

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

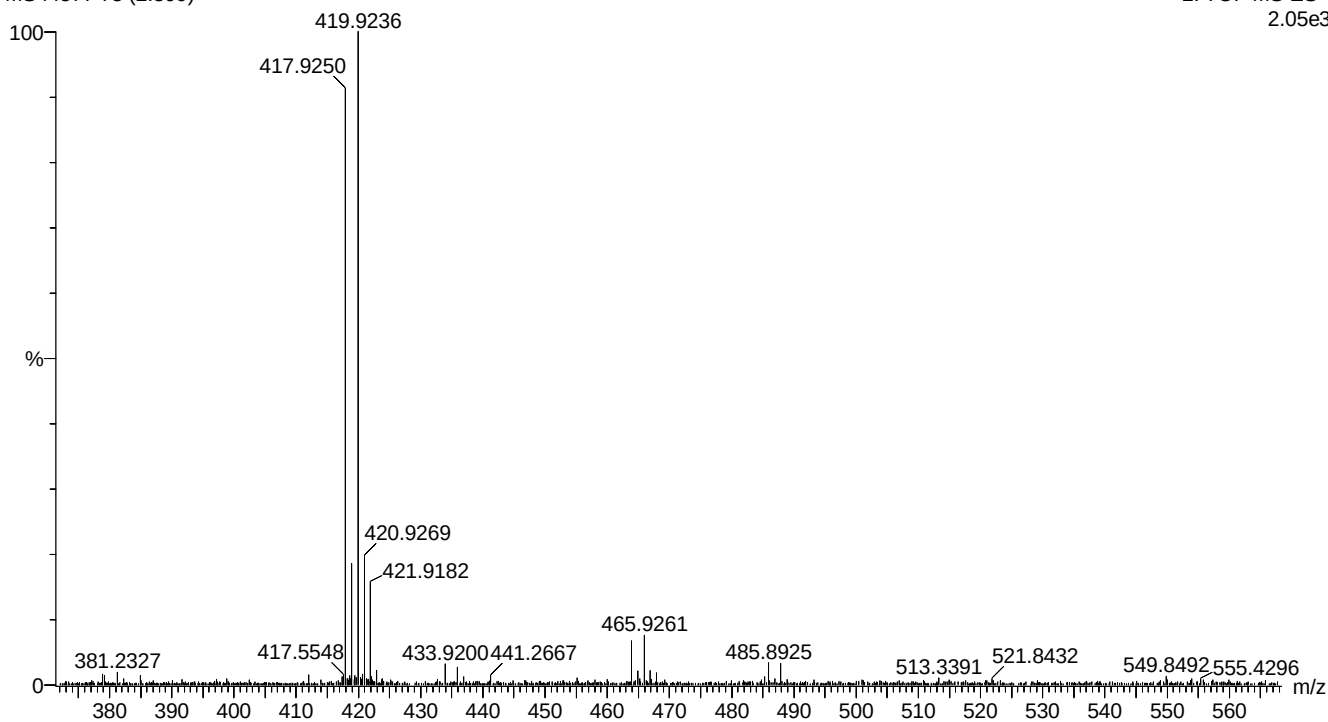
108 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 14-14 H: 0-200 N: 0-10 O: 0-10 S: 3-3 Br: 1-1

J.SHEN JSS 5R

MS44577 78 (2.399)

2: TOF MS ES-
2.05e3

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
417.9250	417.9241	0.9	2.2	8.5	2.2	C14 H13 N 03 S3 Br

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Sample: 18
File:MS44577
Description:J.SHEN JSS 5R

