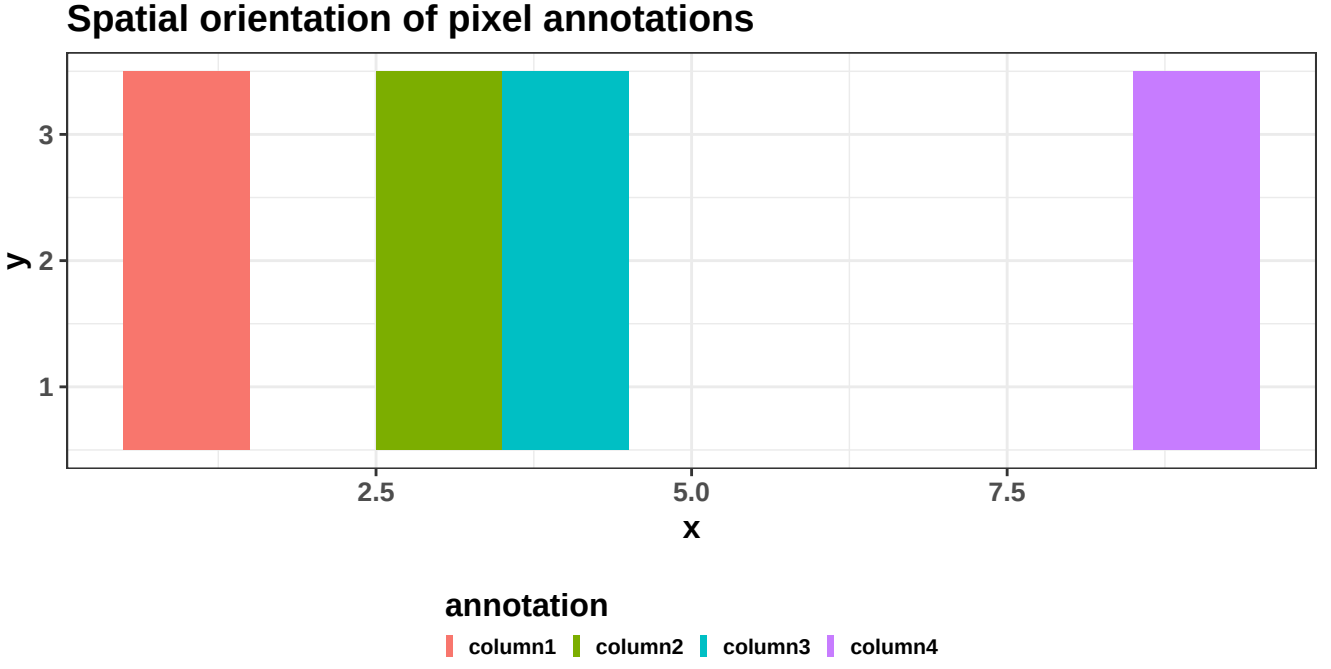
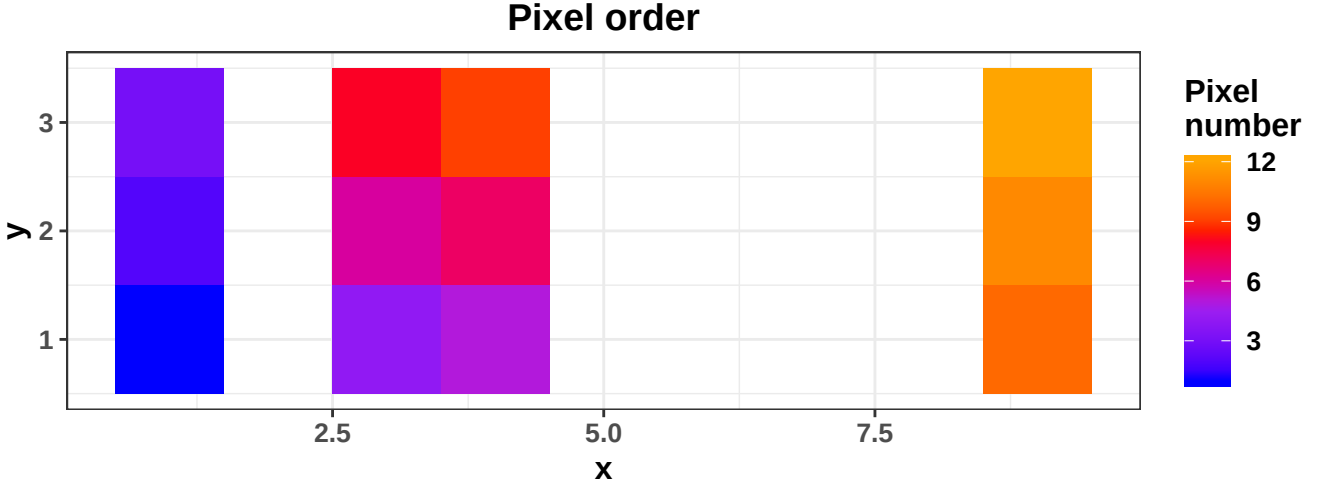
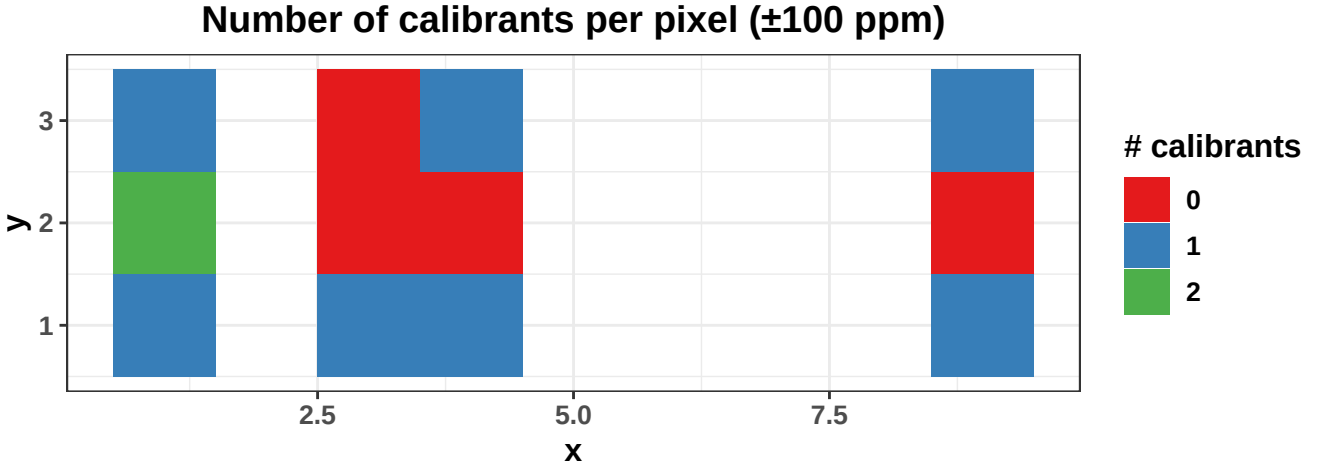
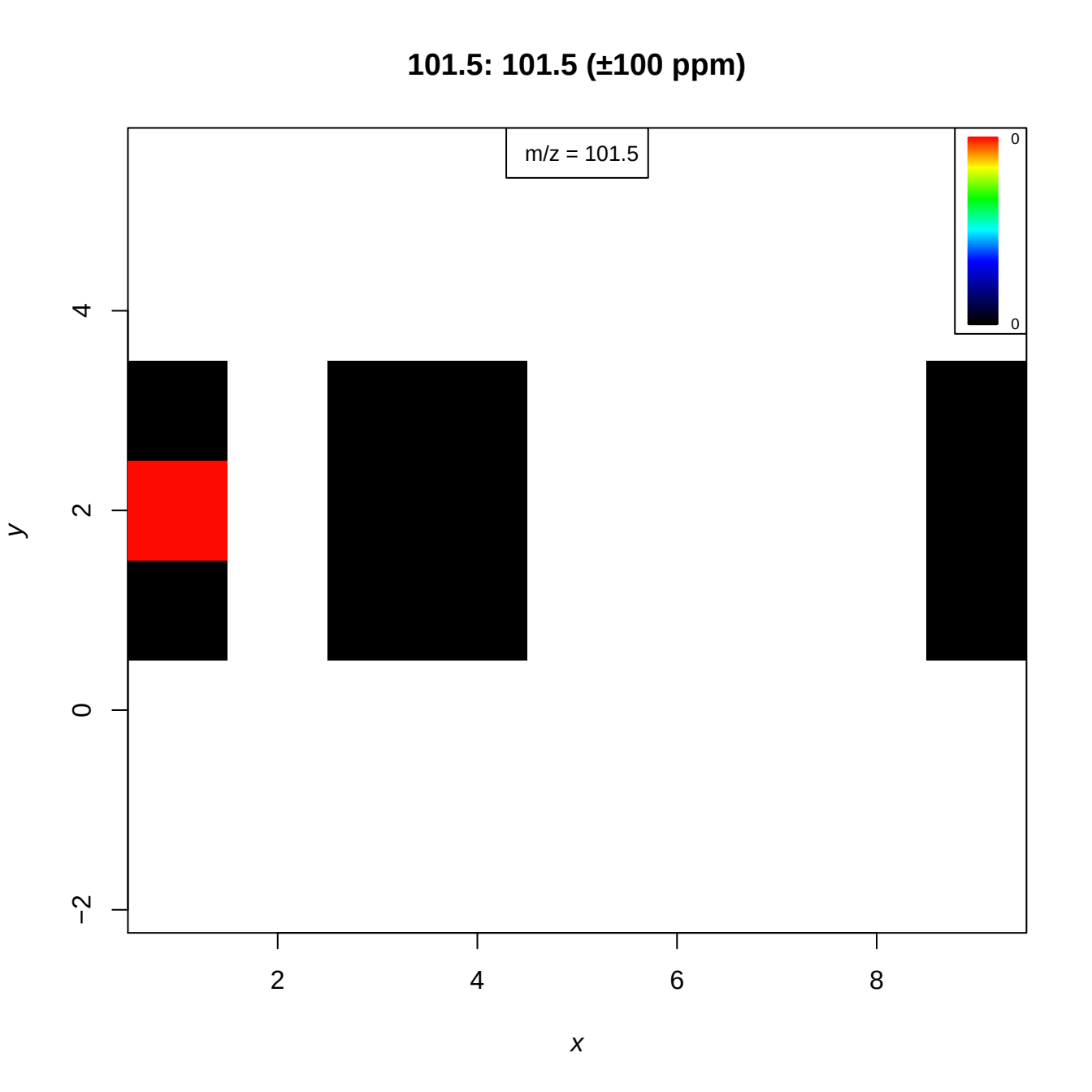
Testfile_rdata

