

Single Mass Analysis

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

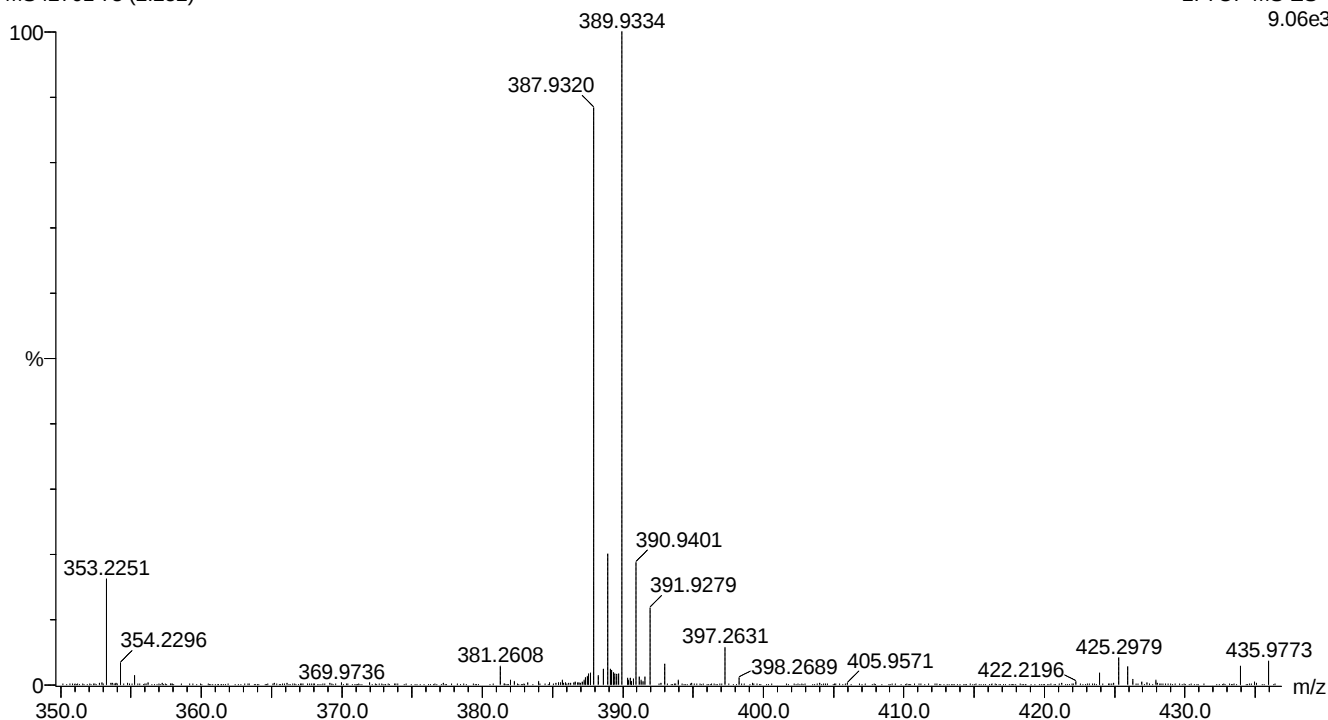
Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 13-13 H: 0-200 N: 0-10 O: 0-10 Na: 0-1 S: 2-2 Br: 1-1

A.ZUBIARRE AZ 161 2
MS42761 73 (2.252)2: TOF MS ES-
9.06e3

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
387.9320	387.9313	0.7	1.8	8.5	59.6	C13 H11 N 04 S2 Br

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Sample: 15
File:MS42761
Description:A.ZUBIARRE AZ 161 2

Vial:2:11
Date:09-Jan-2018

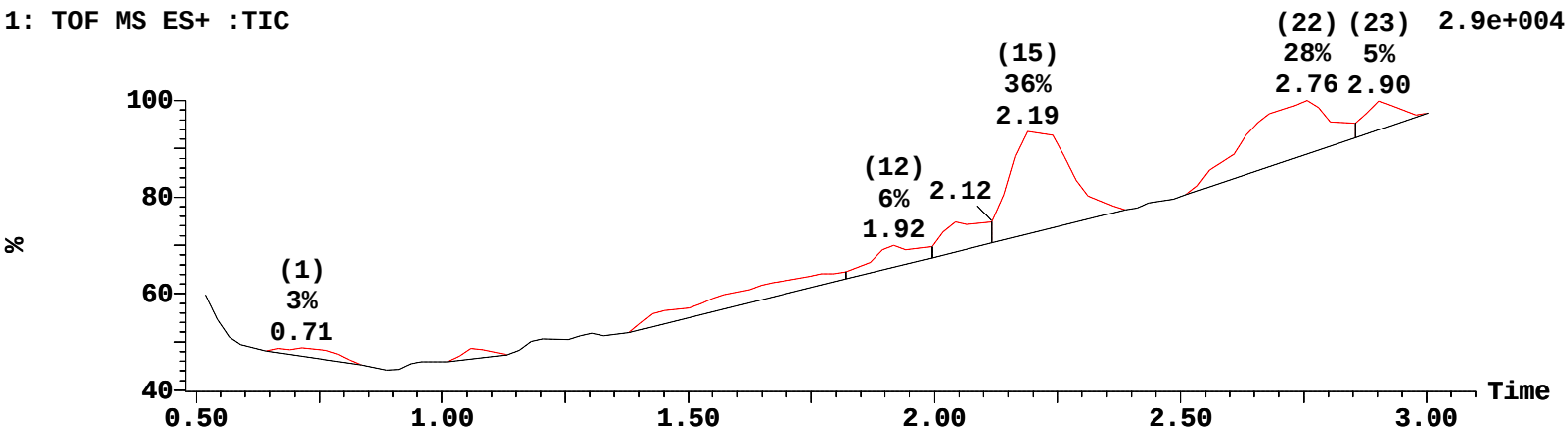
ID:
Time:10:57:57

Printed: Tue Jan 09 11:45:47 2018

Sample Report:

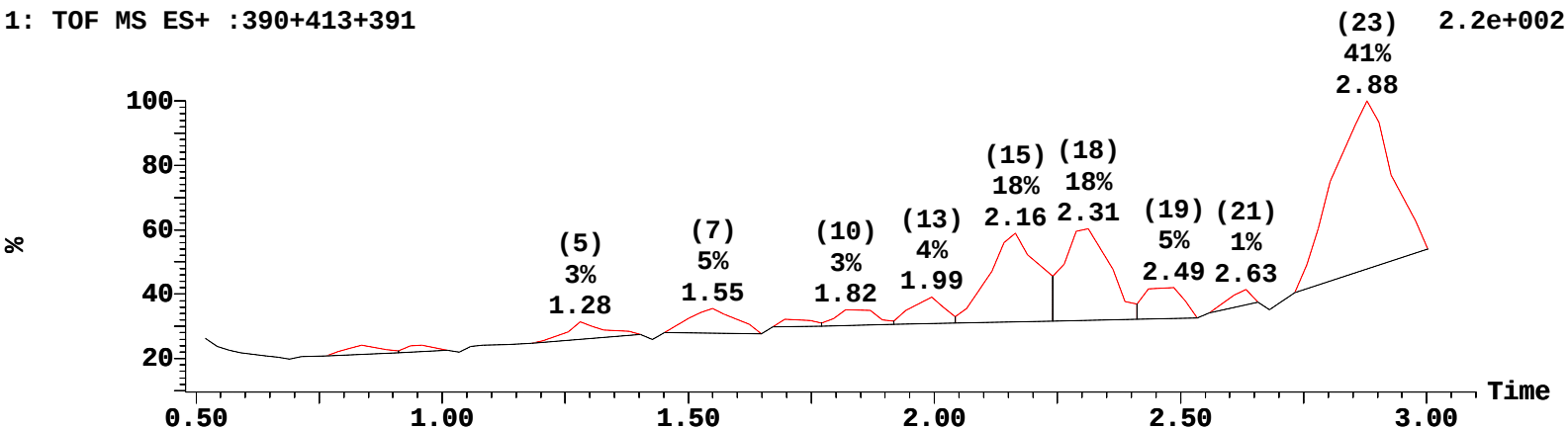
Sample 15 Vial 2:11 ID File MS42761 Date 09-Jan-2018 Time 10:57:57 Description A.ZUBIARRE AZ 161 2

1: TOF MS ES+ :TIC



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.71	7e+001	2.80	0	5e+002	
4		1.06	4e+001	1.69	0	7e+002	
10		1.82	3e+002	12.70	0	4e+002	
12		1.92	1e+002	6.06	0	1e+003	
14		2.12	2e+002	7.20	0	1e+003	
15		2.19	9e+002	36.09	0	6e+003	
22		2.76	7e+002	28.09	0	3e+003	
23		2.90	1e+002	5.37	0	2e+003	

1: TOF MS ES+ :390+413+391



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2		0.84	5e-001	1.28	0	6e+000	
3		0.96	3e-001	0.70	0	4e+000	
5		1.28	1e+000	2.67	0	1e+001	
7		1.55	2e+000	4.77	0	2e+001	
9		1.70	4e-001	0.95	0	5e+000	
10		1.82	1e+000	2.65	0	1e+001	
13		1.99	1e+000	3.64	0	2e+001	
15		2.16	7e+000	18.21	0	6e+001	
18		2.31	7e+000	17.70	0	6e+001	
19		2.49	2e+000	5.11	0	2e+001	
21		2.63	6e-001	1.44	0	1e+001	
23		2.88	2e+001	40.89	0	1e+002	

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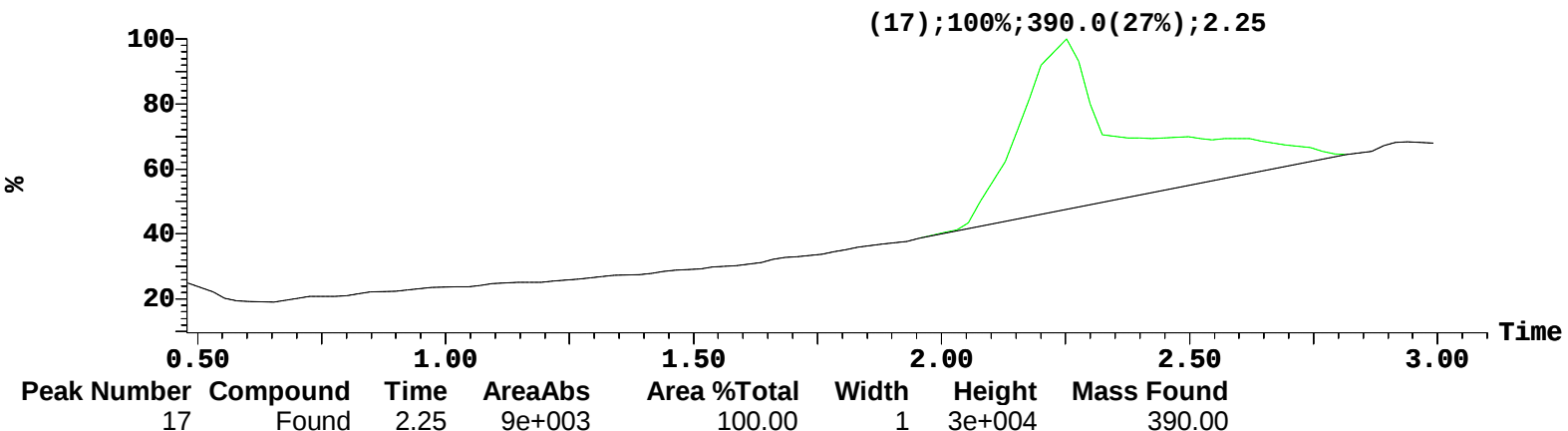
ID:
Time:10:57:57

Printed: Tue Jan 09 11:45:47 2018

Sample Report (continued):

