

Single Mass Analysis

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

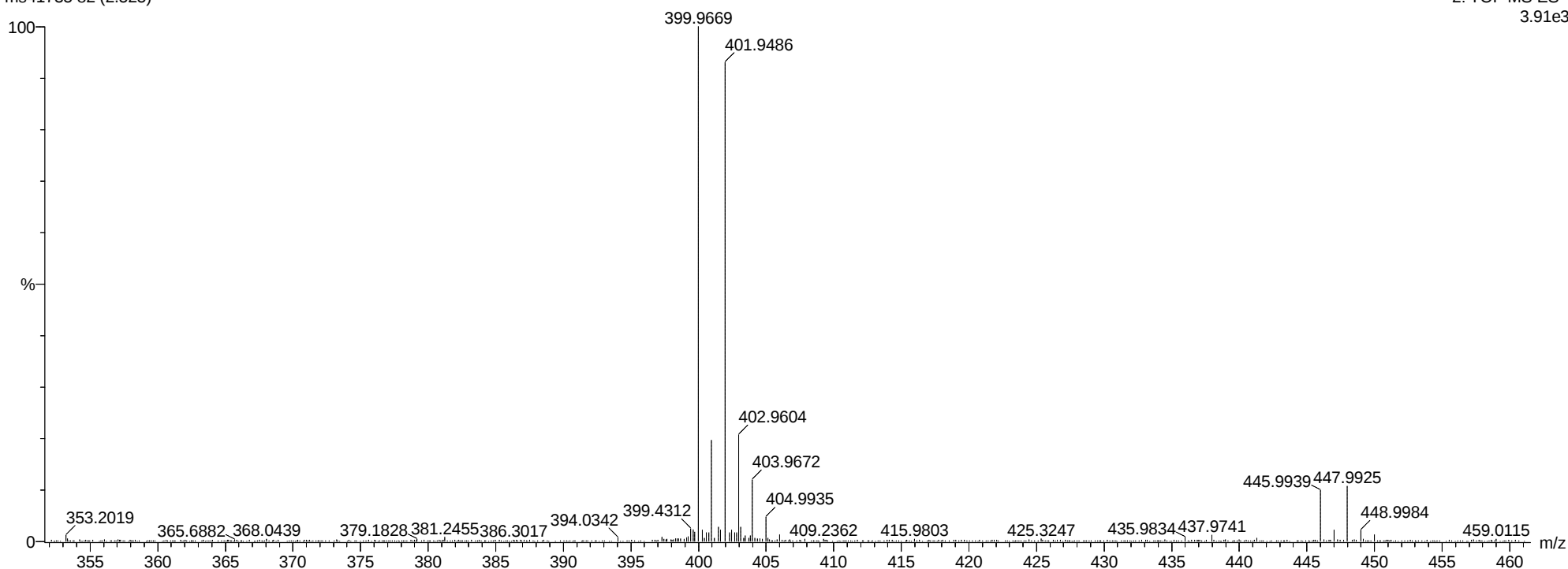
Selected filters: None

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: 15-15 H: 0-200 N: 0-10 O: 0-10 S: 2-2 Br: 1-1

A.ZUBIAURRE AZ 135 1
ms41735 82 (2.525)2: TOF MS ES-
3.91e3

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
399.9669	399.9677	-0.8	-2.0	8.5	49.9	C15 H15 N O3 S2 Br

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Sample: 19
File:ms41735
Description:A.ZUBIAURRE AZ 135 1

