

Single Mass Analysis

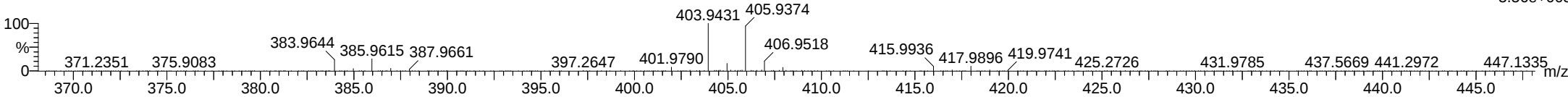
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
675 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 14-14 H: 0-100 N: 0-10 O: 0-14 Na: 0-1 S: 1-3 Br: 1-1 F: 1-1

A.ZUBIARRE AZ 332 1
MS50271 90 (2.767)

ES-ToF

14-Dec-2018
2: TOF MS ES-
5.56e+003



Minimum: -1.5
Maximum: 5.0 10.0 100.0

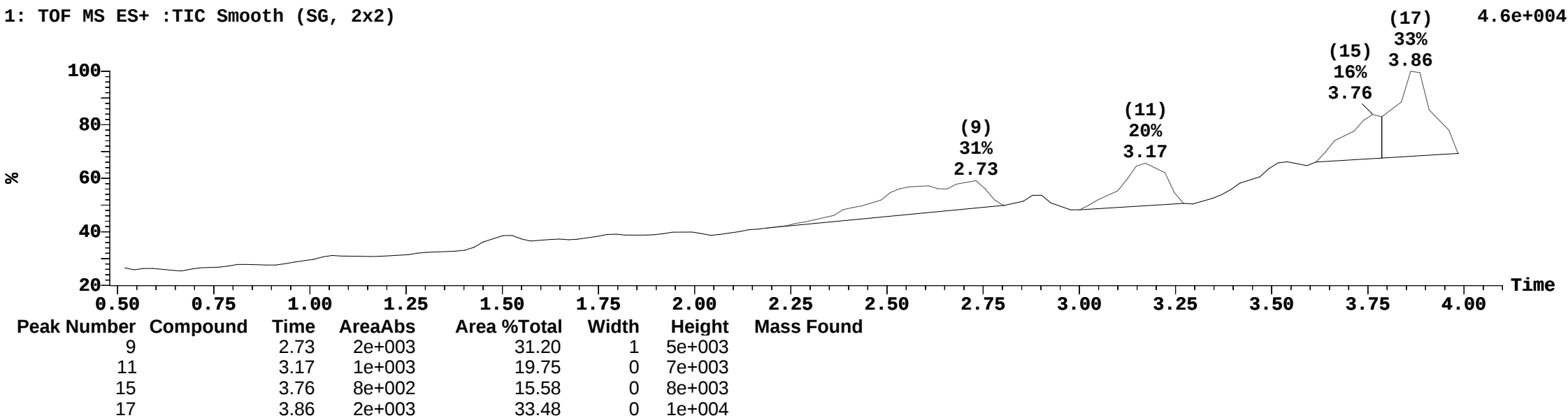
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
403.9431	403.9426	0.5	1.2	8.5	113.8	0.0	C14 H12 N O3 S2 Br F

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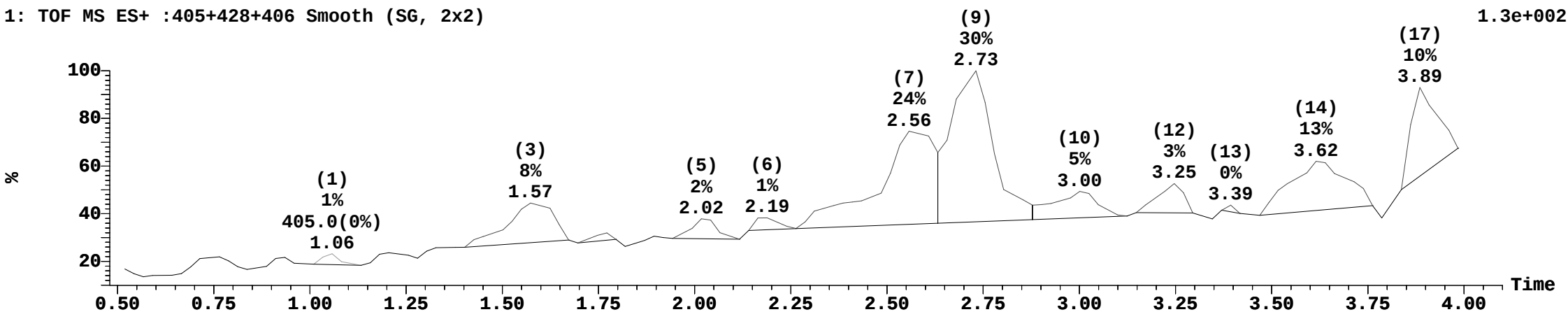
Sample Report:

