

Single Mass Analysis

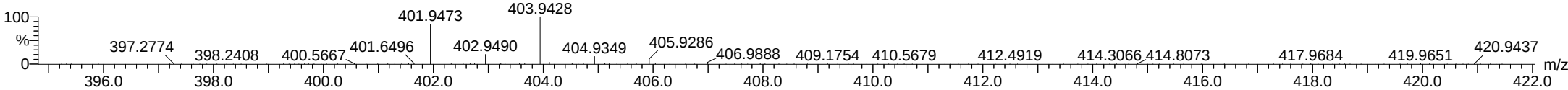
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
446 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 14-14 H: 0-100 N: 0-10 O: 0-10 Na: 0-1 S: 1-2 Br: 1-1

A.ZUBIARRE AZ 319 1
MS49541 76 (2.325)

ES-ToF

09-Nov-2018
2: TOF MS ES-
6.16e+003



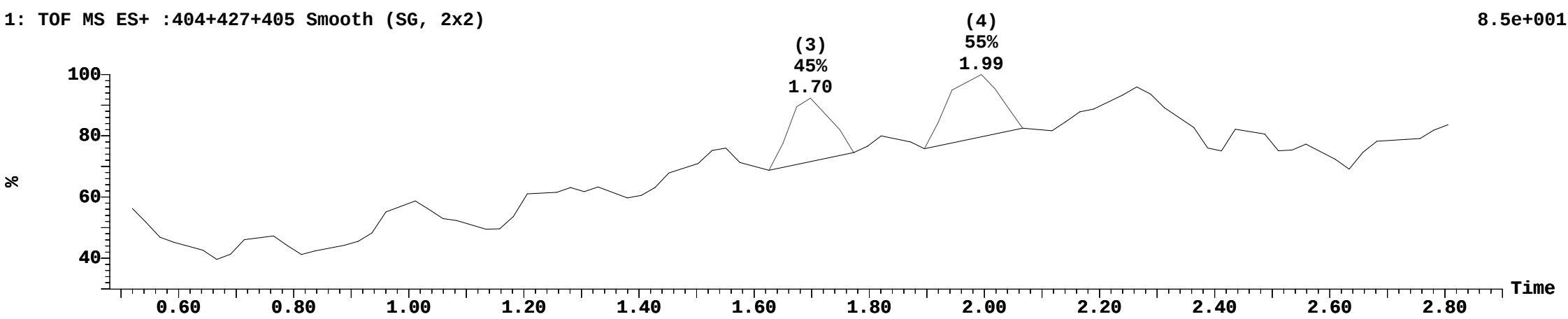
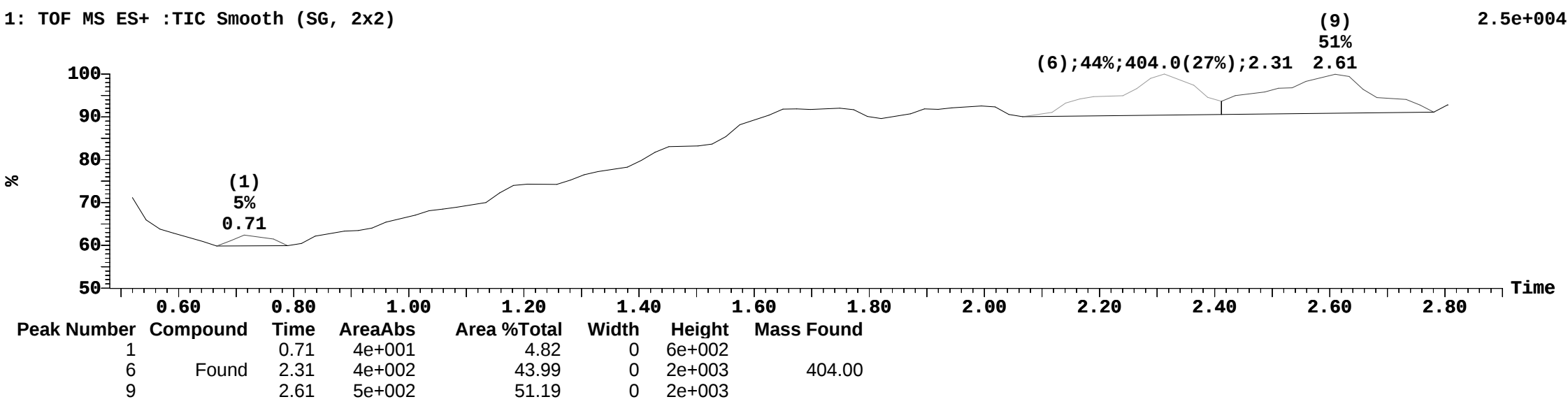
Minimum: -1.5
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula						
401.9473	401.9469	0.4	1.0	8.5	88.4	0.1	C14	H13	N	O4	S2	Br	
	401.9524	-5.1	-12.7	10.5	90.6	2.3	C14	H10	N3	O3	Na	S	Br