Vial:1:16
Date:08-Nov-2017

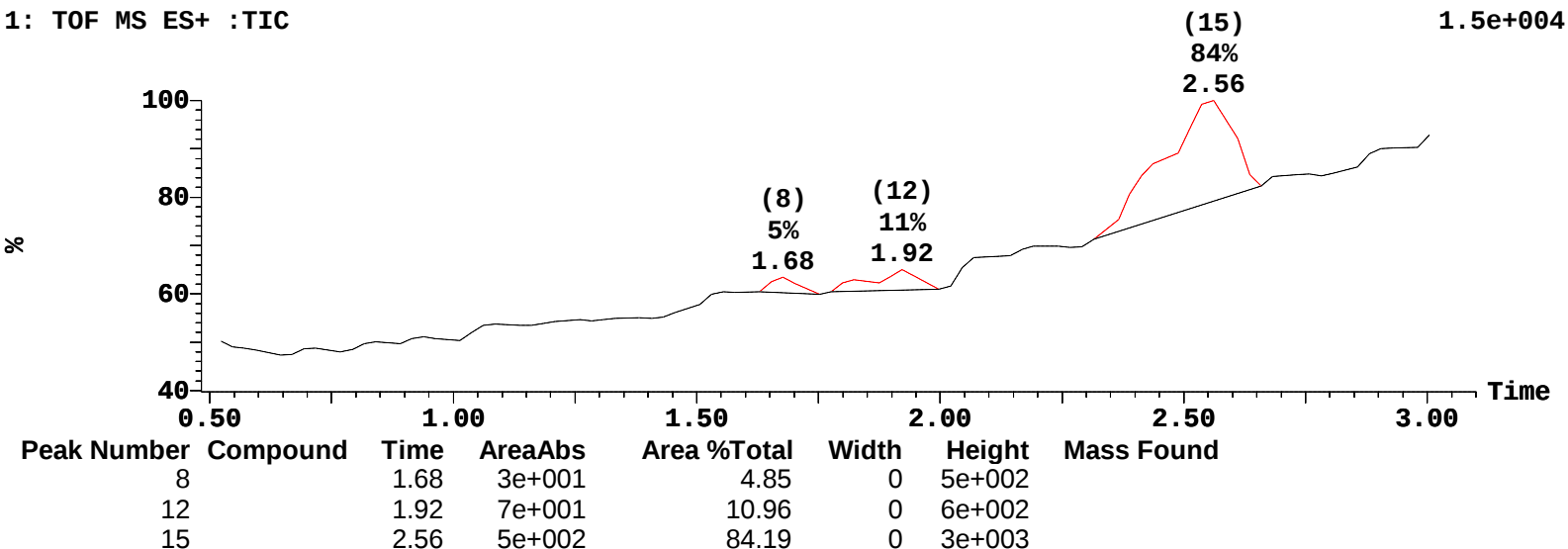
ID:
Time:13:01:18

Printed: Wed Nov 08 14:10:32 2017

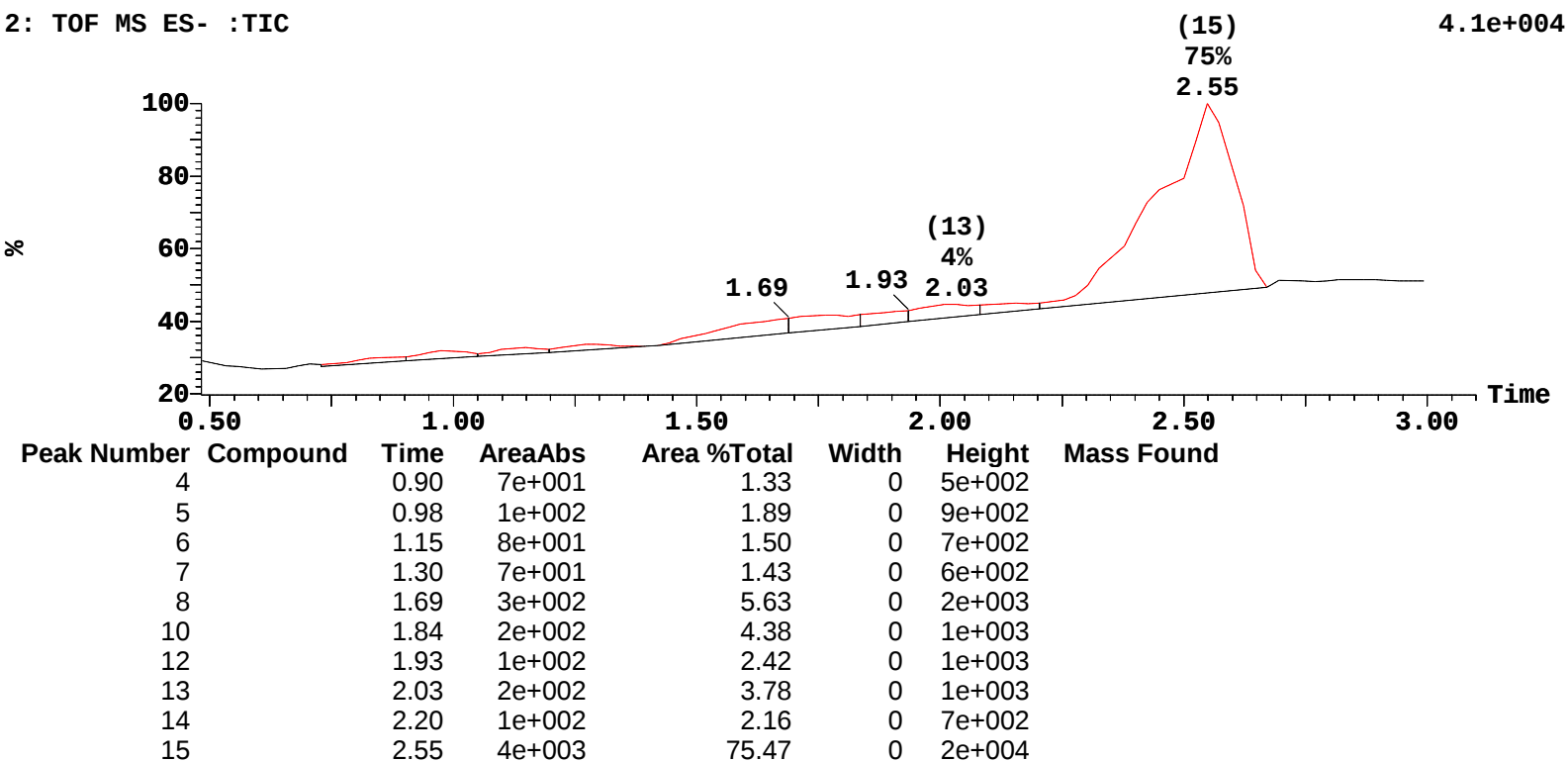
Sample Report:

Sample 19 Vial 1:16 ID File ms41735 Date 08-Nov-2017 Time 13:01:18 Description A.ZUBIAURRE AZ 135 1

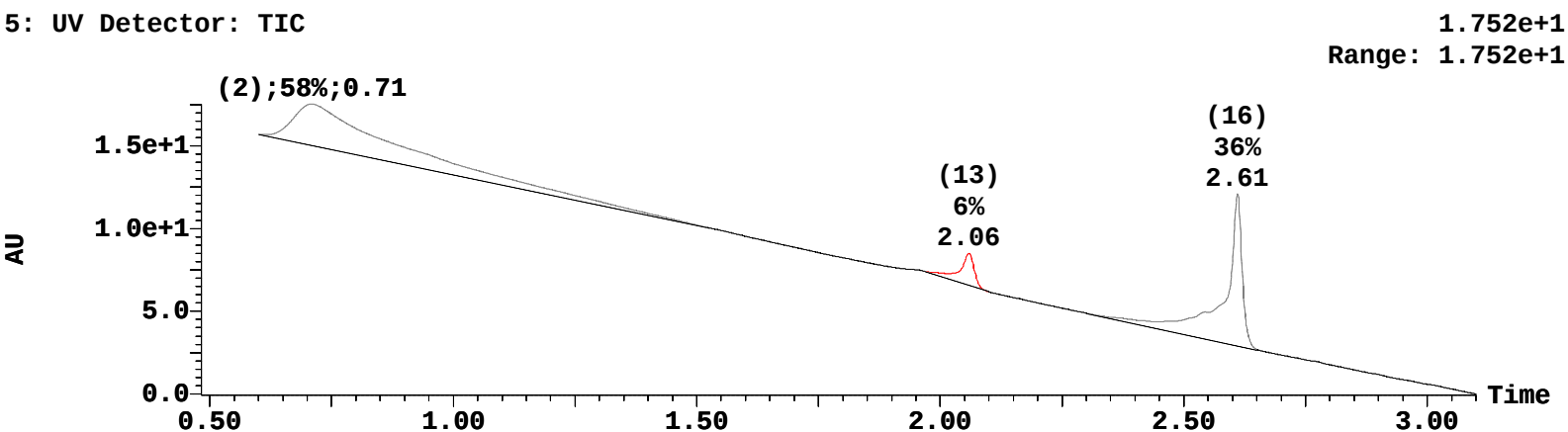
1: TOF MS ES+ :TIC



2: TOF MS ES- :TIC



5: UV Detector: TIC



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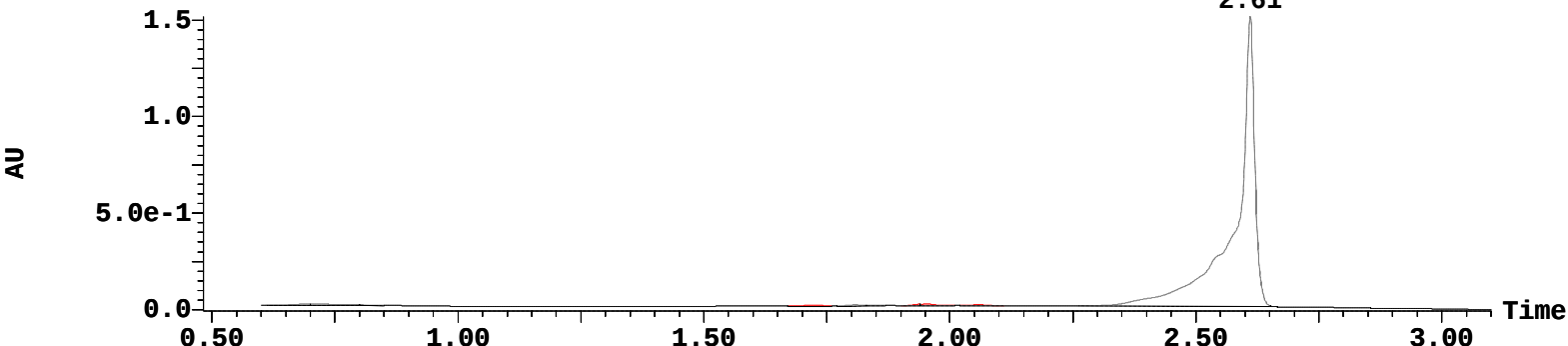
Printed: Wed Nov 08 14:10:32 2017

