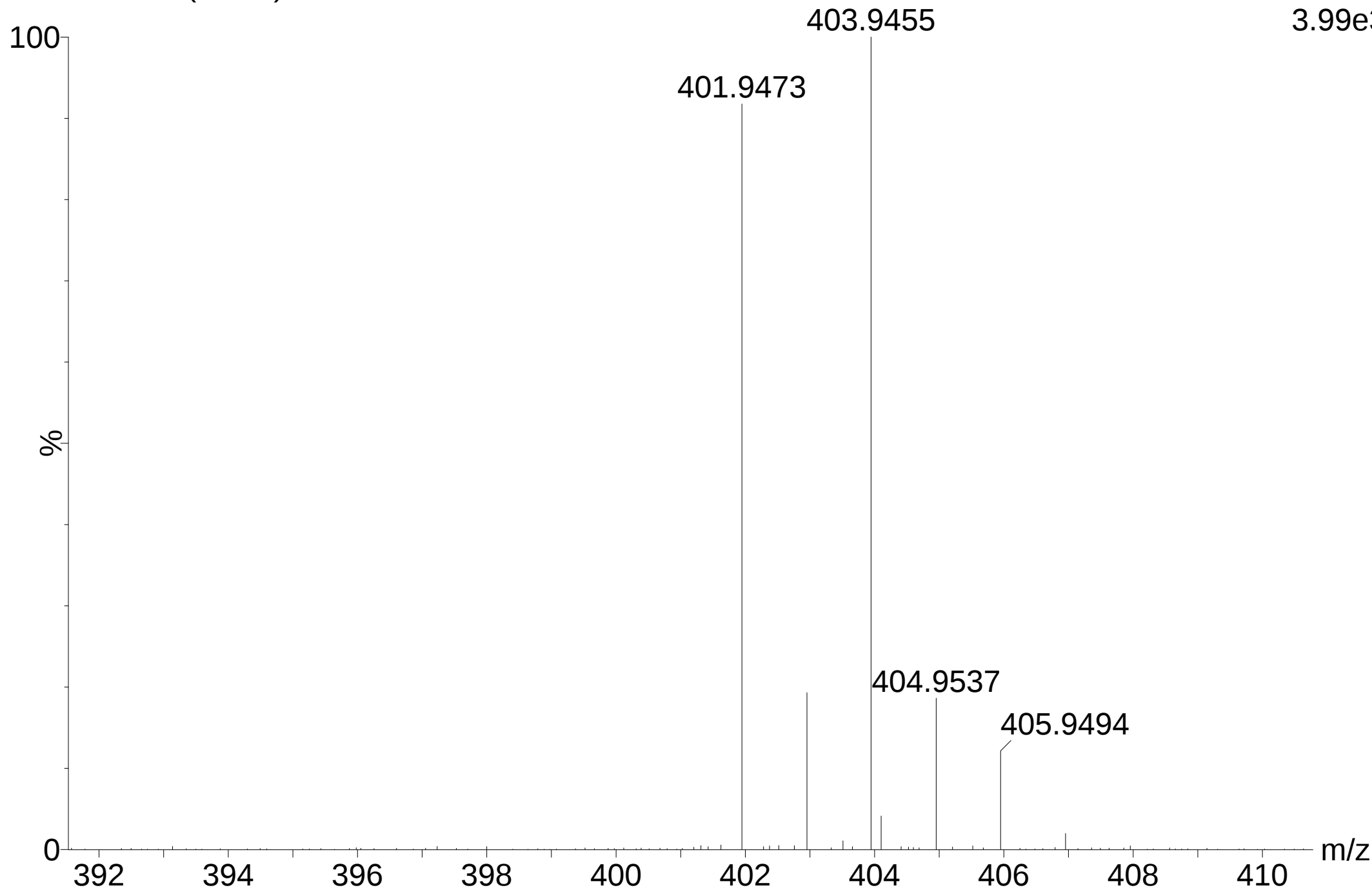


A.ZUBIAURRE AZ321-1
MS49856 78 (2.400)