Vial:1:6
Date:12-Mar-2018

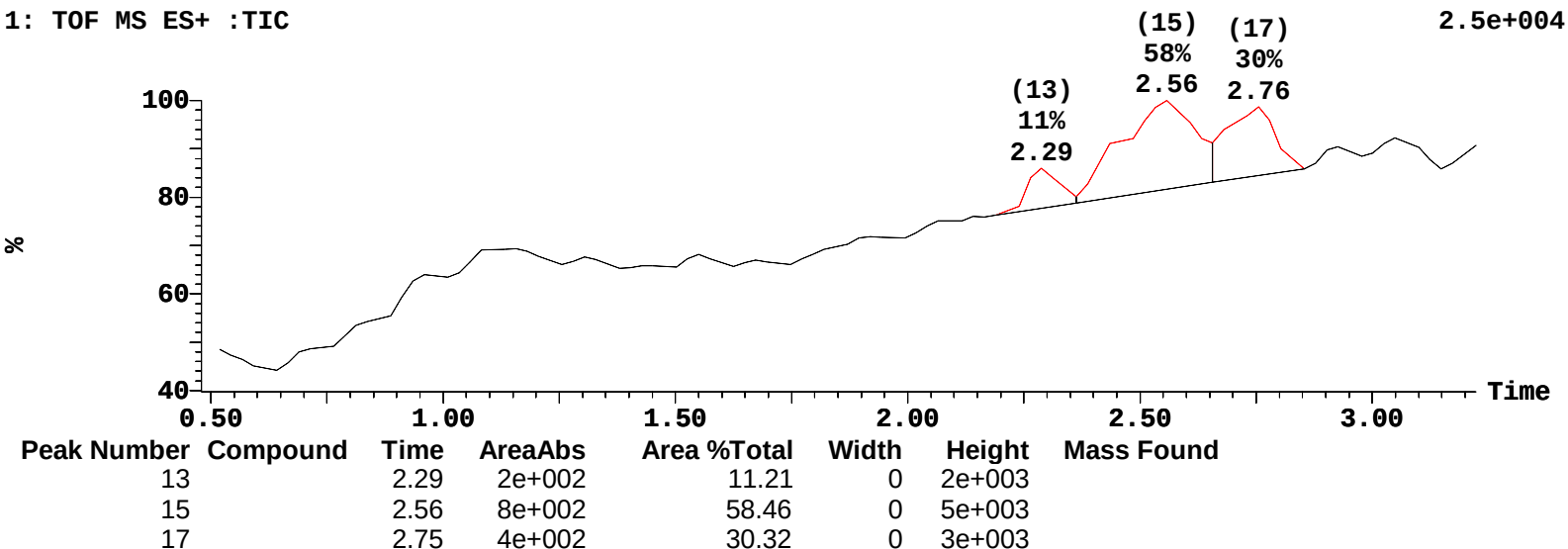
ID:
Time:10:23:21

Printed: Mon Mar 12 13:36:24 2018

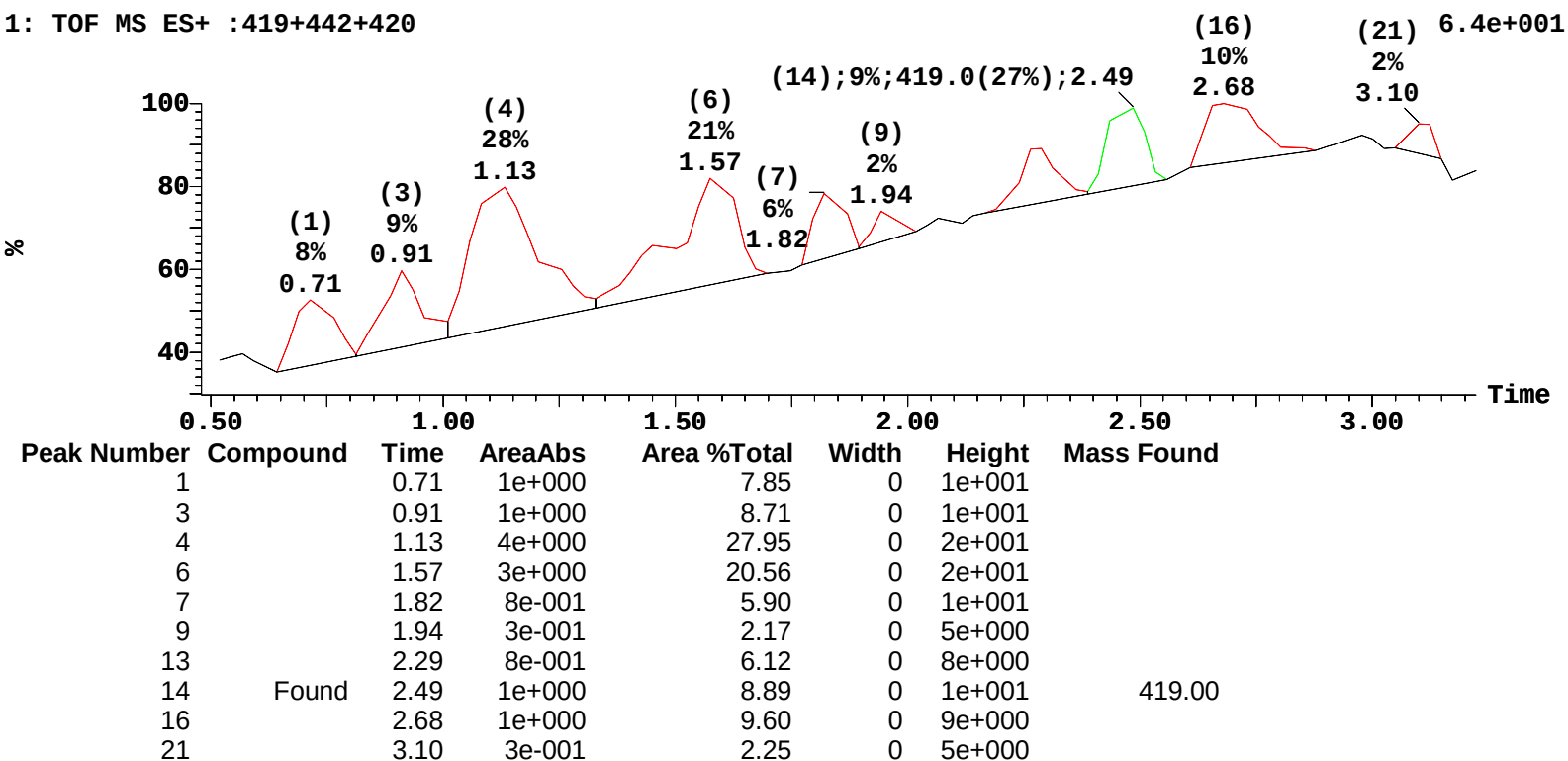
Sample Report:

Sample 18 Vial 1:6 ID File MS44577 Date 12-Mar-2018 Time 10:23:21 Description J.SHEN JSS 5R