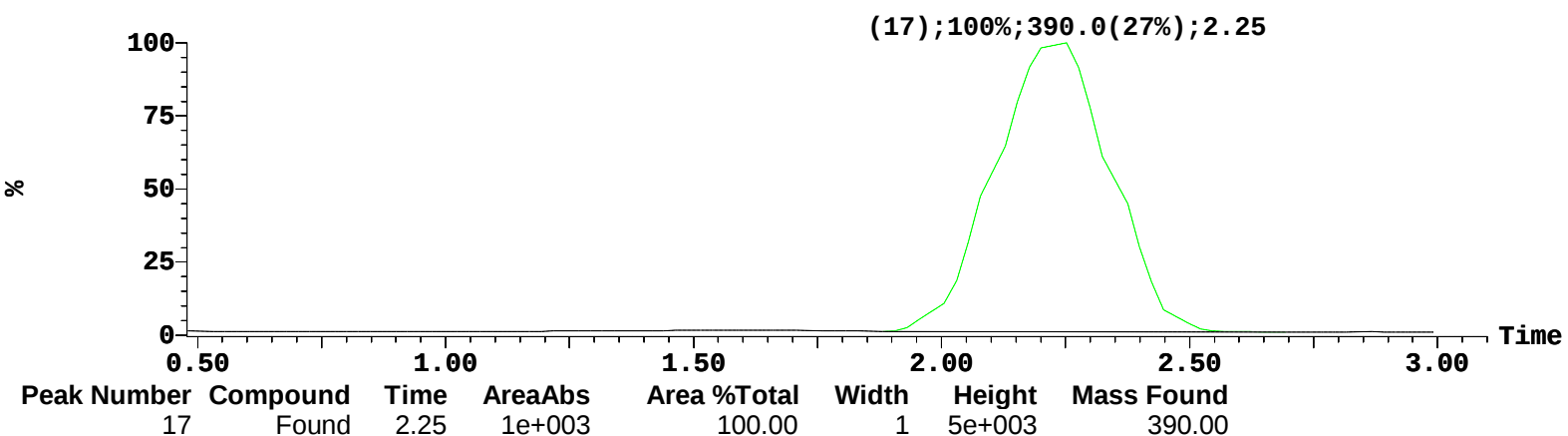
2: TOF MS ES- :TIC

6.3e+004



2: TOF MS ES- :390+435+389

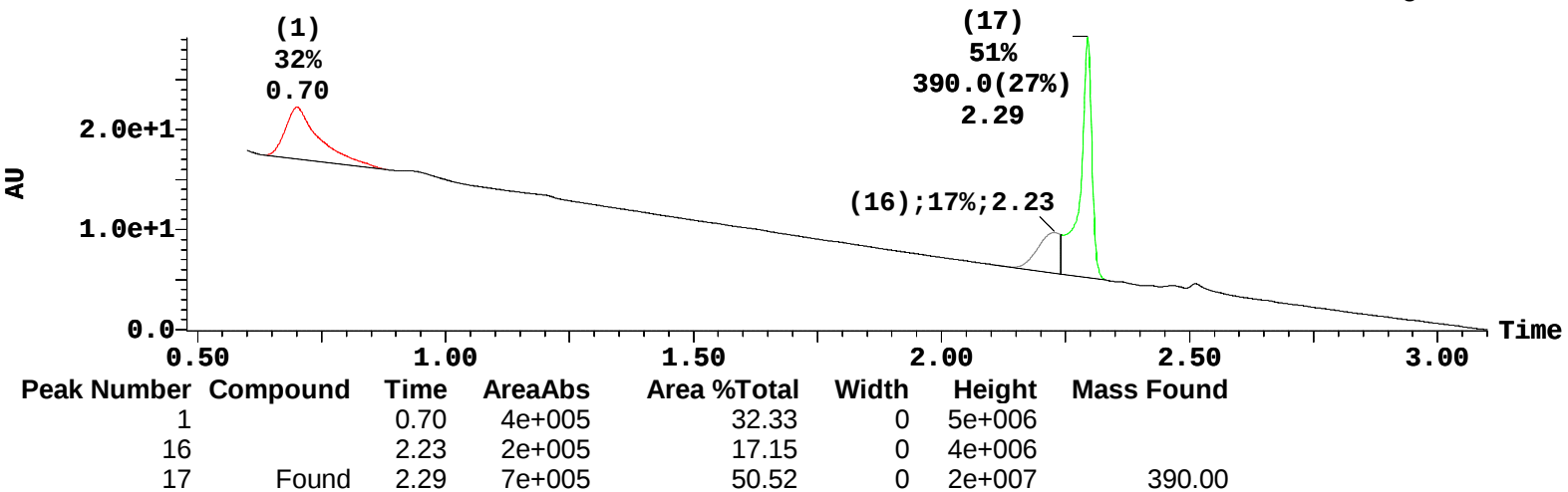
4.9e+003



5: UV Detector: TIC

2.92e+1

Range: 2.92e+1



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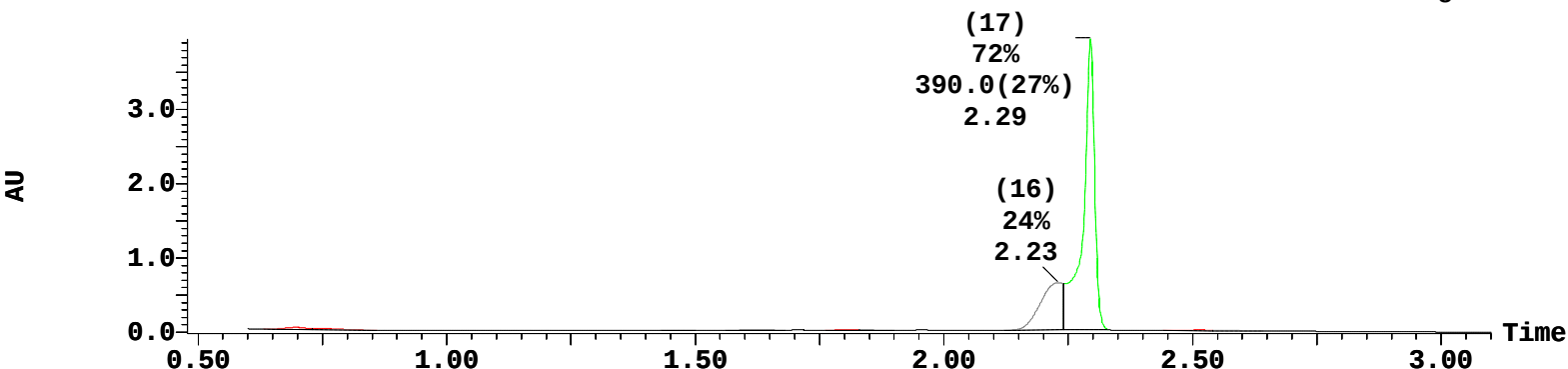
ID:
Time:10:57:57

Printed: Tue Jan 09 11:45:47 2018

Sample Report (continued):