Sample 3 Vial 1:44 ID File MS50271 Date 14-Dec-2018 Time 9::4::9 Description A.ZUBIARRE AZ 332 1

1: TOF MS ES+ :TIC Smooth (SG, 2x2)

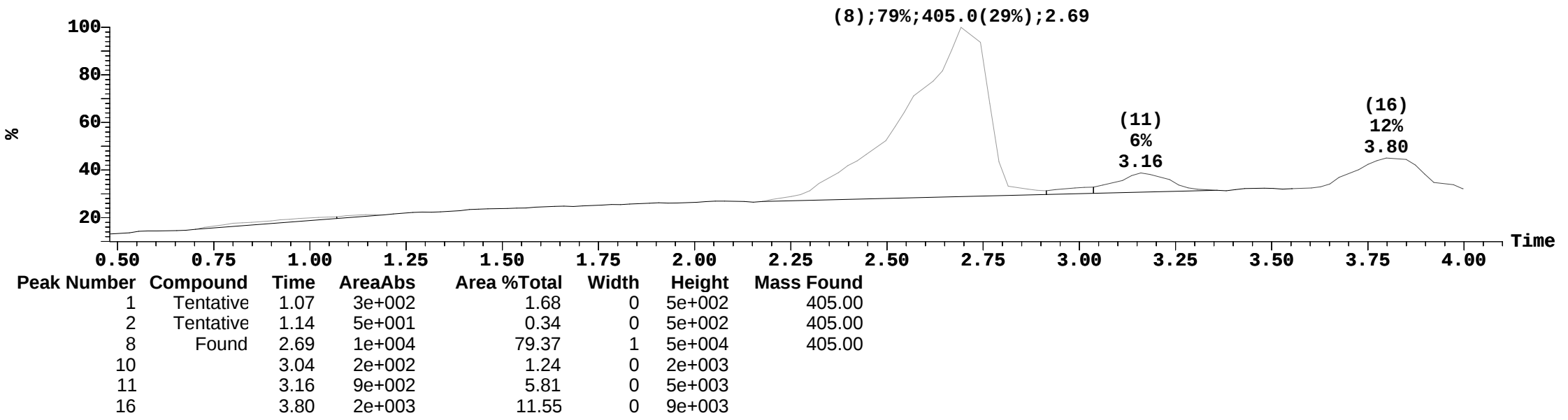


1: TOF MS ES+ :405+428+406 Smooth (SG, 2x2)

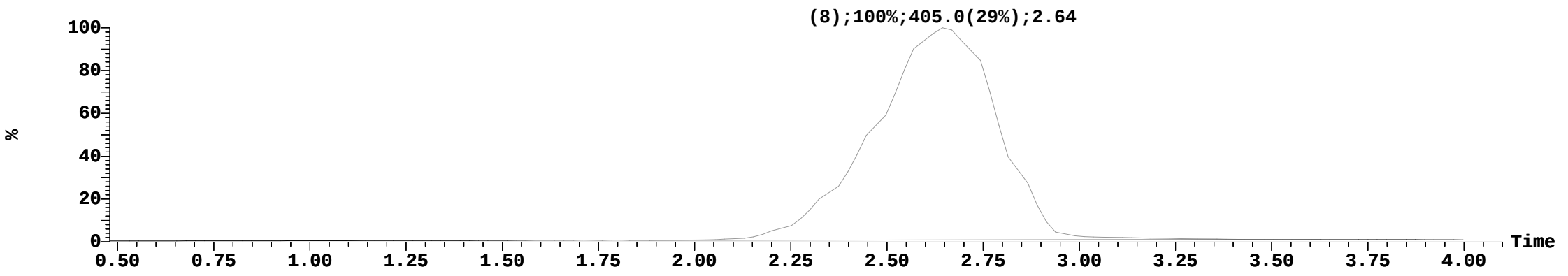


Sample Report (continued):

