

Single Mass Analysis

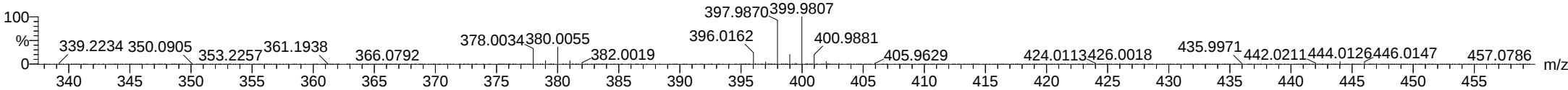
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
659 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 16-16 H: 0-100 N: 0-10 O: 0-14 F: 1-1 Na: 0-1 S: 1-3 Br: 1-1

A.ZUBIARRE AZ 333 1
MS50272 88 (2.691)

ES-ToF

14-Dec-2018
2: TOF MS ES-
8.76e+003



Minimum: -1.5
Maximum: 5.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula						
397.9870	397.9862	0.8	2.0	9.5	92.2	0.0	C16	H14	N	O3	F	S	Br

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Sample: 4
File:MS50272
Description:A.ZUBIARRE AZ 333 1

Vial:1:45
Date:14-Dec-2018

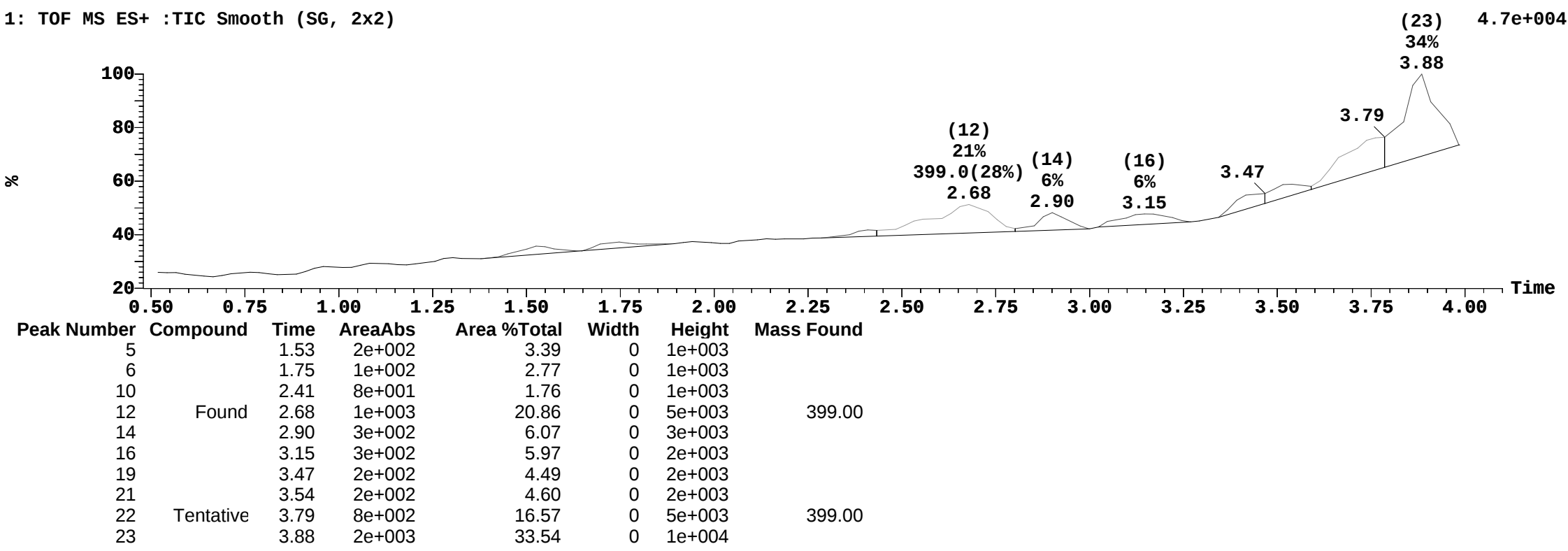
ID:
Time:9::9::8

Printed: Fri Dec 14 10:45:27 2018

Sample Report:

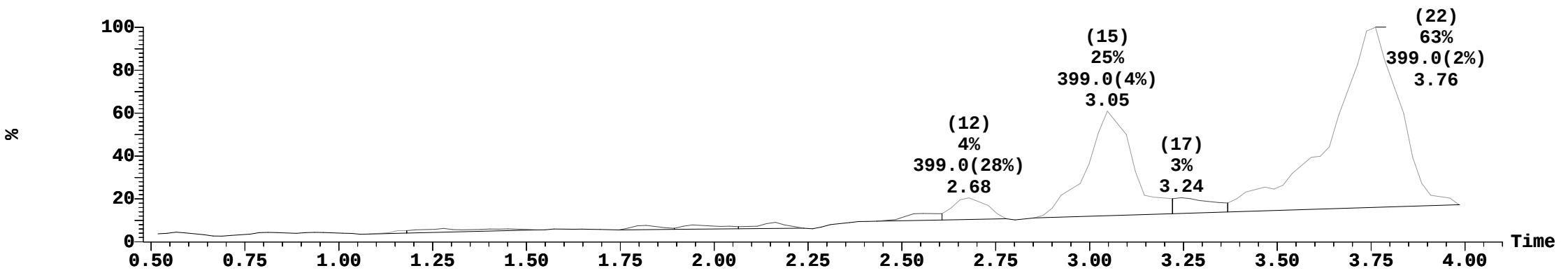
Sample 4 Vial 1:45 ID File MS50272 Date 14-Dec-2018 Time 9::9::8 Description A.ZUBIARRE AZ 333 1

