

Single Mass Analysis

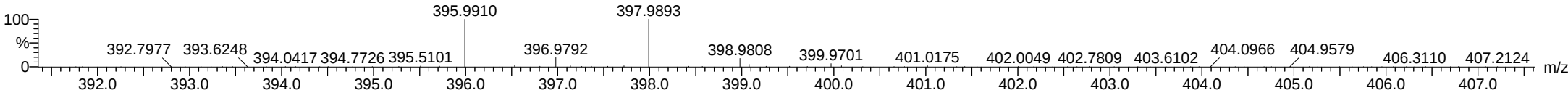
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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 1
MS49543 76 (2.322)

ES-ToF

09-Nov-2018
2: TOF MS ES-
6.25e+003



Minimum: -1.5
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula					
395.9910	395.9905	0.5	1.3	9.5	92.0	0.0	C16	H15	N	O4	S	Br

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Sample: 6
File:MS49543
Description:A.ZUBIARRE AZ 320 1

Vial:1:15
Date:09-Nov-2018

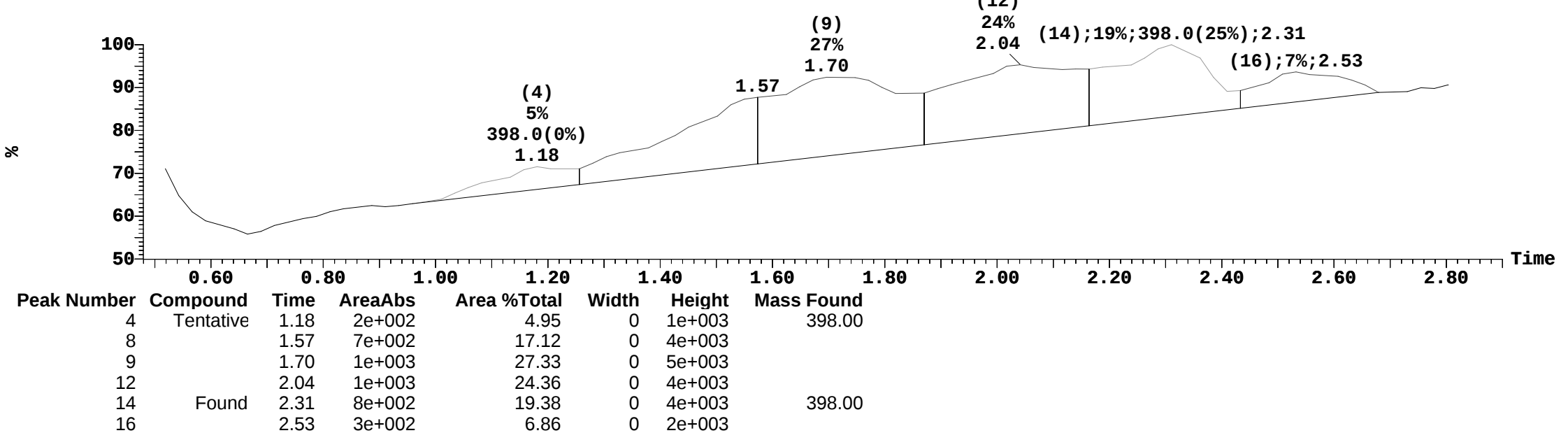
ID:
Time:2::1::2

Printed: Fri Nov 09 15:38:09 2018

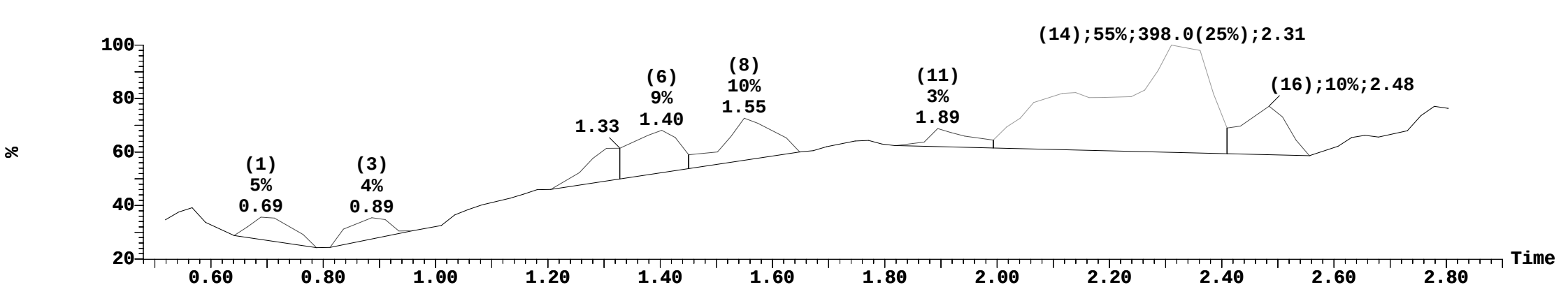
Sample Report:

Sample 6 Vial 1:15 ID File MS49543 Date 09-Nov-2018 Time 2::1::2 Description A.ZUBIARRE AZ 320 1

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



1: TOF MS ES+ :398+421+399 Smooth (SG, 2x2) 9.0e+001



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Vial:1:15
Date:09-Nov-2018

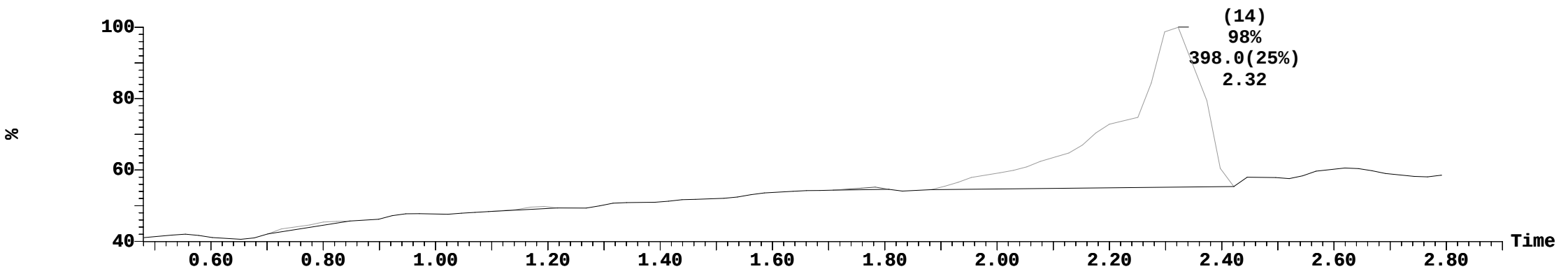
ID:
Time:2::1::2

Printed: Fri Nov 09 15:38:09 2018

Sample Report (continued):

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

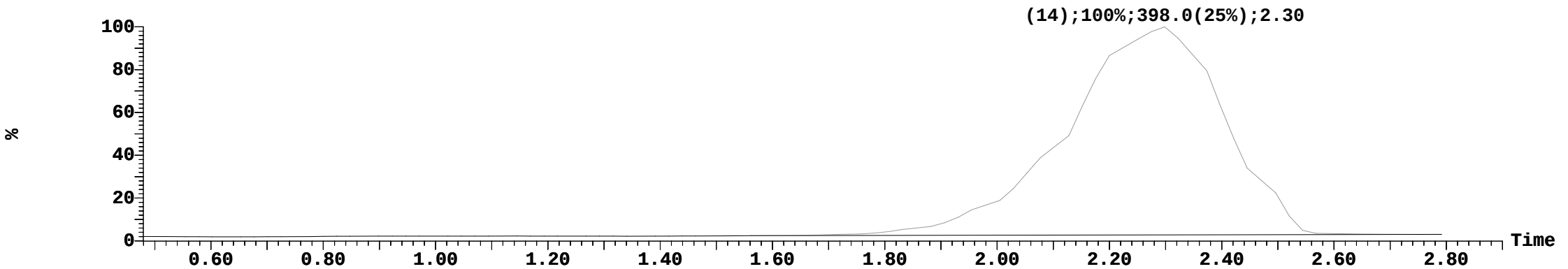
3.9e+004



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2	Tentative	0.85	3e+001	1.10	0		398.00
4	Tentative	1.19	1e+001	0.45	0	2e+002	398.00
10		1.78	1e+001	0.40	0	3e+002	
14	Found	2.32	3e+003	98.05	1	2e+004	398.00

