

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

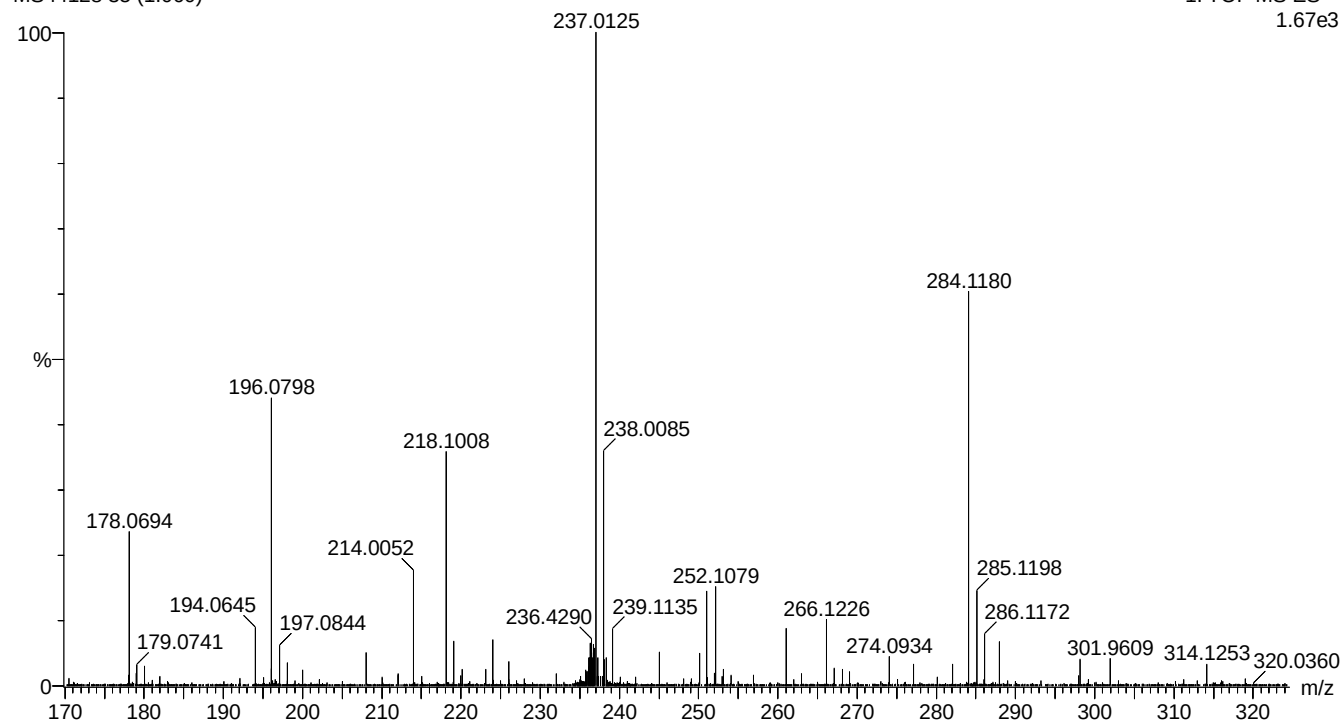
123 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 10-10 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 S: 1-1

J.SHEN JSS3

MS44128 35 (1.060)

1: TOF MS ES+
1.67e3

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
196.0798	196.0796	0.2	1.0	4.5	3.1	C10 H14 N O S

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Sample: 5
File:MS44128
Description:J.SHEN JSS3

Vial:1:19
Date:26-Feb-2018

ID:
Time:10:07:39

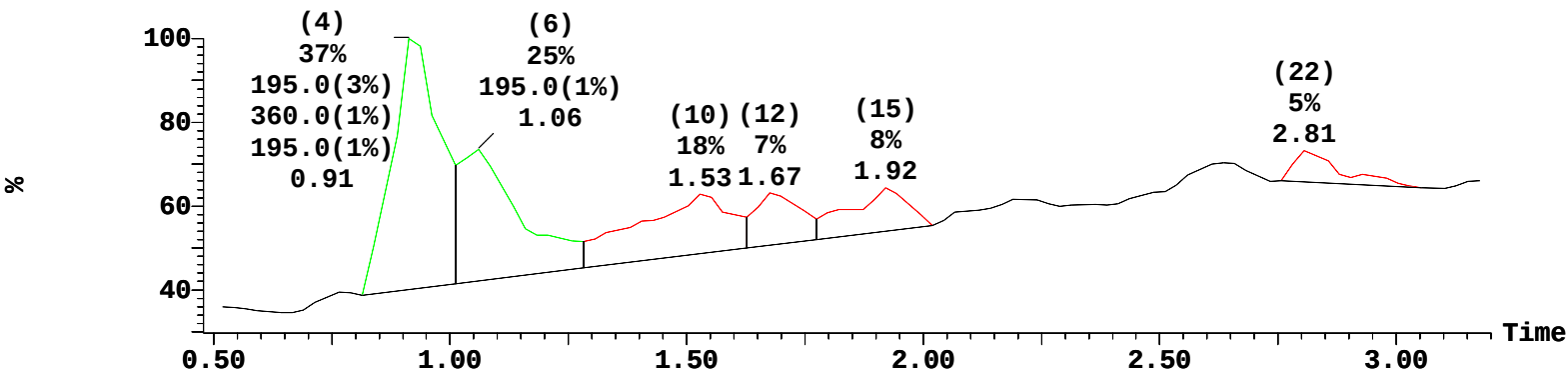
Printed: Mon Feb 26 11:10:17 2018

Sample Report:

Sample 5 Vial 1:19 ID File MS44128 Date 26-Feb-2018 Time 10:07:39 Description J.SHEN JSS3

1: TOF MS ES+ :TIC

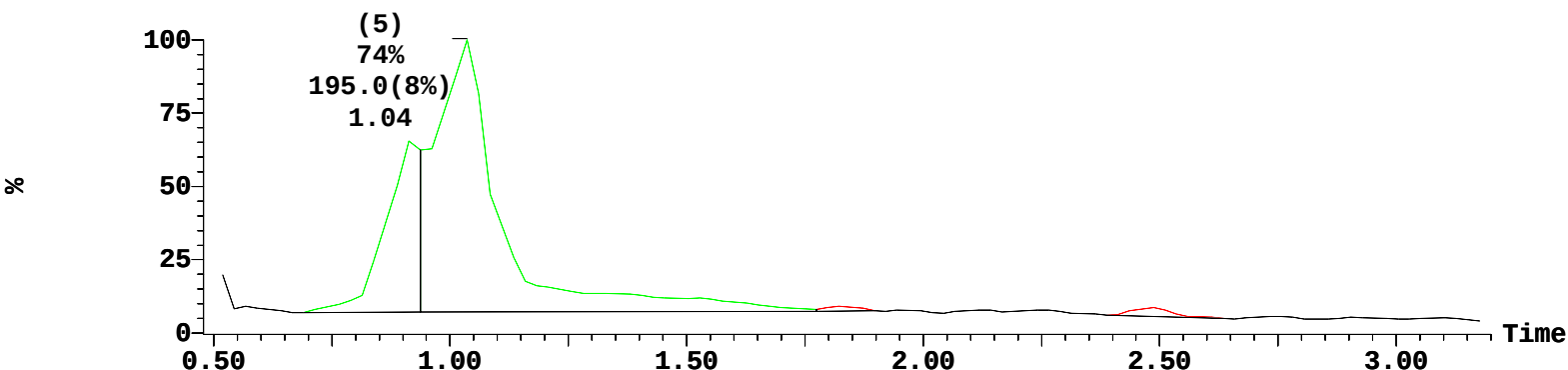
4.1e+004



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
4	Tentative	0.91	3e+003	37.19	0	2e+004	195.00, 360.00
6	Tentative	1.06	2e+003	24.84	0	1e+004	195.00
10		1.53	1e+003	17.77	0	6e+003	
12		1.67	6e+002	7.38	0	5e+003	
15		1.92	6e+002	8.20	0	4e+003	
22		2.81	4e+002	4.62	0	3e+003	