2: TOF MS ES- :TIC Smooth (SG, 2x2) 6.8e+004

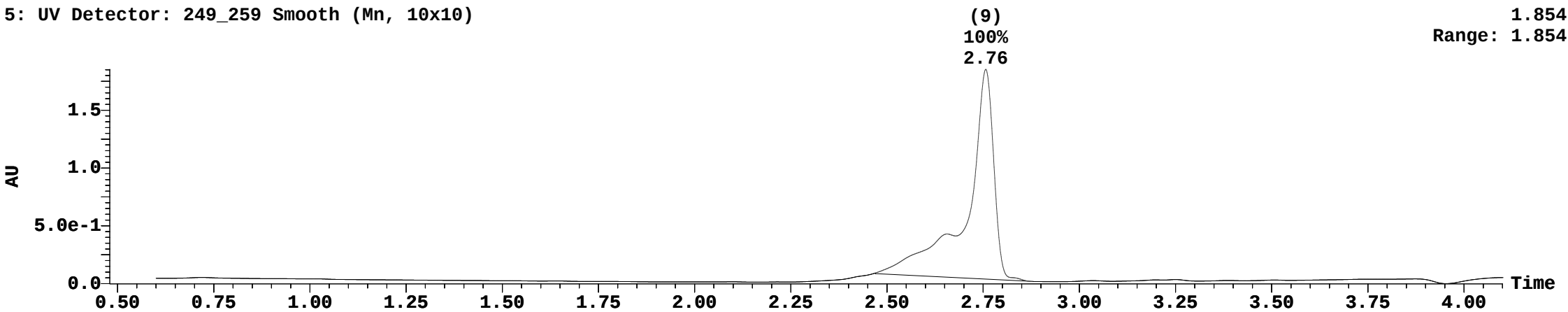


2: TOF MS ES- :405+450+404 Smooth (Mn, 2x3) 9.8e+003



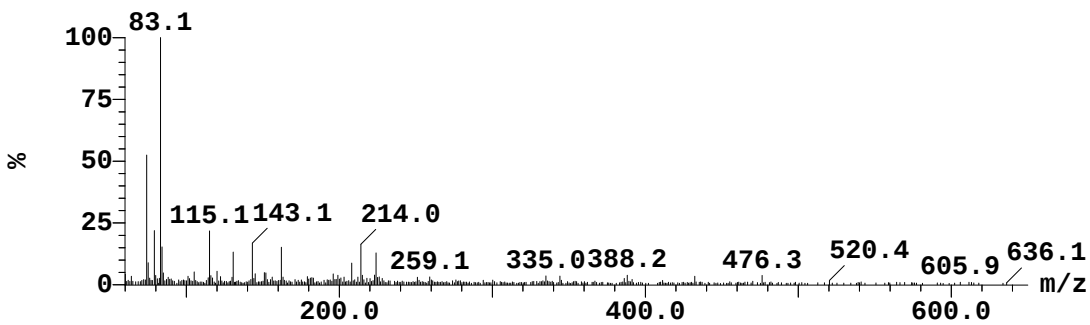
Sample Report (continued):

5: UV Detector: 249_259 Smooth (Mn, 10x10)



Peak ID	Compound	Time	Mass Found
1		1.06	

1:(Time: 1.06) Combine (33:37-(28:29+41))

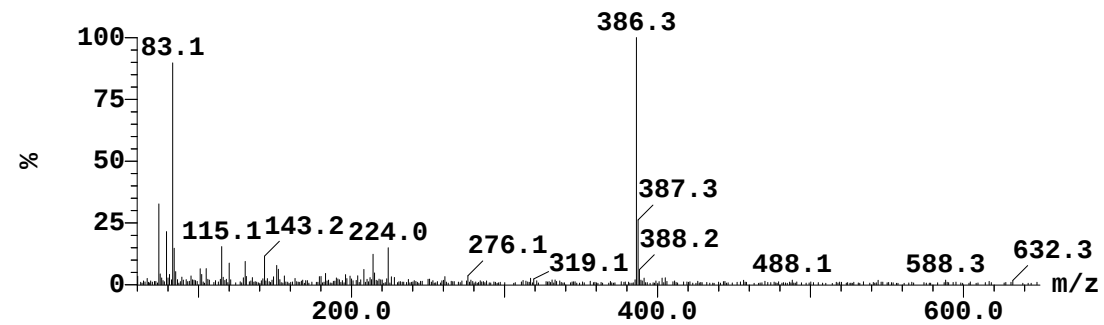


Peak ID	Compound	Time	Mass Found
3		1.57	

3:(Time: 1.57) Combine (50:53-(45:46+58))