5: UV Detector: 244_264

3.953
Range: 3.953

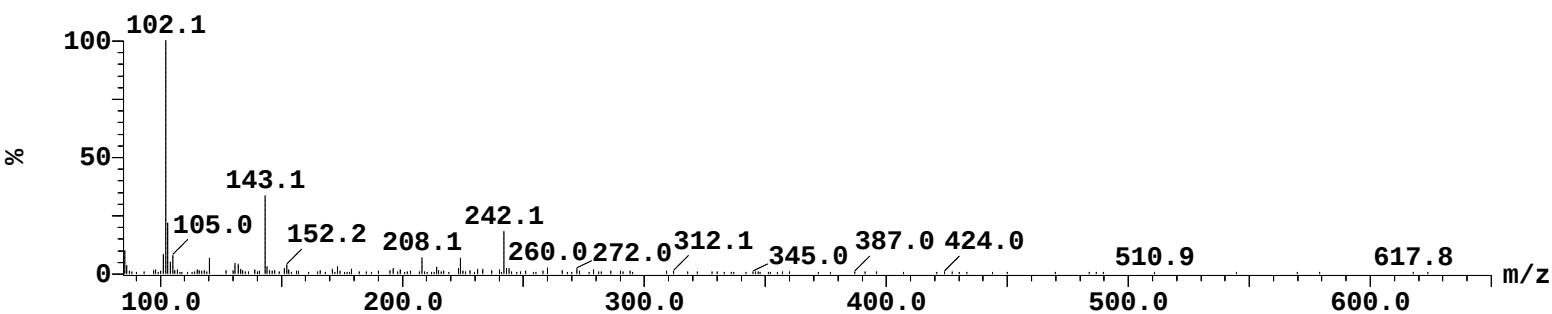


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		0.70	2e+003	1.05	0	3e+004	
1		0.73	1e+003	0.69	0	2e+004	
6		1.50	3e+002	0.20	0	6e+003	
8		1.63	9e+002	0.63	0	1e+004	
10		1.80	5e+002	0.33	0	1e+004	
11		1.84	4e+002	0.24	0	7e+003	
16		2.23	3e+004	23.99	0	6e+005	
17	Found	2.29	1e+005	72.12	0	4e+006	390.00
19		2.51	6e+002	0.41	0	1e+004	
20		2.56	5e+002	0.33	0	1e+004	

Peak ID Compound Time Mass Found
1 0.71

1: (Time: 0.71)

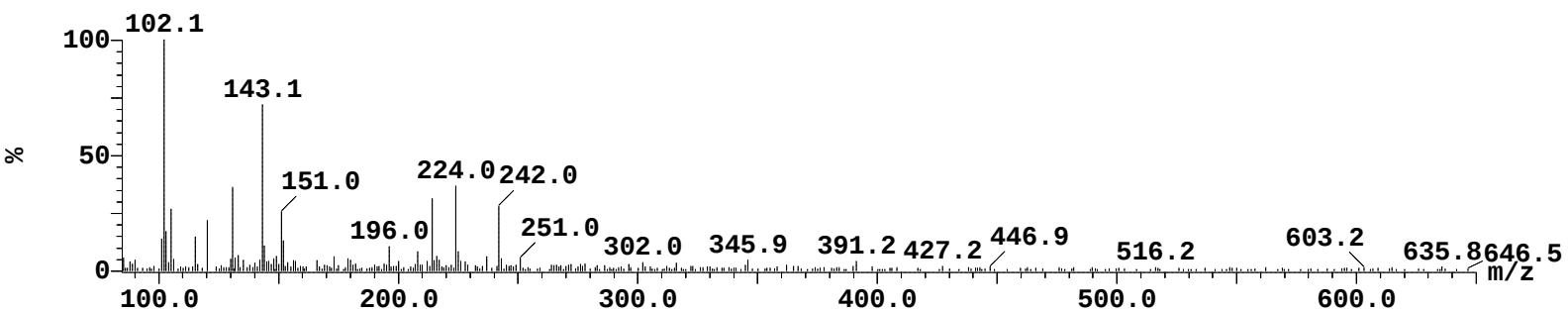
2.8e+003



Peak ID Compound Time Mass Found
2 0.84

2: (Time: 0.84)

1.2e+003



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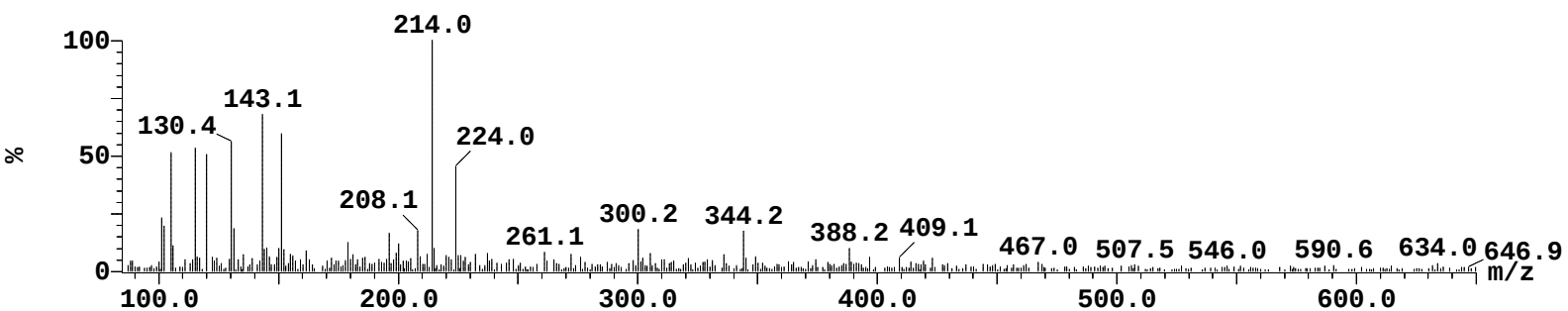
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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3		0.96	
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3: (Time: 0.96)

6.7e+002

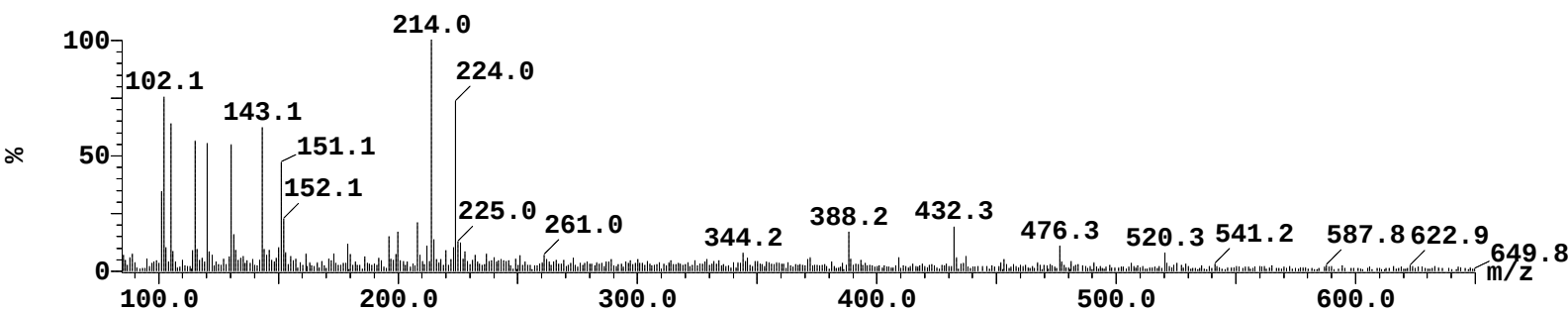


Peak ID	Compound	Time	Mass Found
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4		1.06	
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4: (Time: 1.06)