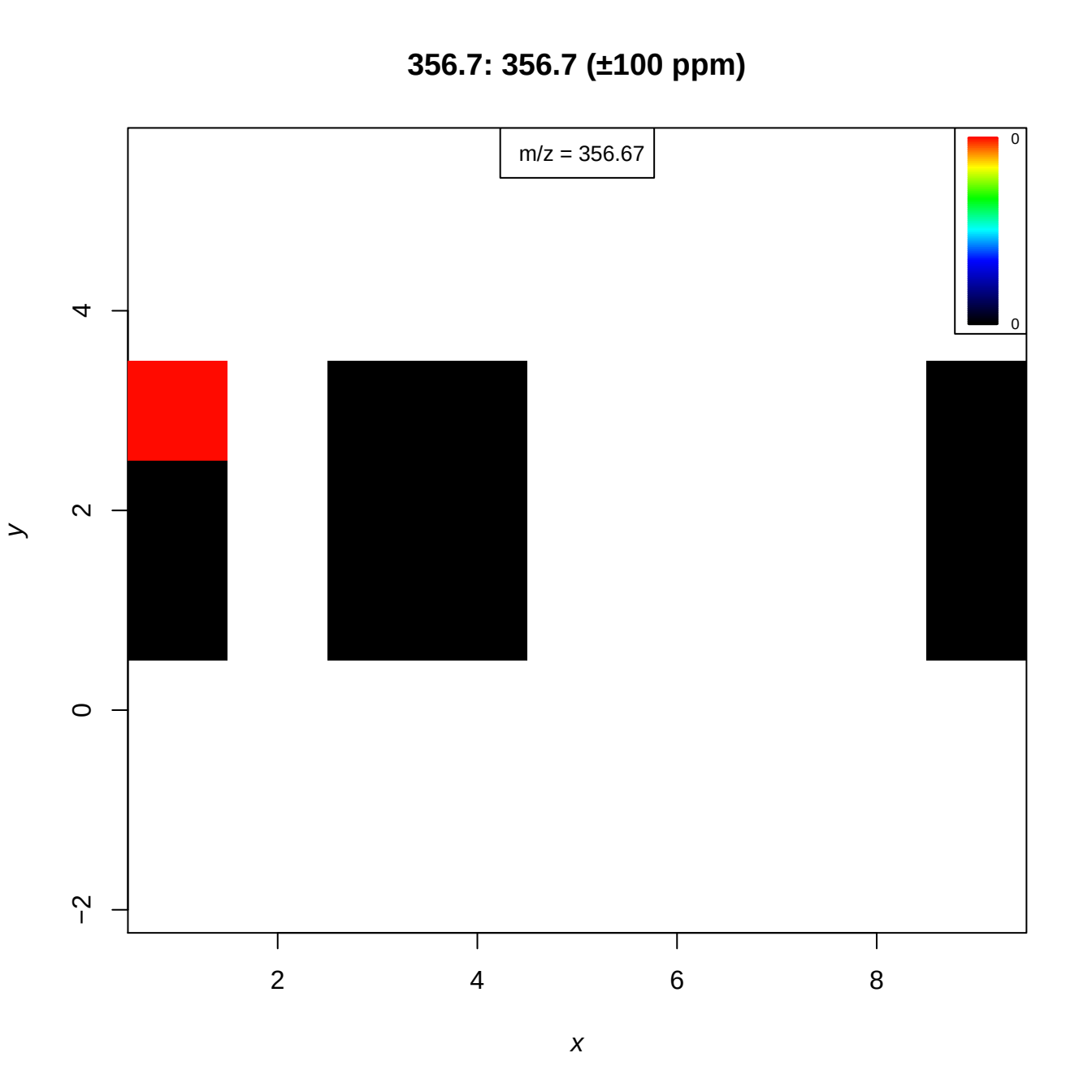
properties	values
Number of m/z features	8399
Range of m/z values	100.08 − 799.92
Number of pixels	12
Range of x coordinates	1 − 9
Range of y coordinates	1 − 3
Range of intensities	0 − 9.24
Number of NA intensities	0
Number of Inf intensities	0
Median of intensities	0
Intensities > 0	31.29 %
Number of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

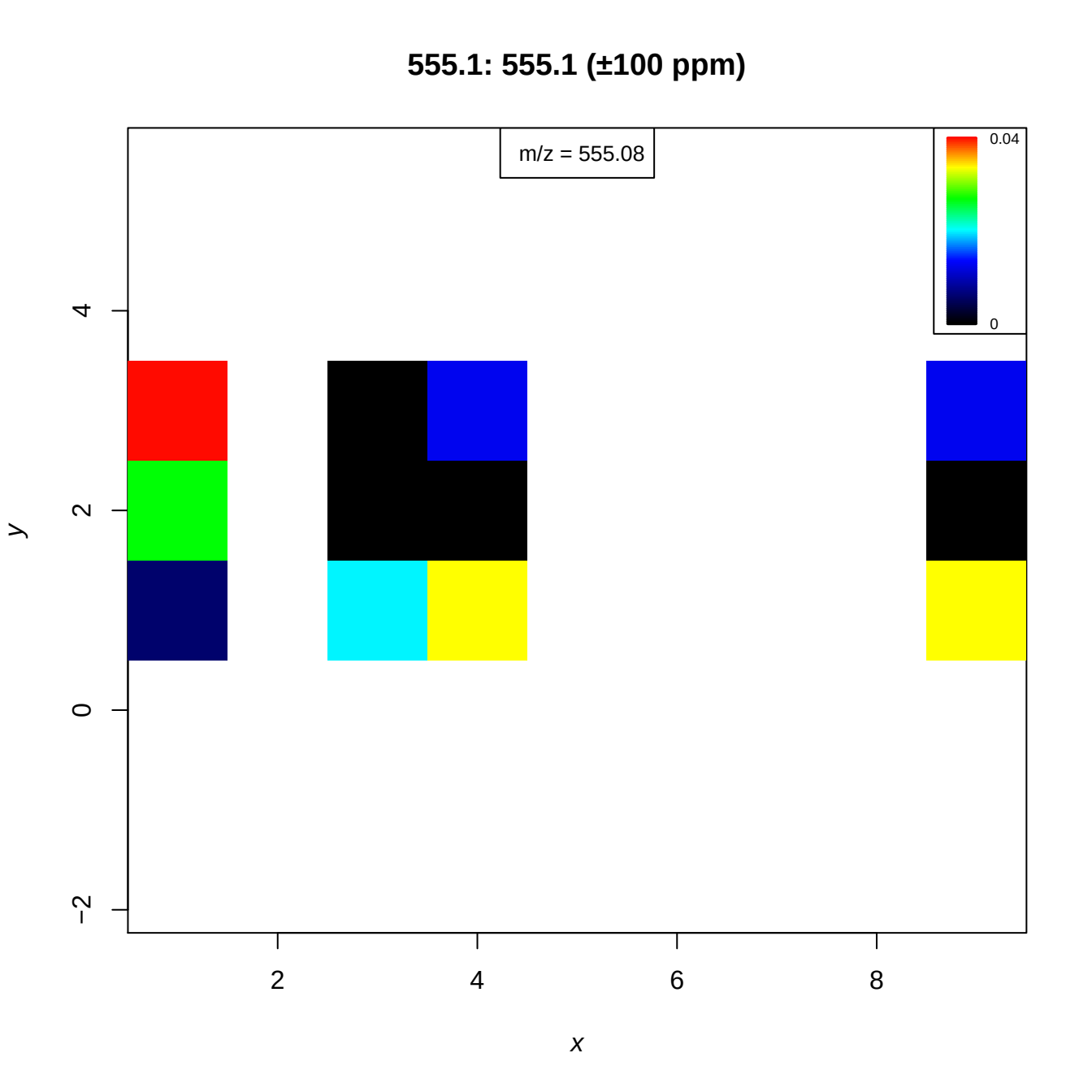

Spatial orientation of pixel annotations
3
2
1
y
2.5
5.0
7.5
x
annotation
column1
column2
column3
column4