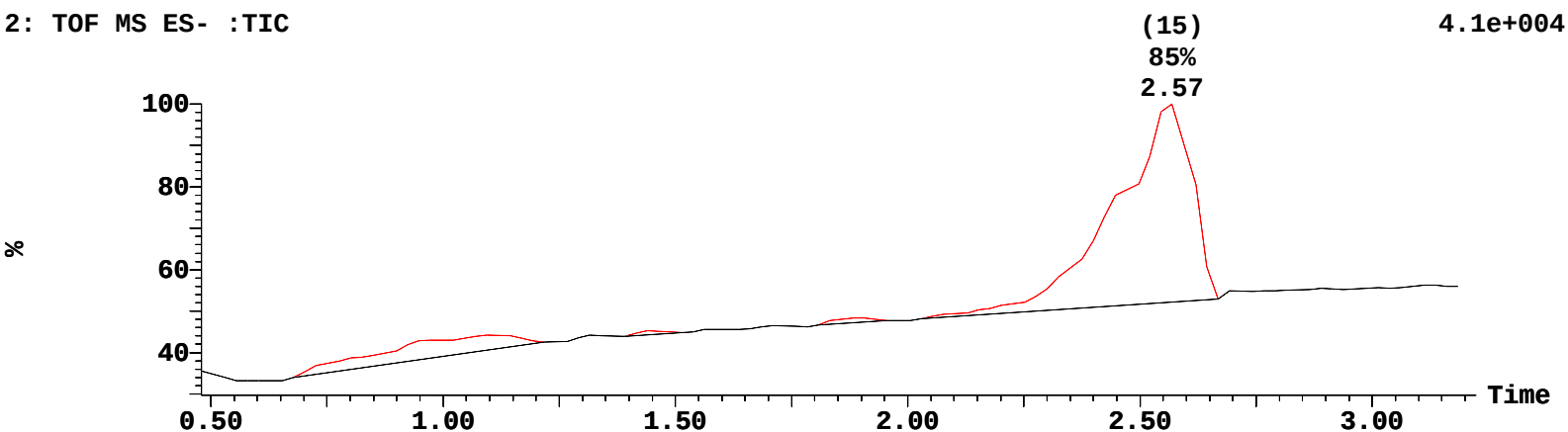
1: TOF MS ES+ :TIC



1: TOF MS ES+ :419+442+420



2: TOF MS ES- :TIC



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ID:
Time:10:23:21

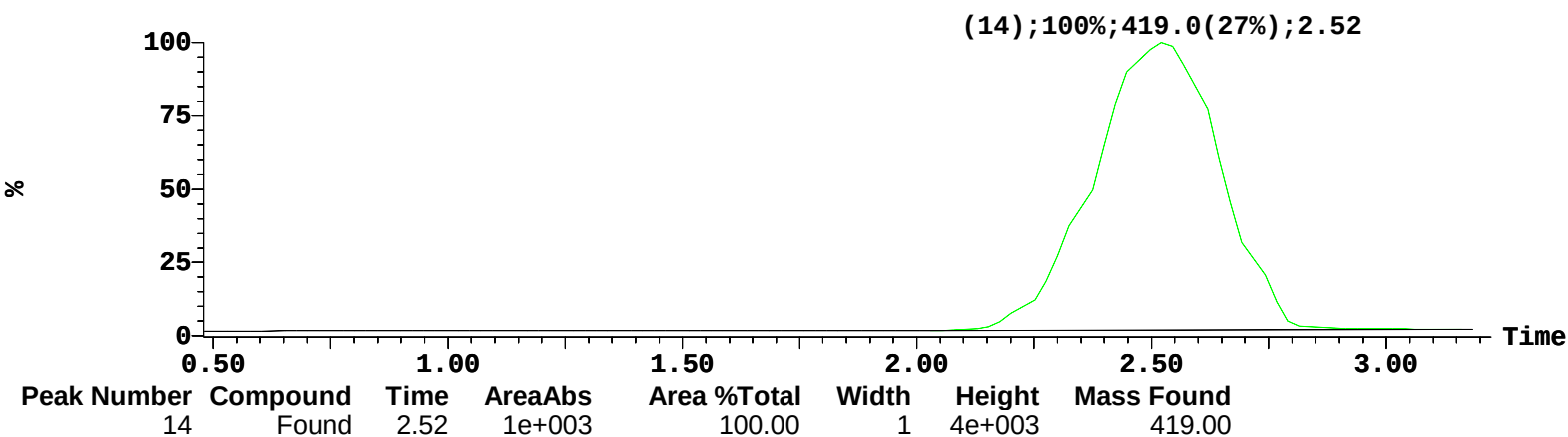
Printed: Mon Mar 12 13:36:24 2018

Sample Report (continued):

Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
4		1.09	6e+002	13.91	1	2e+003	
5		1.44	3e+001	0.56	0	4e+002	
8		1.88	4e+001	0.97	0	5e+002	
15		2.57	4e+003	84.56	1	2e+004	