1.3e+003

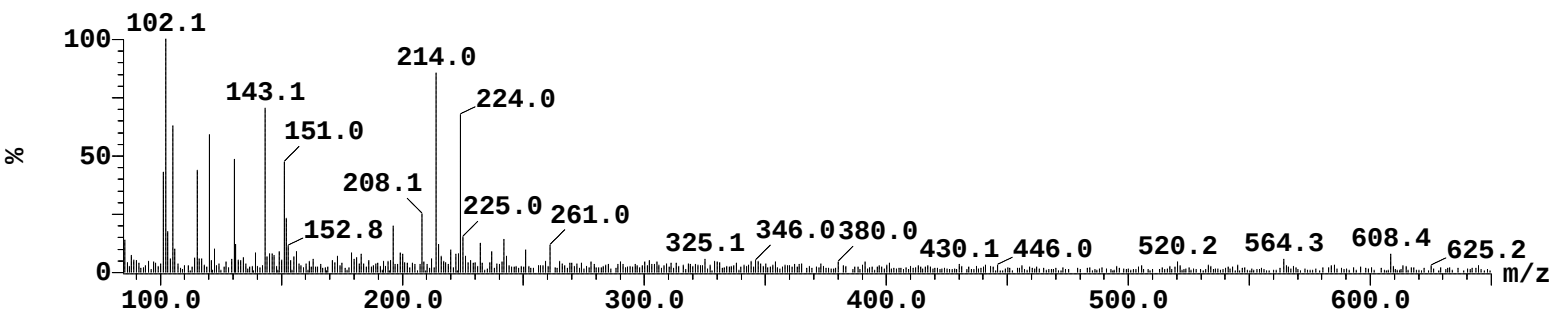


Peak ID	Compound	Time	Mass Found
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5		1.28	
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5: (Time: 1.28)

1.3e+003

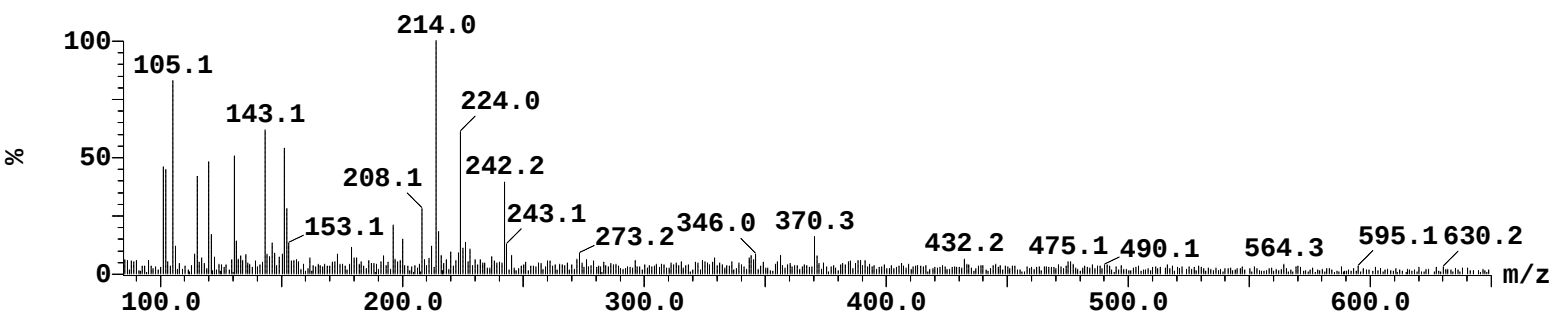


Peak ID	Compound	Time	Mass Found
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7		1.55	
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7: (Time: 1.55)

1.4e+003



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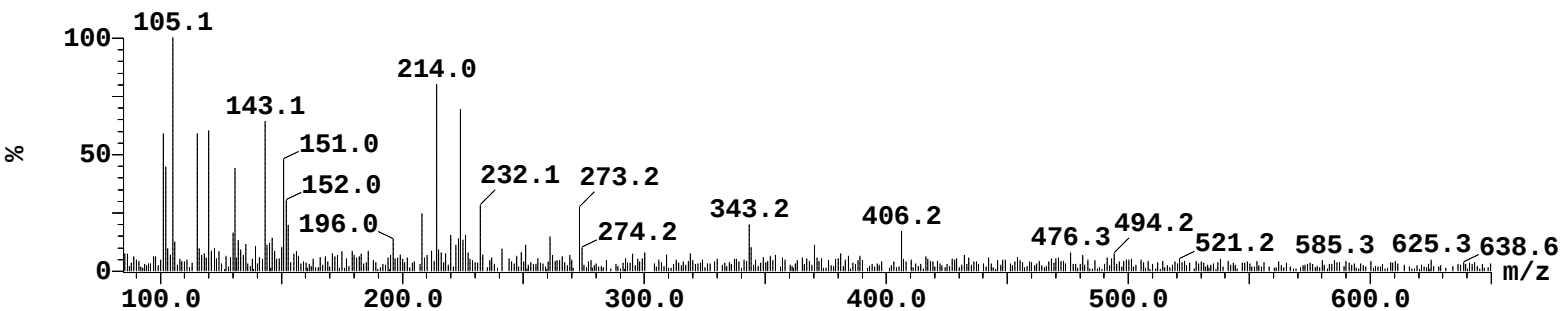
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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9		1.70	
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9: (Time: 1.70)

