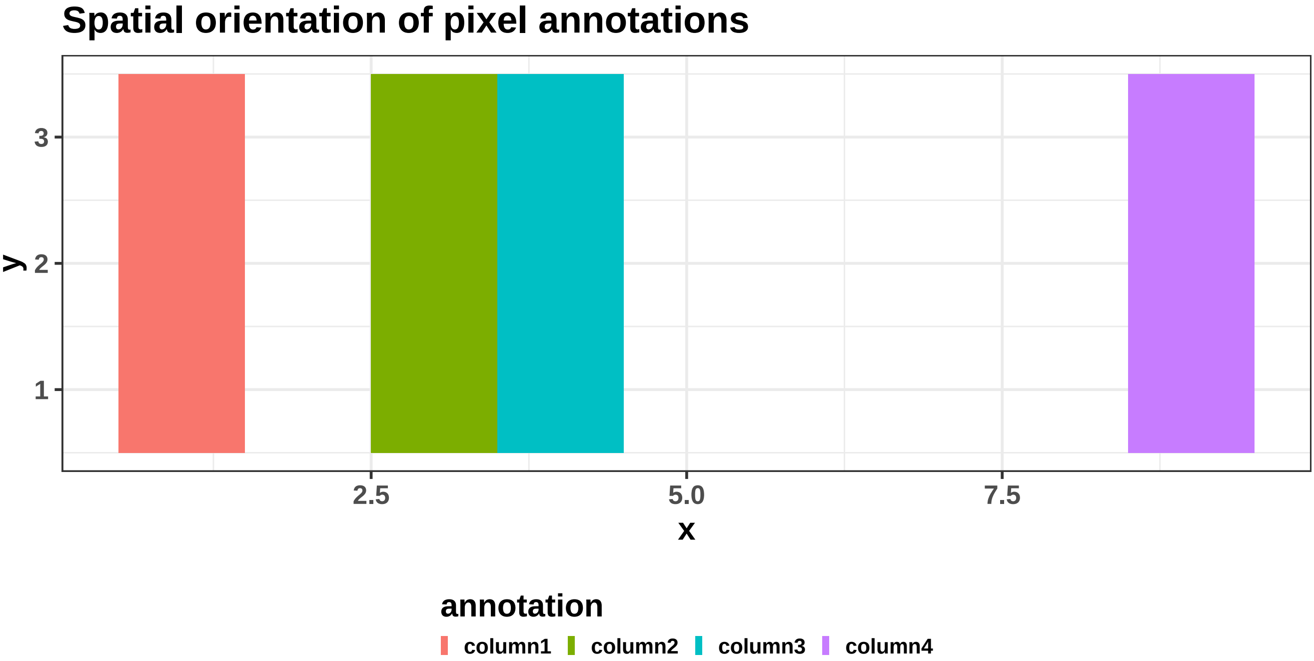
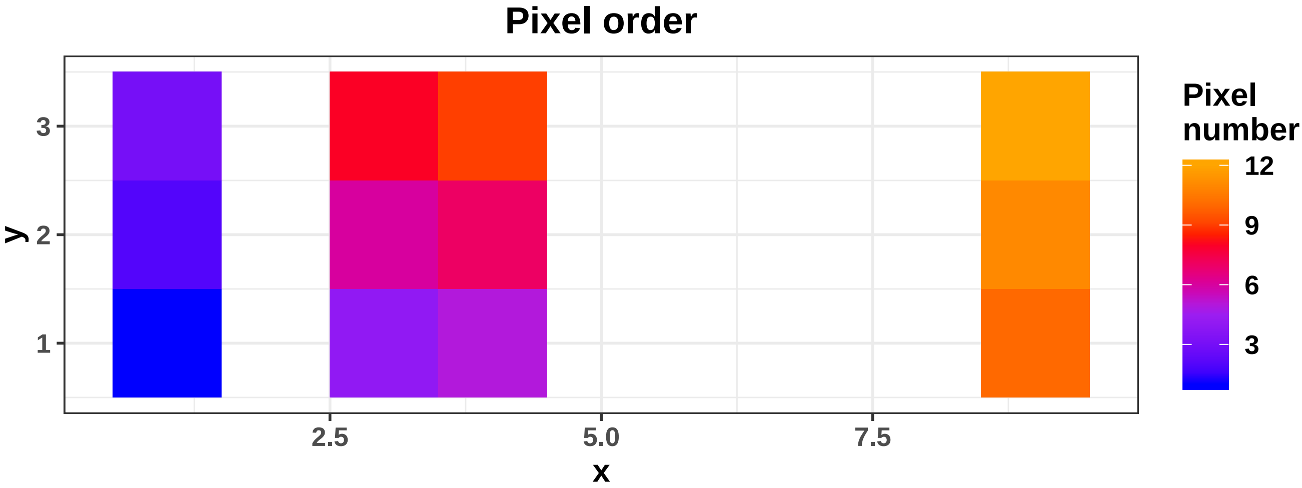
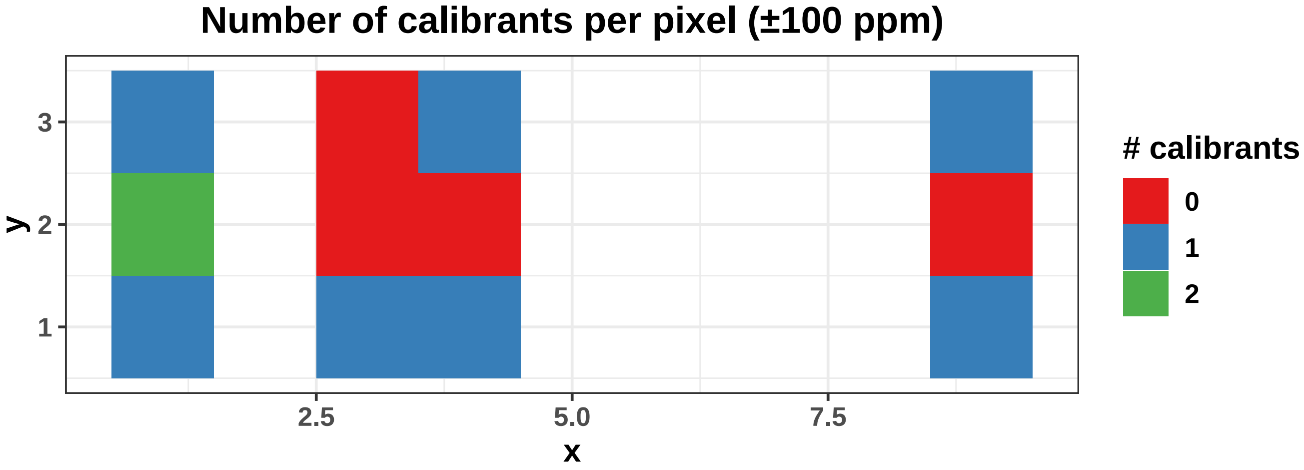
Testfile_rdata

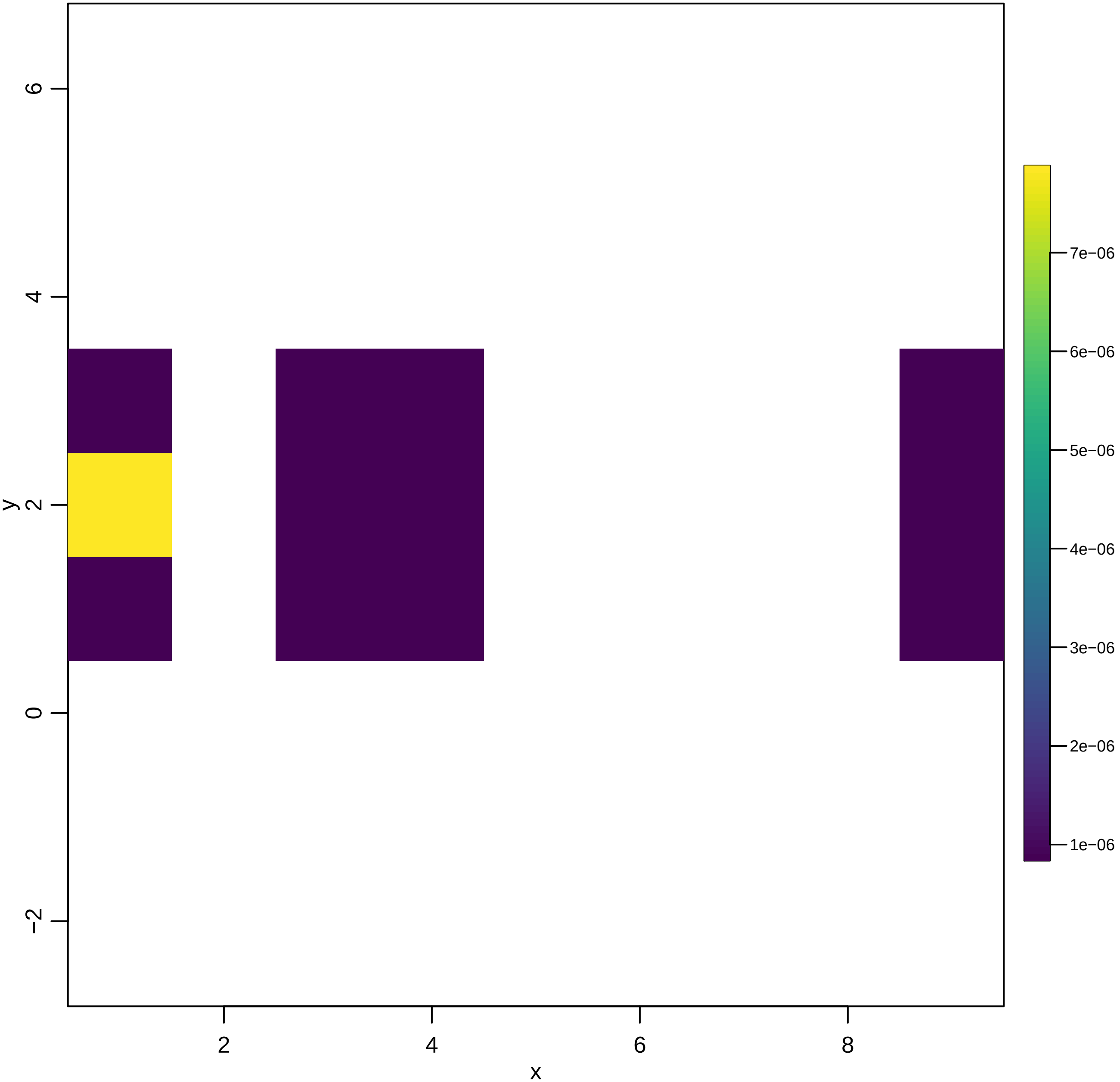
properties	values
Number of m/z features	8399
Range of m/z values	100.08 − 799.92
Number of pixels	12
Range of x coordinates	1 − 9
Range of y coordinates	1 − 3
Range of intensities	0 − 9.24
Number of NA intensities	0
Number of Inf intensities	0
Number of duplicated coordinates	0
Median of intensities	0
Intensities > 0	31.29 %
Number of empty spectra	0
Median TIC ± sd	161.8 ± 47
Median # peaks per spectrum ± sd	2811 ± 424
Centroided	FALSE
input m/z (#valid/#input) in inputcalibrantfile1.tabular	3 / 3

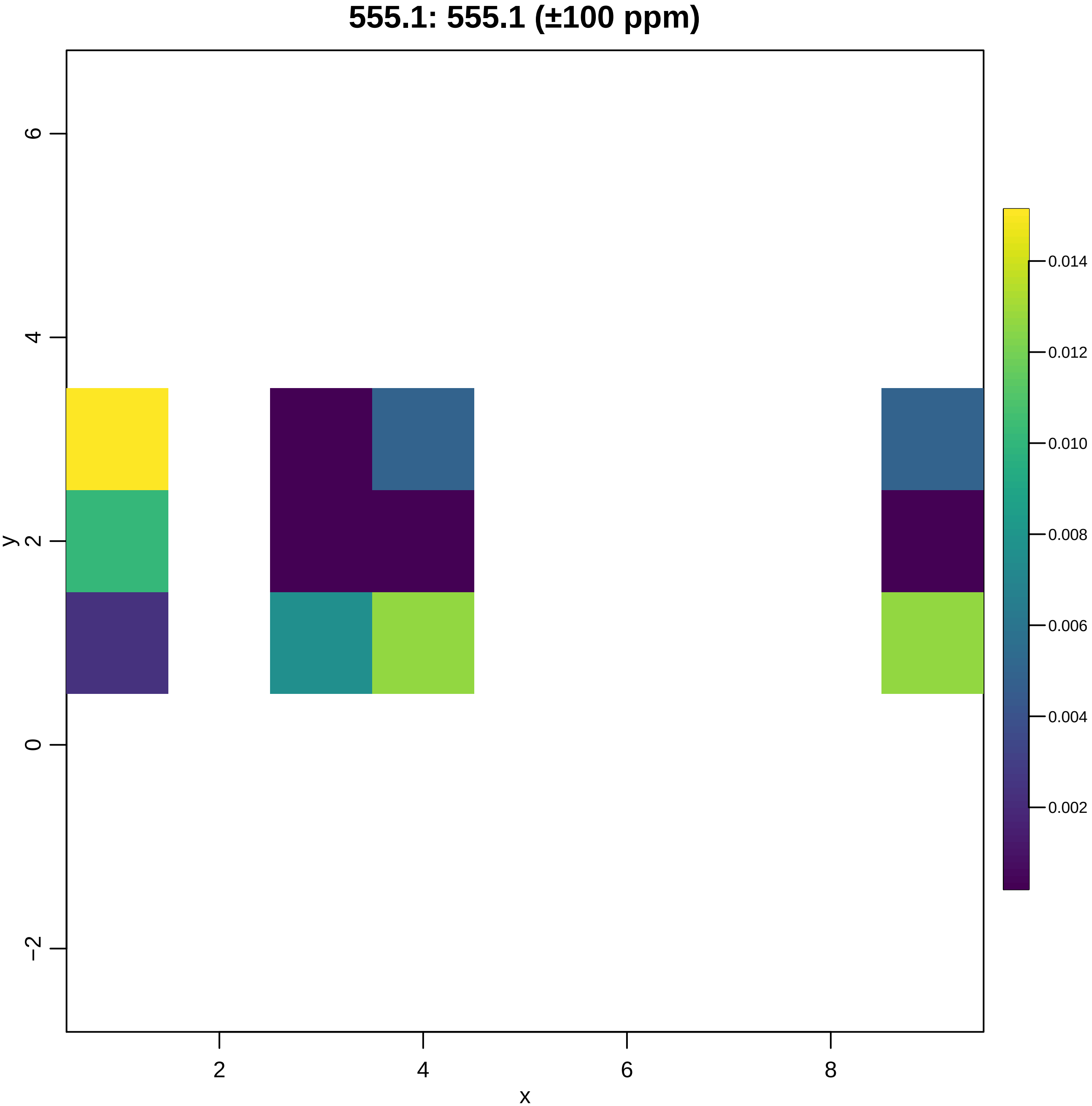

Spatial orientation of pixel annotations
y
3
2
1
2.5
5.0
7.5
x
annotation
column1
column2
column3
column4

