

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

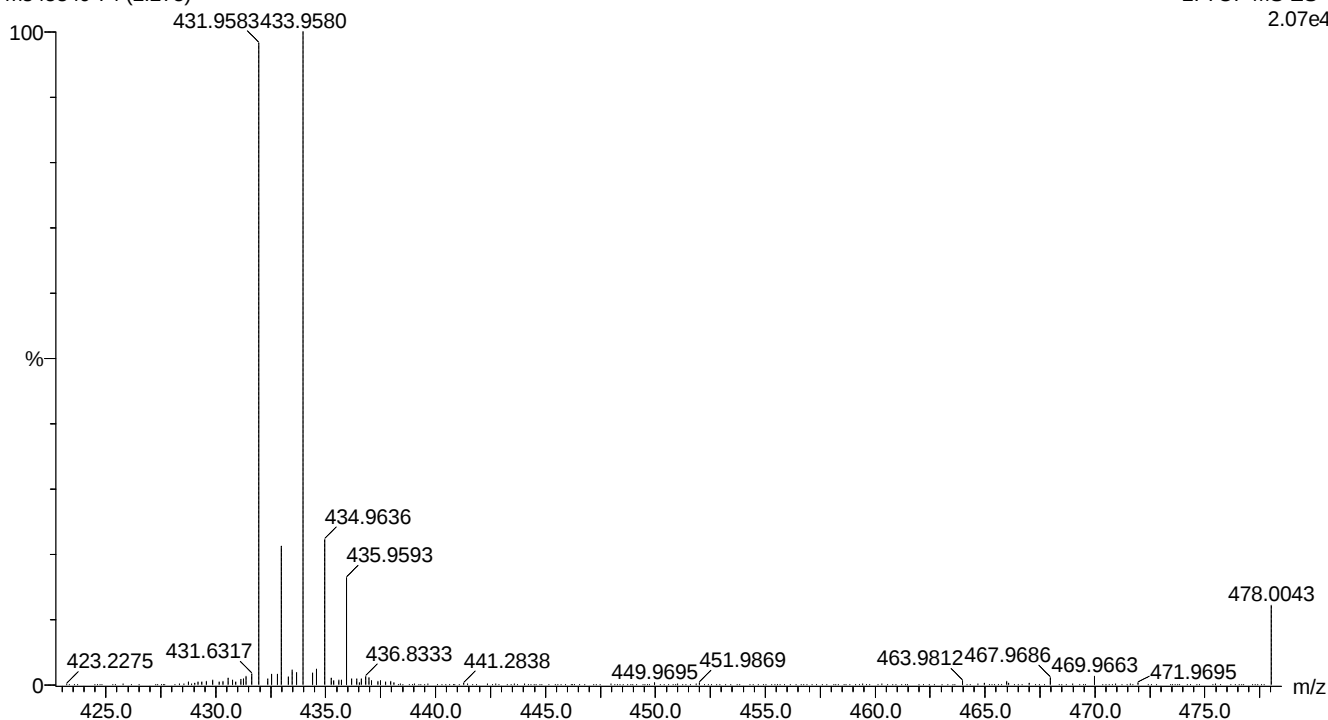
148 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 15-15 H: 0-100 N: 0-10 O: 0-15 S: 2-2 Br: 1-1

X.HU S1 5T

ms45349 74 (2.275)

2: TOF MS ES-
2.07e4

Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
431.9583	431.9575	0.8	1.9	8.5	69.6	C15 H15 N 05 S2 Br

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Sample: 5
File:ms45349
Description:X.HU S1 5T

Vial:1:11
Date:11-Apr-2018

ID:
Time:10:30:34

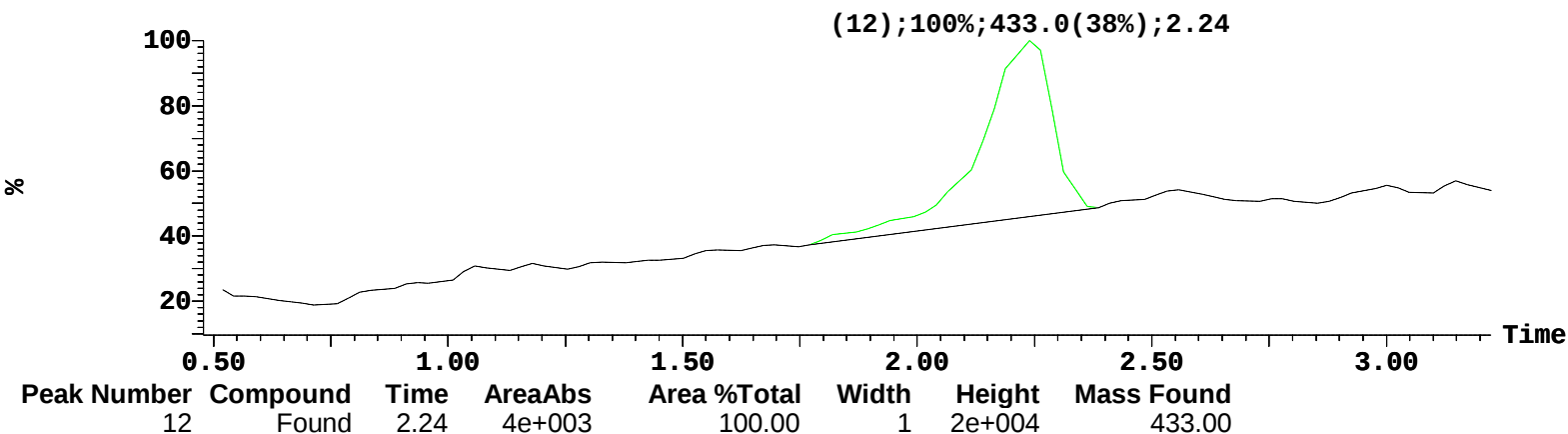
Printed: Wed Apr 11 13:43:18 2018

Sample Report:

Sample 5 Vial 1:11 ID File ms45349 Date 11-Apr-2018 Time 10:30:34 Description X.HU S1 5T

