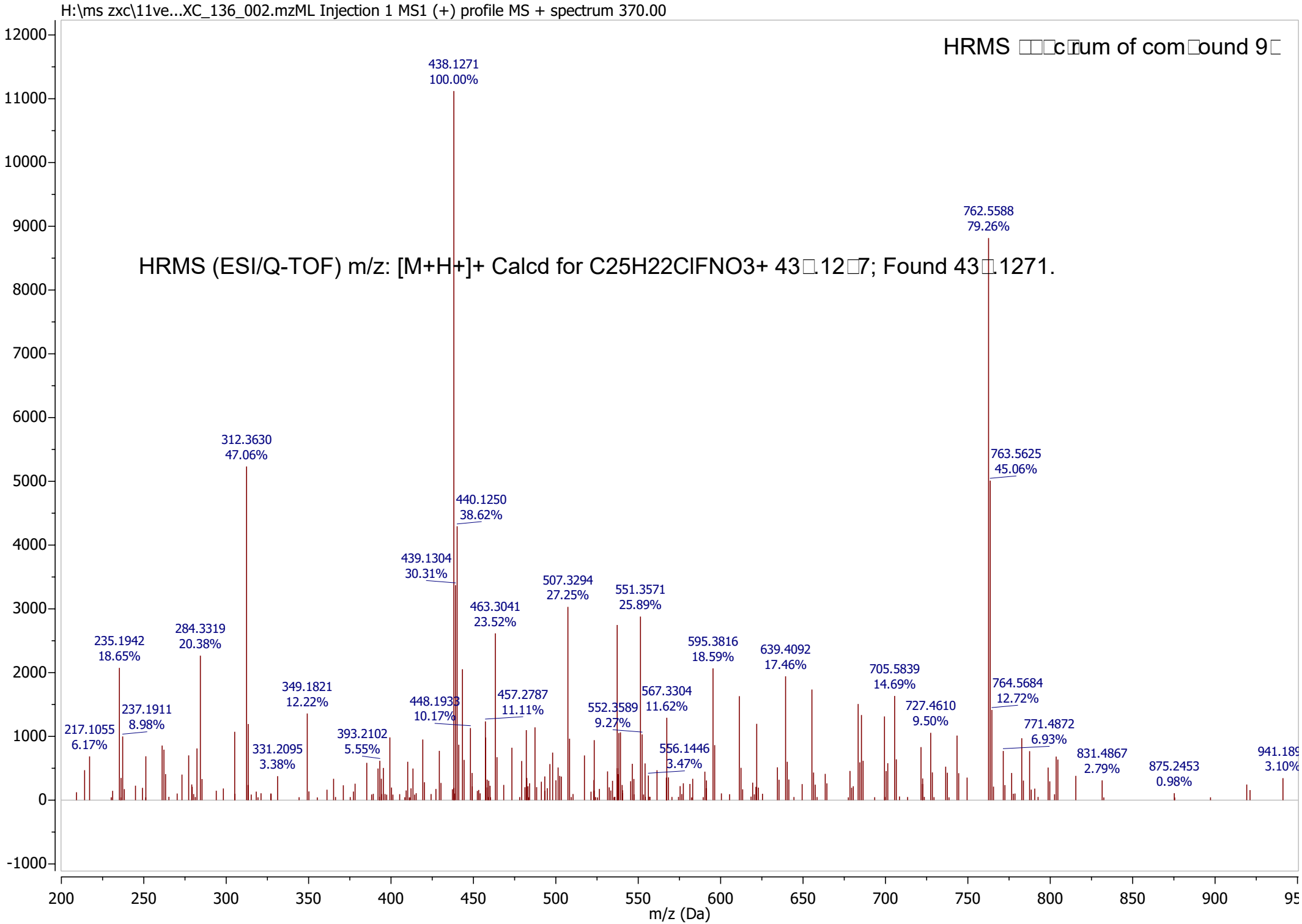

H:\ms zxc\13ve...XC_150_001.mzML Injection 1 MS1 (+) profile MS + spectrum 395.00
HRMS □□□c□rum of com□ound 9l
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C30H24ClFNO4+ 51□.1372; Found 51□.1373.
516.1373
100.00%
518.1357
39.08%
517.1403
33.50%
538.1191
30.02%
615.2416
28.98%
540.1172
11.41%
617.2403
13.01%
616.2455
10.98%
621.8879
7.93%
618.2426
6.17%
528.1570
8.65%
514.3168
3.82%
629.2584
3.27%
312.3626
5.82%
408.0800
4.27%
472.1452
2.41%
552.3599
0.67%
762.5580
5.31%
722.5058
1.92%
804.6035
0.57%
298.2236
1.37%
313.3658
0.92%
388.2535
0.80%
m/z (Da)