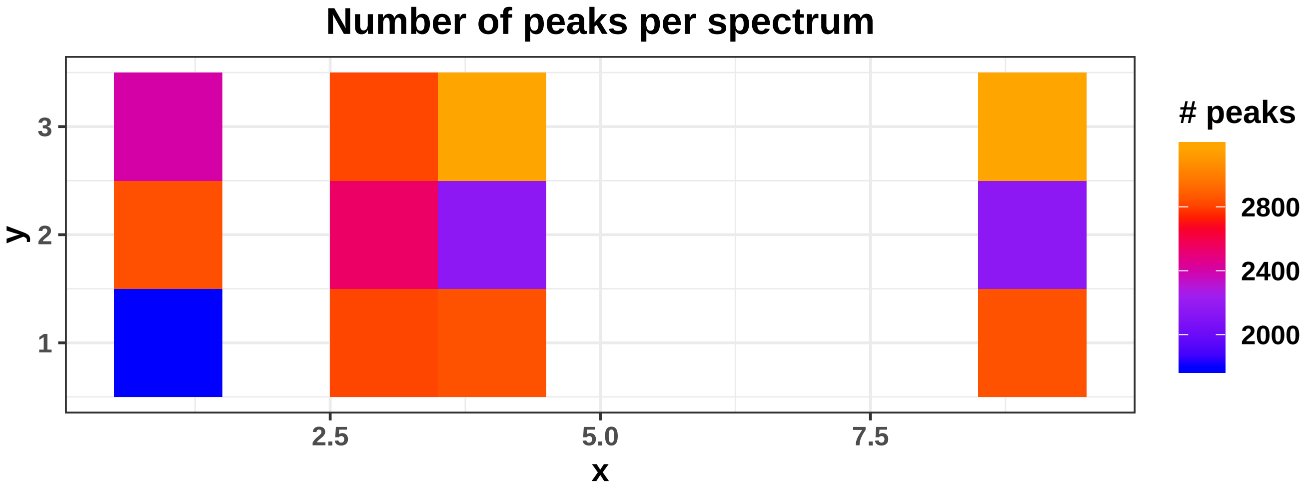

Pixel order
y
3
2
1
2.5
5.0
7.5
x
Pixel number
12
9
6
3

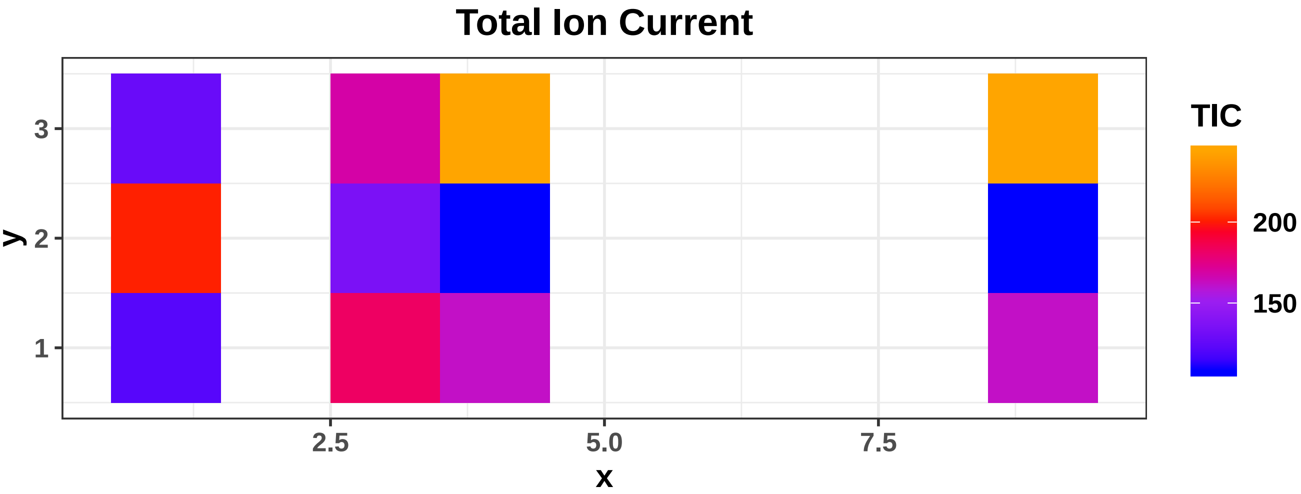

Number of calibrants per pixel (±100 ppm)
y
3
2
1
x
2.5
5.0
7.5
calibrants
0
1
2

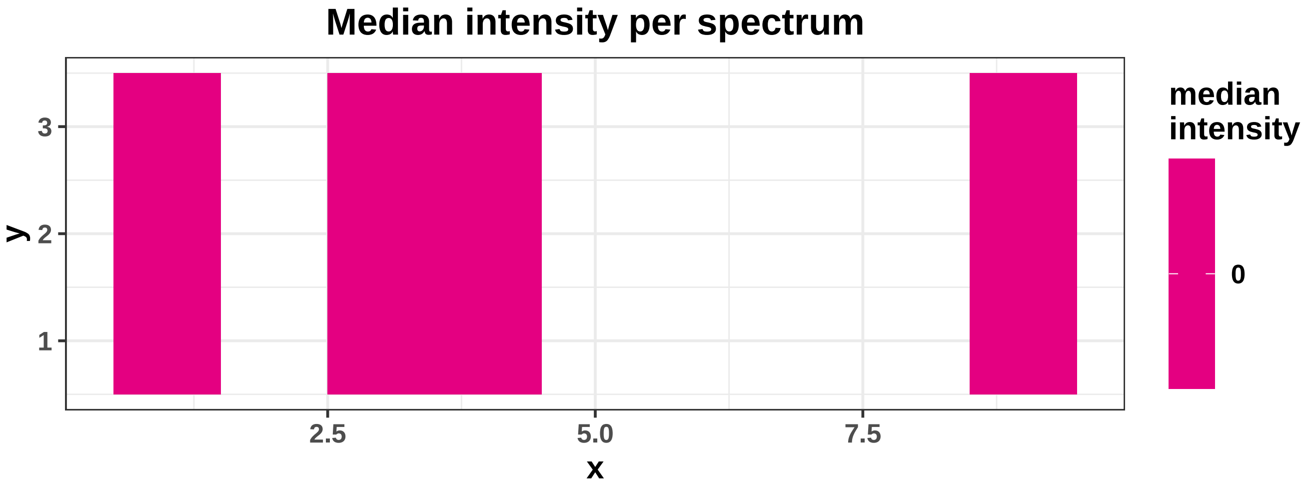
101.5: 101.5 (±100 ppm)

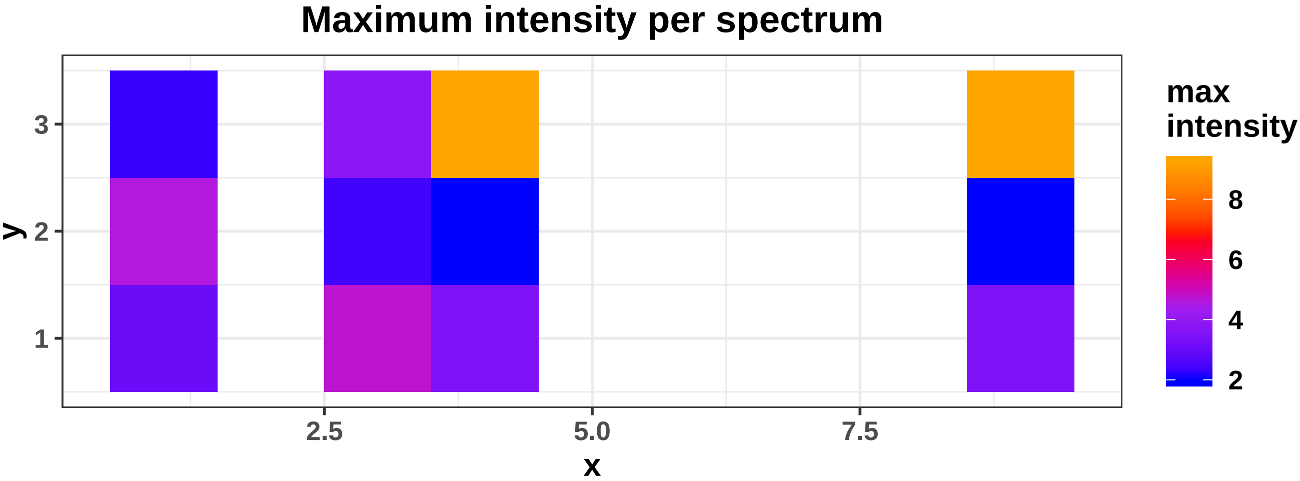



555.1: 555.1 (±100 ppm)
y
6
4
2
0
−2
x
2
4
6
8
0.014
0.012
0.010
0.008
0.006
0.004
0.002