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

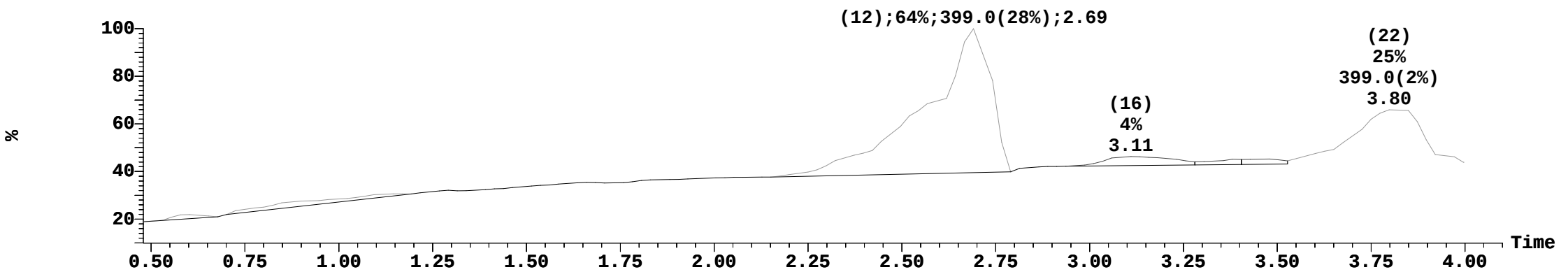


Sample Report (continued):

1: TOF MS ES+ :399+422+400 Smooth (SG, 2x2) 5.7e+002



2: TOF MS ES- :TIC Smooth (SG, 2x2) 4.8e+004

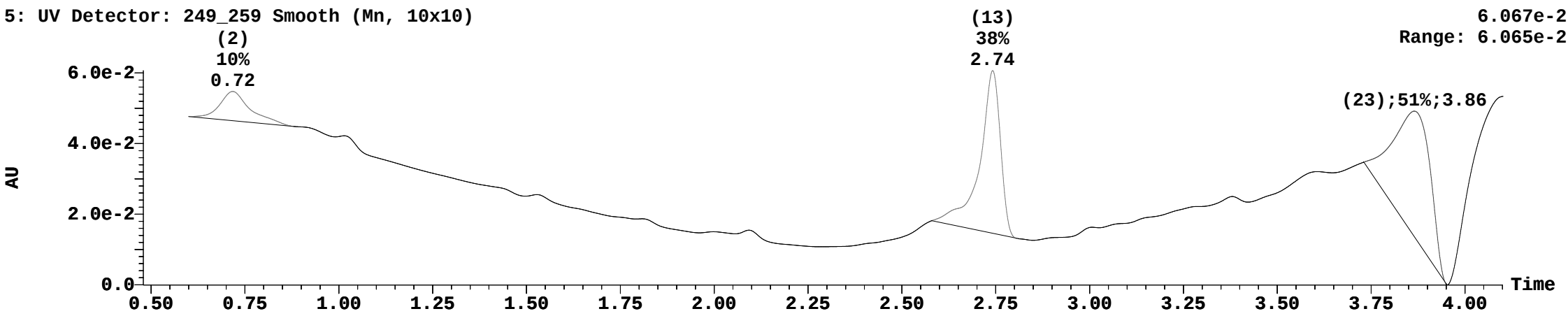
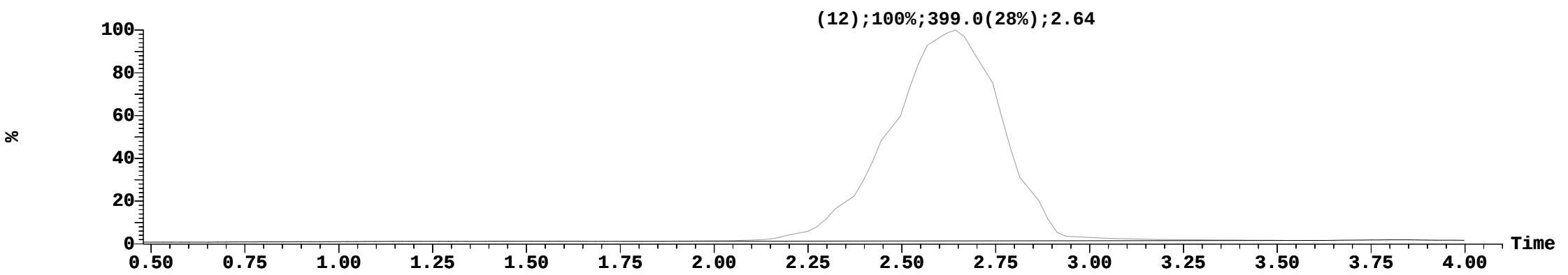


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Tentative	0.60	8e+001	0.83	0	8e+002	399.00
3	Tentative	1.14	3e+002	3.46	0	4e+002	399.00
12	Found	2.69	6e+003	64.10	1	3e+004	399.00
16		3.11	4e+002	4.06	0	2e+003	
18		3.38	1e+002	1.09	0	1e+003	
20		3.48	1e+002	1.27	0	1e+003	
22	Tentative	3.80	2e+003	25.19	0	1e+004	399.00

Sample Report (continued):

2: TOF MS ES- :399+444+398 Smooth (Mn, 2x3)

