

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

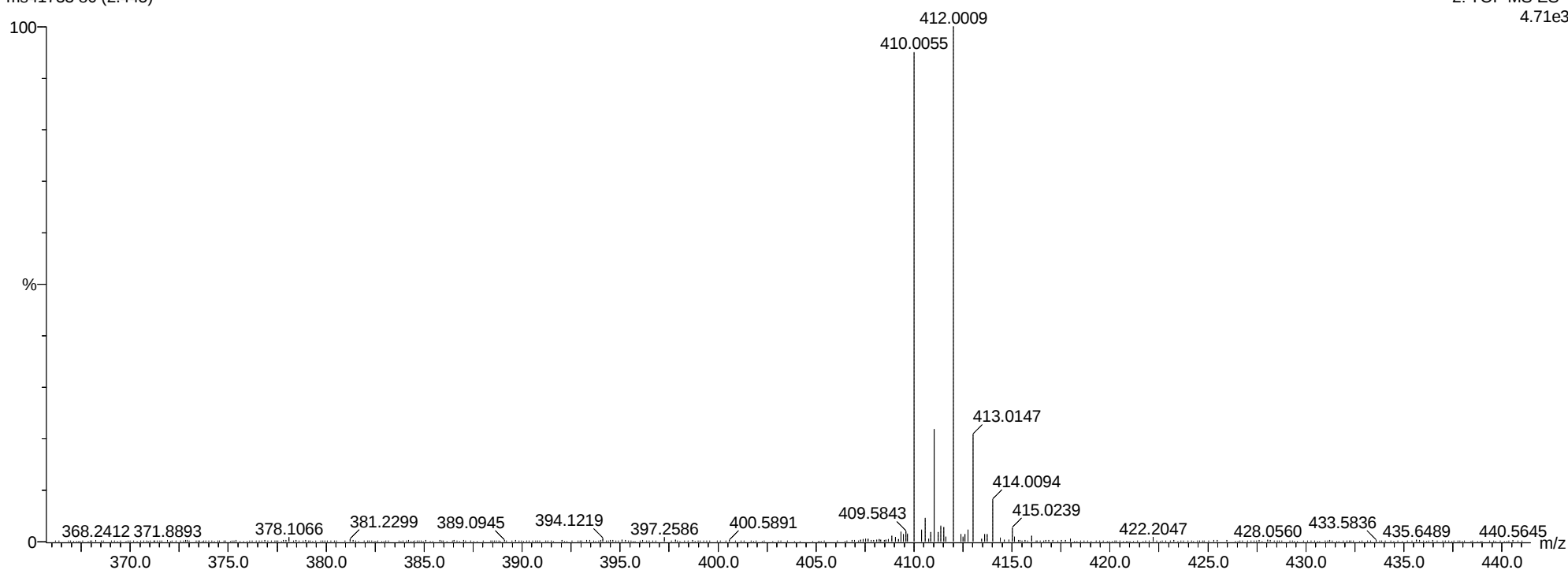
Selected filters: None

Monoisotopic Mass, Even Electron Ions

118 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 17-17 H: 0-200 N: 0-10 O: 0-10 S: 1-1 Br: 1-1

A.ZUBIAURRE AZ 126 1
ms41733 80 (2.445)2: TOF MS ES-
4.71e3

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
410.0055	410.0062	-0.7	-1.7	9.5	9.0	C17 H17 N 04 S Br

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Sample: 17
File:ms41733
Description:A.ZUBIAURRE AZ 126 1