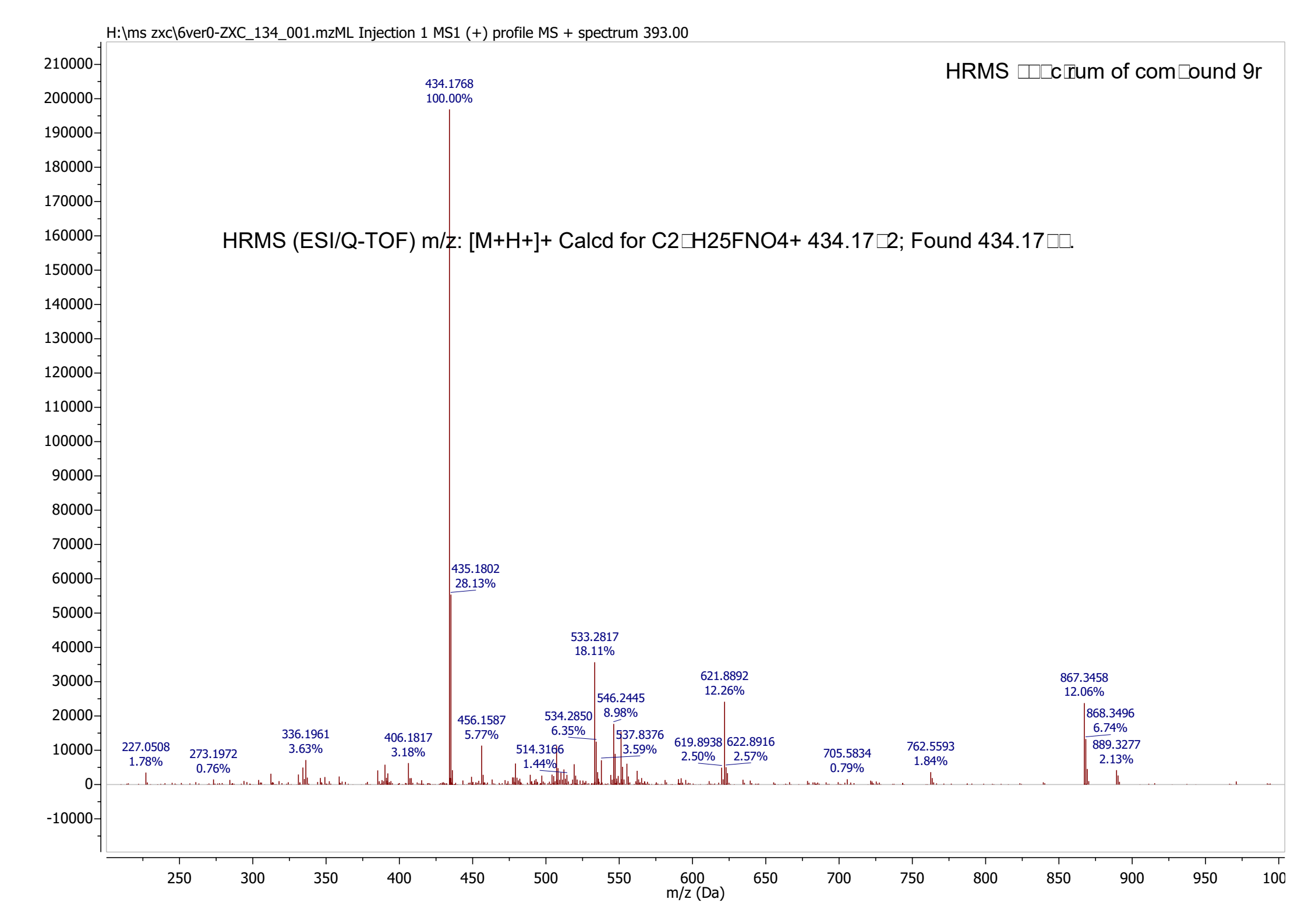

H:\ms zxc\1ver0-ZXC_204_001.mzML Injection 1 MS1 (+) profile MS + spectrum 408.00
HRMS □□□c□um of com□ound 9m
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C30H25ClNO3+ 4□2.1517; Found 4□2.151□.
482.1518
100.00%
581.2567
79.32%
484.1506
38.72%
582.2599
34.63%
483.1552
31.00%
504.1338
24.82%
584.2581
13.12%
555.2471
12.18%
454.1574
7.64%
537.2665
6.27%
595.2712
4.78%
639.4087
3.58%
762.5586
8.90%
683.4344
2.90%
727.4599
2.02%
764.5624
1.23%
815.5099
0.63%
312.3626
6.26%
235.1946
1.92%
349.1824
1.40%
385.2929
1.31%
443.3346
2.73%
985.2785
6.71%
989.2785
2.04%
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
m/z (Da)

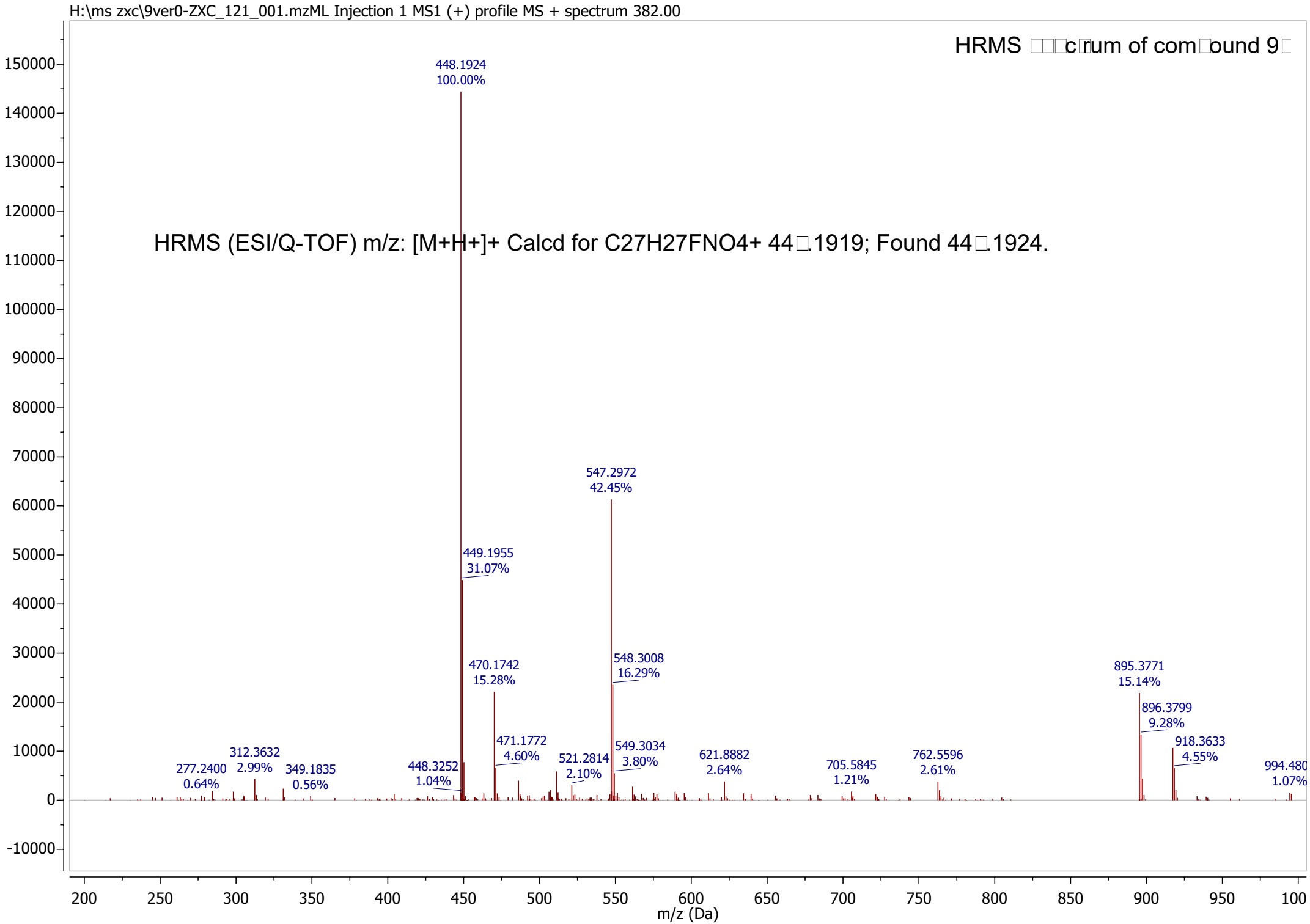

H:\ms zxc\14ve...XC_152_001.mzML Injection 1 MS1 (+) profile MS + spectrum 387.00
HRMS □□□c□um of com□ound 9n
RMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C27H27ClNO4S+ 49□.1344; Found 49□.1344.
496.1344
100.00%
595.2392
49.28%
534.1110
46.70%
498.1325
40.73%
497.1381
29.85%
518.1168
28.03%
621.8884
24.38%
611.2344
22.88%
394.0842
19.52%
512.1297
18.29%
535.1142
14.45%
499.1350
12.71%
613.2330
10.14%
598.2389
7.86%
622.8914
5.17%
762.5588
5.10%
705.9395
3.25%
993.261
3.04%
312.3624
5.24%
395.0881
5.00%
396.0819
6.56%
443.3339
1.86%
500.1345
3.59%
611.3574
2.05%
261.1307
1.34%
306.0007
0.59%
m/z (Da)

