

Single Mass Analysis

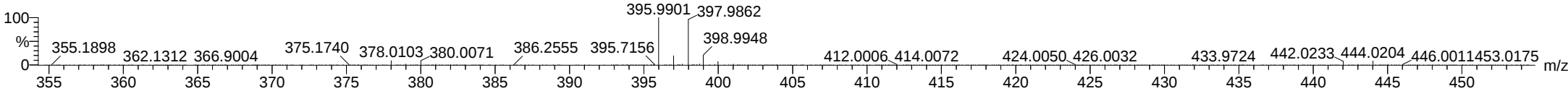
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
228 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 S: 1-2 Br: 1-1

A.ZUBIAURRE AZ322-1
MS49857 77 (2.376)

ES-ToF

2: TOF MS ES-
7.40e+003



Minimum: -1.5

Maximum: 5.0 10.0 100.0

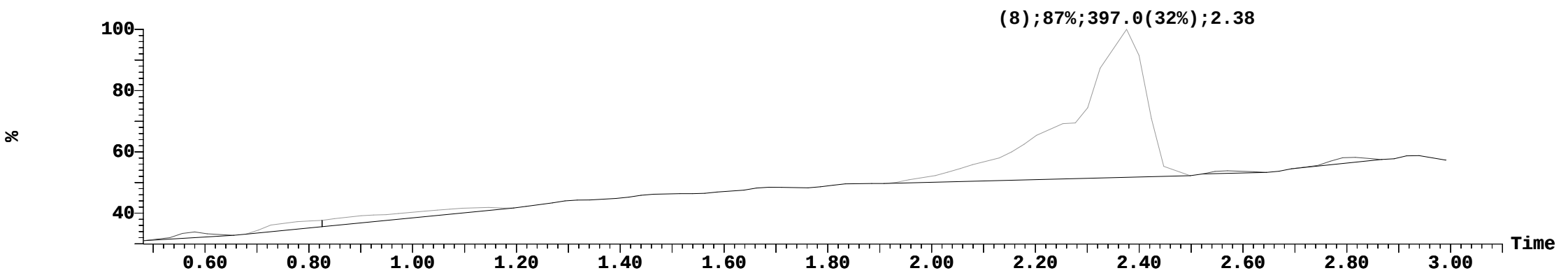
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula					
395.9901	395.9905	-0.4	-1.0	9.5	84.9	0.0	C16	H15	N	O4	S	Br

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Sample Report:

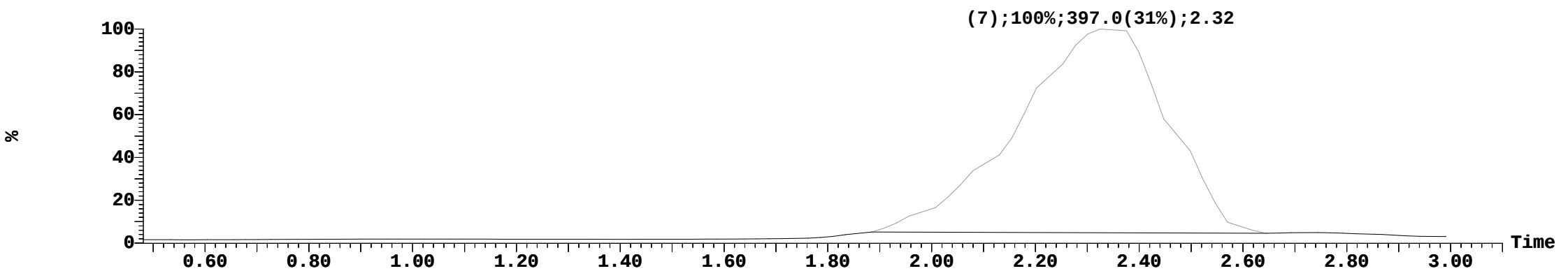
Sample 1 Vial 2:17 ID File MS49857 Date 27-Nov-2018 Time 3::1::4 Description A.ZUBIAURRE AZ322-1

