

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

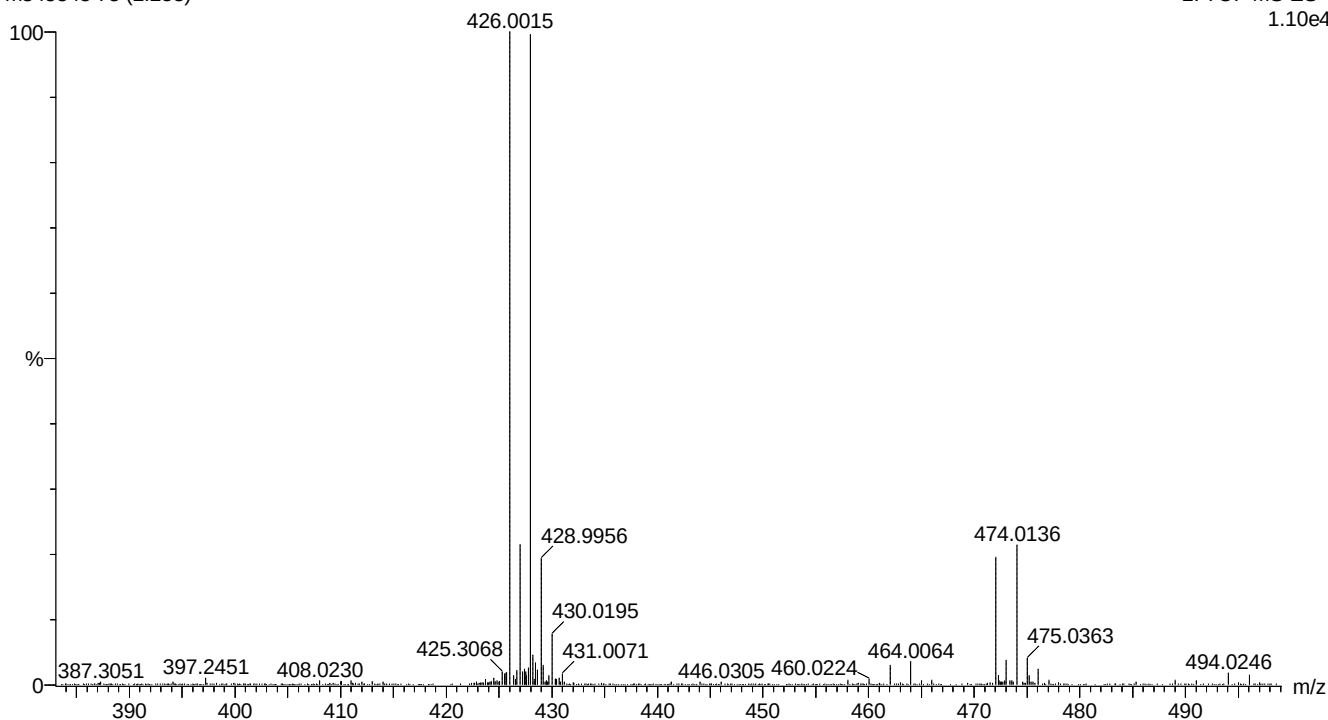
159 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 17-17 H: 0-100 N: 0-10 O: 0-15 S: 1-1 Br: 1-1

X.HU S1 5B

ms45348 73 (2.253)

2: TOF MS ES-
1.10e4

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.0015	426.0011	0.4	0.9	9.5	15.3	C17 H17 N 05 S Br

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Sample: 4
File:ms45348
Description:X.HU S1 5B