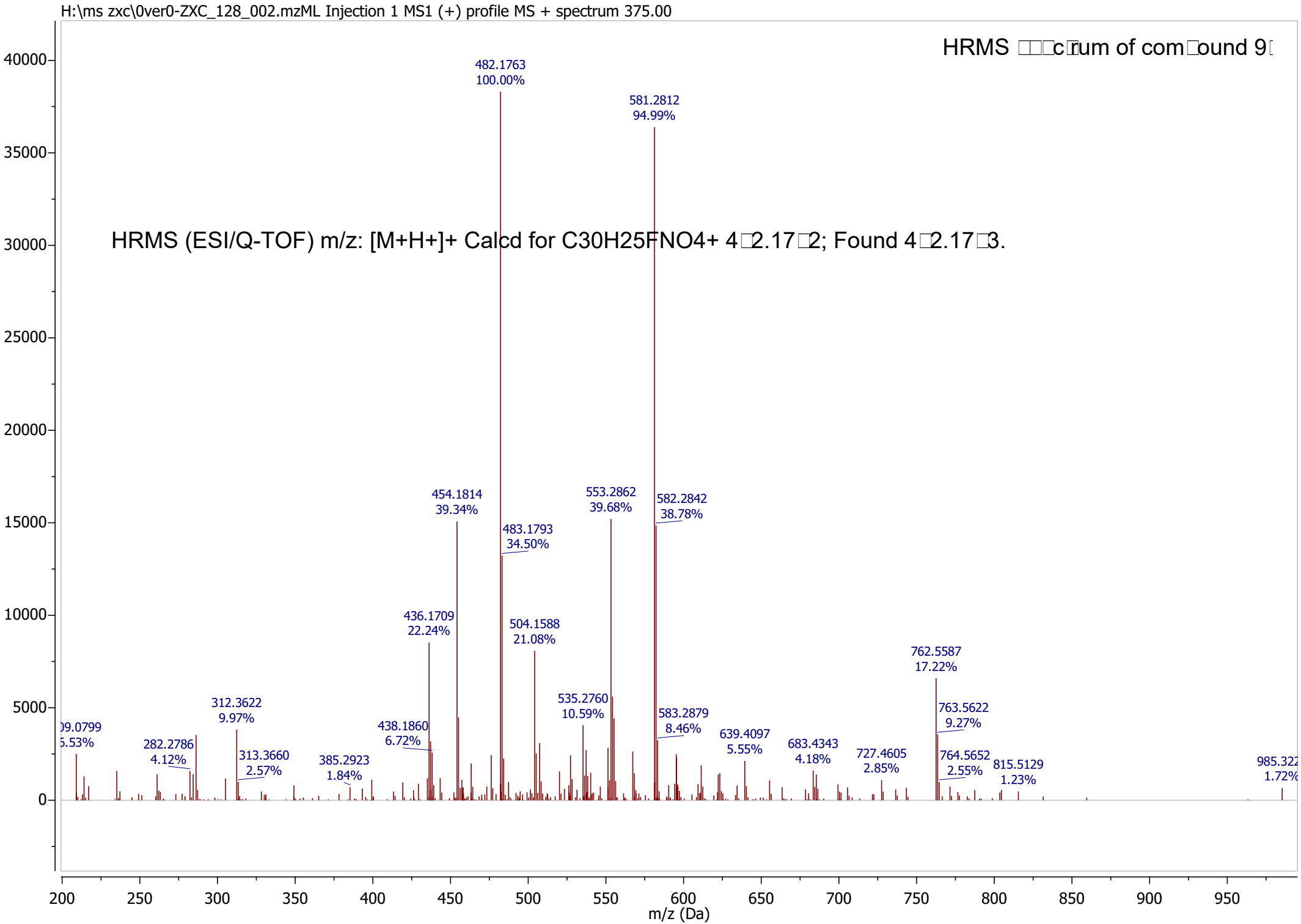

C:\Users\Brr\D...xc\ZXC_106.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□um of com□ound 9o
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C25H22ClNO3Na+ 442.11□0; Found 442.1175.
442.1175 100.00%
420.1353 62.34%
458.0910 47.51%
444.1150 36.76%
526.1675 37.02%
297.0888 22.37%
460.0898 21.12%
421.1389 19.06%
313.0456 17.14%
245.0778 17.86%
558.1050 18.16%
542.1339 14.33%
560.1068 13.19%
295.0126 12.44%
353.0551 11.02%
404.1659 11.86%
626.1844 11.92%
480.0725 9.66%
559.1275 8.41%
644.1549 6.79%
243.0524 8.56%
462.0837 4.84%
355.0506 4.99%
605.2838 3.63%
228.1283 3.77%
632.1857 1.93%
706.4703 2.81%
772.1890 4.45%
861.2456 24.74%
863.2433 18.35%
862.2502 12.63%
845.2704 7.45%
864.2446 9.64%
878.2193 4.60%
843.2624 2.79%
961.2619 3.35%
105.2152 0.84%
145.7686 0.77%
m/z (Da)

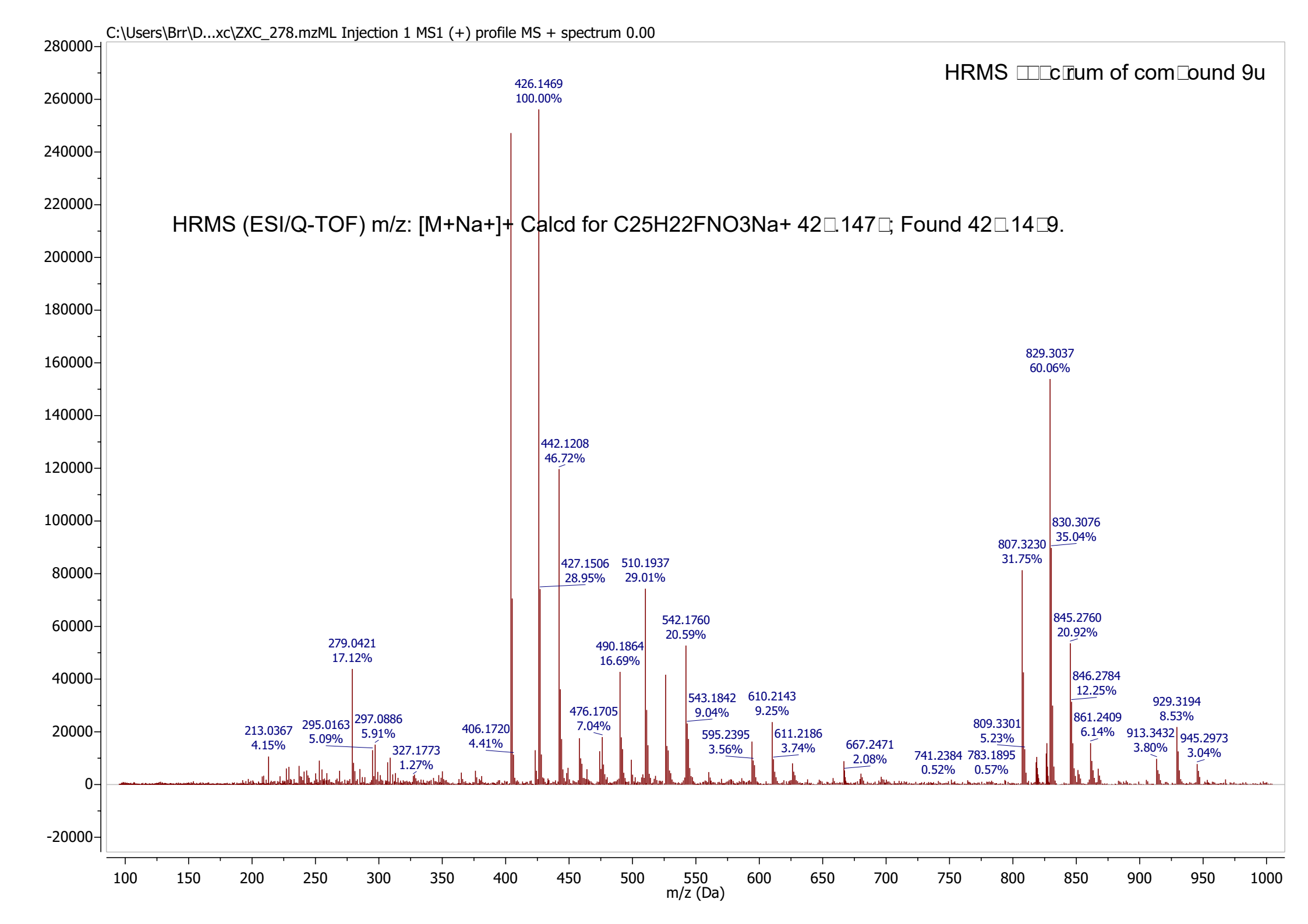

H:\ms zxc\7ver0-ZXC_148_002.mzML Injection 1 MS1 (+) profile MS + spectrum 387.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C24H22ClN2O3+ 421.1313; Found 421.1315.
421.1315
100.00%
423.1293
37.70%
422.1347
27.41%
424.1323
9.26%
286.2027
10.41%
235.1936
5.36%
284.3308
2.12%
328.2498
1.57%
377.1417
5.13%
435.1100
1.86%
473.3456
0.71%
507.3299
3.75%
551.3552
2.85%
595.3824
2.22%
639.4079
1.94%
683.4335
1.53%
727.4609
1.08%
762.5587
9.05%
764.5658
1.19%
841.2556
3.47%
m/z (Da)

