

Single Mass Analysis

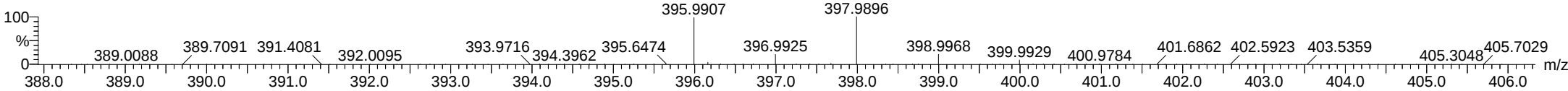
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
444 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 16-16 H: 0-100 N: 0-10 O: 0-10 Na: 0-1 S: 1-2 Br: 1-1

A.ZUBIARRE AZ 320 2
MS49544 74 (2.275)

ES-ToF

09-Nov-2018
2: TOF MS ES-
3.61e+003



Minimum: -1.5
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula						
395.9907	395.9905	0.2	0.5	9.5	75.8	0.0	C16	H15	N	O4	S	Br	

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Sample: 7
File:MS49544
Description:A.ZUBIARRE AZ 320 2

Vial:1:16
Date:09-Nov-2018

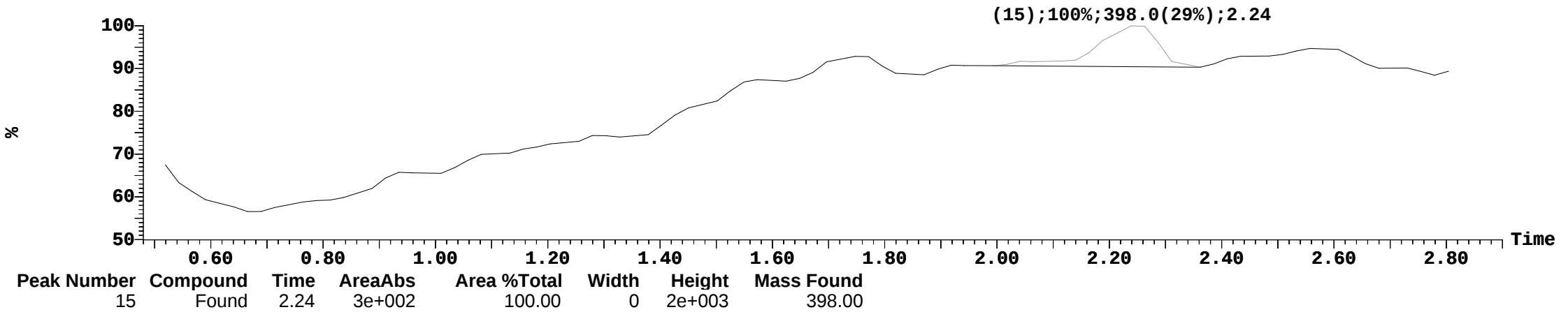
ID:
Time:2::6::5

Printed: Fri Nov 09 15:38:59 2018

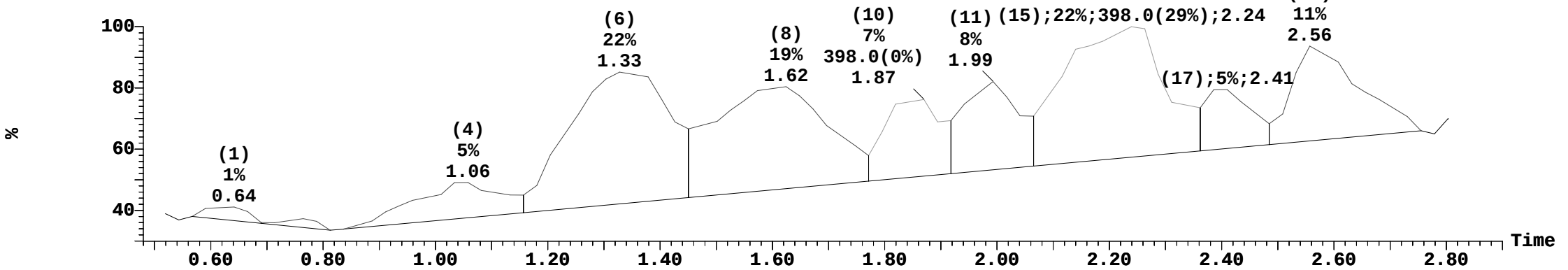
Sample Report:

Sample 7 Vial 1:16 ID File MS49544 Date 09-Nov-2018 Time 2::6::5 Description A.ZUBIARRE AZ 320 2

1: TOF MS ES+ :TIC Smooth (SG, 2x2) 2.5e+004



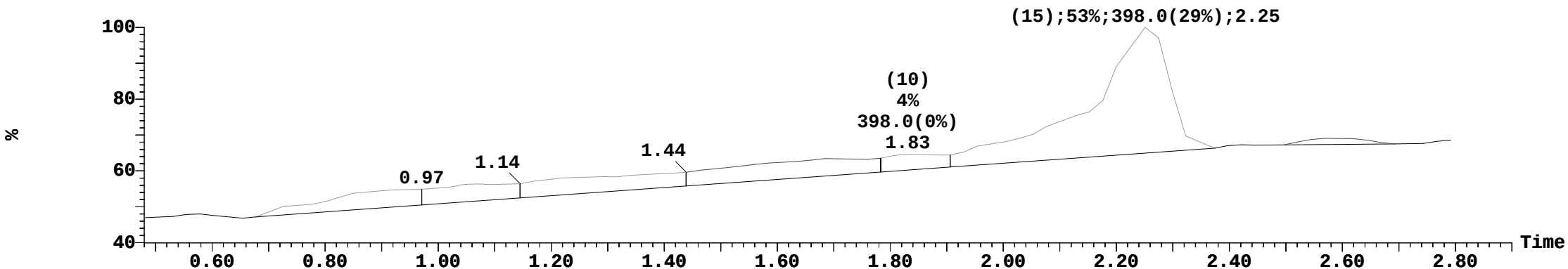
1: TOF MS ES+ :398+421+399 Smooth (SG, 2x2) 8.1e+001



Sample Report (continued):

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

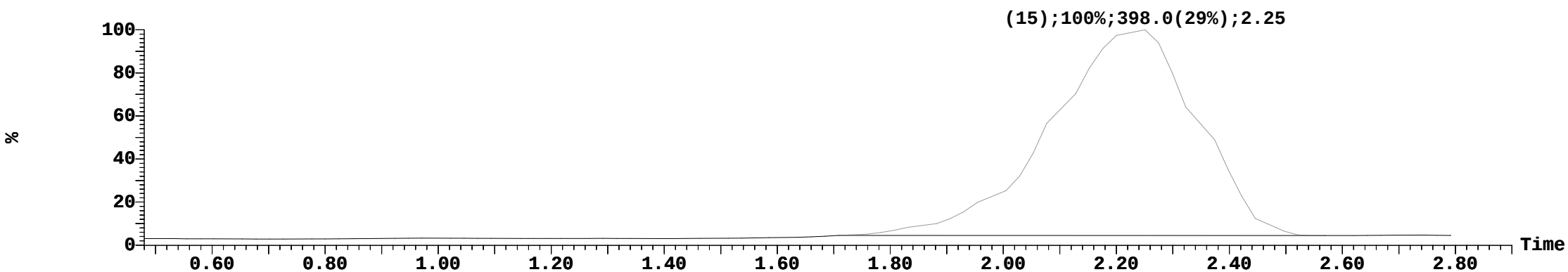
3.3e+004



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
3	Tentative	0.97	3e+002	8.90	0	1e+003	398.00
5	Tentative	1.14	3e+002	6.90	0	1e+003	398.00
7	Tentative	1.44	4e+002	11.14	0	1e+003	398.00
9		1.78	5e+002	13.64	0	1e+003	
10	Tentative	1.83	2e+002	4.44	0	1e+003	398.00
15	Found	2.25	2e+003	53.06	0	1e+004	398.00
18		2.57	7e+001	1.93	0	6e+002	