Vial:1:14
Date:08-Nov-2017

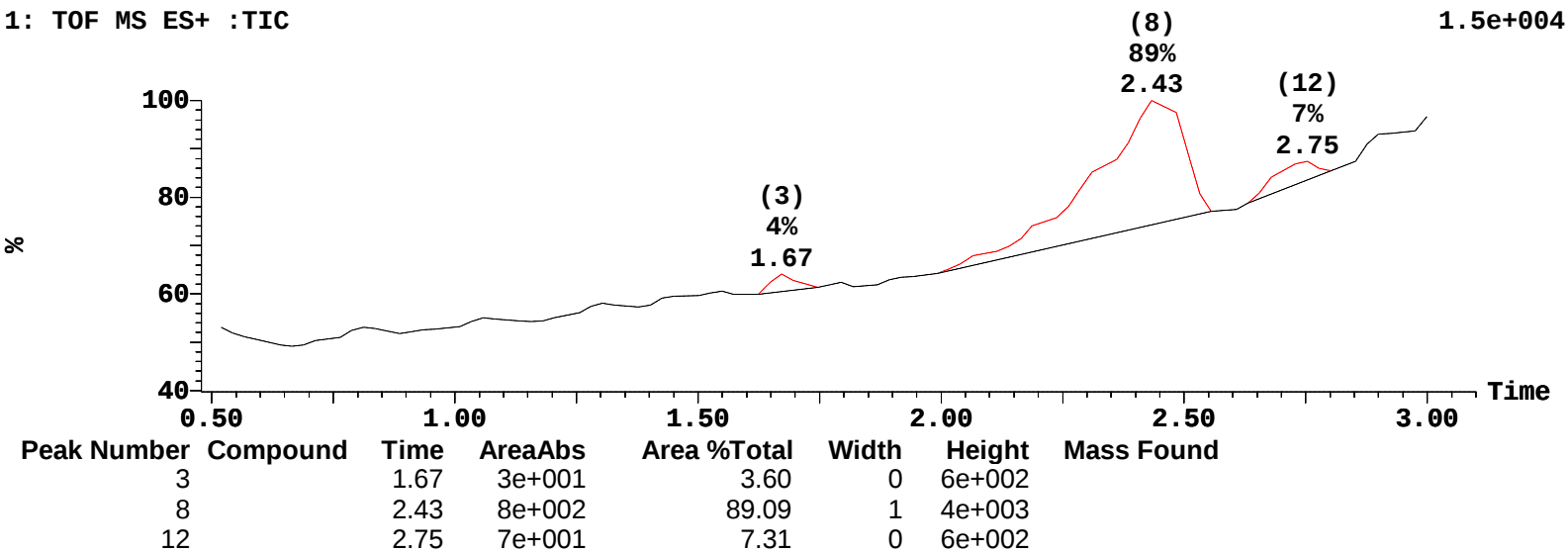
ID:
Time:12:51:28

Printed: Wed Nov 08 14:04:35 2017

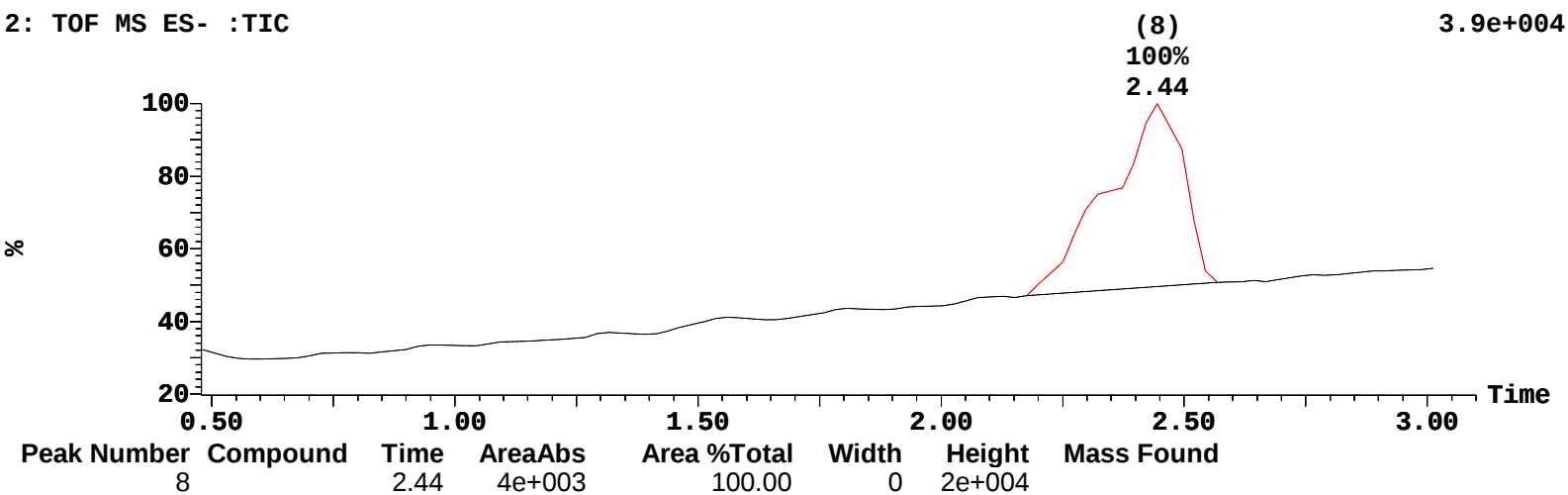
Sample Report:

Sample 17 Vial 1:14 ID File ms41733 Date 08-Nov-2017 Time 12:51:28 Description A.ZUBIAURRE AZ 126 1

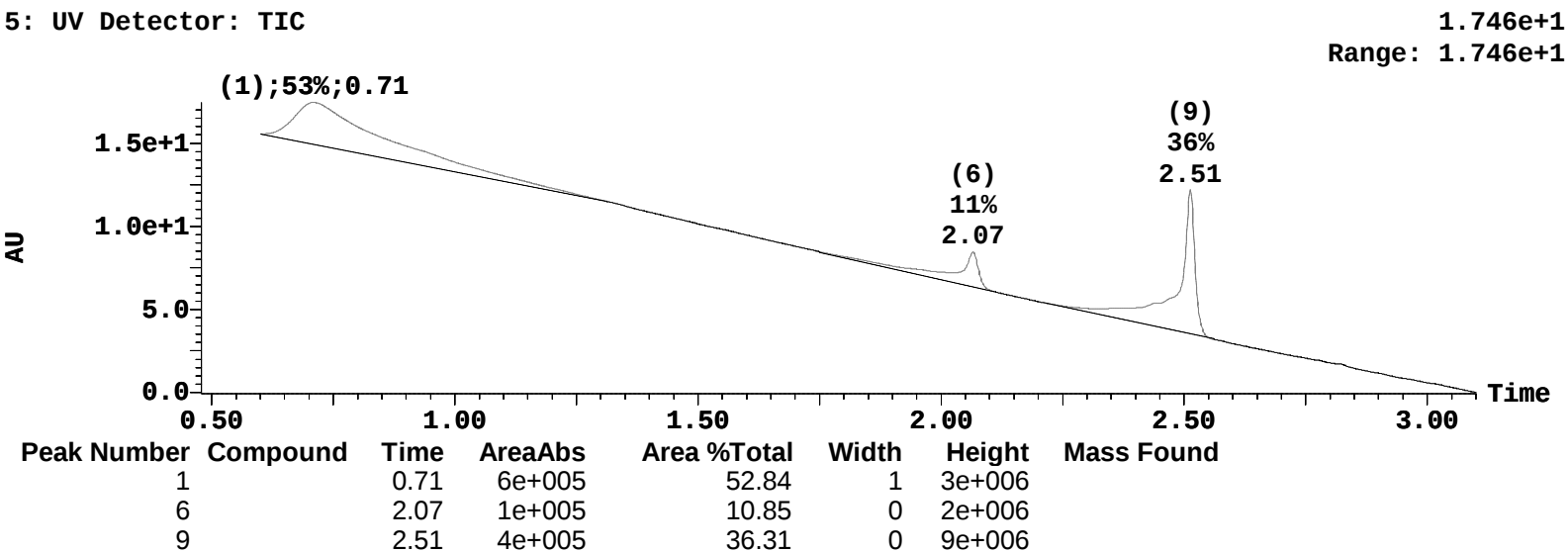
1: TOF MS ES+ :TIC



2: TOF MS ES- :TIC



5: UV Detector: TIC



Sample: 17
File:ms41733
Description:A.ZUBIAURRE AZ 126 1

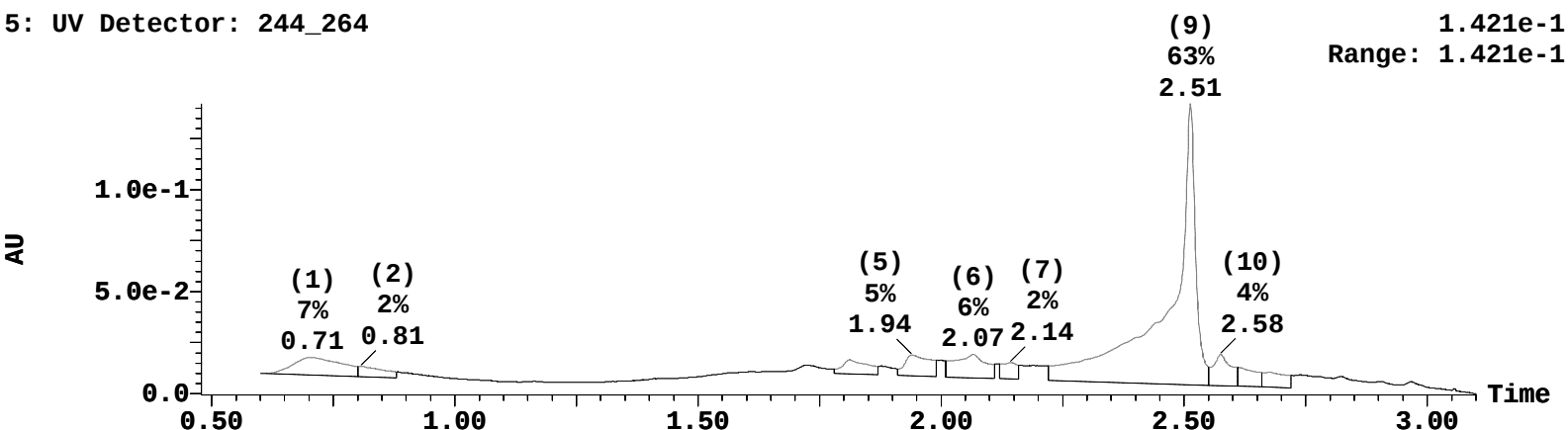
Vial:1:14
Date:08-Nov-2017

ID:
Time:12:51:28

Printed: Wed Nov 08 14:04:35 2017

Sample Report (continued):