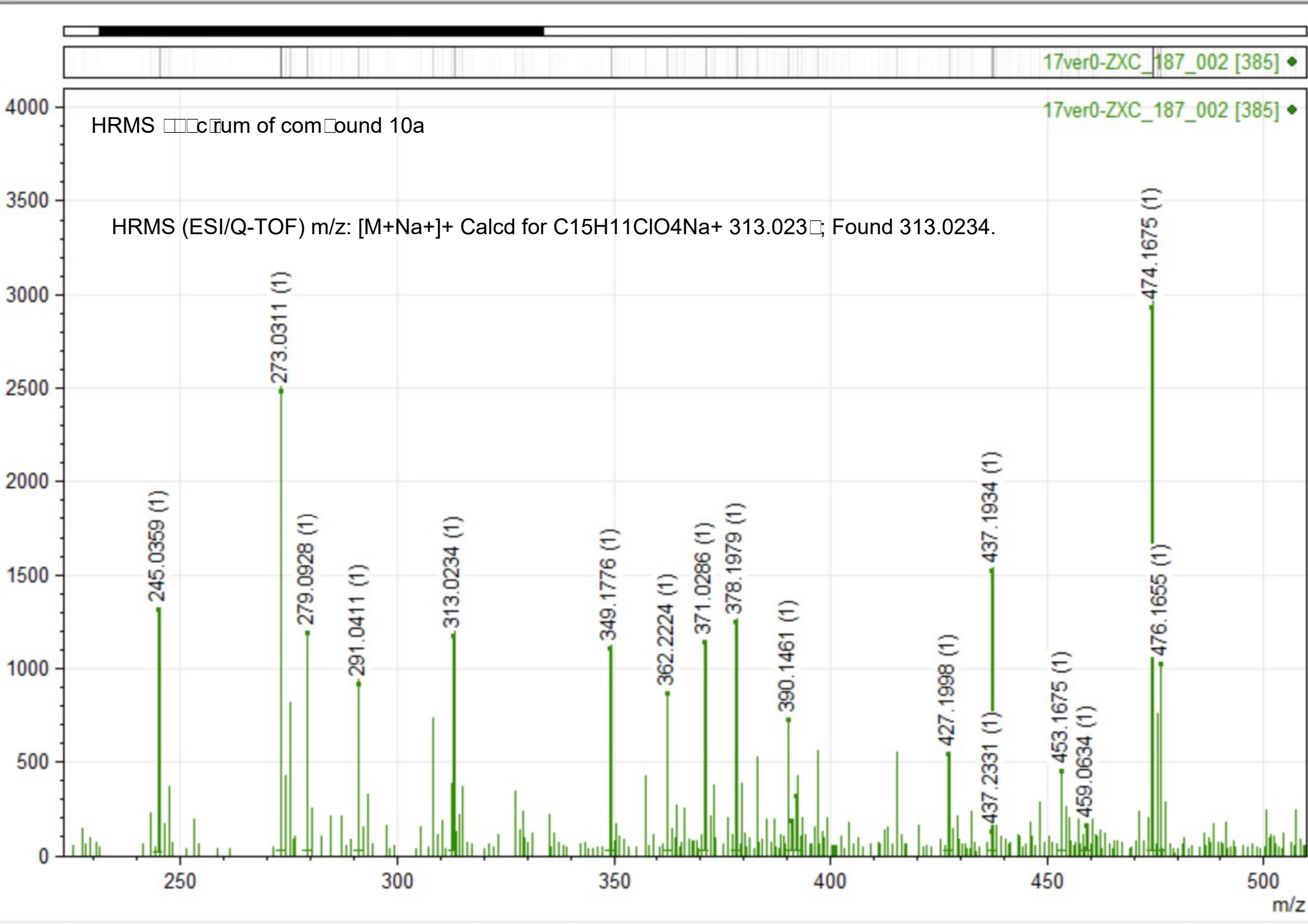

H:\ms zxc\11ve...XC_136_002.mzML Injection 1 MS1 (+) profile MS + spectrum 370.00
HRMS □□□c□rum of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C25H22ClFNO3+ 43□.12□7; Found 43□.1271.
438.1271
100.00%
762.5588
79.26%
312.3630
47.06%
763.5625
45.06%
440.1250
38.62%
439.1304
30.31%
507.3294
27.25%
551.3571
25.89%
463.3041
23.52%
284.3319
20.38%
595.3816
18.59%
639.4092
17.46%
235.1942
18.65%
705.5839
14.69%
764.5684
12.72%
349.1821
12.22%
567.3304
11.62%
448.1933
10.17%
457.2787
11.11%
552.3589
9.27%
727.4610
9.50%
237.1911
8.98%
771.4872
6.93%
217.1055
6.17%
393.2102
5.55%
556.1446
3.47%
831.4867
2.79%
331.2095
3.38%
875.2453
0.98%
941.189
3.10%
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
95
m/z (Da)

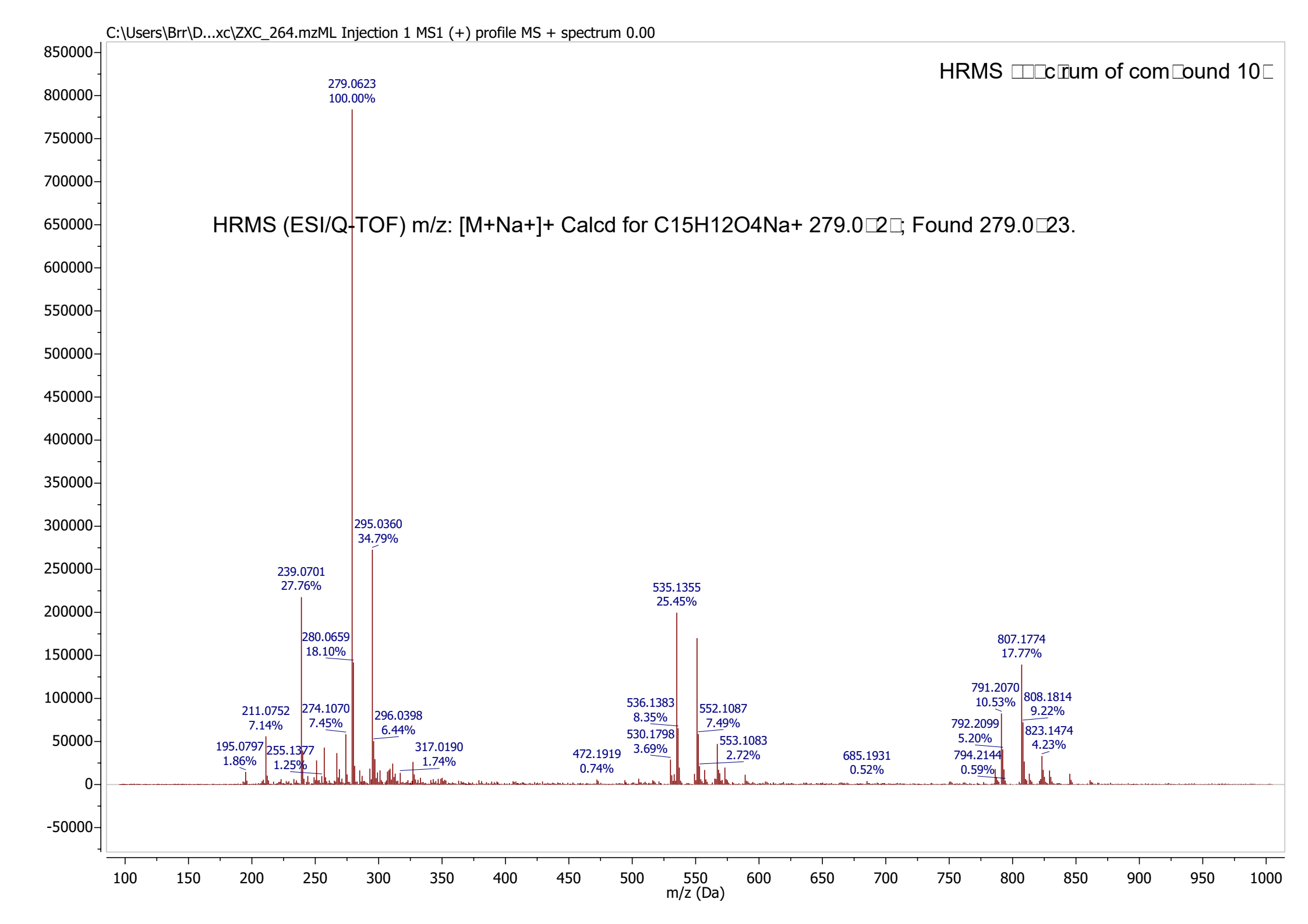

H:\ms zxc\6ver0-ZXC_134_001.mzML Injection 1 MS1 (+) profile MS + spectrum 393.00
HRMS □□□c□um of com□ound 9r
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C2□H25FNO4+ 434.17□2; Found 434.17□□.
434.1768
100.00%
435.1802
28.13%
533.2817
18.11%
621.8892
12.26%
867.3458
12.06%
546.2445
8.98%
868.3496
6.74%
534.2850
6.35%
456.1587
5.77%
537.8376
3.59%
889.3277
2.13%
336.1961
3.63%
406.1817
3.18%
619.8938
2.50%
622.8916
2.57%
514.3166
1.44%
762.5593
1.84%
227.0508
1.78%
705.5834
0.79%
273.1972
0.76%
m/z (Da)