Vial:1:10
Date:11-Apr-2018

ID:
Time:10:25:35

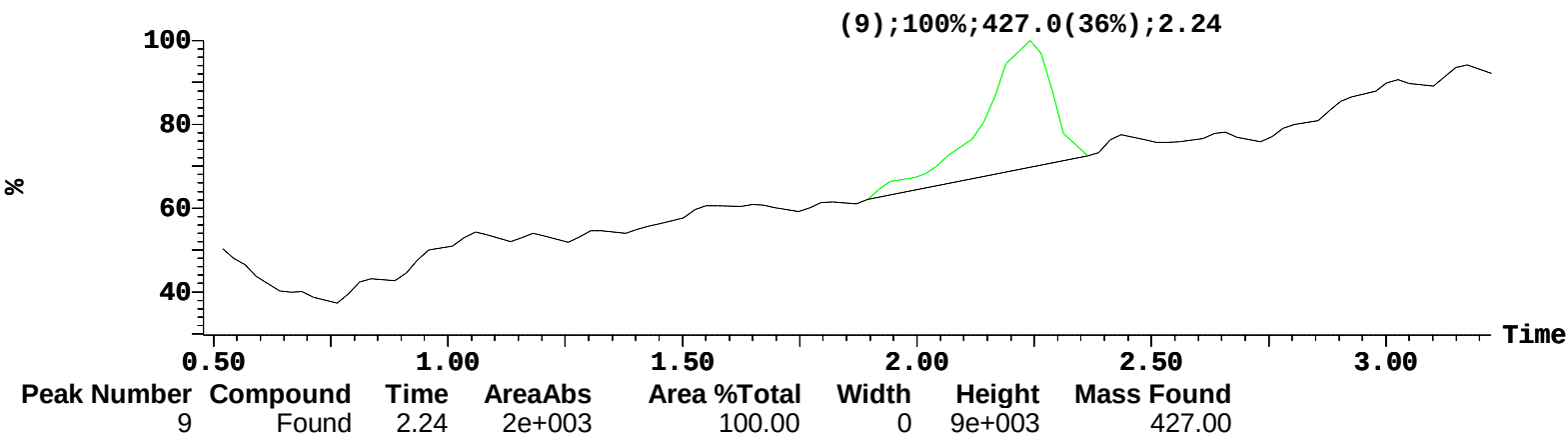
Printed: Wed Apr 11 13:39:39 2018

Sample Report:

Sample 4 Vial 1:10 ID File ms45348 Date 11-Apr-2018 Time 10:25:35 Description X.HU S1 5B