1:TOF MS ES+ 3.5e+003

1:TOF MS ES+ 2.4e+003



Sample: 3
File:MS50271
Description:A.ZUBIARRE AZ 332 1

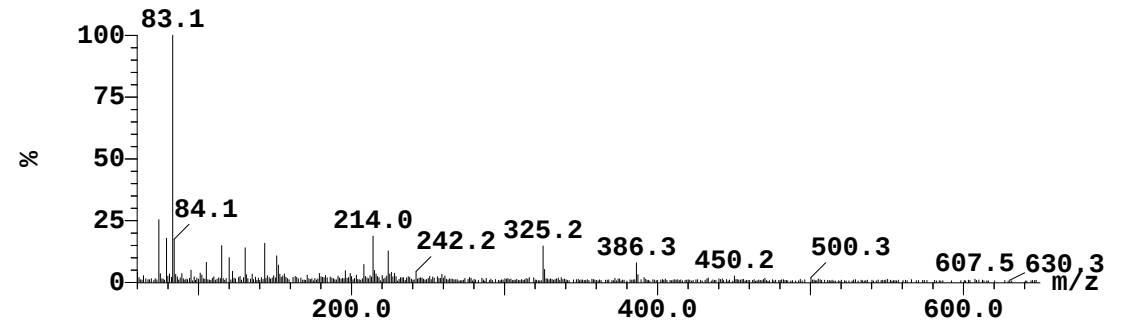
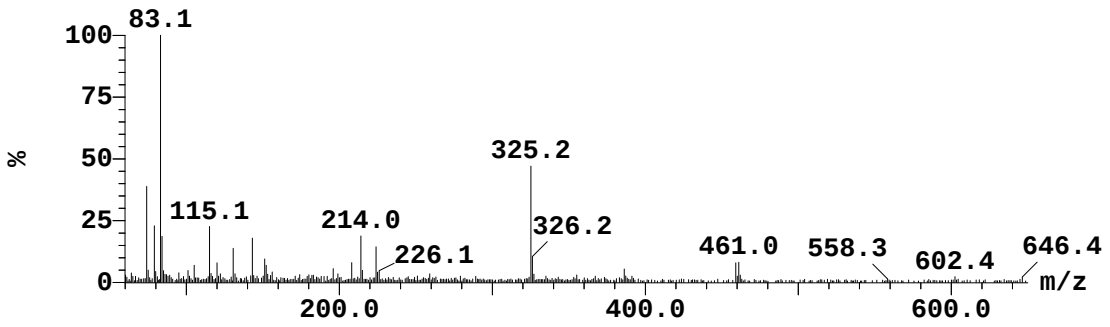
Vial:1:44
Date:14-Dec-2018

ID:
Time:9::4::9

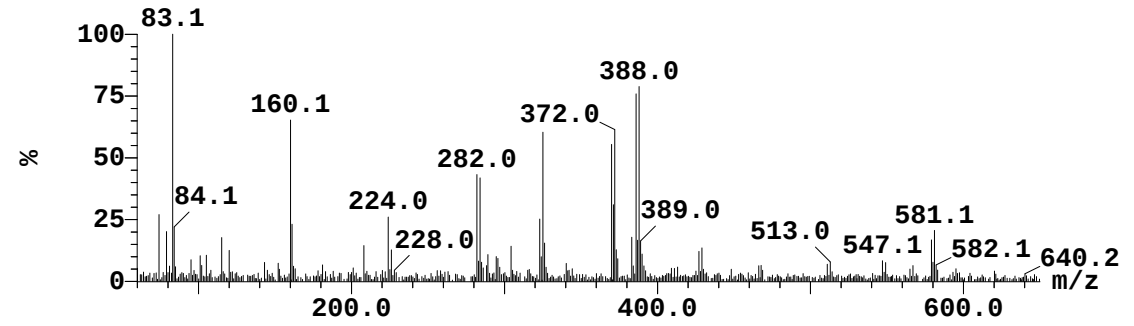
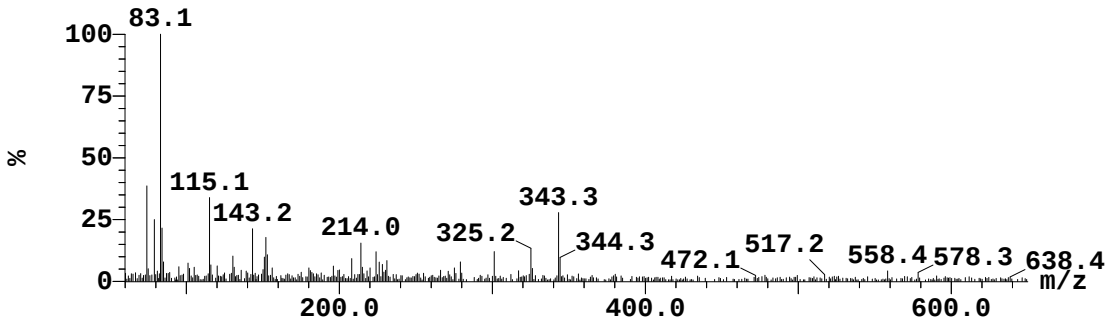
Printed: Fri Dec 14 10:44:13 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
4		1.77		5		2.02	
4:(Time: 1.77) Combine (56:60-(52+64:65))				5:(Time: 2.02) Combine (64:68-(60+72:73))			
1:TOF MS ES+ 3.3e+003				1:TOF MS ES+ 3.7e+003			



Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
6		2.19		7		2.56	
6:(Time: 2.19) Combine (70:73-(65:66+78))				7:(Time: 2.56) Combine (82:85-(77:78+90))			
1:TOF MS ES+ 1.5e+003				1:TOF MS ES+ 1.6e+003			



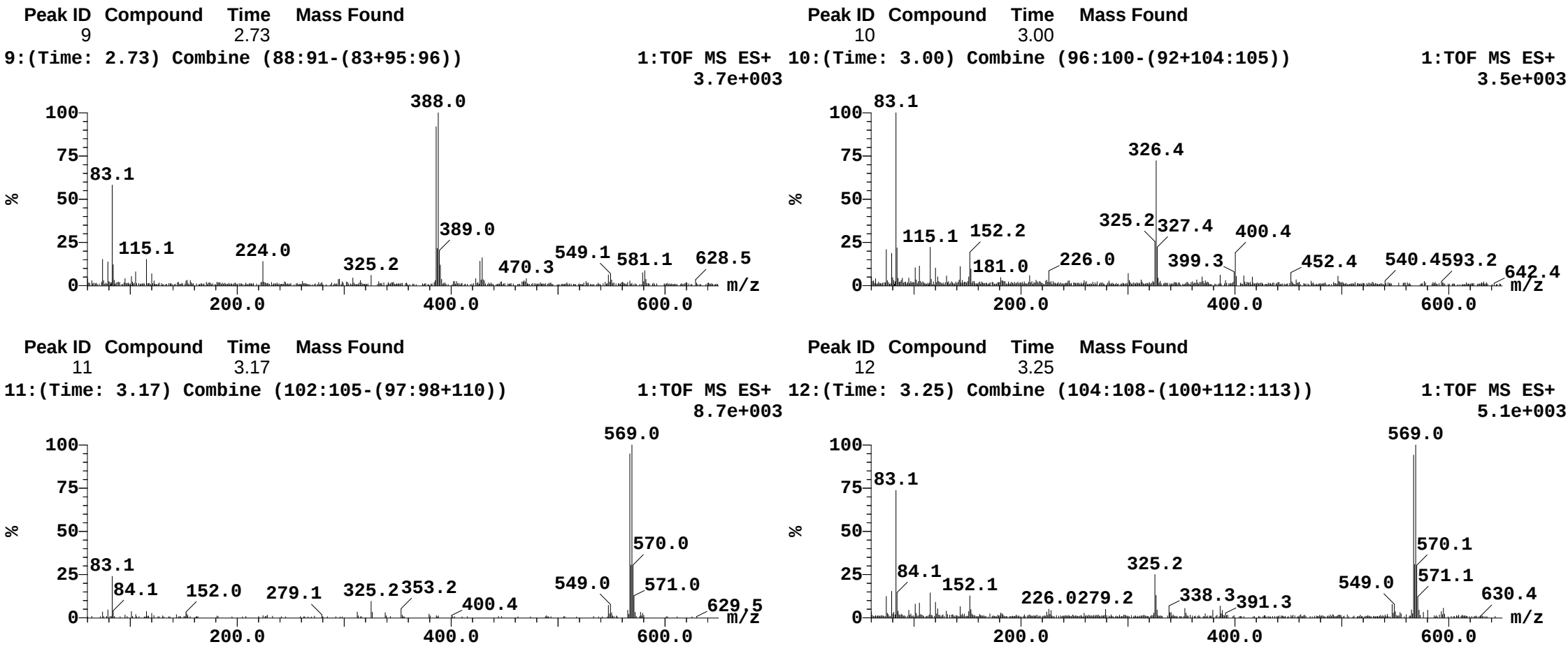
Sample: 3
File:MS50271
Description:A.ZUBIARRE AZ 332 1

