

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

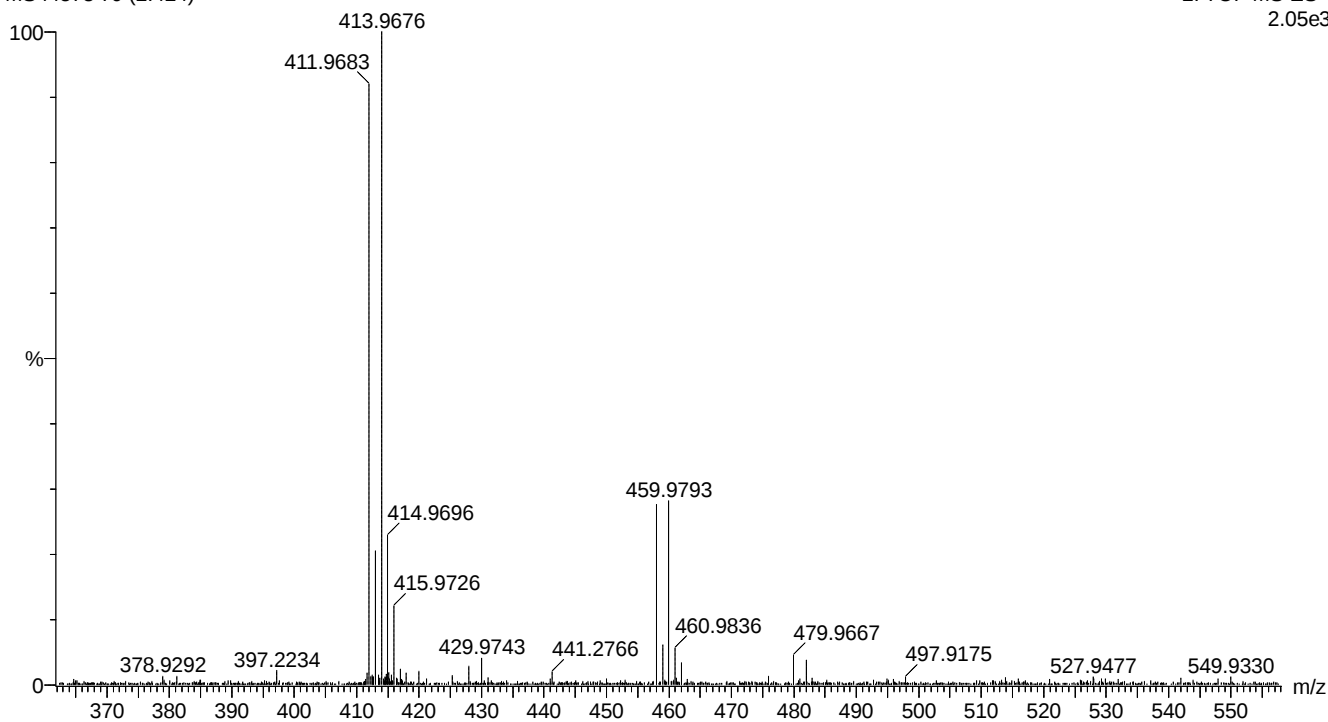
115 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 16-16 H: 0-200 N: 0-10 O: 0-10 S: 2-2 Br: 1-1

J.SHEN JSS 6R

MS44578 79 (2.424)

2: TOF MS ES-
2.05e3

Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
411.9683	411.9677	0.6	1.5	9.5	2.3	C16 H15 N 03 S2 Br

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Sample: 19
File:MS44578
Description:J.SHEN JSS 6R