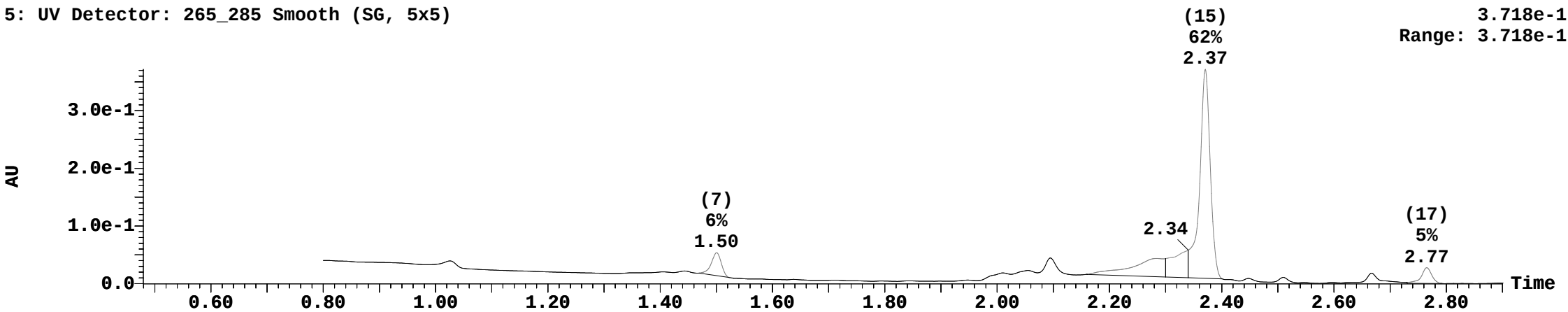
2: TOF MS ES- :398+443+397 Smooth (Mn, 2x3)

3.2e+003



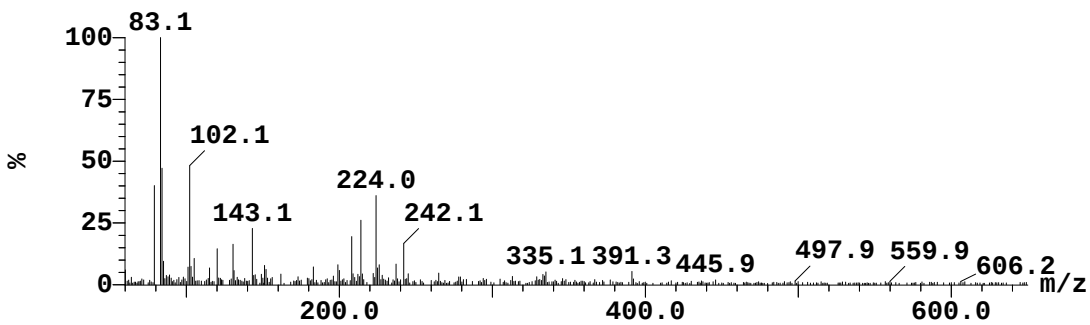
Sample Report (continued):

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



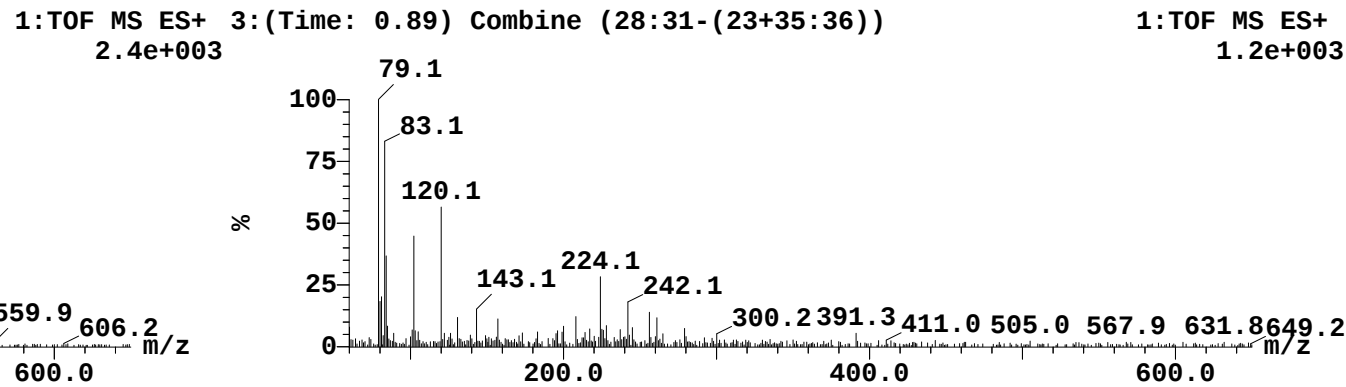
Peak ID	Compound	Time	Mass Found
1		0.69	