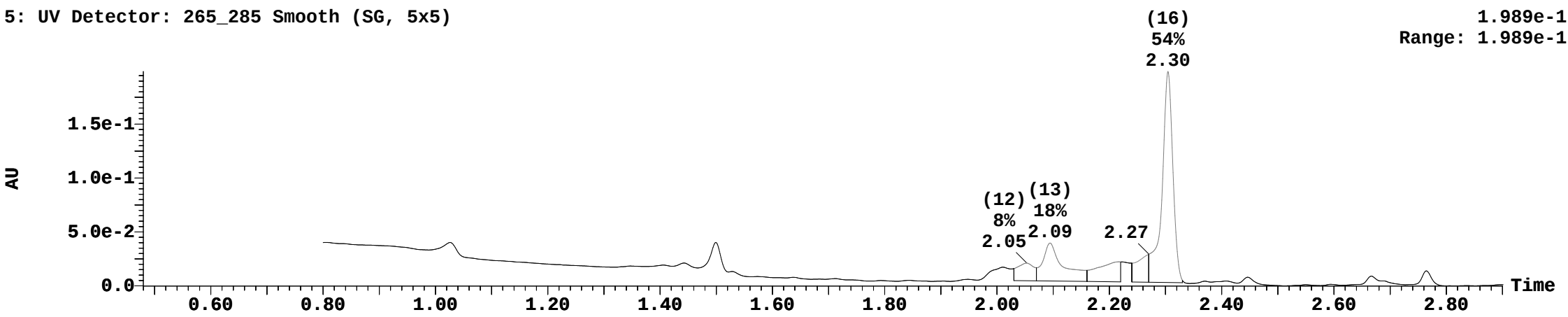
2: TOF MS ES- :398+443+397 Smooth (Mn, 2x3)

2.3e+003



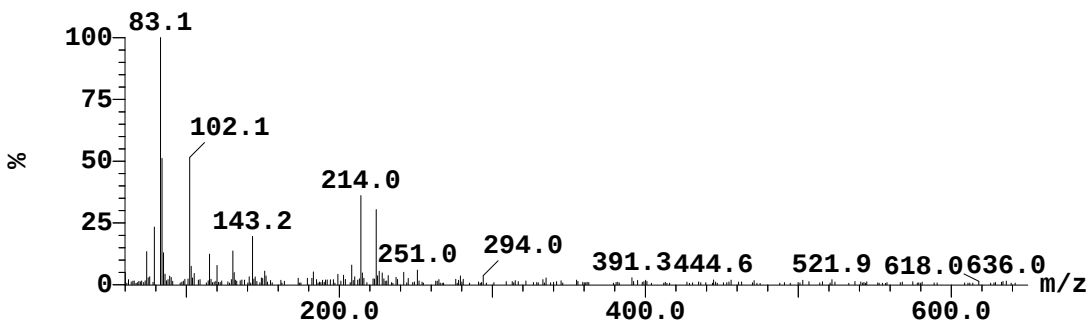
Sample Report (continued):

5: UV Detector: 265_285 Smooth (SG, 5x5)



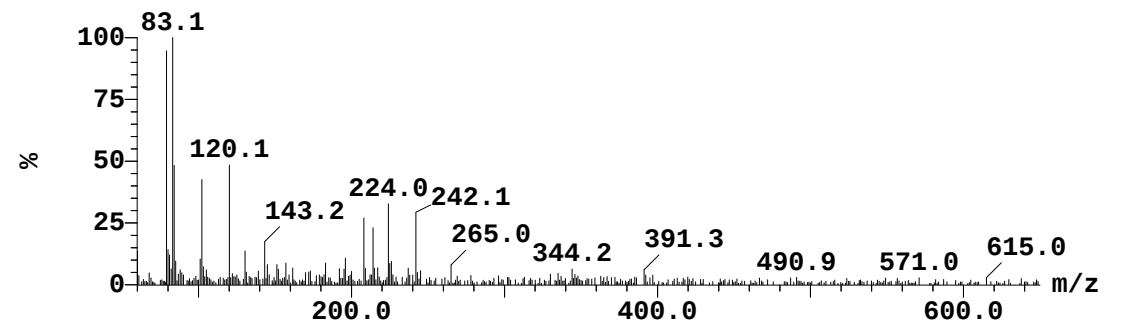
Peak ID	Compound	Time	Mass Found
1		0.64	