This document was created with Win2PDF available at <http://www.win2pdf.com>.
The unregistered version of Win2PDF is for evaluation or non-commercial use only.

Sample Report:

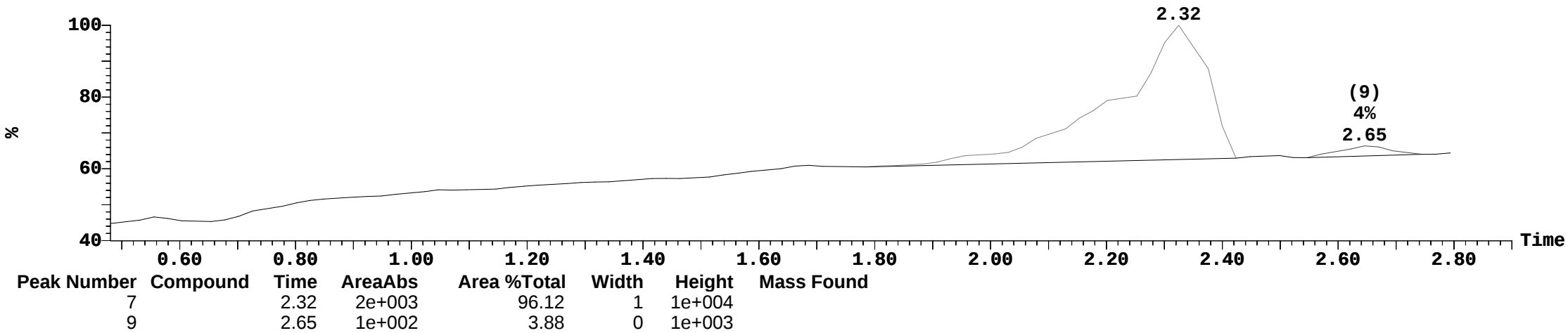
Sample 4 Vial 1:13 ID File MS49541 Date 09-Nov-2018 Time 2::1::5 Description A.ZUBIARRE AZ 319 1



Sample Report (continued):

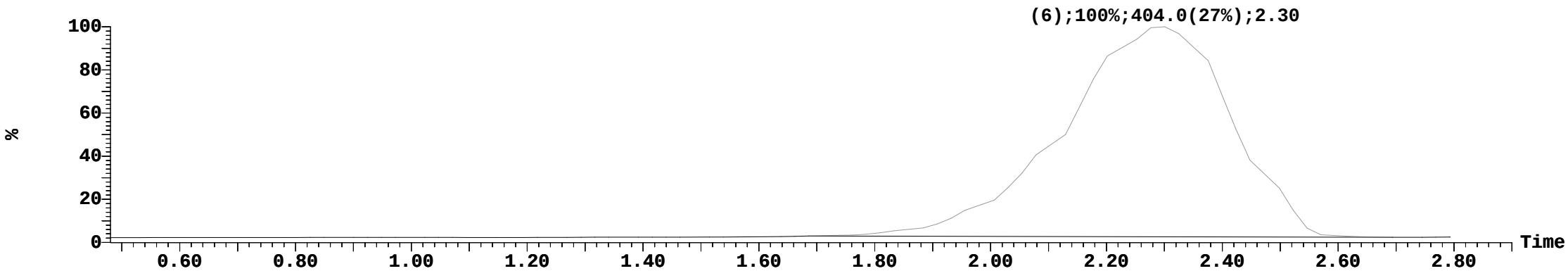
2: TOF MS ES- :TIC Smooth (SG, 2x2)