5.1e+003



Sample: 4
File:MS50272
Description:A.ZUBIARRE AZ 333 1

Vial:1:45
Date:14-Dec-2018

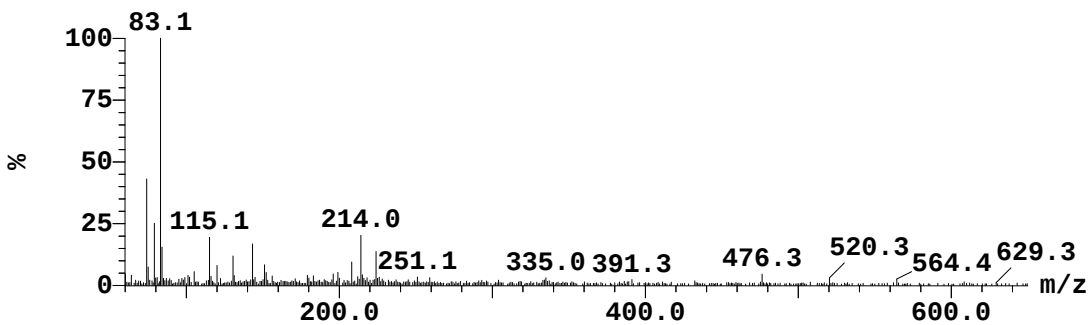
ID:
Time:9::9::8

Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

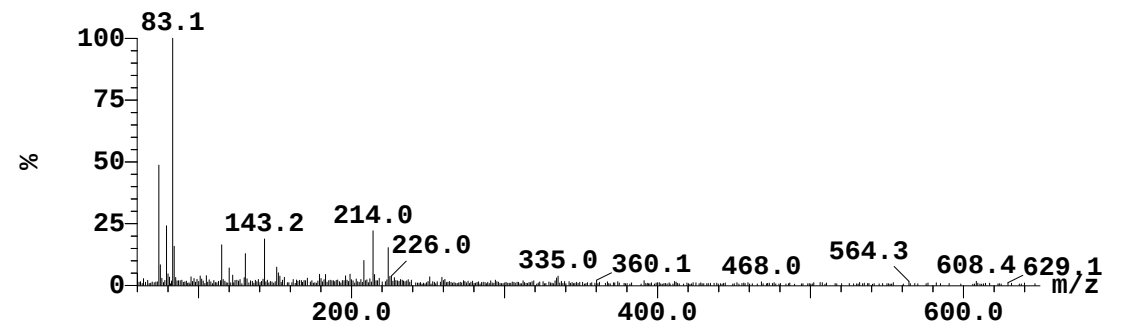
Peak ID	Compound	Time	Mass Found
3		1.18	

3:(Time: 1.18) Combine (37:41-(32:33+45))



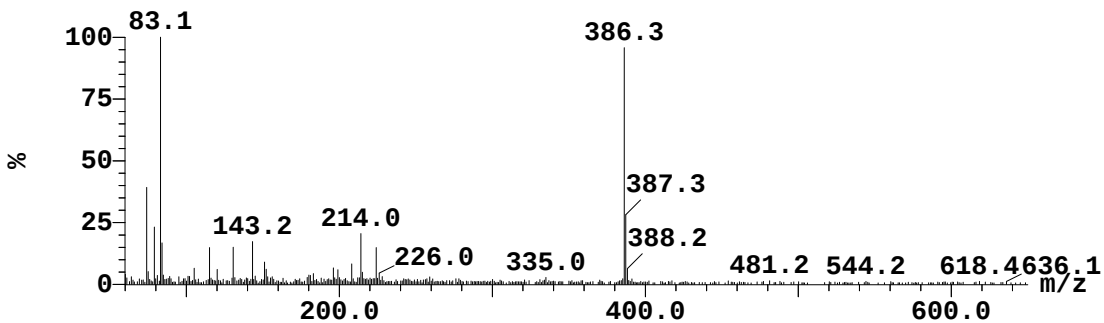
Peak ID	Compound	Time	Mass Found
4		1.28	

1:TOF MS ES+ 4:(Time: 1.28) Combine (40:44-(36+48:49)) 3.1e+003



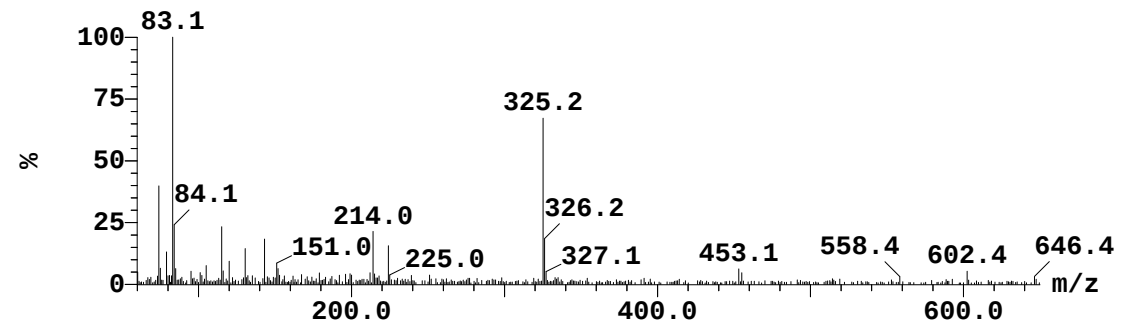
Peak ID	Compound	Time	Mass Found
5		1.53	

5:(Time: 1.53) Combine (48:52-(44+56:57))