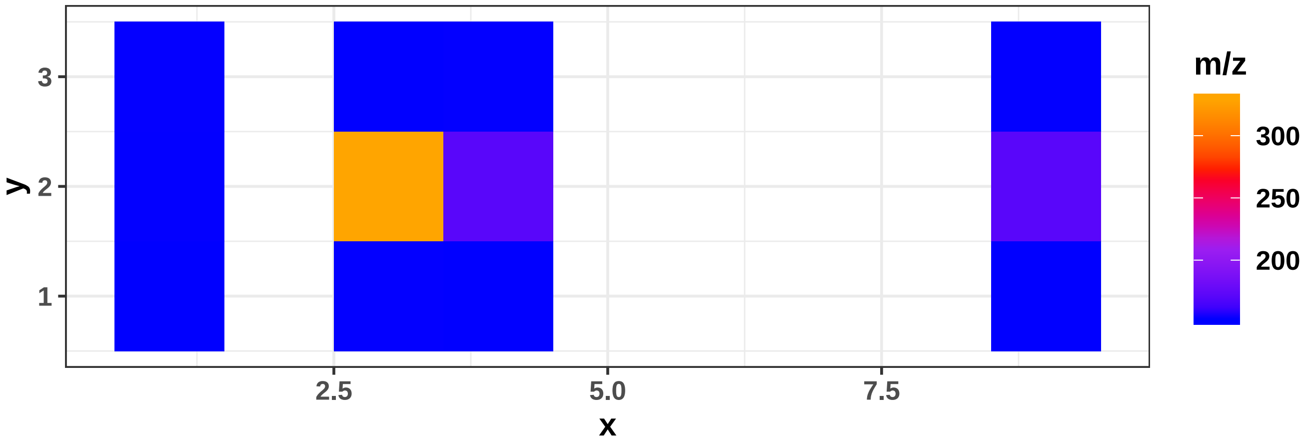

Number of peaks per spectrum
y
3
2
1
x
2.5
5.0
7.5
peaks
2800
2400
2000

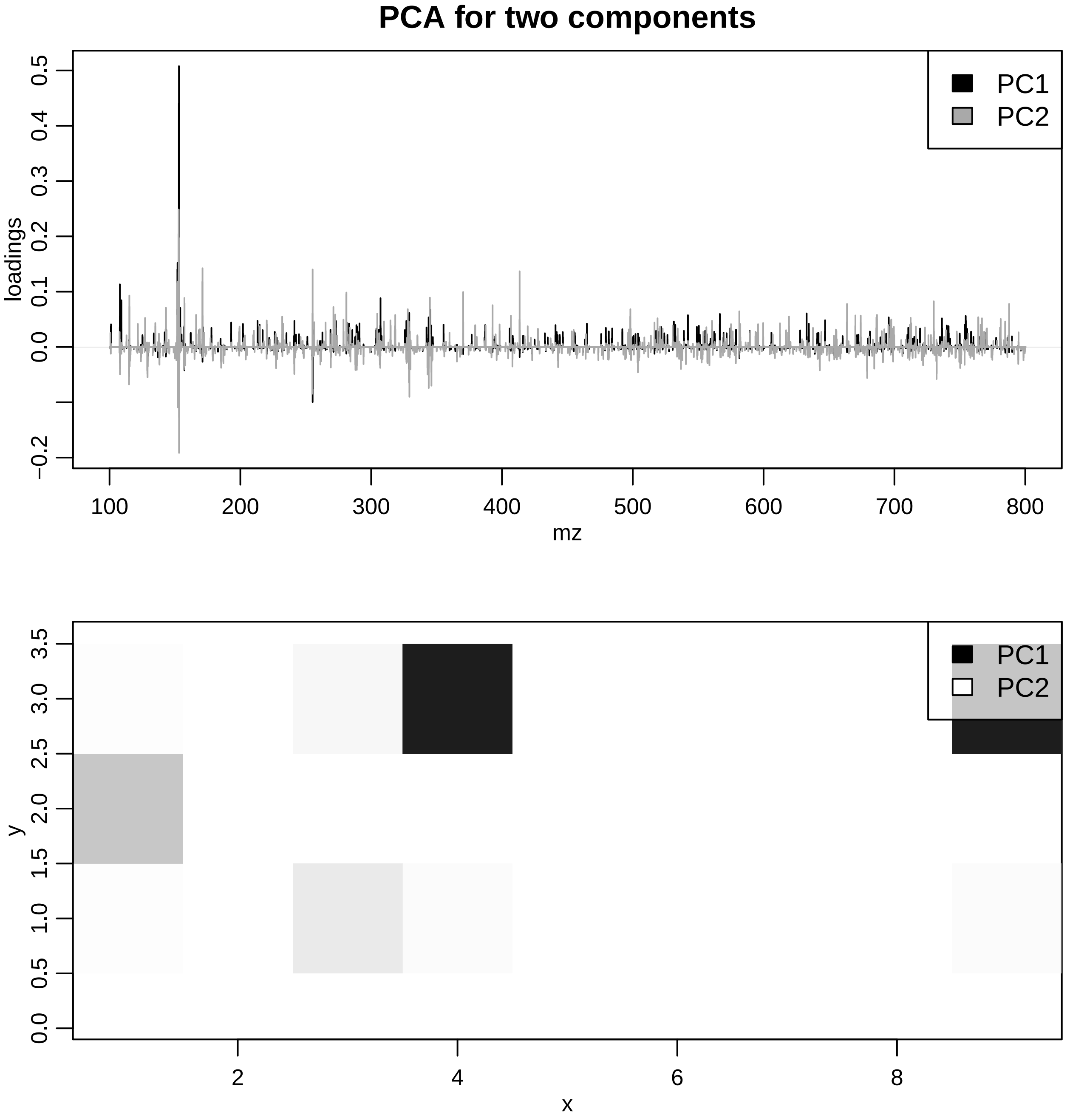

Total Ion Current
y
3
2
1
x
2.5
5.0
7.5
TIC
200
150

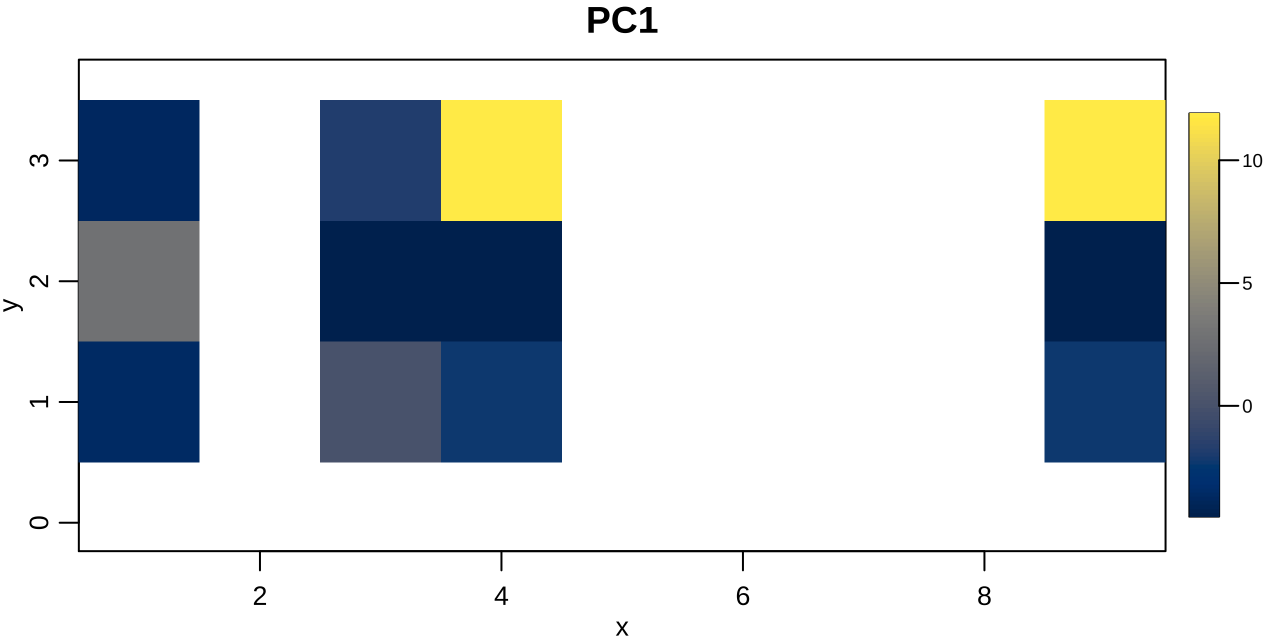

Median intensity per spectrum
y
3
2
1
x
2.5
5.0
7.5
median
intensity
0

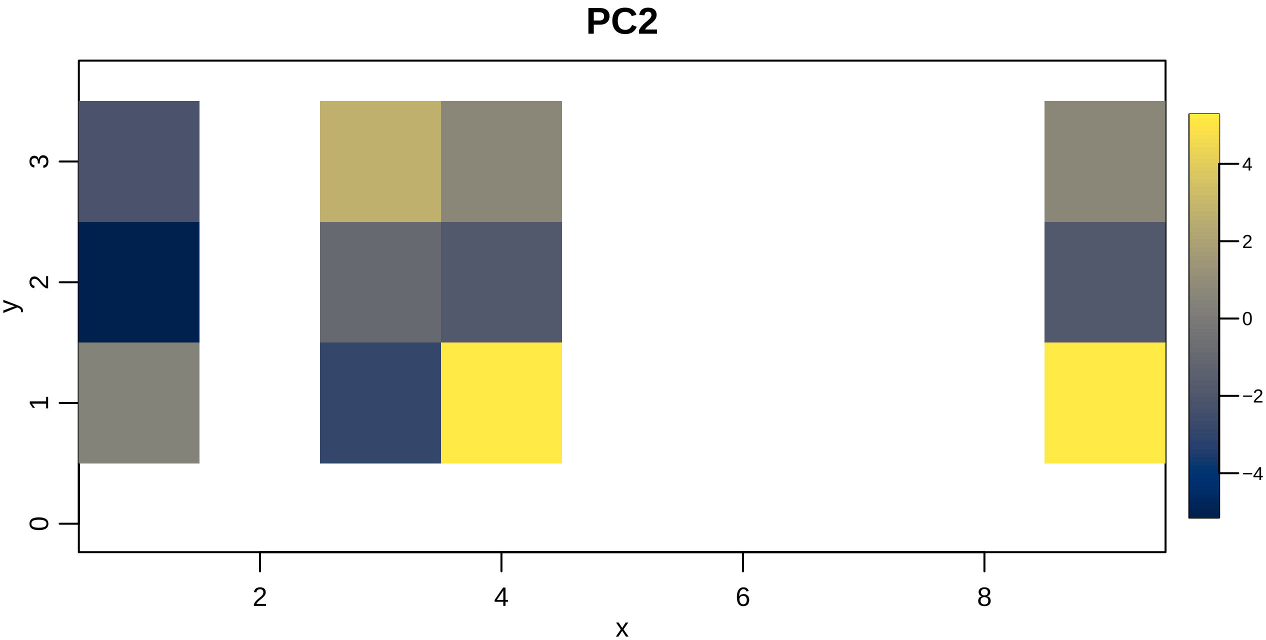

Maximum intensity per spectrum
y
3
2
1
x
2.5
5.0
7.5
max intensity
8
6
4
2

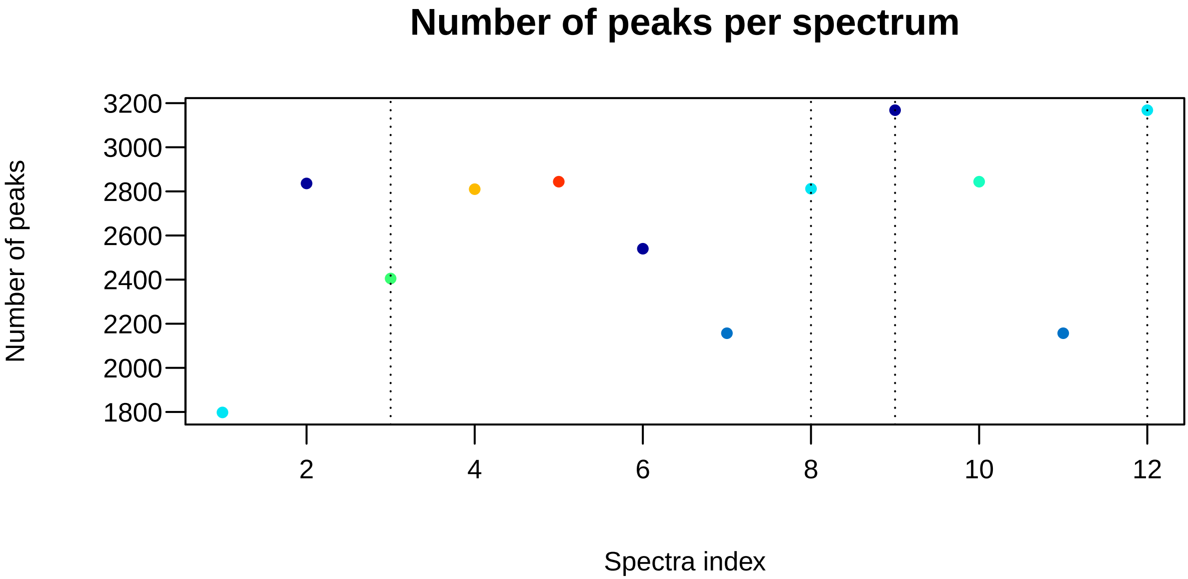
Most abundant m/z in each spectrum

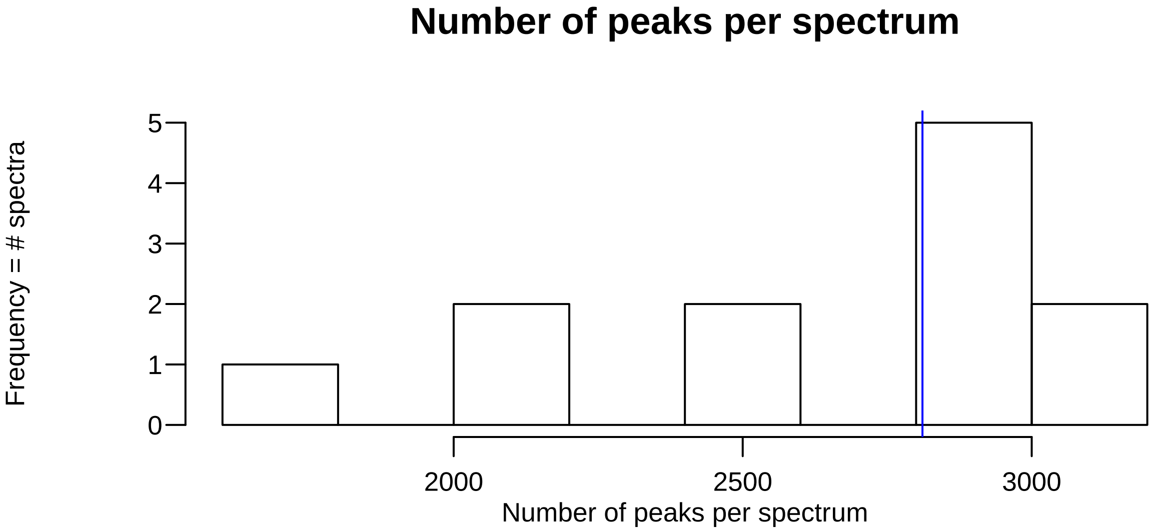


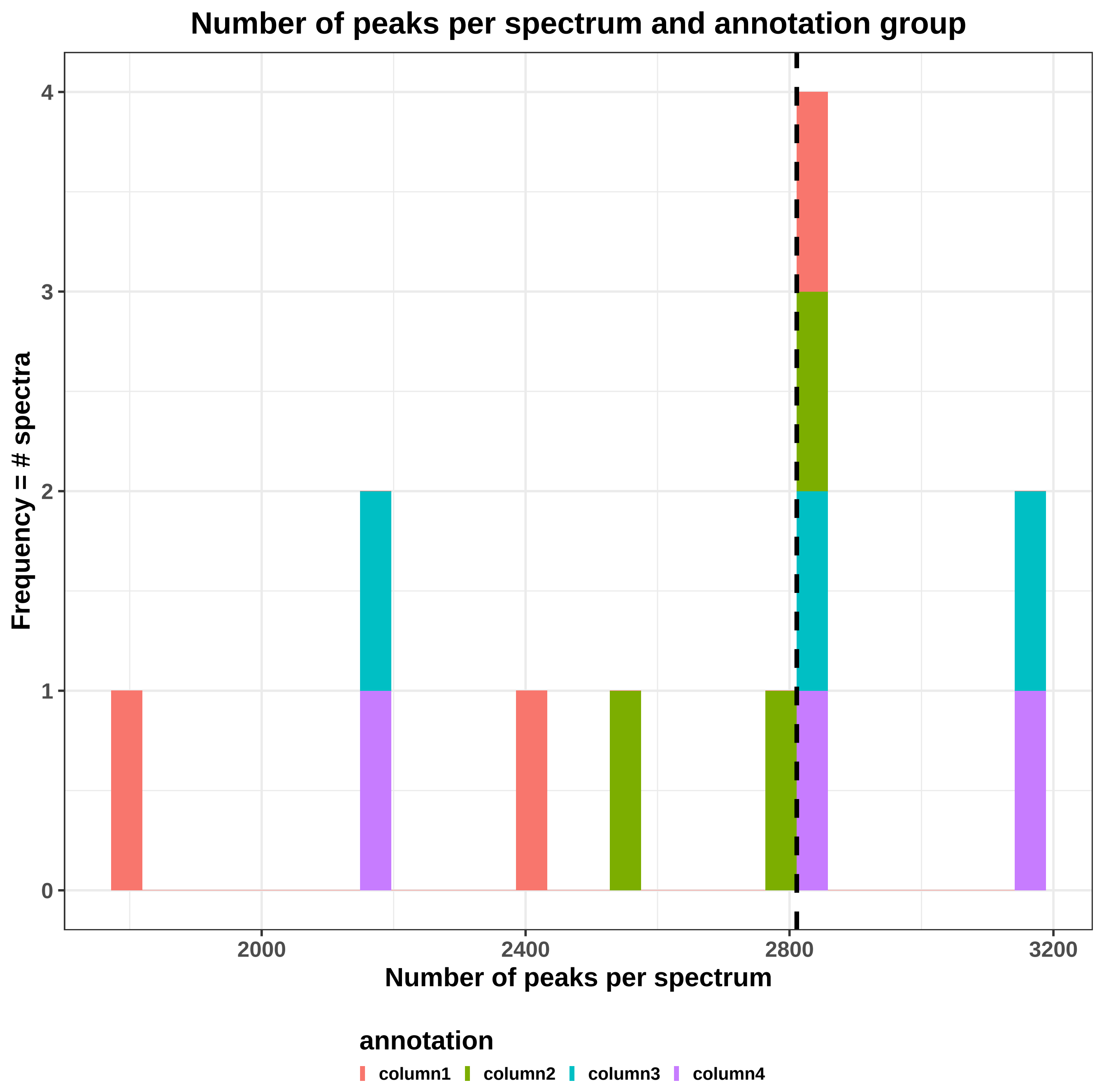

PCA for two components
loadings
0.5
0.4
0.3
0.2
0.1
0.0
−0.2
100
200
300
400
500
600
700
800
mz
PC1
PC2
y
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
8
x
PC1
PC2