Vial:1:7
Date:12-Mar-2018

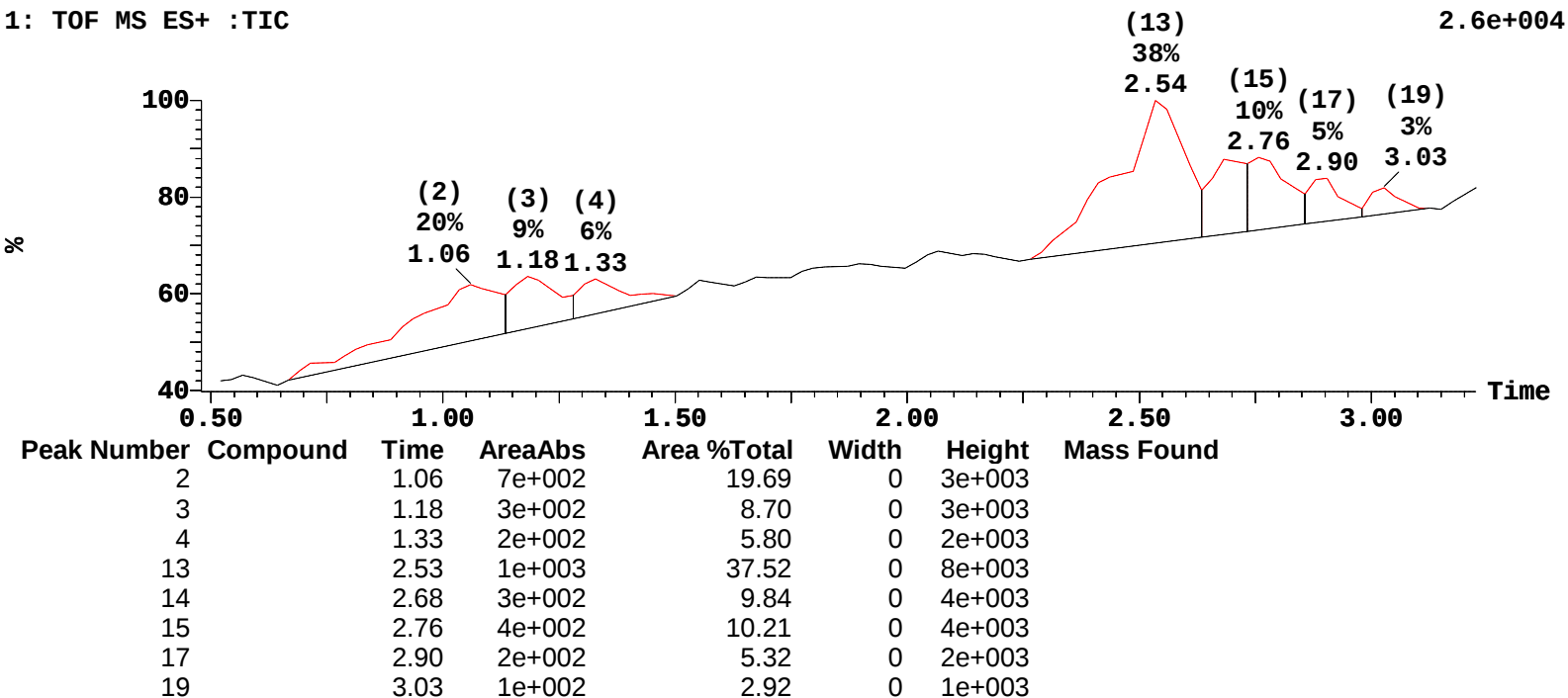
ID:
Time:10:28:18

Printed: Mon Mar 12 13:40:52 2018

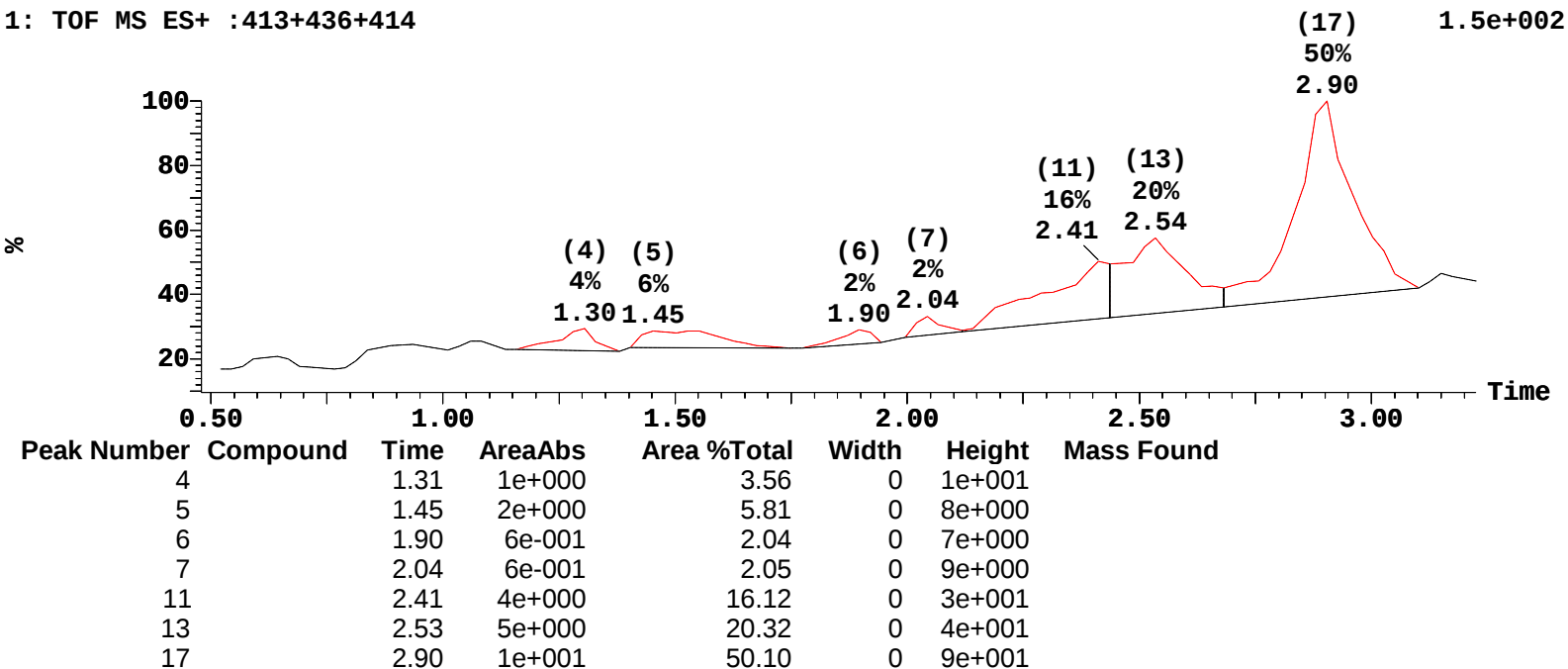
Sample Report:

Sample 19 Vial 1:7 ID File MS44578 Date 