3.5e+004



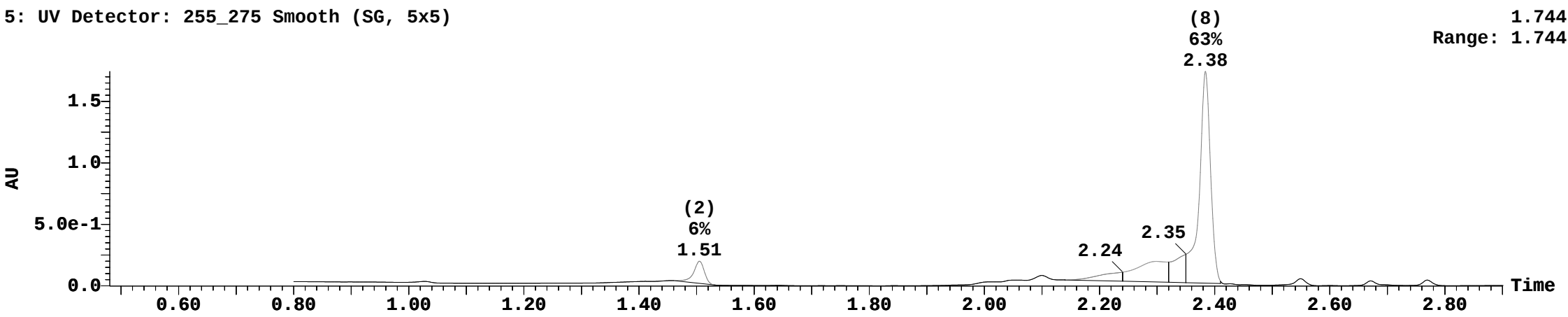
2: TOF MS ES- :404+449+403 Smooth (Mn, 2x3)

3.2e+003



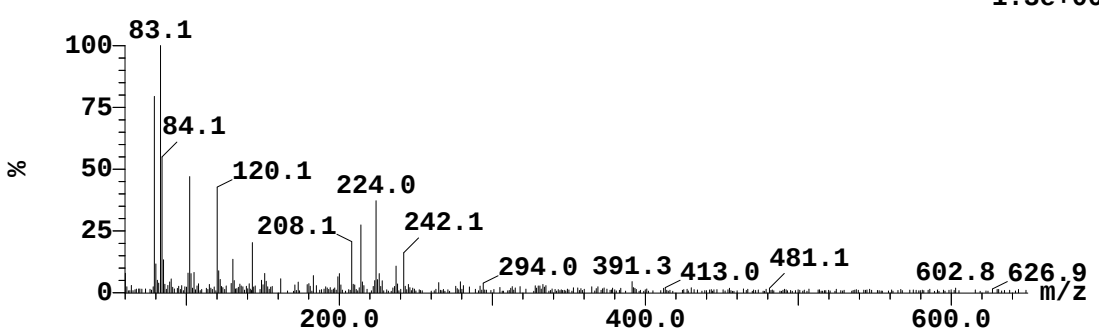
Sample Report (continued):

5: UV Detector: 255_275 Smooth (SG, 5x5)



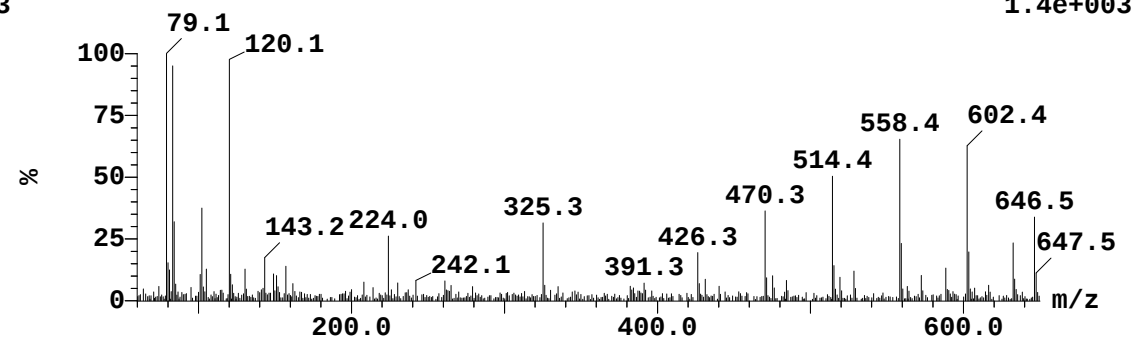
Peak ID	Compound	Time	Mass Found
1		0.71	