2: TOF MS ES- :419+464+418

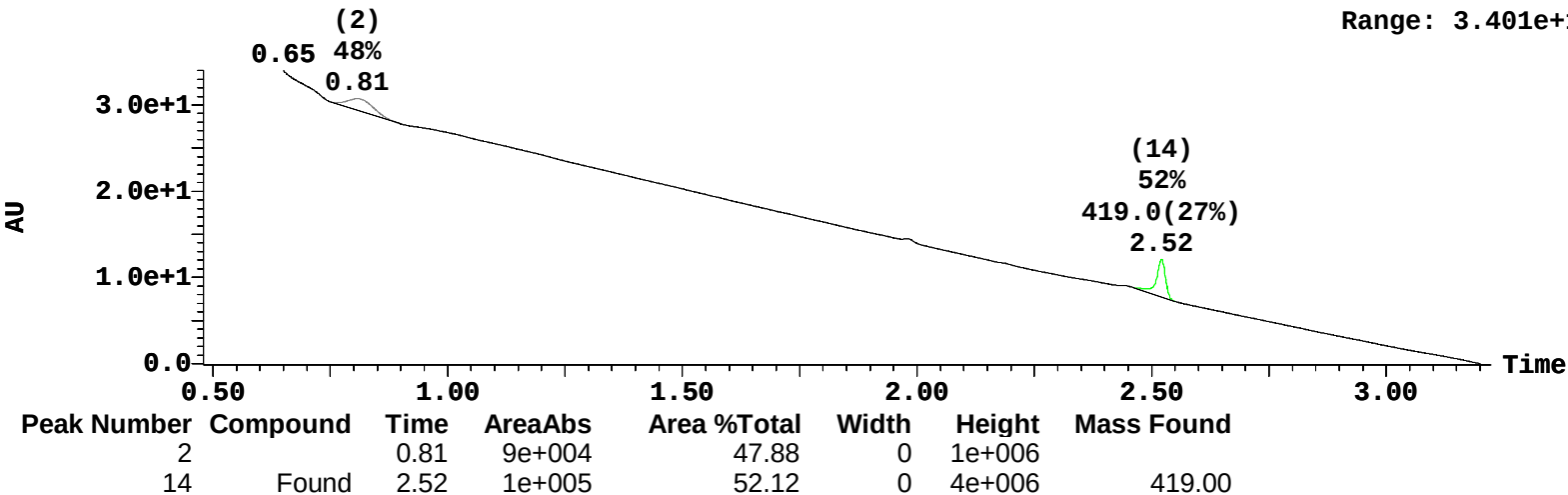
4.1e+003



5: UV Detector: TIC

3.401e+1

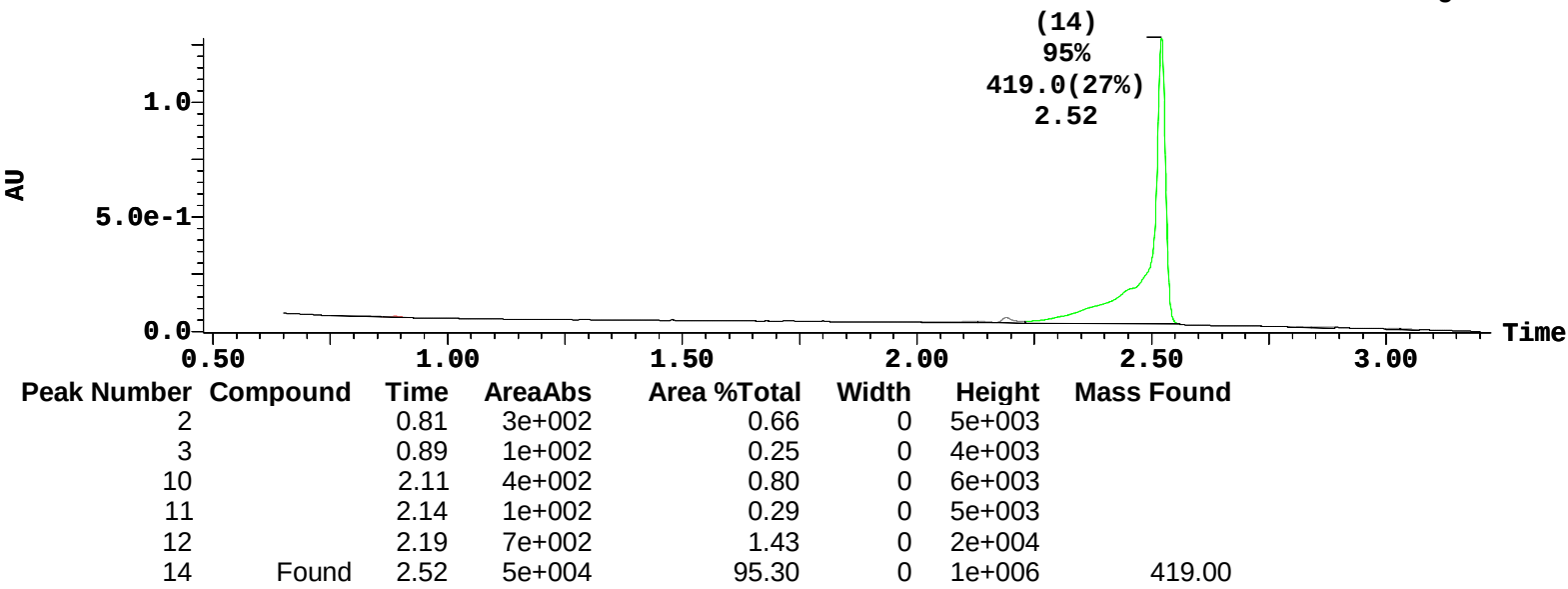
Range: 3.401e+1



5: UV Detector: 244_264

1.279

Range: 1.279



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Sample Report (continued):

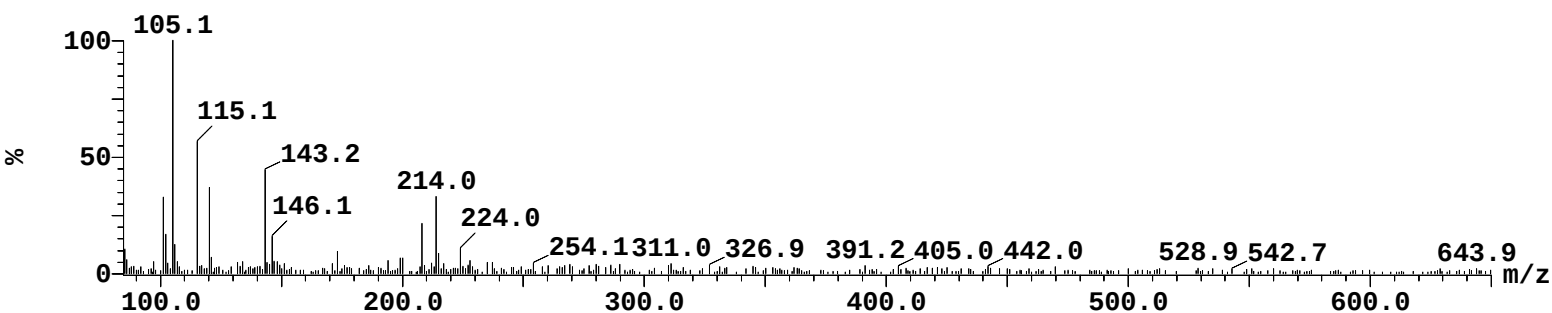
18	2.82	2e+002	0.29	0	4e+003
19	2.88	2e+002	0.37	0	6e+003
20	3.02	2e+002	0.34	0	6e+003
20	3.03	1e+002	0.28	0	5e+003

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

1		0.71	
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1: (Time: 0.71)

9.2e+002

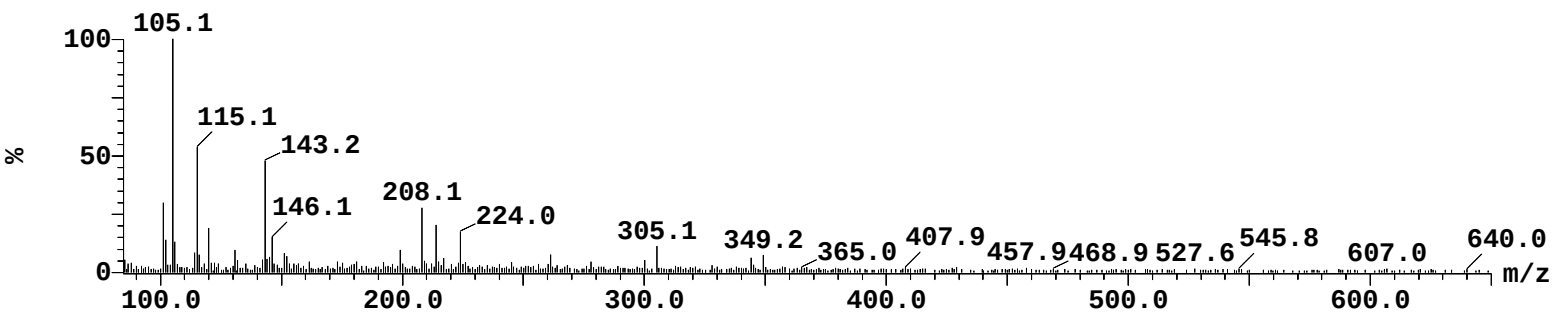


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

3		0.91	
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3: (Time: 0.91)