Sample Report (continued):

Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2		0.71	7e+005	57.65	1	2e+006	
13		2.06	7e+004	5.88	0	2e+006	
16		2.61	4e+005	36.47	0	9e+006	

5: UV Detector: 244_264

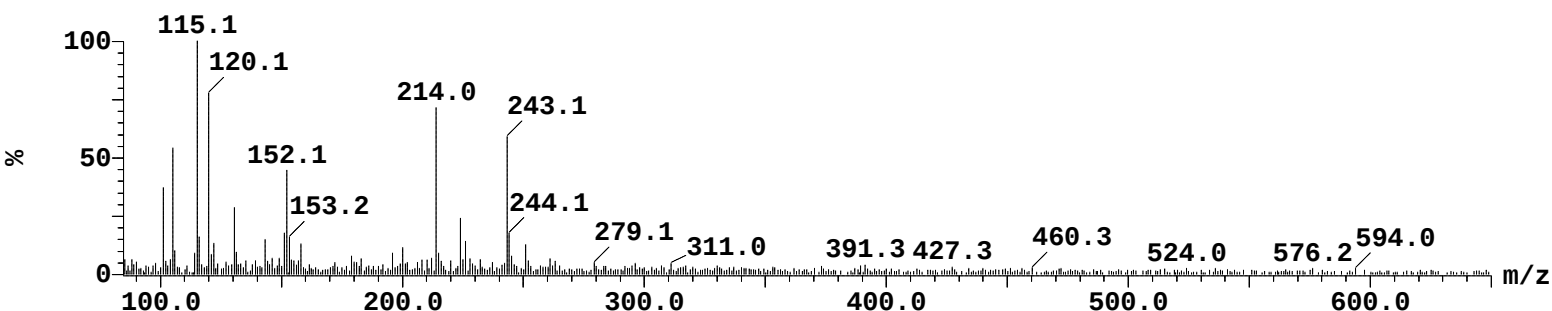
(16) 1.519
96% Range: 1.519
2.61



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.70	3e+002	0.46	0	8e+003	
2		0.71	5e+002	0.72	0	8e+003	
3		0.80	1e+002	0.18	0	3e+003	
8		1.72	3e+002	0.41	0	5e+003	
9		1.81	3e+002	0.42	0	7e+003	
11		1.84	2e+002	0.27	0	5e+003	
12		1.94	2e+002	0.32	0	9e+003	
12		1.96	4e+002	0.63	0	1e+004	
13		2.06	3e+002	0.47	0	7e+003	
16		2.61	7e+004	96.12	0	2e+006	

Peak ID Compound Time Mass Found
8 1.68

8: (Time: 1.68) 1.1e+003



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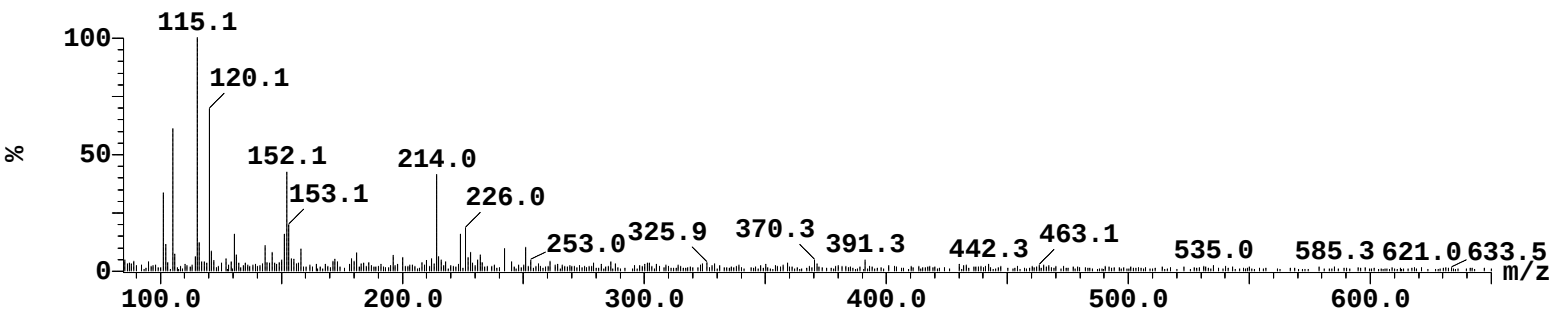
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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12		1.92	
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12: (Time: 1.92)