1: (Time: 0.69) Combine (21:25-(16:17+29))



Peak ID	Compound	Time	Mass Found
3		0.89	

3: (Time: 0.89) Combine (28:31-(23+35:36))



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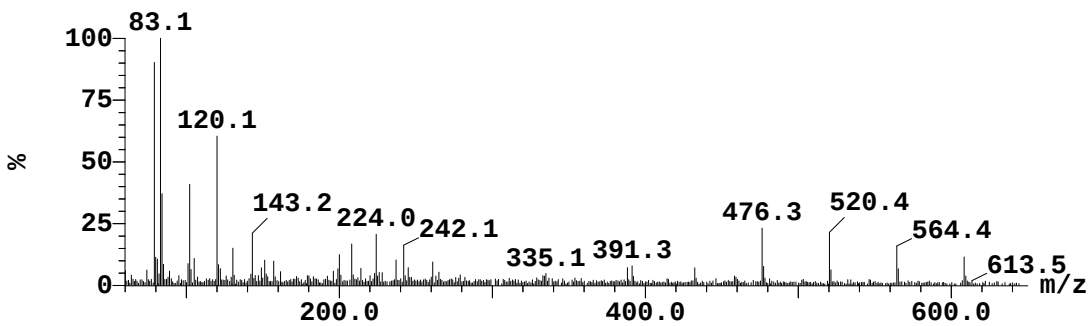
ID:
Time:2::1::2

Printed: Fri Nov 09 15:38:09 2018

Sample Report (continued):

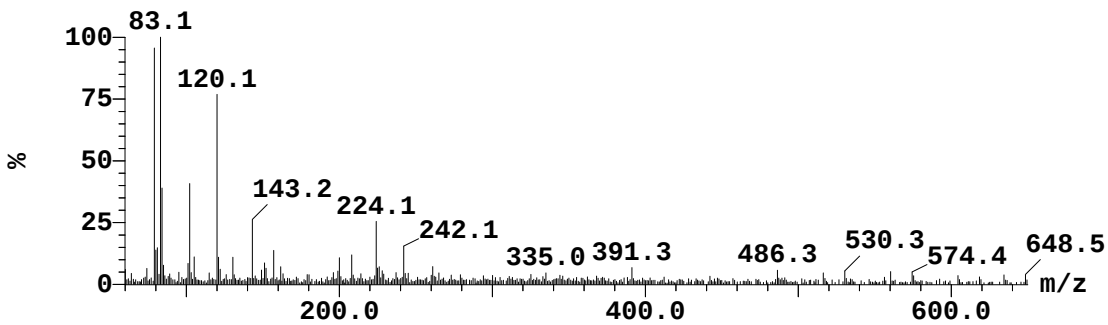
Peak ID	Compound	Time	Mass Found
4		1.18	

4:(Time: 1.18) Combine (37:41-(32:33+45))



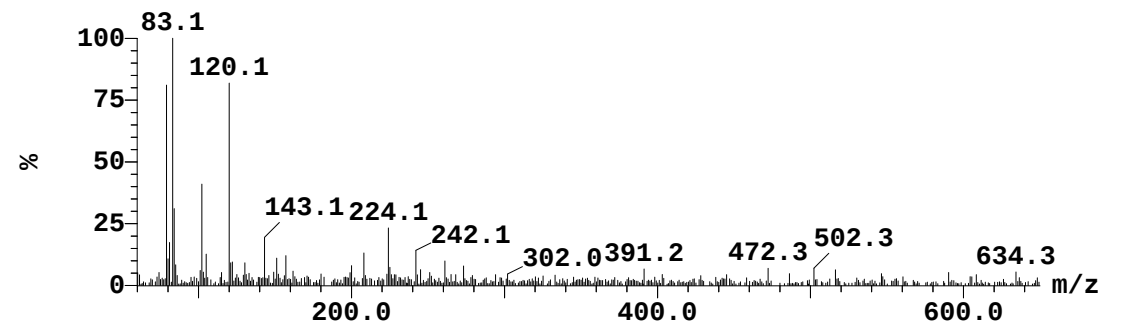
Peak ID	Compound	Time	Mass Found
6		1.40	