1: TOF MS ES+ :195+218+196

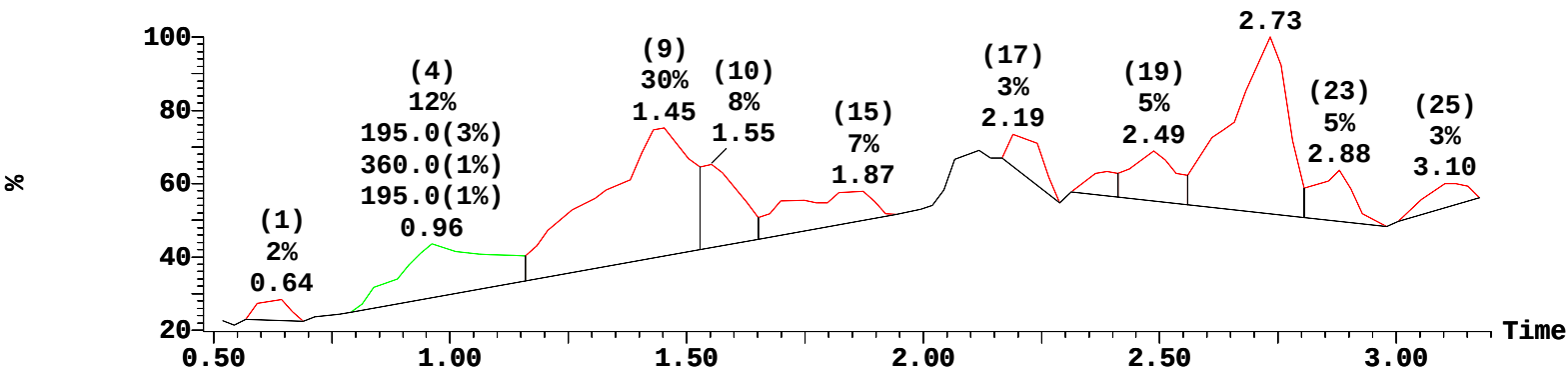
2.0e+003



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
4	Tentative	0.91	9e+001	23.43	0	1e+003	195.00, 360.00
5	Tentative	1.04	3e+002	74.35	1	2e+003	195.00
14		1.82	3e+000	0.66	0	3e+001	
19		2.49	6e+000	1.55	0	6e+001	

1: TOF MS ES+ :360+383+361

1.1e+002



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.64	5e-001	1.63	0	6e+000	
4	Tentative	0.96	4e+000	11.88	0	2e+001	195.00, 360.00

Sample: 5

Vial:1:19

ID:

File:MS44128

Date:26-Feb-2018

Time:10:07:39

Description:J.SHEN JSS3

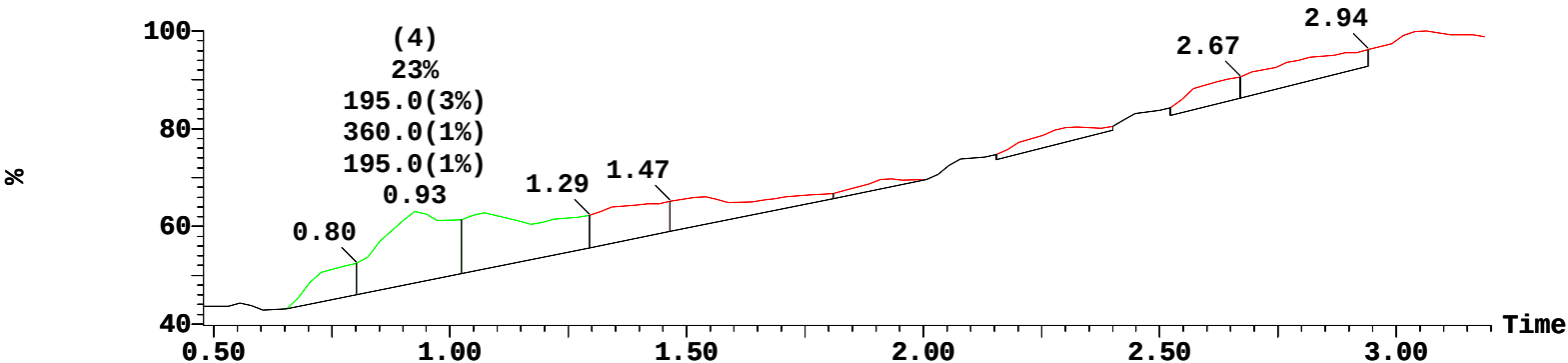
Printed: Mon Feb 26 11:10:17 2018

Sample Report (continued):

9	1.45	9e+000	29.70	0	4e+001
10	1.55	2e+000	7.52	0	3e+001
15	1.87	2e+000	7.29	0	9e+000
17	2.19	1e+000	3.22	0	1e+001
18	2.39	5e-001	1.67	0	7e+000
19	2.49	2e+000	5.40	0	2e+001
21	2.73	7e+000	24.51	0	5e+001
23	2.88	1e+000	4.68	0	2e+001
25	3.10	8e-001	2.51	0	7e+000

2: TOF MS ES- :TIC

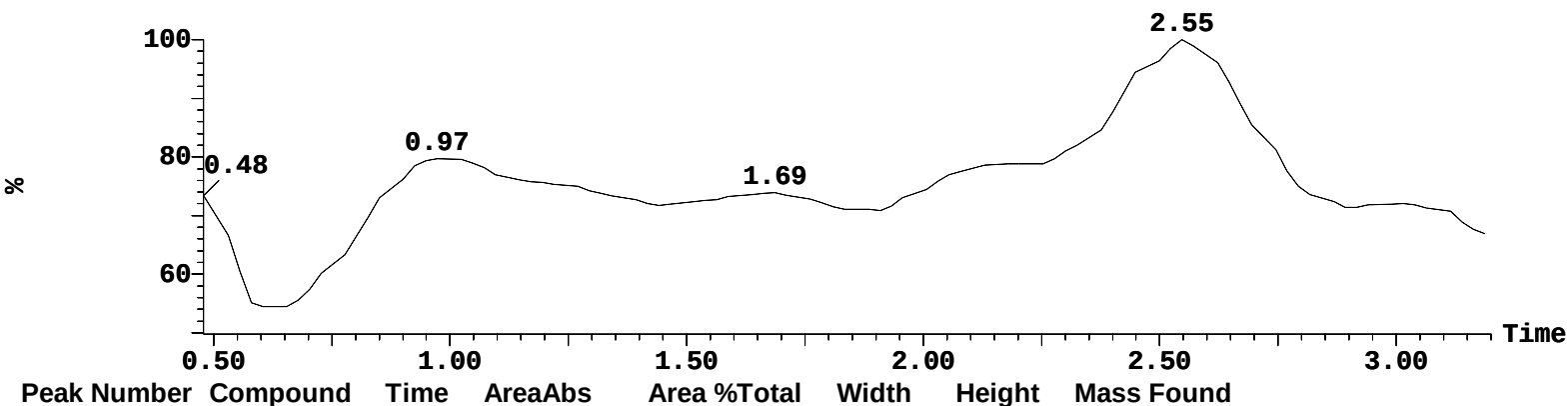
3.1e+004



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2	Tentative	0.80	2e+002	6.23	0	2e+003	195.00, 360.00
4	Tentative	0.92	8e+002	22.65	0	5e+003	195.00, 360.00
6	Tentative	1.07	7e+002	21.06	0	4e+003	195.00
9		1.47	4e+002	10.44	0	2e+003	
13		1.81	4e+002	10.50	0	3e+002	
16		1.93	7e+001	2.12	0	5e+002	
18		2.40	2e+002	4.64	0	2e+002	
20		2.67	2e+002	5.25	0	1e+003	
24		2.94	4e+002	10.58	0	1e+003	
25		3.06	2e+002	6.52	0	1e+003	

2: TOF MS ES- :195+240+194

1.8e+002



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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Sample: 5
File:MS44128
Description:J.SHEN JSS3

Vial:1:19
Date:26-Feb-2018

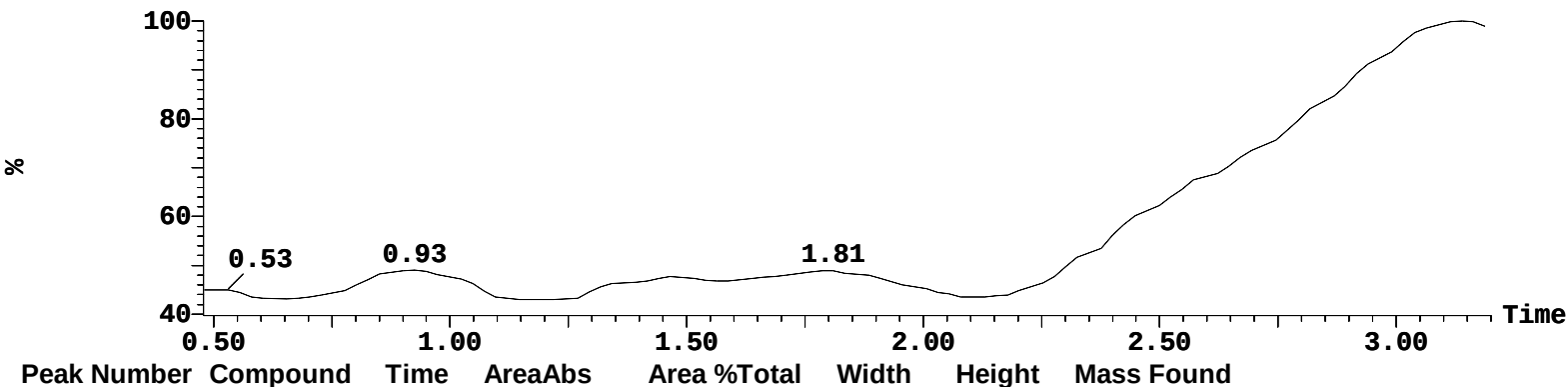
ID:
Time:10:07:39

Printed: Mon Feb 26 11:10:17 2018

Sample Report (continued):