1:(Time: 0.64) Combine (20:23-(15+27:28))



Peak ID	Compound	Time	Mass Found
2		0.76	

1:TOF MS ES+ 2:(Time: 0.76) Combine (24:27-(19+31:32)) 1:TOF MS ES+
1.5e+003 8.5e+002



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Date:09-Nov-2018

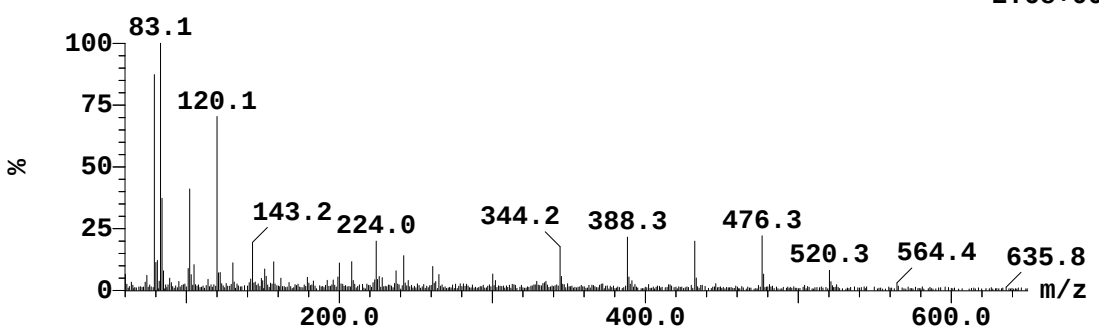
ID:
Time:2::6::5

Printed: Fri Nov 09 15:38:59 2018

Sample Report (continued):

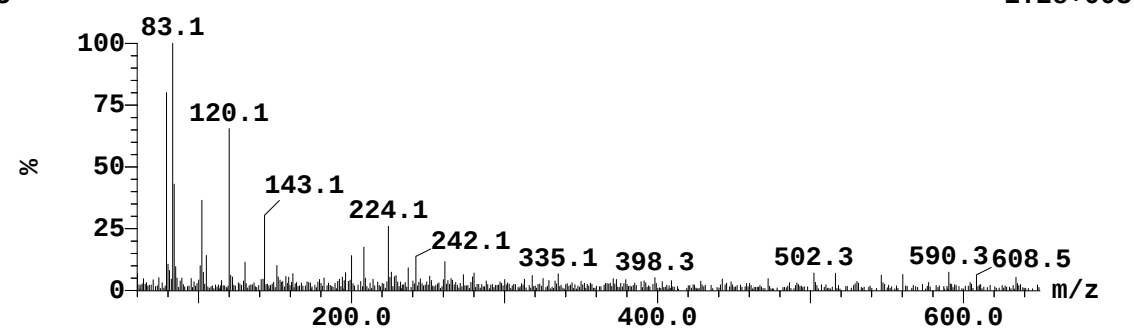
Peak ID	Compound	Time	Mass Found
4		1.06	

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



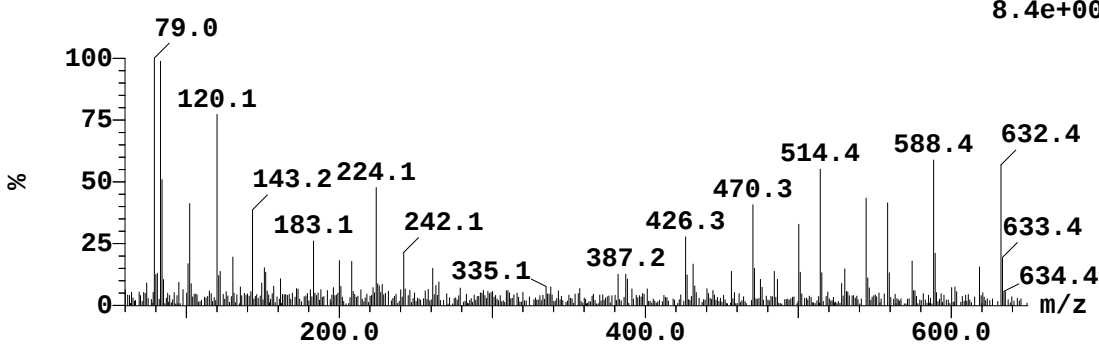
Peak ID	Compound	Time	Mass Found
6		1.33	