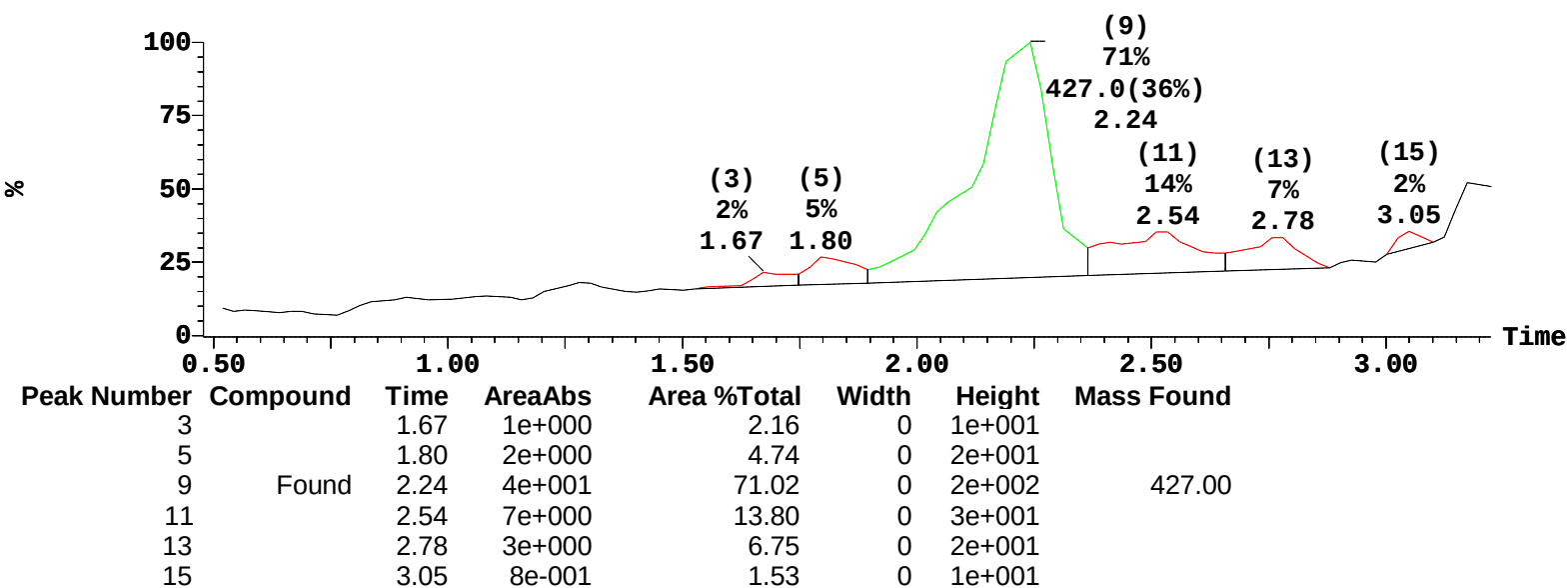
1: TOF MS ES+ :TIC

2.9e+004



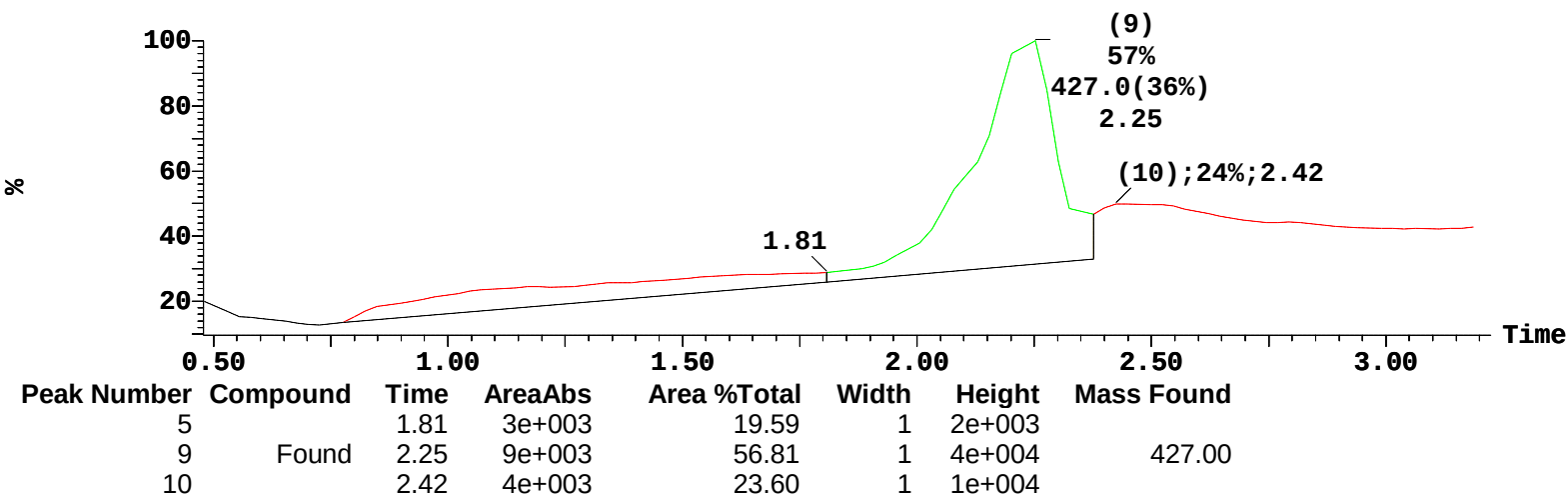
1: TOF MS ES+ :427+450+428

2.3e+002



2: TOF MS ES- :TIC

6.5e+004



Sample: 4
File:ms45348
Description:X.HU S1 5B

Vial:1:10
Date:11-Apr-2018

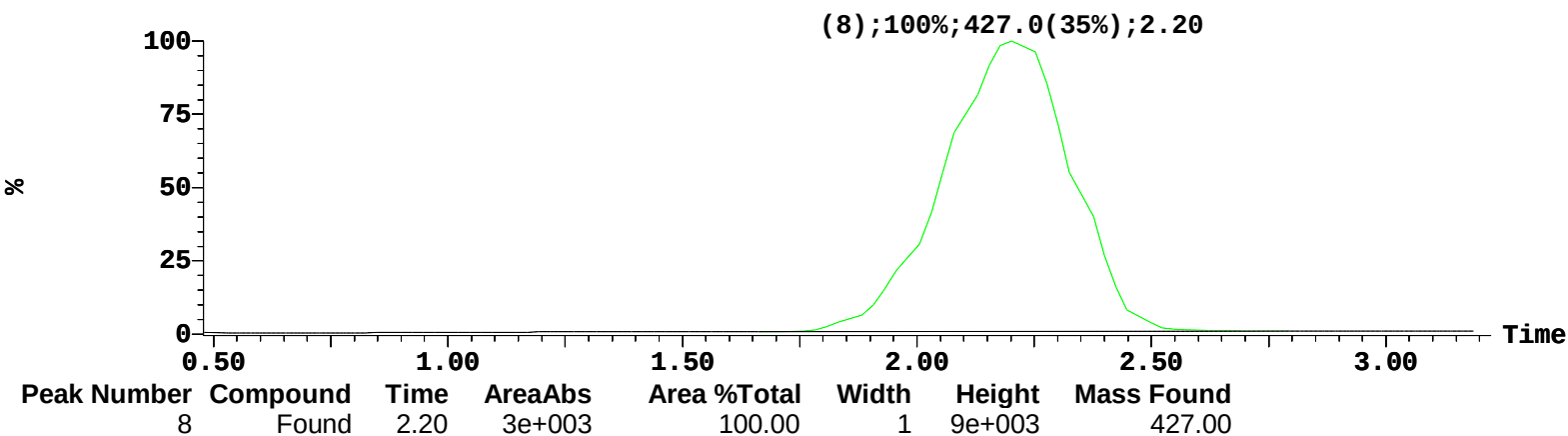
ID:
Time:10:25:35

Printed: Wed Apr 11 13:39:39 2018

Sample Report (continued):

