

Single Mass Analysis

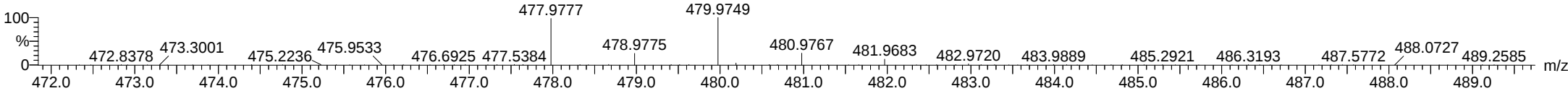
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
237 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-20 H: 0-100 N: 0-10 O: 0-10 Na: 0-1 S: 2-2 Br: 1-1

A.ZUBIARRE AZ 315 1 (VIAL 315 2)
MS49539 92 (2.819)

ES-ToF

09-Nov-2018
2: TOF MS ES-
2.70e+003



Minimum: -1.5
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula						
477.9777	477.9782	-0.5	-1.0	12.5	51.8	0.0	C20	H17	N	O4	S2	Br	

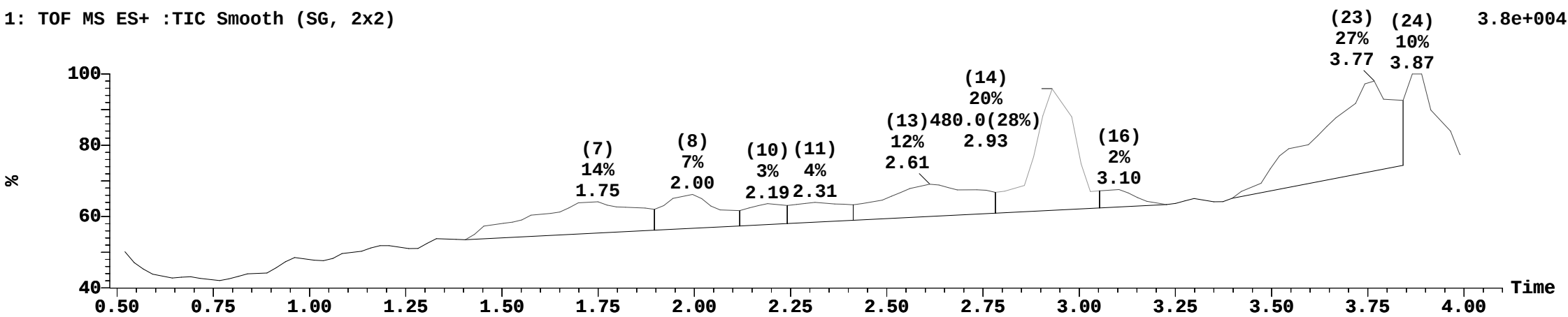
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Printed: Fri Nov 09 15:33:36 2018

Sample Report:

Sample 2 Vial 1:11 ID File MS49539 Date 09-Nov-2018 Time 2::2::5 Description A.ZUBIARRE AZ 315 1 (VIAL 315 2)

1: TOF MS ES+ :TIC Smooth (SG, 2x2)



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
7		1.75	1e+003	13.61	1	3e+003	
8		2.00	6e+002	7.23	0	4e+003	
10		2.19	3e+002	3.07	0	2e+003	
11		2.31	3e+002	4.08	0	2e+003	
13		2.61	1e+003	11.87	0	3e+003	
14	Found	2.93	2e+003	20.24	0	1e+004	480.00
16		3.10	2e+002	2.33	0	2e+003	
23		3.77	2e+003	27.24	0	1e+004	
24		3.87	8e+002	10.35	0	1e+004	

Sample: 2
File:MS49539
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Vial:1:11
Date:09-Nov-2018

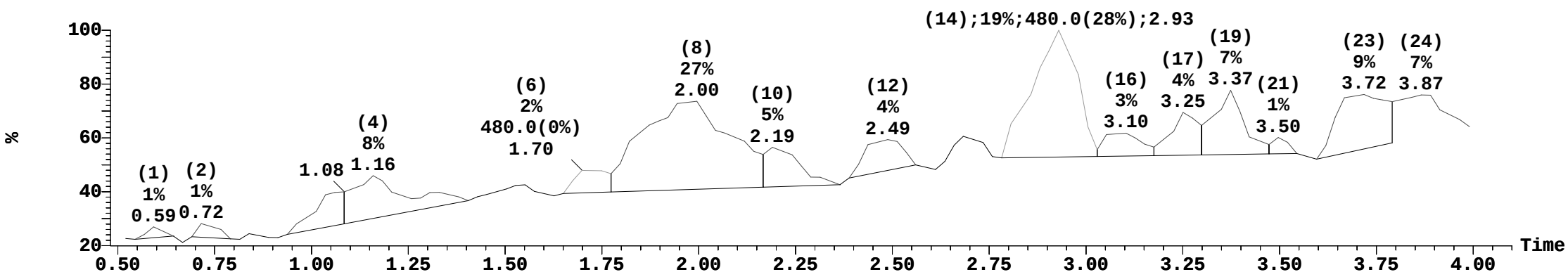
ID:
Time:2::2::5

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Sample Report (continued):

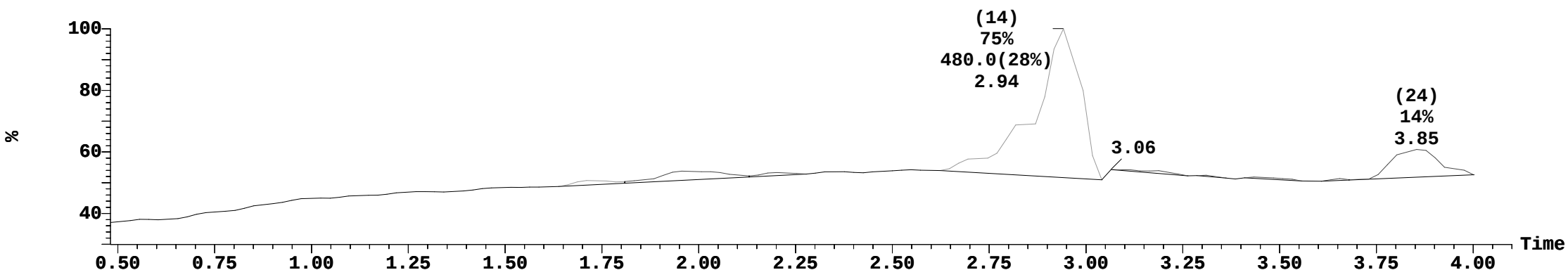
1: TOF MS ES+ :480+503+481 Smooth (SG, 2x2)