Peak ID	Compound	Time	Mass Found
6		1.75	

1:TOF MS ES+ 6:(Time: 1.75) Combine (56:59-(51+63:64)) 3.3e+003



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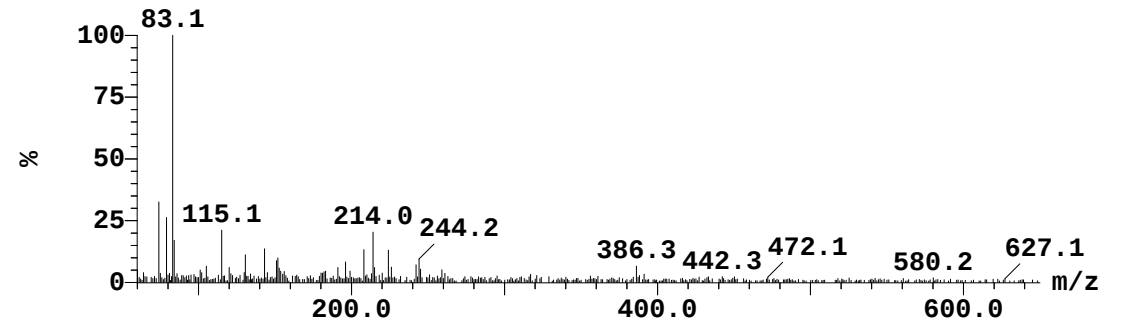
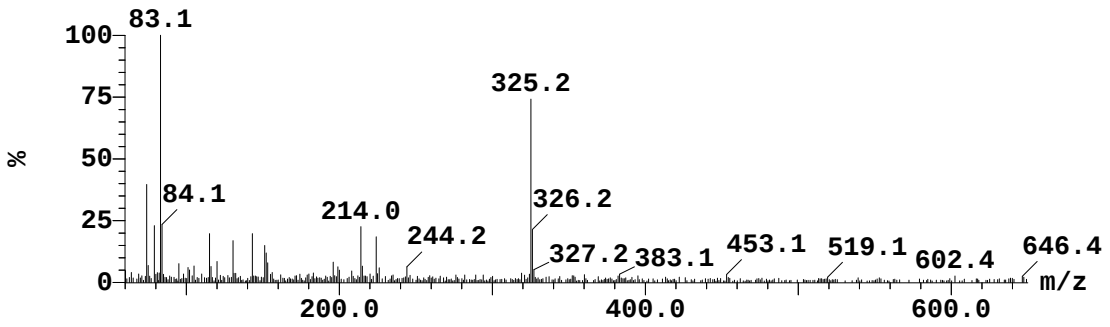
Vial:1:45
Date:14-Dec-2018

ID:
Time:9::9::8

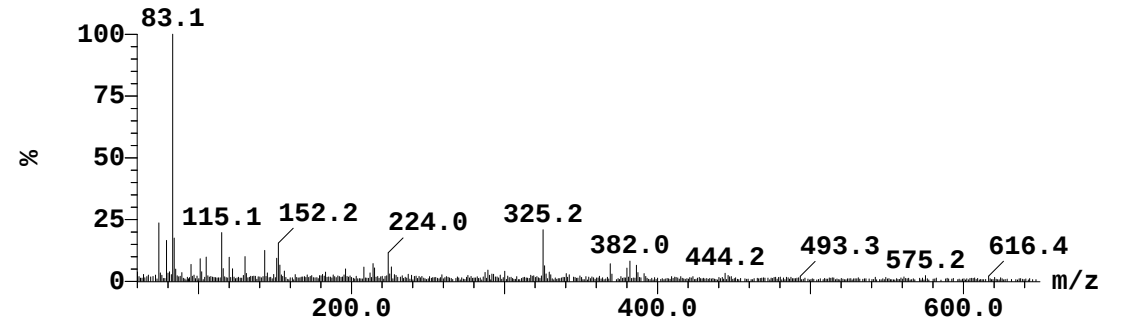
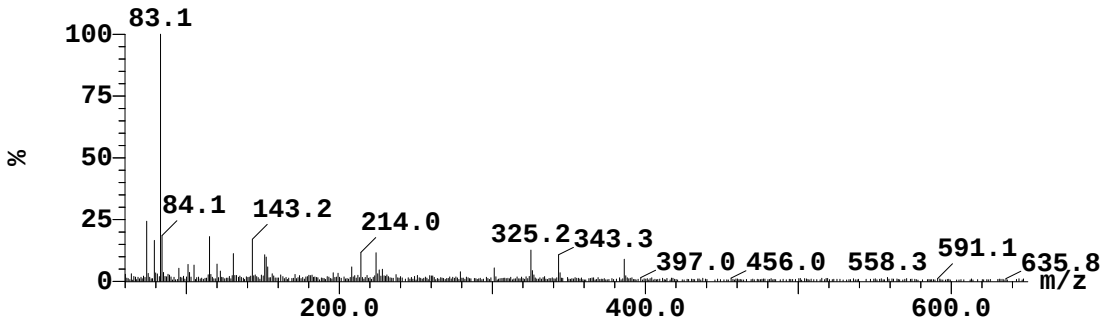
Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
7		1.82		8		1.94	
7:(Time: 1.82) Combine (58:61-(53:54+66))				8:(Time: 1.94) Combine (62:65-(57:58+70))			
1:TOF MS ES+ 1.7e+003				1:TOF MS ES+ 1.7e+003			



Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
9		2.16		10		2.41	
9:(Time: 2.16) Combine (69:73-(64:65+77))				10:(Time: 2.41) Combine (77:81-(72:73+85))			
1:TOF MS ES+ 3.9e+003				1:TOF MS ES+ 3.5e+003			