2: TOF MS ES- :427+472+426

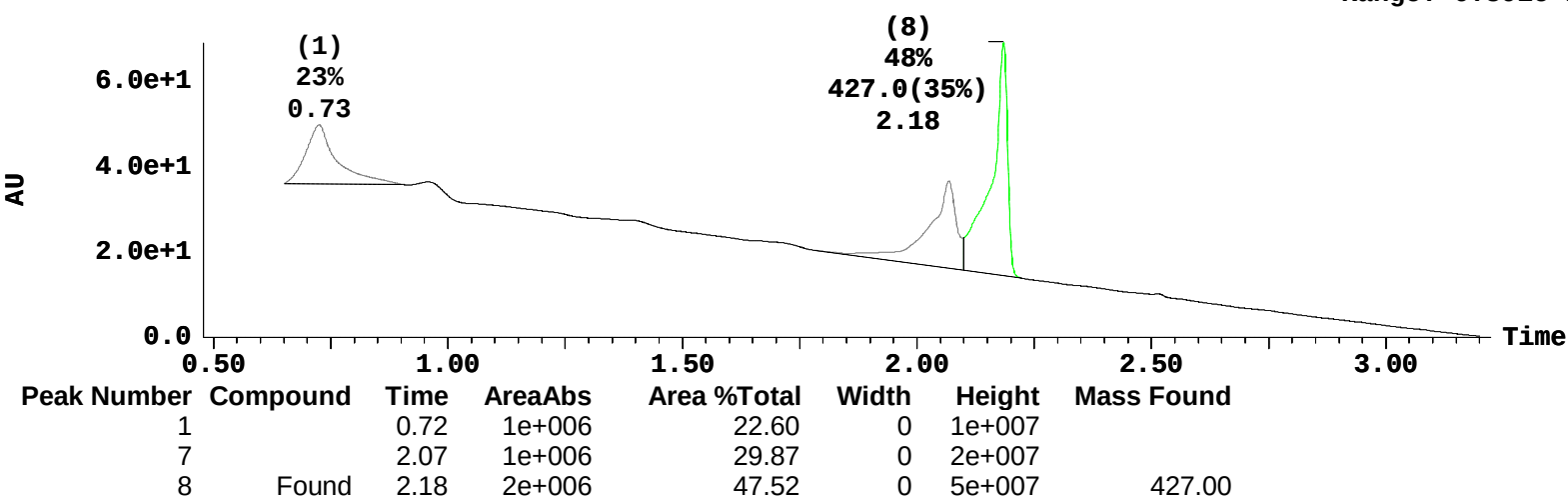
9.5e+003



5: UV Detector: TIC

6.891e+1

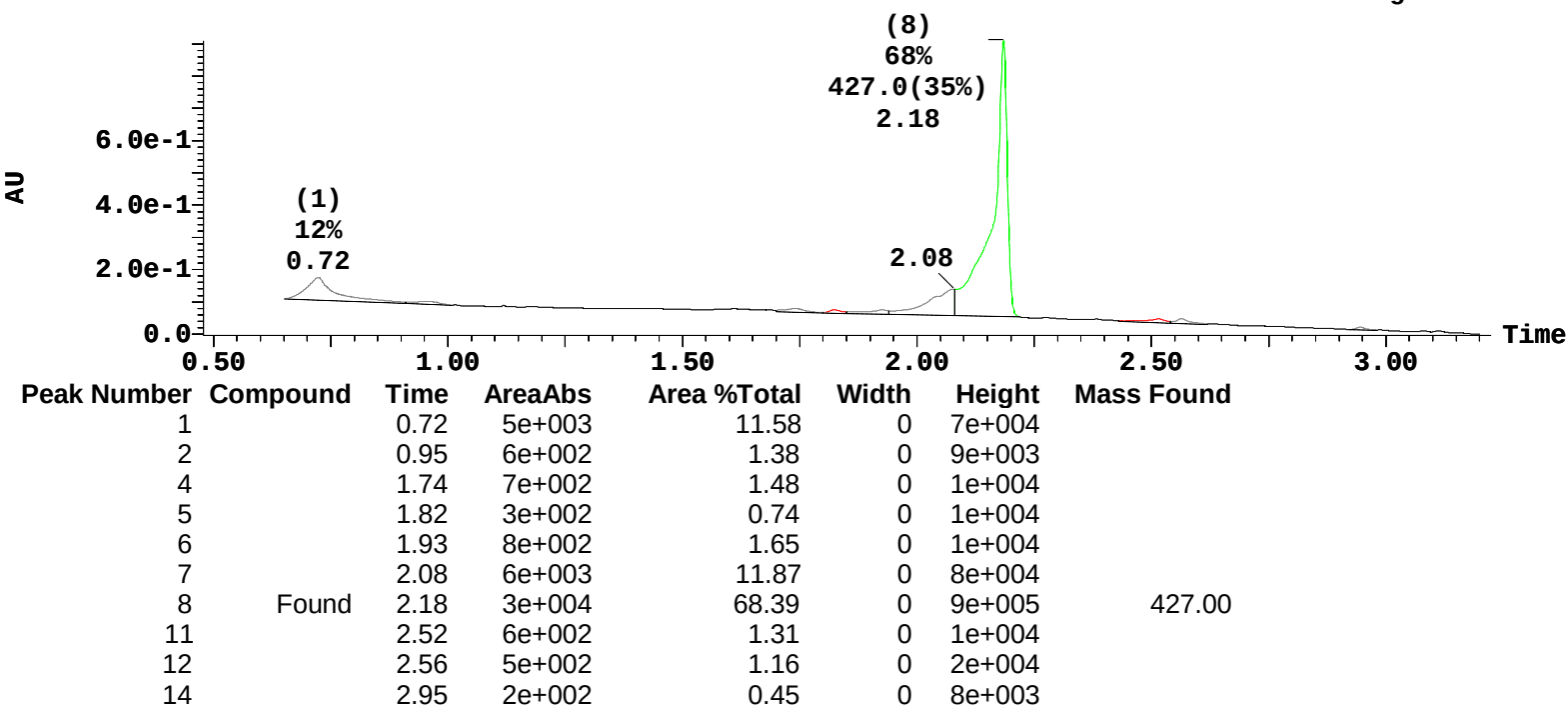
Range: 6.891e+1



5: UV Detector: 244_264

9.09e-1

Range: 9.089e-1



Sample: 4

Vial:1:10

ID:

File:ms45348

Date:11-Apr-2018

Time:10:25:35

Description:X.HU S1 5B

Printed: Wed Apr 11 13:39:39 2018

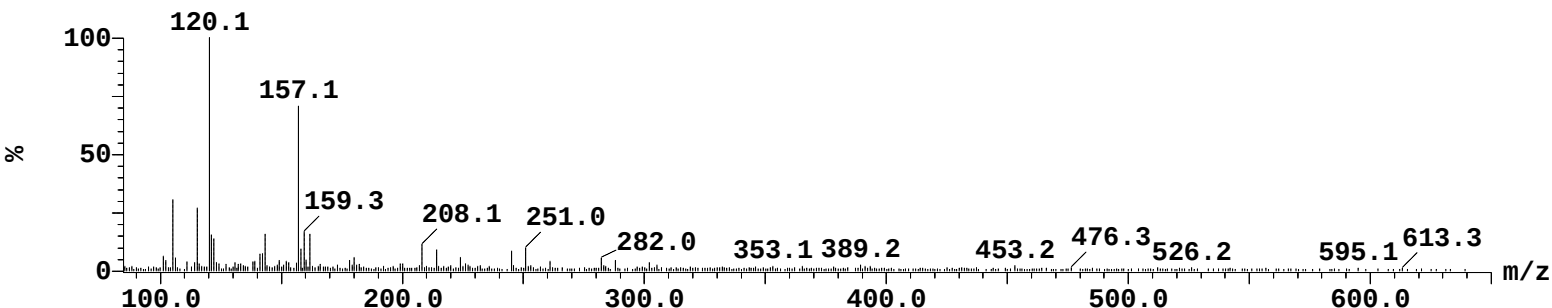