Vial:1:44
Date:14-Dec-2018

ID:
Time:9::4::9

Printed: Fri Dec 14 10:44:13 2018

Sample Report (continued):



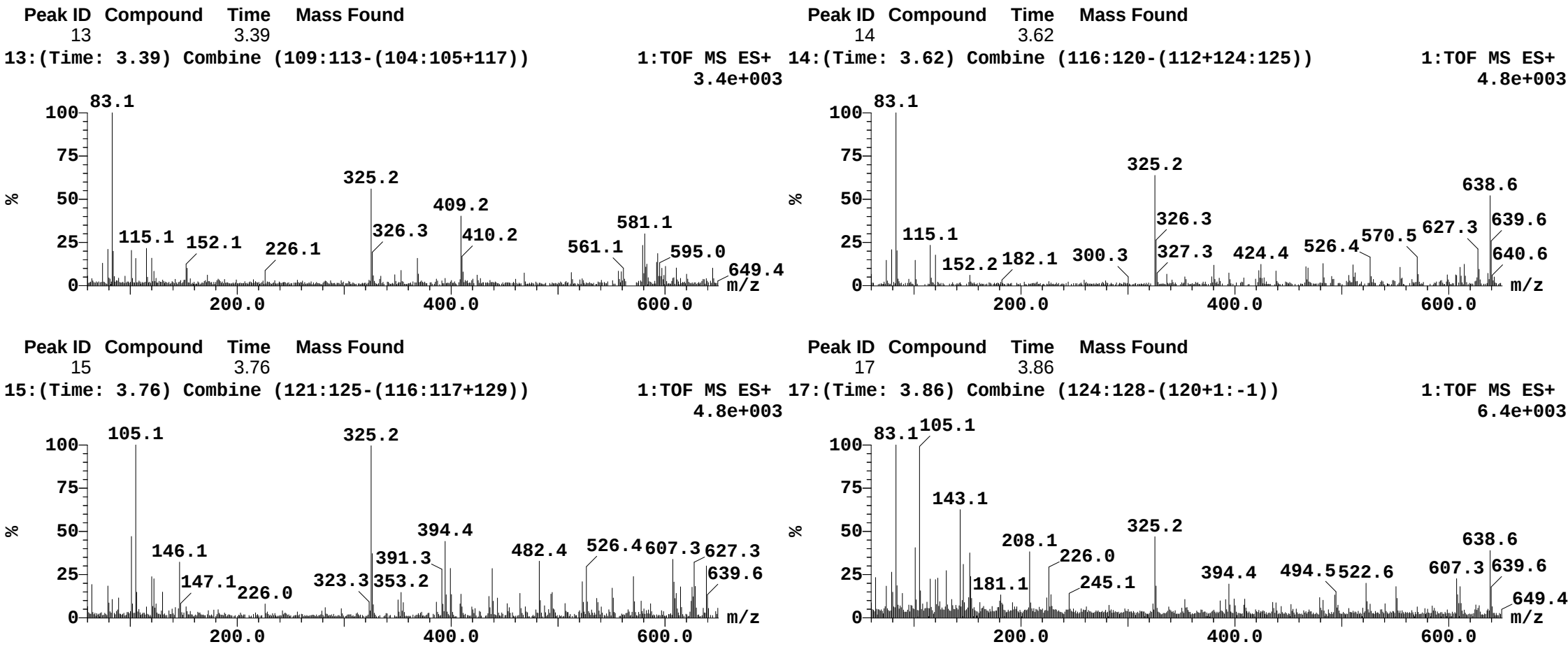
Sample: 3
File:MS50271
Description:A.ZUBIARRE AZ 332 1

Vial:1:44
Date:14-Dec-2018

ID:
Time:9::4::9

Printed: Fri Dec 14 10:44:13 2018

Sample Report (continued):