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Vial:1:45
Date:14-Dec-2018

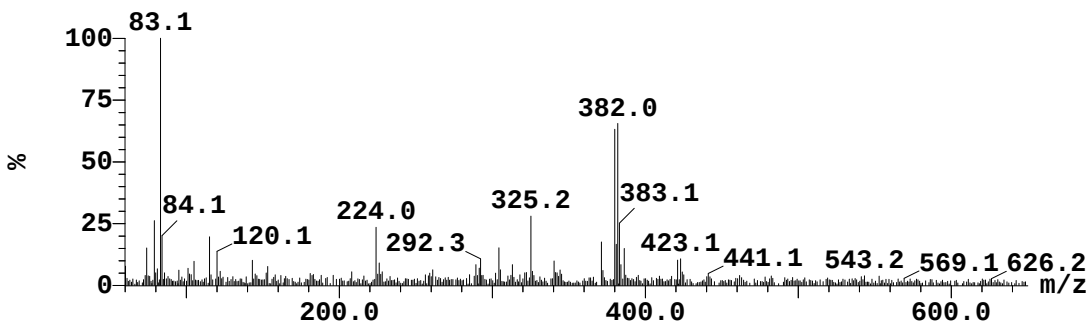
ID:
Time:9::9::8

Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
11		2.56	

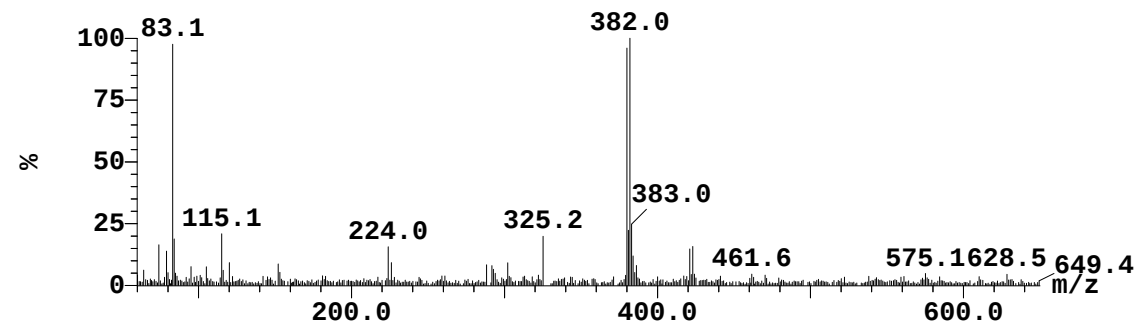
11:(Time: 2.56) Combine (82:85-(77:78+90))



Peak ID	Compound	Time	Mass Found
12		2.68	

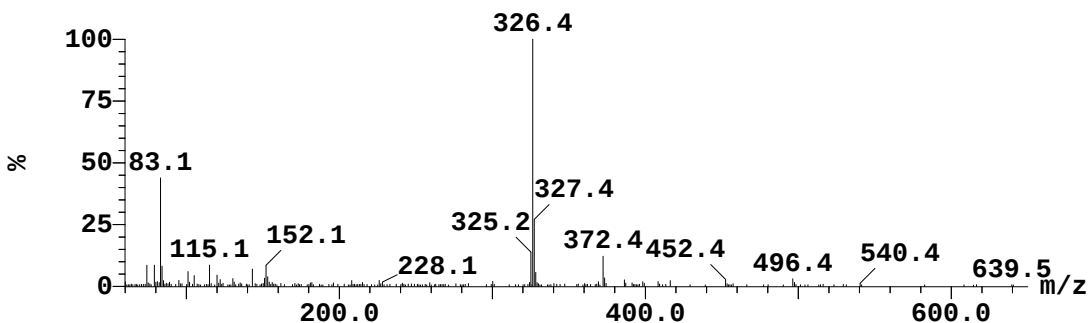
12:(Time: 2.68) Combine (86:89-(81:82+94))

1:TOF MS ES+ 2.3e+003



Peak ID	Compound	Time	Mass Found
14		2.90	

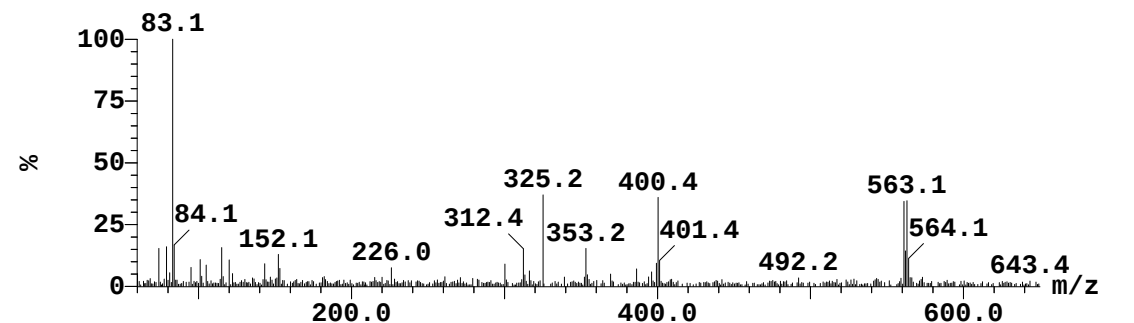
14:(Time: 2.90) Combine (93:97-(88:89+101))



Peak ID	Compound	Time	Mass Found
15	Tentative	3.05	399.00,,400.00

15:(Time: 3.05) Combine (98:101-(93:94+106))