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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3		1.67	
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3: (Time: 1.67)

3.9e+003

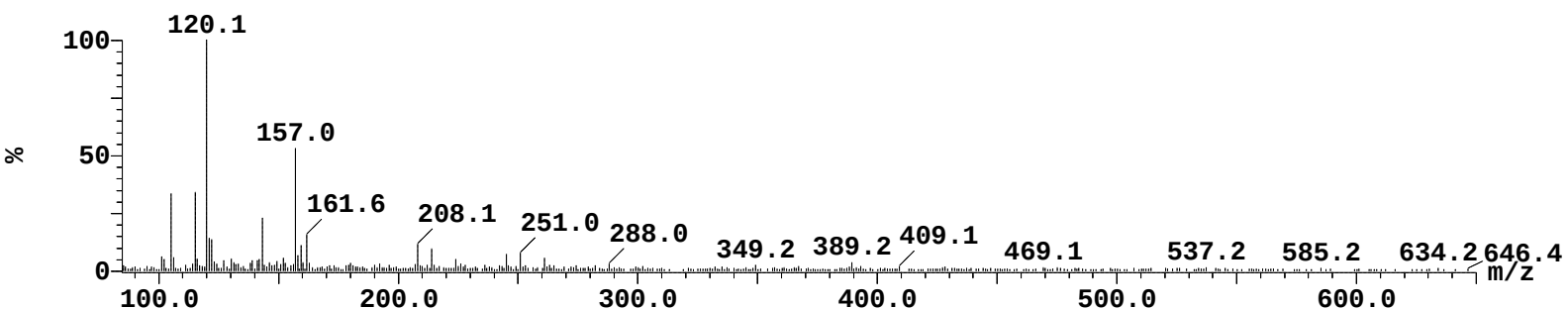


Peak ID	Compound	Time	Mass Found
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5		1.80	
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5: (Time: 1.80)