PC1
y
3
2
1
0
2
4
6
8
x
10
5
0

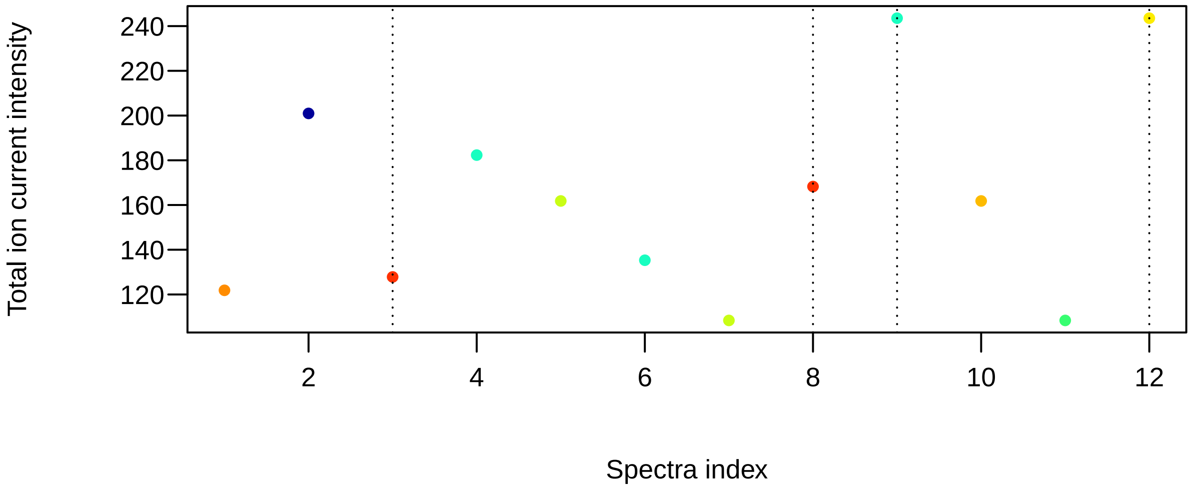

PC2
y
3
2
1
0
2
4
6
8
x
4
2
0
−2
−4


Number of peaks per spectrum

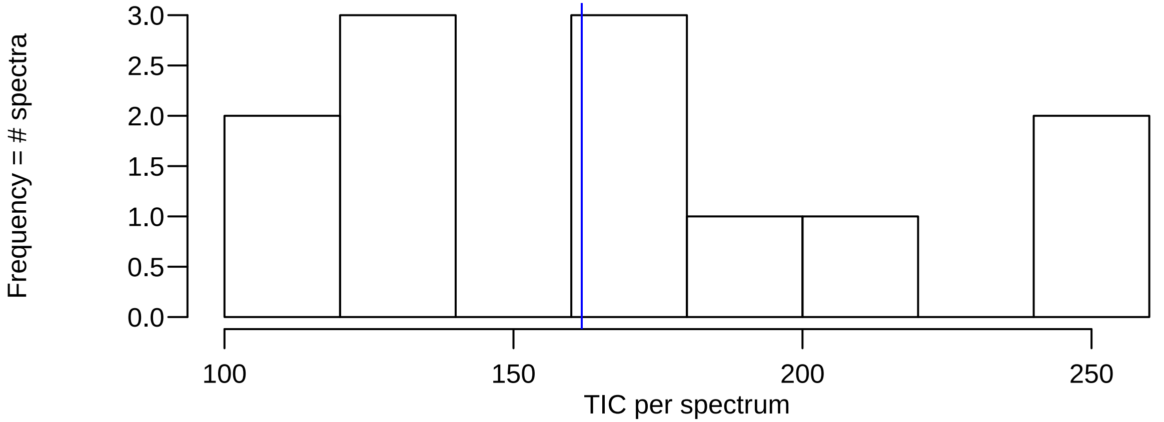

Number of peaks per spectrum

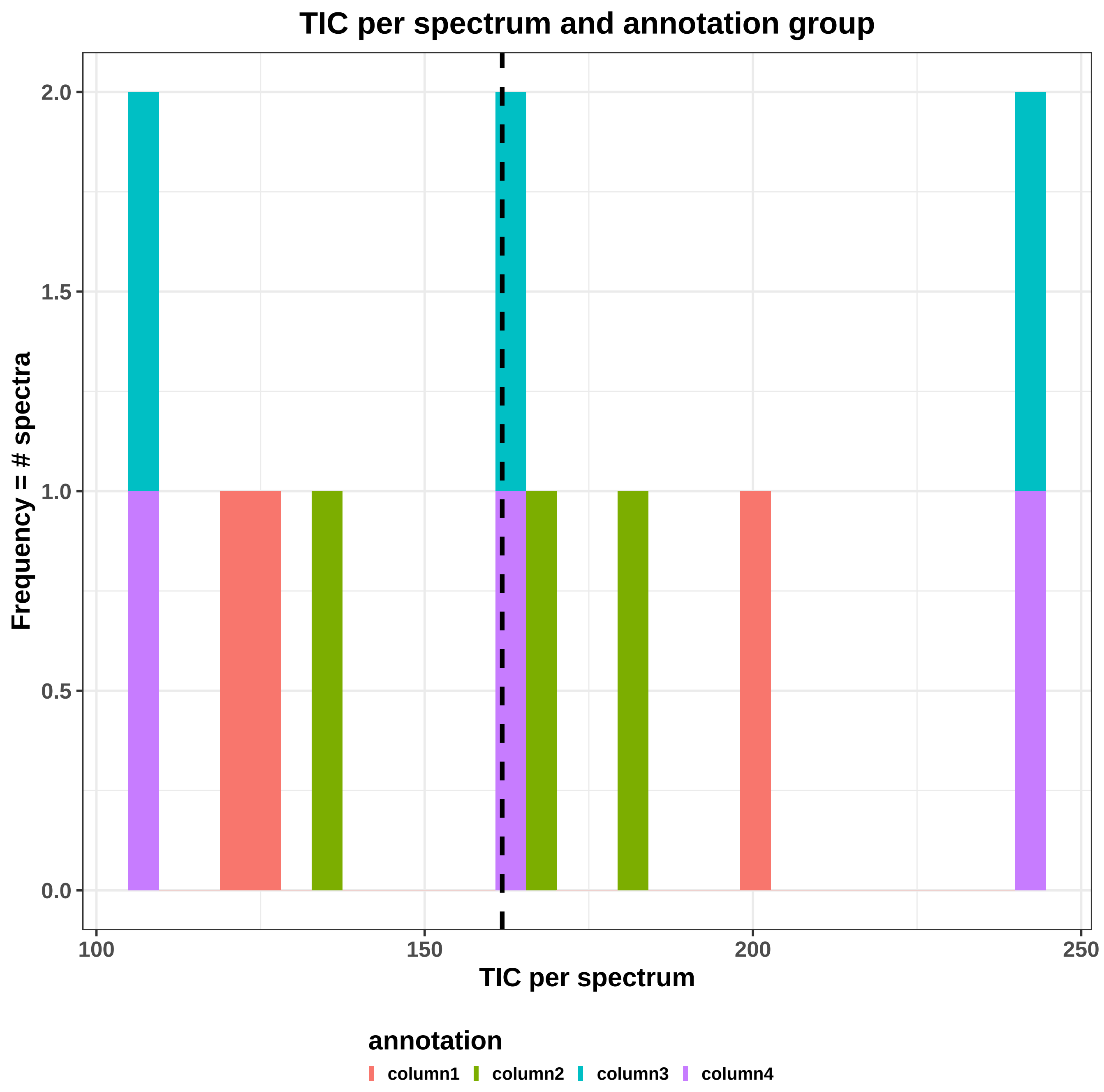

Number of peaks per spectrum and annotation group
Frequency = # spectra
0
1
2
3
4
2000
2400
2800
3200
Number of peaks per spectrum
annotation
column1
column2
column3
column4

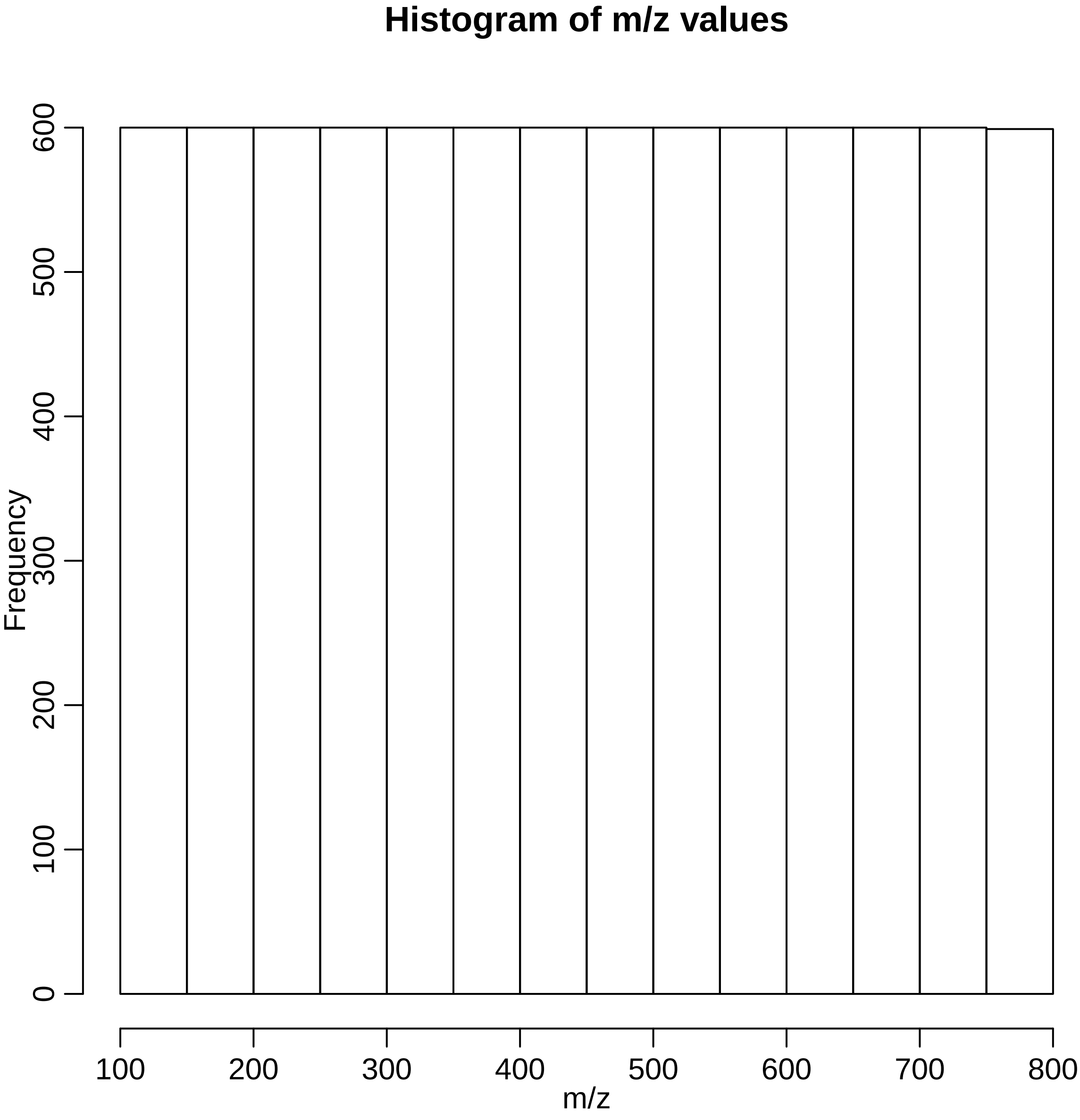
TIC per spectrum



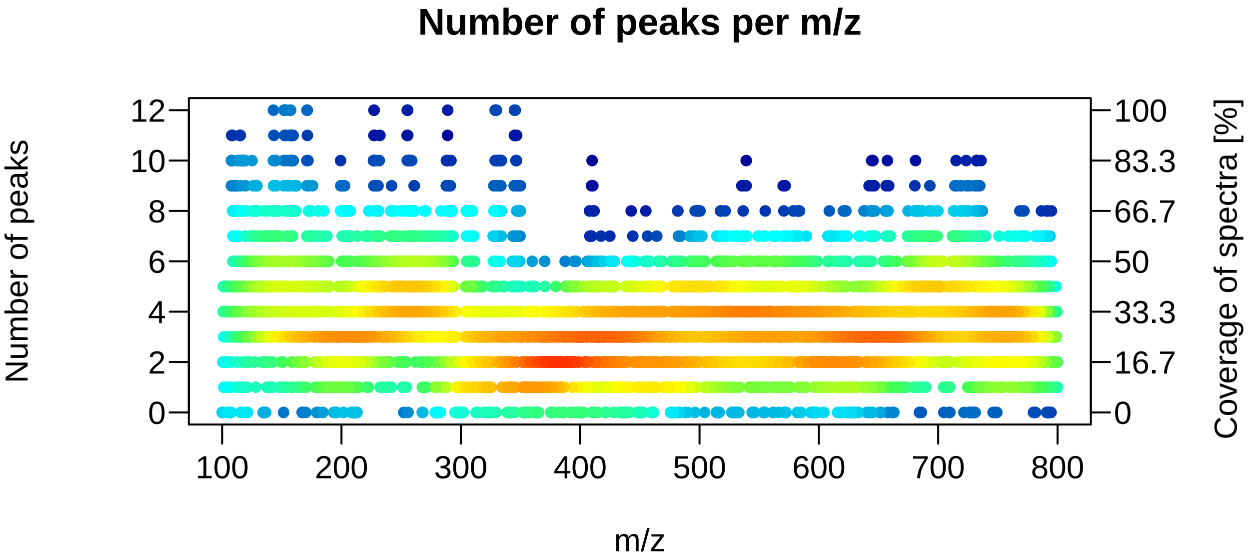
TIC per spectrum

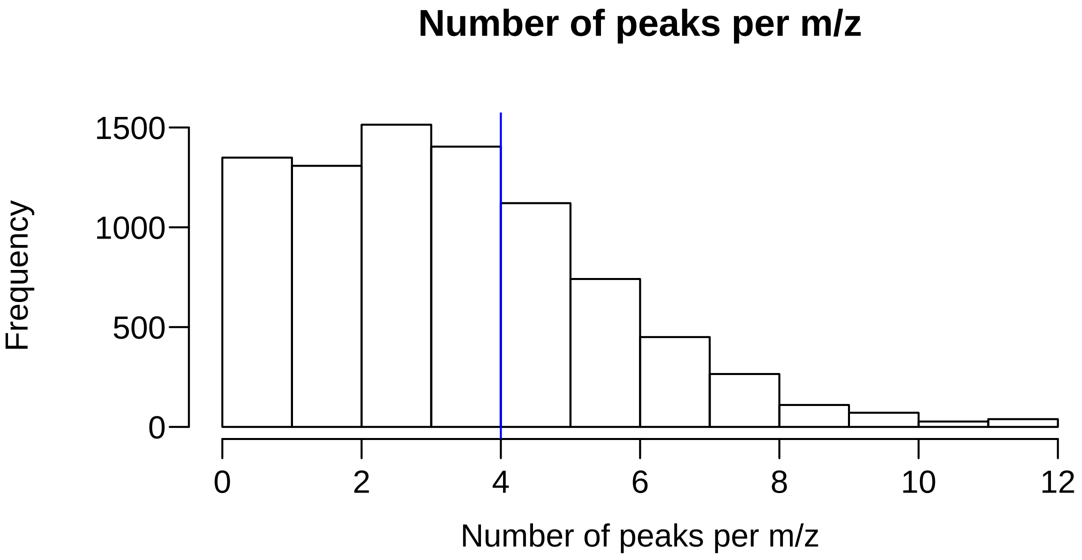


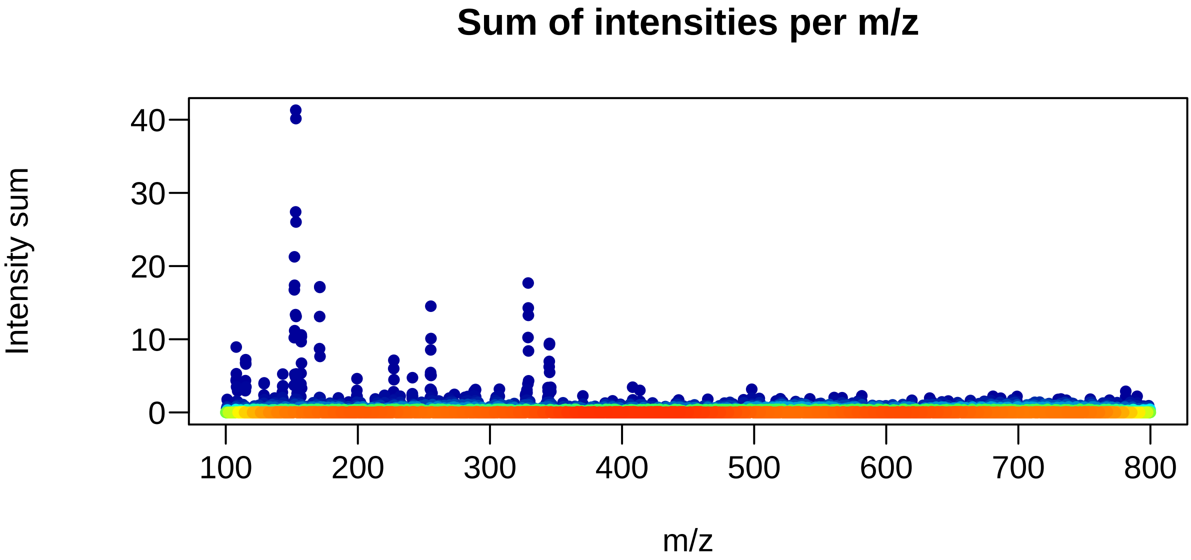

TIC per spectrum and annotation group
Frequency = # spectra
2.0
1.5
1.0
0.5
0.0
100
150
200
250
TIC per spectrum
annotation
column1
column2
column3
column4

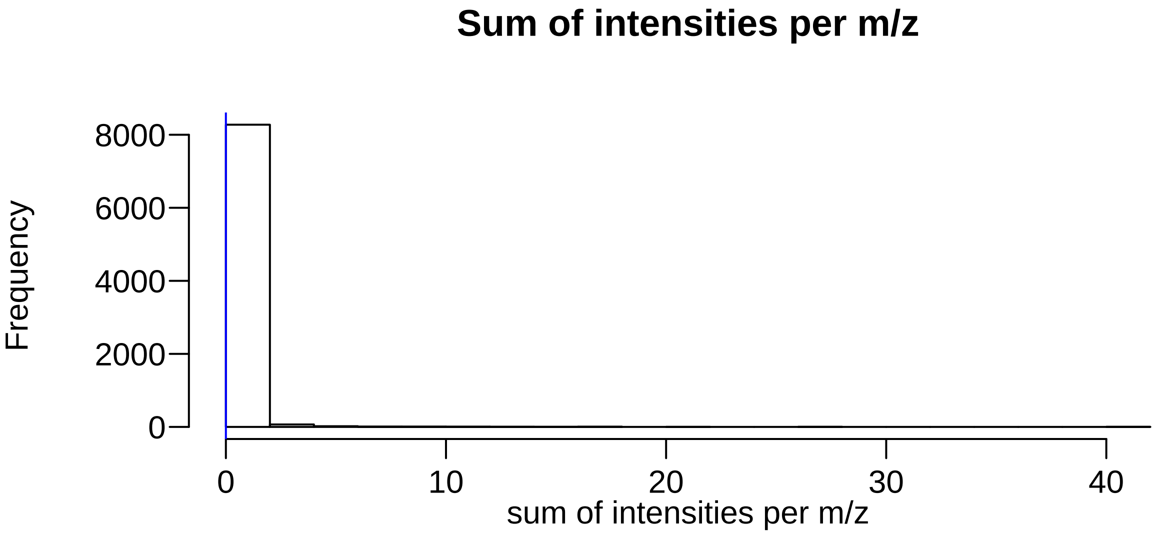


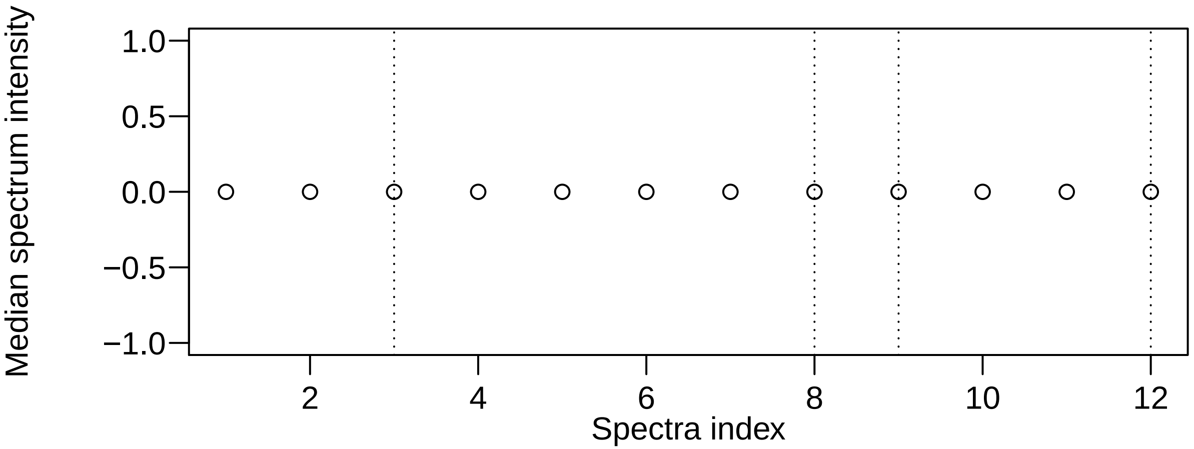
Histogram of m/z values

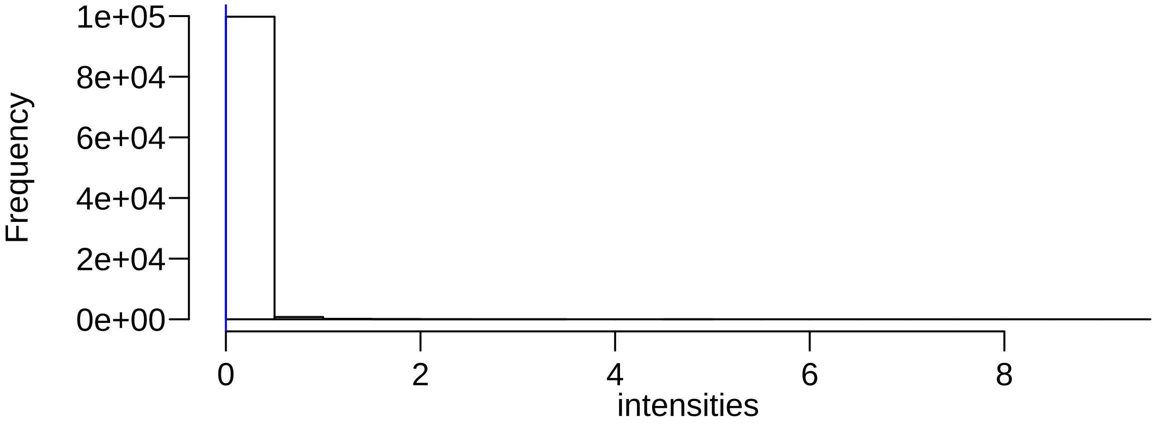

Number of peaks per m/z
Number of peaks
Coverage of spectra [%]
m/z
0
2
4
6
8
10
12
0
16.7
33.3
50
66.7
83.3
100
100
200
300
400
500
600
700
800