1.4e+003

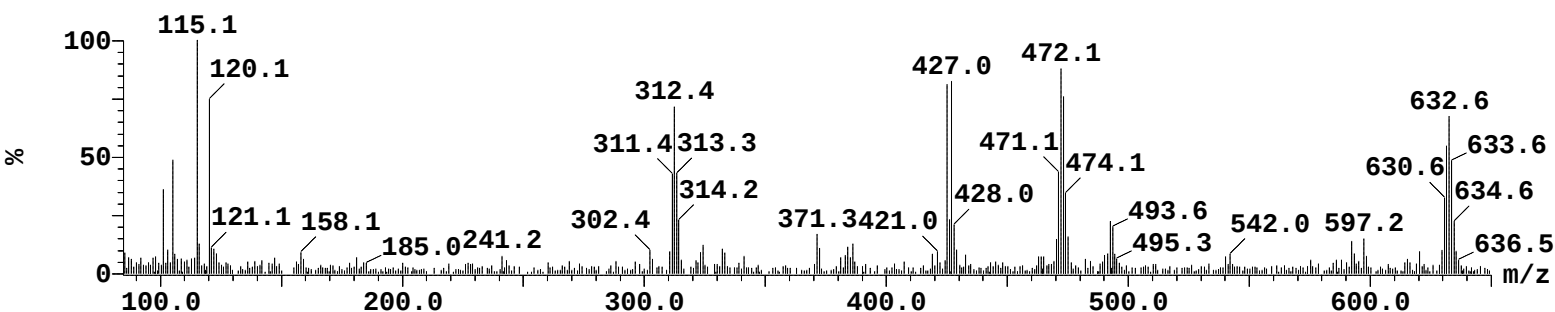


Peak ID	Compound	Time	Mass Found
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15		2.56	
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15: (Time: 2.56)

7.9e+002

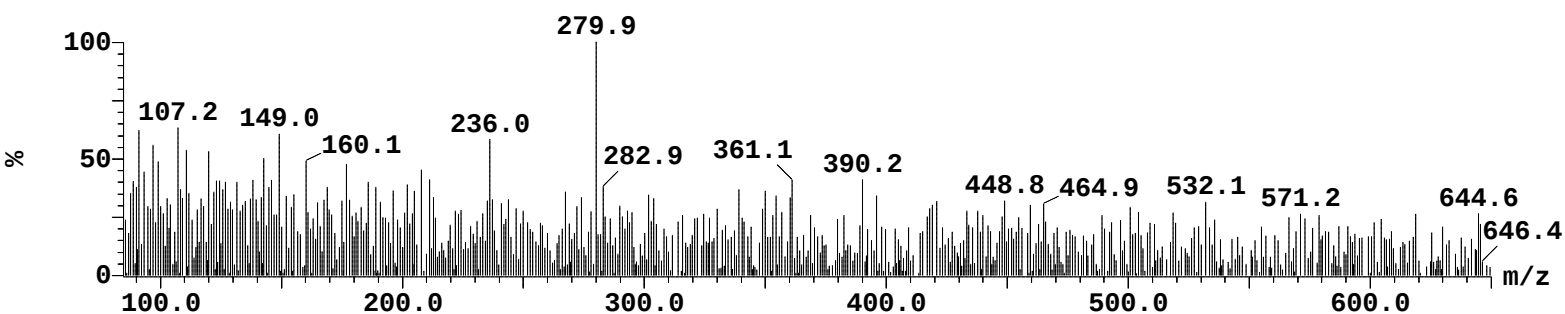


Peak ID	Compound	Time	Mass Found
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4		0.90	
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4: (Time: 0.90)

1.3e+002

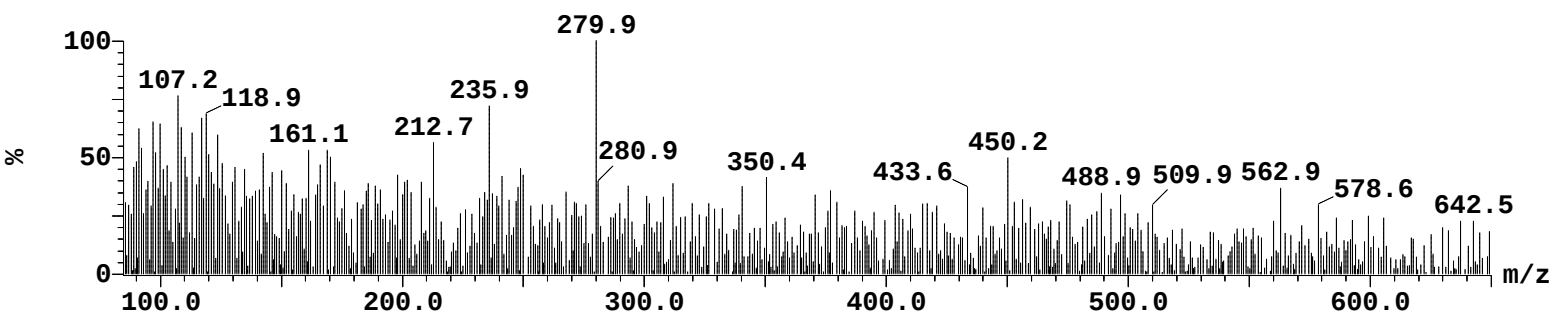


Peak ID	Compound	Time	Mass Found
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5		0.98	
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5: (Time: 0.98)