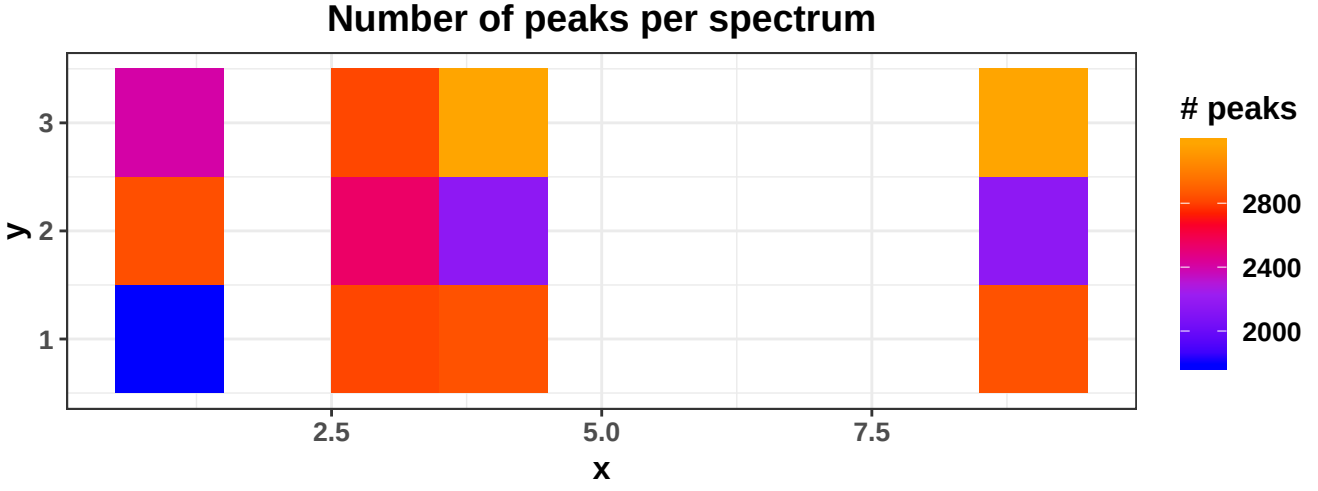

Pixel order
y
3
2
1
2.5
5.0
7.5
x
Pixel number
12
9
6
3

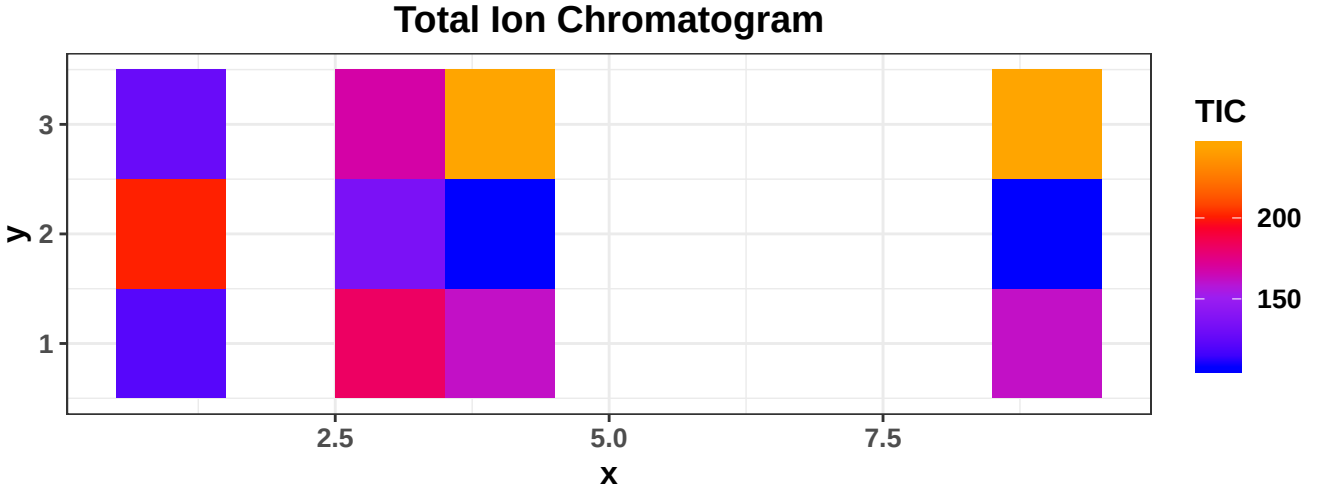

Number of calibrants per pixel (±100 ppm)
y
3
2
1
2.5
5.0
7.5
x
calibrants
0
1
2

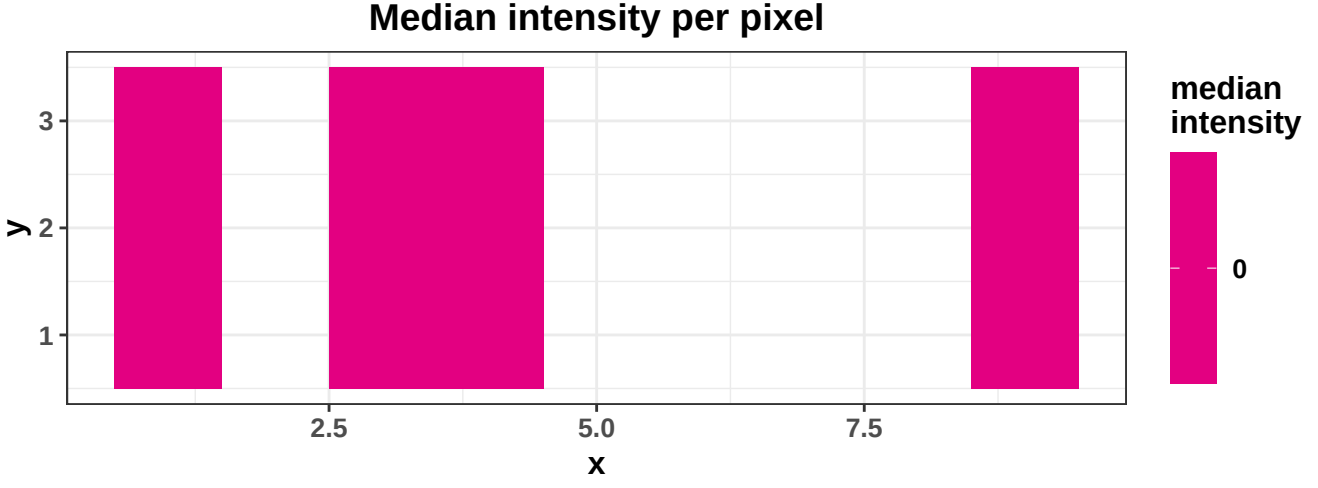

101.5: 101.5 (±100 ppm)
m/z = 101.5
0
0
4
2
0
−2
y
2
4
6
8
x

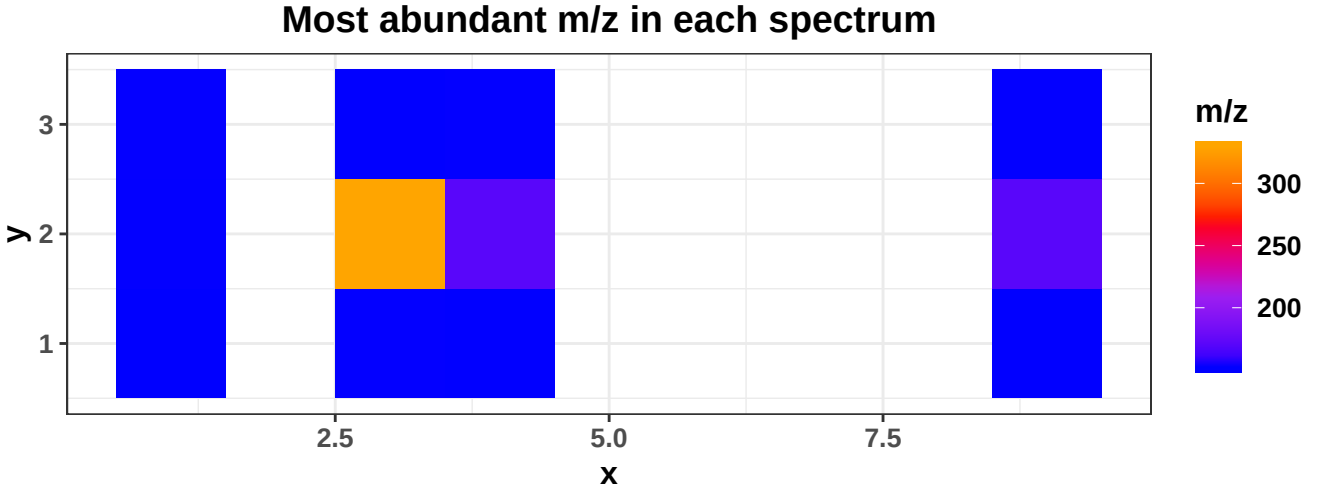

356.7: 356.7 (±100 ppm)
m/z = 356.67
0
0
y
4
2
0
−2
2
4
6
8
x

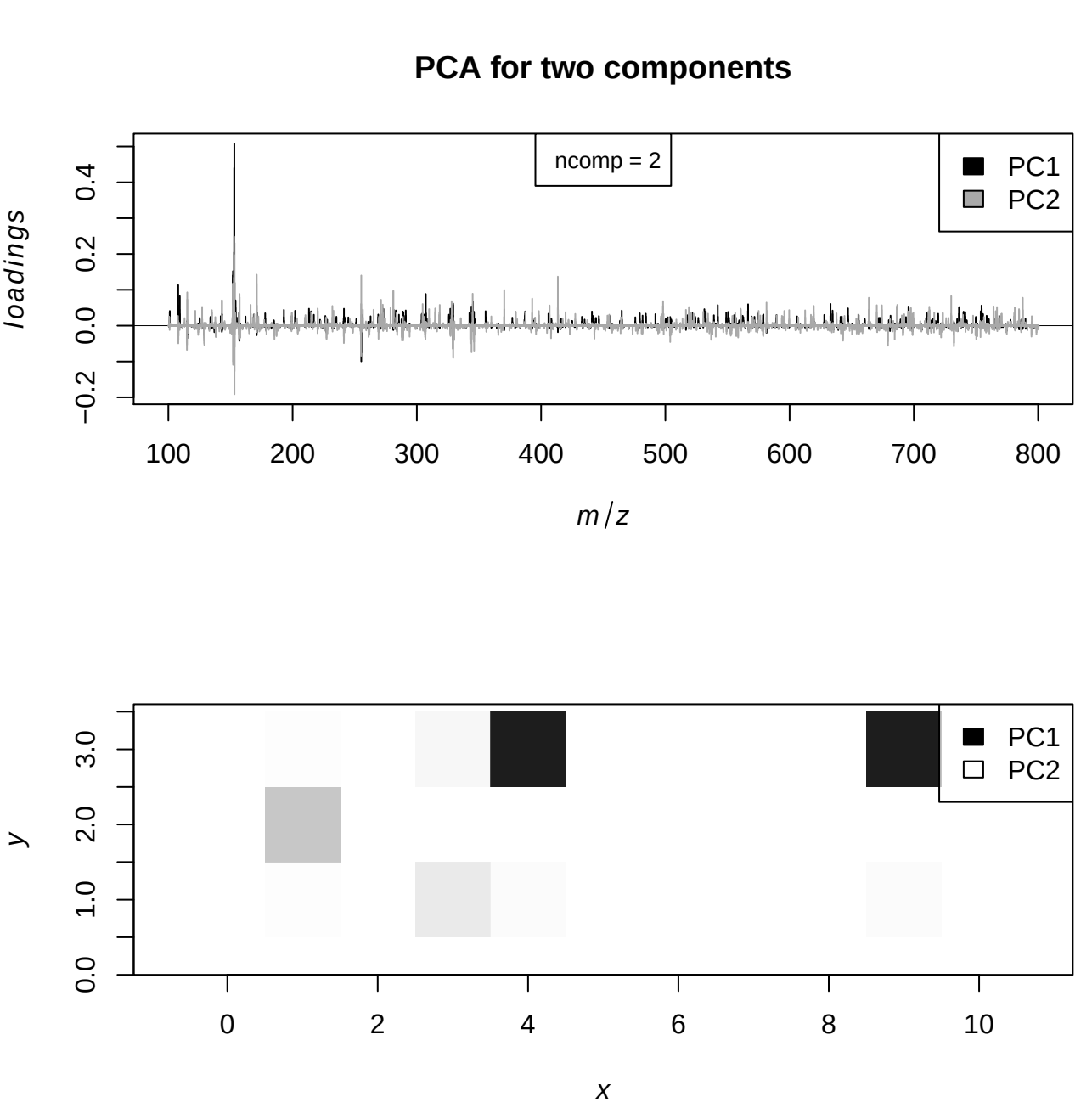

555.1: 555.1 (±100 ppm)
m/z = 555.08
0.04
0
y
x
4
2
0
−2
2
4
6
8

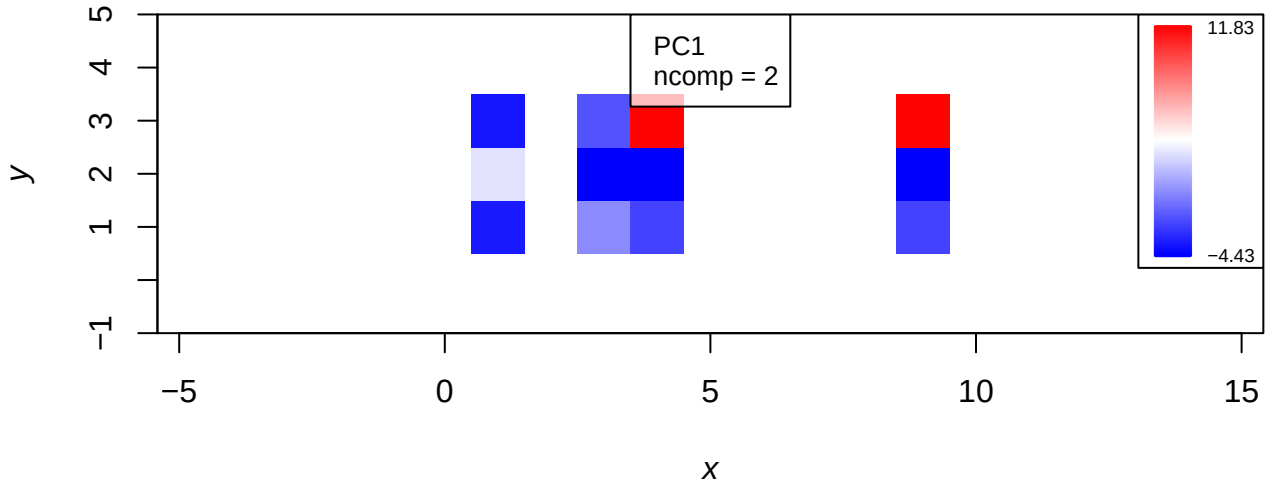