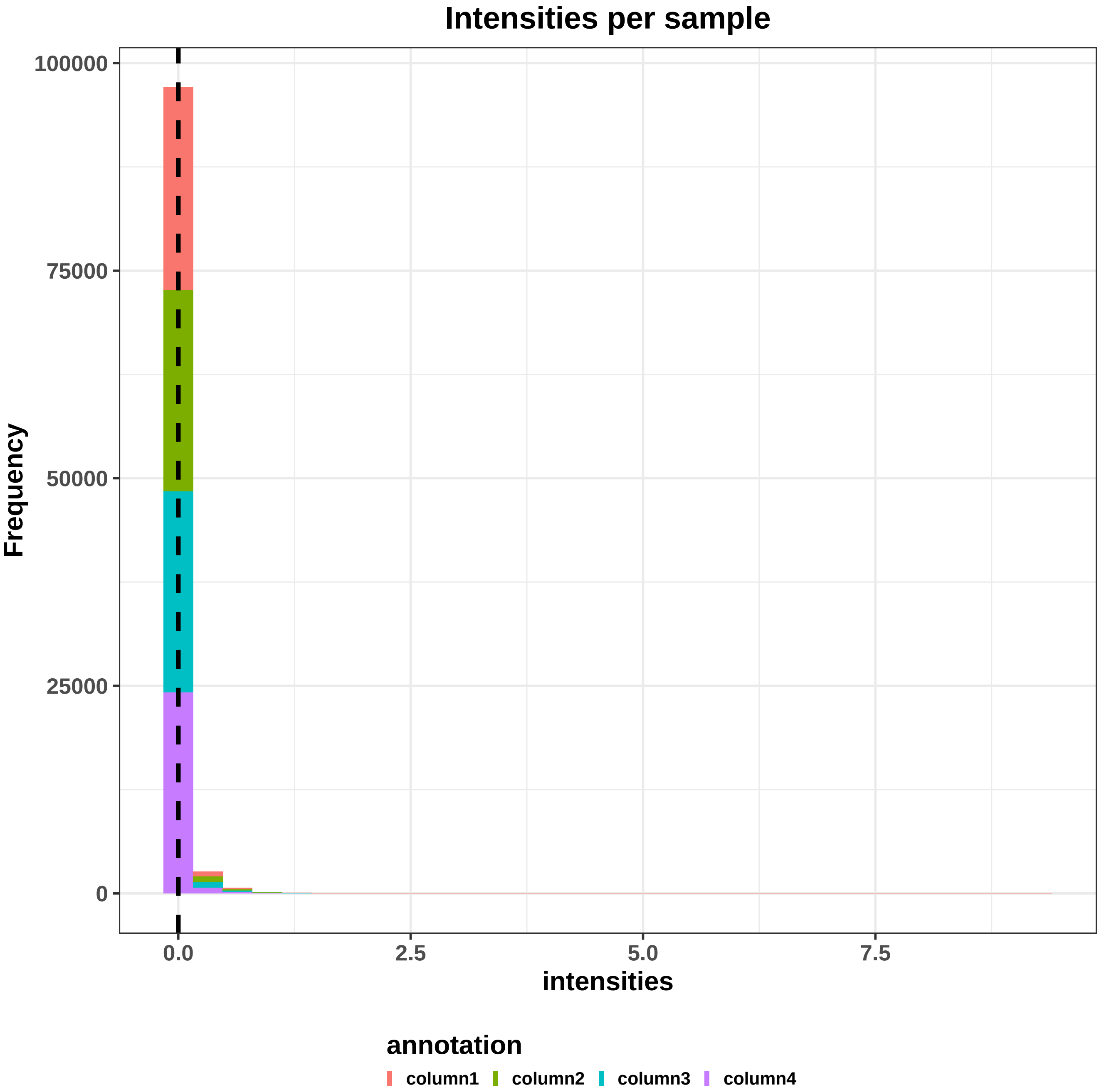

Number of peaks per m/z
Frequency
Number of peaks per m/z
0
500
1000
1500
0
2
4
6
8
10
12

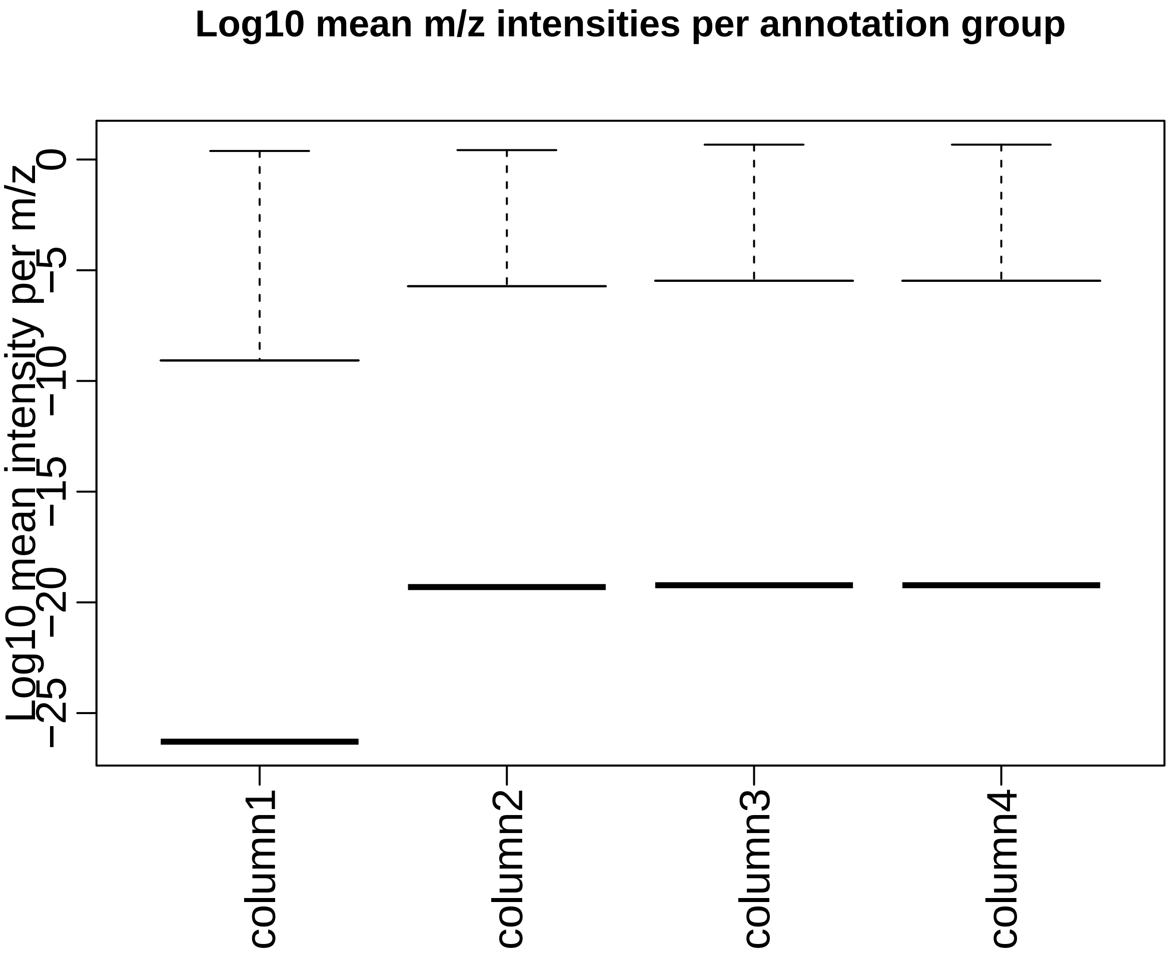

Sum of intensities per m/z
Intensity sum
0
10
20
30
40
m/z
100
200
300
400
500
600
700
800

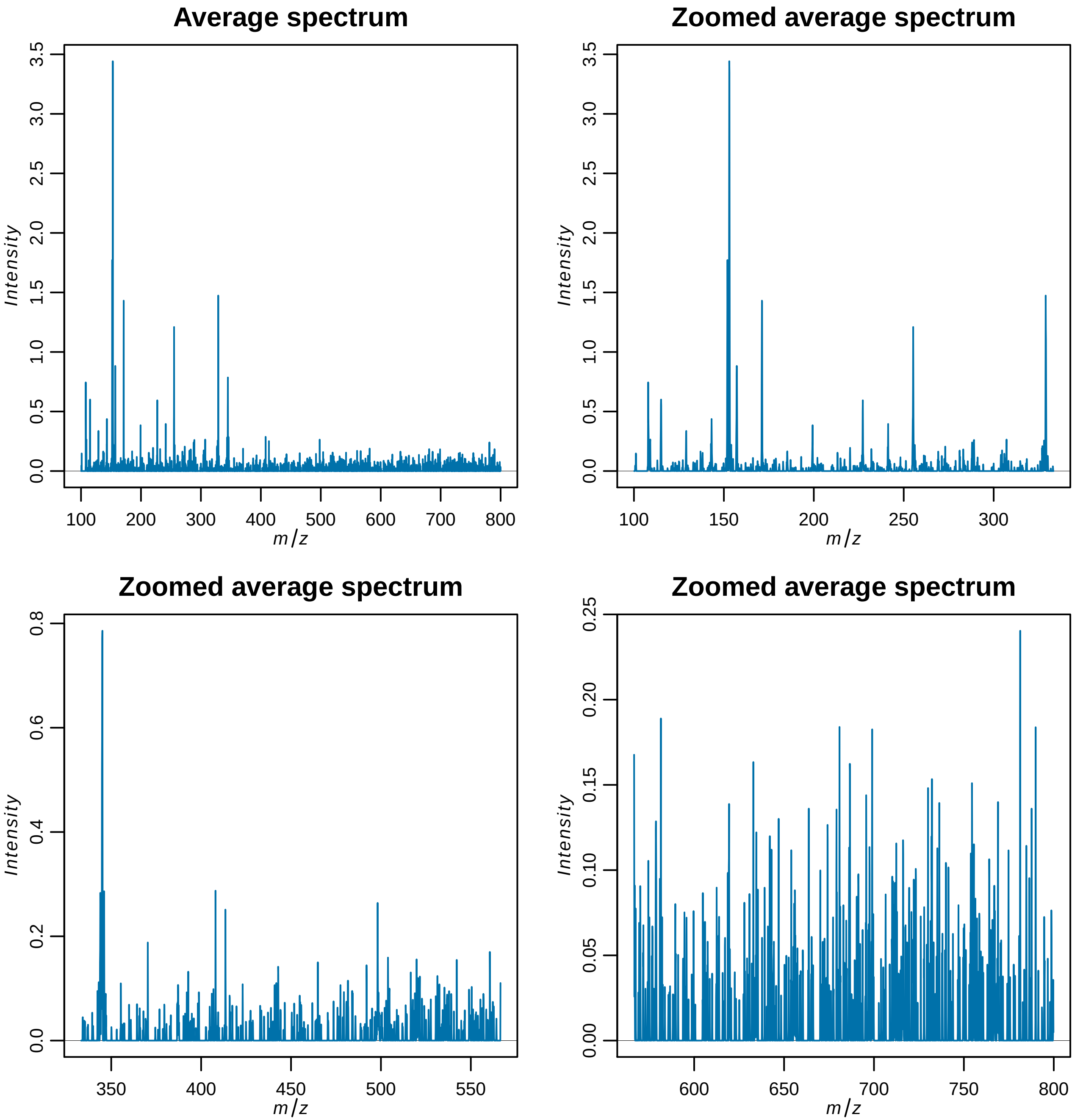

Sum of intensities per m/z
Frequency
0
2000
4000
6000
8000
sum of intensities per m/z
0
10
20
30
40