H:\ms zxc\9ver0-ZXC_121_001.mzML Injection 1 MS1 (+) profile MS + spectrum 382.00
HRMS □□□c□um of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C27H27FNO4+ 44□.1919; Found 44□.1924.
448.1924
100.00%
547.2972
42.45%
449.1955
31.07%
470.1742
15.28%
548.3008
16.29%
895.3771
15.14%
896.3799
9.28%
918.3633
4.55%
471.1772
4.60%
549.3034
3.80%
312.3632
2.99%
277.2400
0.64%
349.1835
0.56%
448.3252
1.04%
521.2814
2.10%
621.8882
2.64%
705.5845
1.21%
762.5596
2.61%
994.480
1.07%
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
100
m/z (Da)

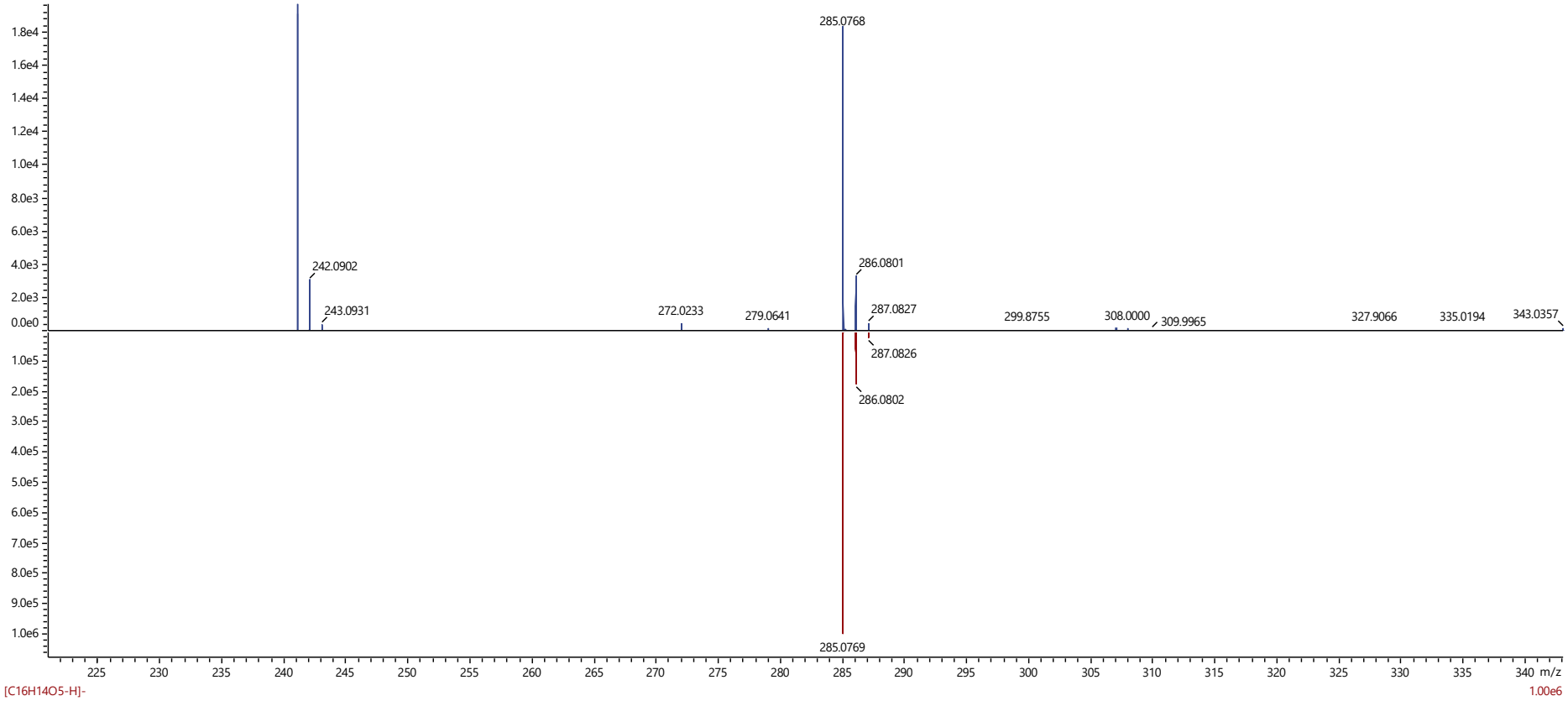

H:\ms zxc\0ver0-ZXC_128_002.mzML Injection 1 MS1 (+) profile MS + spectrum 375.00
HRMS □□□c□um of com□ound 9□
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C30H25FNO4+ 4□2.17□2; Found 4□2.17□3.
482.1763
100.00%
581.2812
94.99%
454.1814
39.34%
553.2862
39.68%
582.2842
38.78%
483.1793
34.50%
436.1709
22.24%
504.1588
21.08%
762.5587
17.22%
535.2760
10.59%
312.3622
9.97%
583.2879
8.46%
763.5622
9.27%
438.1860
6.72%
639.4097
5.55%
683.4343
4.18%
727.4605
2.85%
764.5652
2.55%
815.5129
1.23%
282.2786
4.12%
313.3660
2.57%
385.2923
1.84%
985.322
1.72%
m/z (Da)