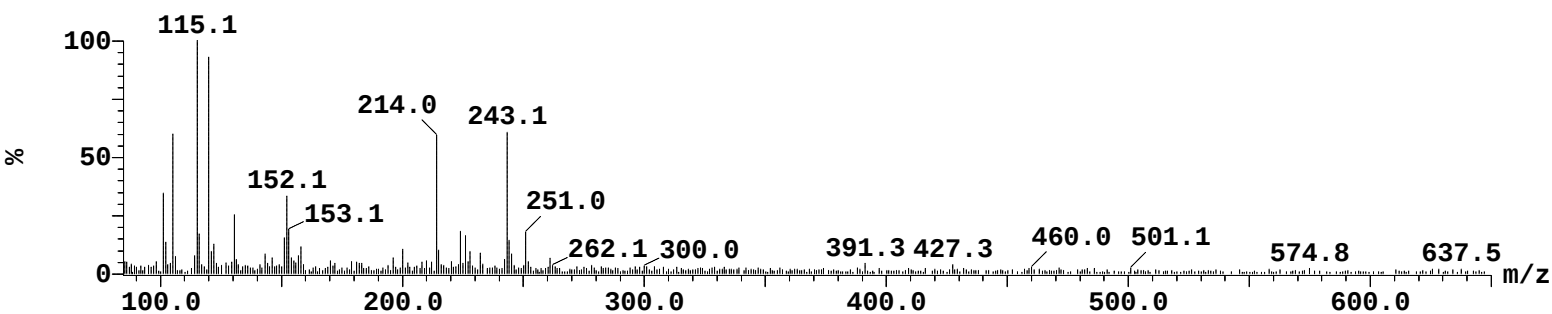
5: UV Detector: 244_264



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.71	1e+003	7.39	0	9e+003	
2		0.81	3e+002	2.36	0	5e+003	
4		1.81	4e+002	3.18	0	7e+003	
5		1.94	7e+002	4.84	0	1e+004	
6		2.07	9e+002	6.41	0	1e+004	
7		2.14	3e+002	2.04	0	8e+003	
9		2.51	9e+003	63.46	0	1e+005	
10		2.58	6e+002	4.48	0	2e+004	
10		2.61	4e+002	3.19	0	9e+003	
11		2.68	4e+002	2.65	0	7e+003	