12-Mar-2018 Time 10:28:18 Description J.SHEN JSS 6R

1: TOF MS ES+ :TIC



1: TOF MS ES+ :413+436+414



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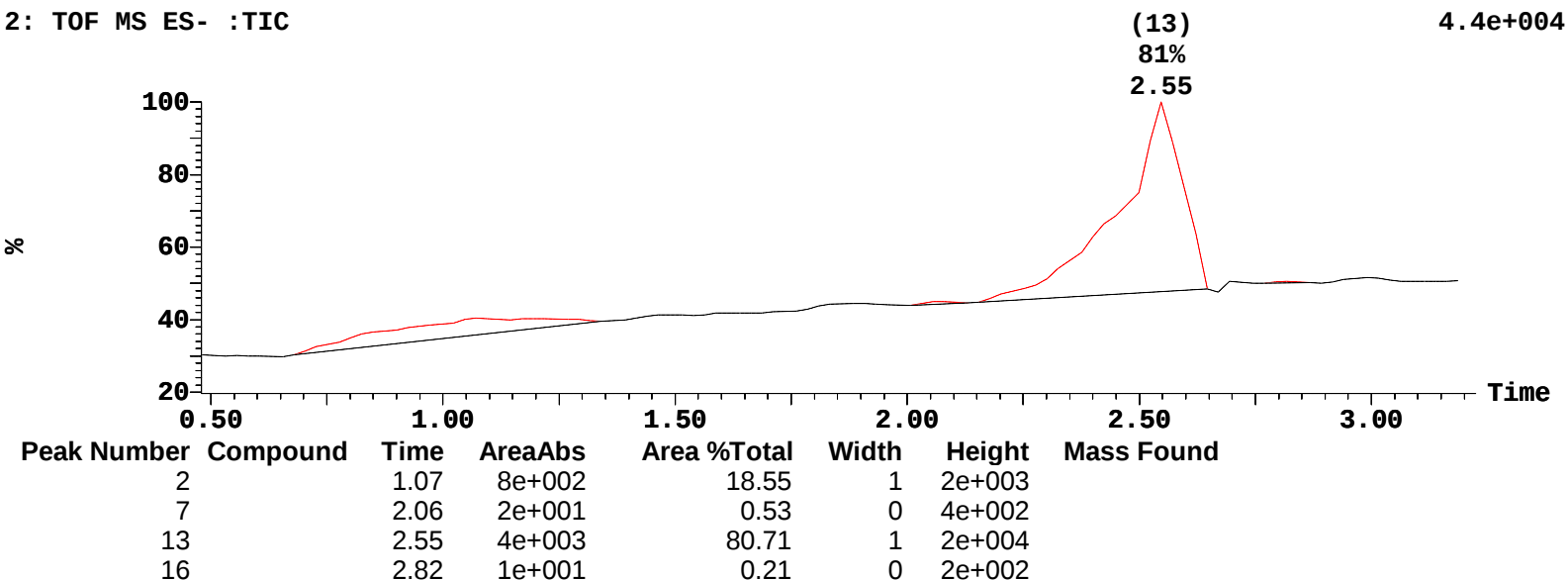
ID:
Time:10:28:18