Sample: 3
File:MS50271
Description:A.ZUBIARRE AZ 332 1

Vial:1:44
Date:14-Dec-2018

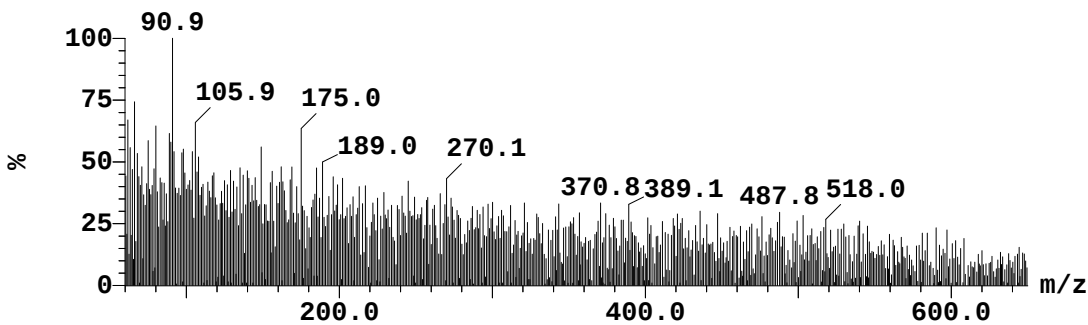
ID:
Time:9::4::9

Printed: Fri Dec 14 10:44:13 2018

Sample Report (continued):

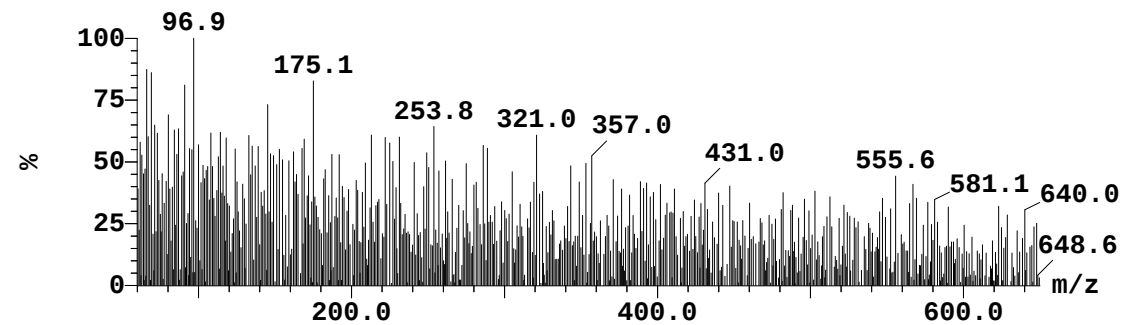
Peak ID	Compound	Time	Mass Found
1	Tentative	1.06	,450.00,404.00

1:(Time: 1.07) Combine (33:37-(28:29+41))



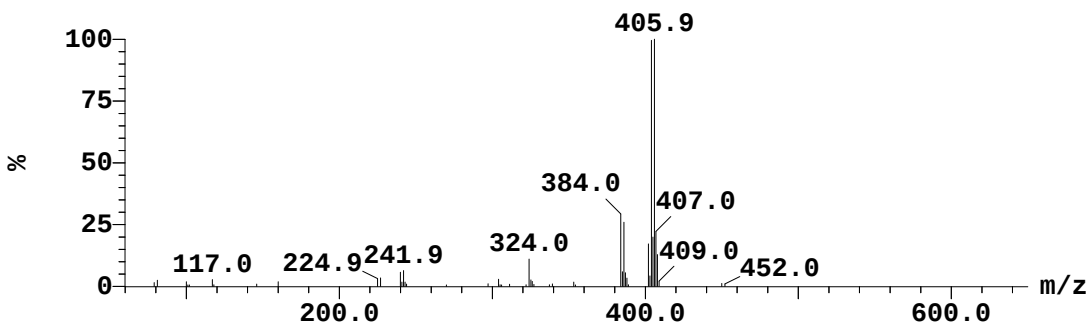
Peak ID	Compound	Time	Mass Found
2	Tentative	1.14	,450.00,404.00

2:TOF MS ES- 2.2e+002
2:(Time: 1.14) Combine (36:39-(31+43:44))