Number of peaks per spectrum
y
3
2
1
2.5
5.0
7.5
x
peaks
2800
2400
2000

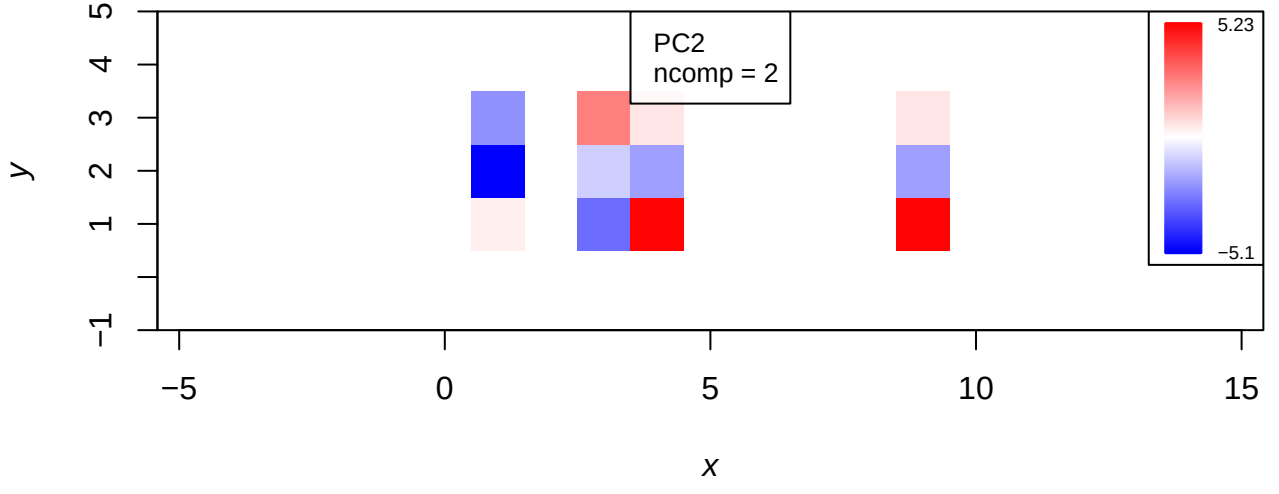

Total Ion Chromatogram
y
3
2
1
2.5
5.0
7.5
x
TIC
200
150

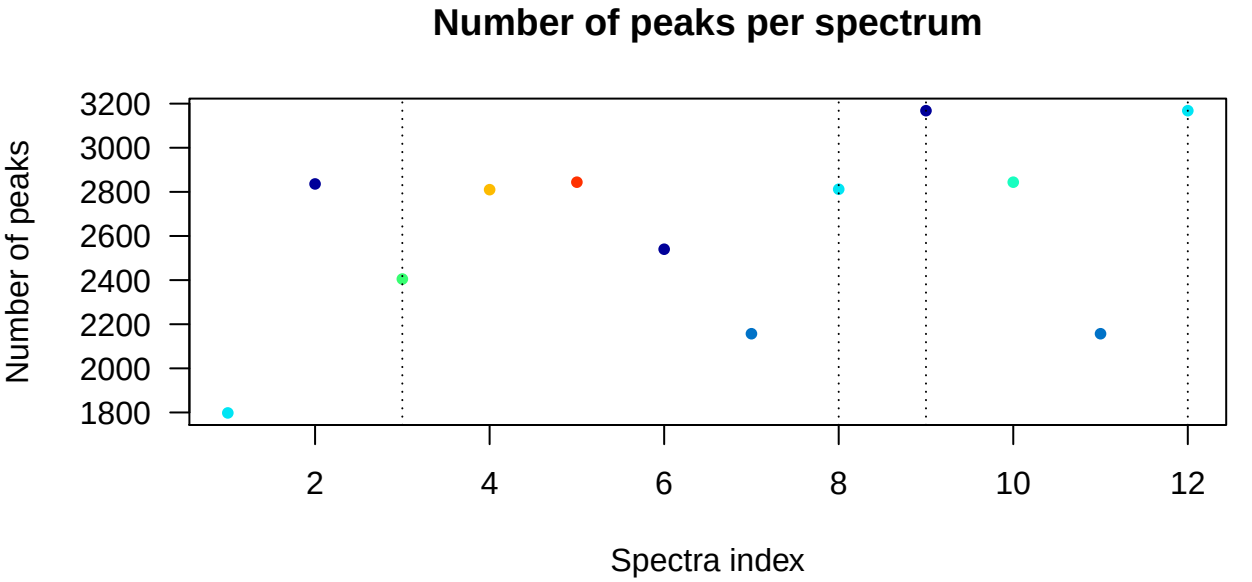

Median intensity per pixel
y
3
2
1
2.5
5.0
7.5
x
median intensity
0

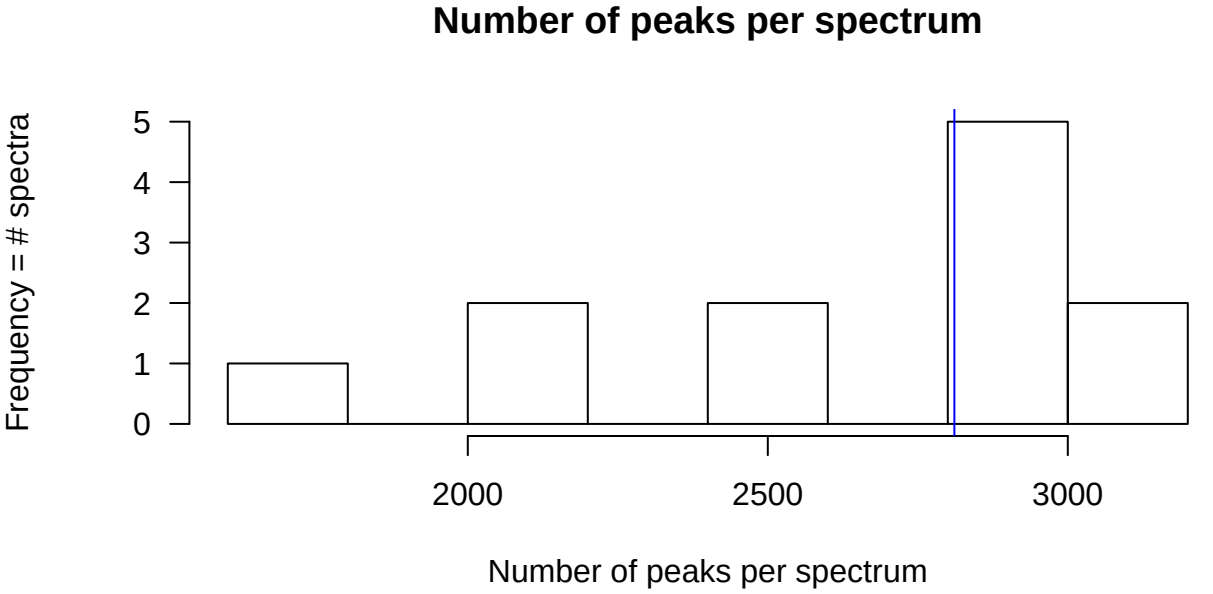

Most abundant m/z in each spectrum
y
3
2
1
2.5
5.0
7.5
x
m/z
300
250
200

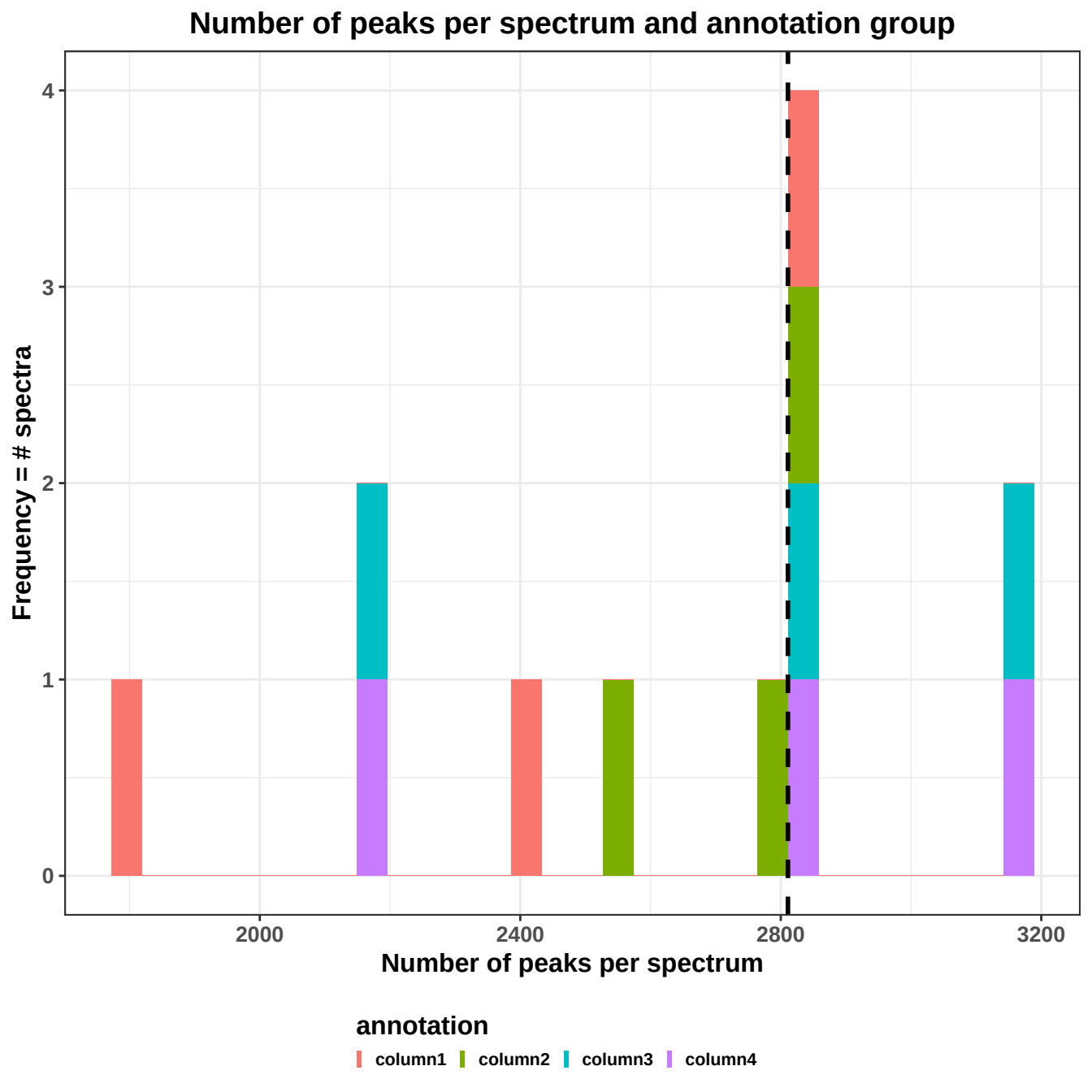

PCA for two components
ncomp = 2
PC1
PC2
loadings
0.4
0.2
0.0
−0.2
100
200
300
400
500
600
700
800
m/z
PC1
PC2
y
3.0
2.0
1.0
0.0
0
2
4
6
8
10
x