2.4e+003

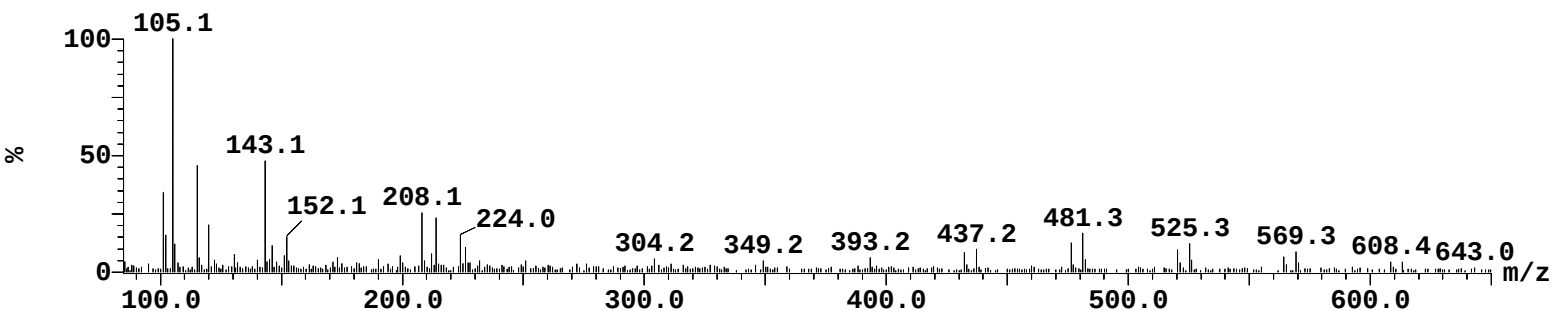


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

4		1.13	
---	--	------	--

4: (Time: 1.13)

1.6e+003



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File: MS44577
Description: J.SHEN JSS 5R

Vial: 1:6
Date: 12-Mar-2018

ID:
Time: 10:23:21

Printed: Mon Mar 12 13:36:24 2018

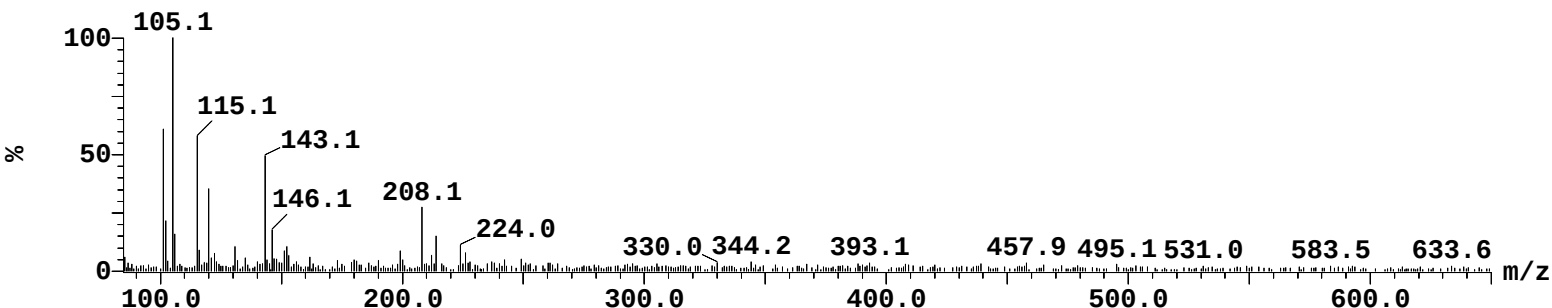
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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6		1.57	
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6: (Time: 1.57)

1.4e+003

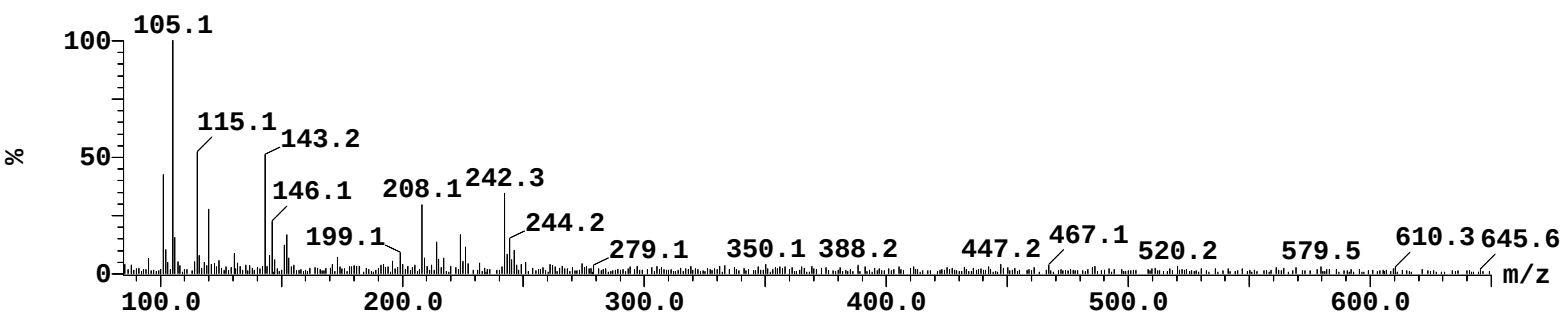


Peak ID	Compound	Time	Mass Found
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7		1.82	
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7: (Time: 1.82)

1.4e+003

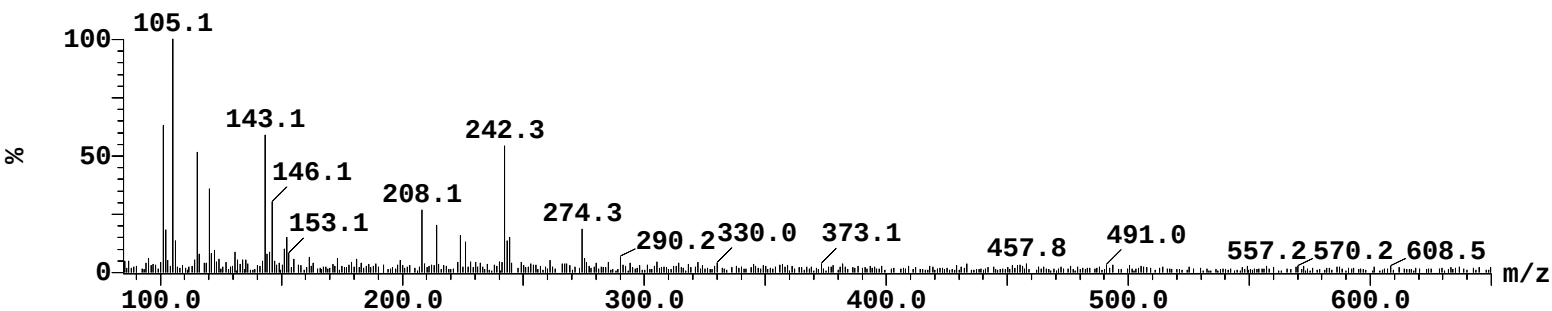


Peak ID	Compound	Time	Mass Found
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9		1.94	
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9: (Time: 1.94)