7.7e+002

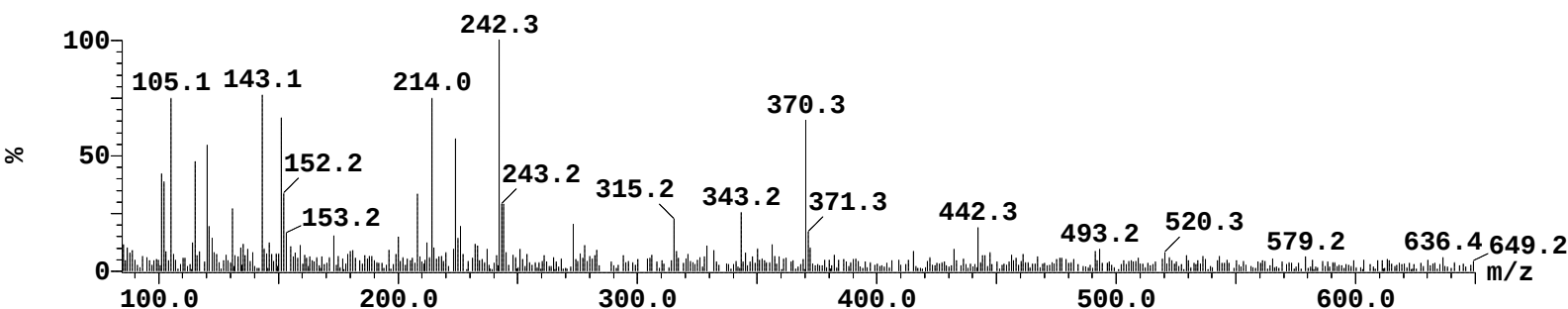


Peak ID	Compound	Time	Mass Found
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10		1.82	
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10: (Time: 1.82)

6.3e+002

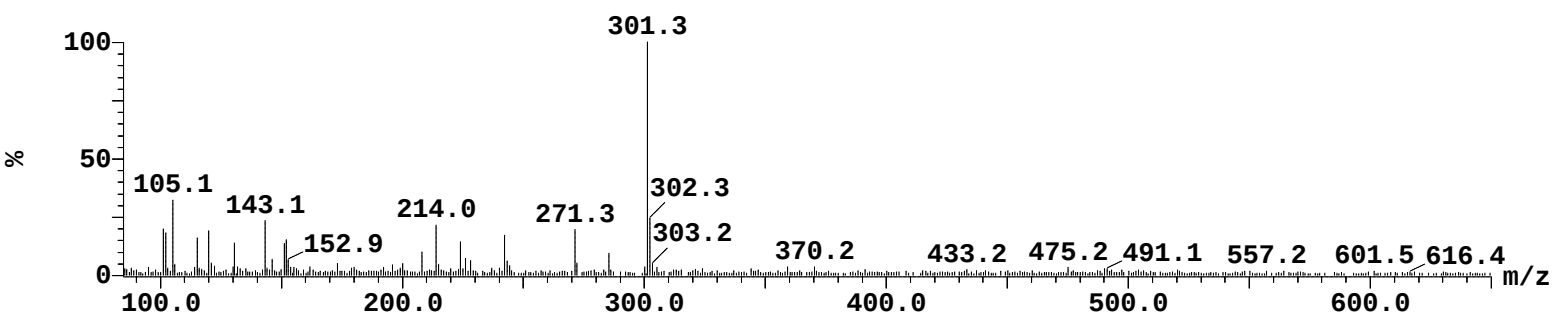


Peak ID	Compound	Time	Mass Found
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12		1.92	
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12: (Time: 1.92)

3.7e+003

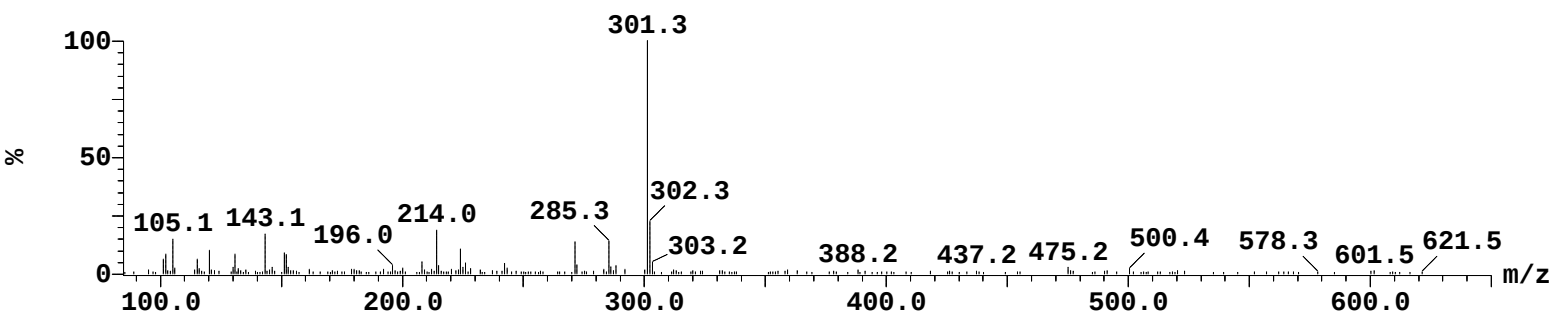


Peak ID	Compound	Time	Mass Found
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13		1.99	
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13: (Time: 1.99)

3.7e+003



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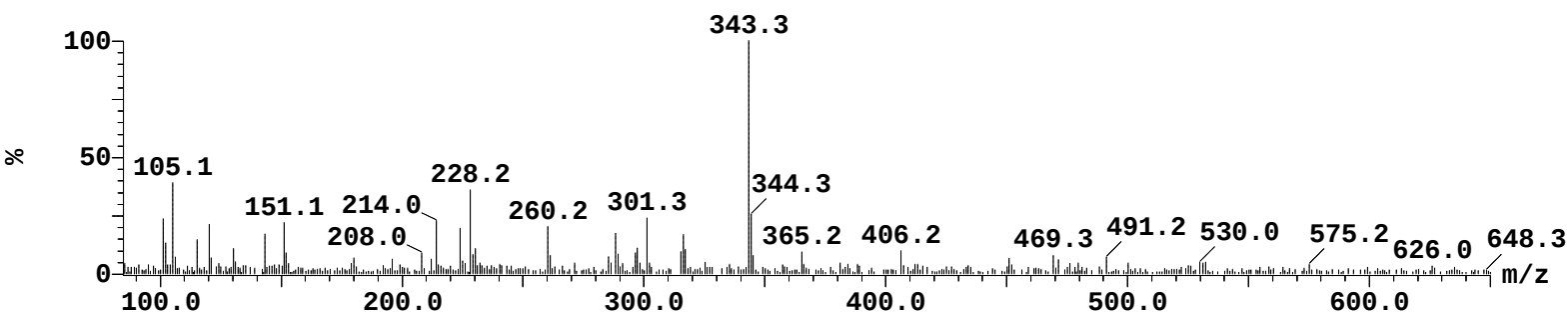
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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14		2.12	
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14: (Time: 2.12)