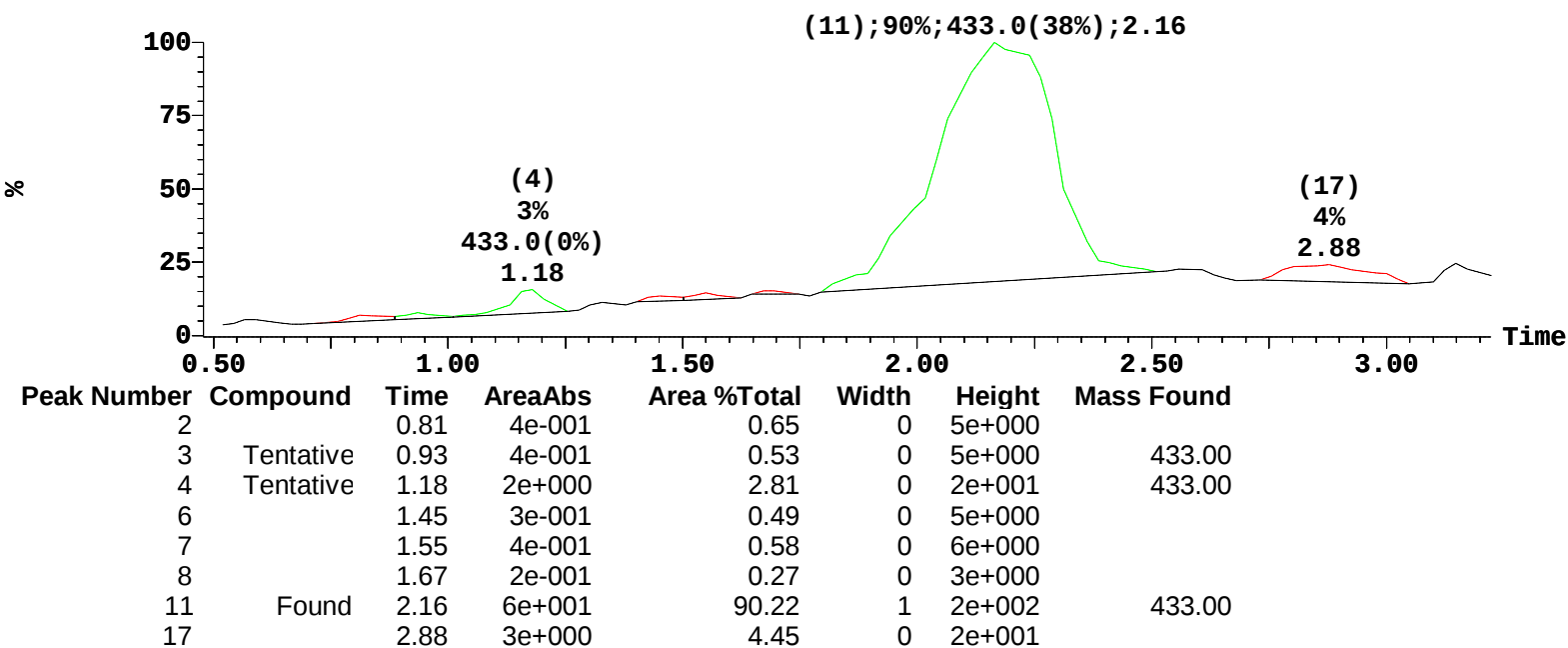
1: TOF MS ES+ :TIC

4.0e+004



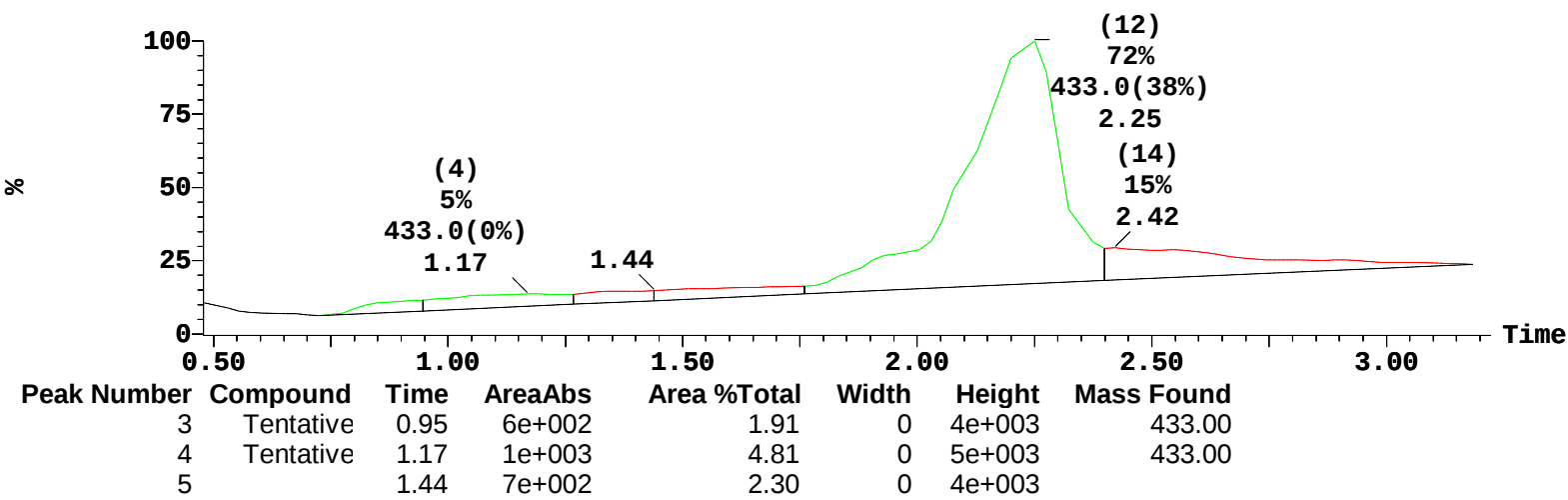
1: TOF MS ES+ :433+456+434

2.7e+002



2: TOF MS ES- :TIC

1.1e+005



Sample: 5
File:ms45349
Description:X.HU S1 5T

Vial:1:11
Date:11-Apr-2018

ID:
Time:10:30:34

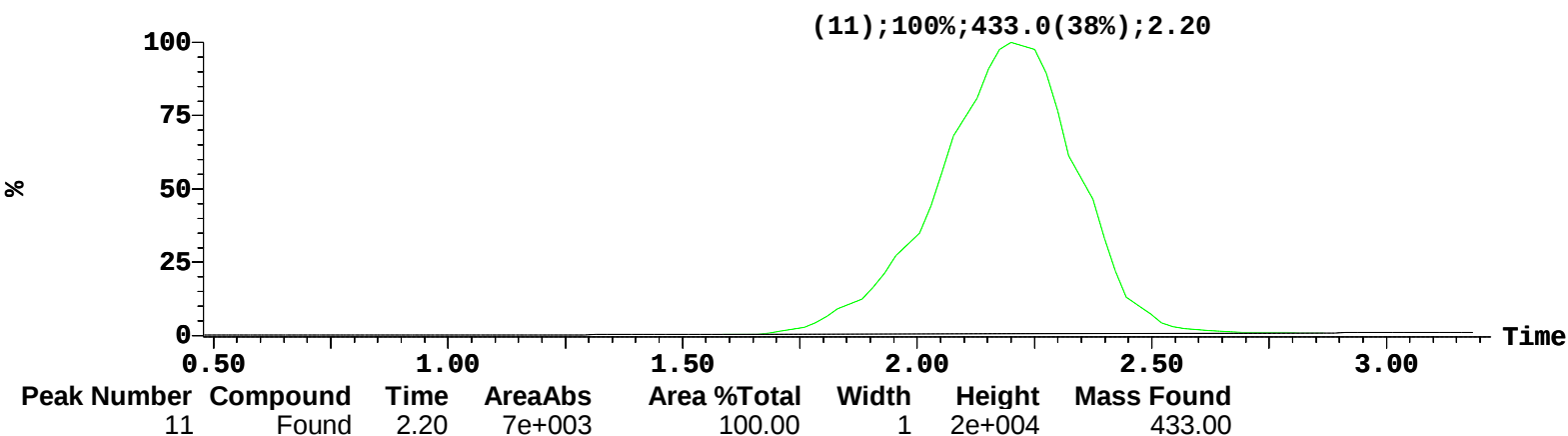
Printed: Wed Apr 11 13:43:18 2018

Sample Report (continued):

9		1.76	1e+003	3.76	0	3e+003	
12	Found	2.25	2e+004	72.36	1	9e+004	433.00
14		2.42	4e+003	14.87	1	1e+004	