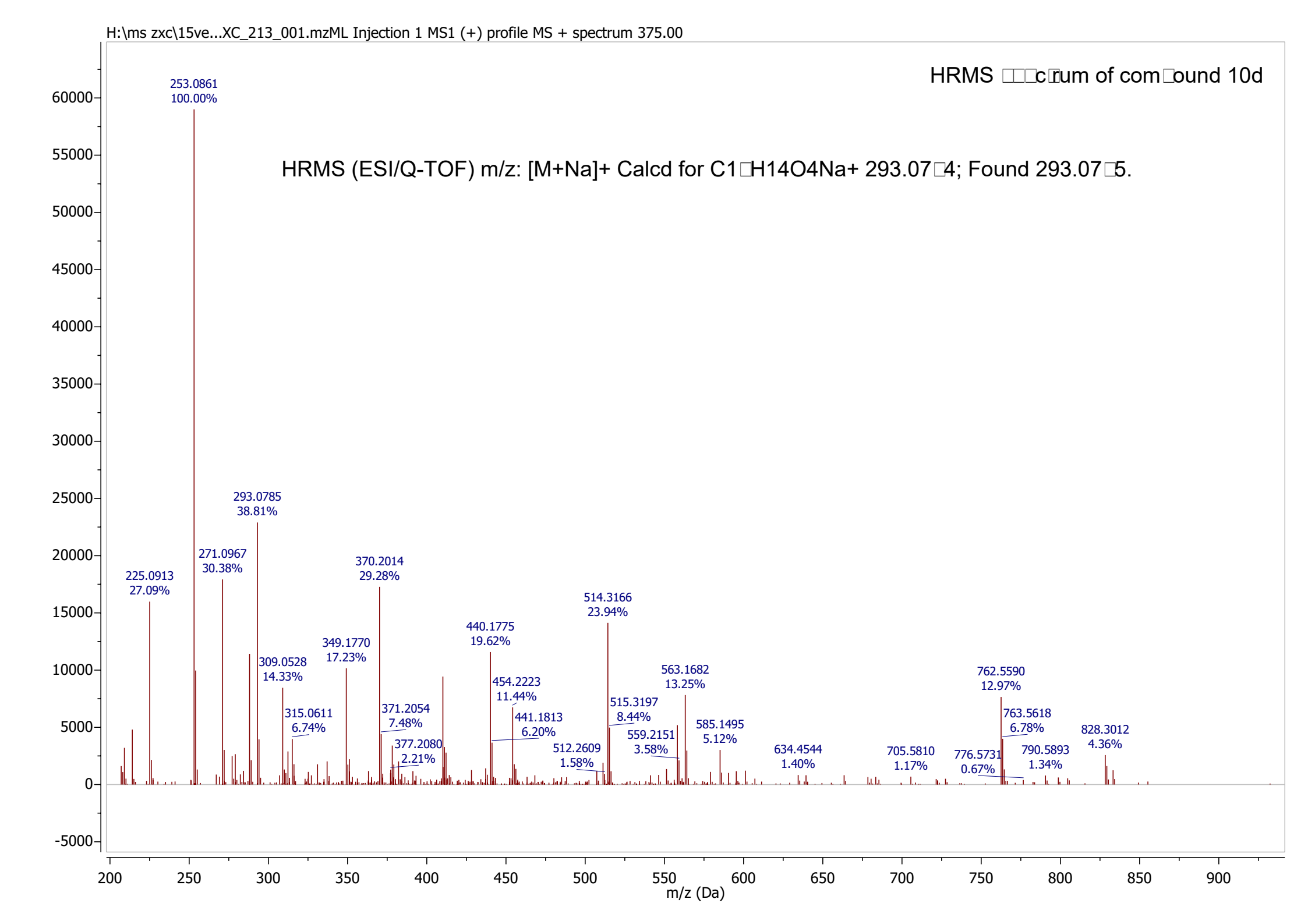

C:\Users\Brr\D...xc\ZXC_278.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□rum of com□ound 9u
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C25H22FNO3Na+ 42□.147□; Found 42□.14□9.
426.1469
100.00%
442.1208
46.72%
427.1506
28.95%
510.1937
29.01%
829.3037
60.06%
830.3076
35.04%
807.3230
31.75%
845.2760
20.92%
542.1760
20.59%
490.1864
16.69%
279.0421
17.12%
846.2784
12.25%
543.1842
9.04%
610.2143
9.25%
476.1705
7.04%
929.3194
8.53%
861.2409
6.14%
809.3301
5.23%
595.2395
3.56%
611.2186
3.74%
913.3432
3.80%
945.2973
3.04%
667.2471
2.08%
213.0367
4.15%
295.0163
5.09%
297.0886
5.91%
406.1720
4.41%
327.1773
1.27%
741.2384
0.52%
783.1895
0.57%
m/z (Da)

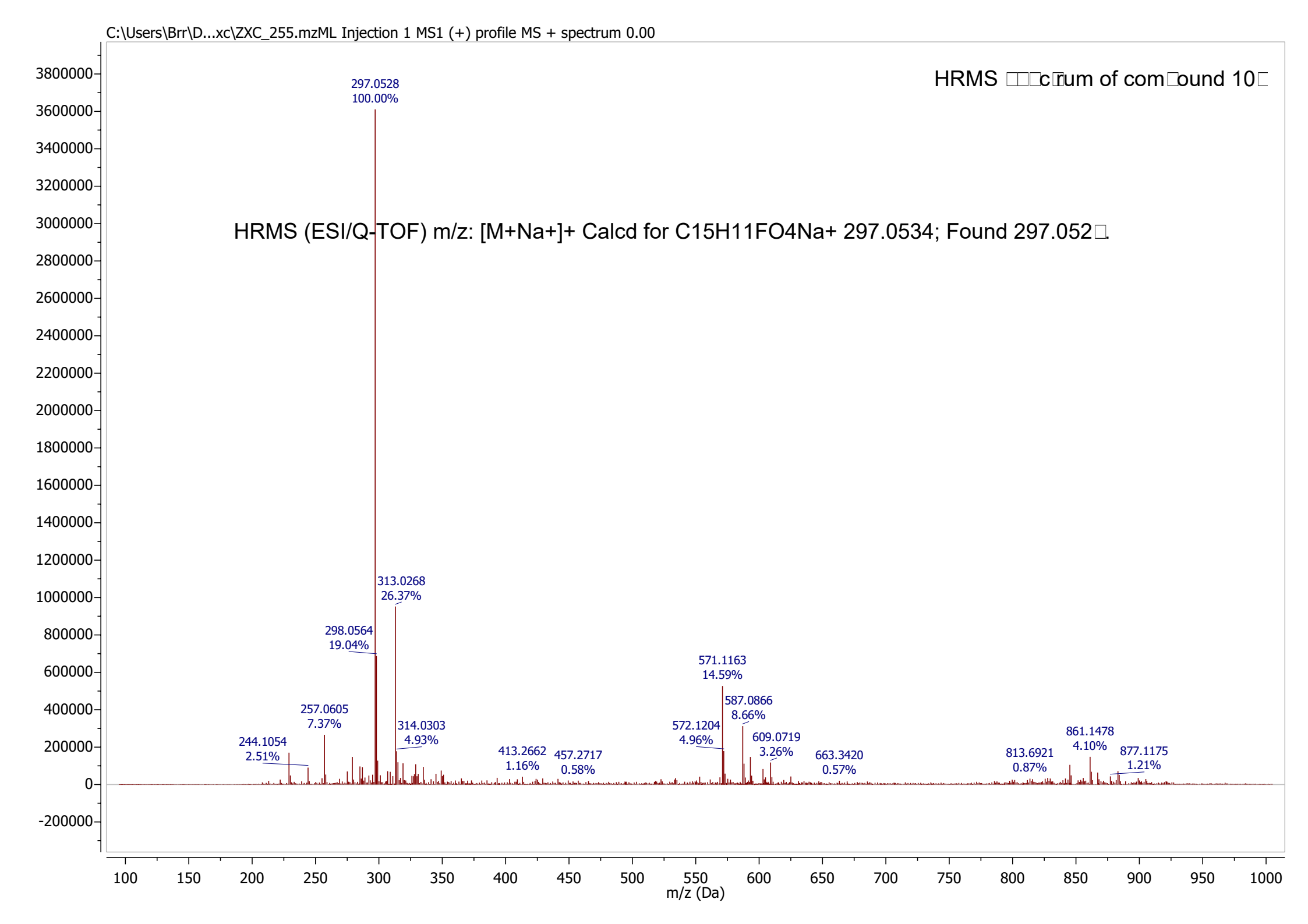

17ver0-ZXC_187_002 [385]
HRMS □□□c□rum of com□ound 10a
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C15H11ClO4Na+ 313.023□; Found 313.0234.
245.0359 (1)
273.0311 (1)
279.0928 (1)
291.0411 (1)
313.0234 (1)
349.1776 (1)
362.2224 (1)
371.0286 (1)
378.1979 (1)
390.1461 (1)
427.1998 (1)
437.1934 (1)
437.2331 (1)
453.1675 (1)
459.0634 (1)
474.1675 (1)
476.1655 (1)
4000
3500
3000
2500
2000
1500
1000
500
0
250
300
350
400
450
500
m/z