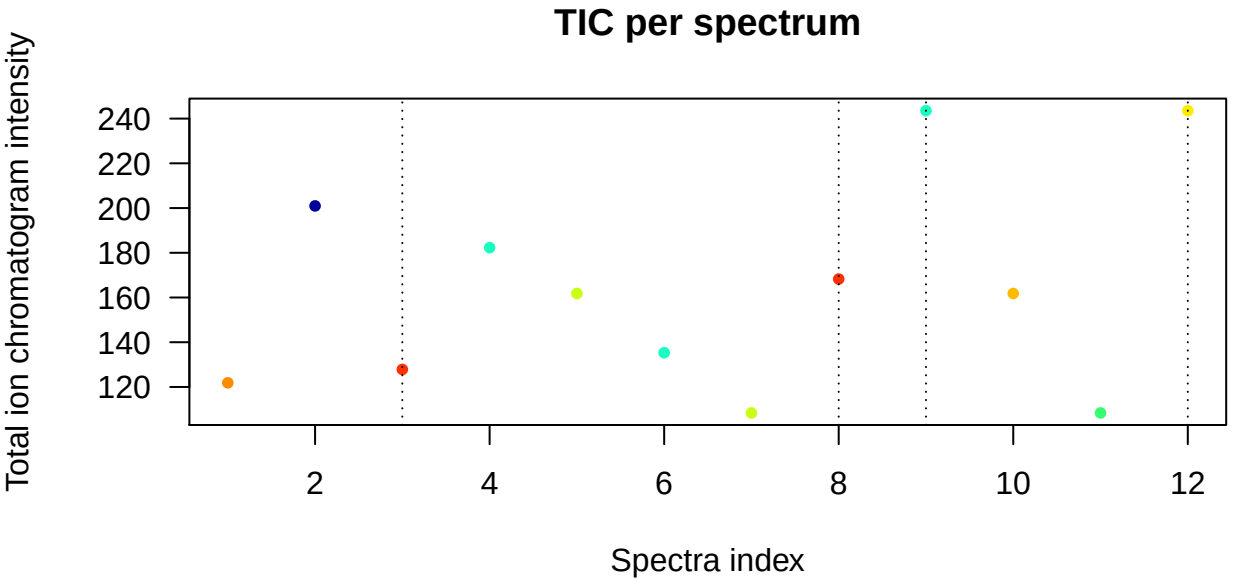

PC1
ncomp = 2
11.83
−4.43
y
x
−1
1
2
3
4
5
−5
0
5
10
15

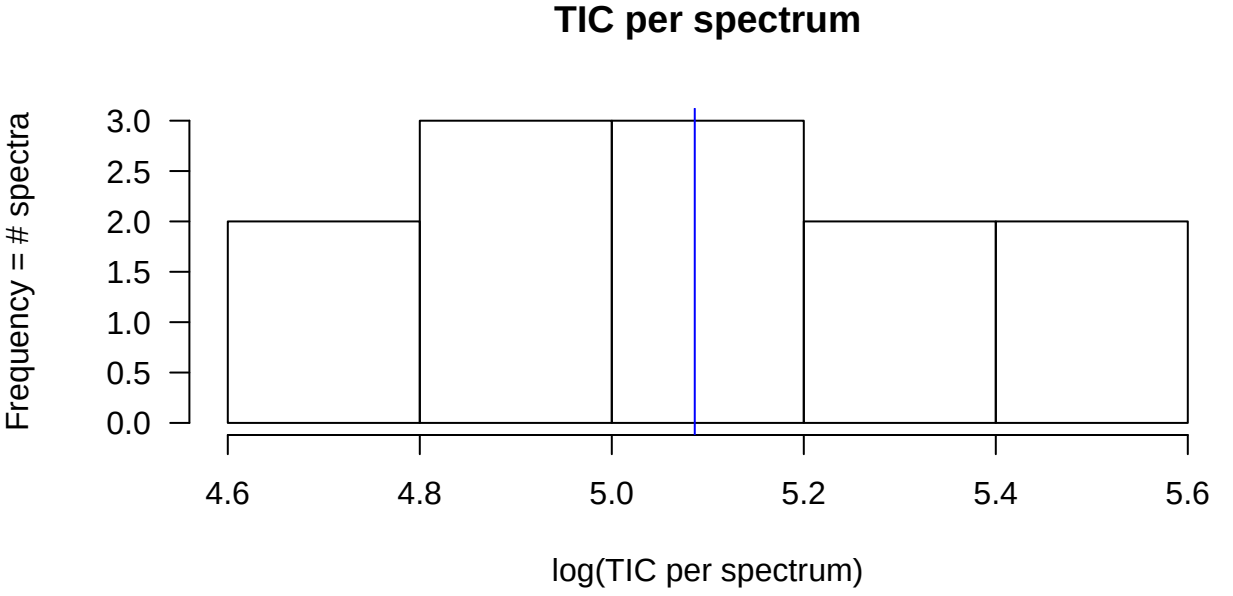

PC2
ncomp = 2
5.23
−5.1
y
x
−1
1
2
3
4
5
−5
0
5
10
15

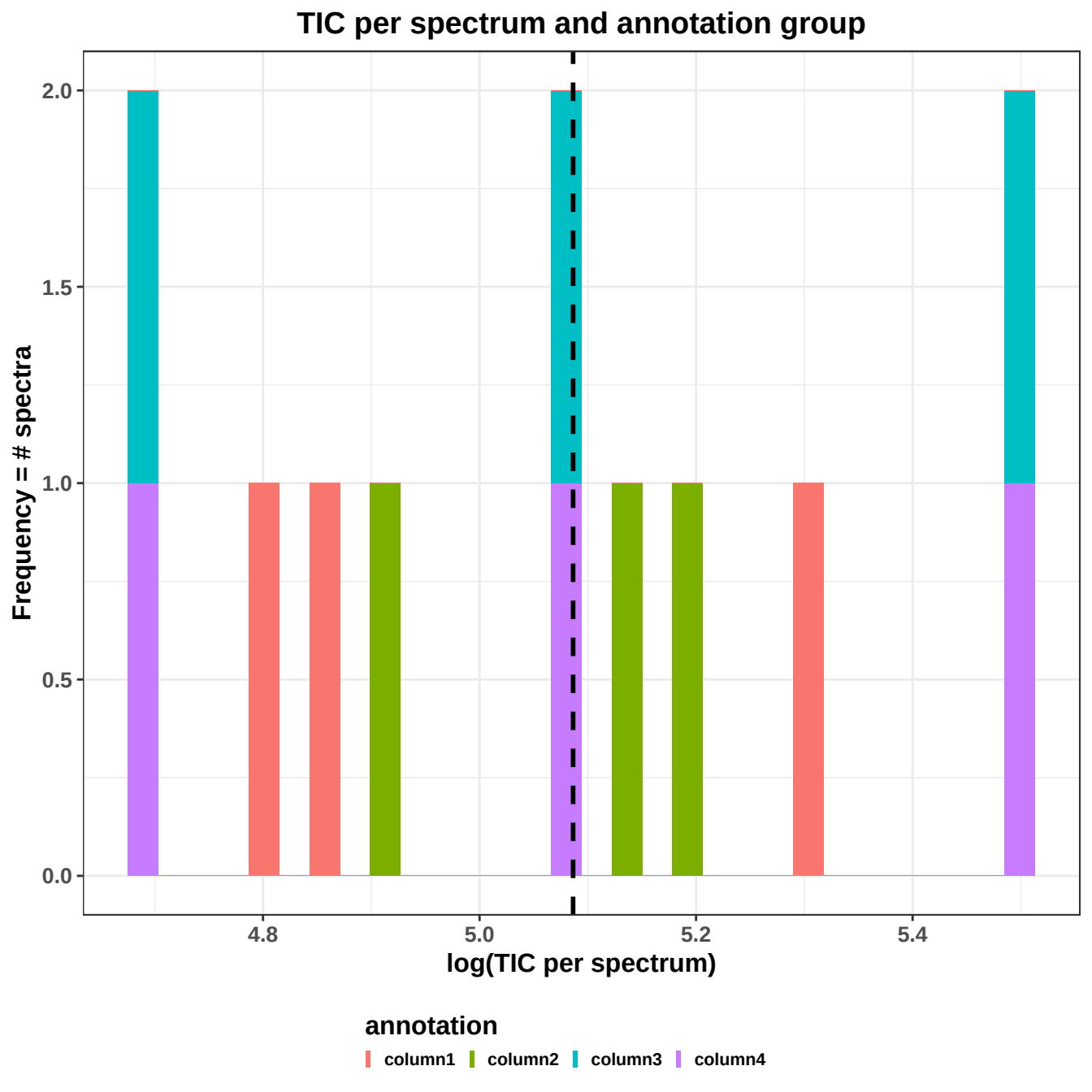

Number of peaks per spectrum
Number of peaks
3200
3000
2800
2600
2400
2200
2000
1800
2
4
6
8
10
12
Spectra index

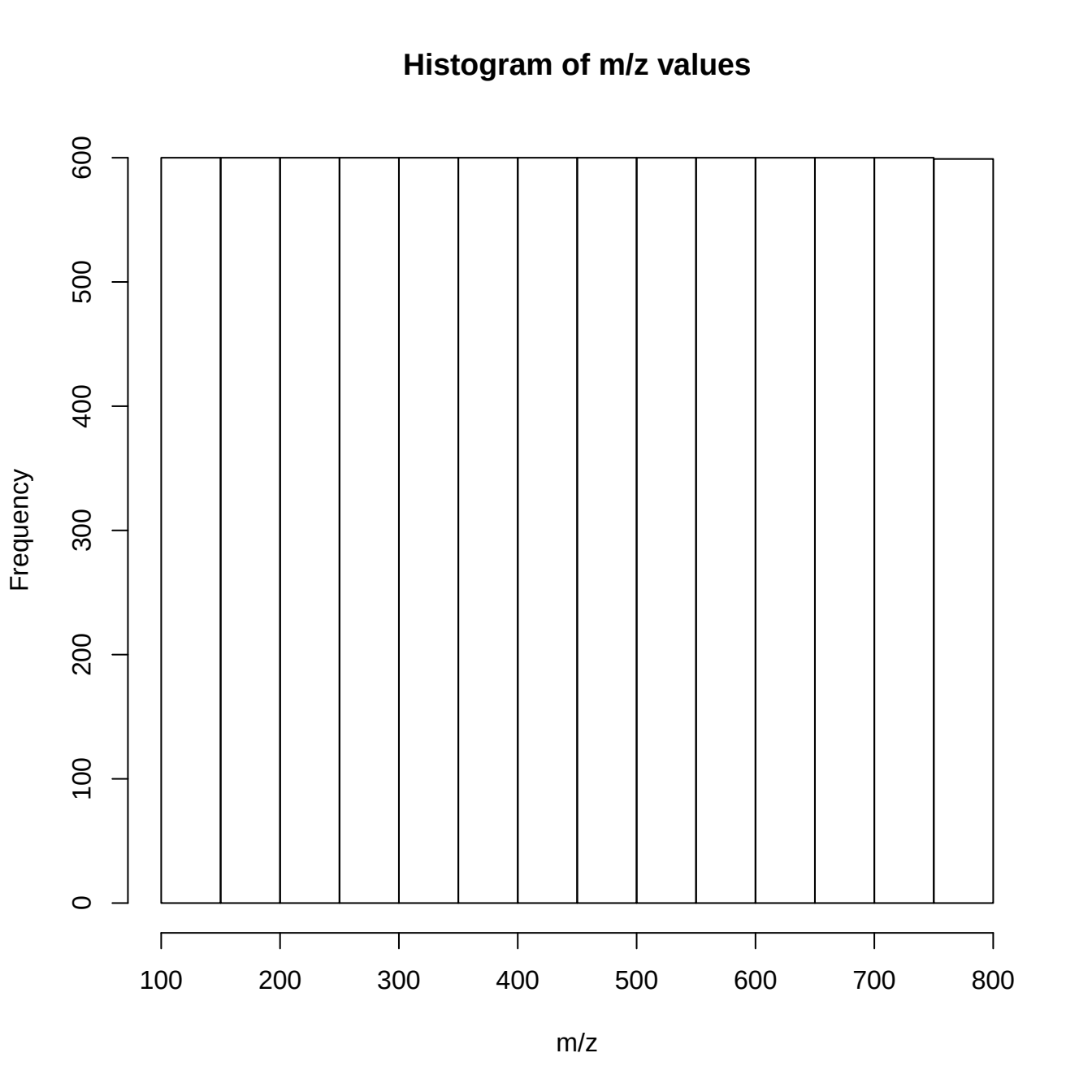

Number of peaks per spectrum
Frequency = # spectra
5
4
3
2
1
0
2000
2500
3000
Number of peaks per spectrum