Printed: Mon Mar 12 13:40:52 2018

Sample Report (continued):

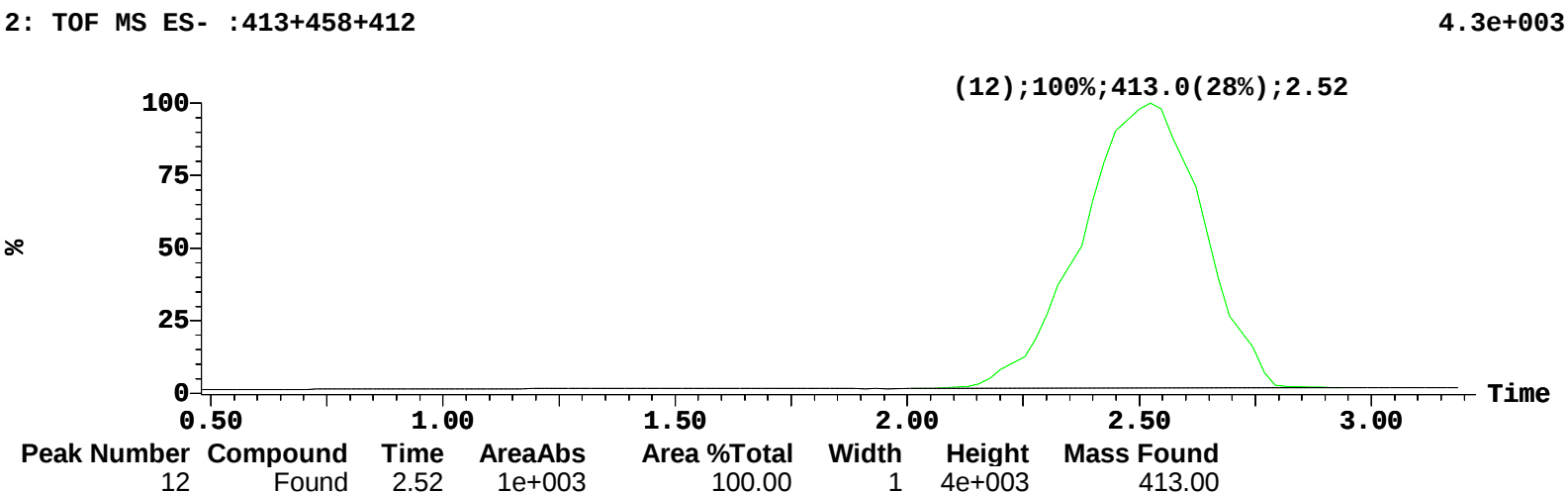
2: TOF MS ES- :TIC

4.4e+004



2: TOF MS ES- :413+458+412

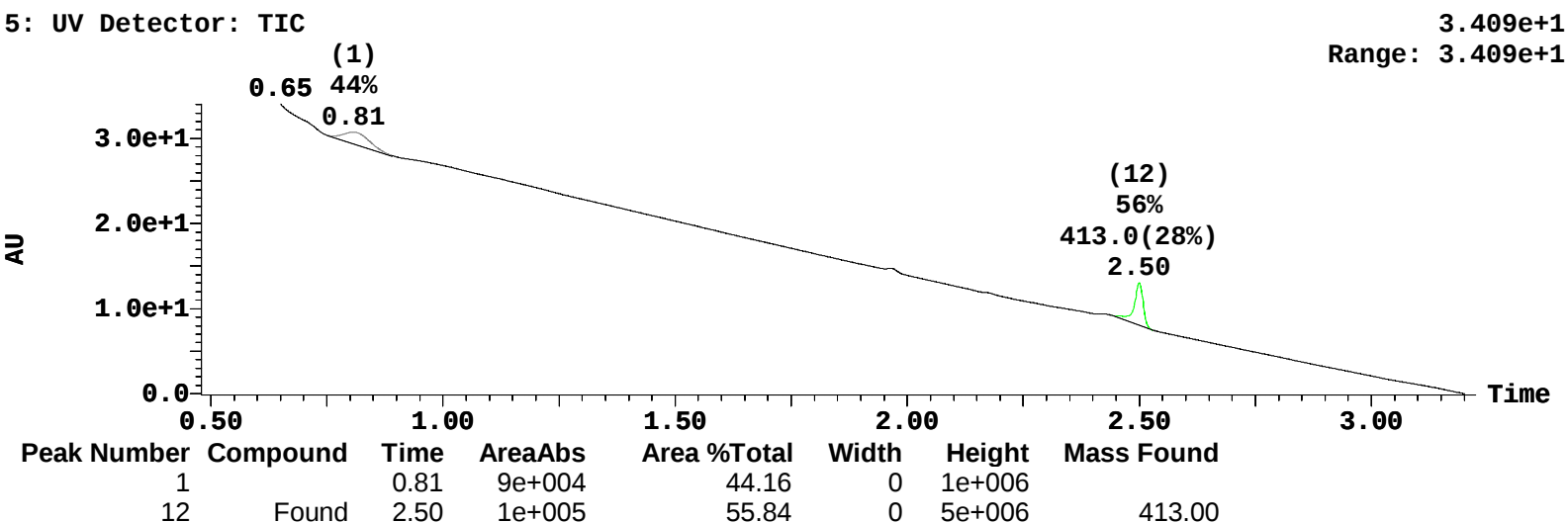
4.3e+003



5: UV Detector: TIC

3.409e+1

Range: 3.409e+1



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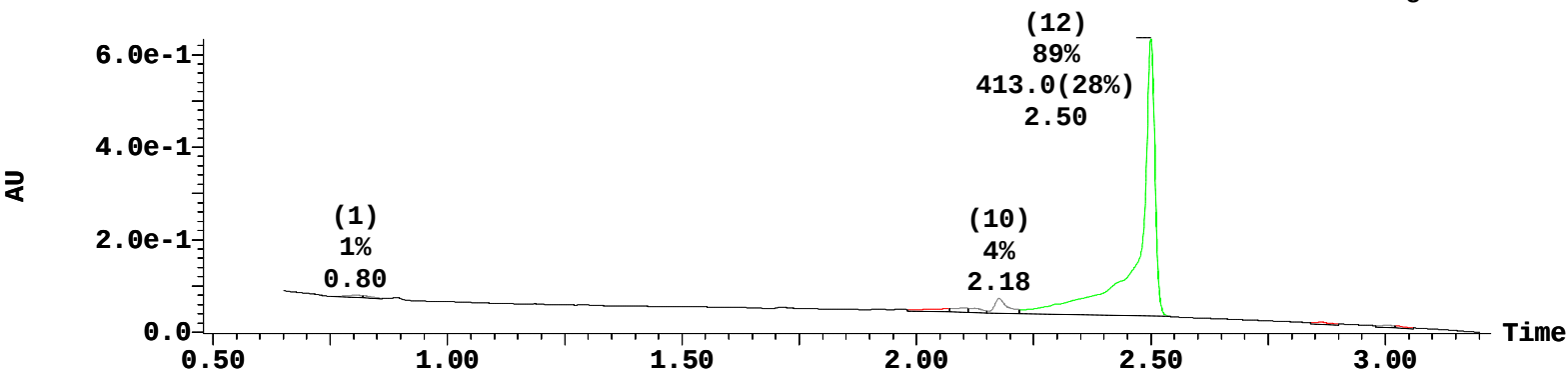
ID:
Time:10:28:18

Printed: Mon Mar 12 13:40:52 2018

Sample Report (continued):

5: UV Detector: 244_264

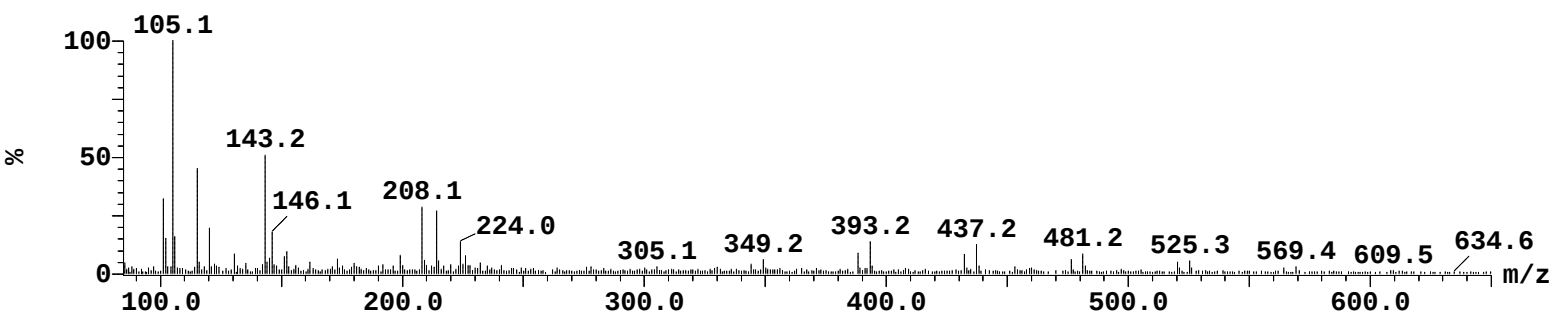
6.34e-1
Range: 6.34e-1



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.80	2e+002	0.68	0	5e+003	
1		0.82	2e+002	0.60	0	5e+003	
7		2.07	5e+002	1.69	0	8e+003	
8		2.10	4e+002	1.35	0	9e+003	
9		2.12	3e+002	1.02	0	9e+003	
10		2.18	1e+003	3.80	0	3e+004	
12	Found	2.50	2e+004	88.91	0	6e+005	413.00
16		2.86	2e+002	0.75	0	5e+003	
18		3.00	2e+002	0.59	0	5e+003	
19		3.02	2e+002	0.61	0	5e+003	