1:(Time: 0.71) Combine (22:25-(17:18+30))



Peak ID	Compound	Time	Mass Found
3		1.70	

1:TOF MS ES+ 3:(Time: 1.70) Combine (54:57-(49:50+62))



Sample: 4

File:MS49541

Description:A.ZUBIARRE AZ 319 1

Vial:1:13

Date:09-Nov-2018

ID:

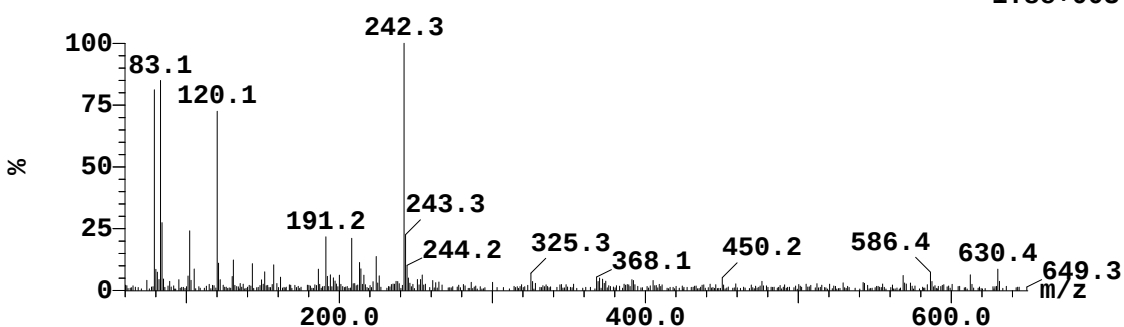
Time:2::1::5

Printed: Fri Nov 09 15:36:11 2018

Sample Report (continued):

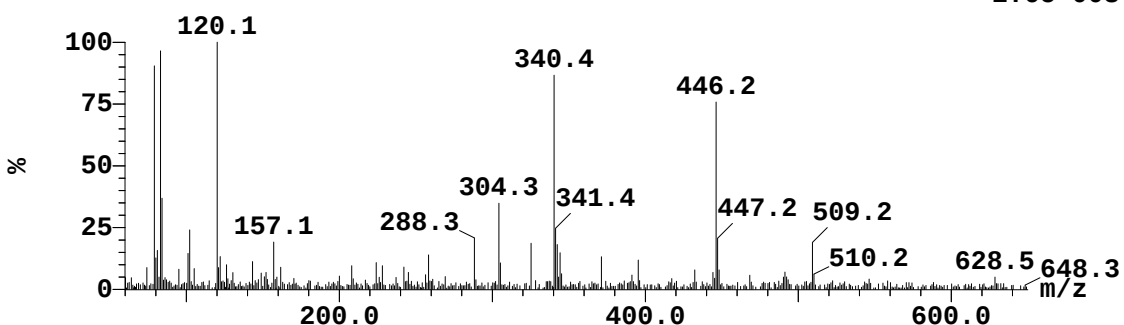
Peak ID	Compound	Time	Mass Found
4		1.99	

4:(Time: 1.99) Combine (64:67-(59+71:72))