Median intensity per spectrum

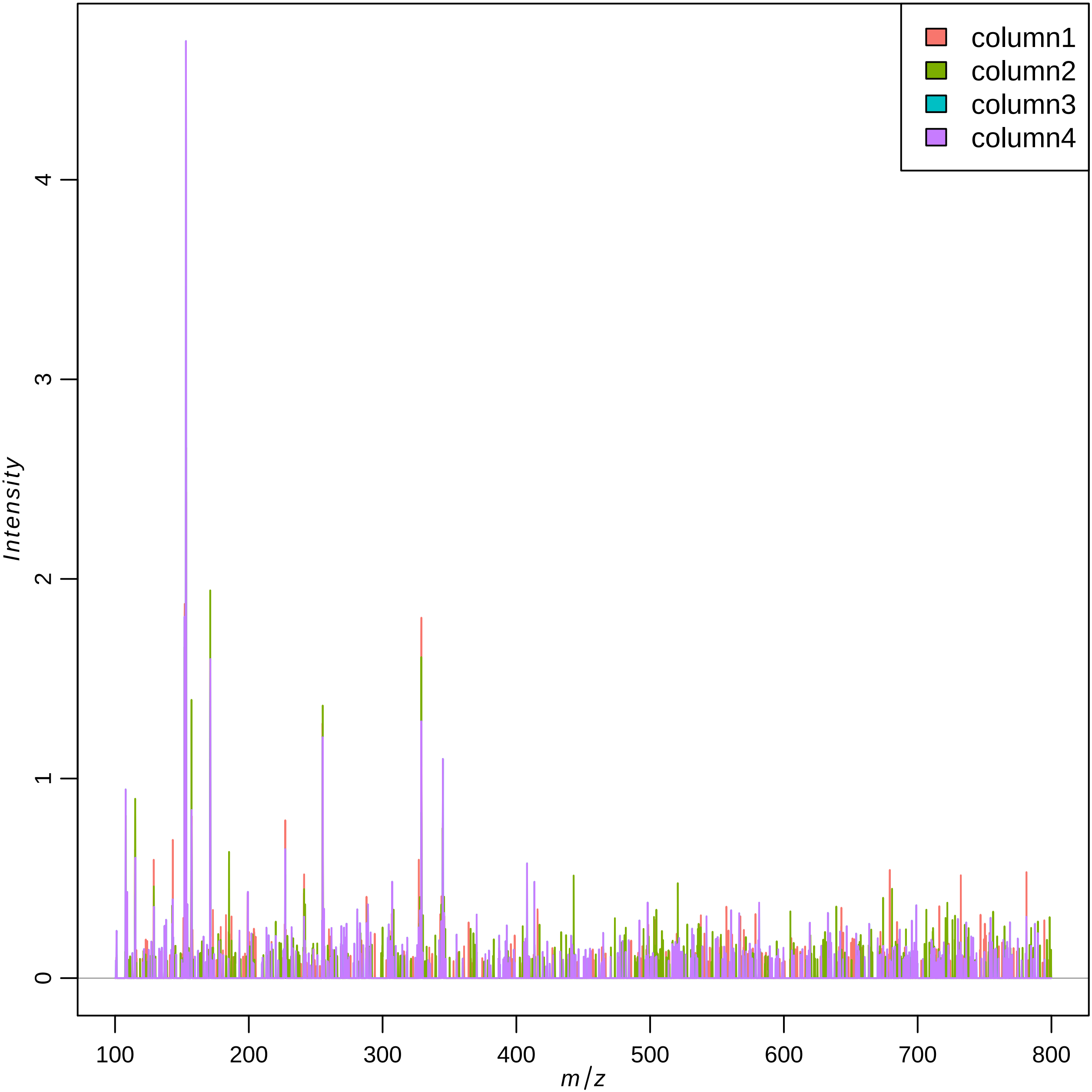

Intensity histogram

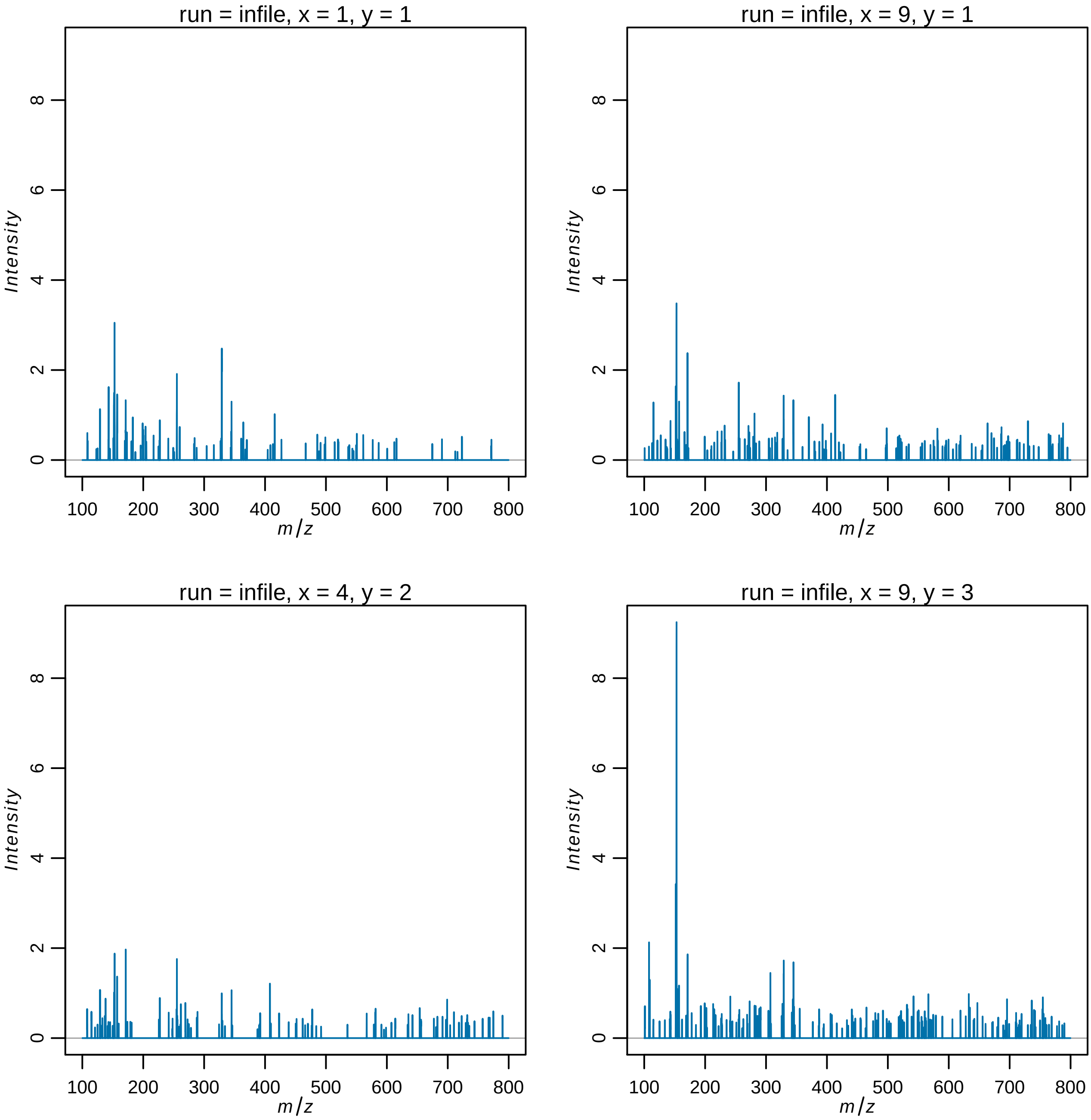

Intensities per sample
Frequency
100000
75000
50000
25000
0
0.0
2.5
5.0
7.5
intensities
annotation
column1
column2
column3
column4

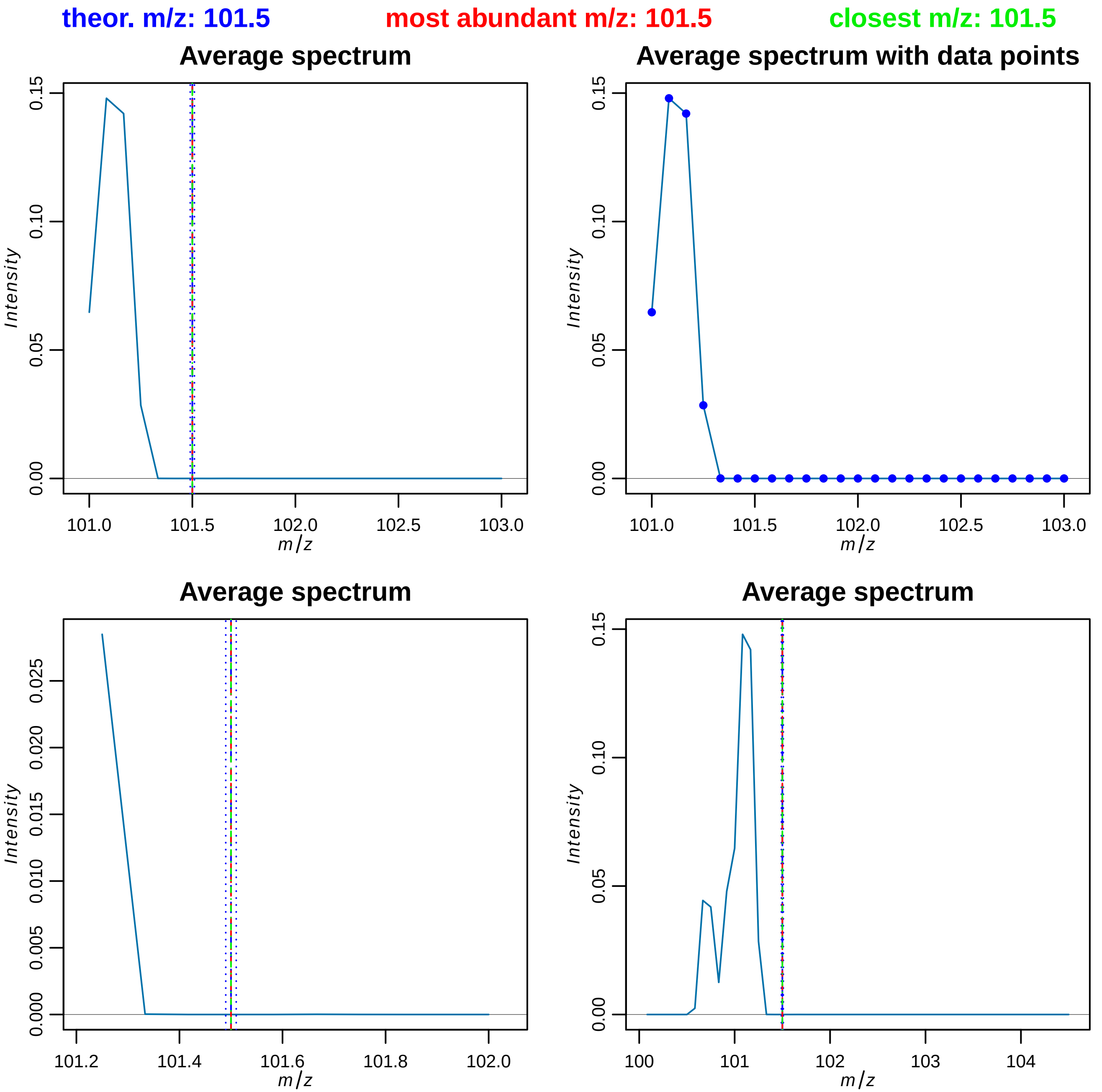

Log10 mean m/z intensities per annotation group
Log10 mean intensity per m/z
0
−5
−10
−15
−20
−25
column1
column2
column3
column4


Average spectrum
Intensity
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
100
200
300
400
500
600
700
800
m/z
Zoomed average spectrum
Intensity
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
100
150
200
250
300
m/z
Zoomed average spectrum
Intensity
0.0
0.2
0.4
0.6
0.8
350
400
450
500
550
m/z
Zoomed average spectrum
Intensity
0.00
0.05
0.10
0.15
0.20
0.25
600
650
700
750
800
m/z

Average mass spectra for annotation groups




run = infile, x = 1, y = 1
run = infile, x = 9, y = 1
run = infile, x = 4, y = 2
run = infile, x = 9, y = 3
Intensity
m/z
0
2
4
6
8
100
200
300
400
500
600
700
800