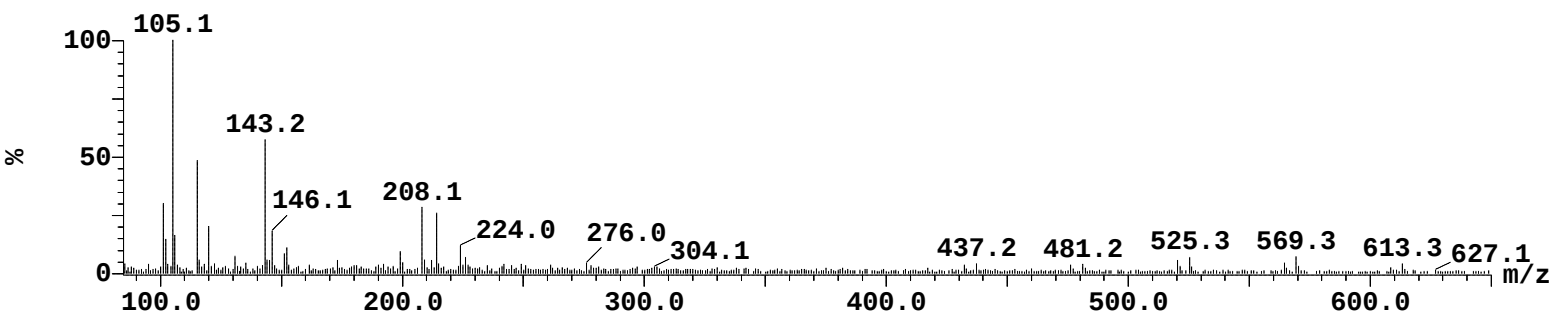
Peak ID Compound Time Mass Found
2 1.06

2: (Time: 1.06) 3.0e+003



Peak ID Compound Time Mass Found
3 1.18

3: (Time: 1.18) 2.9e+003



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Vial: 1:7
Date: 12-Mar-2018

ID:
Time: 10:28:18

Printed: Mon Mar 12 13:40:52 2018

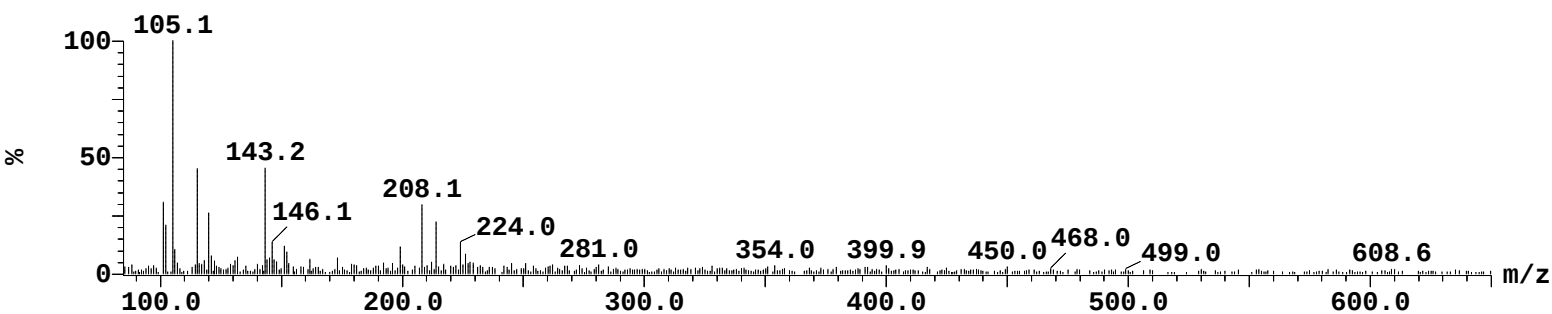
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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4		1.33	
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4: (Time: 1.33)

1.5e+003

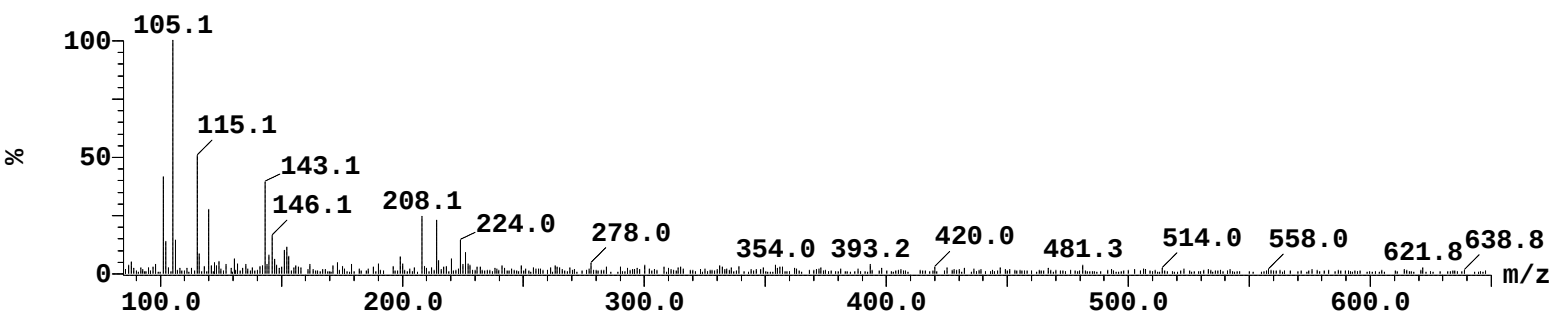


Peak ID	Compound	Time	Mass Found
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5		1.45	
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5: (Time: 1.45)

1.4e+003

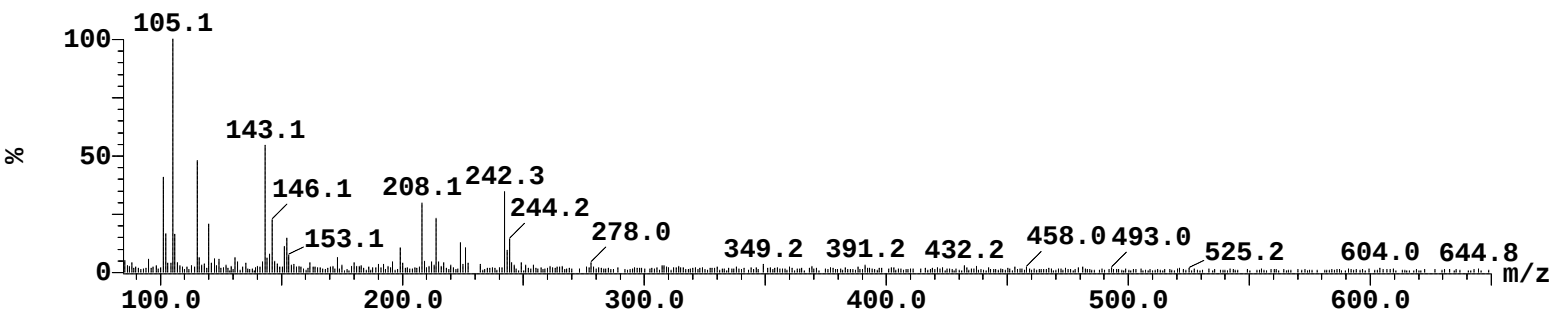


Peak ID	Compound	Time	Mass Found
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6		1.90	
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6: (Time: 1.90)