6:(Time: 1.40) Combine (44:48-(40+52:53))



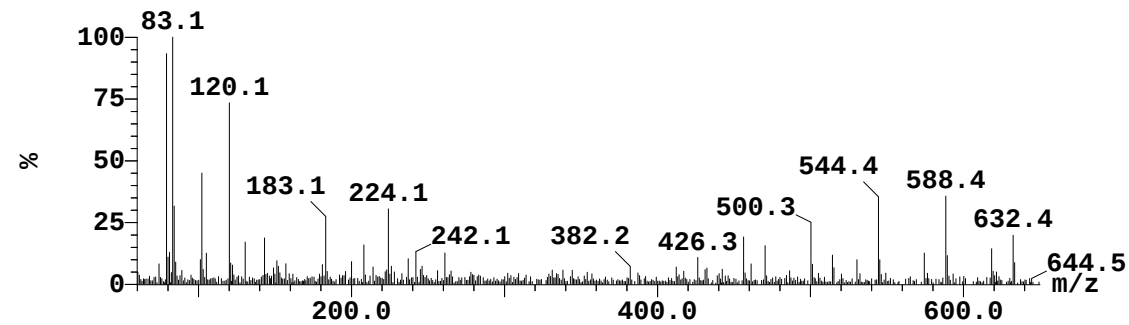
Peak ID	Compound	Time	Mass Found
5		1.33	

1:TOF MS ES+ 5:(Time: 1.33) Combine (42:45-(37:38+50))
2.4e+003



Peak ID	Compound	Time	Mass Found
8		1.57	

1:TOF MS ES+ 8:(Time: 1.57) Combine (50:53-(45:46+58))
1.4e+003



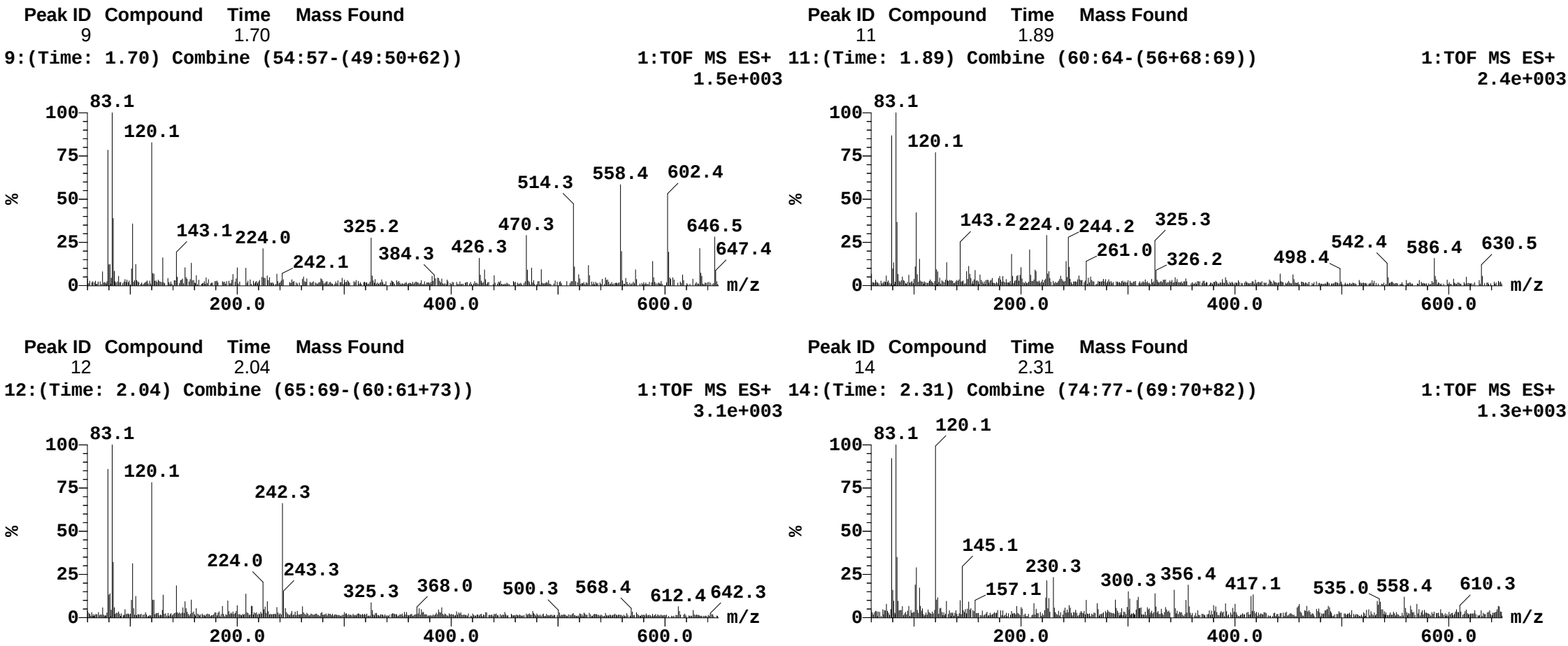
Sample: 6
File:MS49543
Description:A.ZUBIARRE AZ 320 1