2: TOF MS ES- :433+478+432

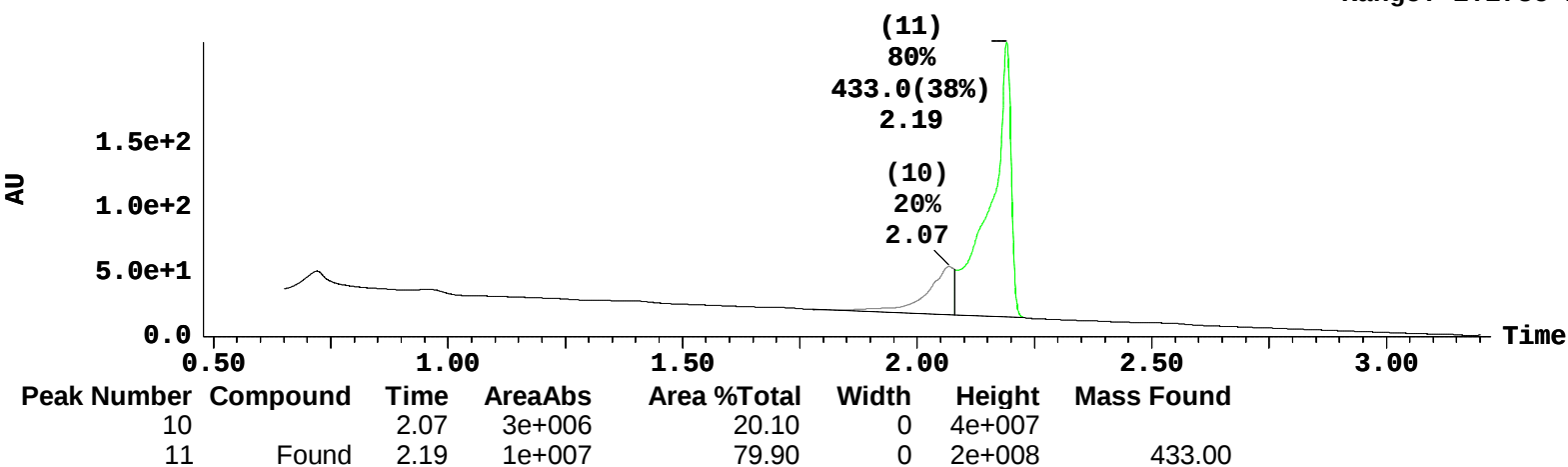
2.1e+004



5: UV Detector: TIC

2.278e+2

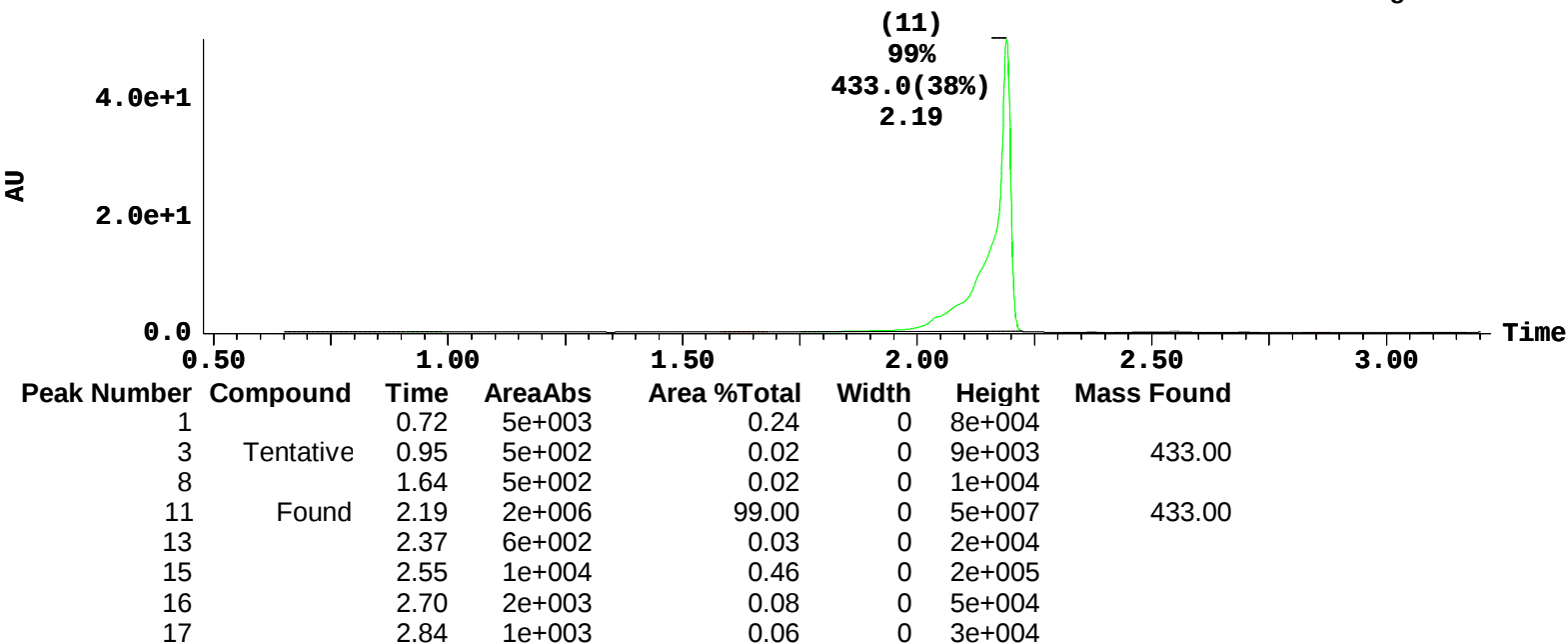
Range: 2.278e+2



5: UV Detector: 244_264

5.023e+1

Range: 5.023e+1



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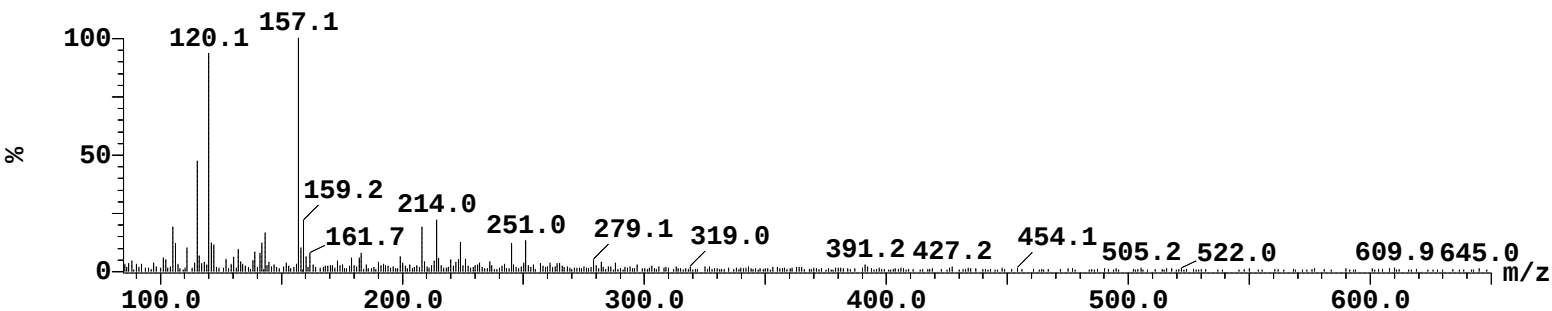
