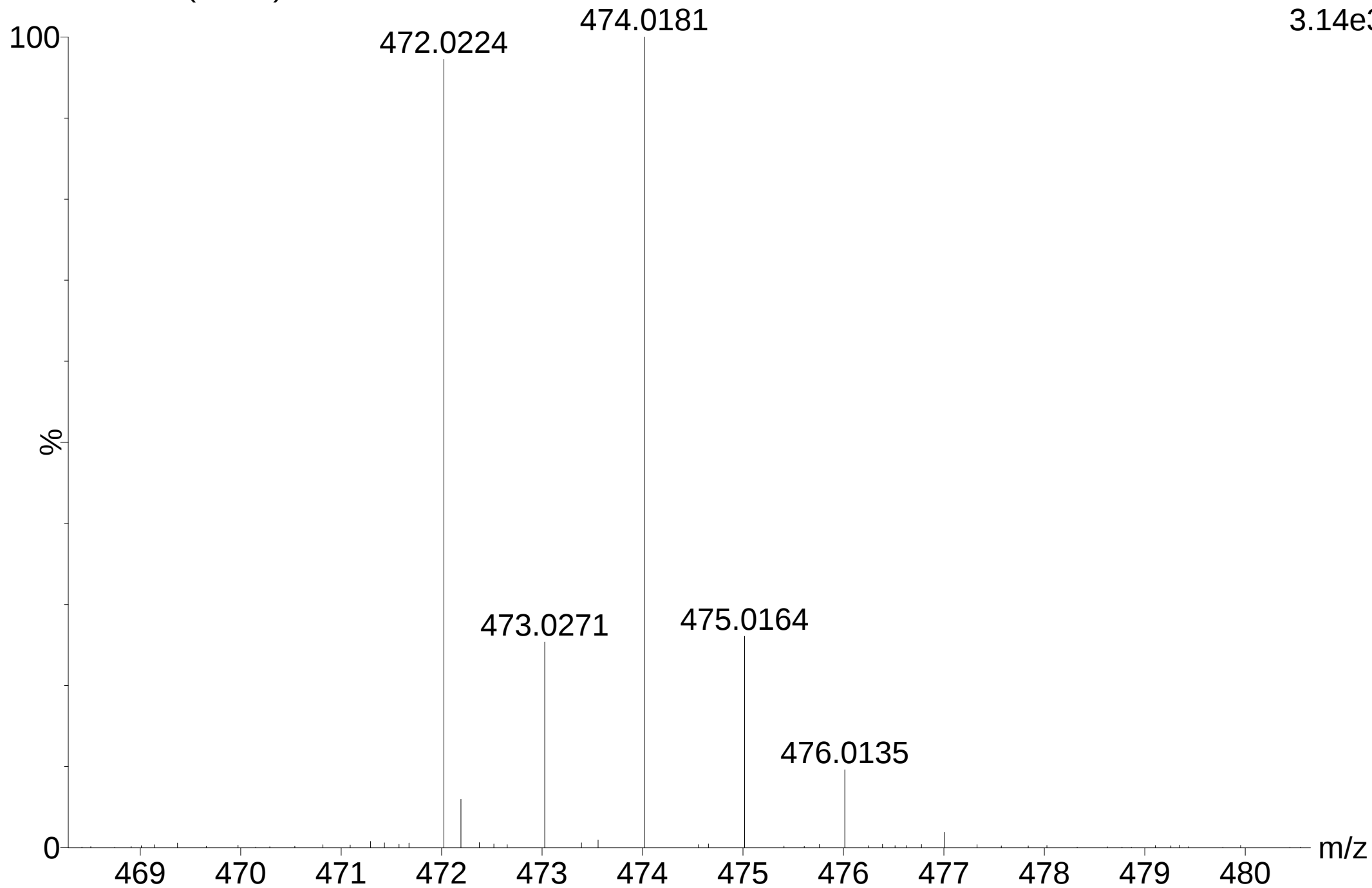


A.ZUBIAURRE AZ316-1P

MS49855 95 (2.912)