Vial:1:15
Date:09-Nov-2018

ID:
Time:2::1::2

Printed: Fri Nov 09 15:38:09 2018

Sample Report (continued):



Sample: 6
File:MS49543
Description:A.ZUBIARRE AZ 320 1

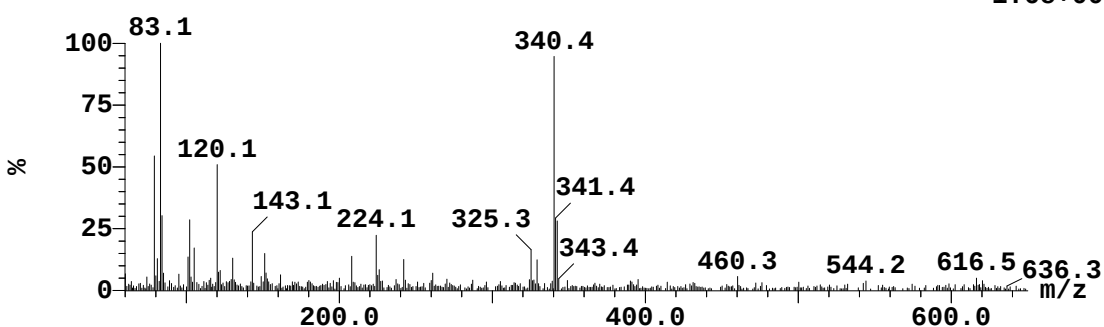
ID:
Time:2::1::2

Printed: Fri Nov 09 15:38:09 2018

Sample Report (continued):

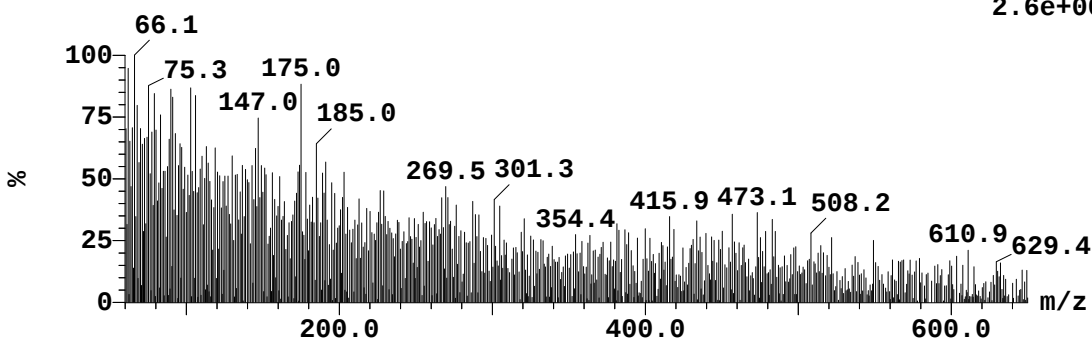
Peak ID	Compound	Time	Mass Found
16		2.53	

16:(Time: 2.48) Combine (80:83-(75+87:88))