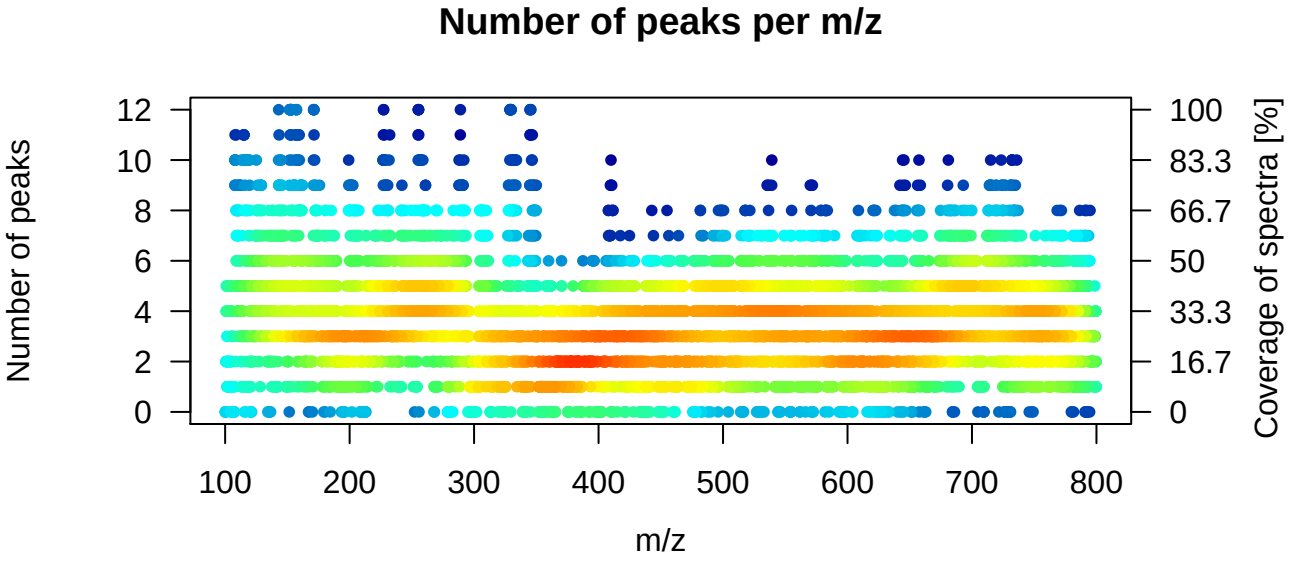

Number of peaks per spectrum and annotation group
Frequency = # spectra
4
3
2
1
0
2000
2400
2800
3200
Number of peaks per spectrum
annotation
column1
column2
column3
column4

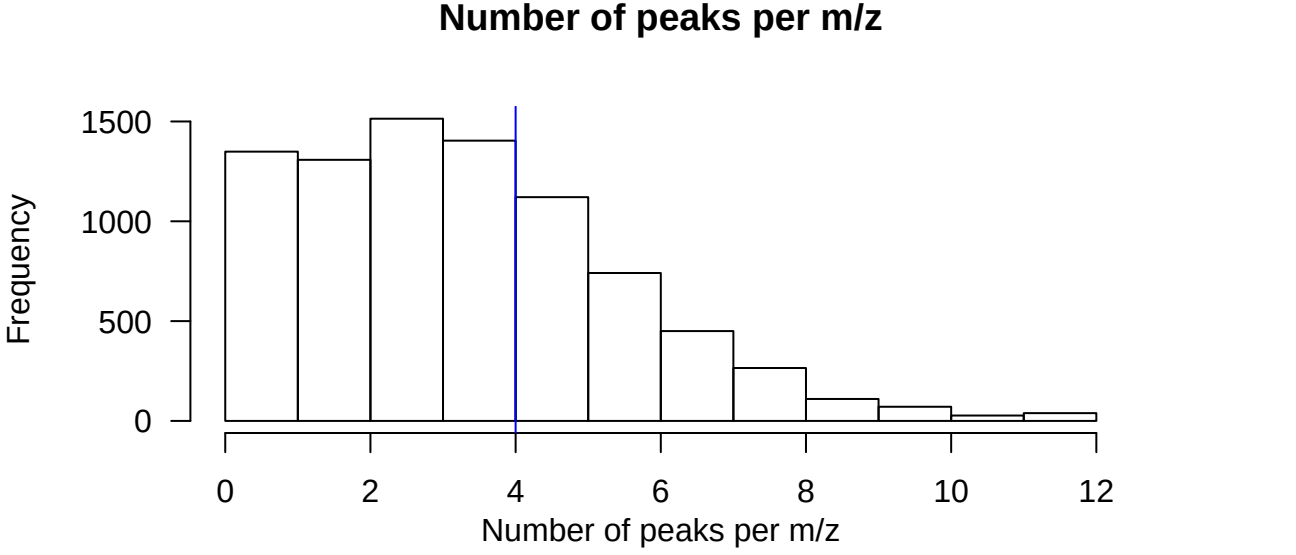

TIC per spectrum
Total ion chromatogram intensity
240
220
200
180
160
140
120
2
4
6
8
10
12
Spectra index

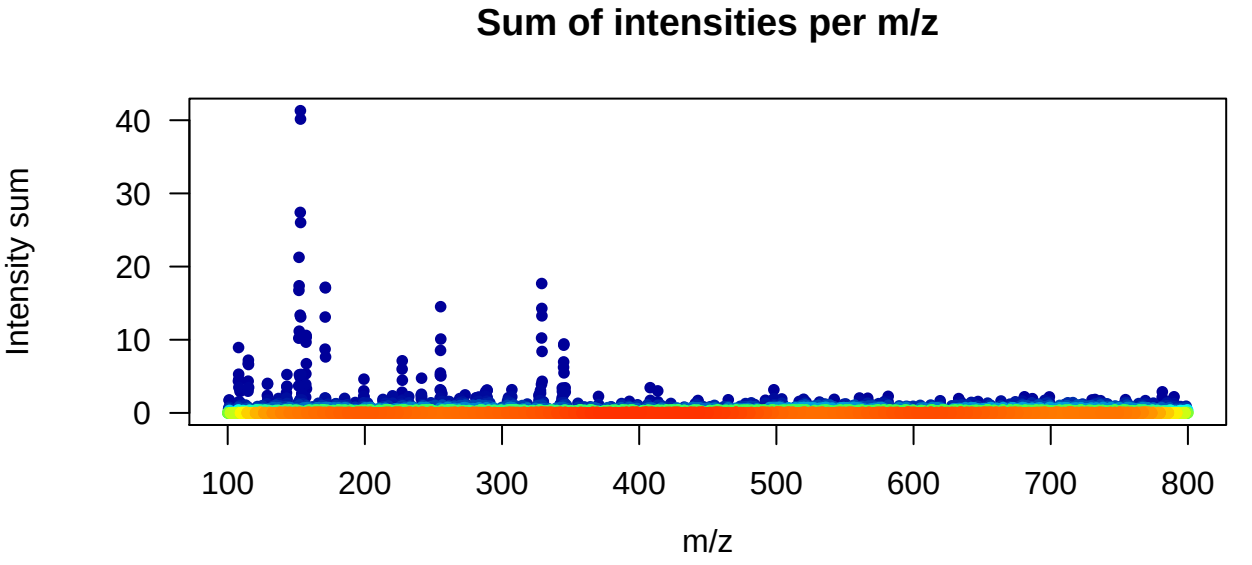

TIC per spectrum
Frequency = # spectra
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.6
4.8
5.0
5.2
5.4
5.6
log(TIC per spectrum)

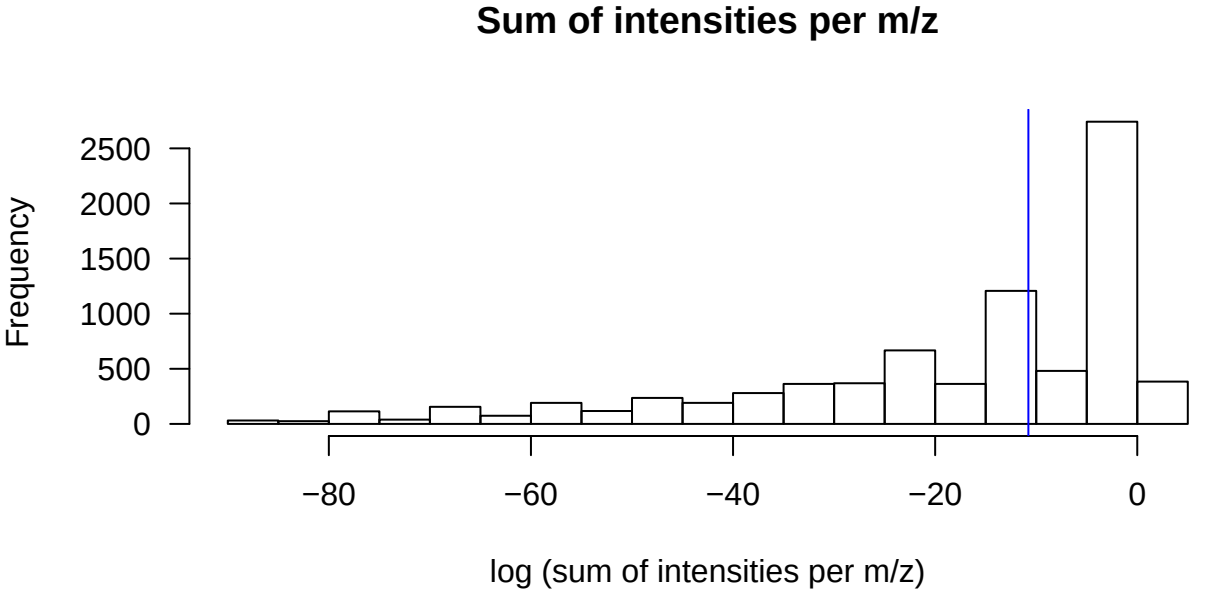

TIC per spectrum and annotation group
Frequency = # spectra
2.0
1.5
1.0
0.5
0.0
4.8
5.0
5.2
5.4
log(TIC per spectrum)
annotation
column1
column2
column3
column4