ES-ToF

2: TOF MS ES-
3.99e3



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Single Mass Analysis

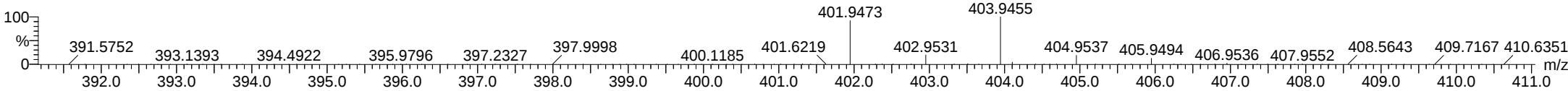
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
113 formula(e) evaluated with 1 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 S: 2-2 Br: 1-1

A.ZUBIAURRE AZ321-1
MS49856 78 (2.400)

ES-ToF

2: TOF MS ES-
3.99e+003



Minimum:
Maximum:

-1.5
100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
401.9473	401.9469	0.4	1.0	8.5	67.6	0.0	C14 H13 N O4 S2 Br

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Sample: 1
File:MS49856
Description:A.ZUBIAURRE AZ321-1

Vial:2:16
Date:27-Nov-2018

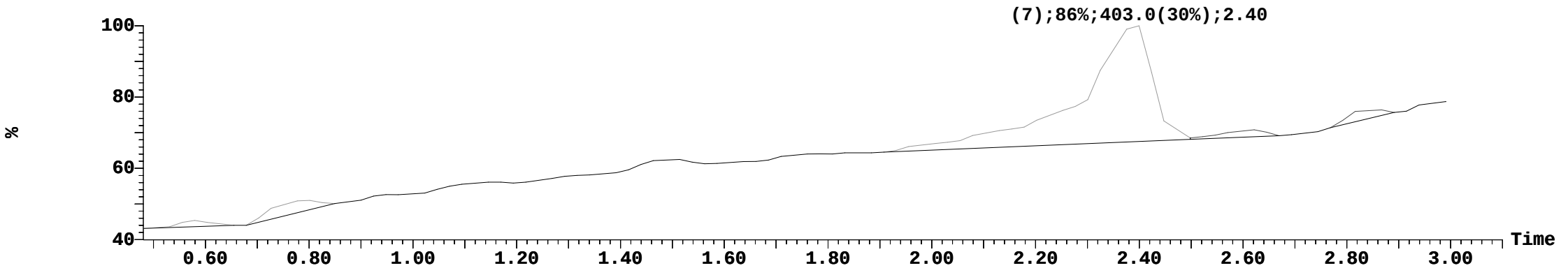
ID:
Time:3::6::3

Printed: Wed Nov 28 10:42:29 2018

Sample Report:

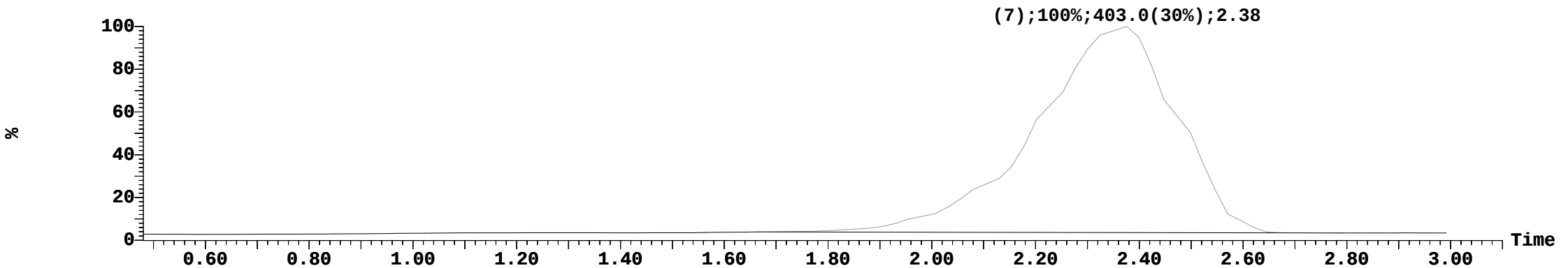
Sample 1 Vial 2:16 ID File MS49856 Date 27-Nov-2018 Time 3::6::3 Description A.ZUBIAURRE AZ321-1