ES-ToF

2: TOF MS ES-
3.14e3



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Single Mass Analysis

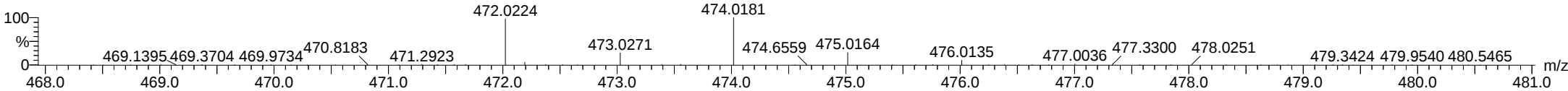
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
238 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 22-22 H: 0-100 N: 0-10 O: 0-10 S: 0-1 Br: 1-1

A.ZUBIAURRE AZ316-1P
MS49855 95 (2.912)

ES-ToF

2: TOF MS ES-
3.14e+003



Minimum: -1.5

Maximum: 5.0 10.0 100.0

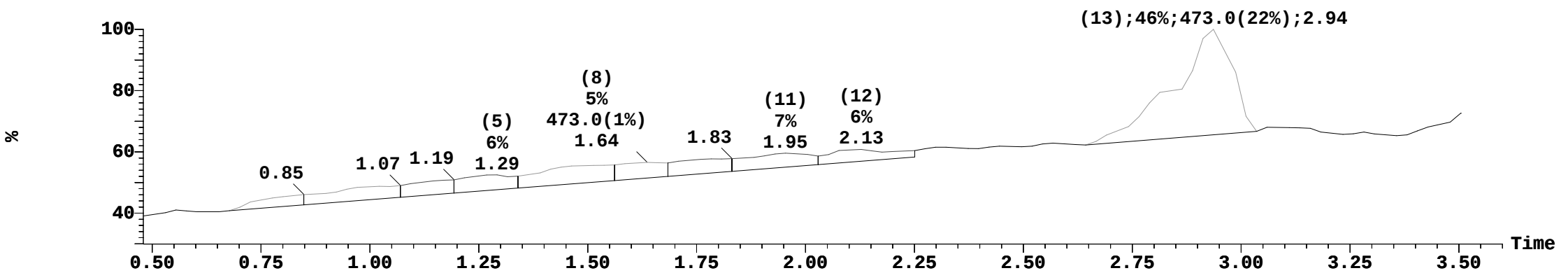
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
472.0224	472.0218	0.6	1.3	13.5	49.2	0.0	C22 H19 N 04 S Br

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Sample Report:

Sample 1 Vial 2:15 ID File MS49855 Date 27-Nov-2018 Time 3::1::5 Description A.ZUBIAURRE AZ316-1P

2: TOF MS ES- :TIC Smooth (SG, 2x2) 3.4e+004

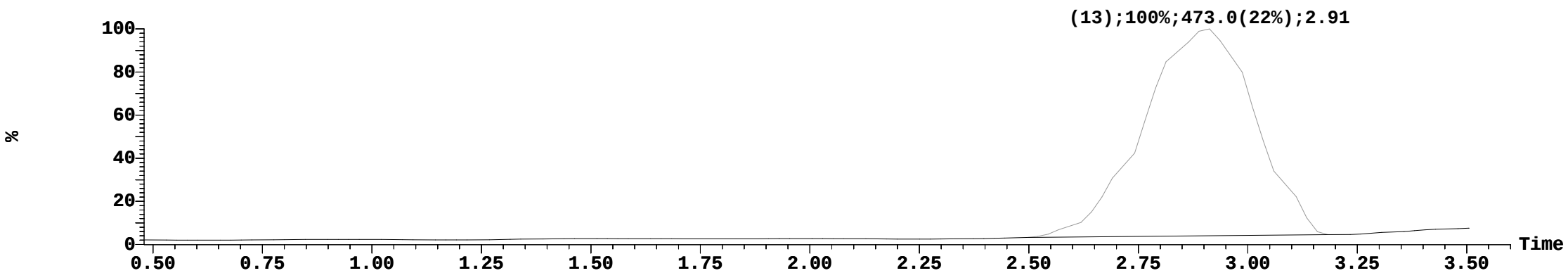


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Tentative	0.85	1e+002	3.55	0	1e+003	473.00
3	Tentative	1.07	3e+002	7.12	0	1e+003	473.00
4		1.19	2e+002	4.52	0	1e+003	
5		1.29	2e+002	5.77	0	2e+003	
7	Tentative	1.56	4e+002	9.69	0	2e+003	473.00
8	Tentative	1.64	2e+002	5.22	0	2e+003	473.00
10		1.83	2e+002	5.67	0	1e+003	
11		1.95	3e+002	6.85	0	2e+003	
12		2.13	2e+002	5.78	0	1e+003	
13	Found	2.94	2e+003	45.82	0	1e+004	473.00