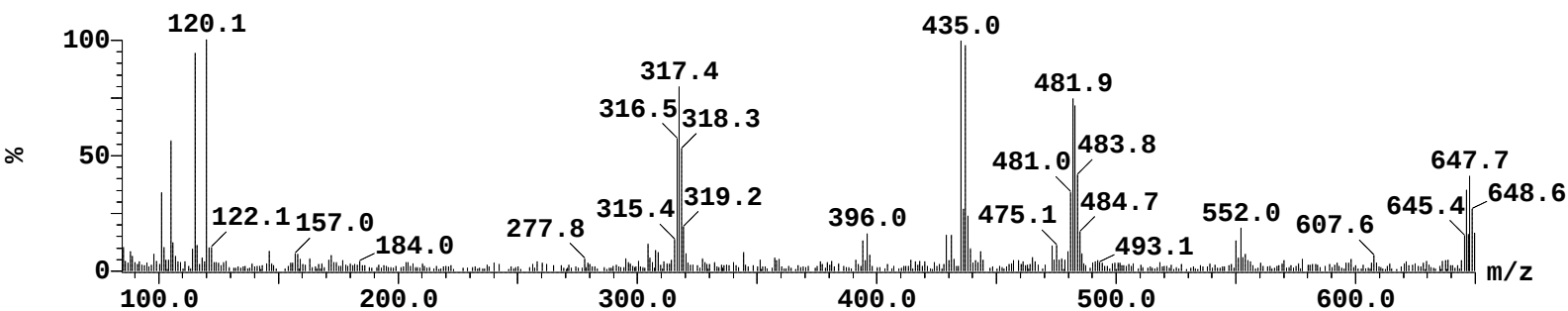
Peak ID Compound Time Mass Found
3 1.67

3: (Time: 1.67) 1.2e+003



Peak ID Compound Time Mass Found
8 2.43

8: (Time: 2.43) 1.0e+003



Sample: 17
File:ms41733
Description:A.ZUBIAURRE AZ 126 1

Vial:1:14
Date:08-Nov-2017

ID:
Time:12:51:28

Printed: Wed Nov 08 14:04:35 2017

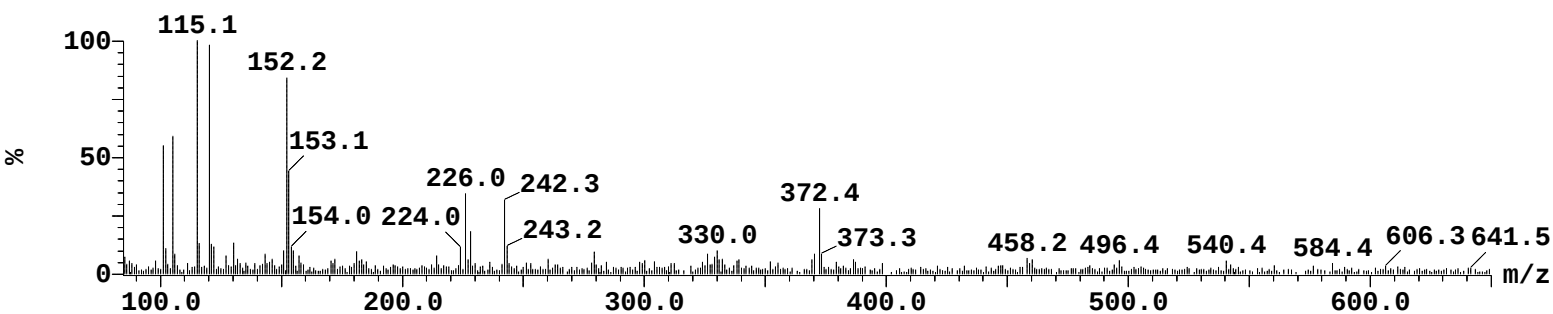
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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12		2.75	
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12: (Time: 2.75)

1.3e+003

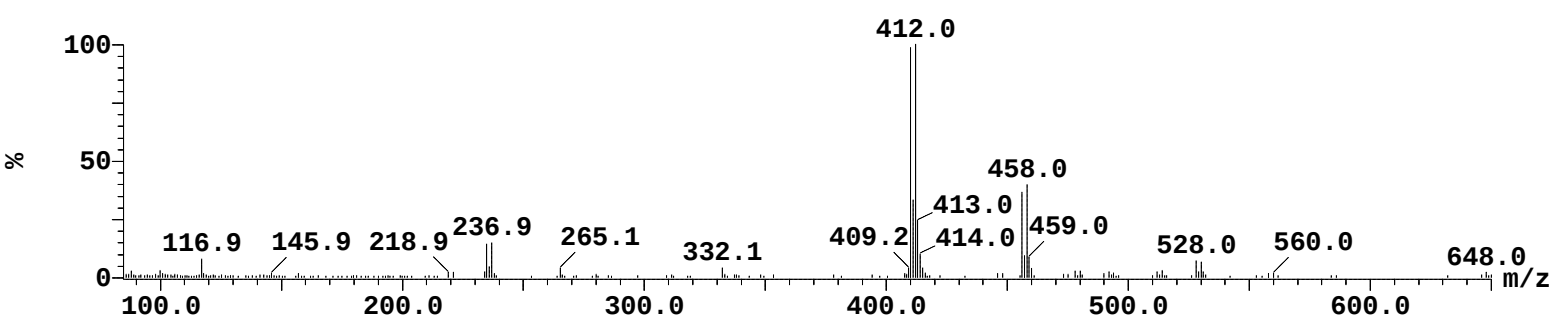


Peak ID	Compound	Time	Mass Found
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8		2.43	
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8: (Time: 2.44)

1.1e+004



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