1.1e+002



2: TOF MS ES- :TIC Smooth (SG, 2x2)

4.4e+004



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
6	Tentative	1.71	7e+001	1.67	0	6e+002	480.00
8		1.96	2e+002	5.95	0	1e+003	
10		2.20	4e+001	0.99	0	4e+002	
14	Found	2.94	3e+003	75.16	0	2e+004	480.00
16		3.06	4e+001	0.93	0		
18		3.31	6e+000	0.16	0	2e+002	
20		3.43	2e+001	0.59	0	2e+002	
22		3.66	1e+001	0.28	0	3e+002	
24		3.85	6e+002	14.26	0	4e+003	

Sample: 2
 File:MS49539
 Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Vial:1:11
 Date:09-Nov-2018

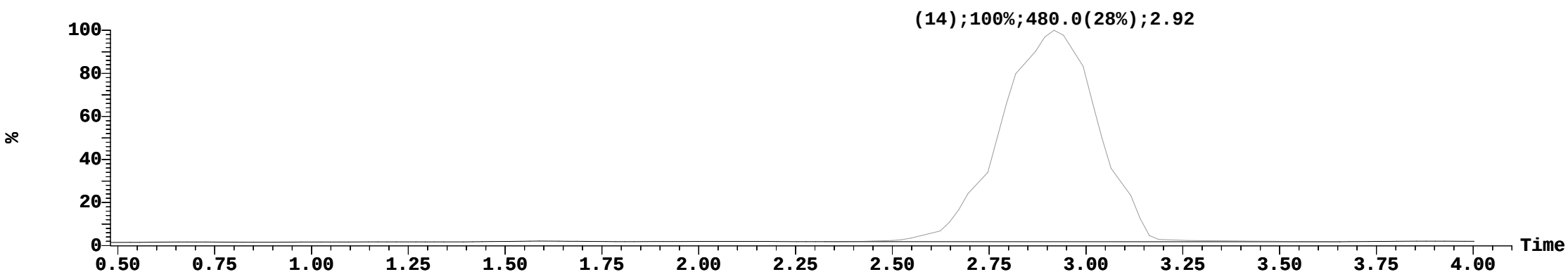
ID:
 Time:2::2::5

Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

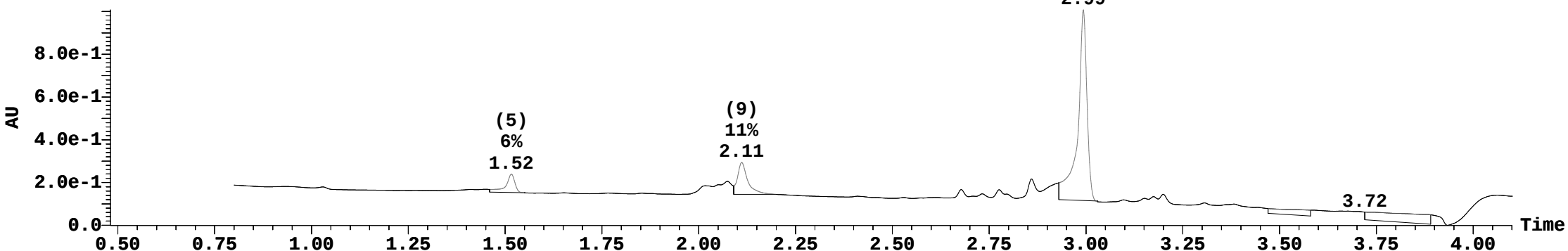
2: TOF MS ES- :480+525+479 Smooth (Mn, 2x3)

3.8e+003



5: UV Detector: 244_264 Smooth (SG, 5x5)

1.008
 Range: 1.008



Sample: 2
File:MS49539
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Vial:1:11
Date:09-Nov-2018

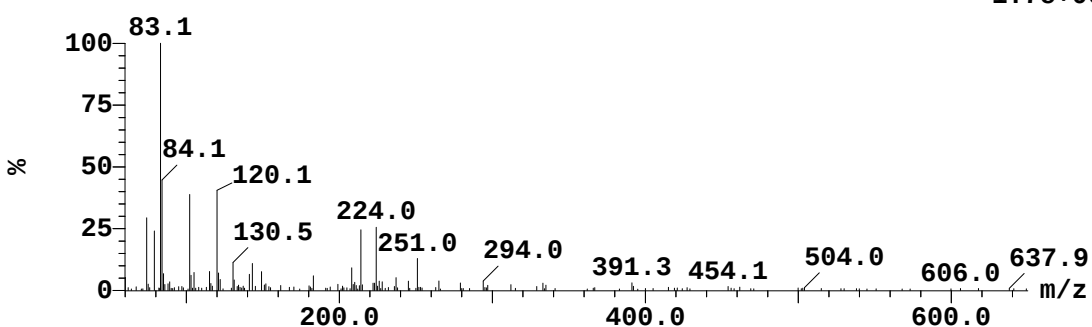
ID:
Time:2::2::5

Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

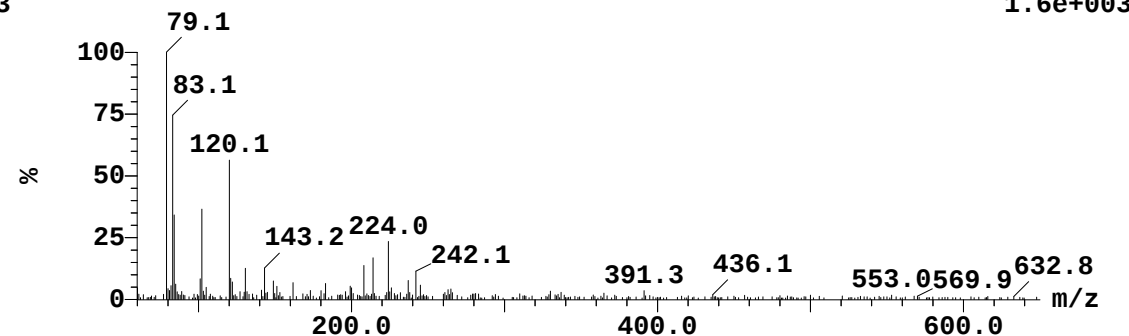
Peak ID	Compound	Time	Mass Found
1		0.59	