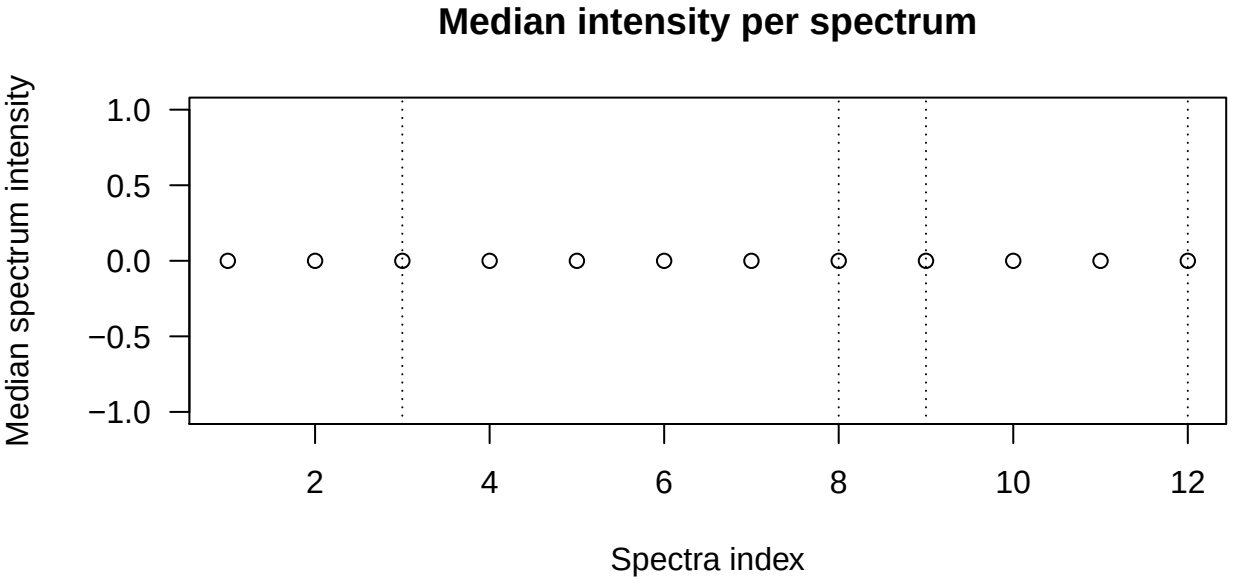

Histogram of m/z values
Frequency
0
100
200
300
400
500
600
100
200
300
400
500
600
700
800
m/z


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

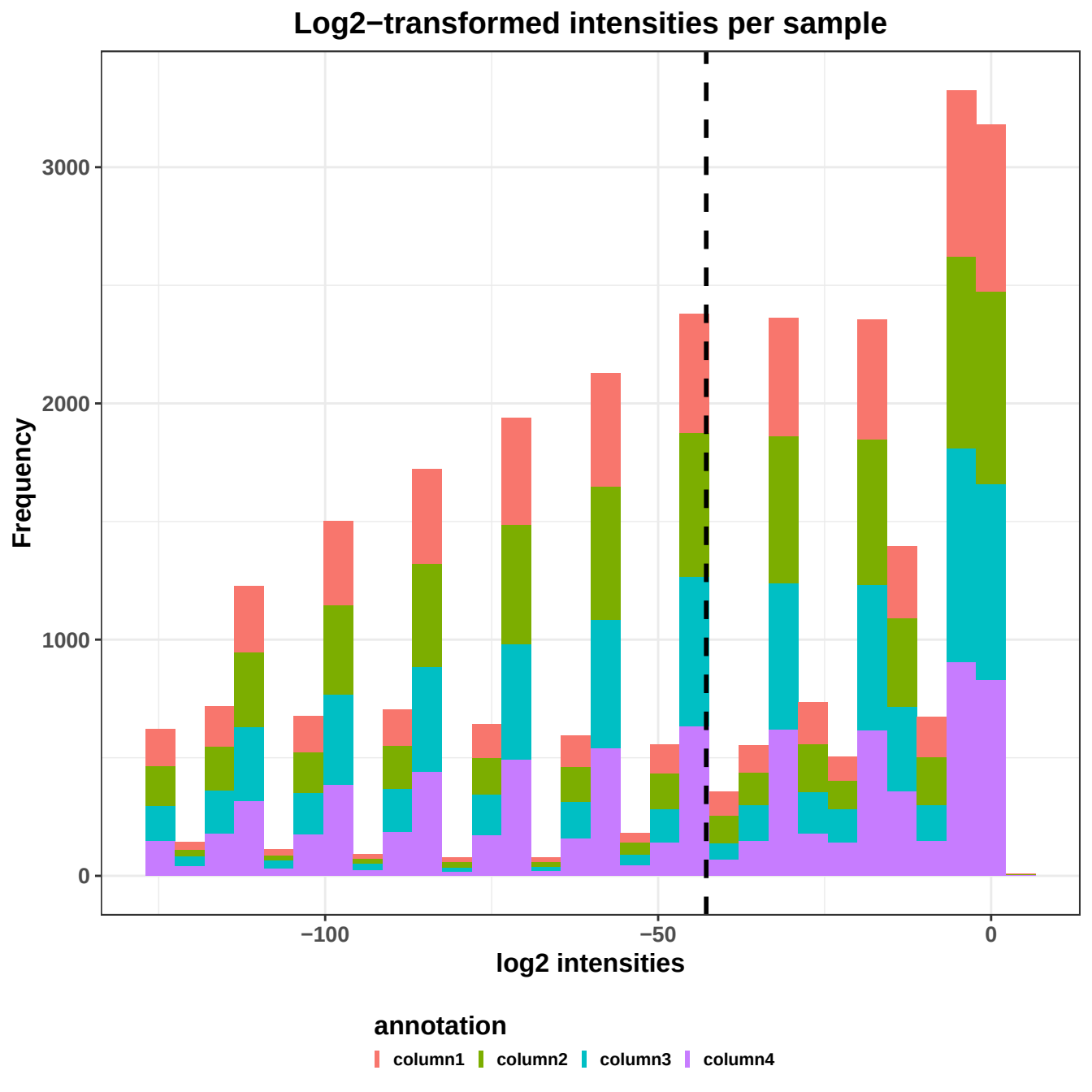

Number of peaks per m/z
Frequency
Number of peaks per m/z
0
500
1000
1500
0
2
4
6
8
10
12


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

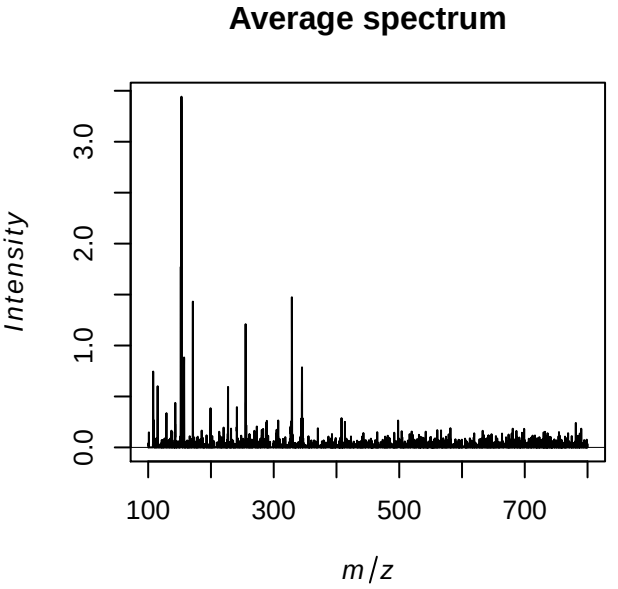

Sum of intensities per m/z
Frequency
0
500
1000
1500
2000
2500
−80
−60
−40
−20
0
log (sum of intensities per m/z)

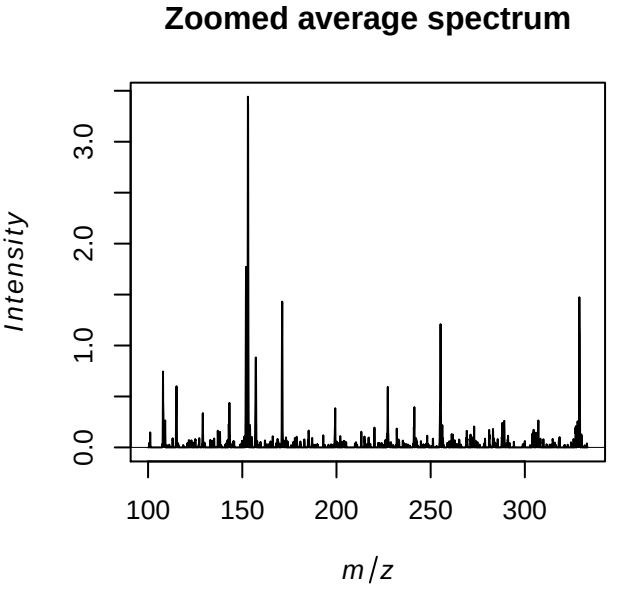

Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
10
12
Spectra index

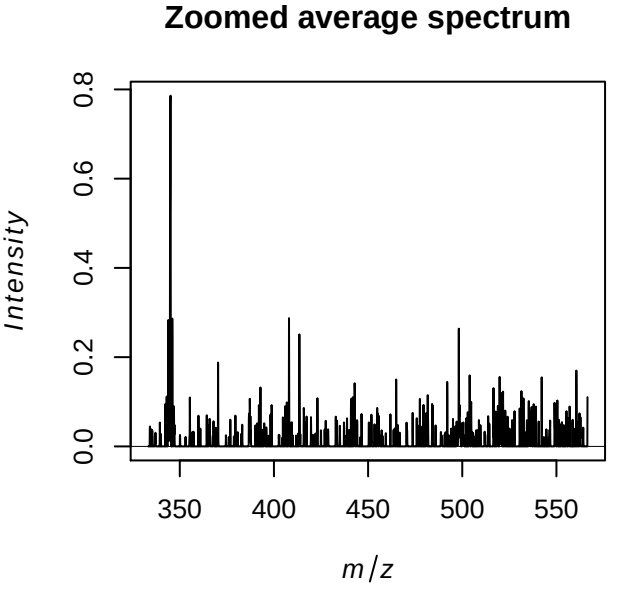
Log2−transformed intensities
Frequency
7000
6000
5000
4000
3000
2000
1000
0
−120
−100
−80
−60
−40
−20
0
log2 intensities

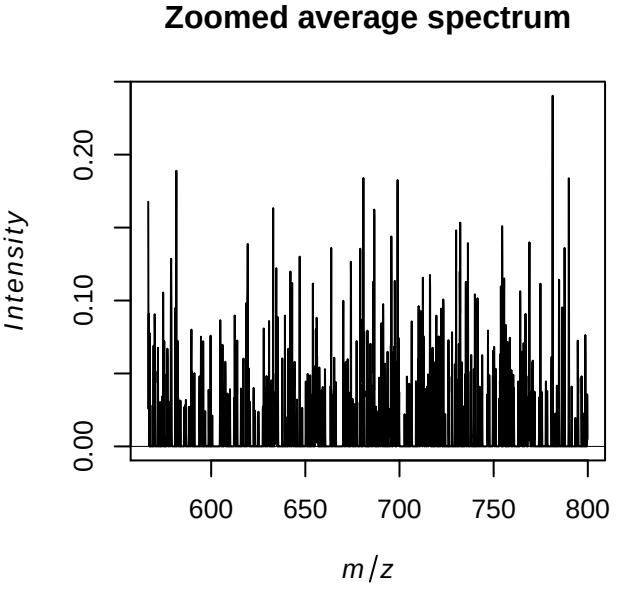

Log2−transformed intensities per sample
Frequency
3000
2000
1000
0
−100
−50
0
log2 intensities
annotation
column1
column2
column3
column4

Mean m/z intensities per annotation group
log2 mean intensity per m/z
0
−20
−40
−60
−80
column1
column2
column3
column4