1.4e+002



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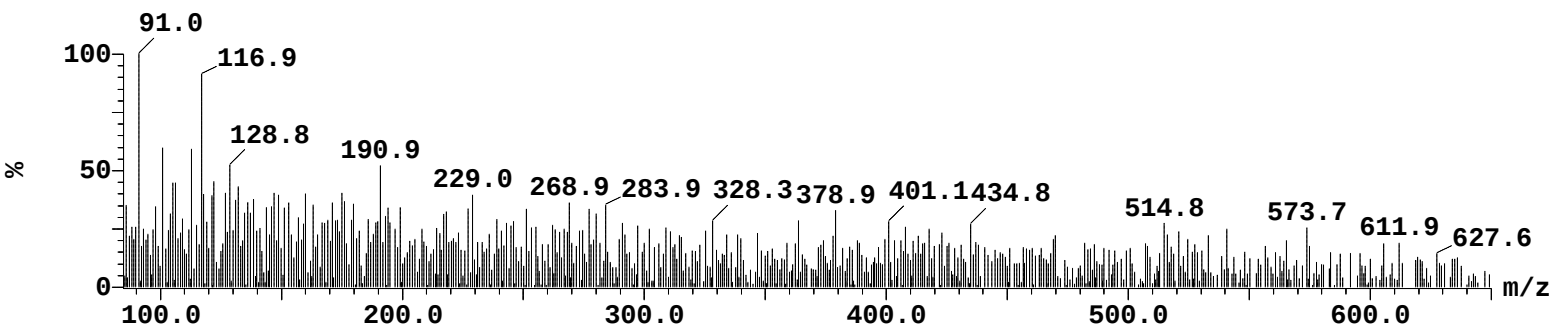
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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6		1.15	
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6: (Time: 1.15)

1.6e+002

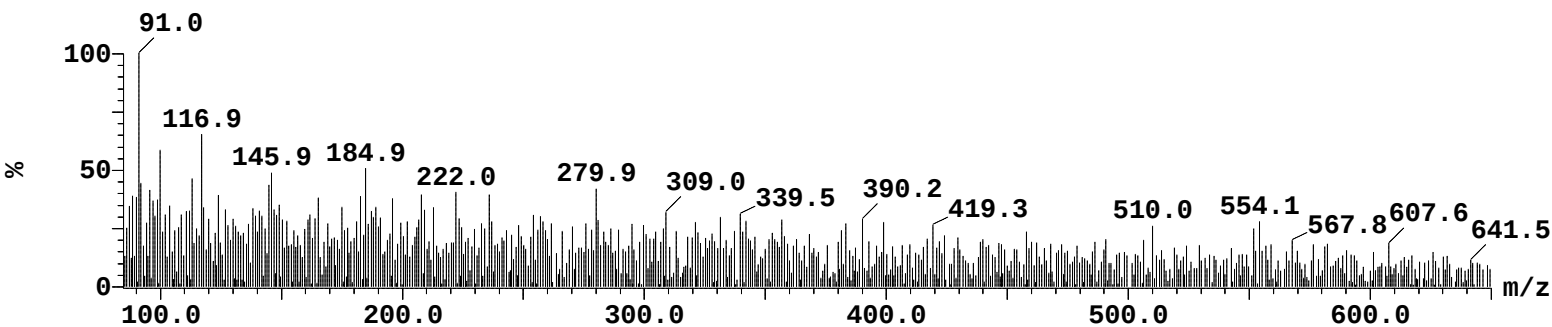


Peak ID	Compound	Time	Mass Found
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7		1.30	
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7: (Time: 1.30)

2.7e+002

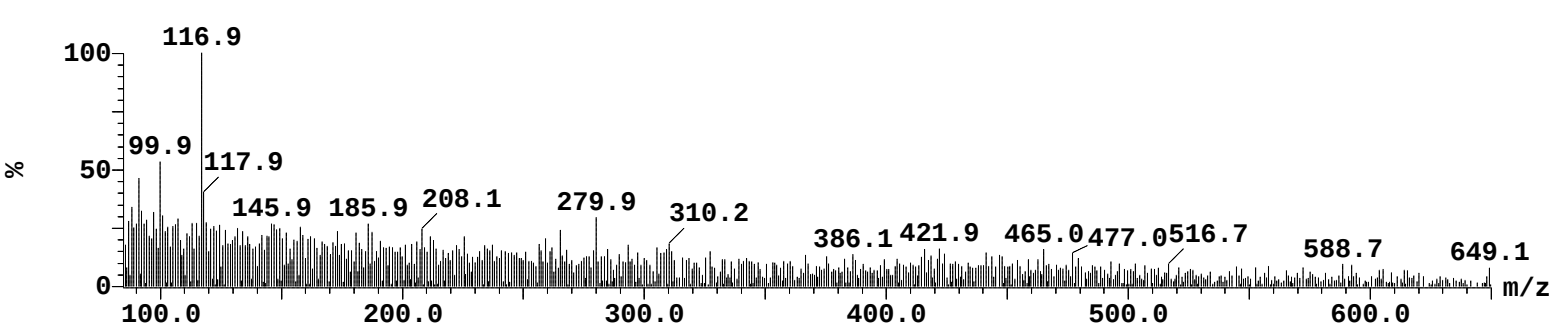


Peak ID	Compound	Time	Mass Found
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8		1.68	
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8: (Time: 1.69)