Sample Report (continued):

2: TOF MS ES- :473+518+472 Smooth (Mn, 2x3)

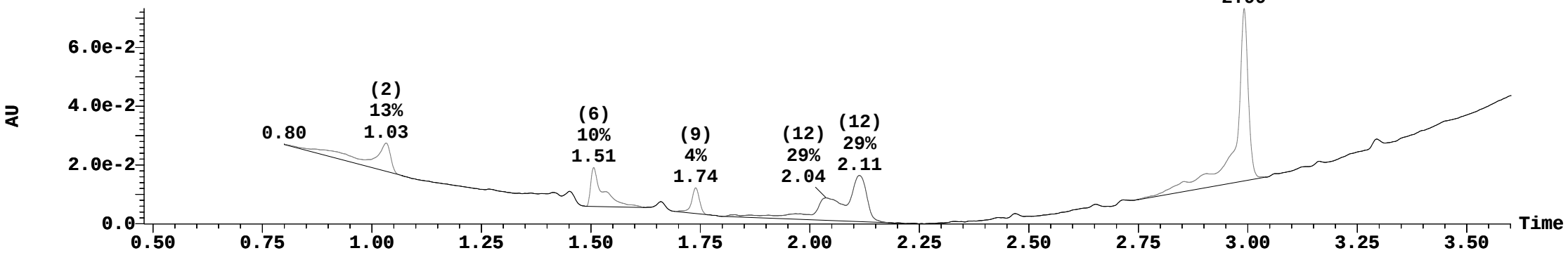
2.6e+003



5: UV Detector: 267.5_282.5 Smooth (SG, 5x5)

7.329e-2

Range: 7.328e-2



Sample: 1

Vial:2:15

ID:

File:MS49855

Date:27-Nov-2018

Time:3::1::5

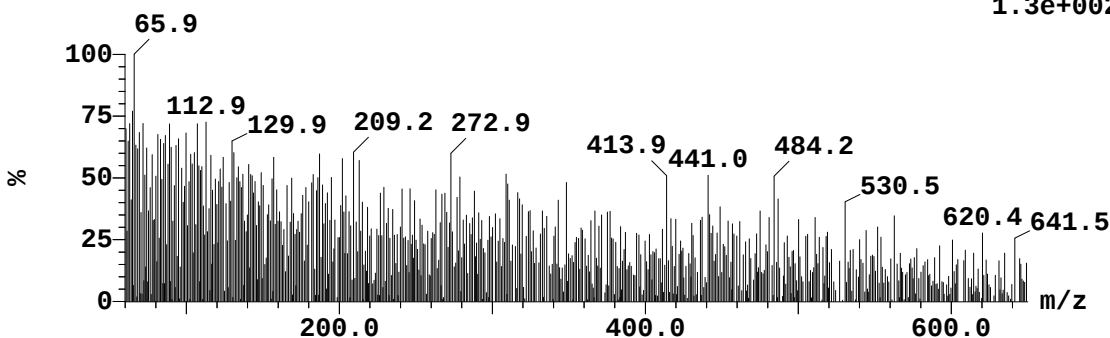
Description:A.ZUBIAURRE AZ316-1P

Printed: Wed Nov 28 10:40:53 2018

Sample Report (continued):