1.2e+003

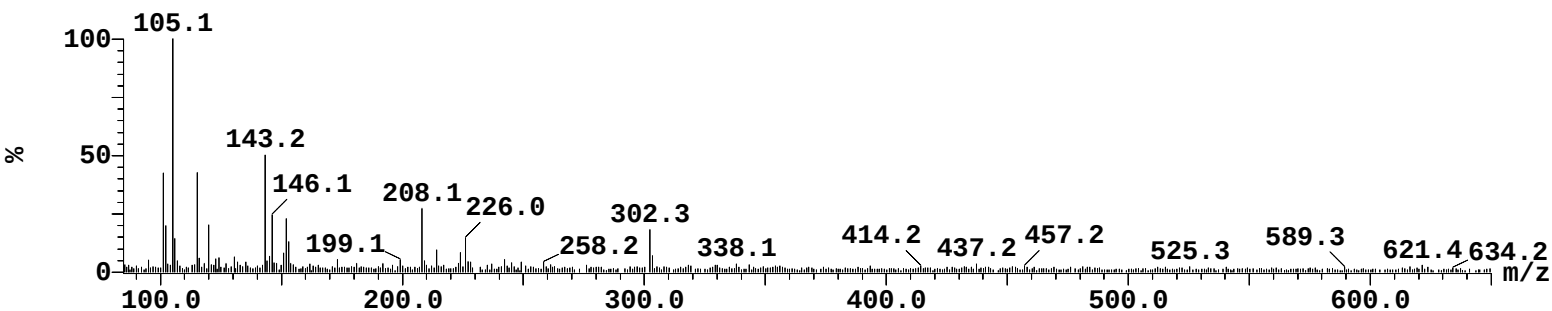


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

13		2.29	
----	--	------	--

13: (Time: 2.29)

3.3e+003



Sample: 18
File: MS44577
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Vial: 1:6
Date: 12-Mar-2018

ID:
Time: 10:23:21

Printed: Mon Mar 12 13:36:24 2018

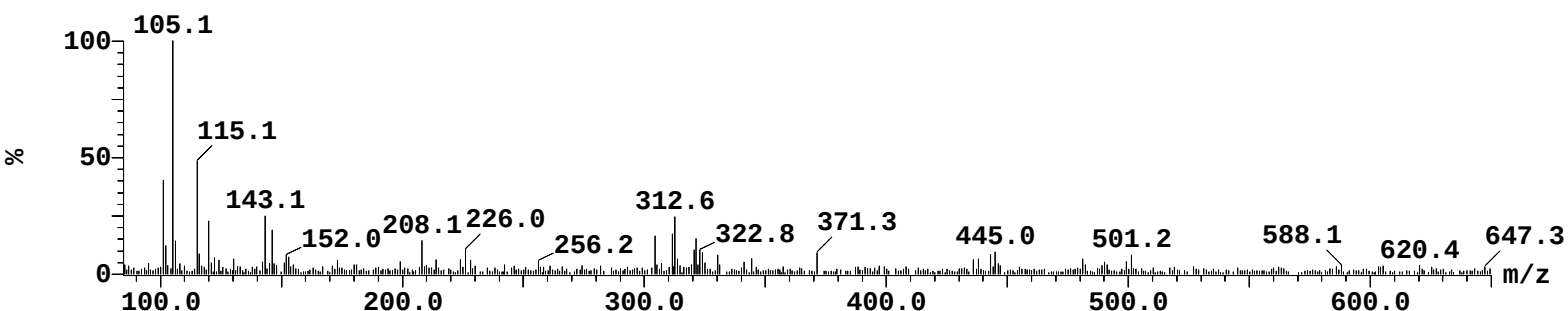
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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14		2.49	
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14: (Time: 2.49)

1.9e+003

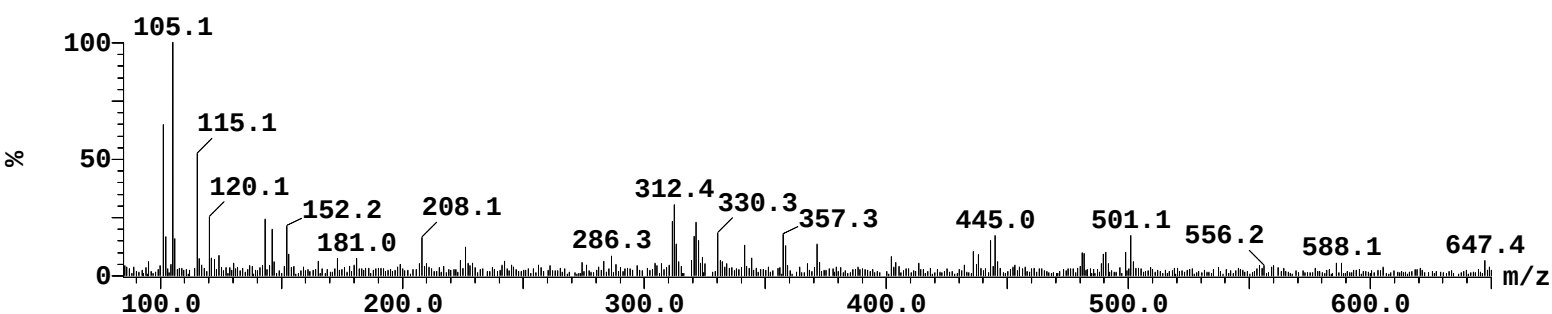


Peak ID	Compound	Time	Mass Found
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15		2.56	
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15: (Time: 2.56)