1:(Time: 0.59) Combine (18:21-(13:14+26))



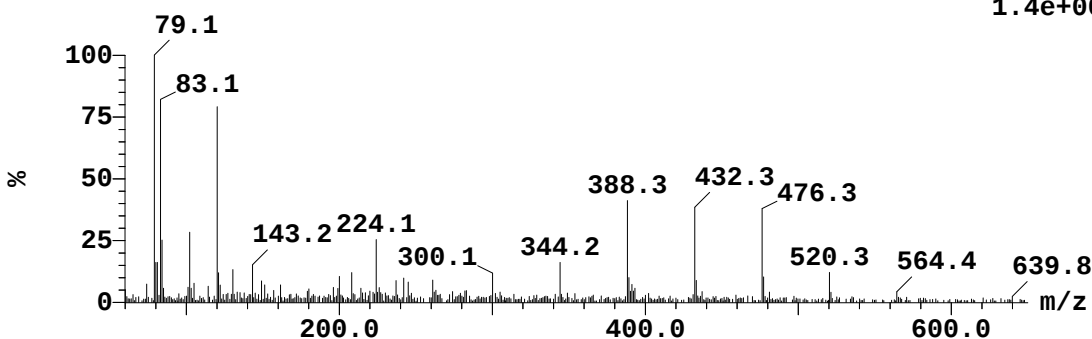
Peak ID	Compound	Time	Mass Found
2		0.72	

1:TOF MS ES+ 2:(Time: 0.72) Combine (22:25-(17:18+30)) 1.7e+003



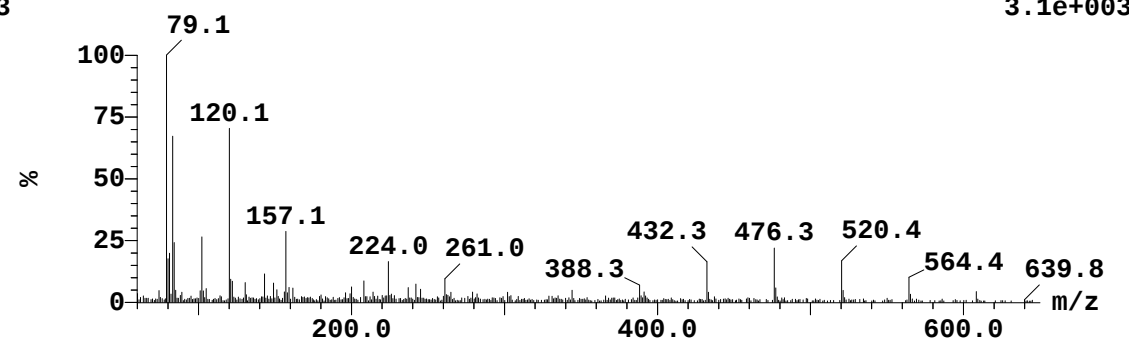
Peak ID	Compound	Time	Mass Found
3		1.08	

3:(Time: 1.08) Combine (34:37-(29:30+42))



Peak ID	Compound	Time	Mass Found
4		1.16	

1:TOF MS ES+ 4:(Time: 1.16) Combine (36:40-(32+44:45)) 3.1e+003



Sample: 2
File:MS49539
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

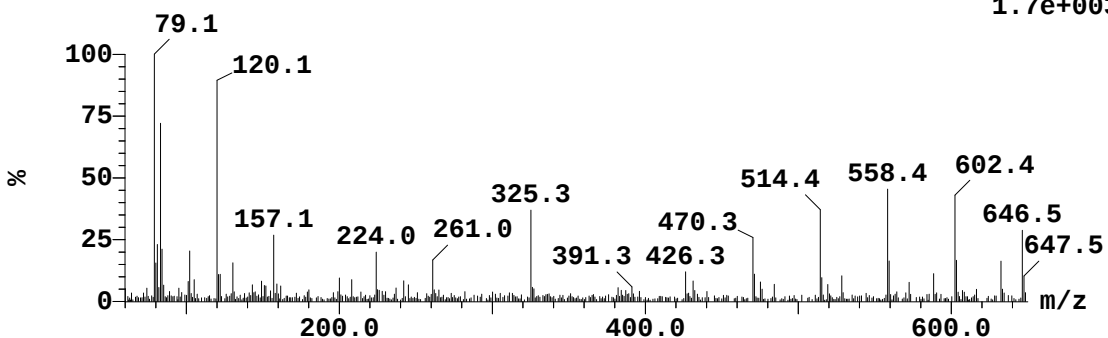
Vial:1:11
Date:09-Nov-2018

ID:
Time:2::2::5

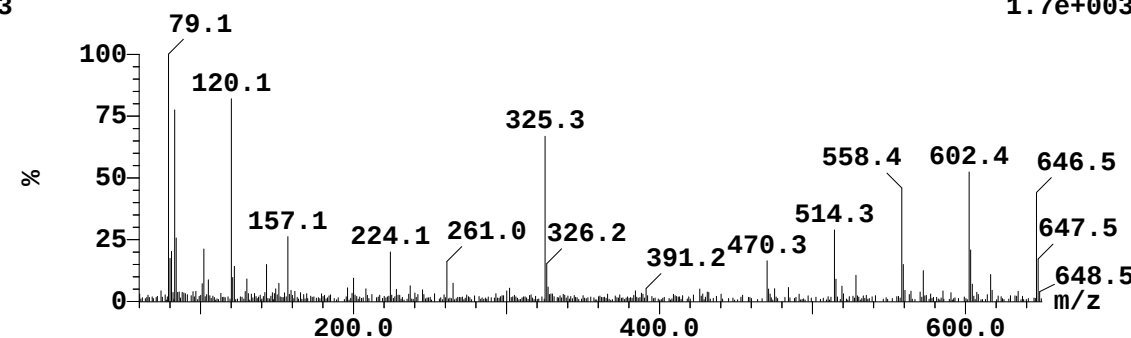
Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