6.0e+002

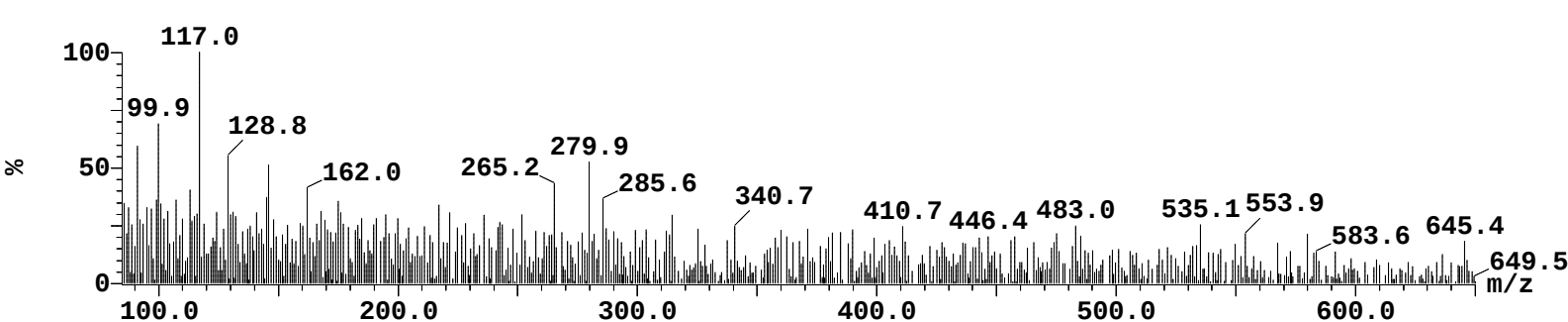


Peak ID	Compound	Time	Mass Found
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10		1.84	
----	--	------	--

10: (Time: 1.84)

2.4e+002



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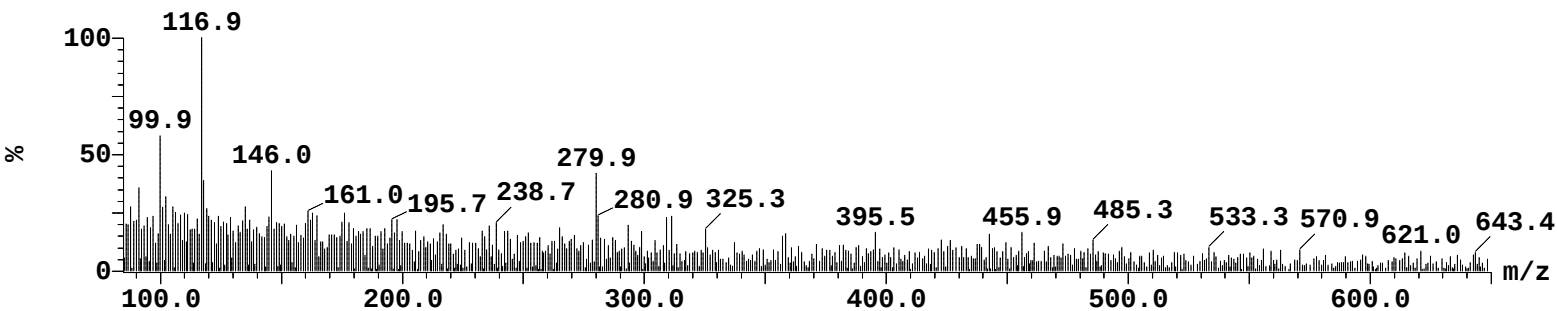
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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12		1.92	
----	--	------	--

12: (Time: 1.93)