1:TOF MS ES+ 1.9e+003



Sample: 4
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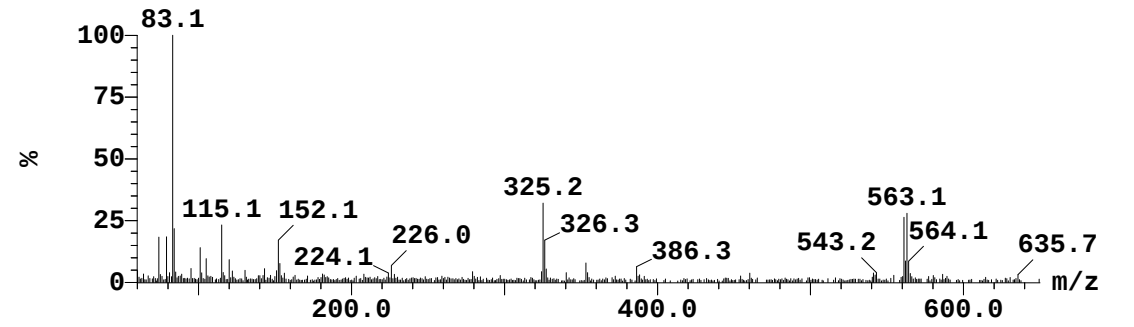
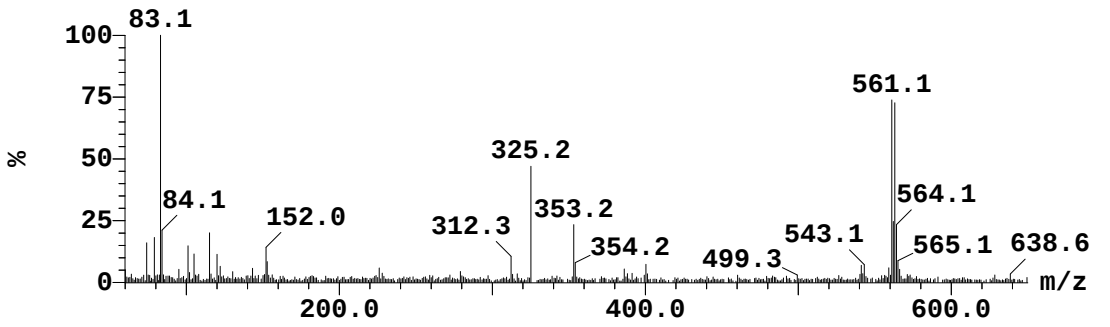
Vial:1:45
Date:14-Dec-2018

ID:
Time:9::9::8

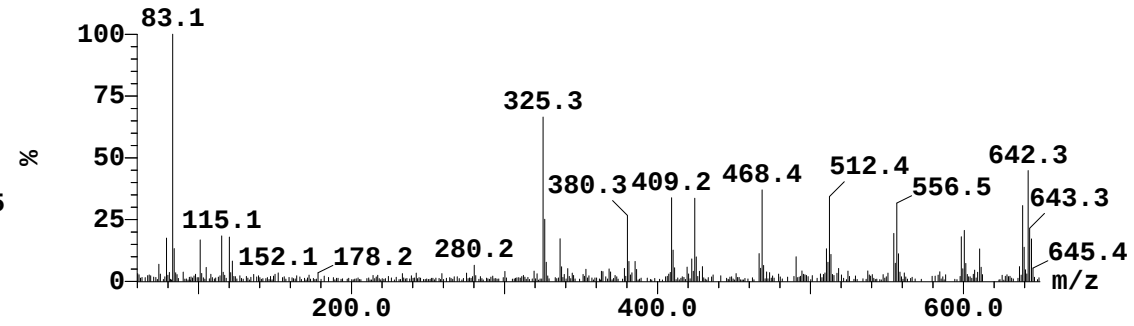
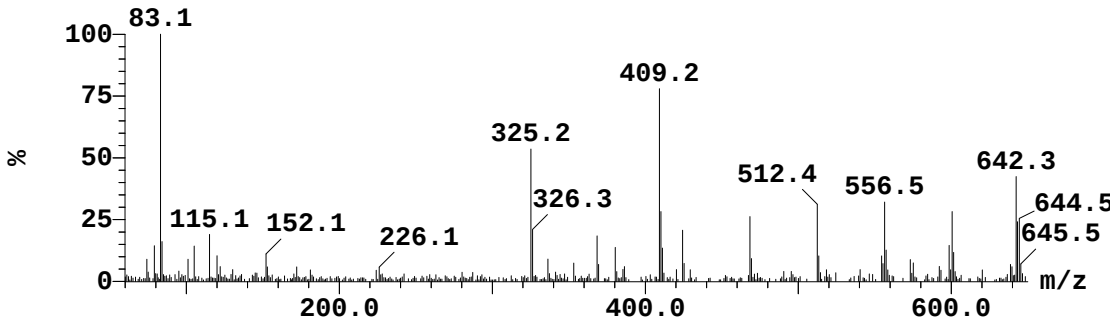
Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
16		3.15		17		3.24	
16:(Time: 3.15) Combine (101:105-(96:97+109))				17:(Time: 3.24) Combine (104:108-(100+112:113))			
1:TOF MS ES+ 3.4e+003				1:TOF MS ES+ 3.5e+003			



Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
19		3.47		21		3.54	
19:(Time: 3.47) Combine (112:115-(107+119:120))				21:(Time: 3.54) Combine (114:117-(109:110+122))			
1:TOF MS ES+ 2.0e+003				1:TOF MS ES+ 2.0e+003			



Sample: 4
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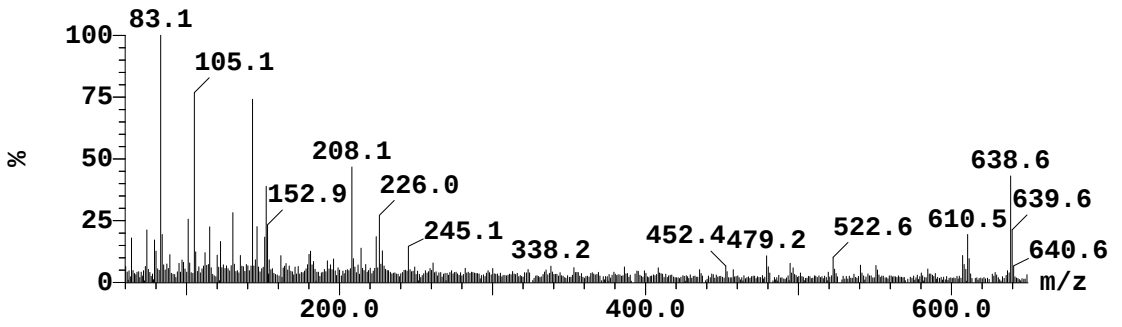
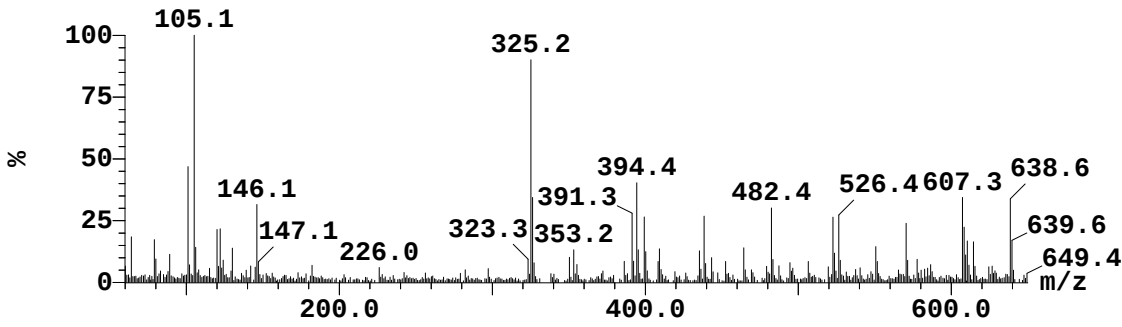
Vial:1:45
Date:14-Dec-2018