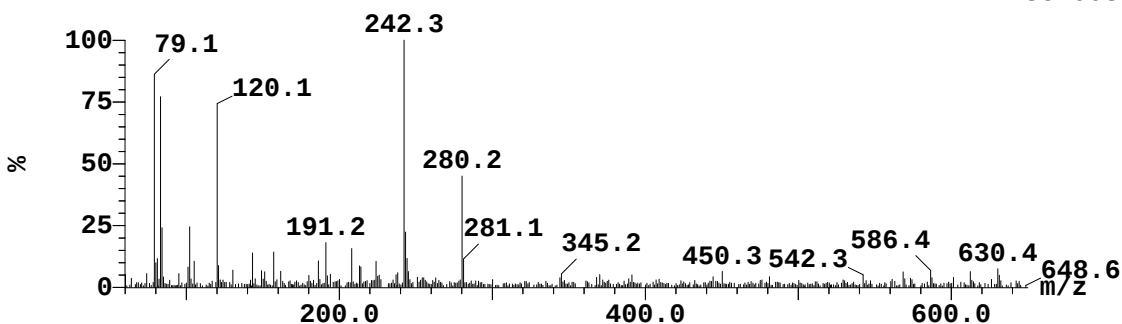
Peak ID Compound Time Mass Found
6
1.70
6:(Time: 1.70) Combine (54:57-(49:50+62))



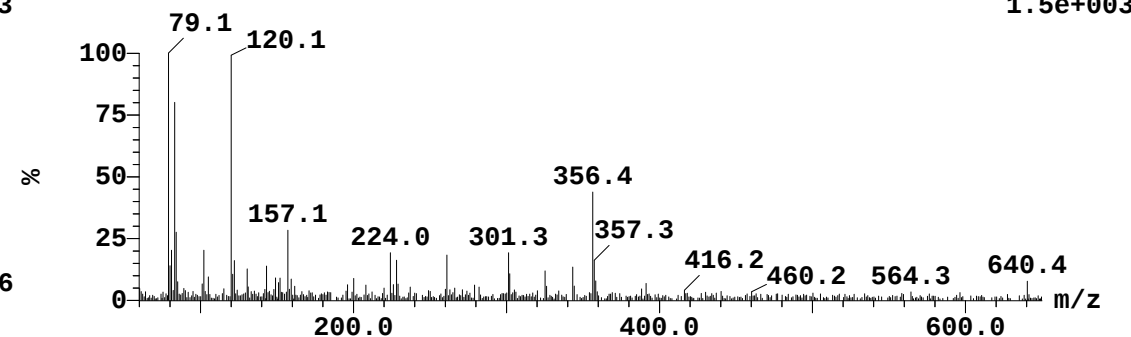
Peak ID Compound Time Mass Found
7
1.75
7:(Time: 1.75) Combine (56:59-(51+63:64))



Peak ID Compound Time Mass Found
8
2.00
8:(Time: 2.00) Combine (64:67-(59+71:72))



Peak ID Compound Time Mass Found
10
2.19
10:(Time: 2.19) Combine (70:73-(65:66+78))



Sample: 2

Vial:1:11

ID:

File:MS49539

Date:09-Nov-2018

Time:2::2::5

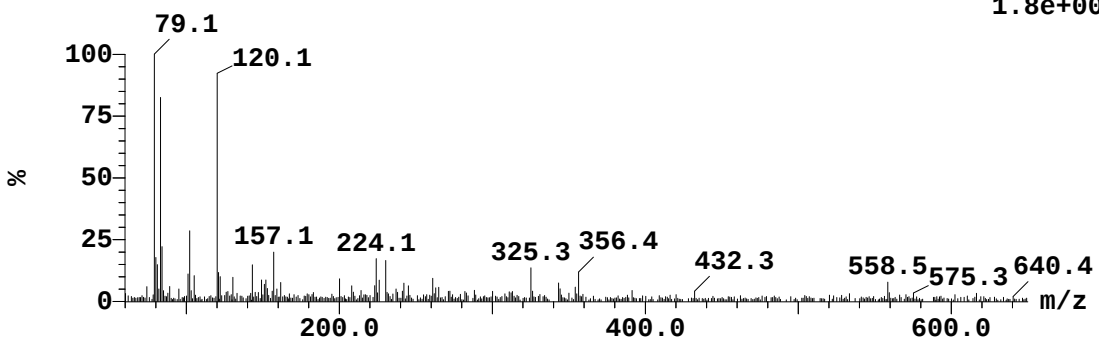
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

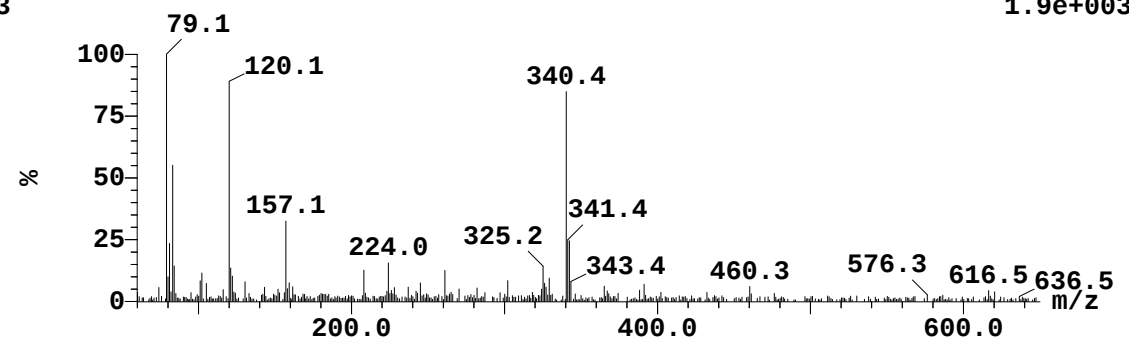
Peak ID	Compound	Time	Mass Found
11		2.31	