Sample Report (continued):

18	3.10	5e+002	0.02	0	2e+004
19	3.14	2e+003	0.07	0	5e+004

Peak ID	Compound	Time	Mass Found
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2: (Time: 0.81)

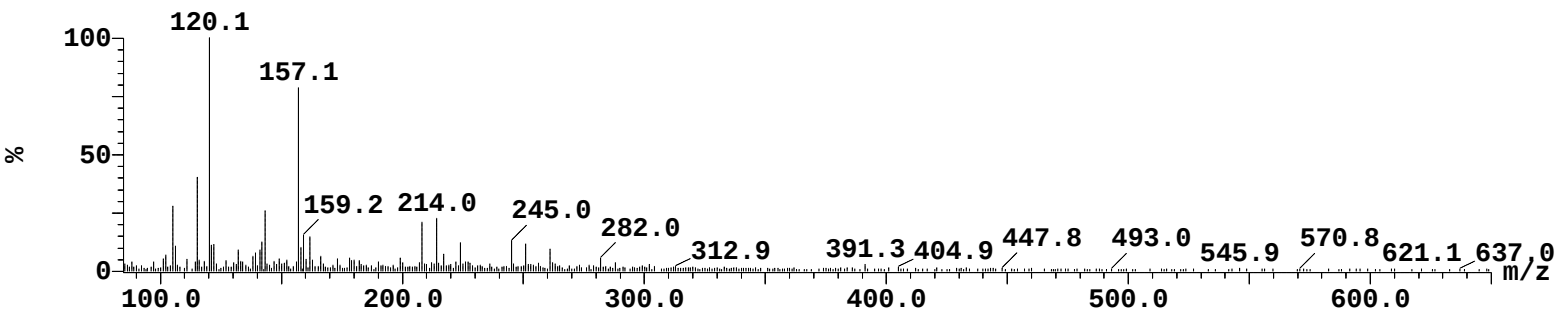
1.5e+003



Peak ID	Compound	Time	Mass Found
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3: (Time: 0.93)