ID:
Time:9::9::8

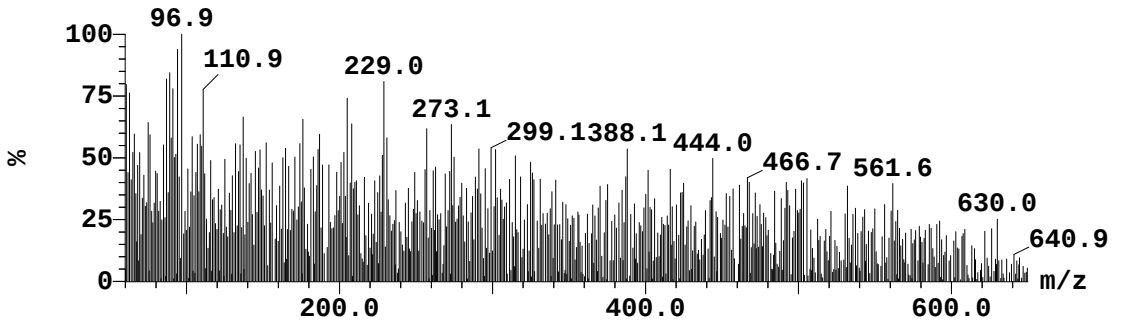
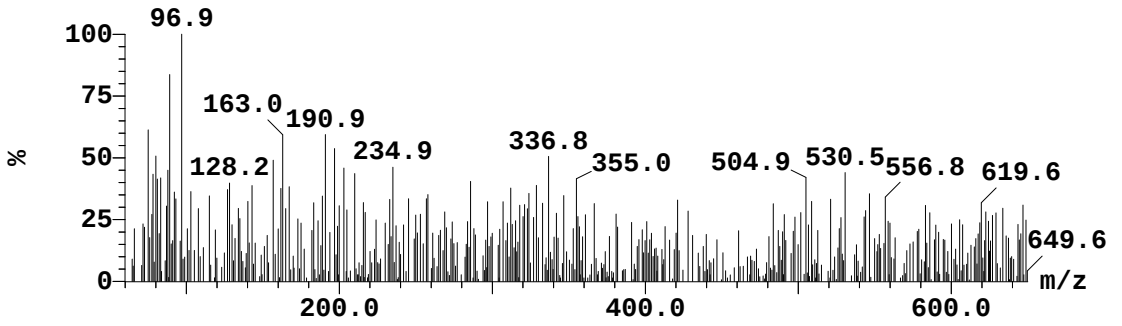
Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
22	Tentative	3.79	,422.00,400.00	23		3.88	
22:(Time: 3.76) Combine (121:125-(116:117+129))				23:(Time: 3.88) Combine (125:129-(120:121+1:-1))			
1:TOF MS ES+ 4.9e+003				1:TOF MS ES+ 5.8e+003			



Peak ID	Compound	Time	Mass Found	Peak ID	Compound	Time	Mass Found
1	Tentative	0.60	399.00,,398.00	3	Tentative	1.18	,444.00,398.00
1:(Time: 0.60) Combine (18:21-(13:14+26))				3:(Time: 1.14) Combine (36:39-(31+43:44))			
2:TOF MS ES- 7.6e+001				2:TOF MS ES- 1.0e+002			