3.6e+003

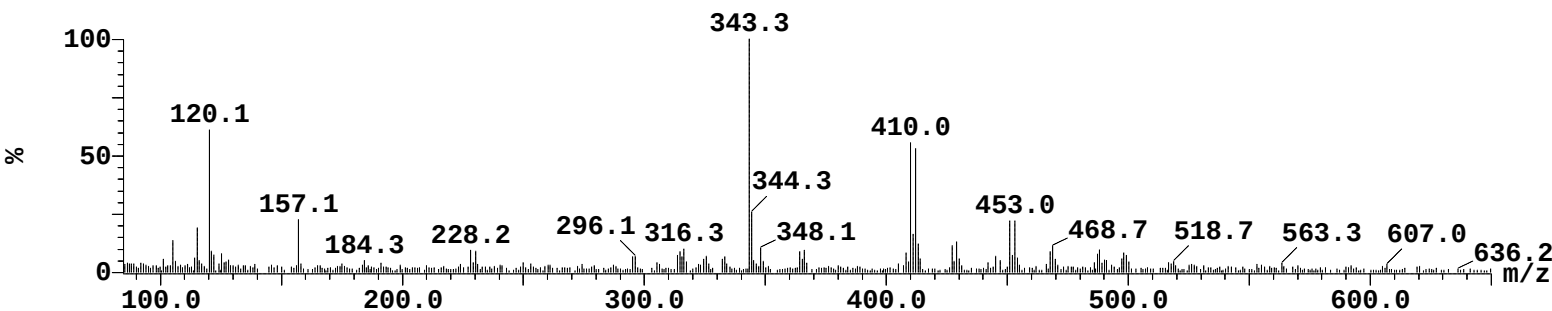


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

9		2.24	
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9: (Time: 2.24)

2.9e+003

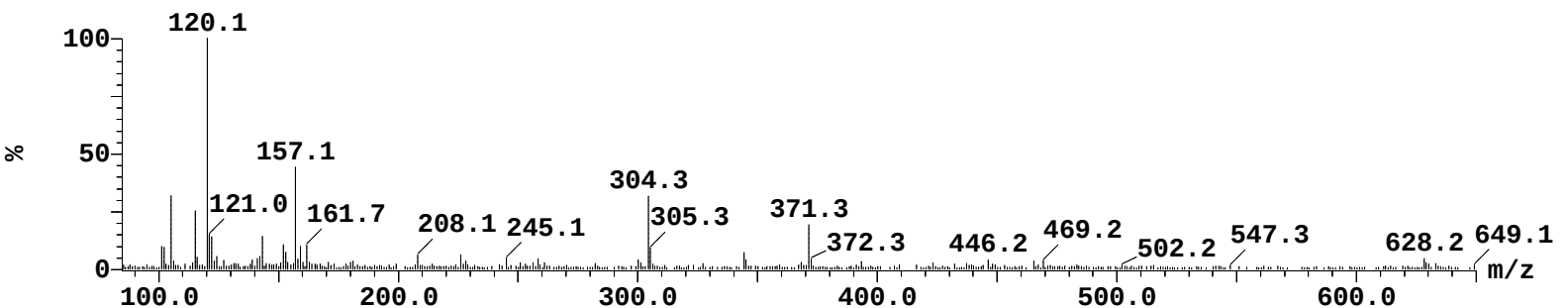


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

11		2.54	
----	--	------	--

11: (Time: 2.54)

4.6e+003



Sample: 4
File:ms45348
Description:X.HU S1 5B

Vial:1:10
Date:11-Apr-2018

ID:
Time:10:25:35

Printed: Wed Apr 11 13:39:39 2018

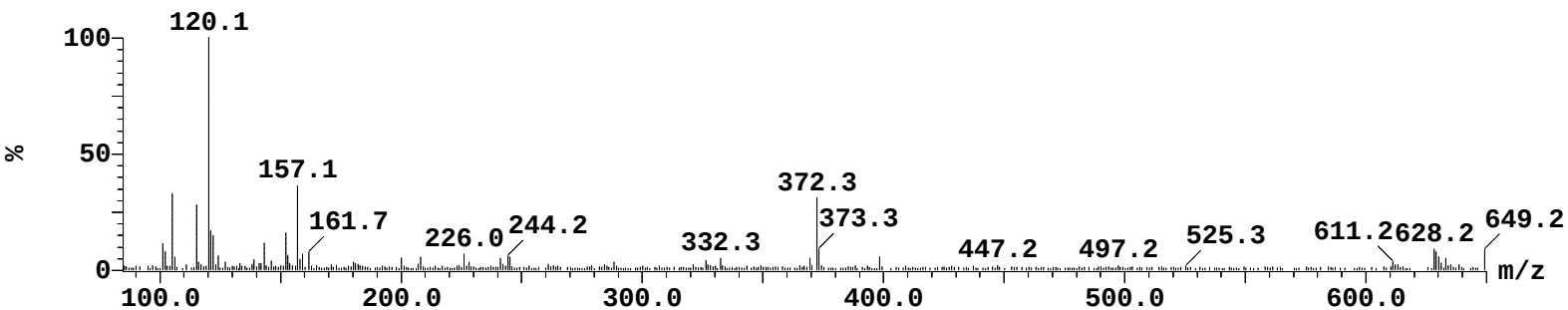
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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13		2.78	
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13: (Time: 2.78)