6.3e+002

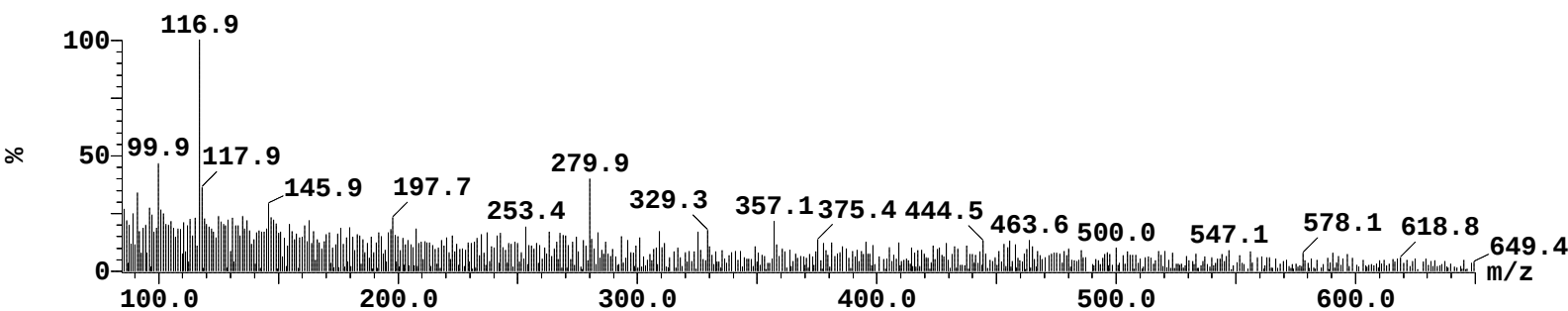


Peak ID	Compound	Time	Mass Found
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13		2.03	
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13: (Time: 2.03)

7.2e+002

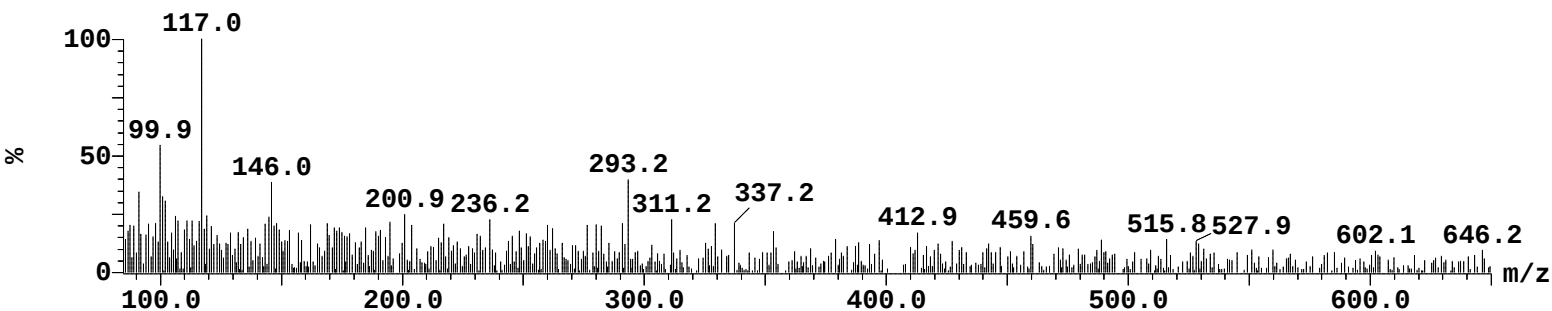


Peak ID	Compound	Time	Mass Found
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14		2.20	
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14: (Time: 2.20)

4.1e+002

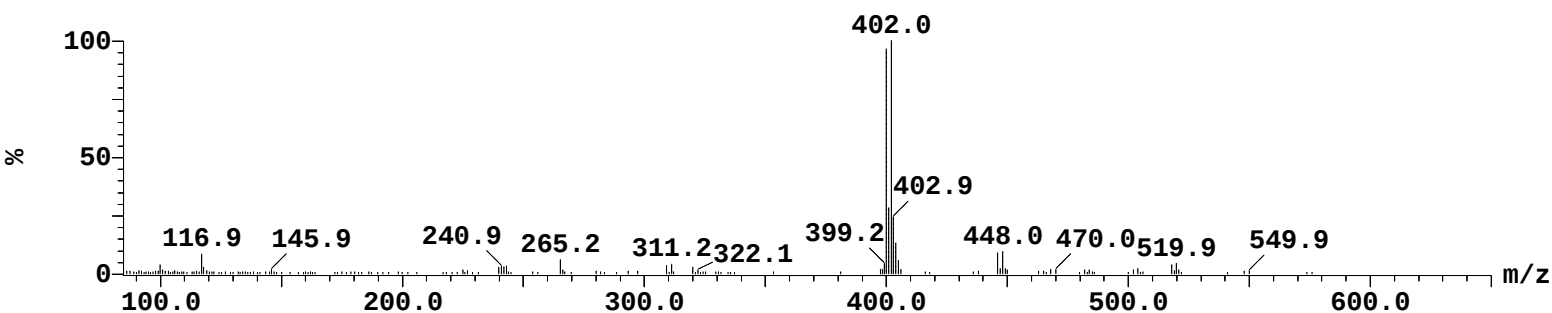


Peak ID	Compound	Time	Mass Found
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15		2.56	
----	--	------	--

15: (Time: 2.55)

1.9e+004



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