1.6e+003

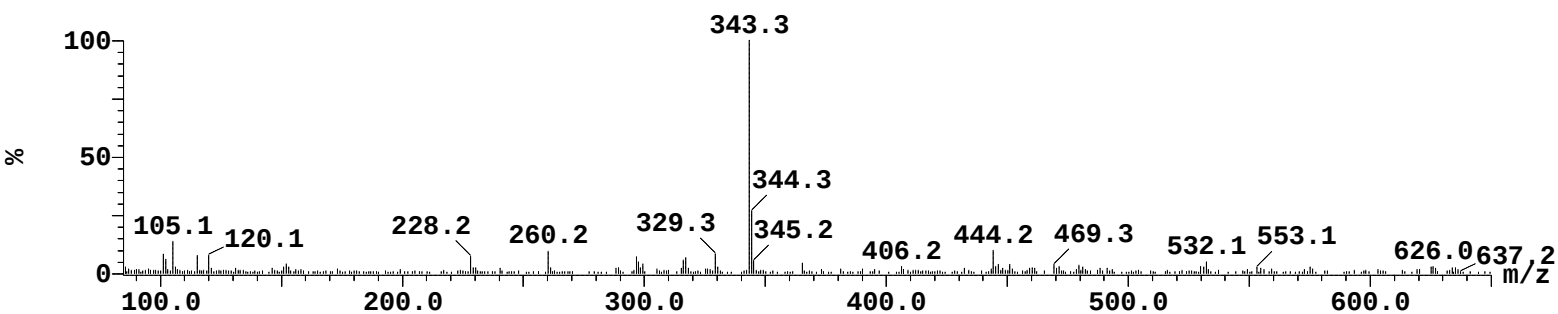


Peak ID	Compound	Time	Mass Found
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15		2.19	
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15: (Time: 2.19)

5.6e+003

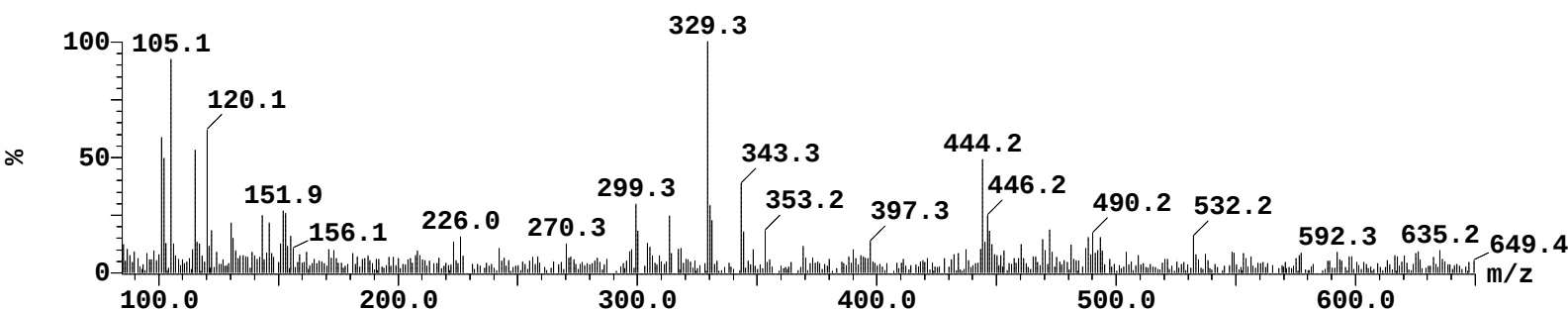


Peak ID	Compound	Time	Mass Found
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18		2.31	
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18: (Time: 2.31)

9.1e+002

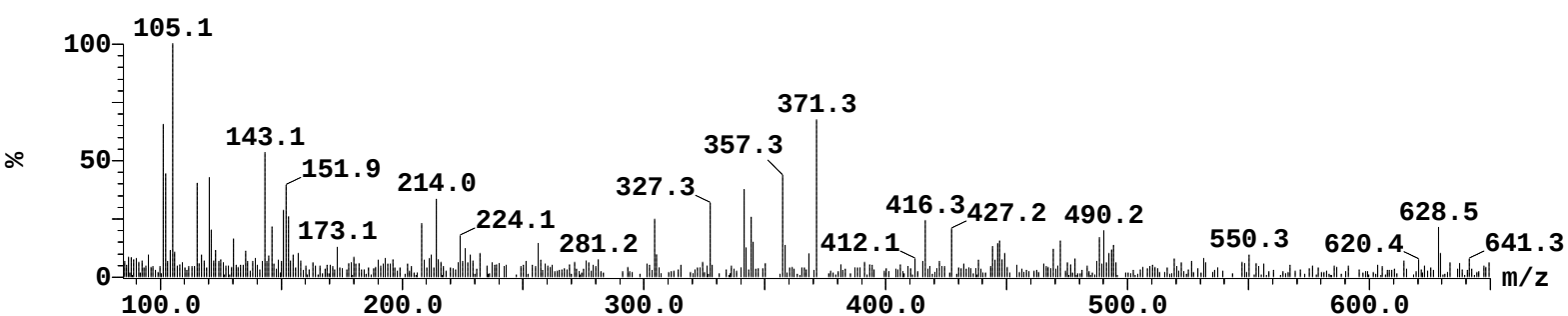


Peak ID	Compound	Time	Mass Found
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19		2.49	
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19: (Time: 2.49)