2: TOF MS ES- :360+405+359

1.6e+002

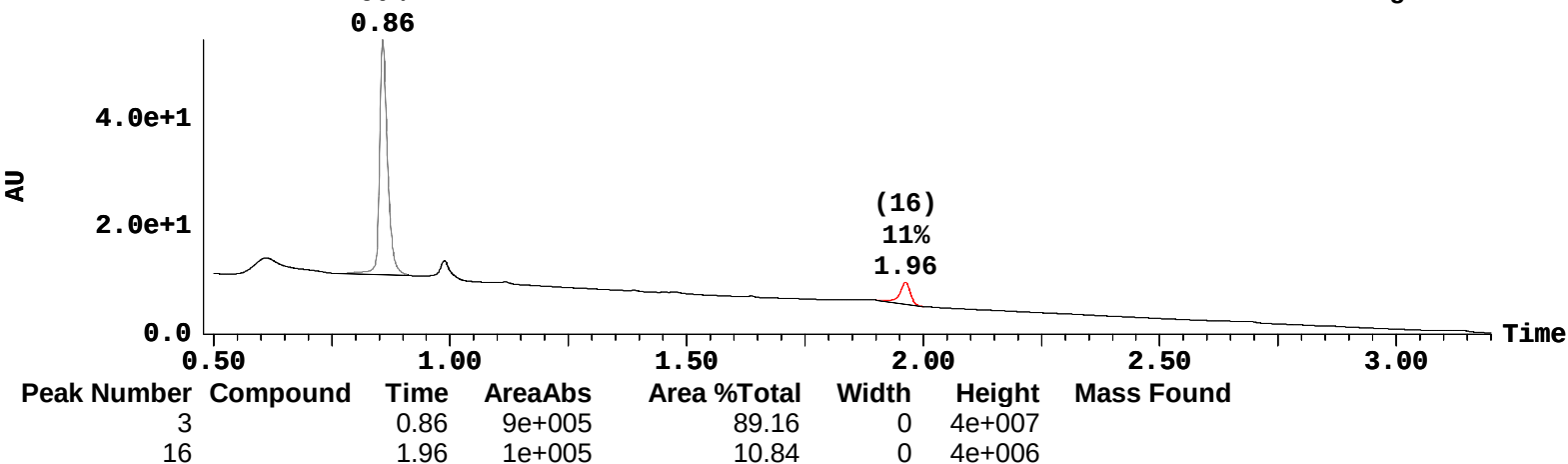


5: UV Detector: TIC

(3)

5.454e+1

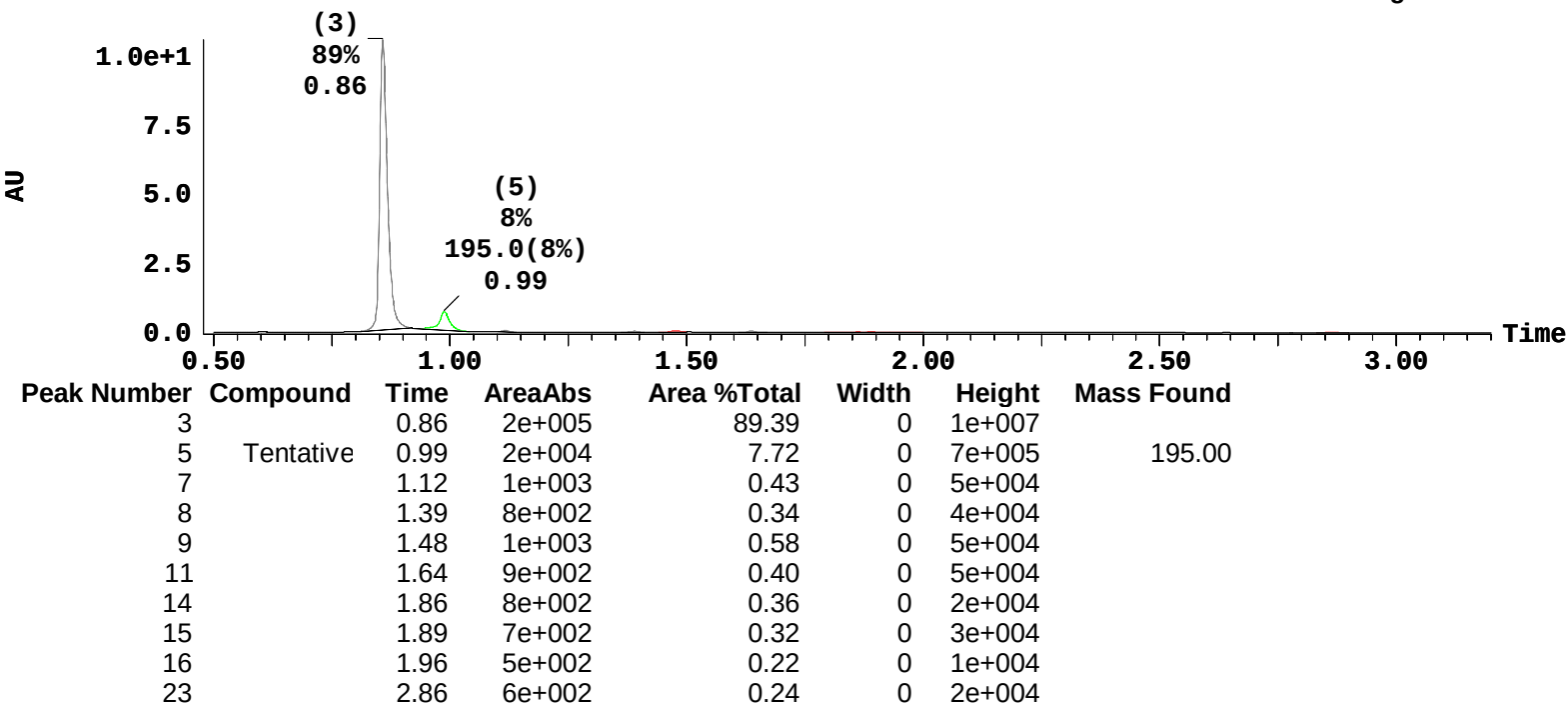
Range: 5.454e+1



5: UV Detector: 244_264

1.062e+1

Range: 1.062e+1



Sample: 5
File: MS44128
Description: J.SHEN JSS3

Vial: 1:19
Date: 26-Feb-2018

ID:
Time: 10:07:39

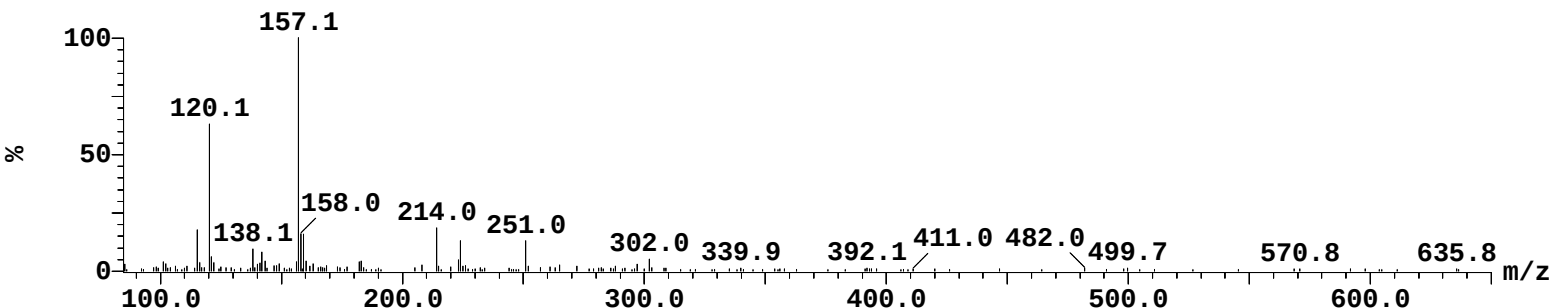
Printed: Mon Feb 26 11:10:17 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
1		0.64	

1: (Time: 0.64)