1:TOF MS ES+ 6:(Time: 1.33) Combine (42:45-(37:38+50)) 1:TOF MS ES+ 2.6e+003 1.2e+003



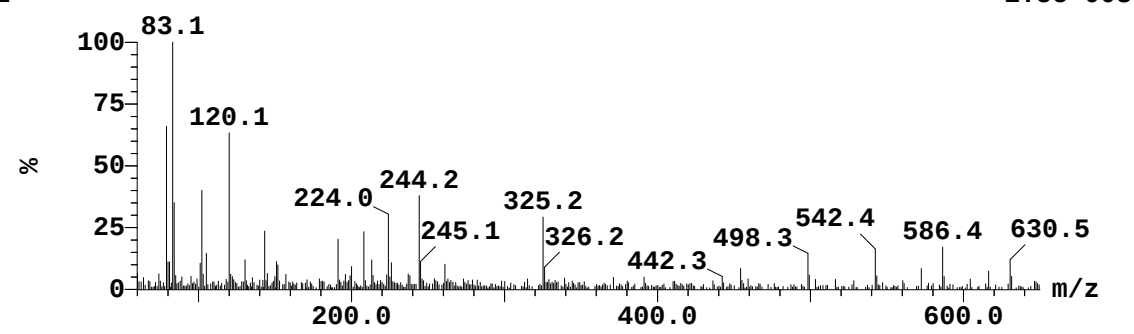
Peak ID	Compound	Time	Mass Found
8		1.62	

8:(Time: 1.62) Combine (52:55-(47+59:60))



Peak ID	Compound	Time	Mass Found
10		1.87	

1:TOF MS ES+ 10:(Time: 1.87) Combine (60:63-(55+67:68)) 1:TOF MS ES+ 8.4e+002 1.5e+003