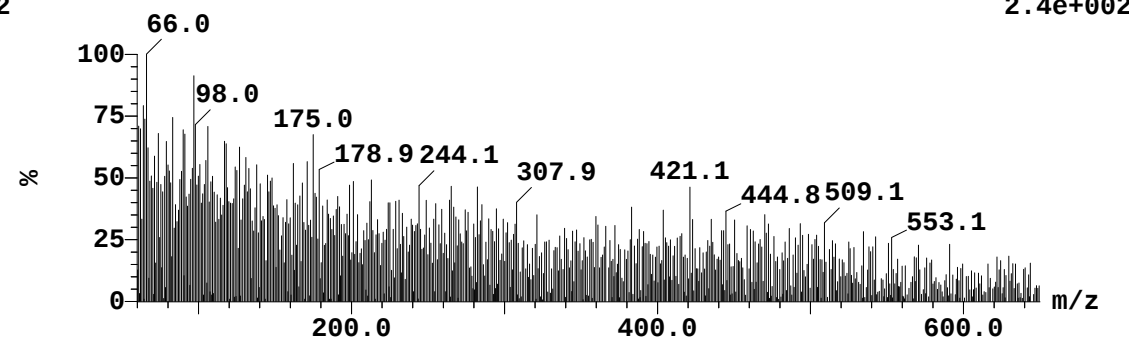
Peak ID	Compound	Time	Mass Found
1	Tentative	0.85	,518.00,472.00

1:(Time: 0.85) Combine (26:29-(21:22+34))



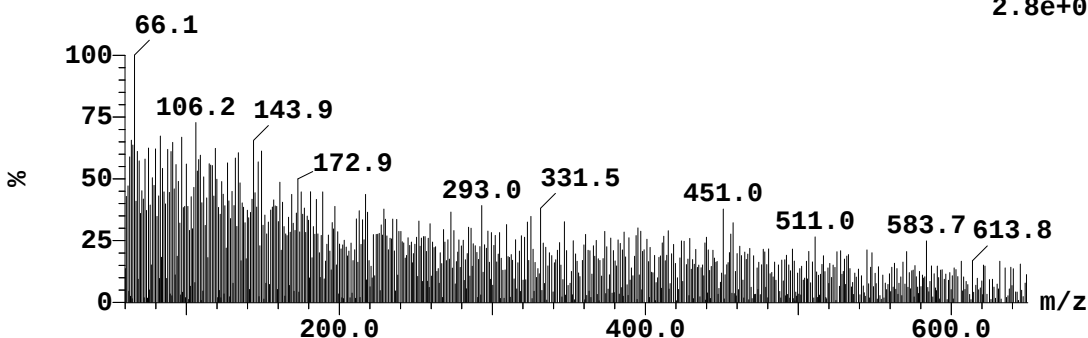
Peak ID	Compound	Time	Mass Found
3	Tentative	1.07	,518.00,472.00

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



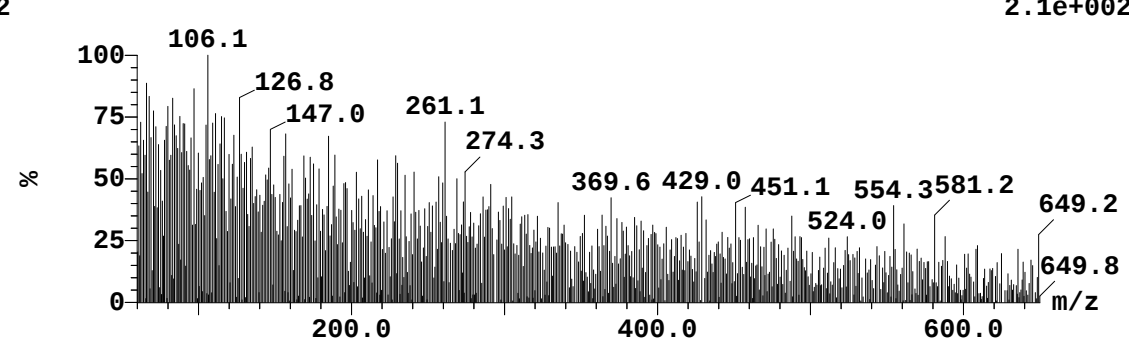
Peak ID	Compound	Time	Mass Found
4		1.19	

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



Peak ID	Compound	Time	Mass Found
5		1.29	

5:(Time: 1.29) Combine (40:44-(36+48:49))