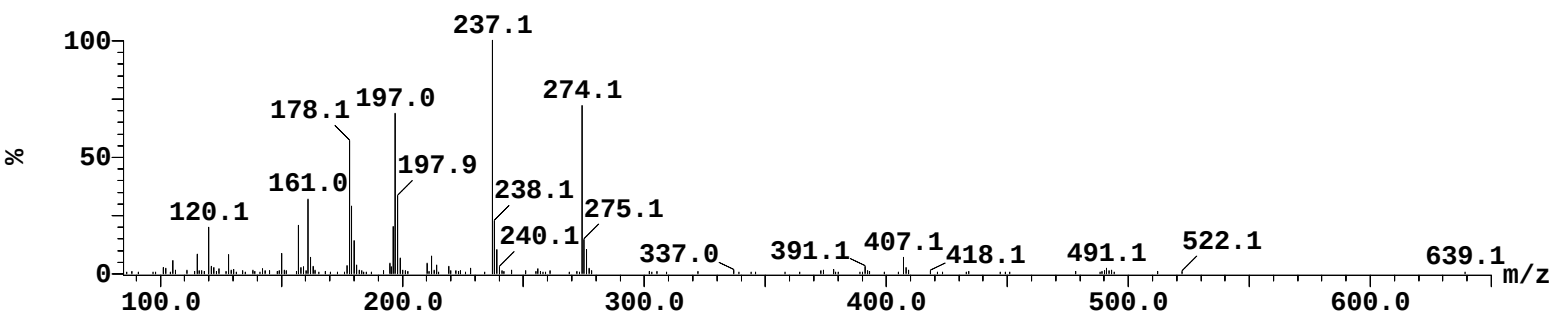
1.7e+003



Peak ID	Compound	Time	Mass Found
4	Tentative	0.91	195.00

4: (Time: 0.91)

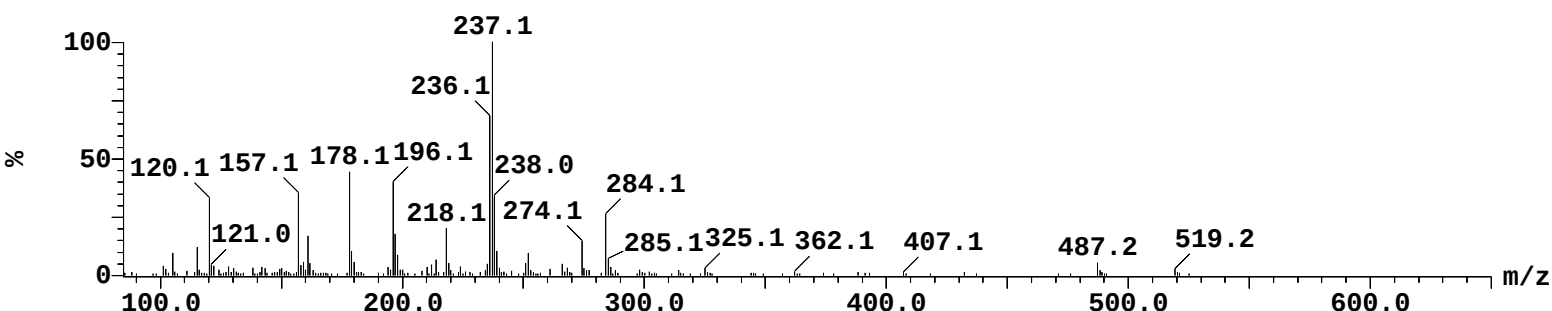
1.3e+004



Peak ID	Compound	Time	Mass Found
5	Tentative	1.04	195.00

5: (Time: 1.04)

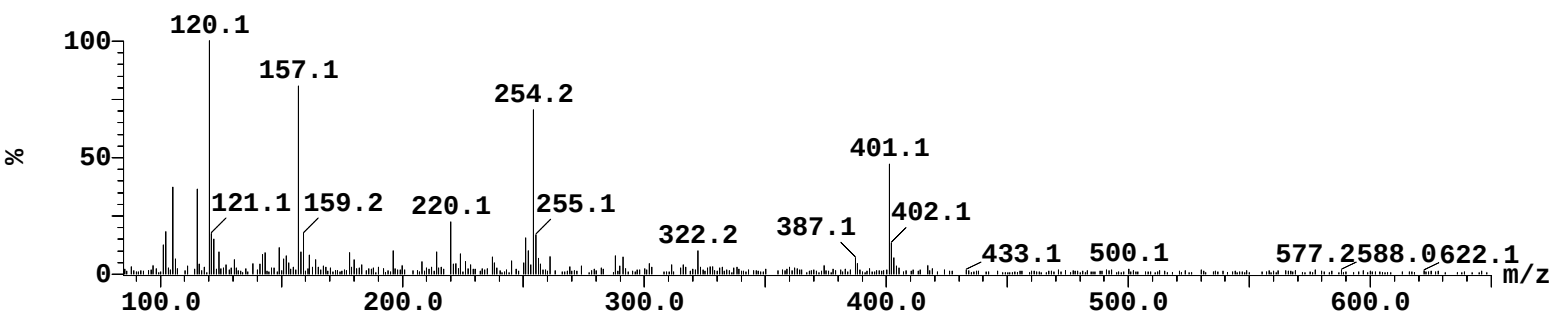
1.0e+004



Peak ID	Compound	Time	Mass Found
9		1.45	

9: (Time: 1.45)

2.2e+003



Sample: 5
File: MS44128
Description: J.SHEN JSS3

Vial: 1:19
Date: 26-Feb-2018

ID:
Time: 10:07:39

Printed: Mon Feb 26 11:10:17 2018

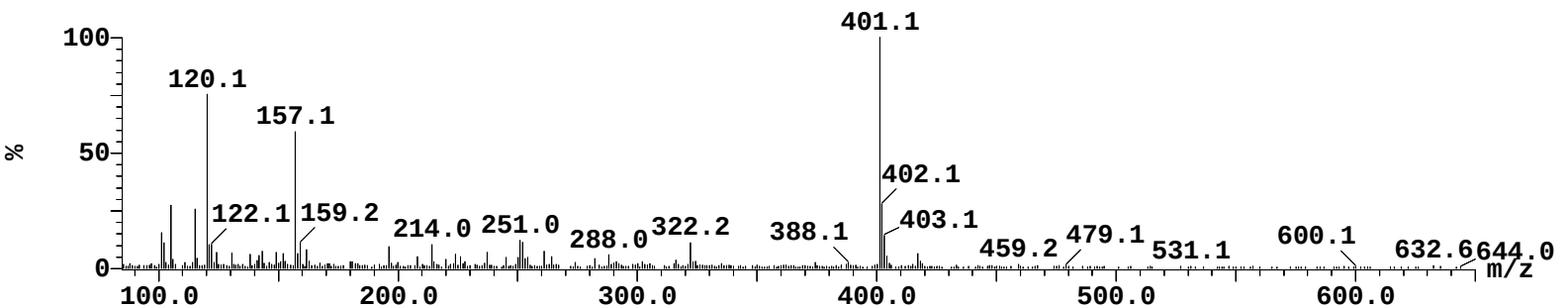
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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10		1.53	
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10: (Time: 1.53)

5.0e+003

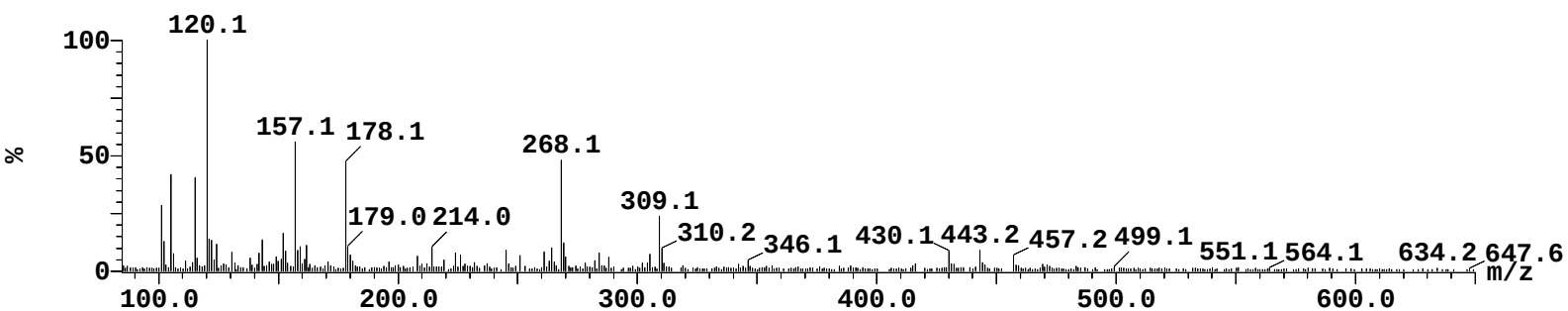


Peak ID	Compound	Time	Mass Found
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12		1.67	
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12: (Time: 1.67)