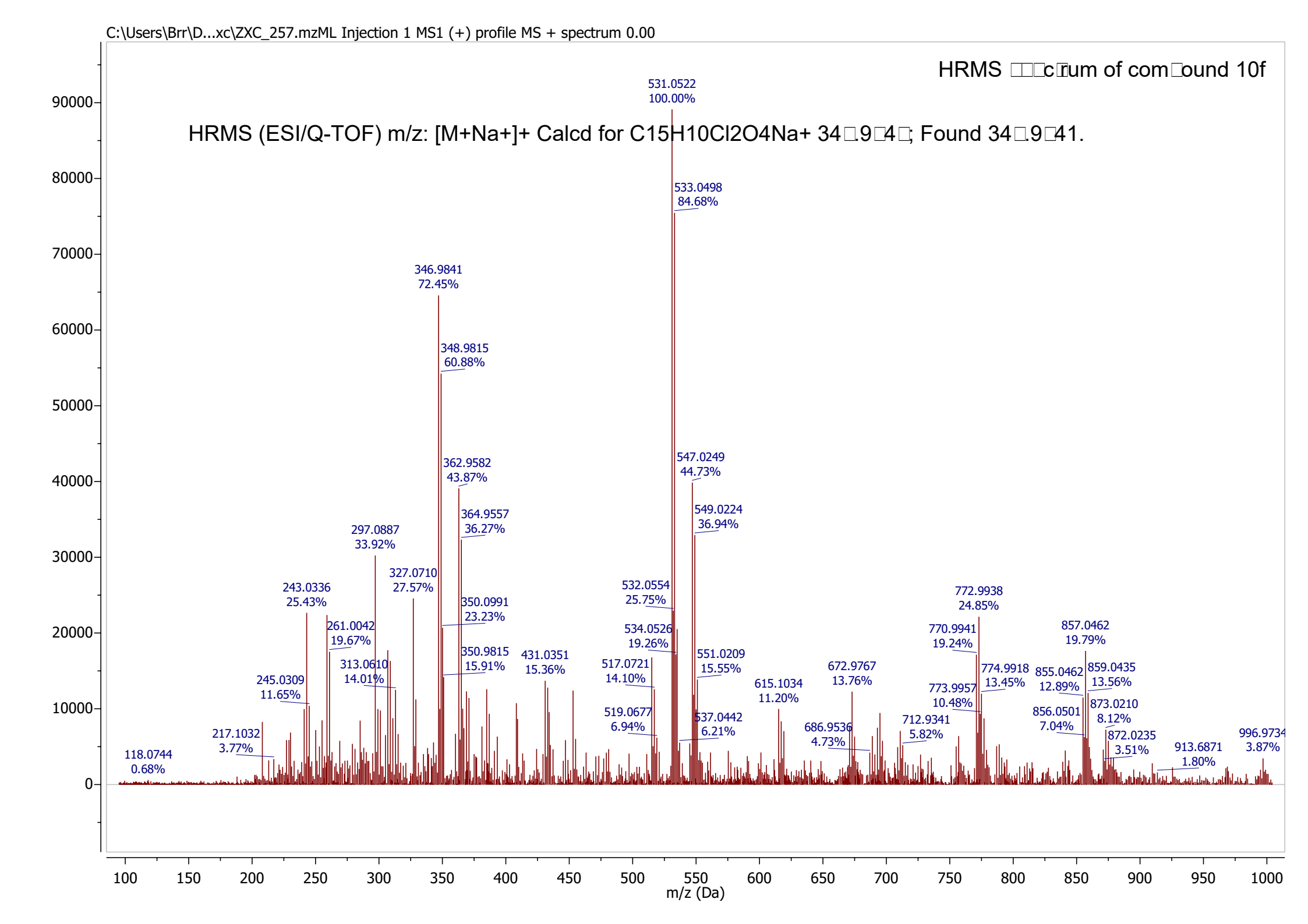

C:\Users\Brr\D...xc\ZXC_264.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□um of com□ound 10□
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C15H12O4Na+ 279.0□2□; Found 279.0□23.
279.0623
100.00%
295.0360
34.79%
239.0701
27.76%
280.0659
18.10%
535.1355
25.45%
807.1774
17.77%
791.2070
10.53%
808.1814
9.22%
211.0752
7.14%
274.1070
7.45%
296.0398
6.44%
536.1383
8.35%
552.1087
7.49%
792.2099
5.20%
823.1474
4.23%
530.1798
3.69%
553.1083
2.72%
195.0797
1.86%
255.1377
1.25%
317.0190
1.74%
472.1919
0.74%
685.1931
0.52%
794.2144
0.59%
m/z (Da)

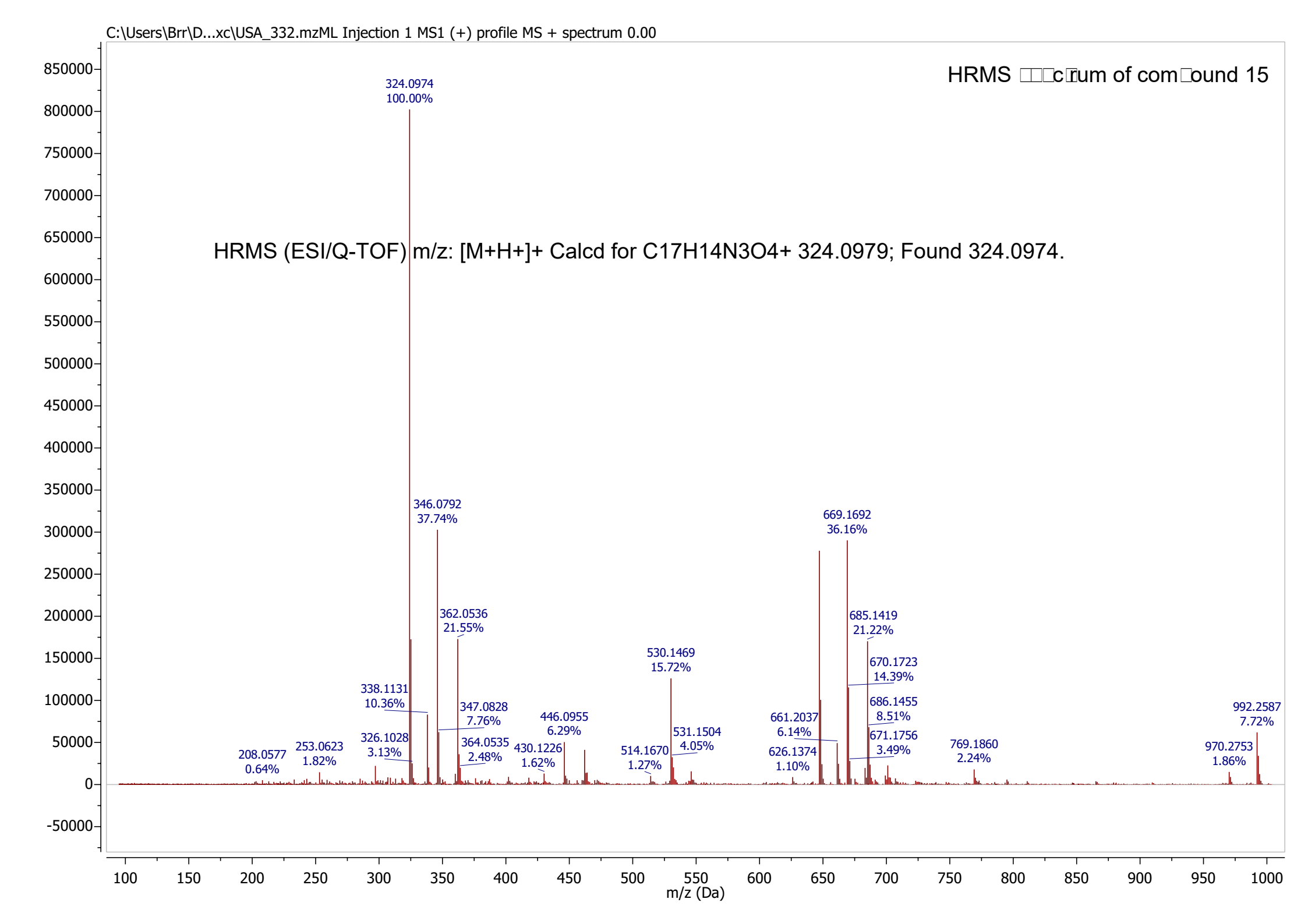
HRMS (ESI/Q-TOF) m/z: [M-H]- Calcd for C1□H13O5- 2□5.07□9; Found 2□5.07□□.