2: TOF MS ES- :TIC Smooth (SG, 2x2) 3.1e+004



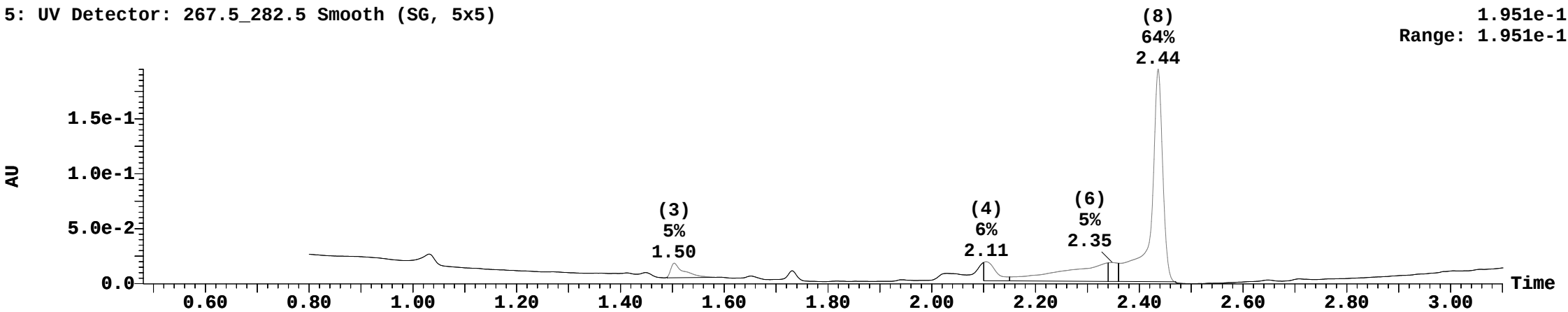
Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Tentative	0.58	4e+001	1.96	0	5e+002	403.00
2	Tentative	0.80	1e+002	5.68	0	8e+002	403.00
7	Found	2.40	2e+003	86.05	1	1e+004	403.00
9		2.62	6e+001	3.14	0	6e+002	
10		2.87	6e+001	3.17	0	5e+002	

2: TOF MS ES- :403+448+402 Smooth (Mn, 2x3) 2.2e+003



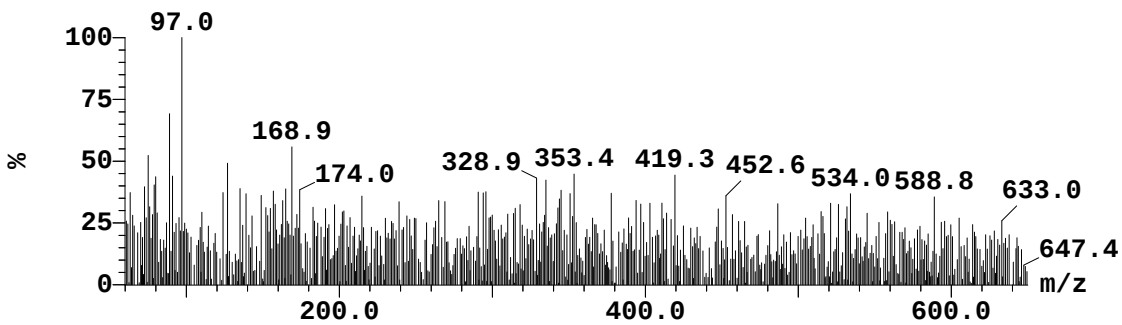
Sample Report (continued):

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



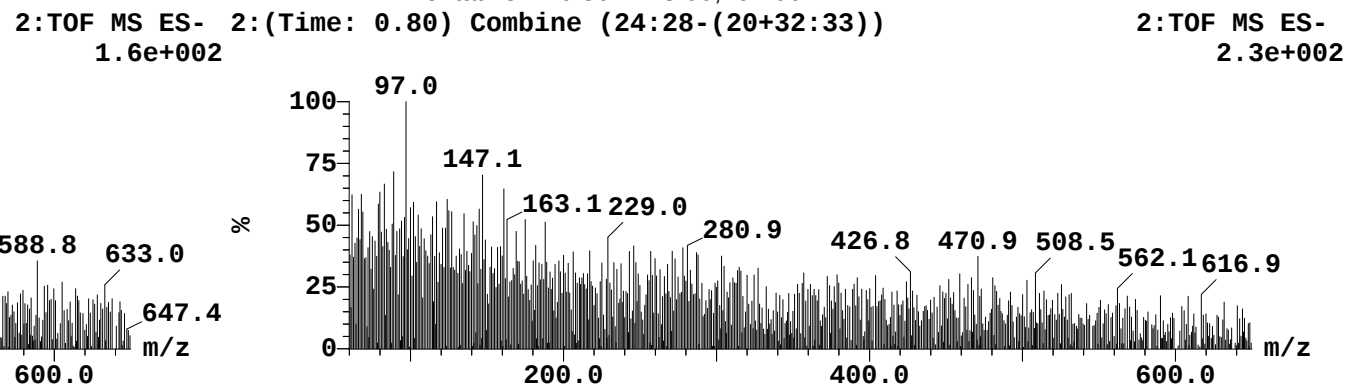
Peak ID	Compound	Time	Mass Found
1	Tentative	0.58	,448.00,402.00