4.2e+003

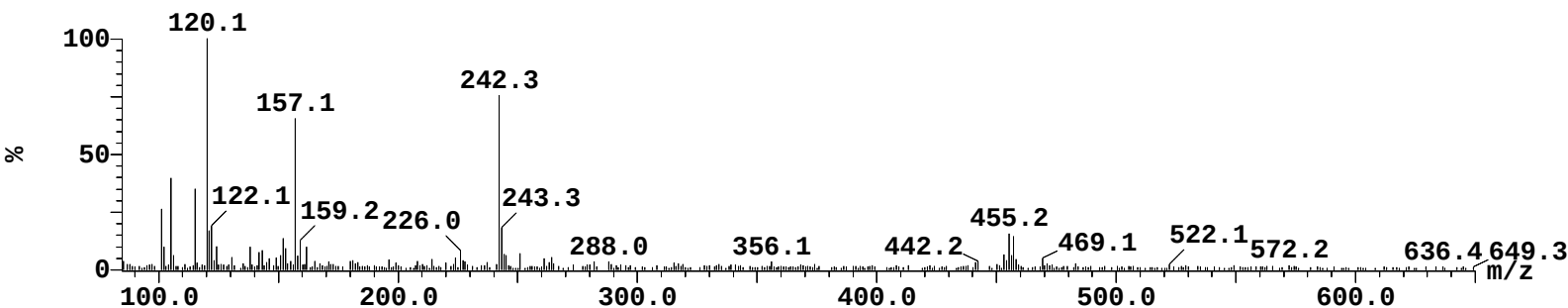


Peak ID	Compound	Time	Mass Found
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14		1.82	
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14: (Time: 1.82)

2.4e+003

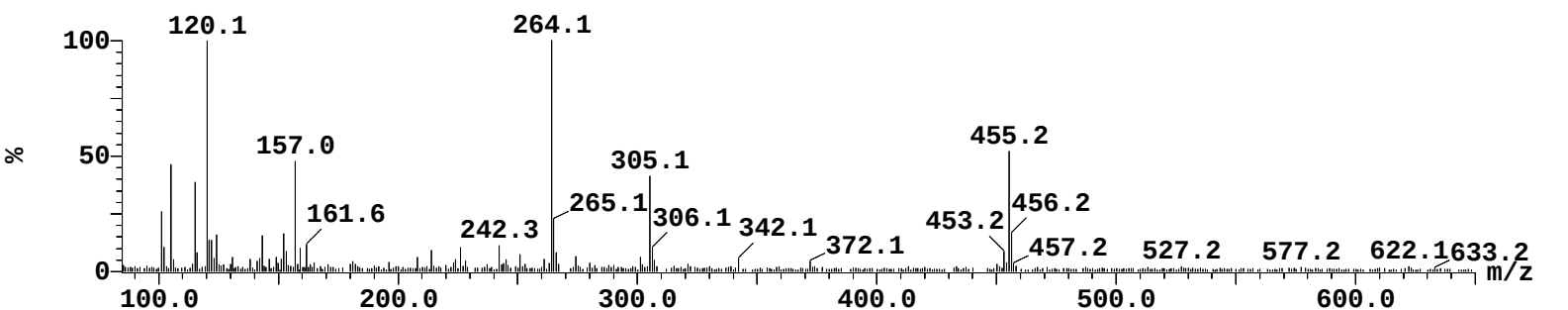


Peak ID	Compound	Time	Mass Found
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15		1.92	
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15: (Time: 1.92)

3.9e+003



Sample: 5
File:MS44128
Description:J.SHEN JSS3

Vial:1:19
Date:26-Feb-2018

ID:
Time:10:07:39

Printed: Mon Feb 26 11:10:17 2018

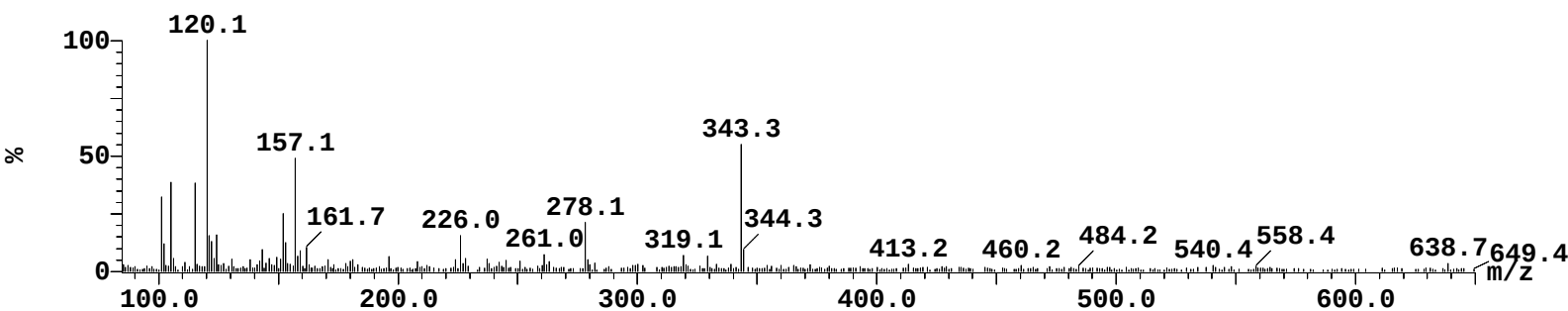
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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17		2.19	
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17: (Time: 2.19)

2.6e+003

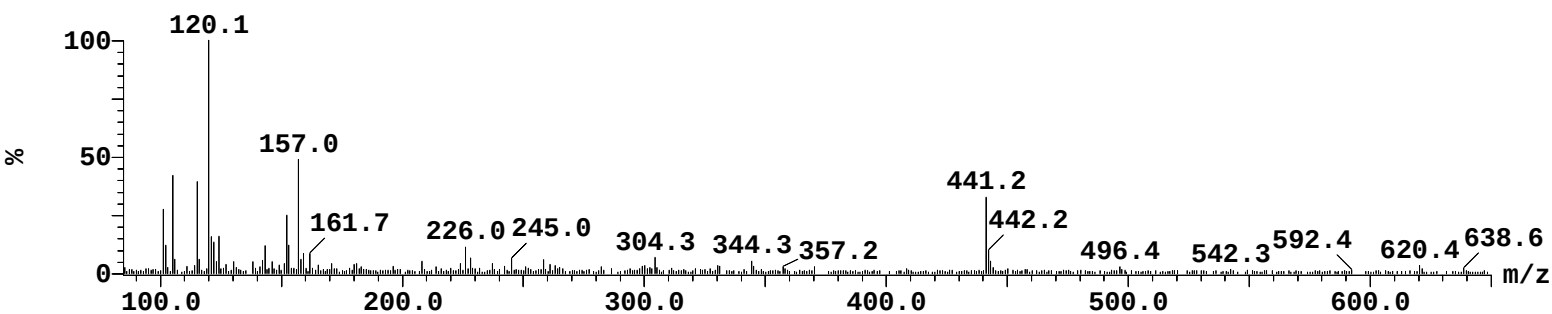


Peak ID	Compound	Time	Mass Found
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18		2.39	
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18: (Time: 2.39)

4.3e+003

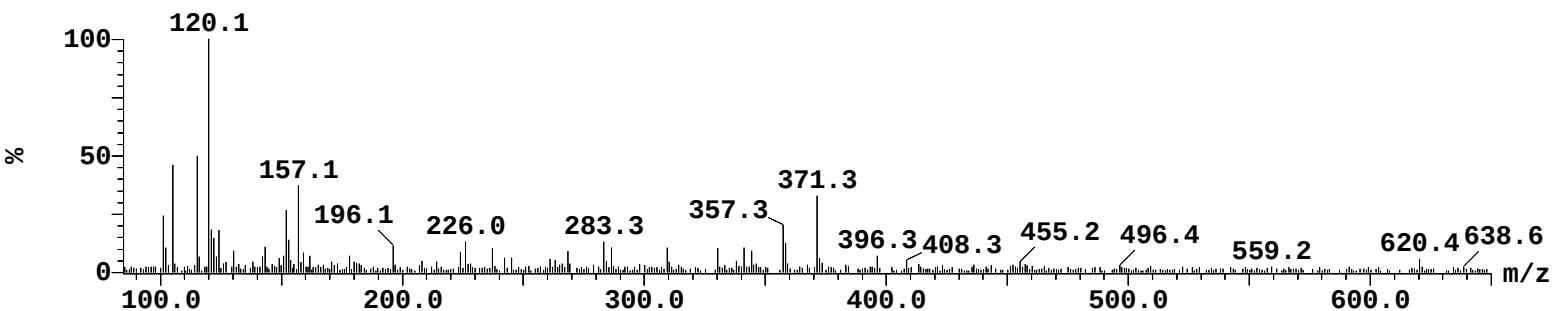


Peak ID	Compound	Time	Mass Found
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19		2.49	
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19: (Time: 2.49)