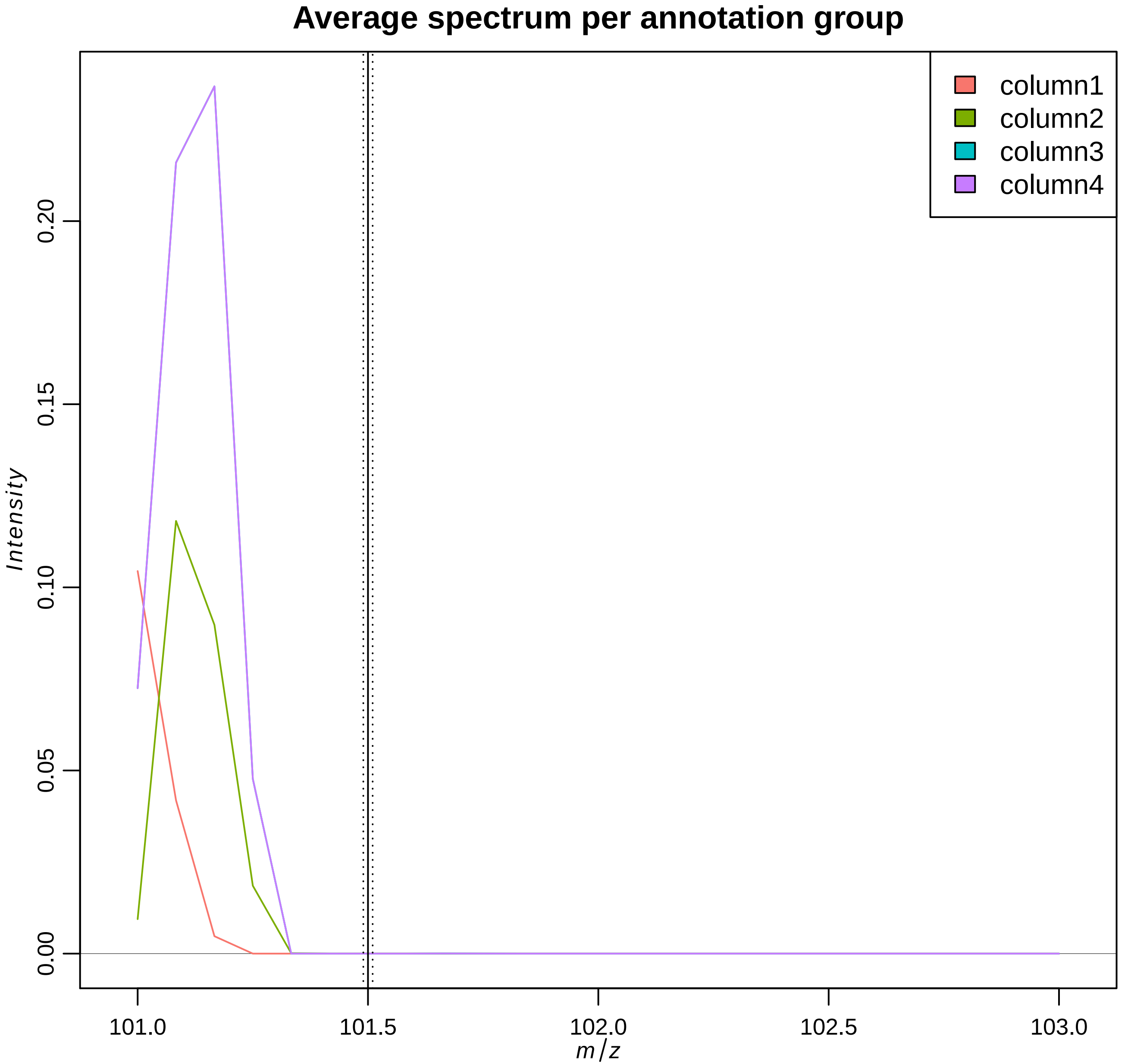


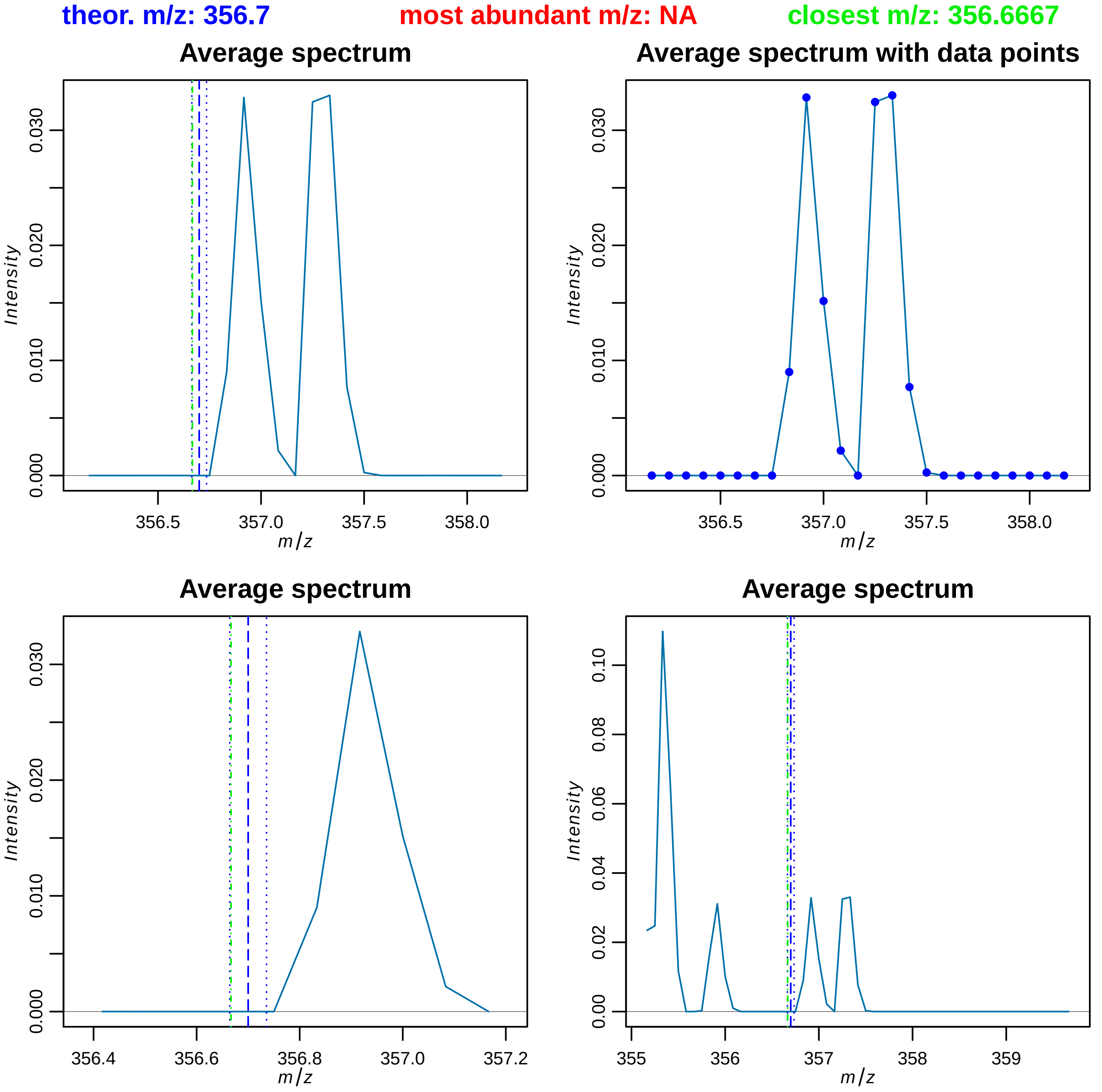
Average spectrum

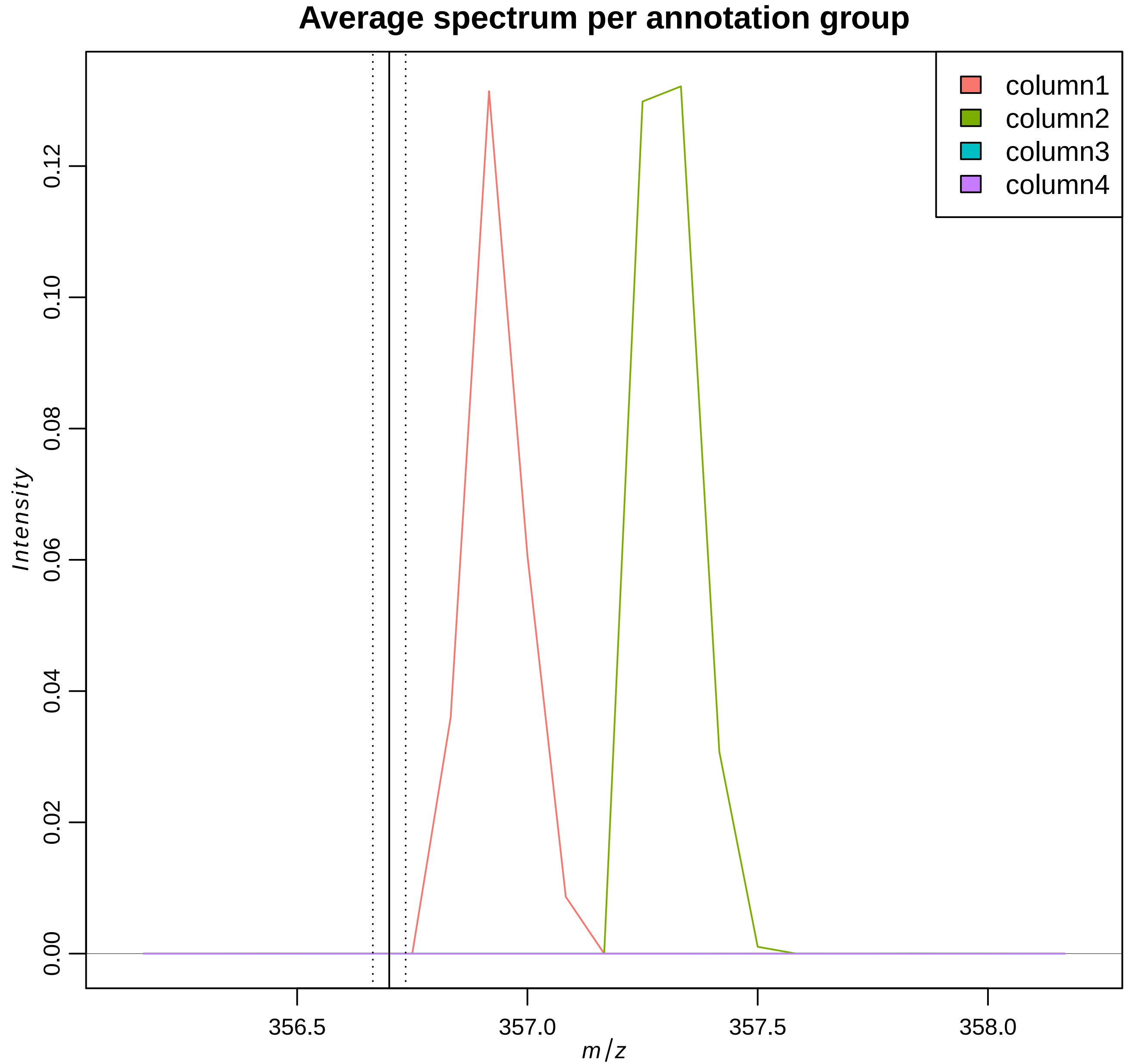
Average spectrum with data points

Average spectrum

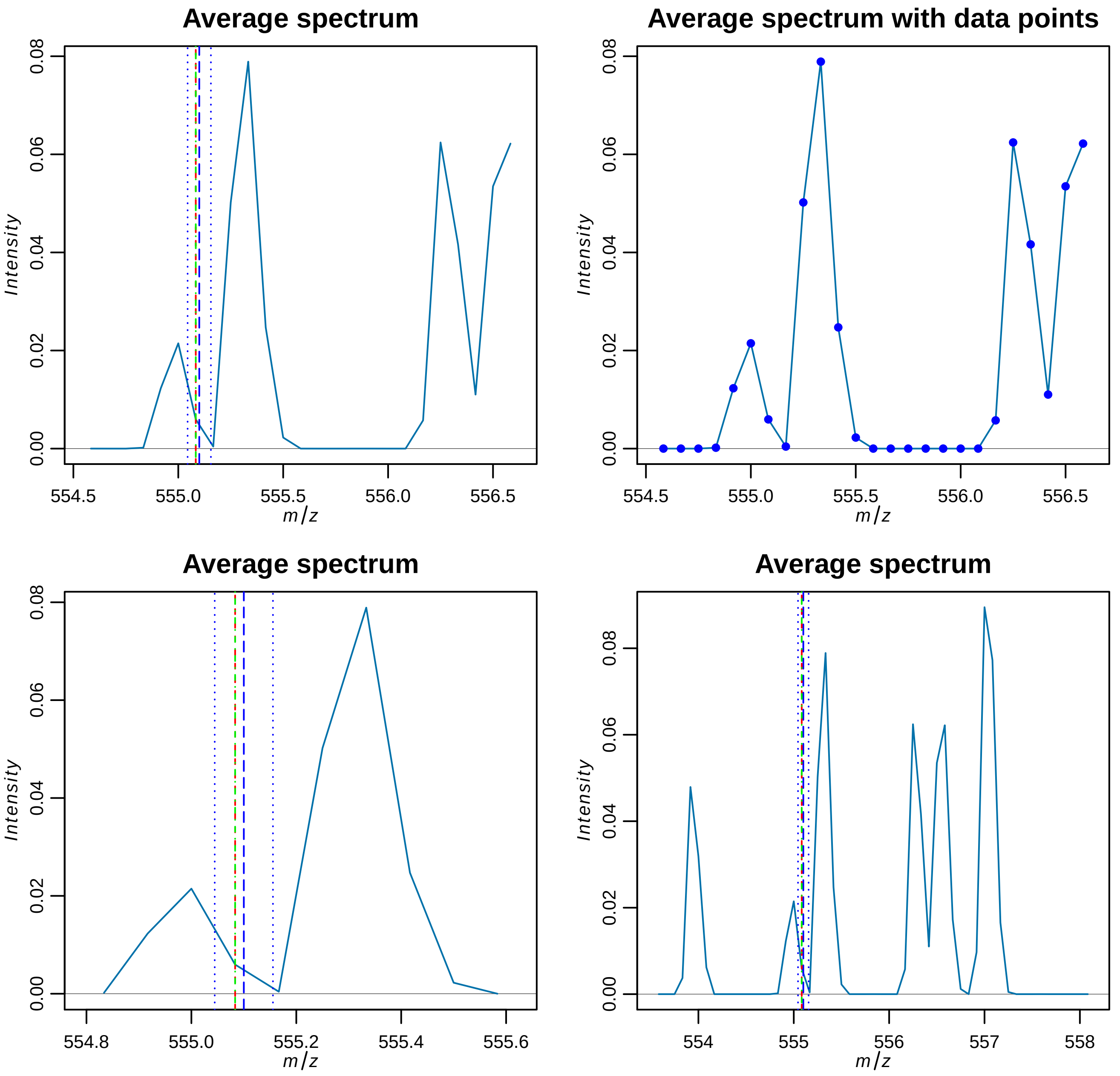
Average spectrum

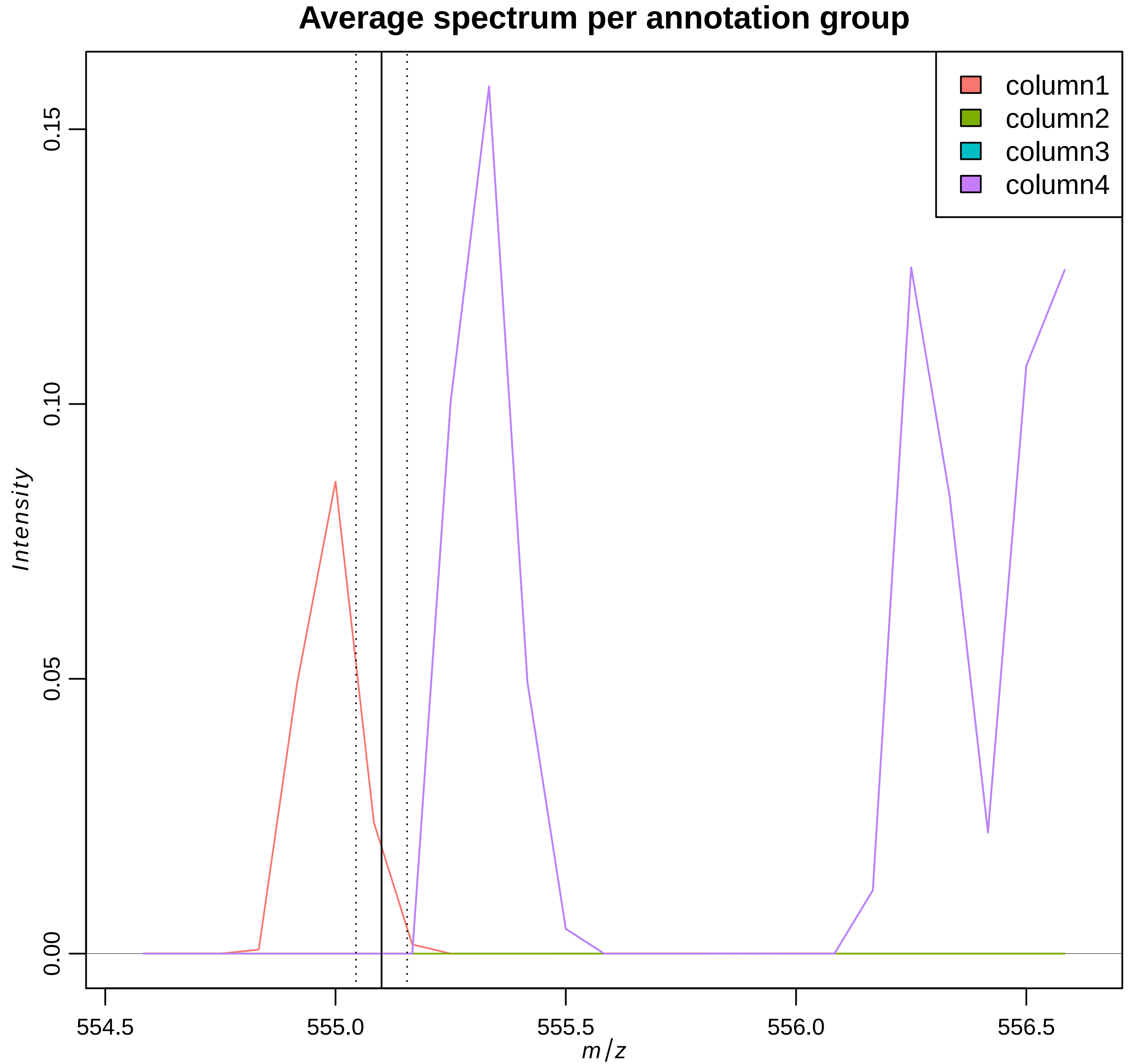

Average spectrum per annotation group
column1
column2
column3
column4
Intensity
0.00
0.05
0.10
0.15
0.20
m/z
101.0
101.5
102.0
102.5
103.0

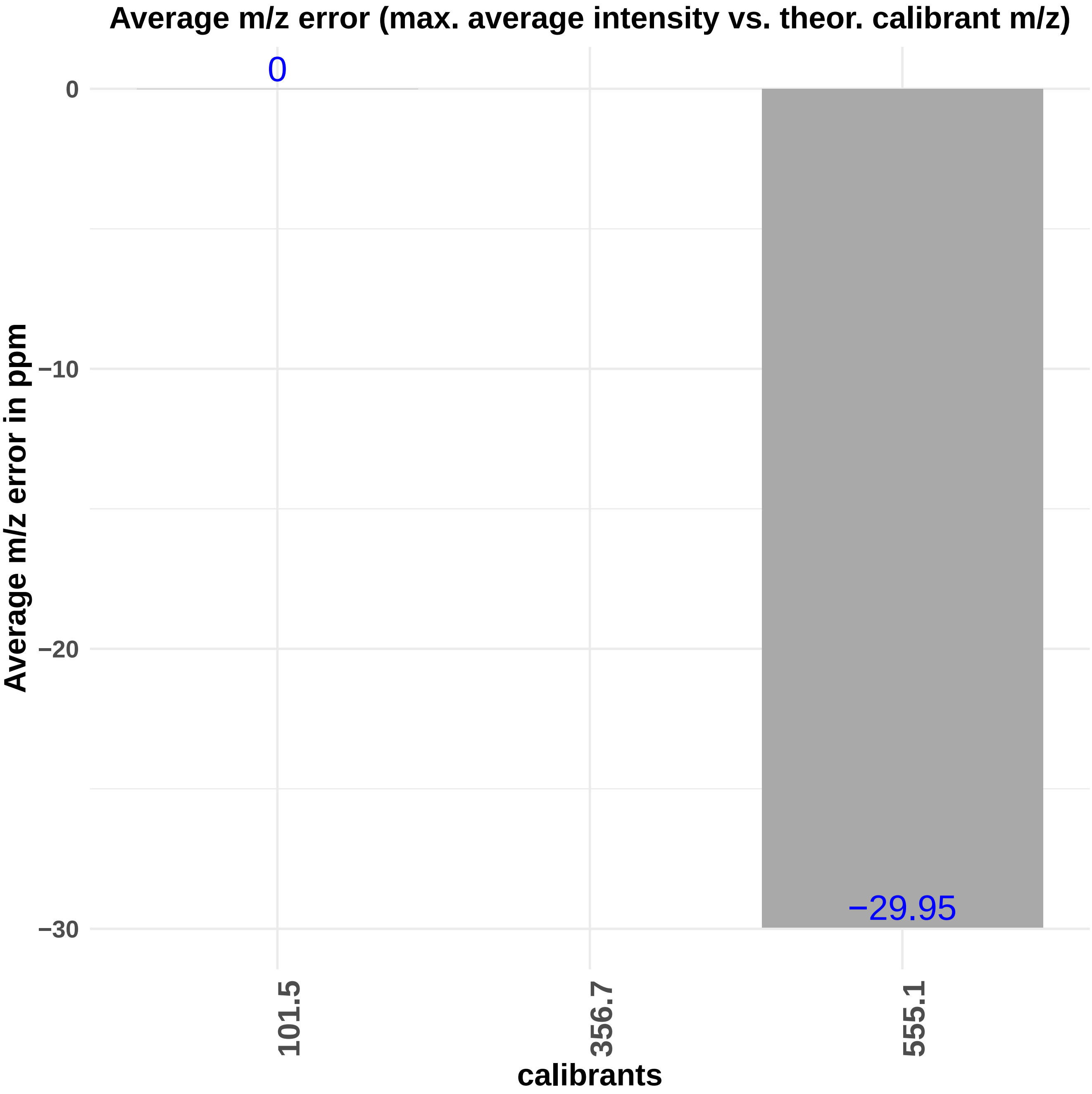

theor. m/z: 356.7
most abundant m/z: NA
closest m/z: 356.6667
Average spectrum
Intensity
0.000
0.010
0.020
0.030
356.5
357.0
357.5
358.0
m/z
Average spectrum with data points
Intensity
0.000
0.010
0.020
0.030
356.5
357.0
357.5
358.0
m/z
Average spectrum
Intensity
0.000
0.010
0.020
0.030
356.4
356.6
356.8
357.0
357.2
m/z
Average spectrum
Intensity
0.00
0.02
0.04
0.06
0.08
0.10
355
356
357
358
359
m/z