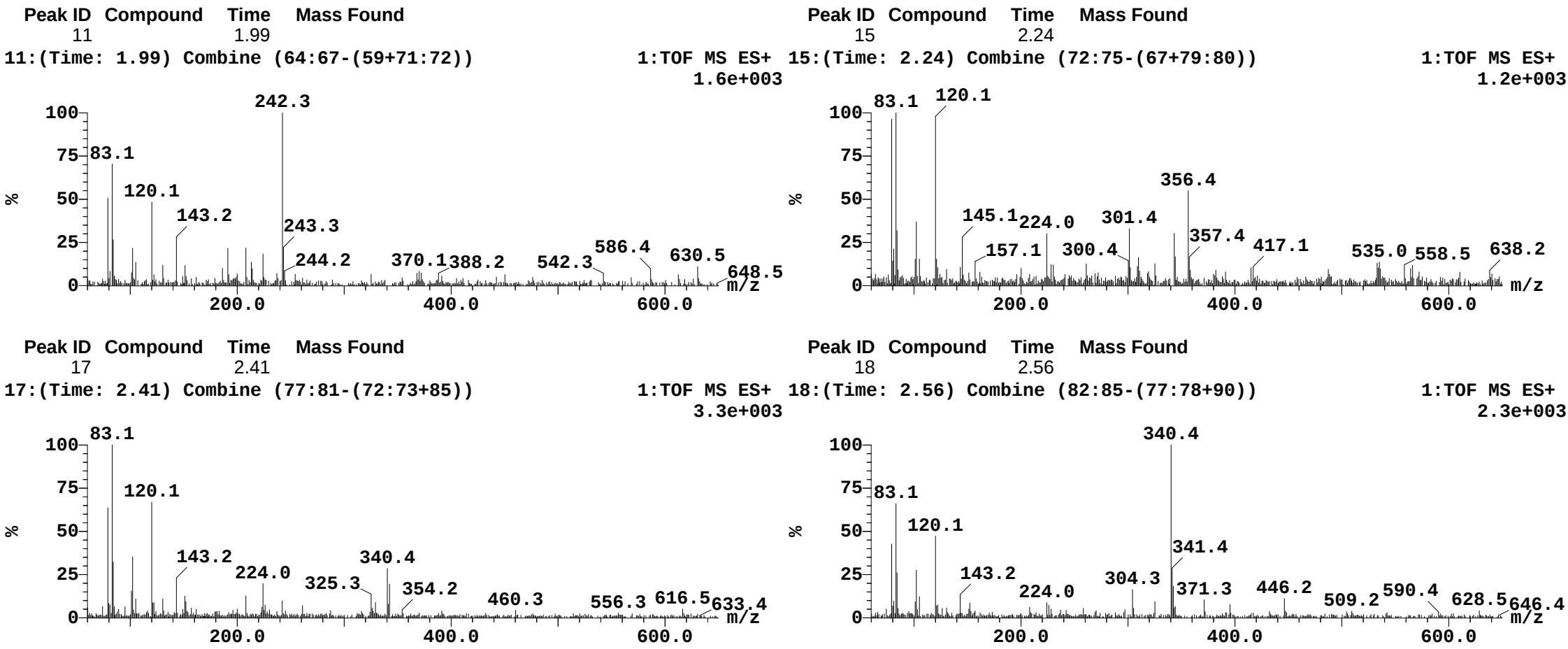
Sample: 7
File:MS49544
Description:A.ZUBIARRE AZ 320 2

Vial:1:16
Date:09-Nov-2018

ID:
Time:2::6::5

Printed: Fri Nov 09 15:38:59 2018

Sample Report (continued):



Sample: 7

File:MS49544

Description:A.ZUBIARRE AZ 320 2

Vial:1:16

Date:09-Nov-2018

ID:

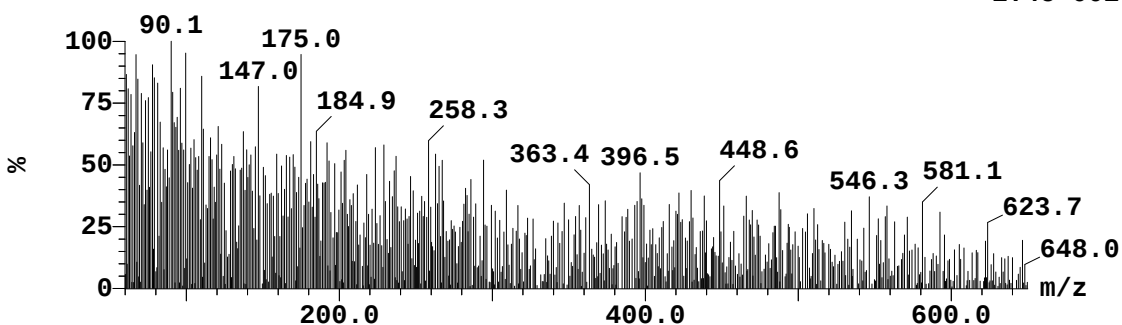
Time:2::6::5

Printed: Fri Nov 09 15:38:59 2018

Sample Report (continued):