1.9e+003

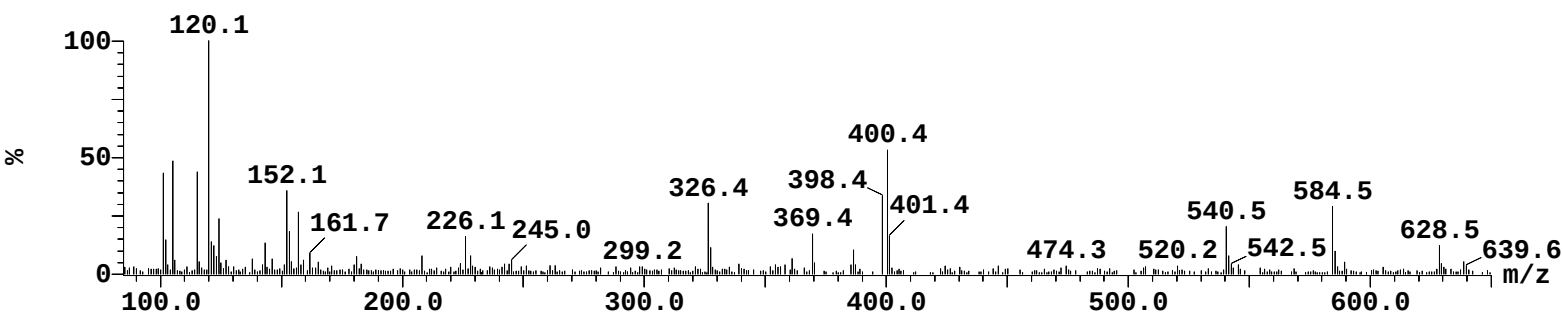


Peak ID	Compound	Time	Mass Found
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21		2.73	
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21: (Time: 2.73)

2.2e+003



Sample: 5
File:MS44128
Description:J.SHEN JSS3

Vial:1:19
Date:26-Feb-2018

ID:
Time:10:07:39

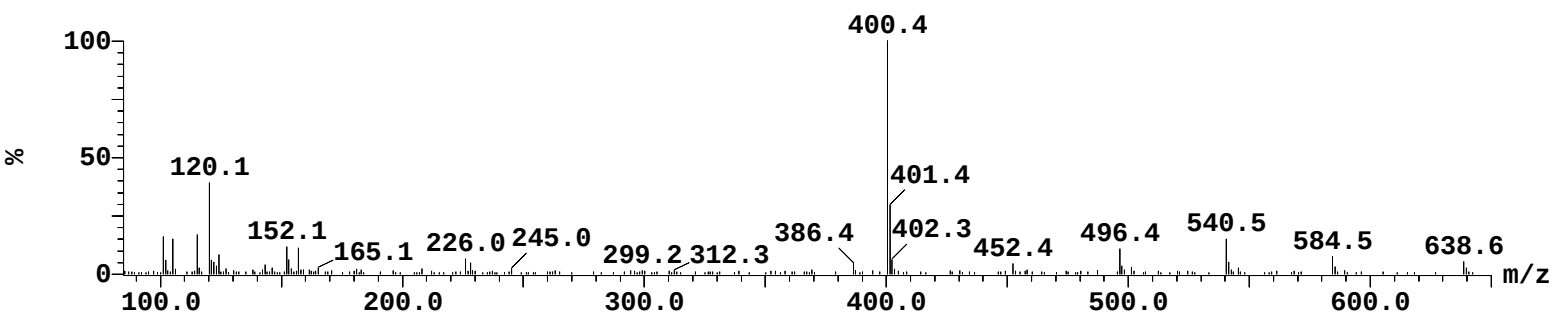
Printed: Mon Feb 26 11:10:17 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
22		2.81	

22: (Time: 2.81)

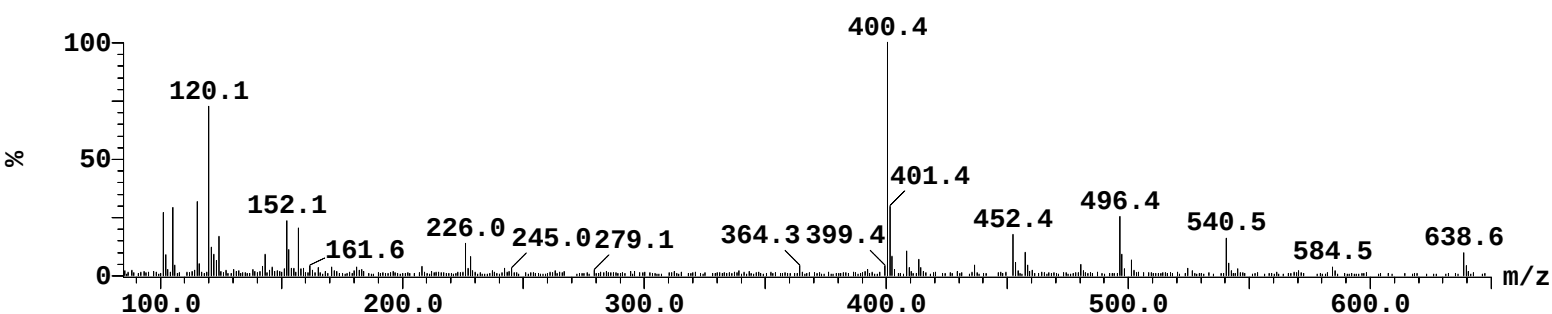
6.2e+003



Peak ID	Compound	Time	Mass Found
23		2.88	

23: (Time: 2.88)

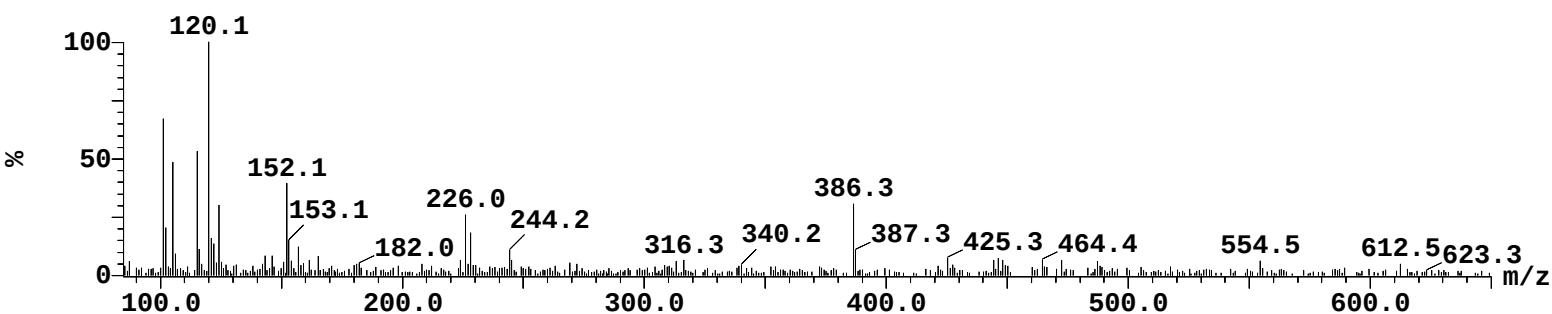
5.7e+003



Peak ID	Compound	Time	Mass Found
25		3.10	

25: (Time: 3.10)

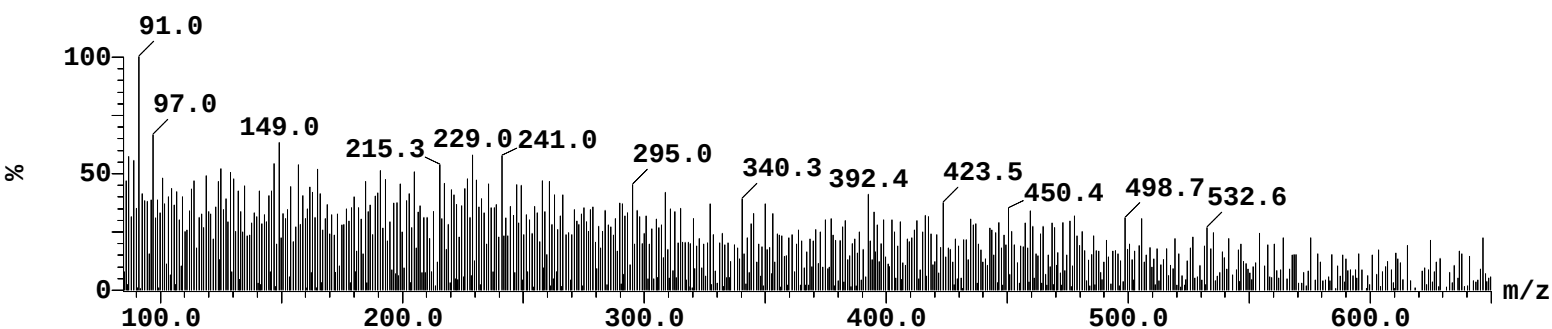
1.8e+003



Peak ID	Compound	Time	Mass Found
2	Tentative	0.80	195.00, 360.00

2: (Time: 0.80)