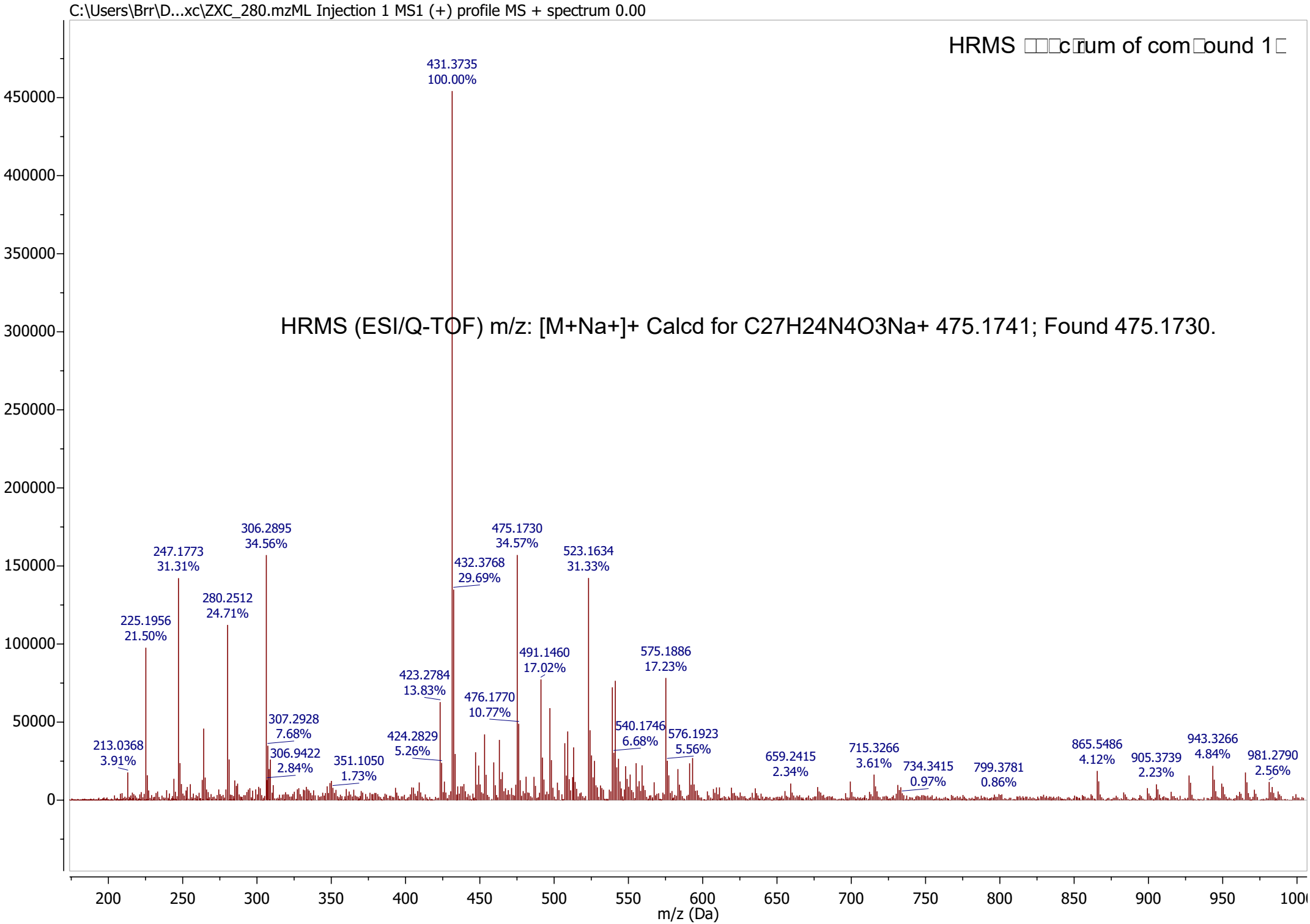



H:\ms zxc\15ve...XC_213_001.mzML Injection 1 MS1 (+) profile MS + spectrum 375.00
HRMS □□□c□um of com□ound 10d
HRMS (ESI/Q-TOF) m/z: [M+Na]+ Calcd for C1□H14O4Na+ 293.07□4; Found 293.07□5.
253.0861
100.00%
293.0785
38.81%
271.0967
30.38%
225.0913
27.09%
370.2014
29.28%
514.3166
23.94%
440.1775
19.62%
349.1770
17.23%
309.0528
14.33%
563.1682
13.25%
762.5590
12.97%
454.2223
11.44%
315.0611
6.74%
371.2054
7.48%
515.3197
8.44%
441.1813
6.20%
763.5618
6.78%
585.1495
5.12%
828.3012
4.36%
559.2151
3.58%
377.2080
2.21%
512.2609
1.58%
634.4544
1.40%
705.5810
1.17%
776.5731
0.67%
790.5893
1.34%
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z (Da)


C:\Users\Brr\D...xc\ZXC_255.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□rum of com□ound 10□
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C15H11FO4Na+ 297.0534; Found 297.052□.
297.0528
100.00%
313.0268
26.37%
298.0564
19.04%
257.0605
7.37%
314.0303
4.93%
244.1054
2.51%
413.2662
1.16%
457.2717
0.58%
571.1163
14.59%
587.0866
8.66%
572.1204
4.96%
609.0719
3.26%
663.3420
0.57%
861.1478
4.10%
813.6921
0.87%
877.1175
1.21%
m/z (Da)


C:\Users\Brr\D...xc\ZXC_257.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□rum of com□ound 10f
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C15H10Cl2O4Na+ 34□.9□4□; Found 34□.9□41.
531.0522
100.00%
533.0498
84.68%
346.9841
72.45%
348.9815
60.88%
362.9582
43.87%
547.0249
44.73%
364.9557
36.27%
549.0224
36.94%
297.0887
33.92%
327.0710
27.57%
243.0336
25.43%
532.0554
25.75%
350.0991
23.23%
261.0042
19.67%
534.0526
19.26%
772.9938
24.85%
770.9941
19.24%
857.0462
19.79%
350.9815
15.91%
431.0351
15.36%
313.0610
14.01%
517.0721
14.10%
551.0209
15.55%
774.9918
13.45%
859.0435
13.56%
245.0309
11.65%
615.1034
11.20%
672.9767
13.76%
855.0462
12.89%
773.9957
10.48%
873.0210
8.12%
217.1032
3.77%
519.0677
6.94%
537.0442
6.21%
712.9341
5.82%
856.0501
7.04%
686.9536
4.73%
872.0235
3.51%
996.9734
3.87%
913.6871
1.80%
118.0744
0.68%
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z (Da)


C:\Users\Brr\D...xc\USA_332.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□um of com□ound 15
HRMS (ESI/Q-TOF) m/z: [M+H+]+ Calcd for C17H14N3O4+ 324.0979; Found 324.0974.
324.0974
100.00%
346.0792
37.74%
362.0536
21.55%
338.1131
10.36%
347.0828
7.76%
326.1028
3.13%
364.0535
2.48%
208.0577
0.64%
253.0623
1.82%
430.1226
1.62%
446.0955
6.29%
514.1670
1.27%
530.1469
15.72%
531.1504
4.05%
669.1692
36.16%
685.1419
21.22%
670.1723
14.39%
686.1455
8.51%
671.1756
3.49%
661.2037
6.14%
626.1374
1.10%
769.1860
2.24%
970.2753
1.86%
992.2587
7.72%
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z (Da)


C:\Users\Brr\D...xc\ZXC_280.mzML Injection 1 MS1 (+) profile MS + spectrum 0.00
HRMS □□□c□um of com□ound 1□
HRMS (ESI/Q-TOF) m/z: [M+Na+]+ Calcd for C27H24N4O3Na+ 475.1741; Found 475.1730.
431.3735
100.00%
475.1730
34.57%
306.2895
34.56%
523.1634
31.33%
247.1773
31.31%
432.3768
29.69%
280.2512
24.71%
225.1956
21.50%
491.1460
17.02%
575.1886
17.23%
423.2784
13.83%
476.1770
10.77%
307.2928
7.68%
540.1746
6.68%
576.1923
5.56%
424.2829
5.26%
213.0368
3.91%
306.9422
2.84%
351.1050
1.73%
659.2415
2.34%
715.3266
3.61%
734.3415
0.97%
799.3781
0.86%
865.5486
4.12%
905.3739
2.23%
943.3266
4.84%
981.2790
2.56%
m/z (Da)