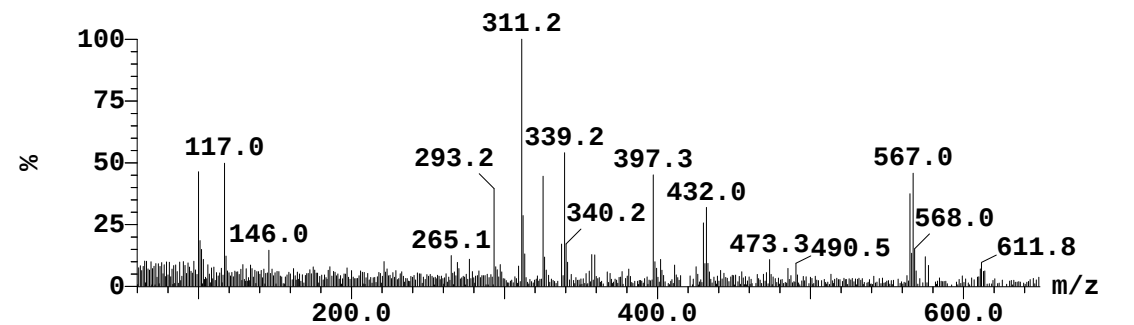
Peak ID	Compound	Time	Mass Found
8	Found	2.69	,450.00,404.00

8:(Time: 2.64) Combine (84:88-(80+92:93))



Peak ID	Compound	Time	Mass Found
10		3.00	

2:TOF MS ES- 4.3e+004
10:(Time: 3.04) Combine (97:101-(92:93+105))



Sample: 3
File:MS50271
Description:A.ZUBIARRE AZ 332 1

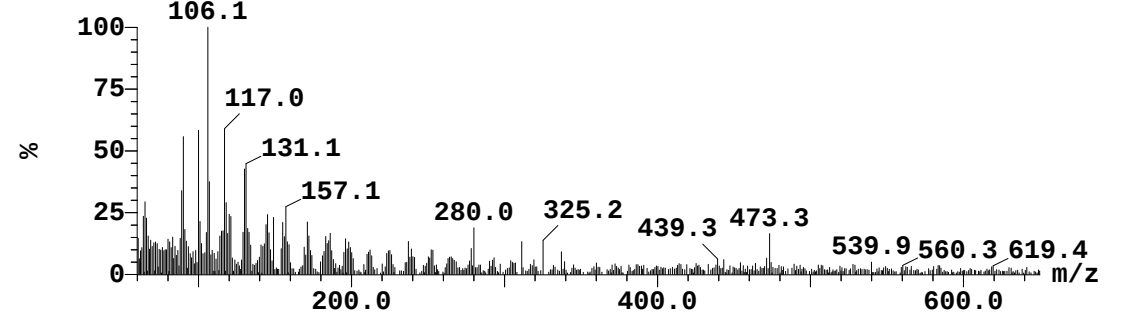
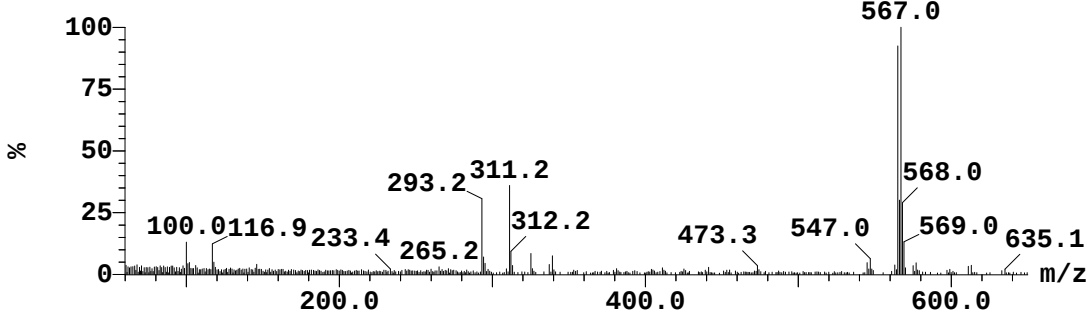
Vial:1:44
Date:14-Dec-2018

ID:
Time:9::4::9

Printed: Fri Dec 14 10:44:13 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
11		3.17		16		3.80	
11:(Time: 3.16) Combine (101:105-(96:97+109))				16:(Time: 3.80) Combine (122:125-(117:118+130))			
2:TOF MS ES- 5.8e+003				2:TOF MS ES- 1.9e+003			



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