

Single Mass Analysis

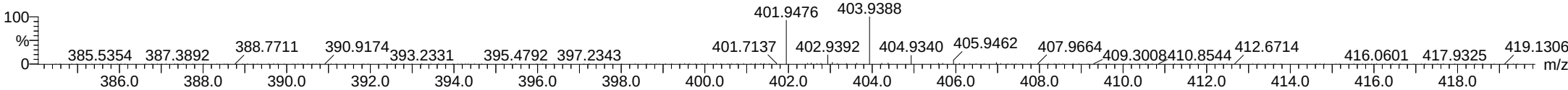
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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 2
MS49542 74 (2.277)

ES-ToF

09-Nov-2018
2: TOF MS ES-
4.07e+003



Minimum: -1.5
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula						
401.9476	401.9469	0.7	1.7	8.5	95.7	0.5	C14	H13	N	O4	S2	Br	
	401.9524	-4.8	-11.9	10.5	96.2	1.0	C14	H10	N3	O3	Na	S	Br

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Sample: 5
File:MS49542
Description:A.ZUBIARRE AZ 319 2

Vial:1:14
Date:09-Nov-2018

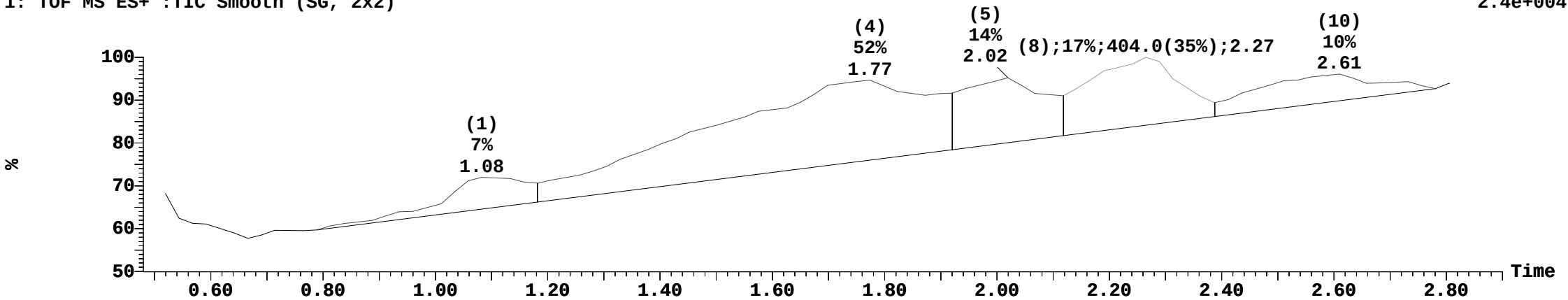
ID:
Time:2::6::8

Printed: Fri Nov 09 15:37:04 2018

Sample Report:

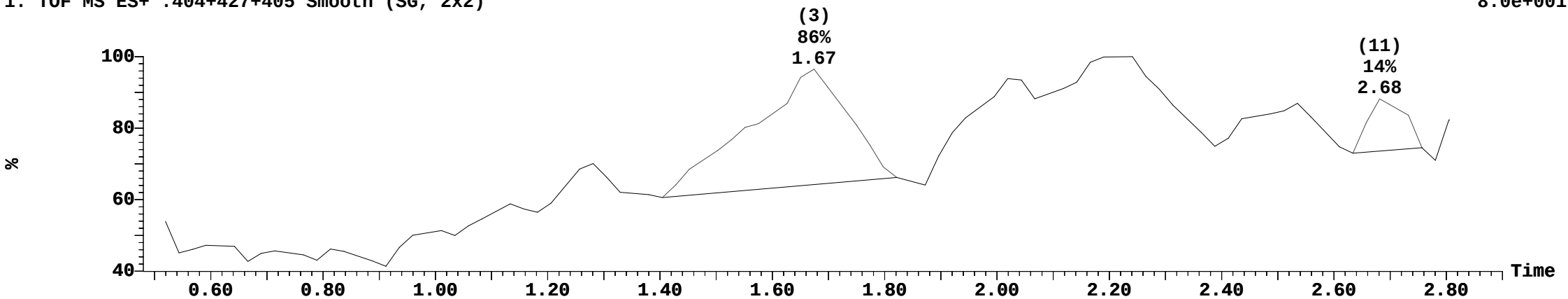
Sample 5 Vial 1:14 ID File MS49542 Date 09-Nov-2018 Time 2::6::8 Description A.ZUBIARRE AZ 319 2