11:(Time: 2.31) Combine (74:77-(69:70+82))



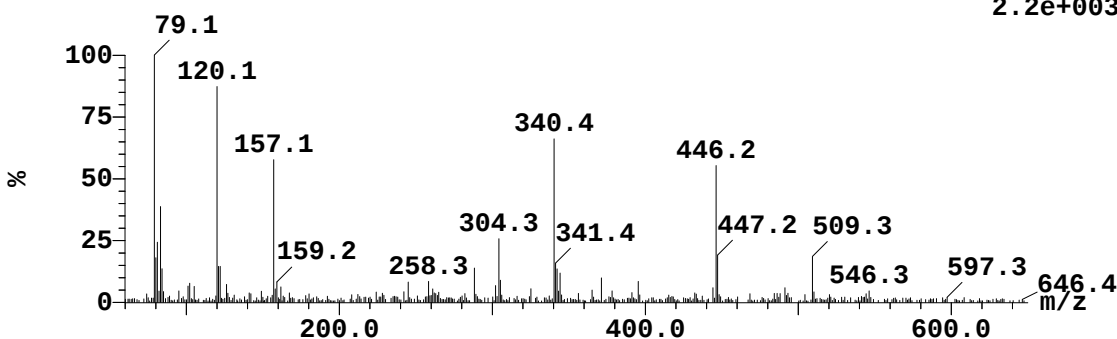
Peak ID	Compound	Time	Mass Found
12		2.49	

12:(Time: 2.49) Combine (80:83-(75+87:88))



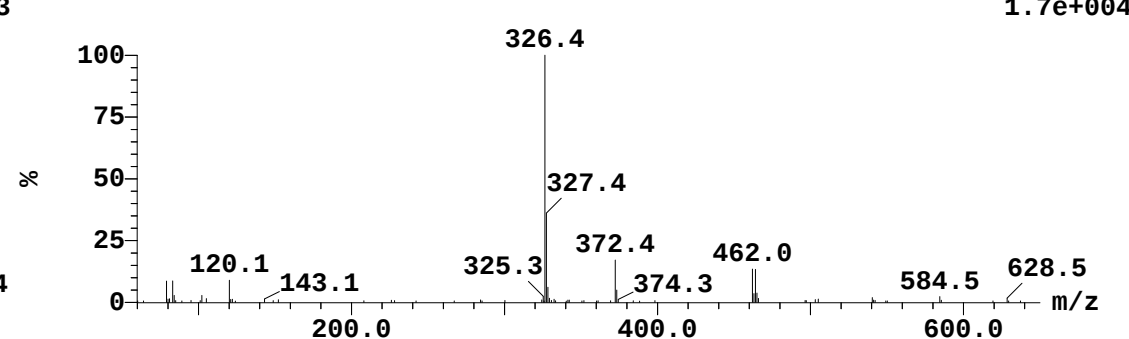
Peak ID	Compound	Time	Mass Found
13		2.61	

13:(Time: 2.61) Combine (84:87-(79+91:92))



Peak ID	Compound	Time	Mass Found
14		2.93	

14:(Time: 2.93) Combine (94:97-(89:90+102))



Sample: 2
File:MS49539
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Vial:1:11
Date:09-Nov-2018

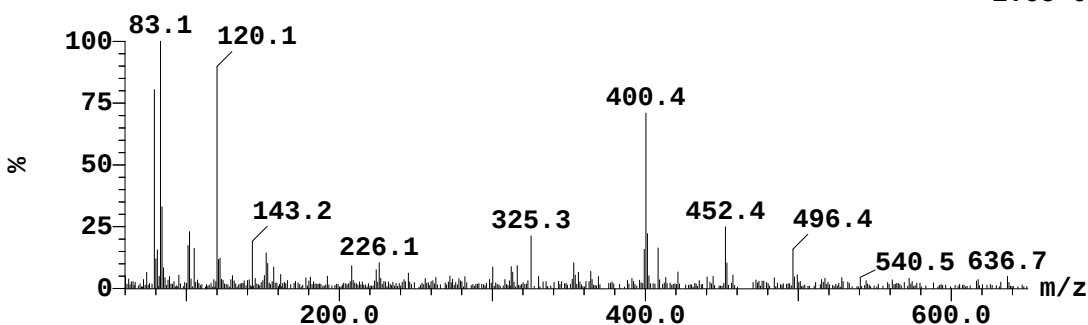
ID:
Time:2::2::5

Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

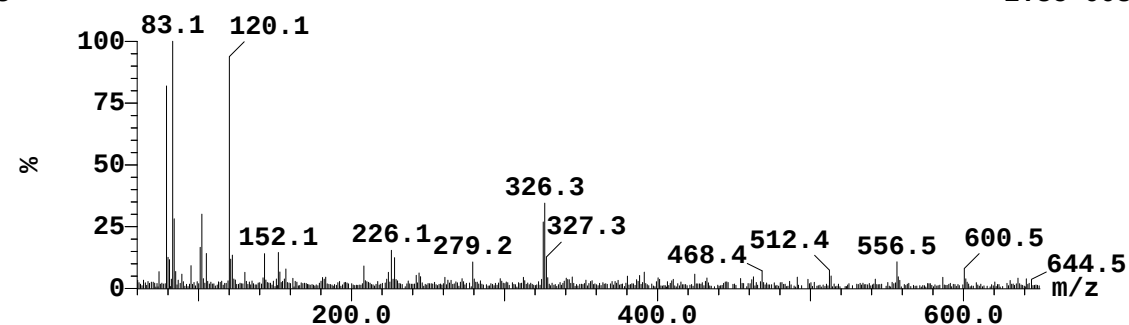
Peak ID	Compound	Time	Mass Found
16		3.10	

16:(Time: 3.10) Combine (100:103-(95+107:108))