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Vial:1:45
Date:14-Dec-2018

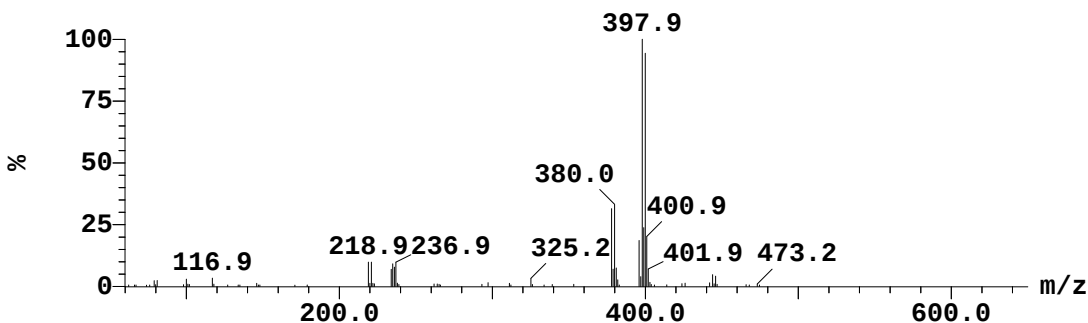
ID:
Time:9::9::8

Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

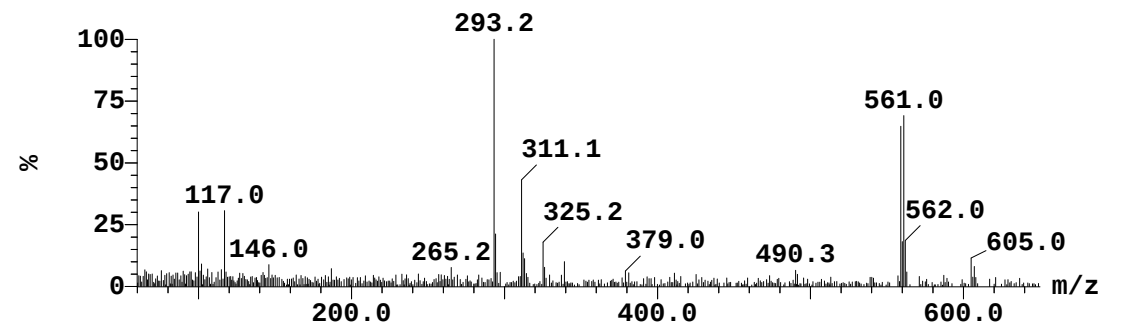
Peak ID	Compound	Time	Mass Found
12	Found	2.68	,444.00,398.00

12:(Time: 2.64) Combine (84:88-(80+92:93))



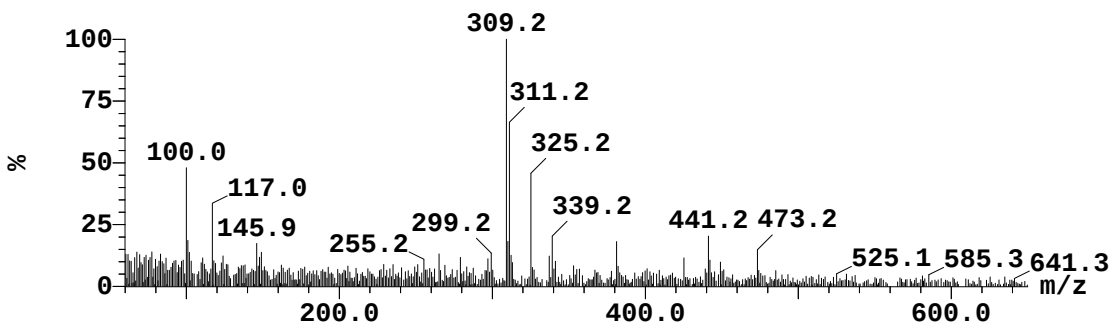
Peak ID	Compound	Time	Mass Found
16		3.15	

2:TOF MS ES- 16:(Time: 3.11) Combine (100:103-(95+107:108)) 2.5e+004 2:TOF MS ES- 1.6e+003



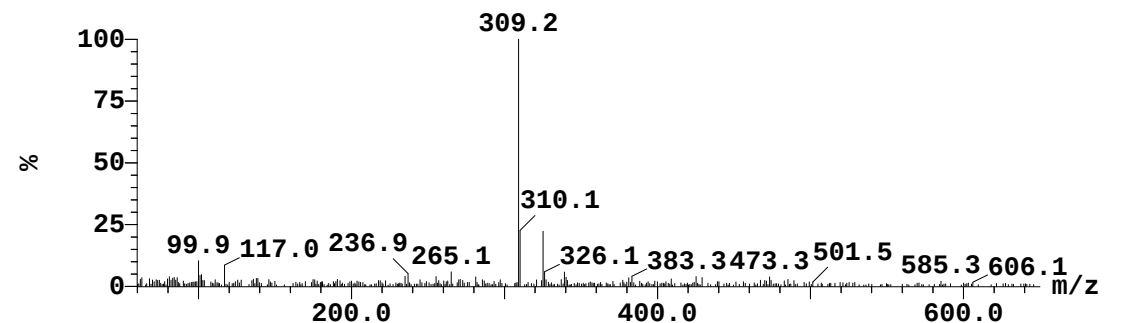
Peak ID	Compound	Time	Mass Found
18		3.38	

18:(Time: 3.38) Combine (108:112-(104+116:117))



Peak ID	Compound	Time	Mass Found
20		3.48	

2:TOF MS ES- 20:(Time: 3.48) Combine (112:115-(107+119:120)) 1.4e+003 2:TOF MS ES- 2.6e+003



Sample: 4
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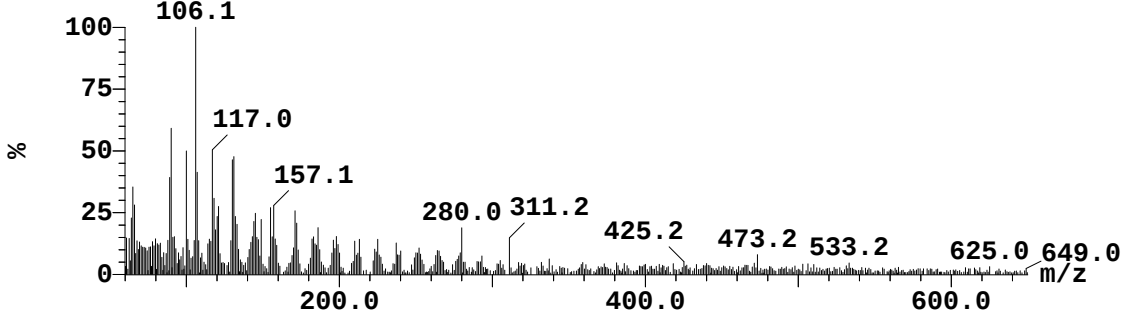
Vial:1:45
Date:14-Dec-2018

ID:
Time:9::9::8

Printed: Fri Dec 14 10:45:27 2018

Sample Report (continued):

Peak ID	Compound	Time	Mass Found
22		3.79	
22:(Time: 3.80) Combine (122:125-(117:118+130))			2:T0F MS ES- 2.1e+003



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