2.6e+003

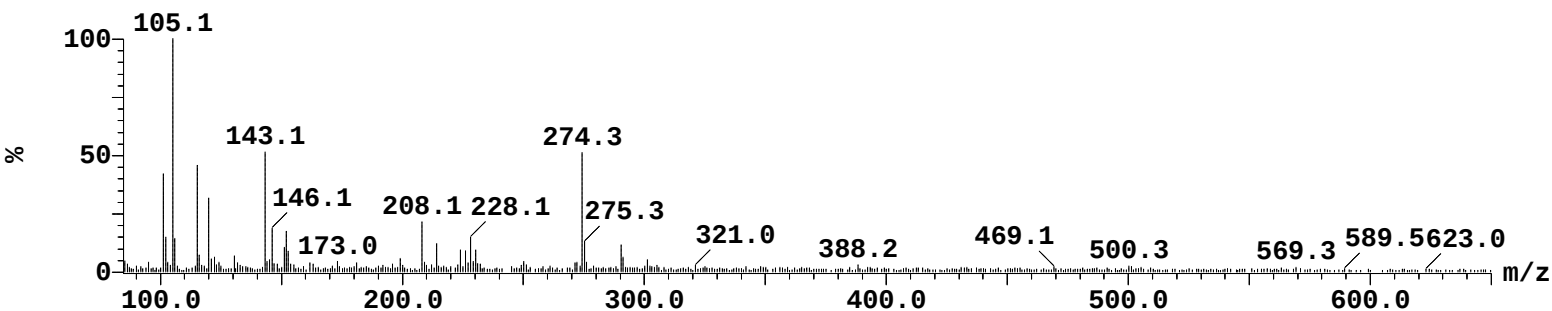


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

7		2.04	
---	--	------	--

7: (Time: 2.04)

2.9e+003



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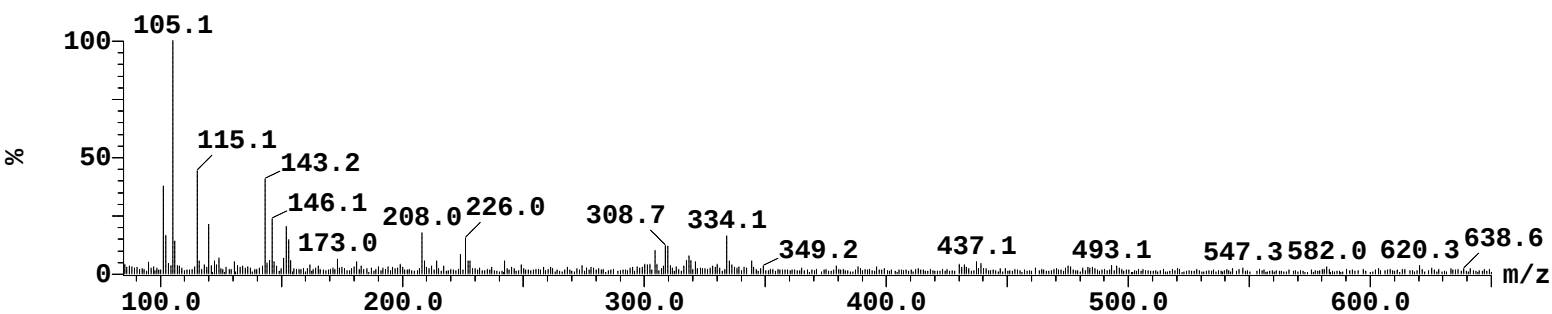
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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11		2.41	
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11: (Time: 2.41)

3.4e+003

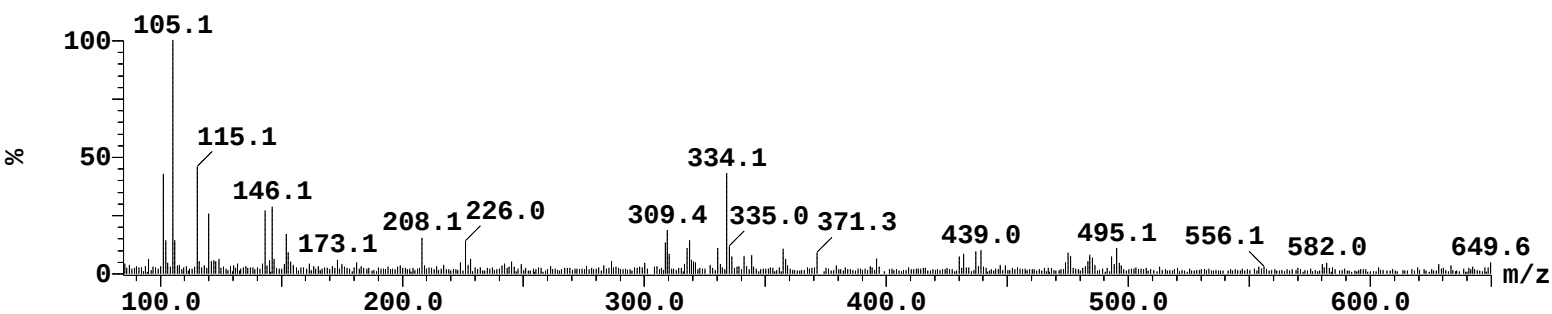


Peak ID	Compound	Time	Mass Found
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13		2.53	
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13: (Time: 2.53)

3.6e+003

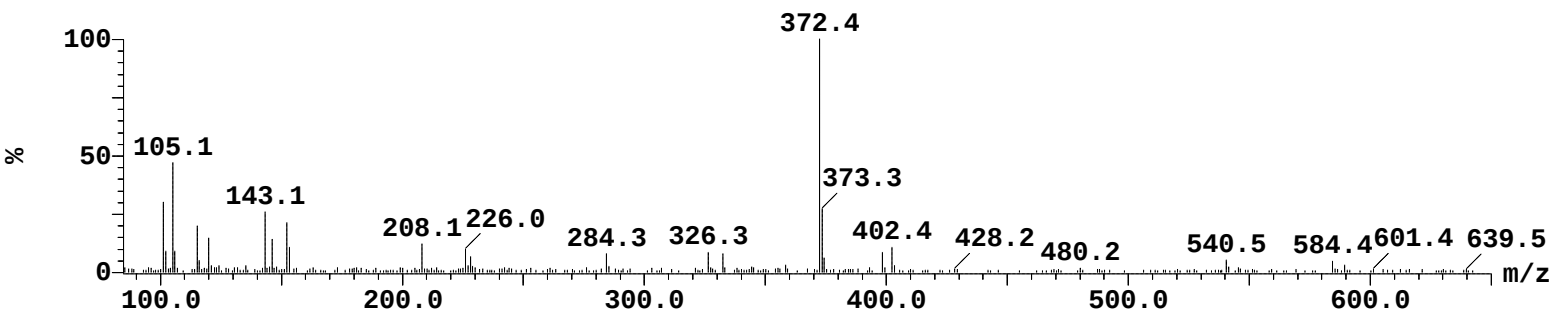


Peak ID	Compound	Time	Mass Found
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14		2.68	
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14: (Time: 2.68)