2.4e+002



Sample: 5
File: MS44128
Description: J.SHEN JSS3

Vial: 1:19
Date: 26-Feb-2018

ID:
Time: 10:07:39

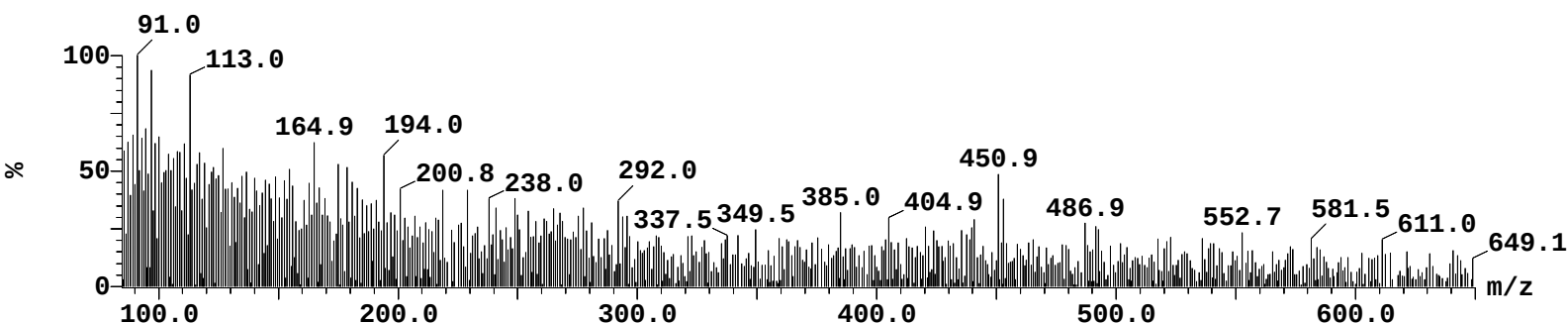
Printed: Mon Feb 26 11:10:17 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
4	Found	0.91	195.00, 360.00

4: (Time: 0.92)

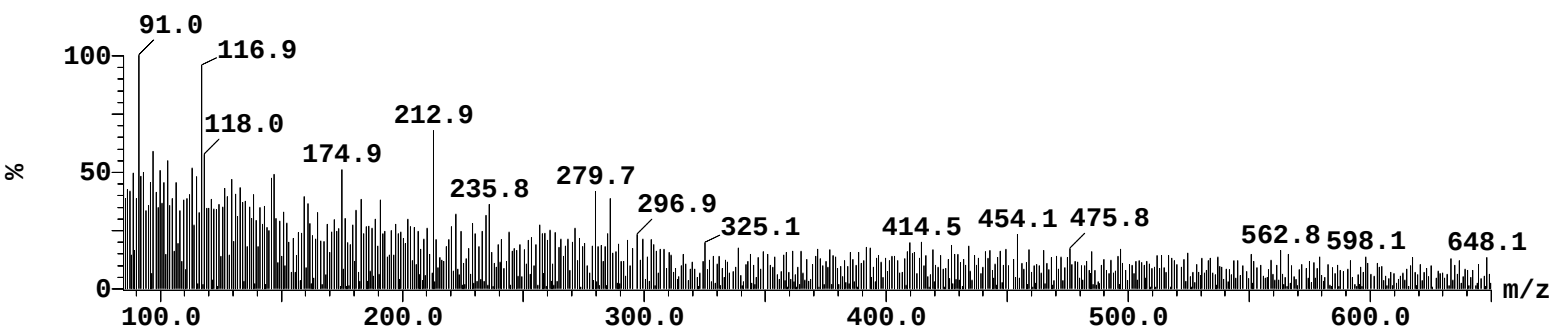
3.6e+002



Peak ID	Compound	Time	Mass Found
6	Tentative	1.06	195.00

6: (Time: 1.07)

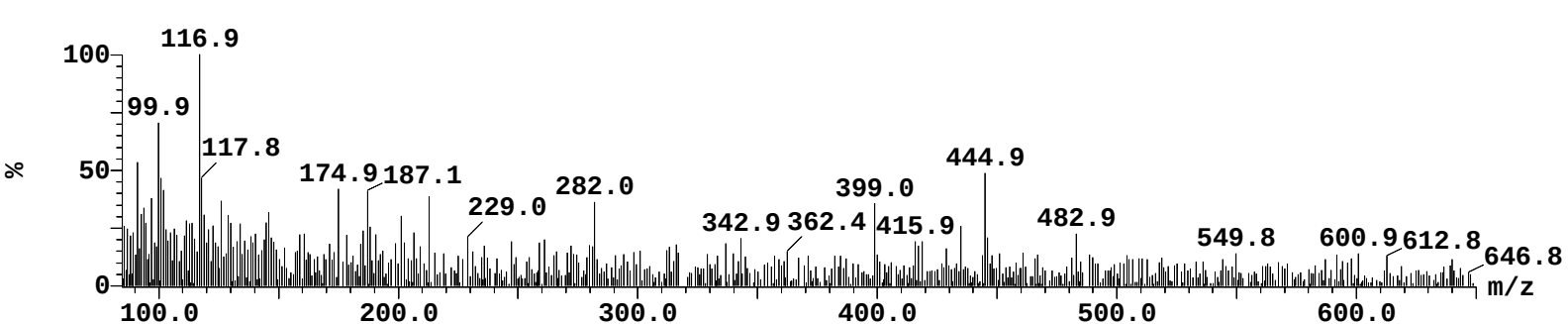
4.4e+002



Peak ID	Compound	Time	Mass Found
9		1.45	

9: (Time: 1.47)

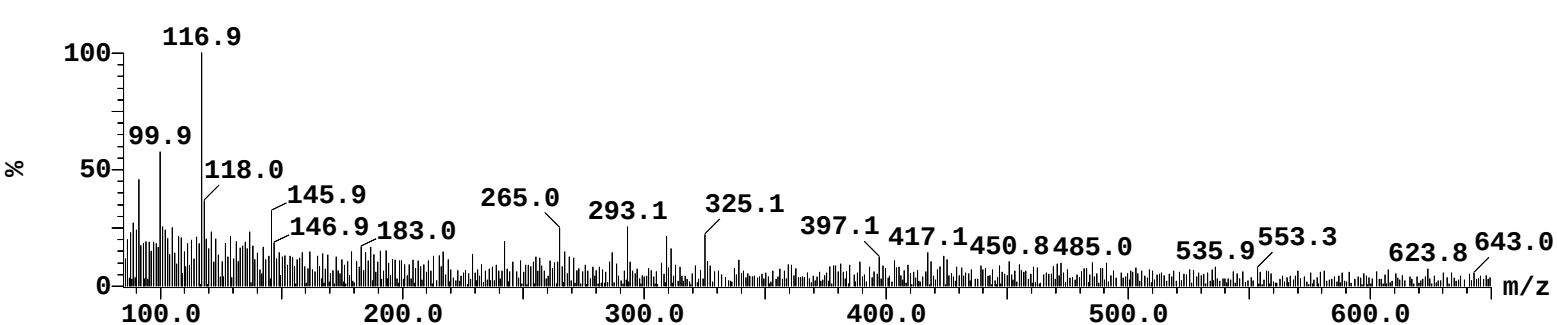
4.1e+002



Peak ID	Compound	Time	Mass Found
13		1.81	

13: (Time: 1.81)