2: TOF MS ES- :TIC Smooth (SG, 2x2) 4.1e+004



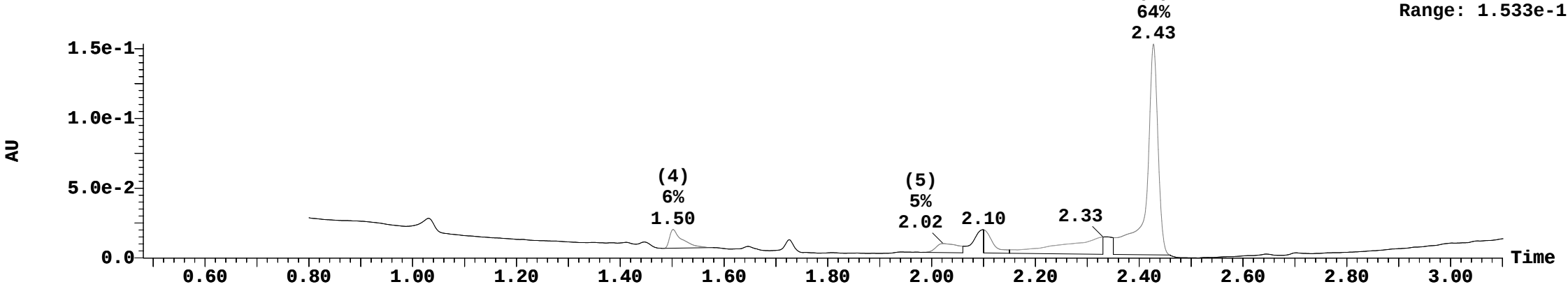
Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.58	6e+001	1.45	0	7e+002	
2	Tentative	0.83	1e+002	2.92	0	8e+002	397.00
3	Tentative	1.15	3e+002	6.64	0	4e+002	397.00
8	Found	2.38	3e+003	86.83	1	2e+004	397.00
10		2.57	3e+001	0.66	0	3e+002	
11		2.82	6e+001	1.50	0	6e+002	

2: TOF MS ES- :397+442+396 Smooth (Mn, 2x3) 3.8e+003

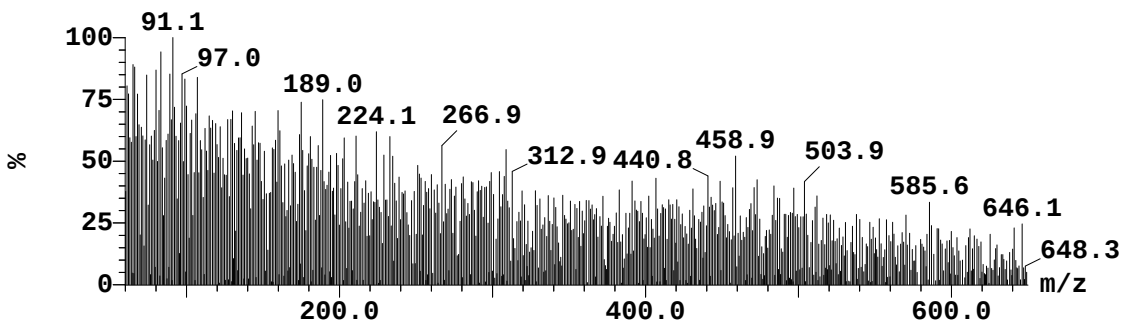
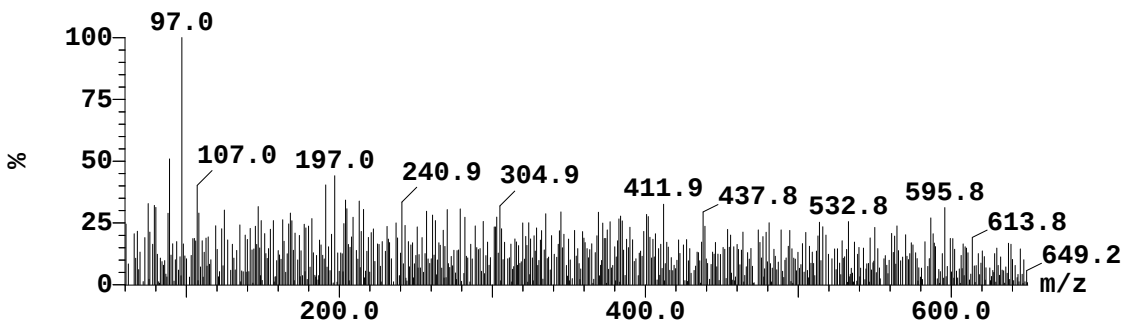


Sample Report (continued):

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



Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
1		0.58		2	Tentative	0.83	,442.00,396.00
1: (Time: 0.58) Combine (17:21-(12:13+25))				2: (Time: 0.83) Combine (25:29-(20:21+33))			
2: TOF MS ES- 2.0e+002				2: TOF MS ES- 1.8e+002			