3.1e+003

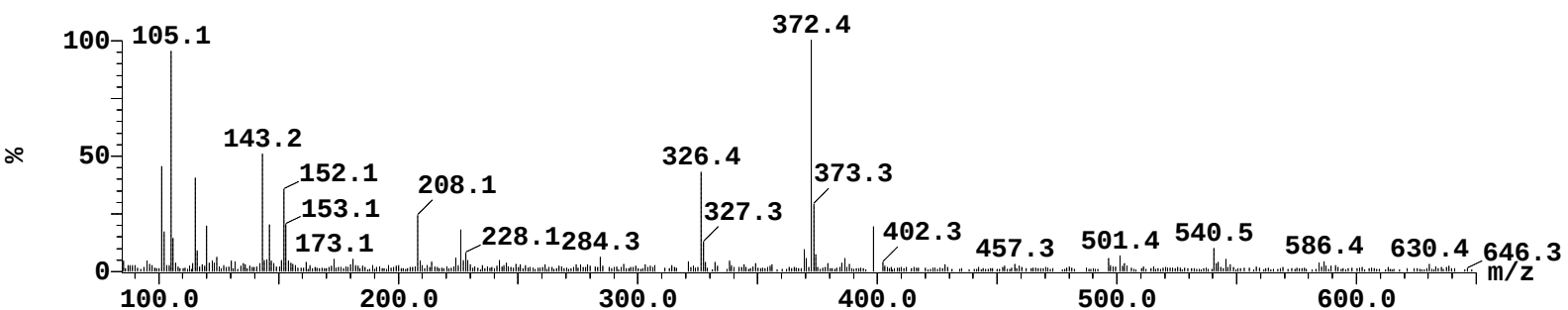


Peak ID	Compound	Time	Mass Found
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15		2.76	
----	--	------	--

15: (Time: 2.76)

3.4e+003



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ID:
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Printed: Mon Mar 12 13:40:52 2018

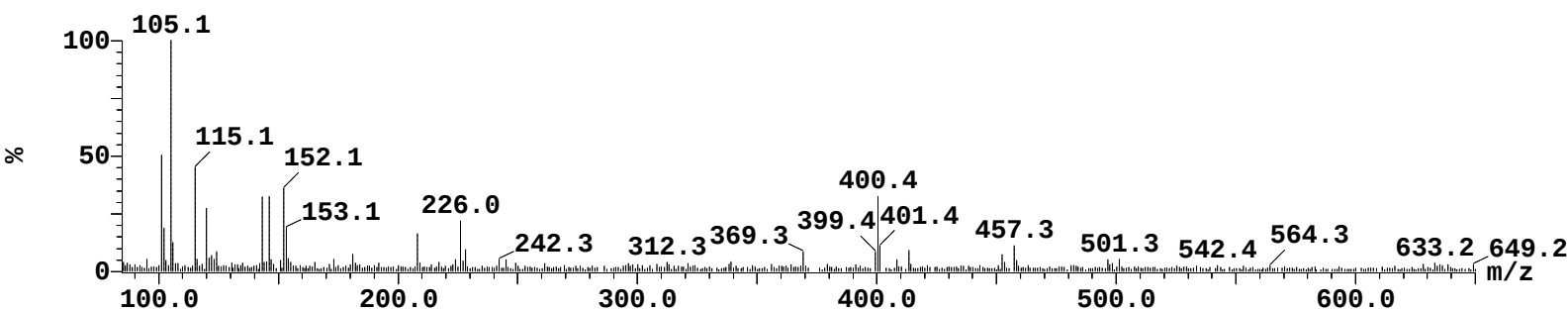
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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17		2.90	
----	--	------	--

17: (Time: 2.90)

2.9e+003

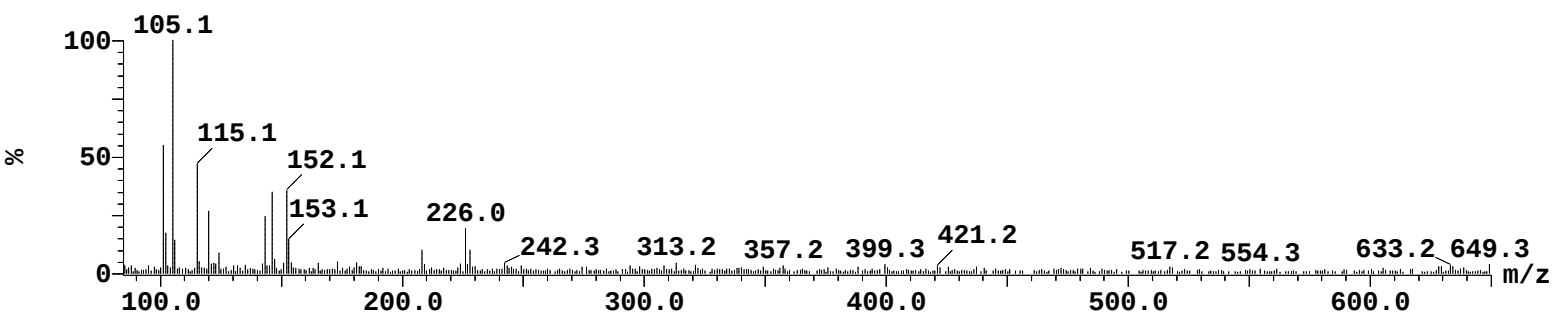


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

19		3.03	
----	--	------	--

19: (Time: 3.03)