8.4e+002



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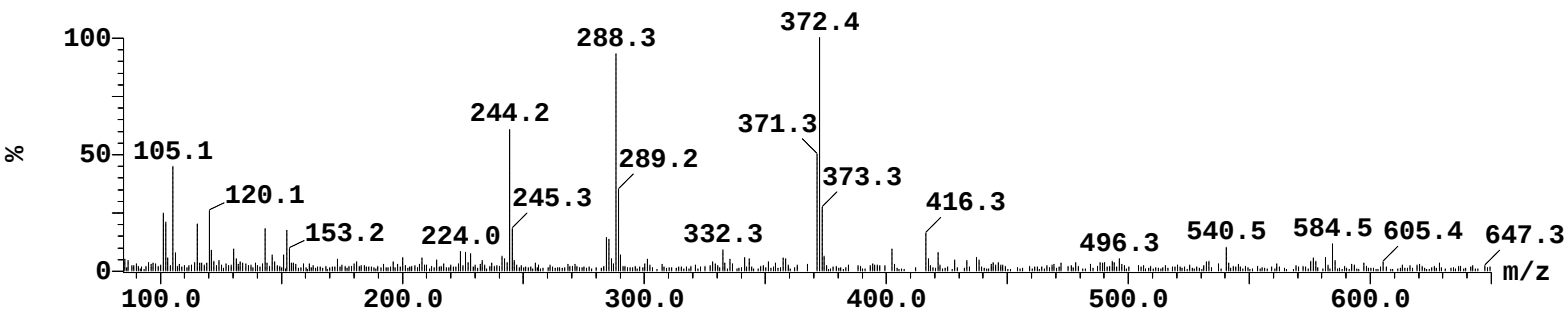
Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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21		2.63	
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21:(Time: 2.63)

3.5e+003

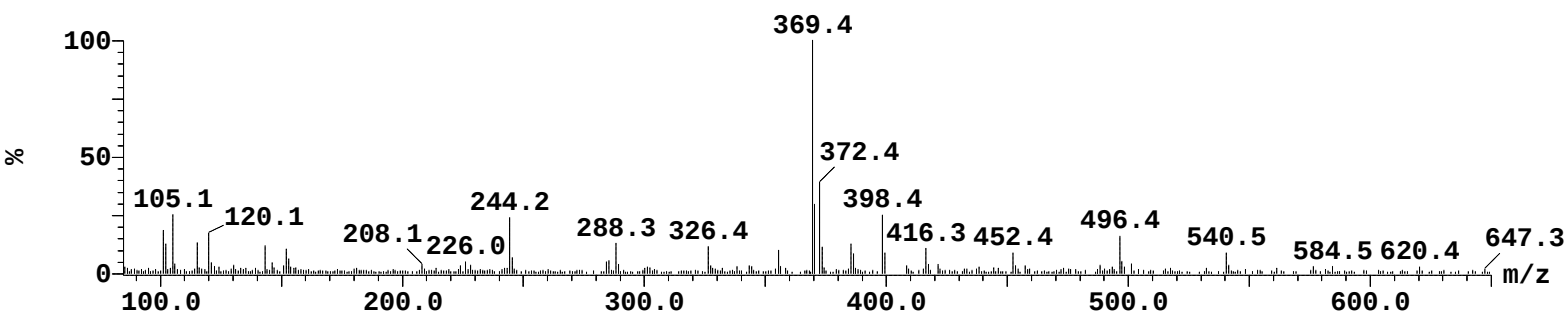


Peak ID	Compound	Time	Mass Found
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22		2.76	
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22:(Time: 2.76)

5.9e+003

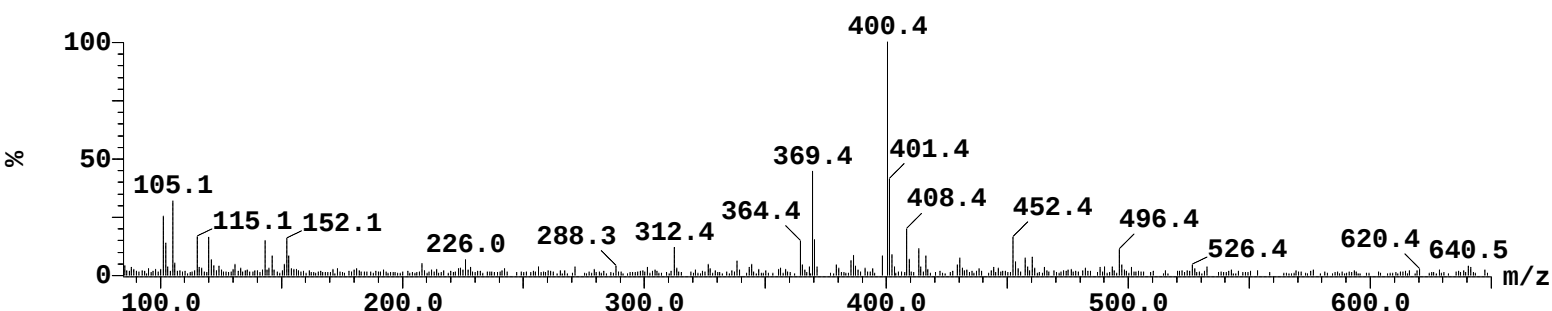


Peak ID	Compound	Time	Mass Found
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23		2.90	
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23:(Time: 2.88)

4.7e+003

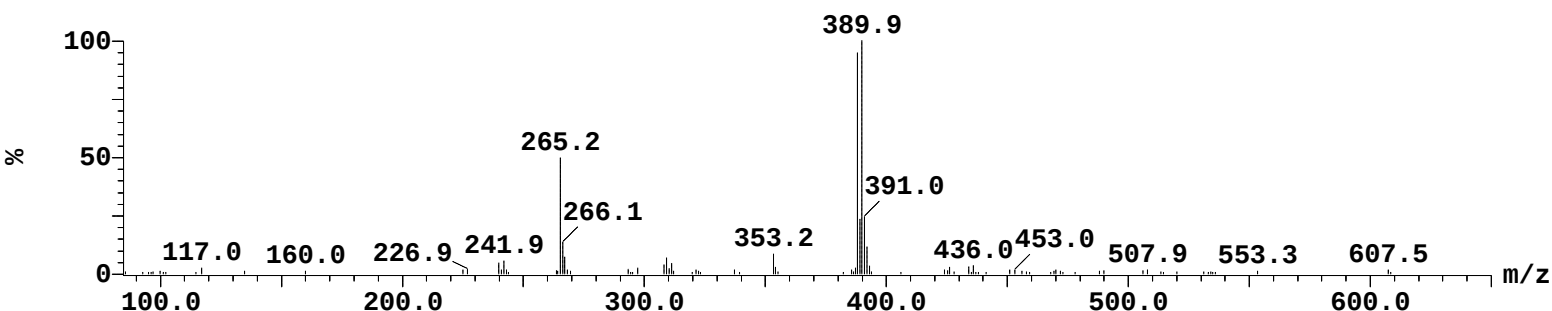


Peak ID	Compound	Time	Mass Found
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17	Found	2.25	390.00
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17:(Time: 2.25)

2.2e+004



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