4.8e+003

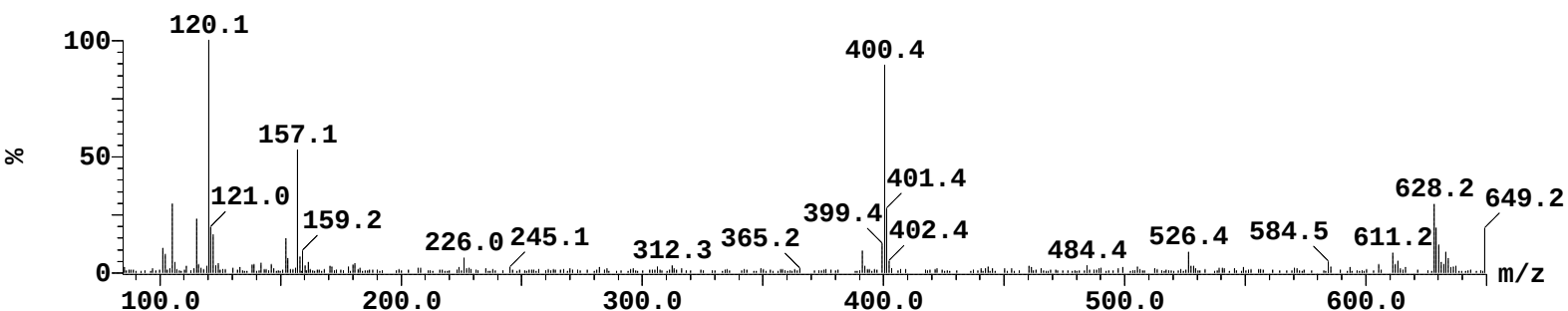


Peak ID	Compound	Time	Mass Found
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15		3.05	
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15: (Time: 3.05)

3.1e+003

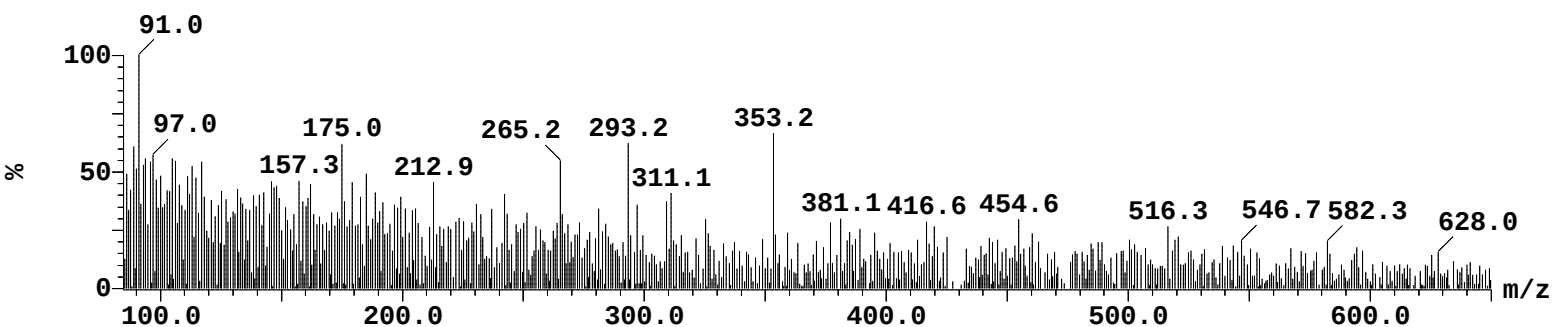


Peak ID	Compound	Time	Mass Found
---------	----------	------	------------

5		1.80	
---	--	------	--

5: (Time: 1.81)