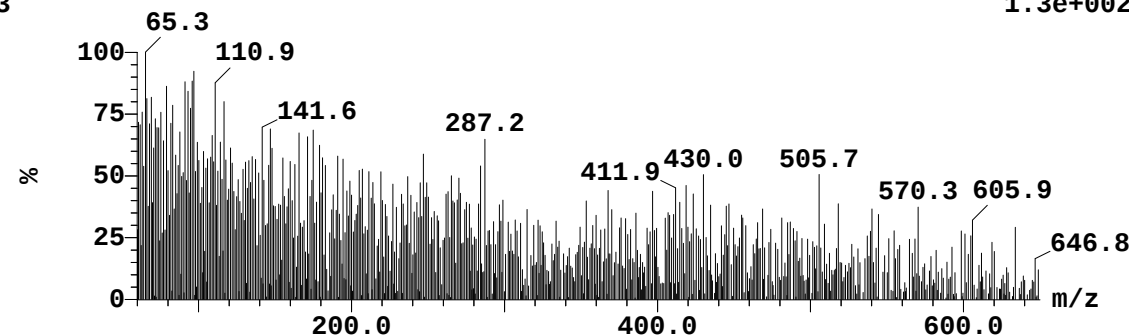
Peak ID	Compound	Time	Mass Found
4	Tentative	1.18	,443.00,397.00

4:(Time: 1.19) Combine (37:41-(32:33+45))



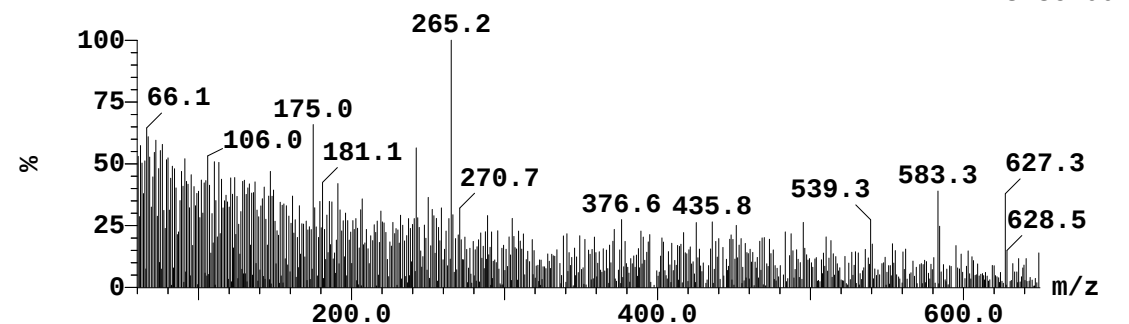
Peak ID	Compound	Time	Mass Found
2	Tentative	0.85	,443.00,397.00

1:TOF MS ES+ 2:(Time: 0.85) Combine (26:29-(21:22+34))



Peak ID	Compound	Time	Mass Found
10		1.78	

2:TOF MS ES- 10:(Time: 1.78) Combine (56:60-(52+64:65))



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ID:
Time:2::1::2

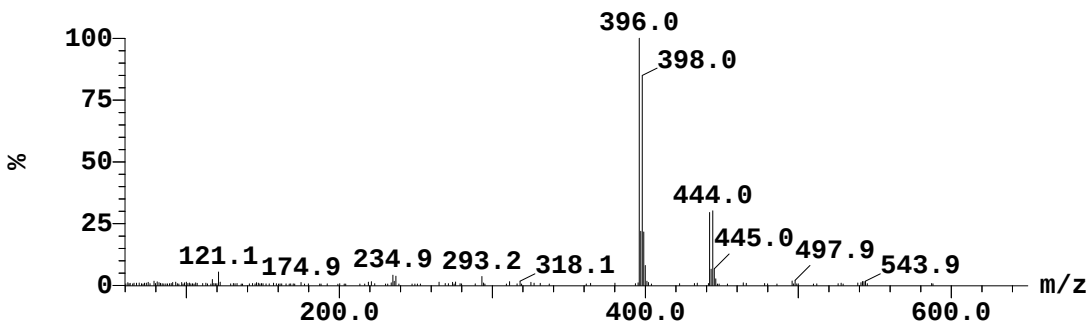
Printed: Fri Nov 09 15:38:09 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
14	Found	2.31	,443.00,397.00

14:(Time: 2.30) Combine (73:77-(68:69+81))

2:T0F MS ES-
1.7e+004



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