Sample: 1
File:MS49855
Description:A.ZUBIAURRE AZ316-1P

Vial:2:15
Date:27-Nov-2018

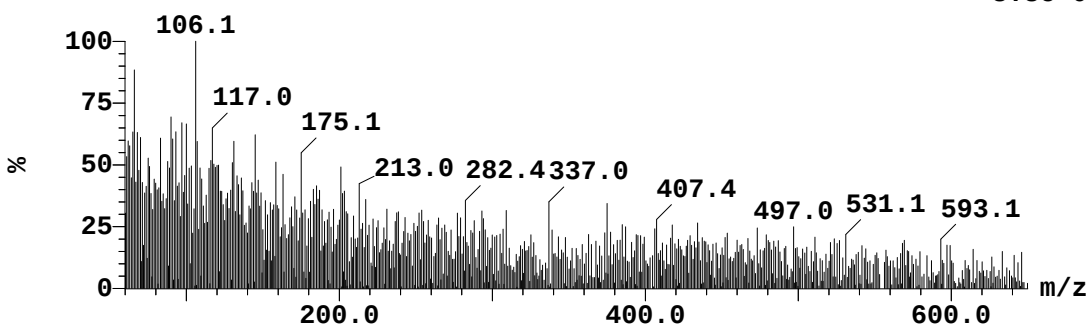
ID:
Time:3::1::5

Printed: Wed Nov 28 10:40:53 2018

Sample Report (continued):

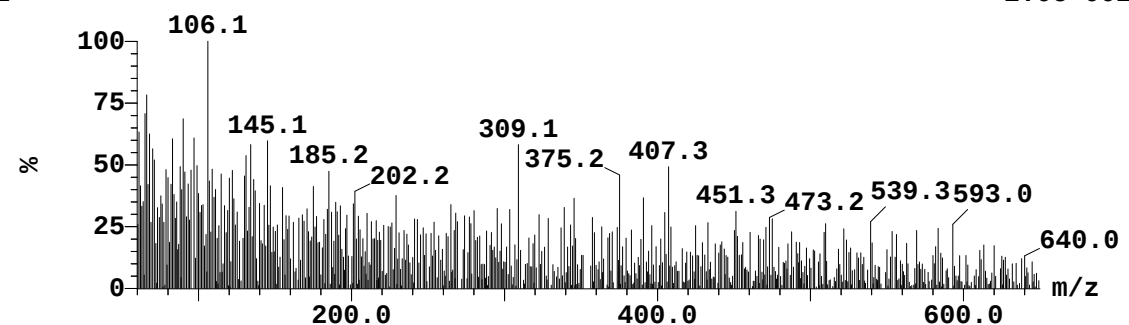
Peak ID	Compound	Time	Mass Found
7	Tentative	1.56	,518.00,472.00

7:(Time: 1.56) Combine (49:53-(44:45+57))



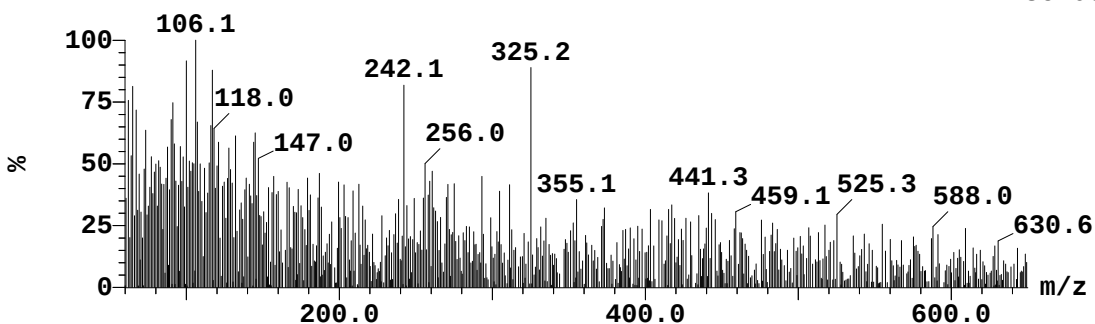
Peak ID	Compound	Time	Mass Found
8	Tentative	1.64	,518.00,472.00

2:TOF MS ES- 8:(Time: 1.64) Combine (52:55-(47+59:60)) 3.3e+002 2:TOF MS ES- 2.0e+002