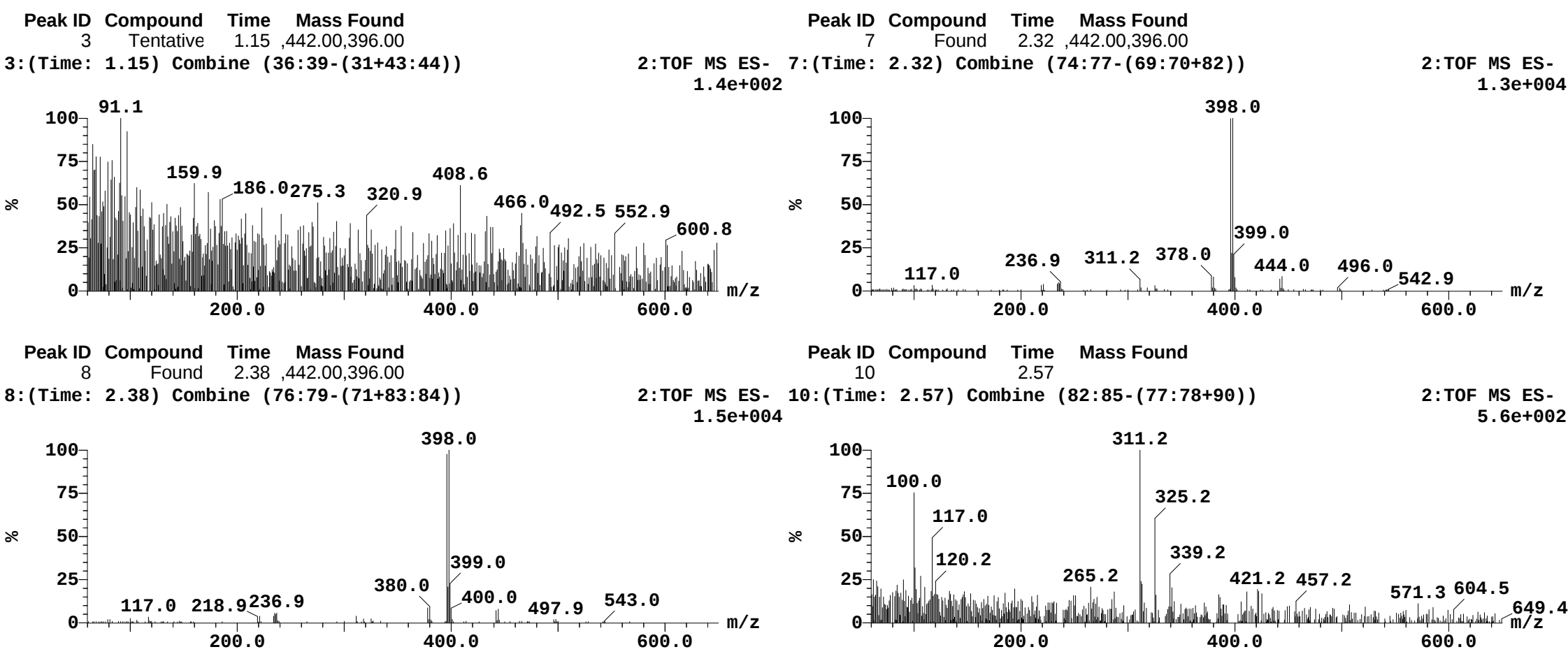
Sample: 1
File:MS49857
Description:A.ZUBIAURRE AZ322-1

Vial:2:17
Date:27-Nov-2018

ID:
Time:3::1::4

Printed: Wed Nov 28 10:43:27 2018

Sample Report (continued):



Sample: 1

File:MS49857

Description:A.ZUBIAURRE AZ322-1

Vial:2:17

Date:27-Nov-2018

ID:

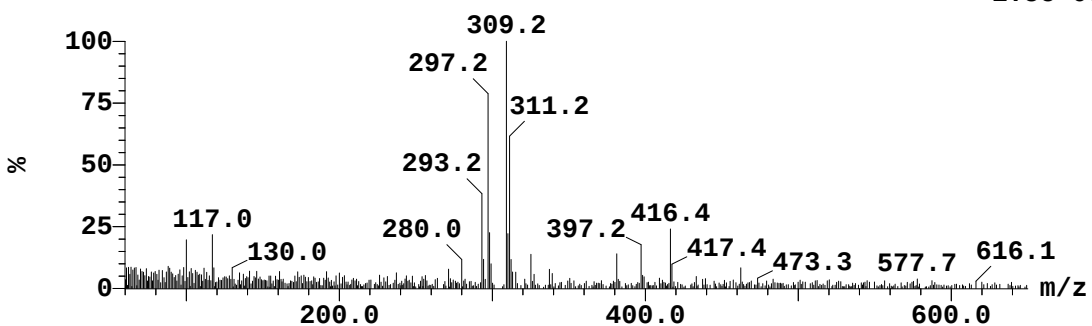
Time:3::1::4

Printed: Wed Nov 28 10:43:27 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
11		2.82	

11:(Time: 2.82) Combine (90:93-(85:86+98))

2:T0F MS ES-
1.5e+003

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