Peak ID	Compound	Time	Mass Found
9		2.61	

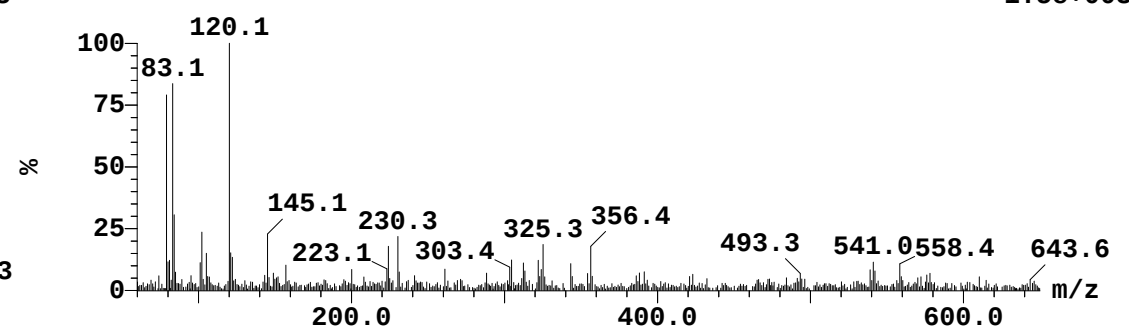
9:(Time: 2.61) Combine (84:87-(79+91:92))



Peak ID	Compound	Time	Mass Found
6		2.31	

1:TOF MS ES+ 6:(Time: 2.31) Combine (74:77-(69:70+82))

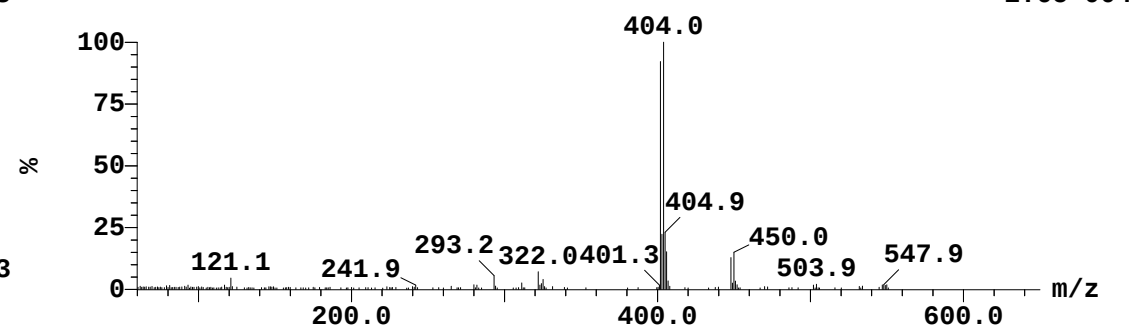
1.8e+003



Peak ID	Compound	Time	Mass Found
6	Found	2.31	,449.00,403.00

1:TOF MS ES+ 6:(Time: 2.30) Combine (73:77-(68:69+81))

1.6e+003



Sample: 4
File:MS49541
Description:A.ZUBIARRE AZ 319 1

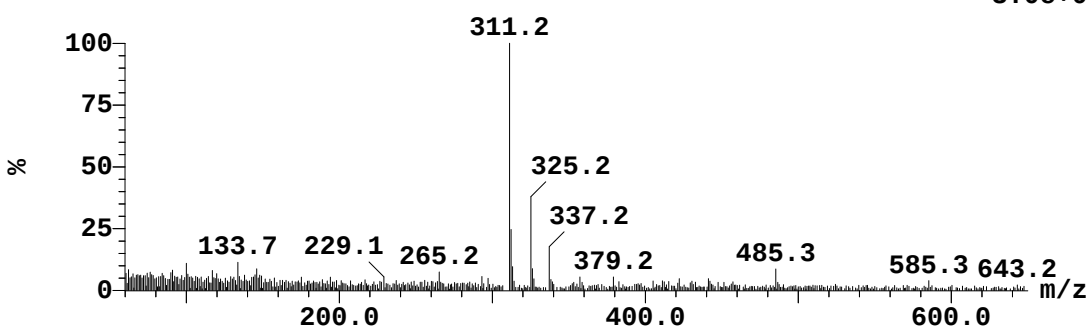
Vial:1:13
Date:09-Nov-2018

ID:
Time:2::1::5

Printed: Fri Nov 09 15:36:11 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
9		2.61	
9:(Time: 2.65) Combine (84:88-(80+92:93))			
			2:T0F MS ES- 3.0e+003



This document was created with Win2PDF available at <http://www.win2pdf.com>.
The unregistered version of Win2PDF is for evaluation or non-commercial use only.