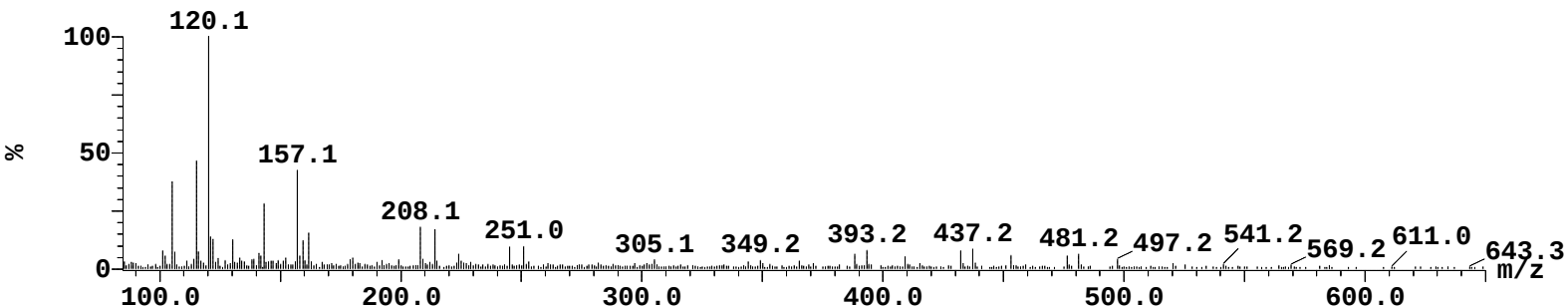
2.2e+003



Peak ID	Compound	Time	Mass Found
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4: (Time: 1.18)

2.6e+003



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Date:11-Apr-2018

ID:
Time:10:30:34

Printed: Wed Apr 11 13:43:18 2018

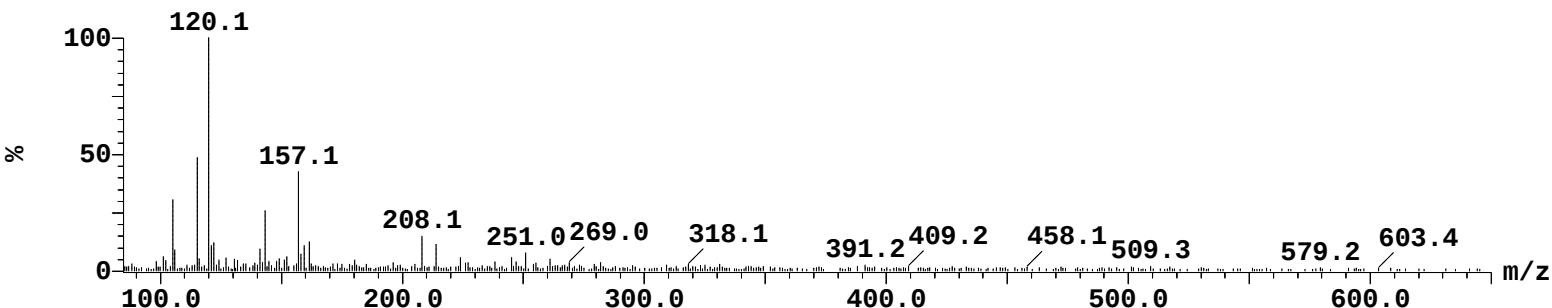
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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6
1.45

6: (Time: 1.45)

1.6e+003

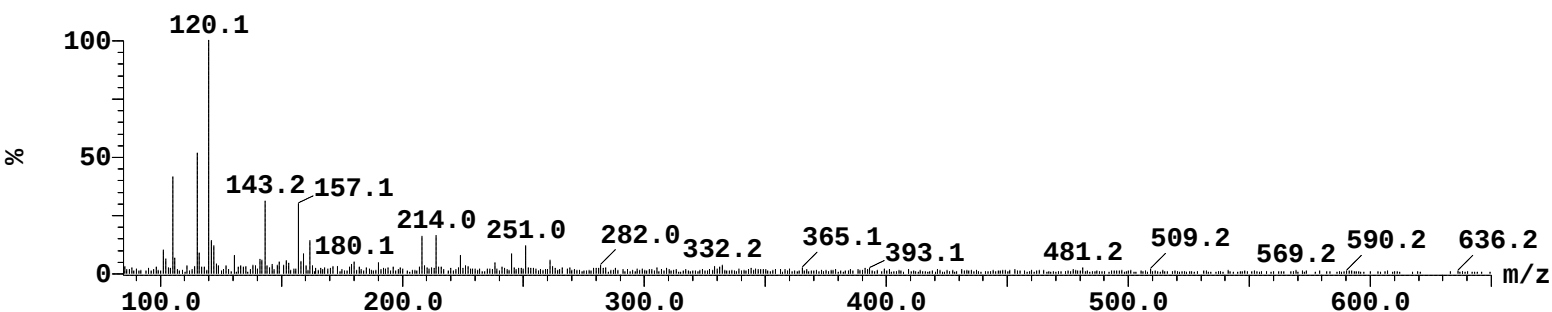


Peak ID	Compound	Time	Mass Found
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7
1.55

7: (Time: 1.55)

2.7e+003

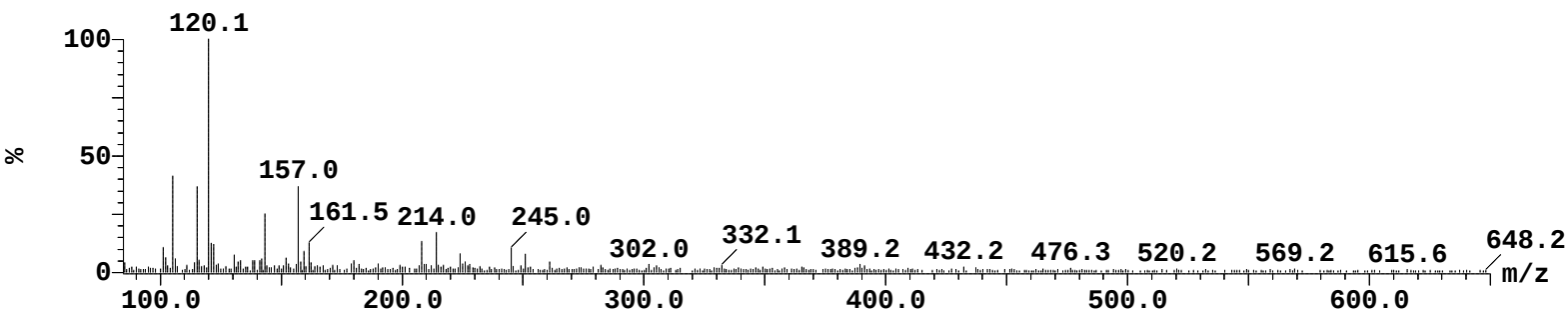


Peak ID	Compound	Time	Mass Found
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8
1.67