1: (Time: 0.58) Combine (17:21-(12:13+25))



Peak ID	Compound	Time	Mass Found
2	Tentative	0.80	448.00,402.00

2: (Time: 0.80) Combine (24:28-(20+32:33))



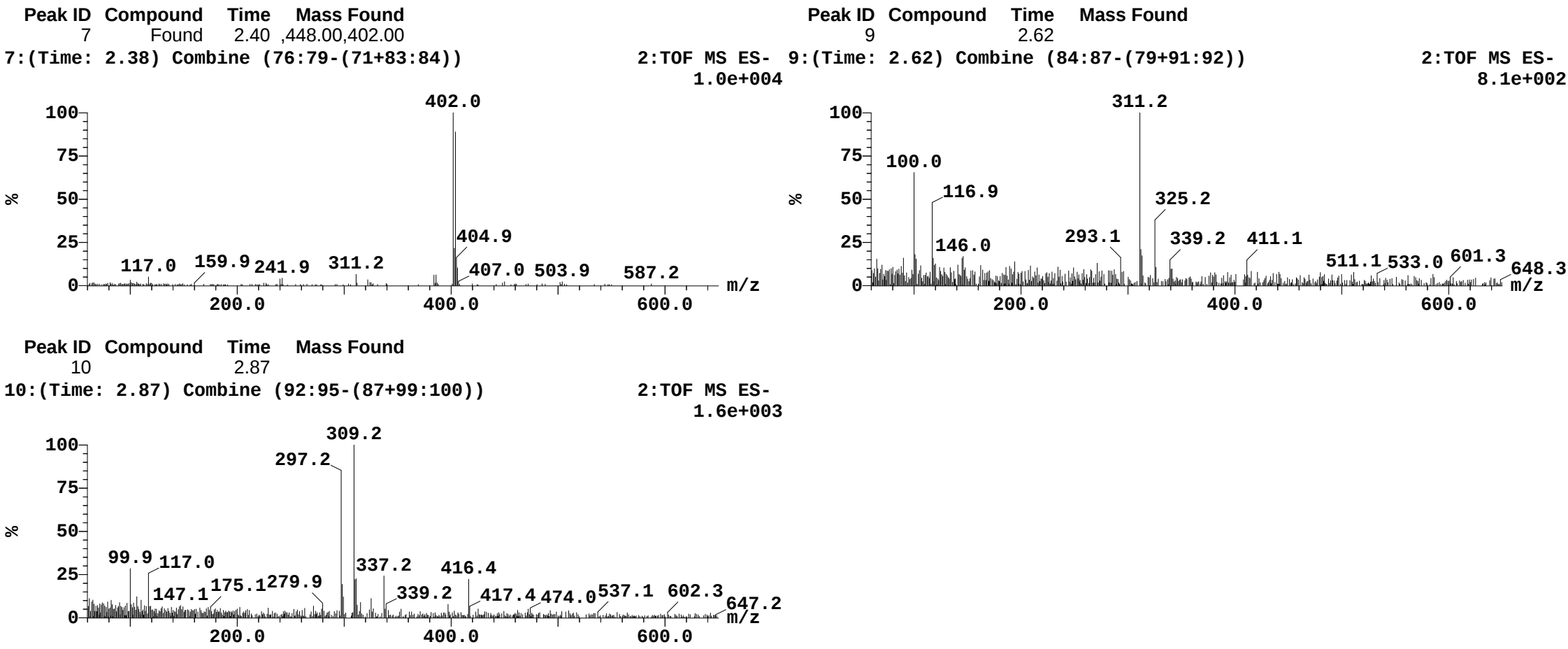
Sample: 1
File:MS49856
Description:A.ZUBIAURRE AZ321-1

Vial:2:16
Date:27-Nov-2018

ID:
Time:3::6::3

Printed: Wed Nov 28 10:42:29 2018

Sample Report (continued):



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