1: TOF MS ES+ :TIC Smooth (SG, 2x2) 2.4e+004



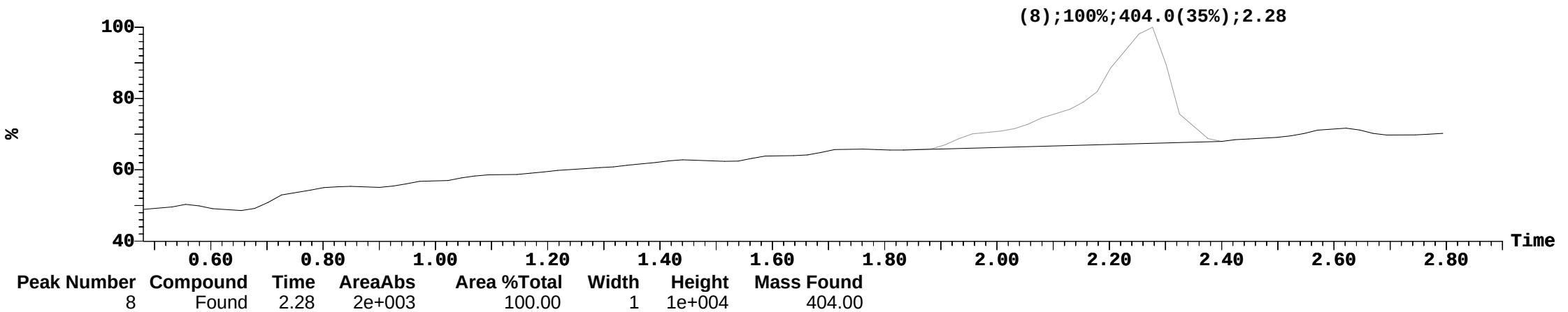
Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		1.08	3e+002	7.14	0	2e+003	
4		1.77	2e+003	51.51	1	5e+003	
5		2.02	6e+002	14.39	0	4e+003	
8	Found	2.27	7e+002	17.31	0	4e+003	404.00
10		2.61	4e+002	9.66	0	2e+003	

1: TOF MS ES+ :404+427+405 Smooth (SG, 2x2) 8.0e+001

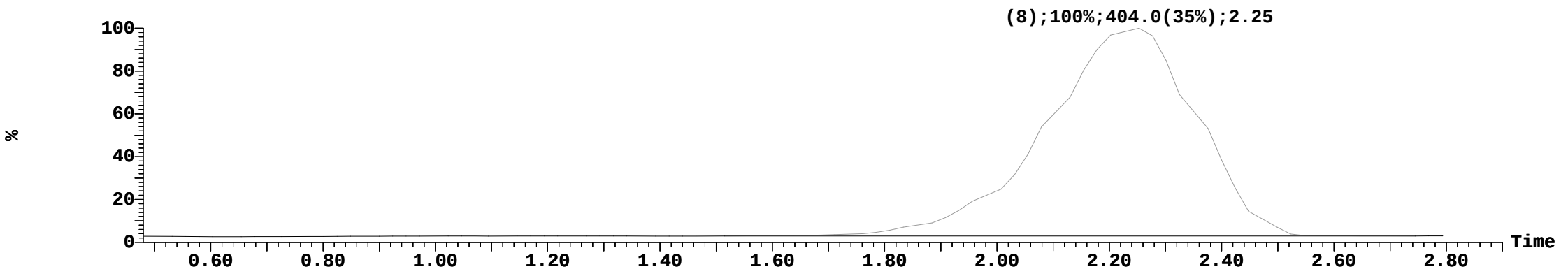


Sample Report (continued):