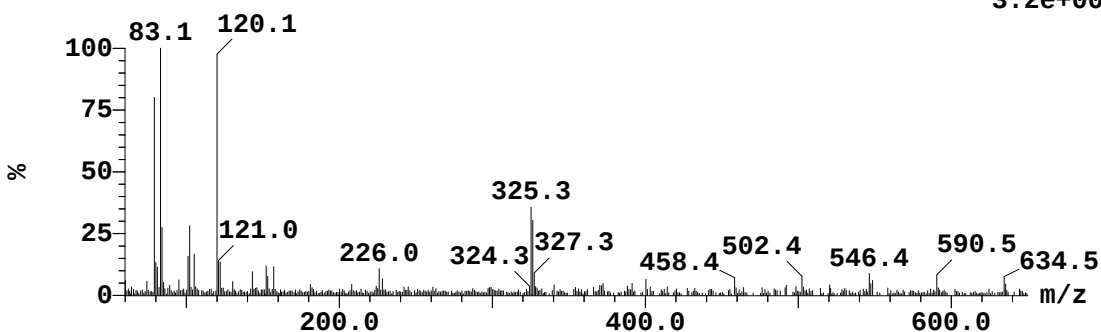
Peak ID	Compound	Time	Mass Found
17		3.25	

17:(Time: 3.25) Combine (104:108-(100+112:113))



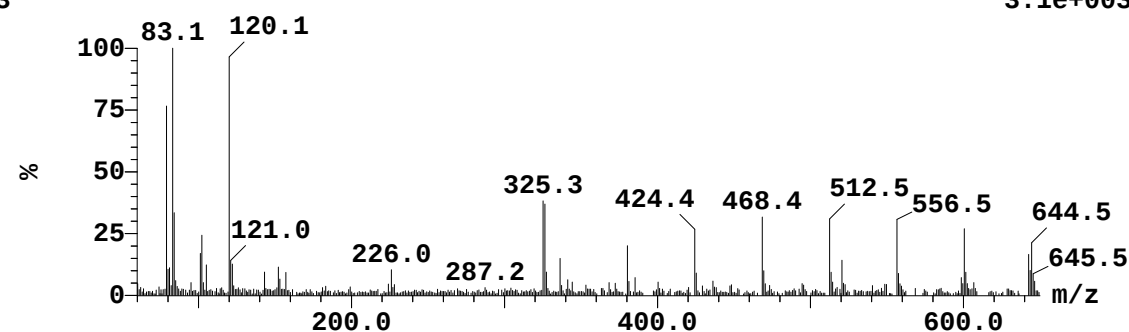
Peak ID	Compound	Time	Mass Found
19		3.37	

19:(Time: 3.37) Combine (108:112-(104+116:117))



Peak ID	Compound	Time	Mass Found
21		3.50	

21:(Time: 3.50) Combine (112:116-(108+120:121))



Sample: 2

Vial:1:11

ID:

File:MS49539

Date:09-Nov-2018

Time:2::2::5

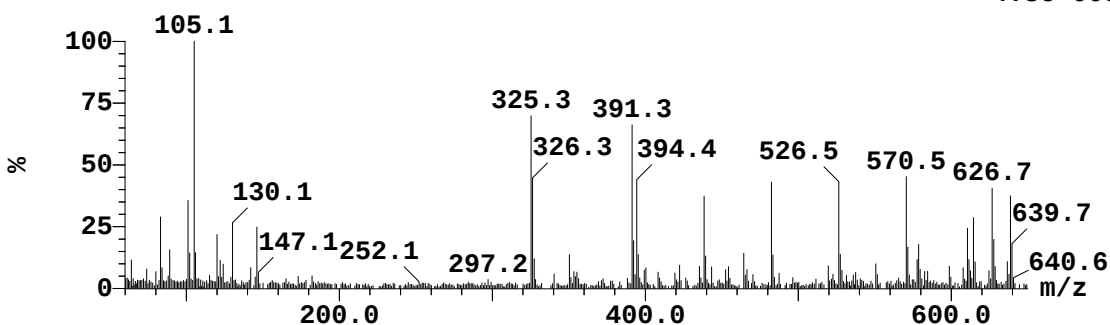
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
23		3.77	

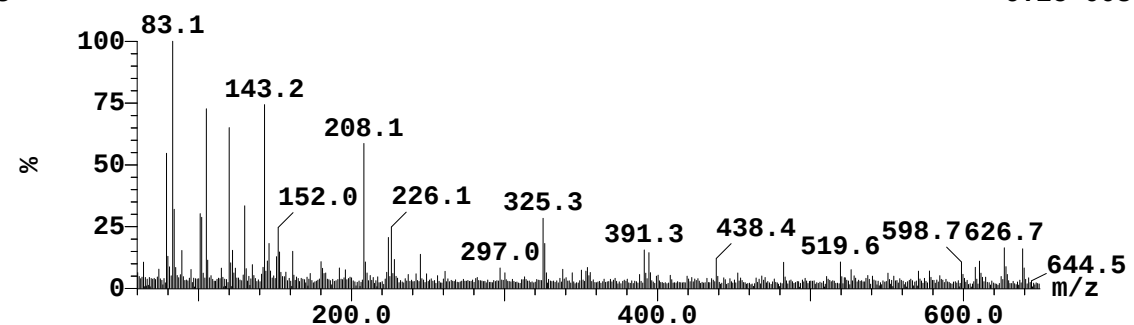
23:(Time: 3.77) Combine (121:125-(116:117+129))