1.7e+003

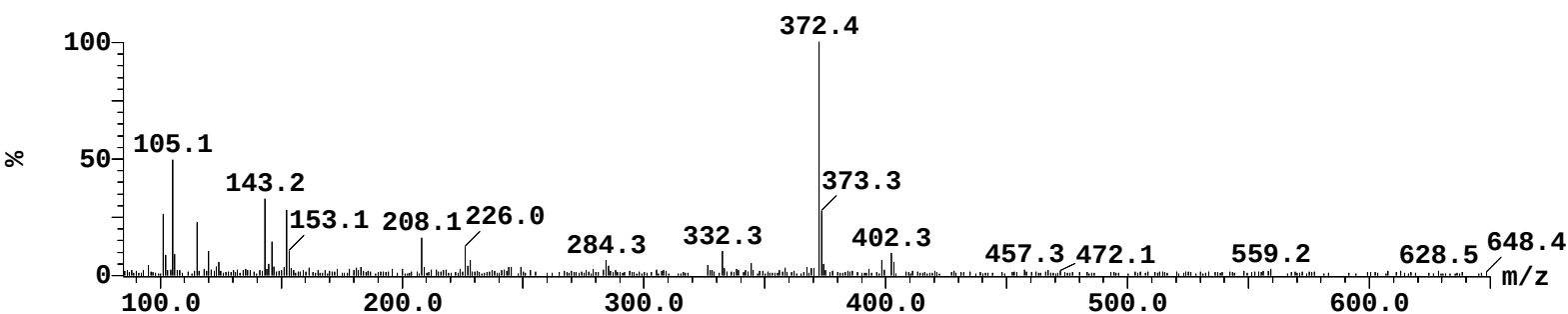


Peak ID	Compound	Time	Mass Found
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16		2.68	
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16: (Time: 2.68)

2.7e+003

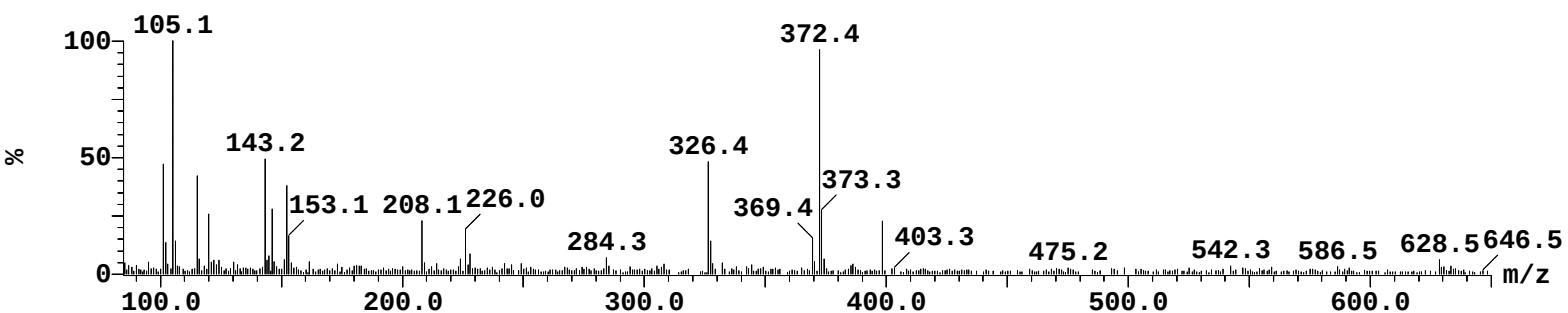


Peak ID	Compound	Time	Mass Found
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17		2.75	
----	--	------	--

17: (Time: 2.75)

3.3e+003



Sample: 18
File: MS44577
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Vial: 1:6
Date: 12-Mar-2018

ID:
Time: 10:23:21

Printed: Mon Mar 12 13:36:24 2018

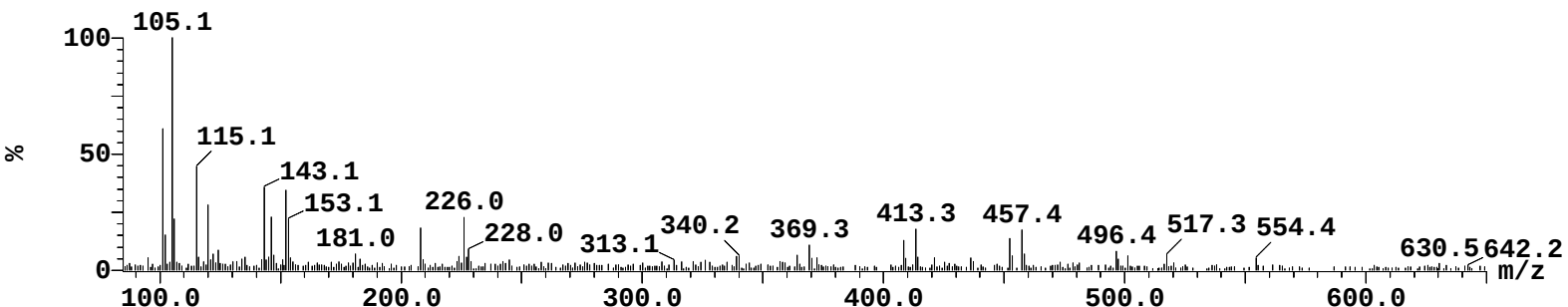
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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21		3.10	
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21: (Time: 3.10)

1.6e+003

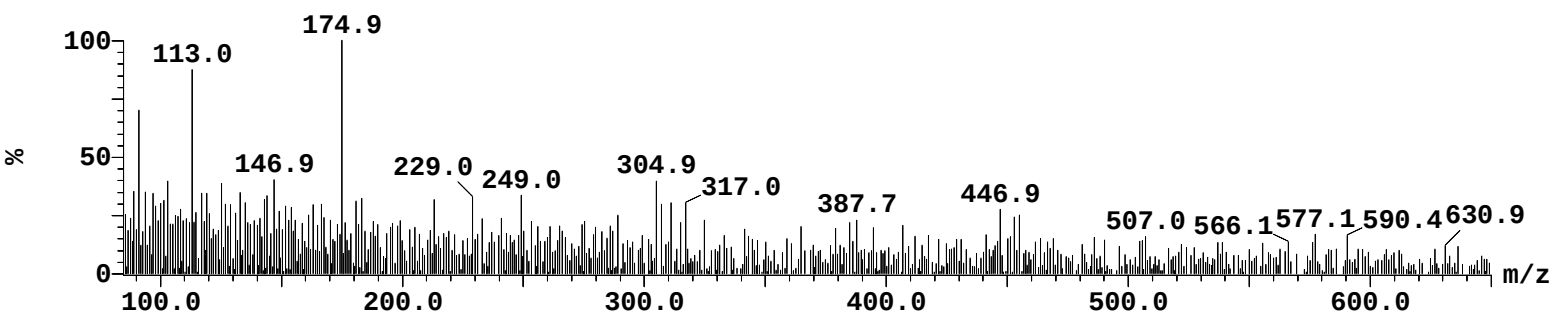


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

4		1.13	
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4: (Time: 1.09)