9.9e+002



Sample: 5
File: MS44128
Description: J.SHEN JSS3

Vial: 1:19
Date: 26-Feb-2018

ID:
Time: 10:07:39

Printed: Mon Feb 26 11:10:17 2018

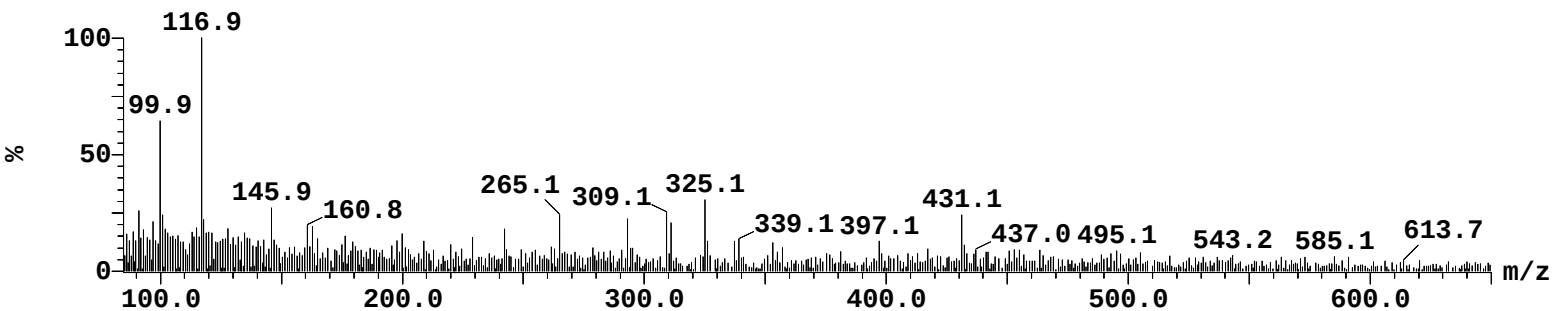
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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16		1.93	
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16: (Time: 1.93)

1.2e+003

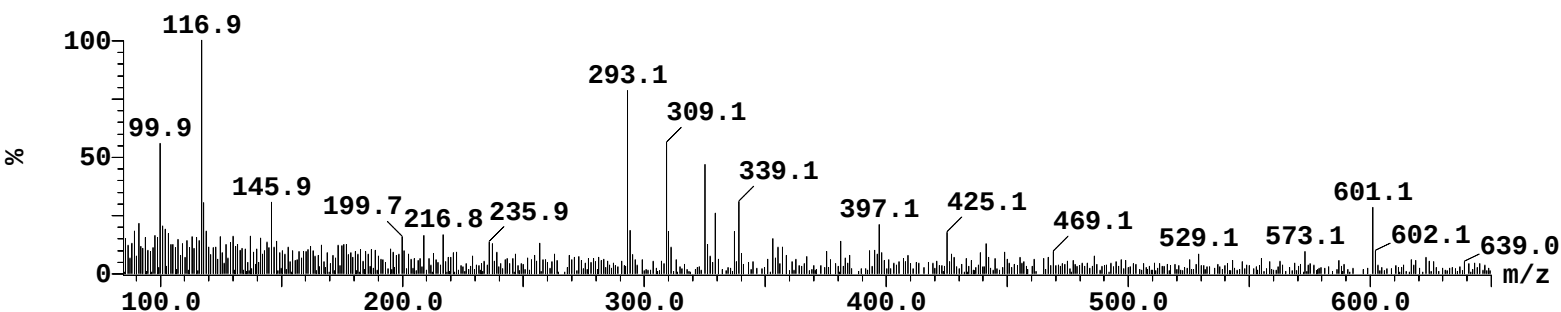


Peak ID	Compound	Time	Mass Found
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18		2.39	
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18: (Time: 2.40)

1.4e+003

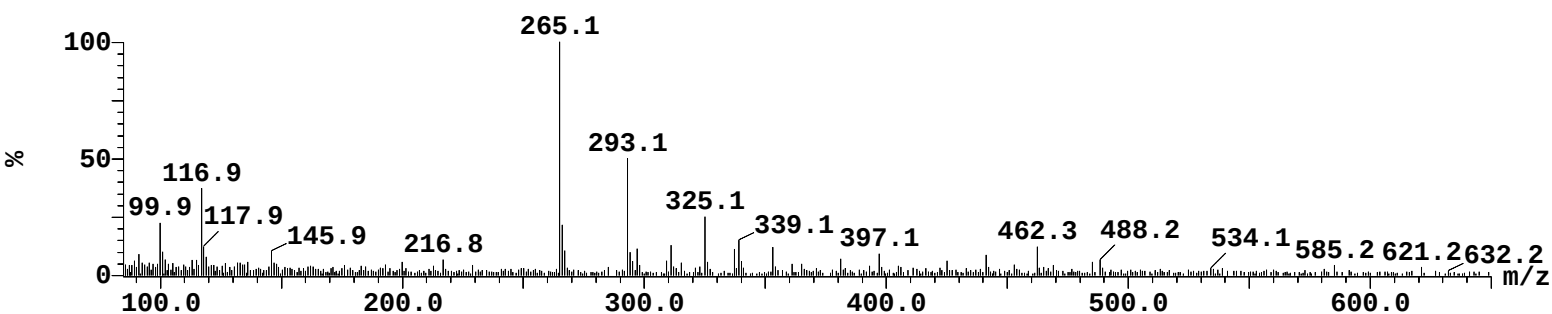


Peak ID	Compound	Time	Mass Found
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20		2.67	
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20: (Time: 2.67)

4.2e+003

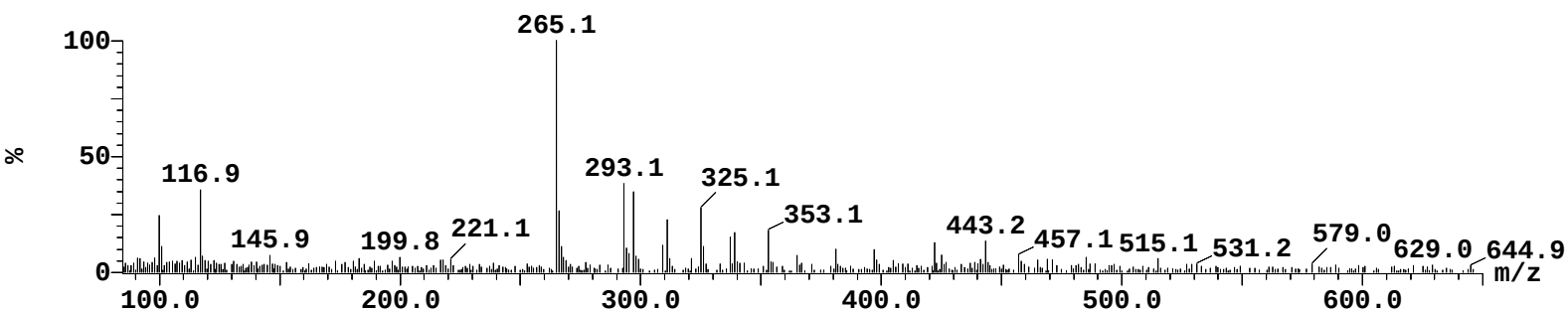


Peak ID	Compound	Time	Mass Found
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24		2.94	
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24: (Time: 2.94)

2.1e+003



Sample: 5

Vial:1:19

ID:

File:MS44128

Date:26-Feb-2018

Time:10:07:39

Description:J.SHEN JSS3

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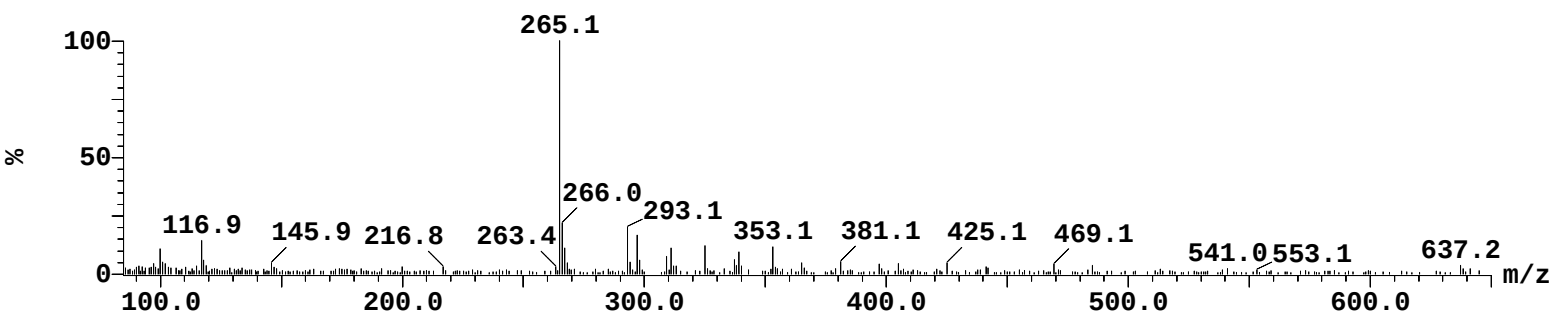
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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25		3.10	
----	--	------	--

25: (Time: 3.06)

4.4e+003



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