3.5e+002

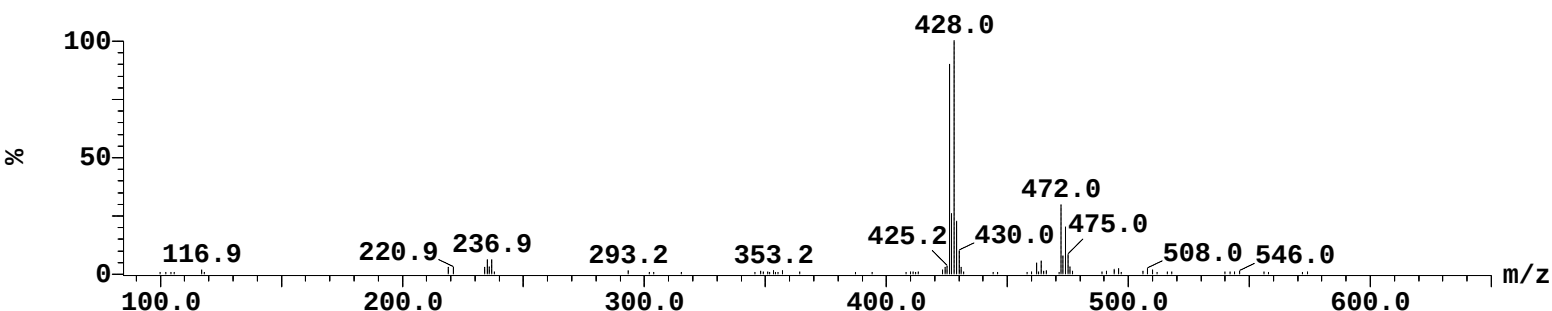


Peak ID	Compound	Time	Mass Found
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8	Found	2.20	427.00
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8: (Time: 2.20)

3.2e+004



Sample: 4
File:ms45348
Description:X.HU S1 5B

Vial:1:10
Date:11-Apr-2018

ID:
Time:10:25:35

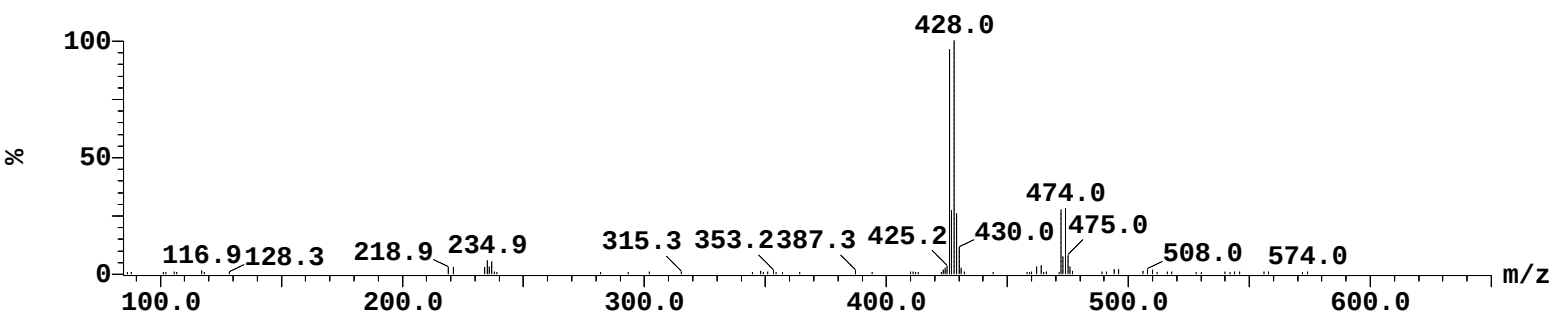
Printed: Wed Apr 11 13:39:39 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
9	Found	2.24	427.00

9: (Time: 2.25)

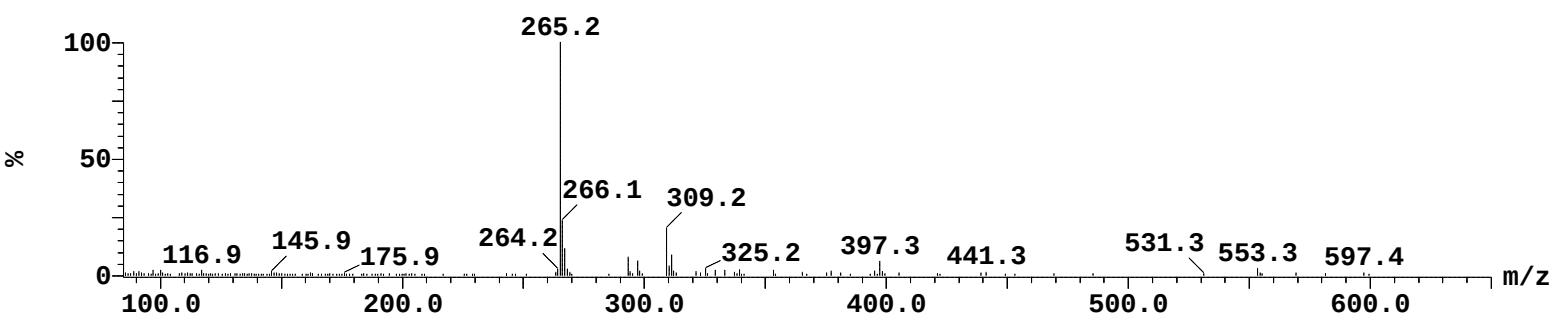
2.9e+004



Peak ID	Compound	Time	Mass Found
10		2.42	

10: (Time: 2.42)

1.9e+004



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