2: TOF MS ES- :TIC Smooth (SG, 2x2) 3.2e+004



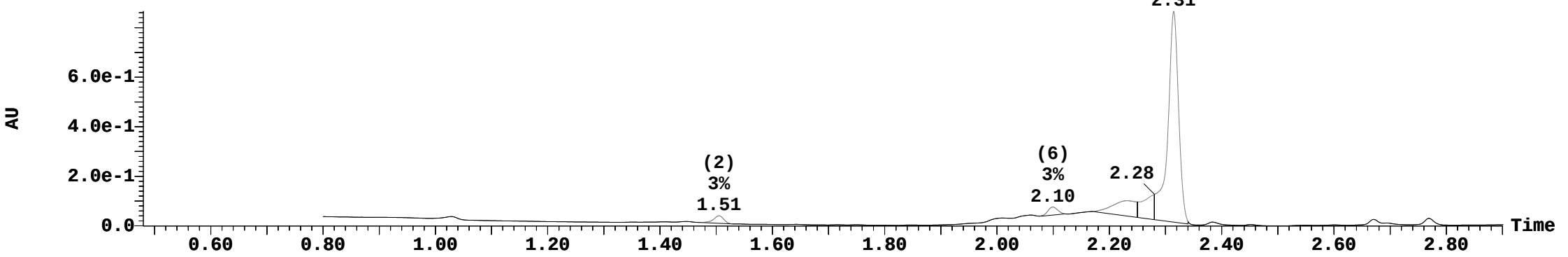
2: TOF MS ES- :404+449+403 Smooth (Mn, 2x3) 2.6e+003



Sample Report (continued):

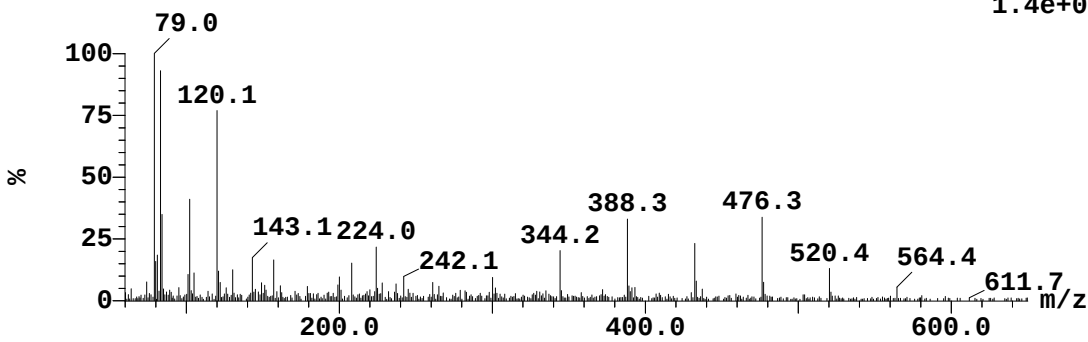
5: UV Detector: 255_275 Smooth (SG, 5x5)