Peak ID	Compound	Time	Mass Found
24		3.87	

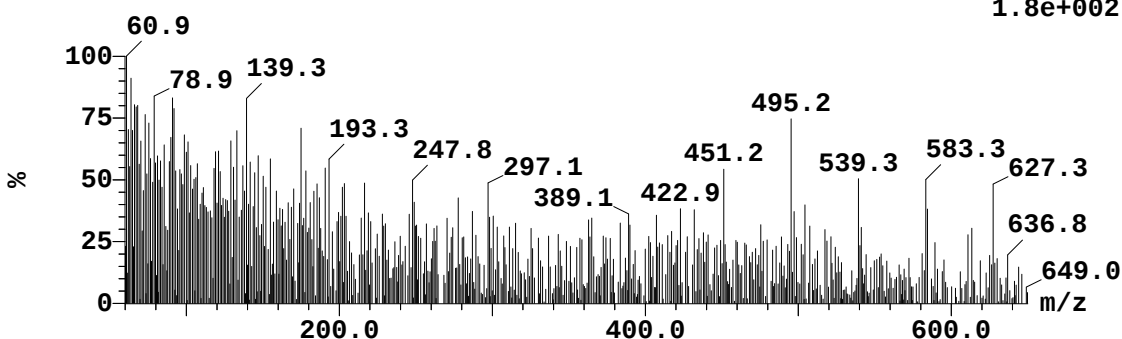
24:(Time: 3.87) Combine (124:128-(120+1:-1))

1:TOF MS ES+ 6.2e+003



Peak ID	Compound	Time	Mass Found
6	Tentative	1.70	,525.00,479.00

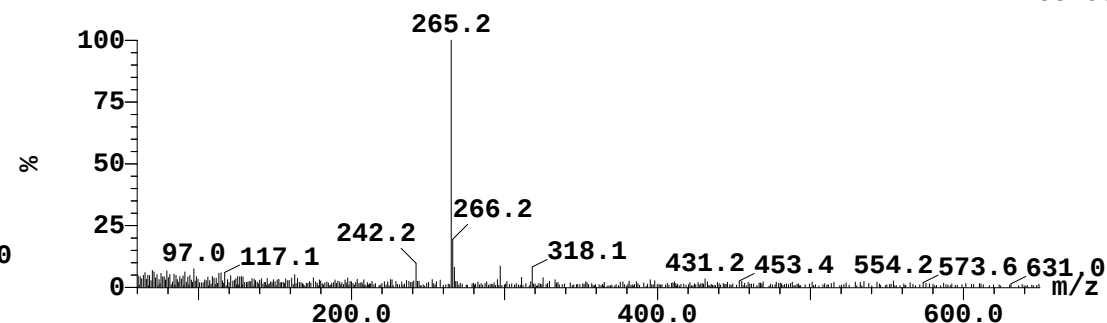
6:(Time: 1.71) Combine (54:57-(49:50+62))



Peak ID	Compound	Time	Mass Found
8		2.00	

8:(Time: 1.96) Combine (62:65-(57:58+70))

2:TOF MS ES- 2.6e+003



Sample: 2

File:MS49539

Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

Vial:1:11

Date:09-Nov-2018

ID:

Time:2::2::5

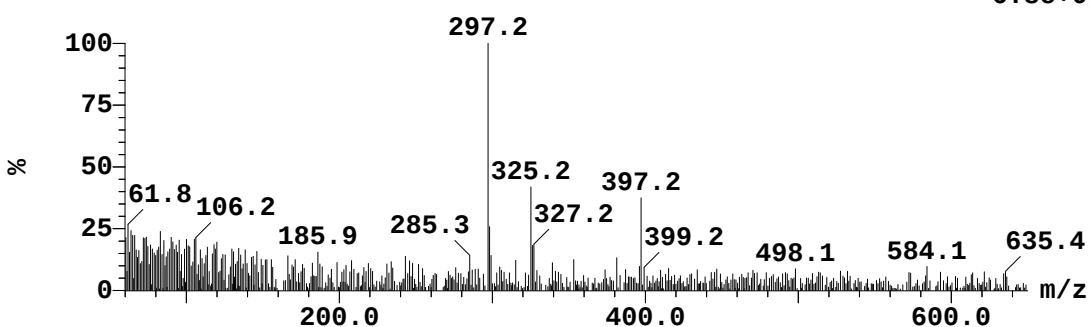
Printed: Fri Nov 09 15:33:36 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
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10		2.19	
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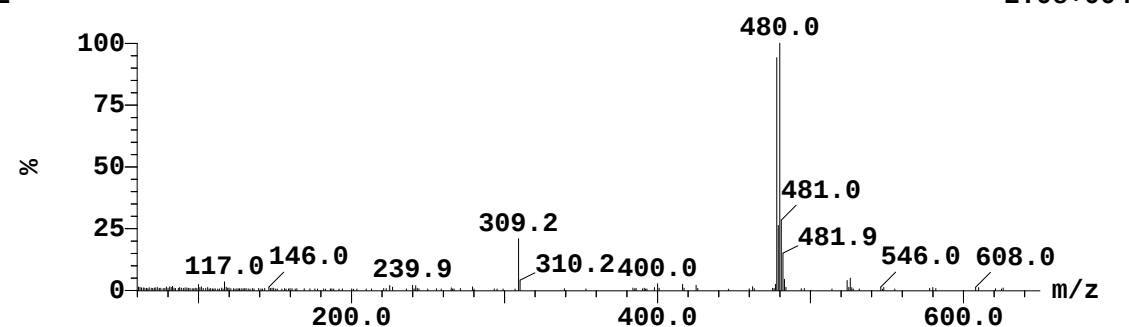
10:(Time: 2.20) Combine (70:73-(65:66+78))



Peak ID	Compound	Time	Mass Found
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14	Found	2.93	,525.00,479.00
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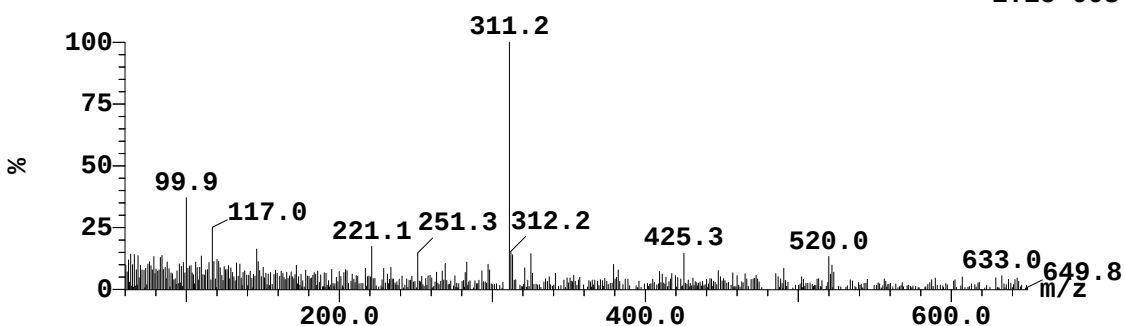
14:(Time: 2.92) Combine (93:97-(88:89+101))