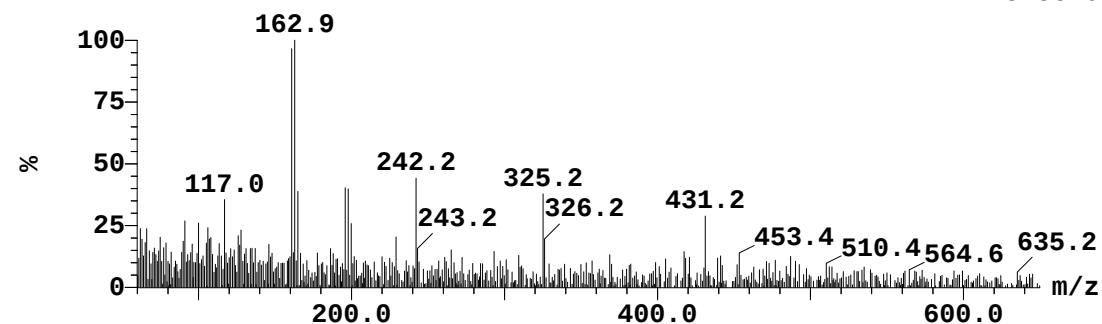
Peak ID	Compound	Time	Mass Found
10		1.83	

10:(Time: 1.83) Combine (58:61-(53:54+66))



Peak ID	Compound	Time	Mass Found
11		1.95	

2:TOF MS ES- 11:(Time: 1.95) Combine (62:65-(57:58+70)) 1.8e+002 2:TOF MS ES- 5.5e+002



Sample: 1
File:MS49855
Description:A.ZUBIAURRE AZ316-1P

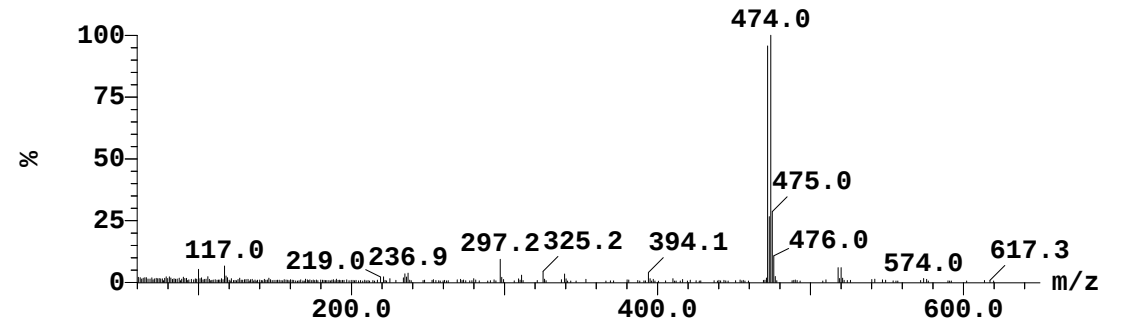
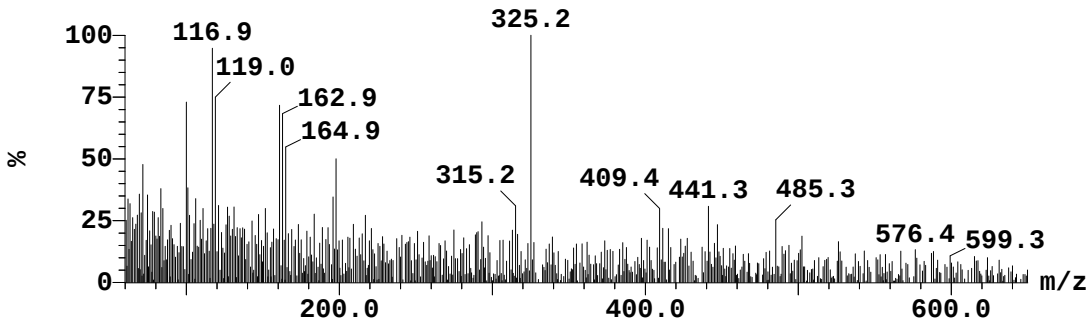
Vial:2:15
Date:27-Nov-2018

ID:
Time:3::1::5

Printed: Wed Nov 28 10:40:53 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
12		2.13		13	Found	2.94	,518.00,472.00
12:(Time: 2.13) Combine (68:71-(63+75:76))				13:(Time: 2.91) Combine (93:97-(88:89+101))			
2:TOF MS ES- 3.3e+002				2:TOF MS ES- 1.3e+004			



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