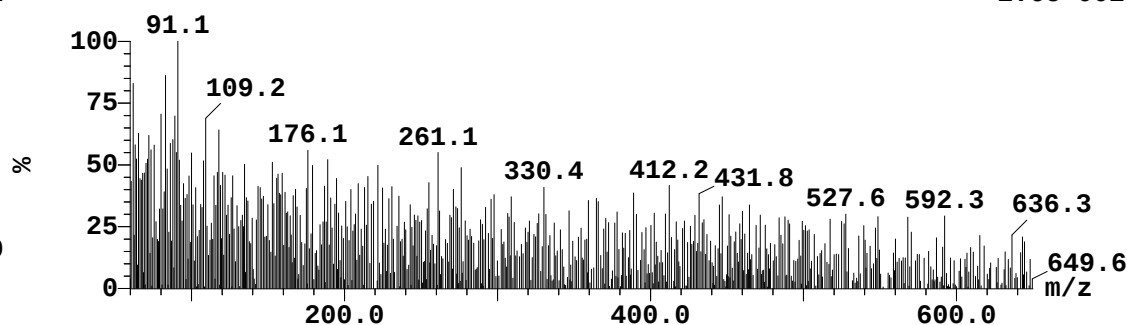
Peak ID	Compound	Time	Mass Found
3	Tentative	0.97	,443.00,397.00

3:(Time: 0.97) Combine (30:33-(25:26+38))



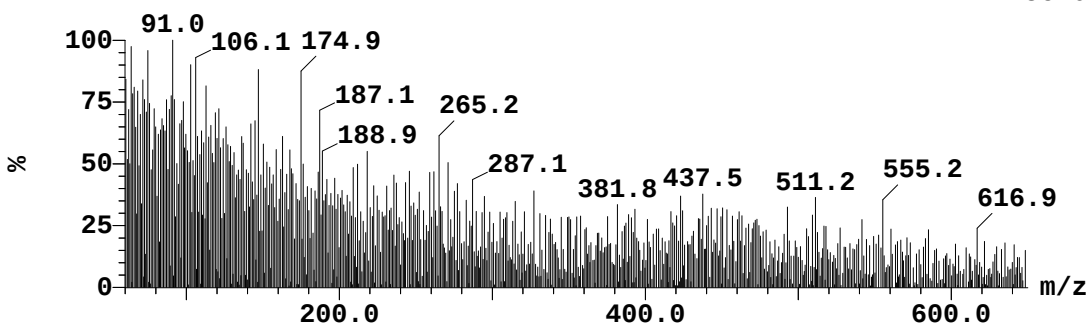
Peak ID	Compound	Time	Mass Found
5	Tentative	1.14	,443.00,397.00

5:(Time: 1.14) Combine (36:39-(31+43:44))



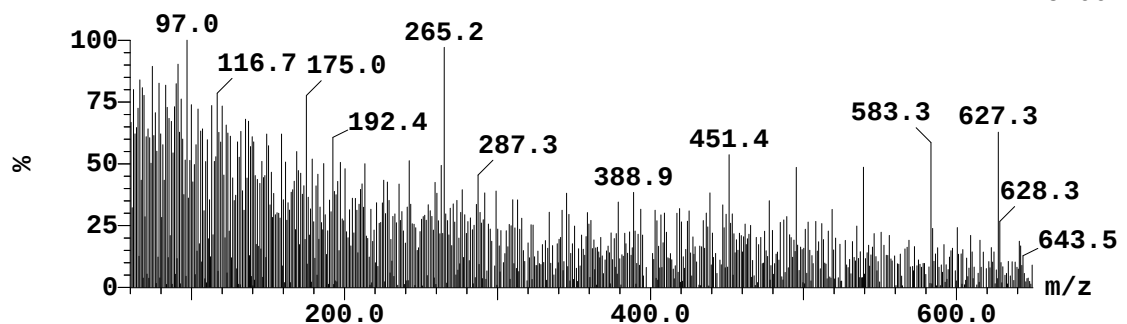
Peak ID	Compound	Time	Mass Found
7	Tentative	1.44	,443.00,397.00

7:(Time: 1.44) Combine (45:49-(40:41+53))



Peak ID	Compound	Time	Mass Found
9		1.78	

9:(Time: 1.78) Combine (56:60-(52+64:65))