8.663e-1
Range: 8.662e-1



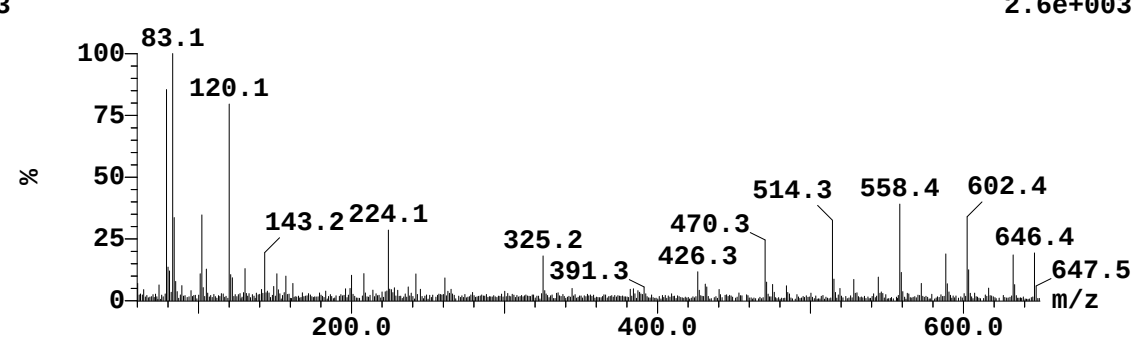
Peak ID	Compound	Time	Mass Found
1		1.08	

1: (Time: 1.08) Combine (34:37-(29:30+42))



Peak ID	Compound	Time	Mass Found
3		1.67	

1: TOF MS ES+ 3: (Time: 1.67) Combine (53:57-(48:49+61))



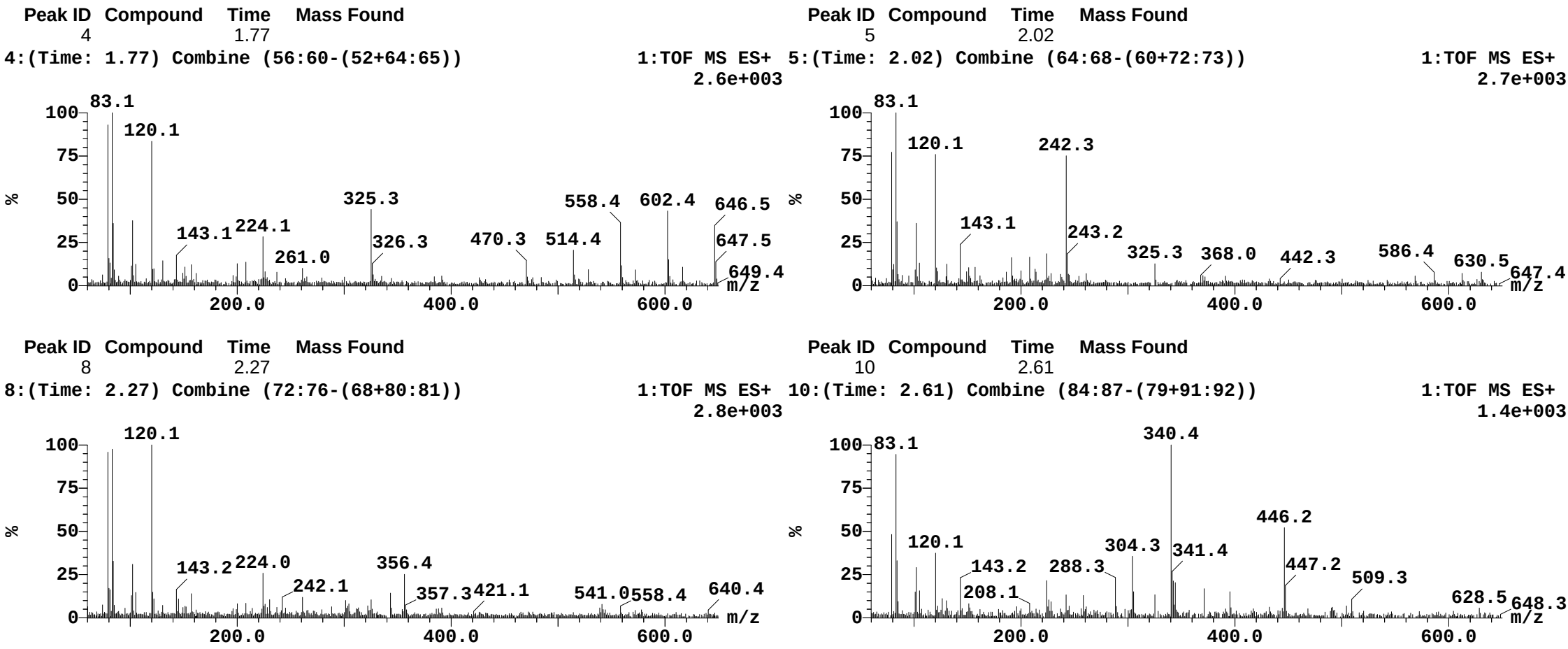
Sample: 5
File:MS49542
Description:A.ZUBIARRE AZ 319 2