8: (Time: 1.67)

3.0e+003

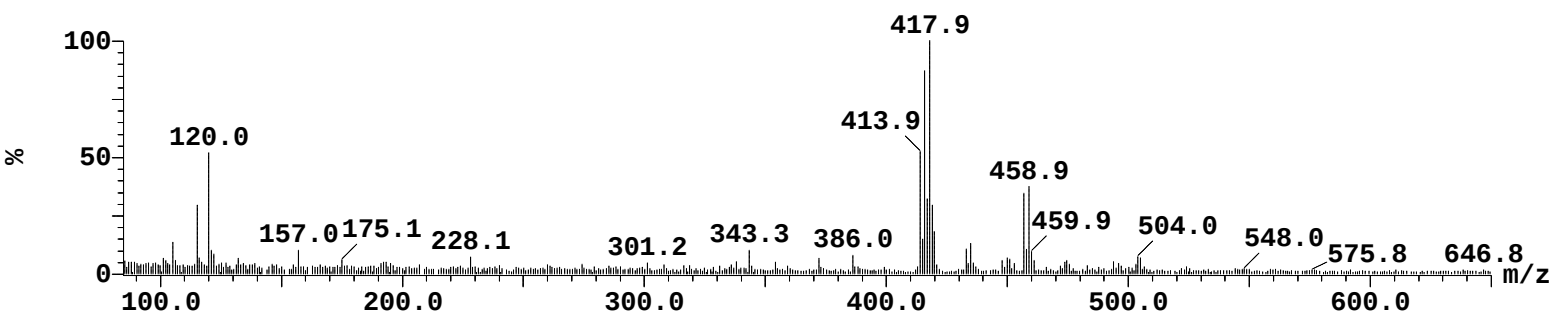


Peak ID	Compound	Time	Mass Found
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11
2.16

11: (Time: 2.16)

5.9e+003



Sample: 5
File:ms45349
Description:X.HU S1 5T

Vial:1:11
Date:11-Apr-2018

ID:
Time:10:30:34

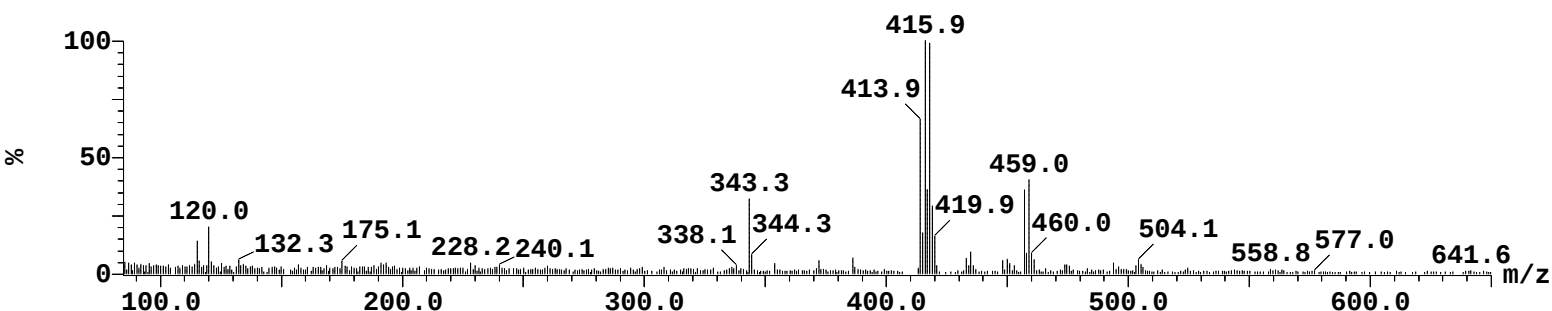
Printed: Wed Apr 11 13:43:18 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
12		2.24	

12: (Time: 2.24)

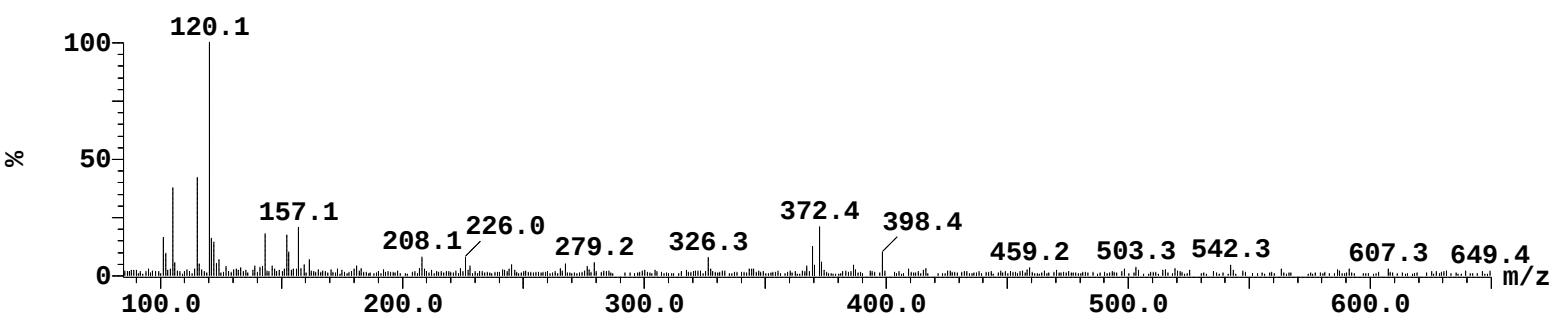
5.9e+003



Peak ID	Compound	Time	Mass Found
17		2.88	

17: (Time: 2.88)