Sample: 7
File:MS49544
Description:A.ZUBIARRE AZ 320 2

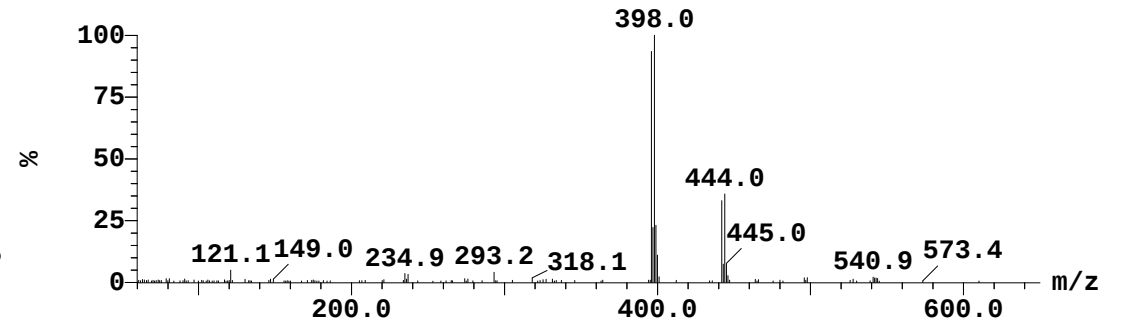
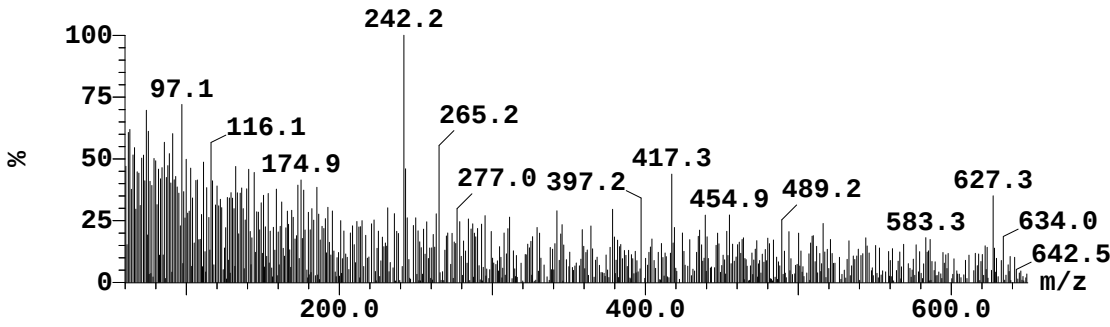
Vial:1:16
Date:09-Nov-2018

ID:
Time:2::6::5

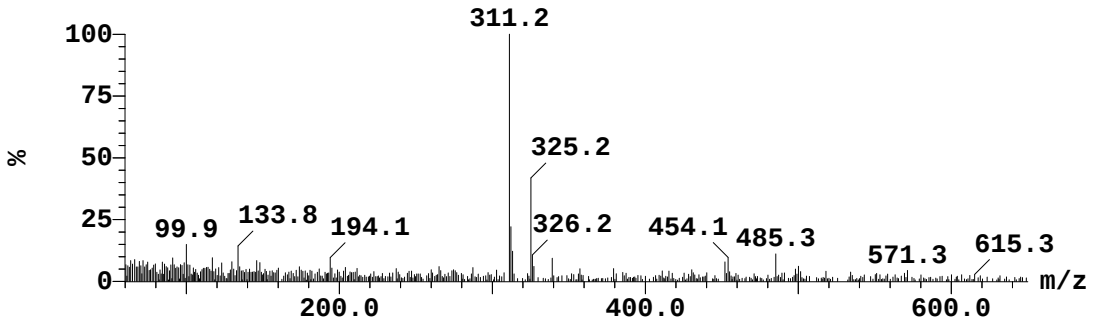
Printed: Fri Nov 09 15:38:59 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
10	Tentative	1.87	443.00,397.00	15	Found	2.24	,443.00,397.00
10:(Time: 1.83) Combine (58:61-(53:54+66))				15:(Time: 2.25) Combine (72:75-(67+79:80))			
2:TOF MS ES- 2.4e+002				2:TOF MS ES- 1.0e+004			



Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
18		2.56					
18:(Time: 2.57) Combine (82:85-(77:78+90))				2:TOF MS ES- 1.6e+003			



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