Vial:1:14
Date:09-Nov-2018

ID:
Time:2::6::8

Printed: Fri Nov 09 15:37:04 2018

Sample Report (continued):



Sample: 5
File:MS49542
Description:A.ZUBIARRE AZ 319 2

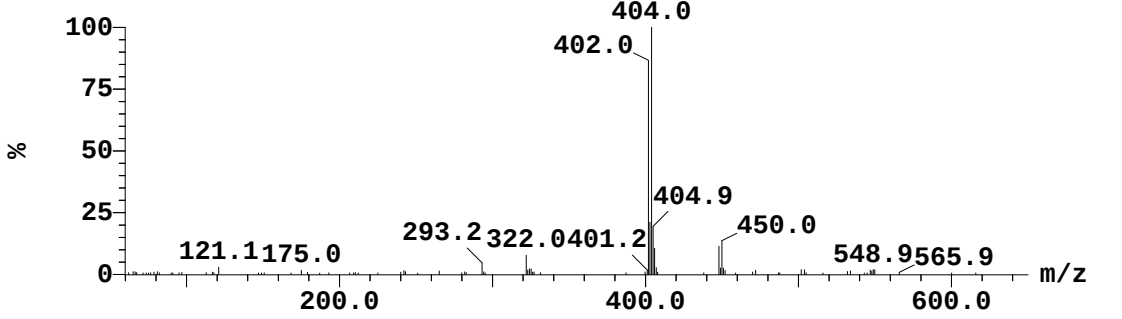
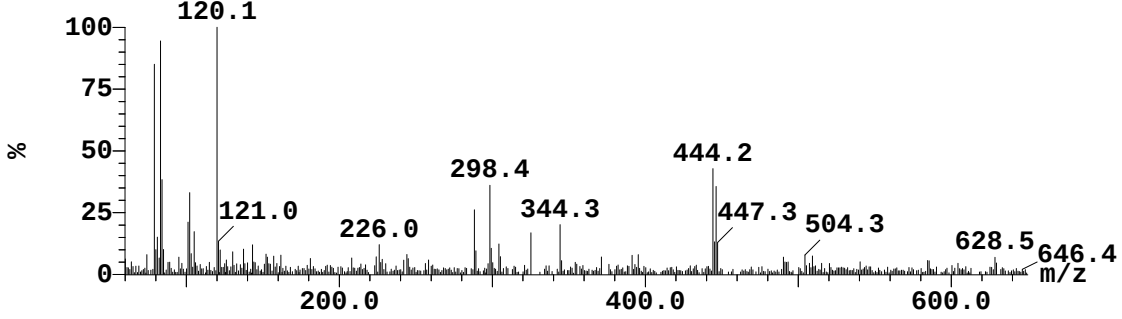
Vial:1:14
Date:09-Nov-2018

ID:
Time:2::6::8

Printed: Fri Nov 09 15:37:04 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
11		2.68		8	Found	2.27	,449.00,403.00
11:(Time: 2.68) Combine (86:89-(81:82+94))				8:(Time: 2.25) Combine (72:75-(67+79:80))			
1:TOF MS ES+ 1.3e+003				2:TOF MS ES- 1.2e+004			



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