Peak ID	Compound	Time	Mass Found
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16		3.10	
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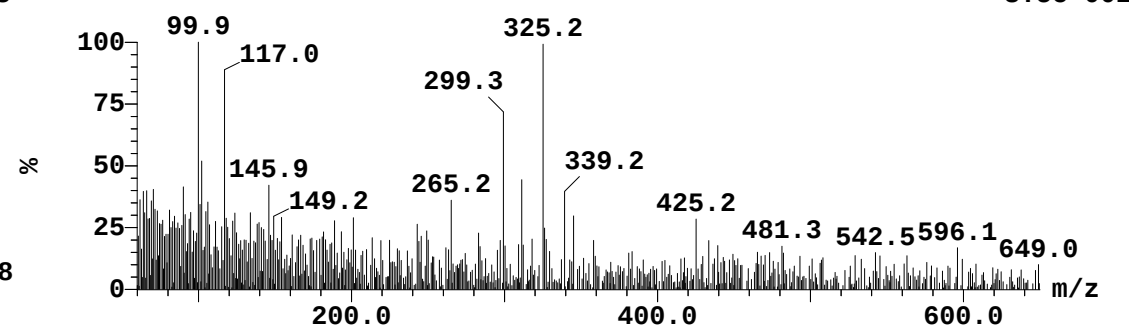
16:(Time: 3.06) Combine (98:101-(93:94+106))



Peak ID	Compound	Time	Mass Found
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18		3.31	
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18:(Time: 3.31) Combine (106:109-(101:102+114))



Sample: 2

Vial:1:11

ID:

File:MS49539

Date:09-Nov-2018

Time:2::2::5

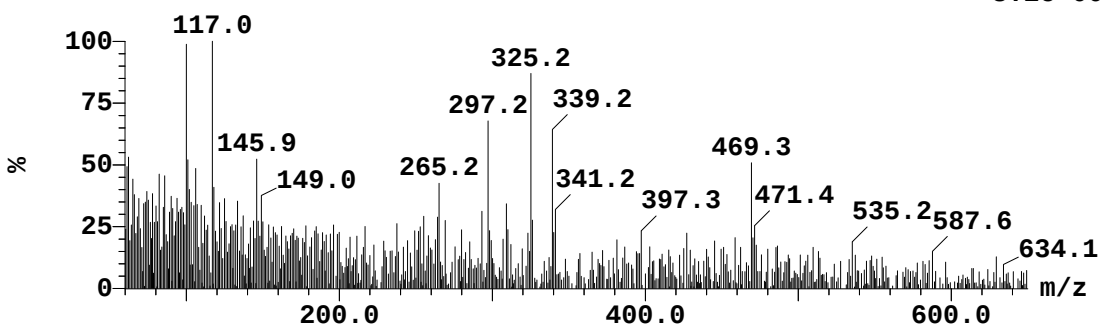
Description:A.ZUBIARRE AZ 315 1 (VIAL 315 2)

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Sample Report (continued):

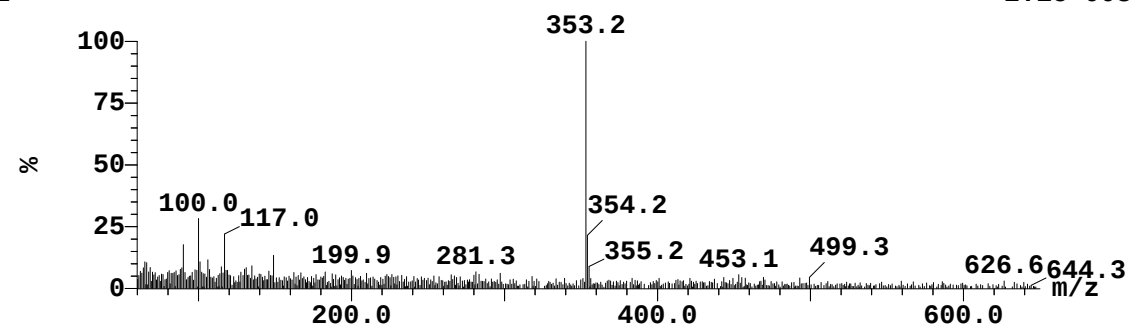
Peak ID	Compound	Time	Mass Found
20		3.43	

20:(Time: 3.43) Combine (110:113-(105:106+118))



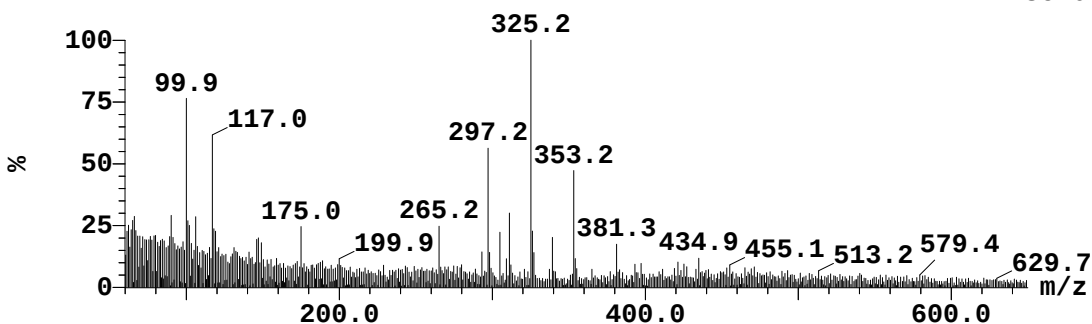
Peak ID	Compound	Time	Mass Found
22		3.66	

22:(Time: 3.66) Combine (117:121-(112:113+125))



Peak ID	Compound	Time	Mass Found
24		3.87	

24:(Time: 3.85) Combine (124:127-(119+1:-1))



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