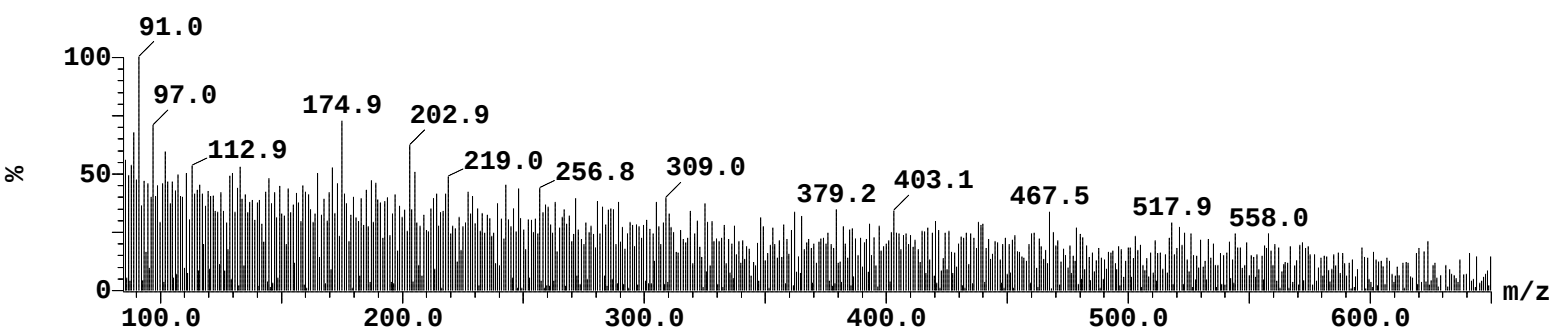
3.7e+003



Peak ID	Compound	Time	Mass Found
3	Tentative	0.93	433.00

3: (Time: 0.95)

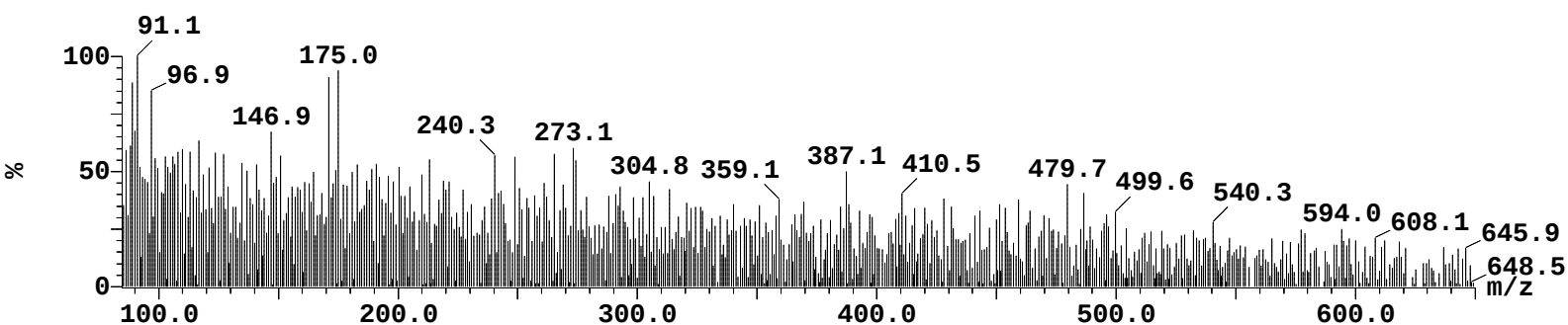
2.6e+002



Peak ID	Compound	Time	Mass Found
4	Tentative	1.18	433.00

4: (Time: 1.17)

2.0e+002



Sample: 5
File:ms45349
Description:X.HU S1 5T

Vial:1:11
Date:11-Apr-2018

ID:
Time:10:30:34

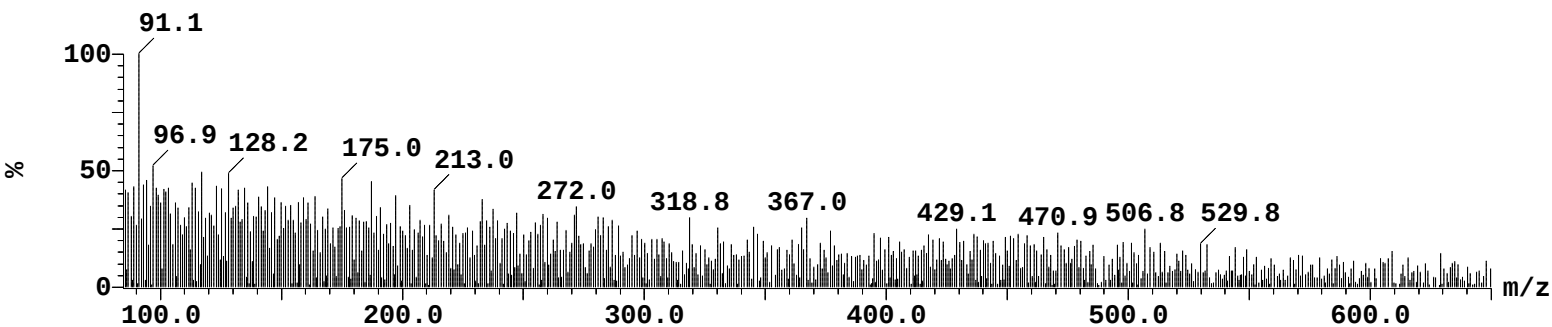
Printed: Wed Apr 11 13:43:18 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
5		1.44	

5: (Time: 1.44)

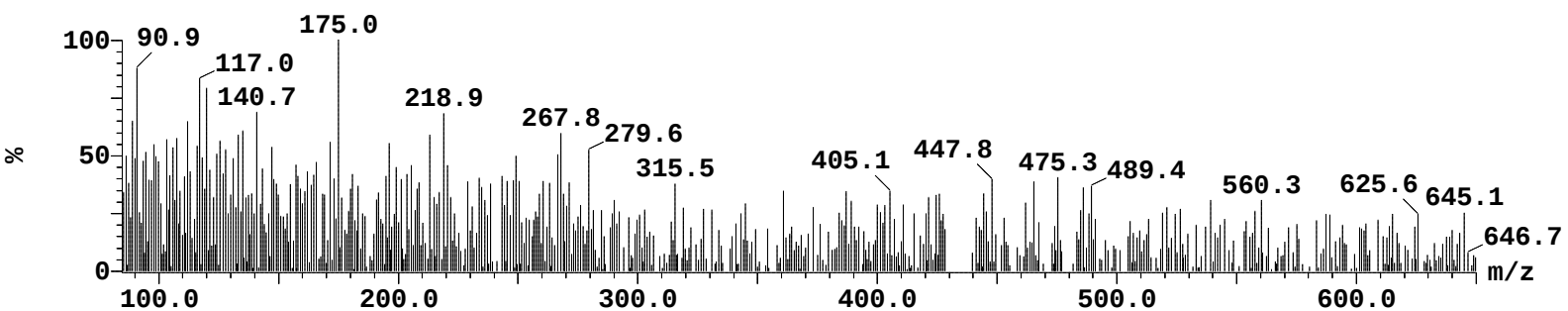
3.5e+002



Peak ID	Compound	Time	Mass Found
9		1.76	

9: (Time: 1.76)