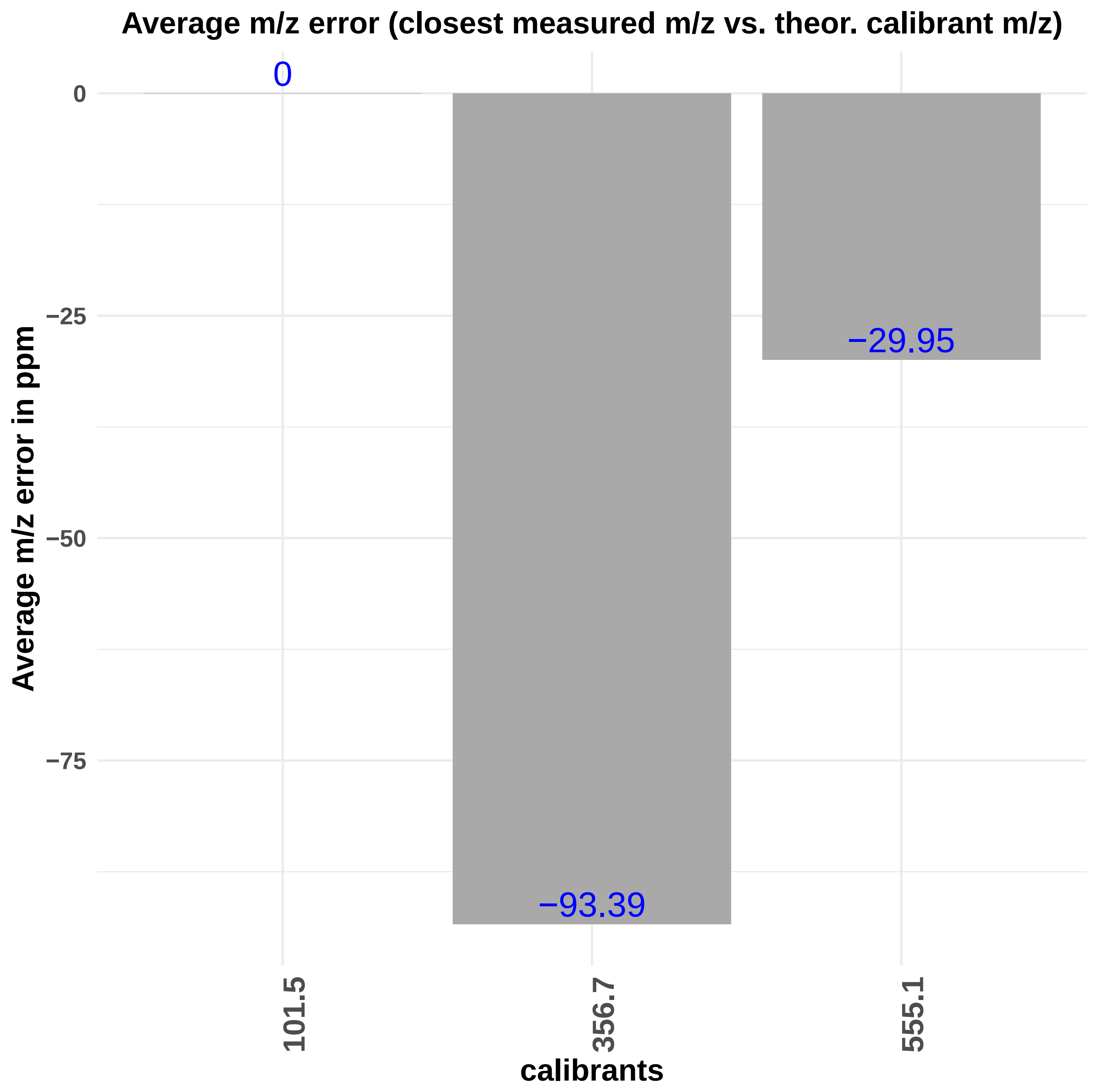

Average spectrum per annotation group
column1
column2
column3
column4
Intensity
0.00
0.02
0.04
0.06
0.08
0.10
0.12
356.5
357.0
357.5
358.0
m/z

theor. m/z: 555.1 **most abundant m/z: 555.0834** **closest m/z: 555.0834**

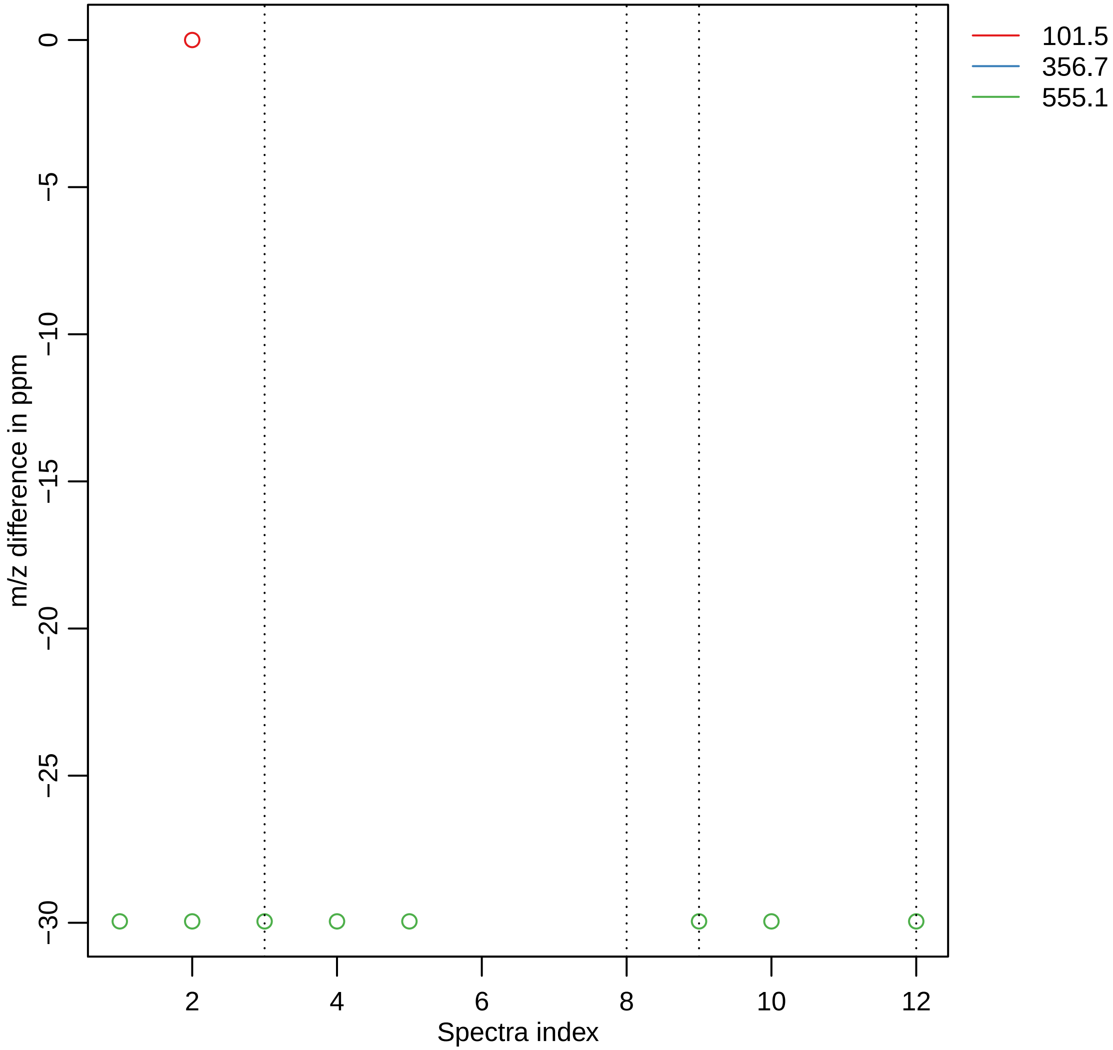



Average spectrum per annotation group
Intensity
0.00
0.05
0.10
0.15
m/z
554.5
555.0
555.5
556.0
556.5
column1
column2
column3
column4

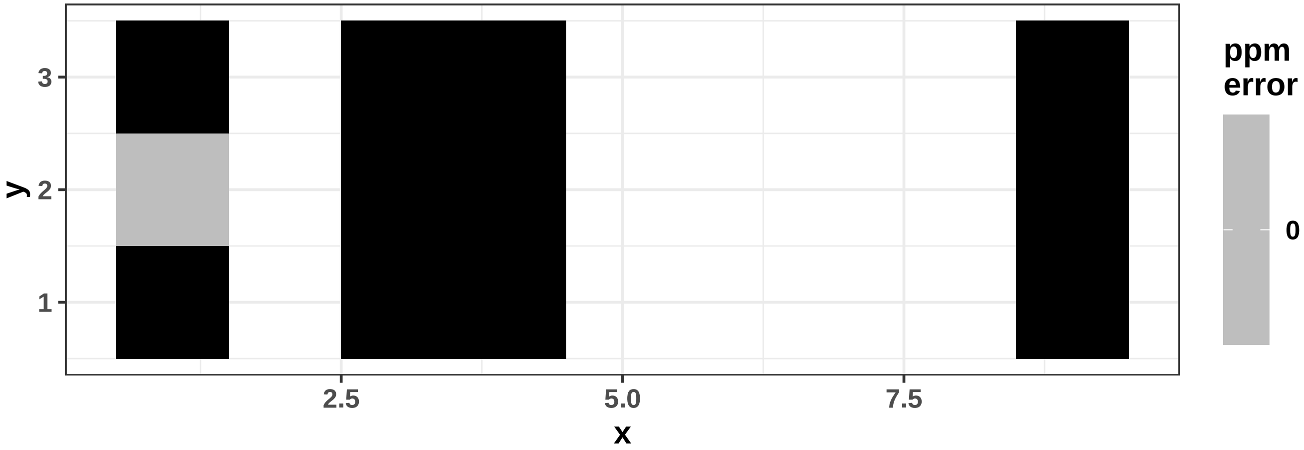

Average m/z error (max. average intensity vs. theor. calibrant m/z)
Average m/z error in ppm
0
−10
−20
−30
0
−29.95
101.5
356.7
555.1
calibrants

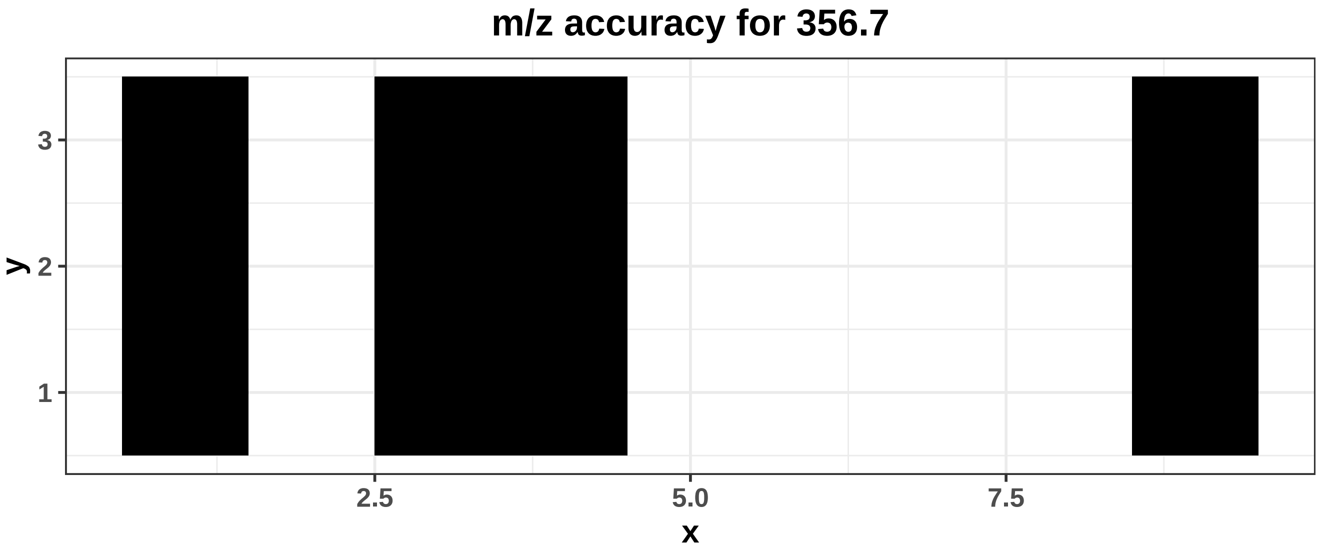

Average m/z error (closest measured m/z vs. theor. calibrant m/z)
Average m/z error in ppm
0
−25
−50
−75
0
−93.39
−29.95
101.5
356.7
555.1
calibrants

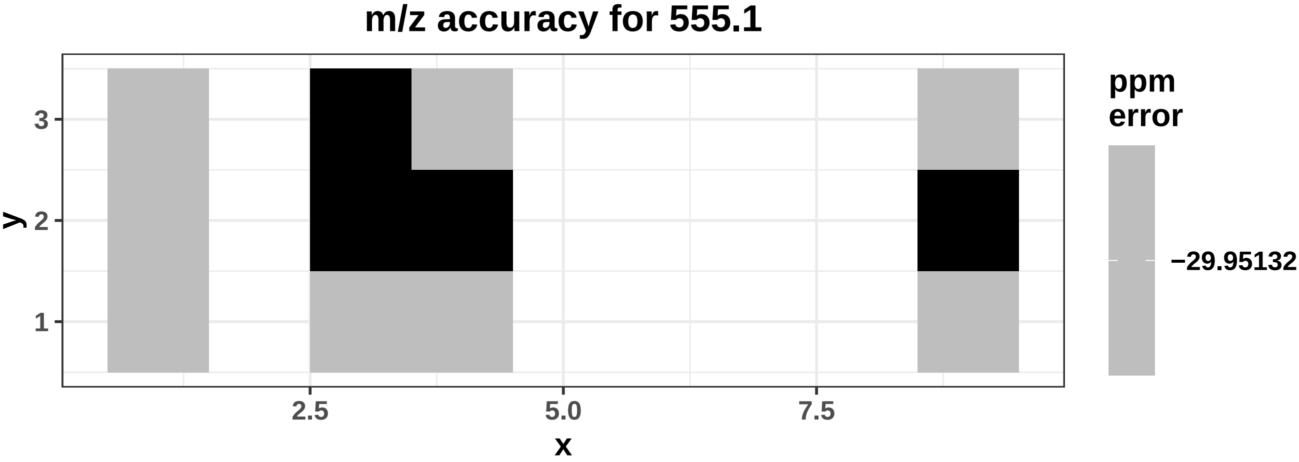
Difference m/z with max. average intensity vs. theor. m/z (per spectrum)



m/z accuracy for 101.5




m/z accuracy for 356.7
y
3
2
1
2.5
5.0
7.5
x


m/z accuracy for 555.1
y
3
2
1
x
2.5
5.0
7.5
ppm error
−29.95132