3.4e+003

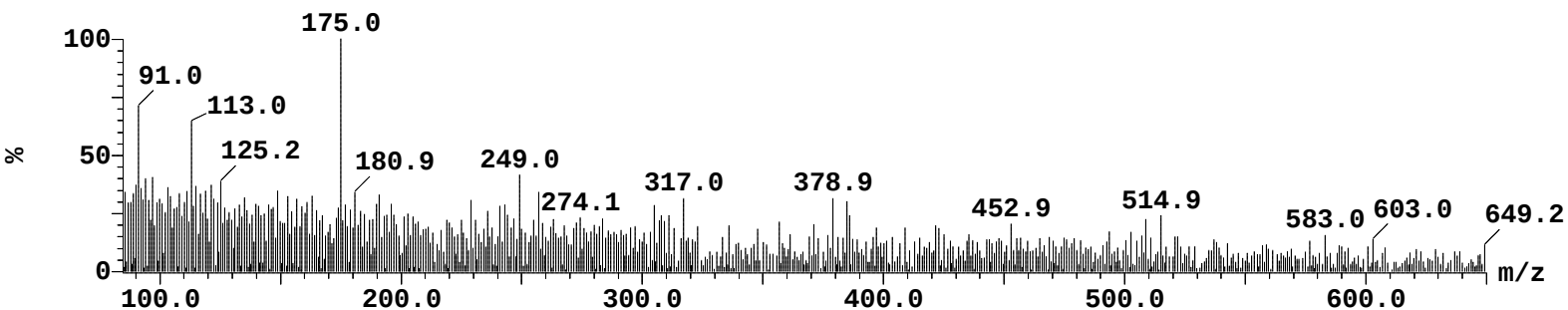


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

2		1.06	
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2: (Time: 1.07)

4.8e+002

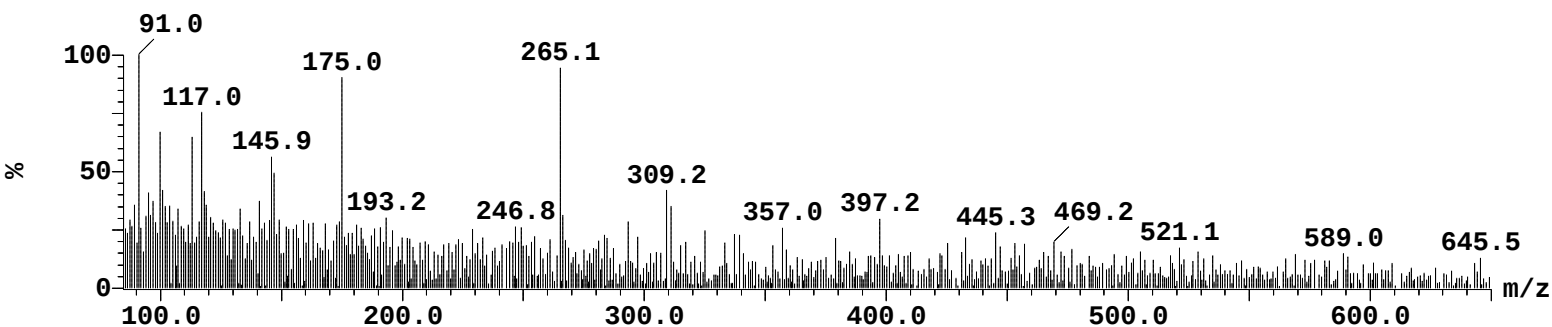


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

7		2.04	
---	--	------	--

7: (Time: 2.06)

5.1e+002



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Vial: 1:7
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ID:
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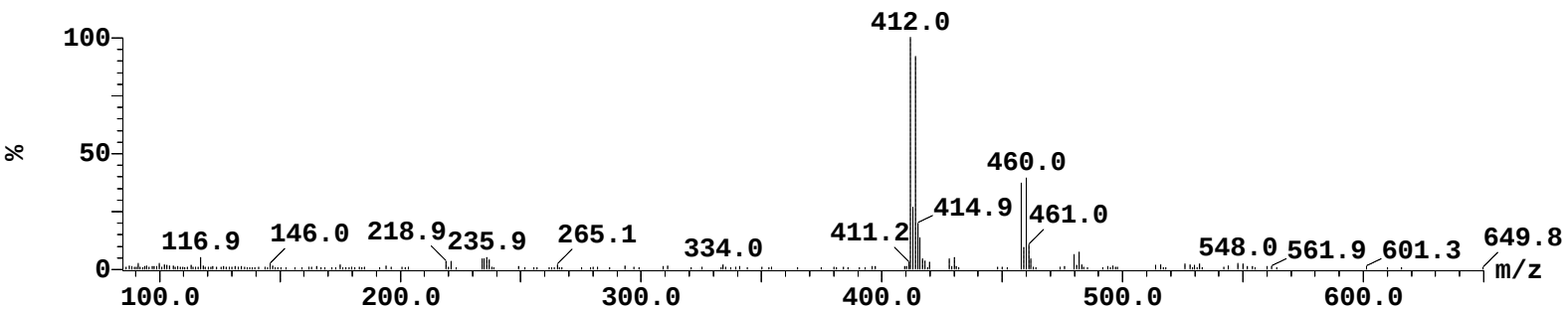
Printed: Mon Mar 12 13:40:52 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
12	Found	2.52	413.00

12: (Time: 2.52)

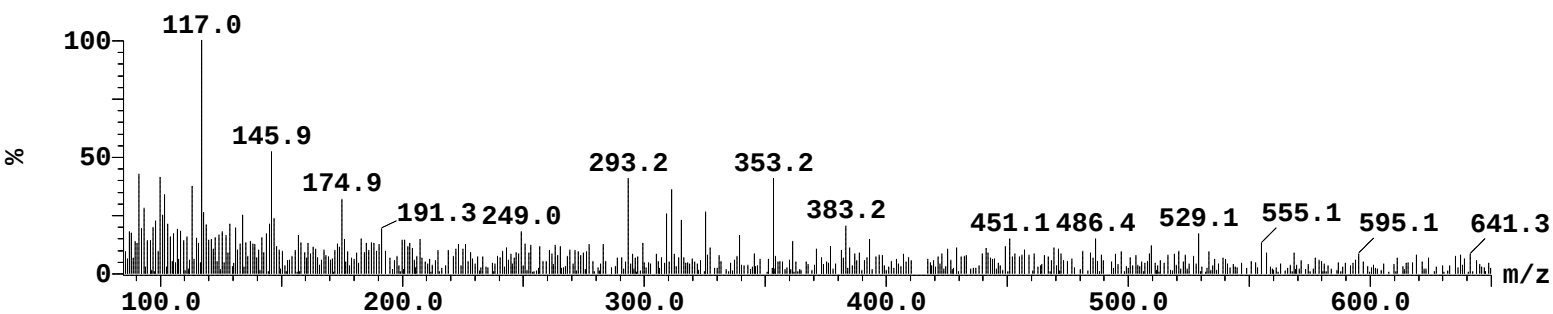
1.8e+004



Peak ID	Compound	Time	Mass Found
16		2.82	

16: (Time: 2.82)

5.9e+002



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