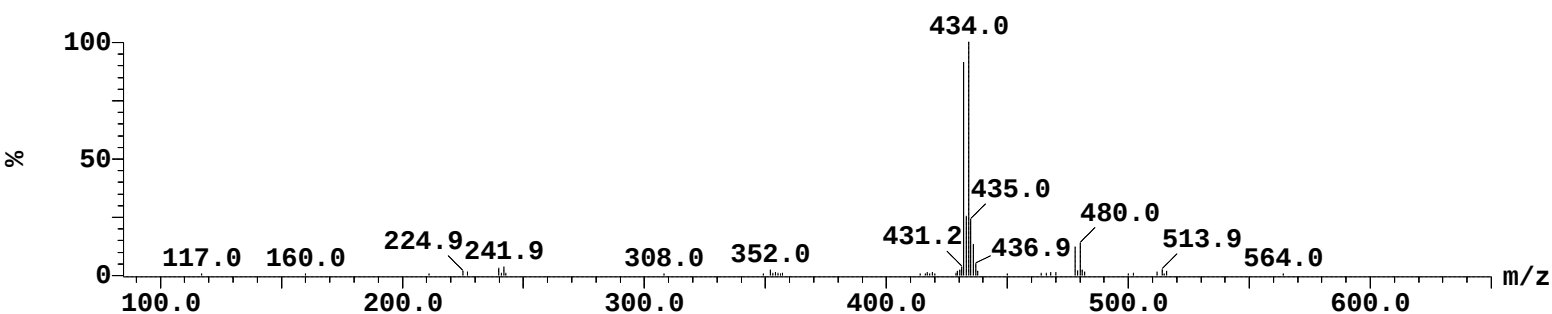
1.7e+002



Peak ID	Compound	Time	Mass Found
11	Found	2.16	433.00

11: (Time: 2.20)

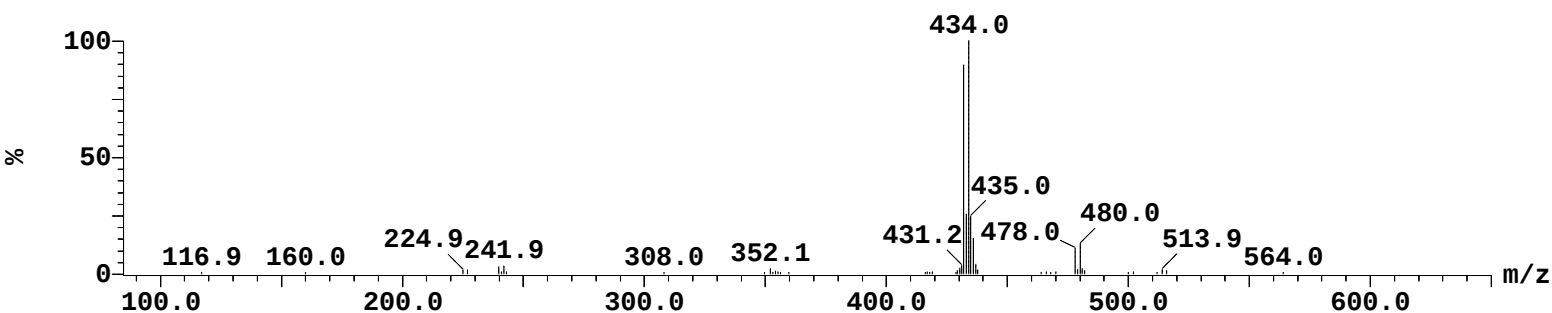
7.4e+004



Peak ID	Compound	Time	Mass Found
12	Found	2.24	433.00

12: (Time: 2.25)

7.6e+004



Openlynx Report -

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Sample: 5
File:ms45349
Description:X.HU S1 5T

Vial:1:11
Date:11-Apr-2018

ID:
Time:10:30:34

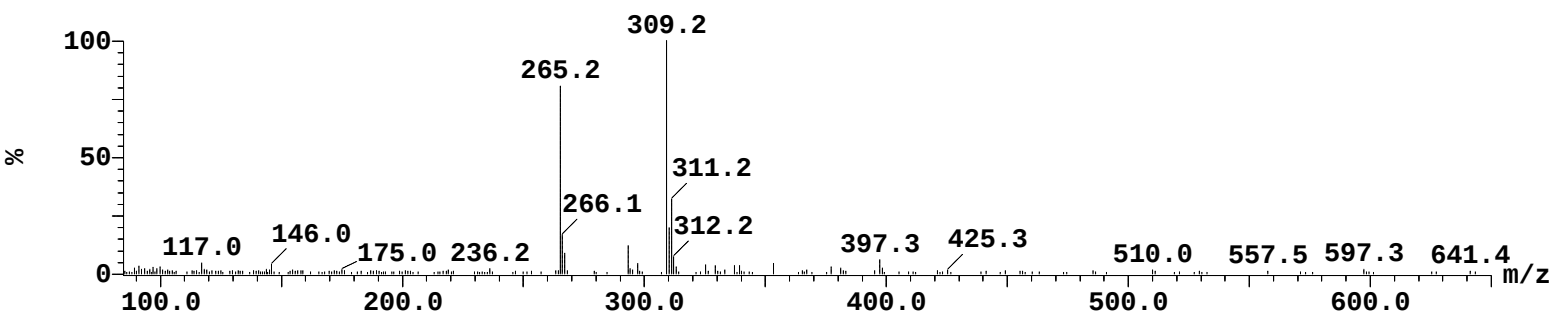
Printed: Wed Apr 11 13:43:18 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
14		2.42	

14: (Time: 2.42)

1.0e+004



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