3.2e+002

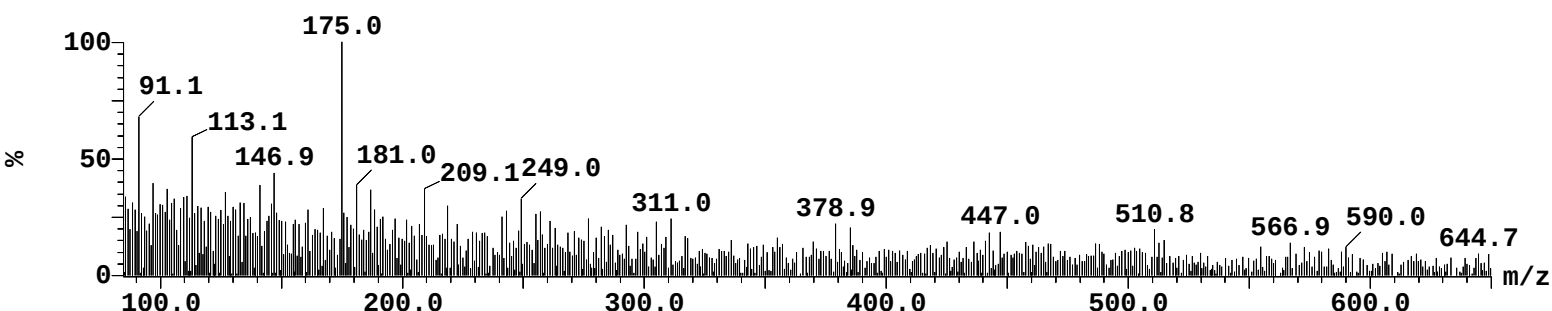


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

5		1.44	
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5: (Time: 1.44)

5.6e+002

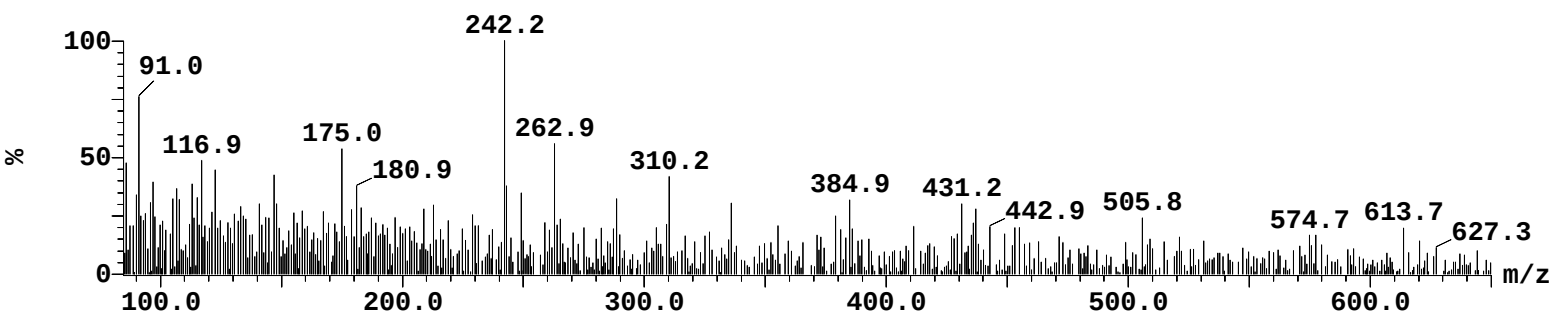


Peak ID	Compound	Time	Mass Found
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8		1.88	
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8: (Time: 1.88)

3.3e+002



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Date:12-Mar-2018

ID:
Time:10:23:21

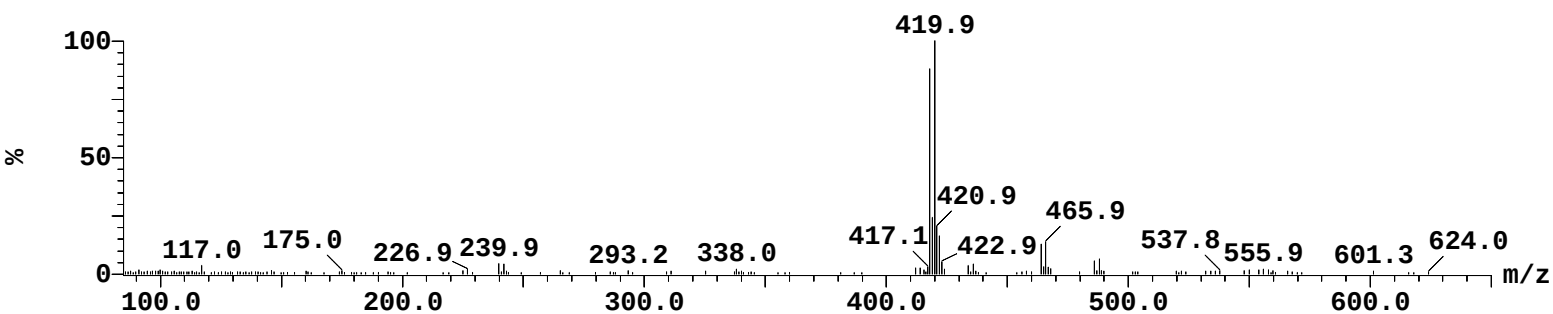
Printed: Mon Mar 12 13:36:24 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
14	Found	2.49	419.00

14: (Time: 2.52)

2.2e+004



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