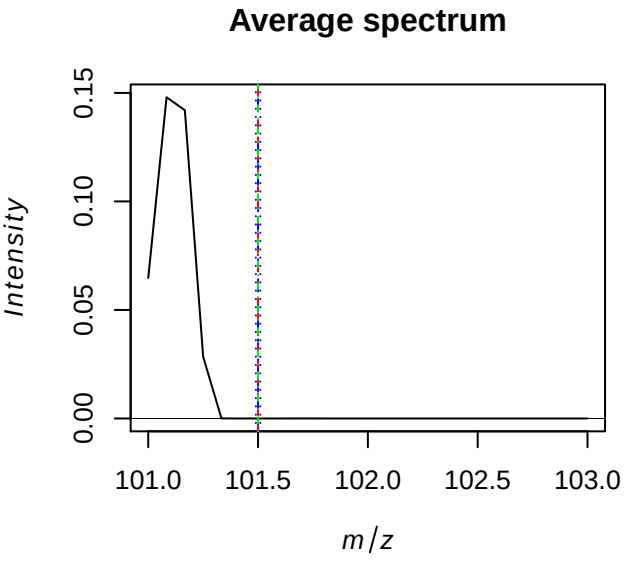

Average spectrum
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z

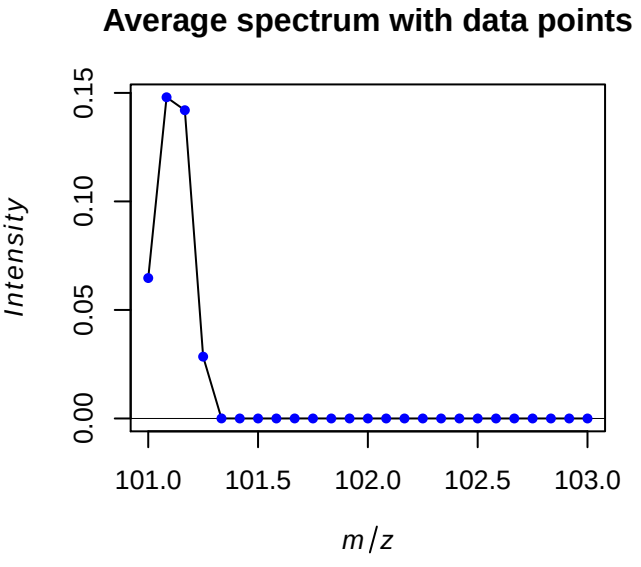

Zoomed average spectrum
Intensity
0.0
1.0
2.0
3.0
100
150
200
250
300
m/z

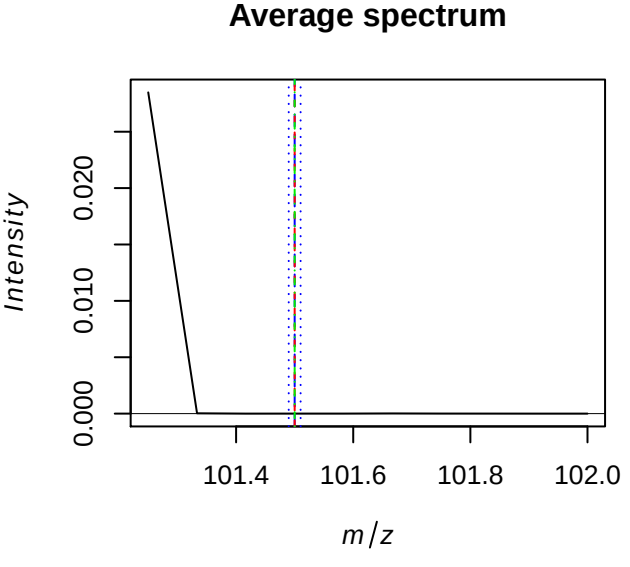

Zoomed average spectrum
Intensity
0.0
0.2
0.4
0.6
0.8
350
400
450
500
550
m/z

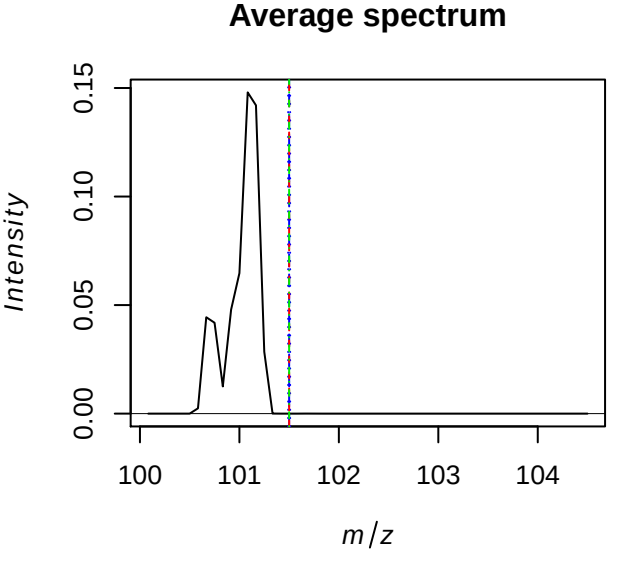

Zoomed average spectrum
Intensity
0.00
0.10
0.20
600
650
700
750
800
m/z

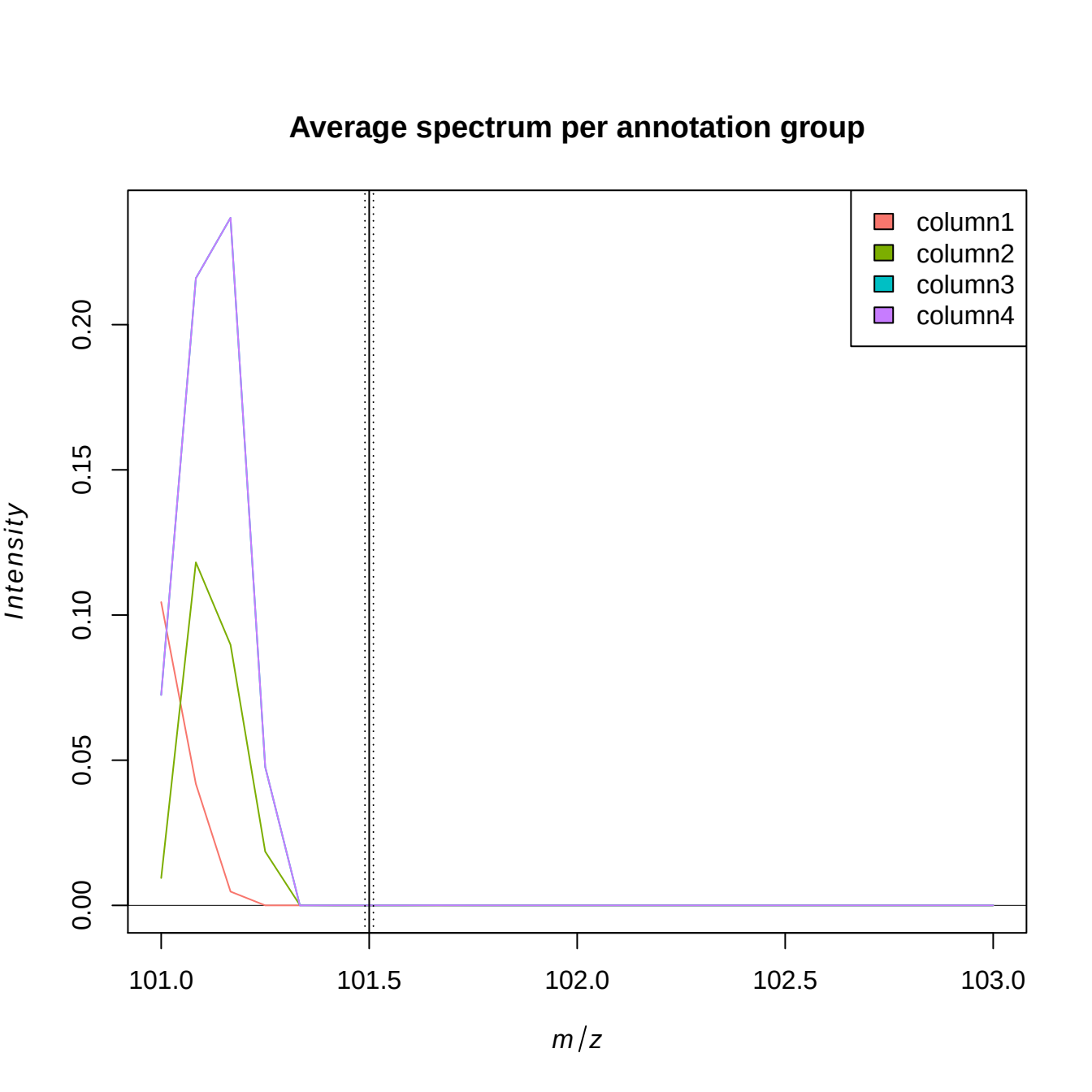
theor. m/z: 101.5 most abundant m/z: 101.5 closest m/z: 101.5



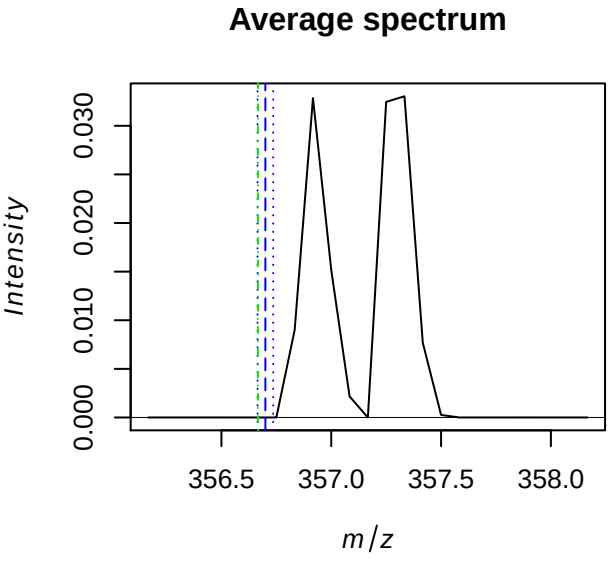


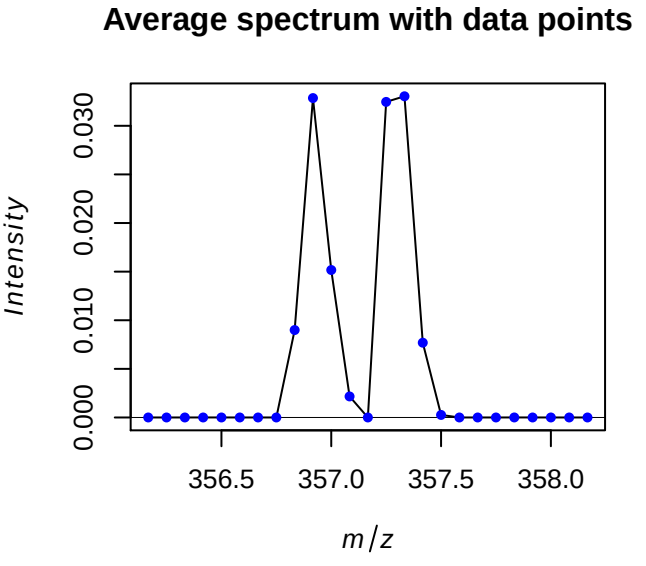


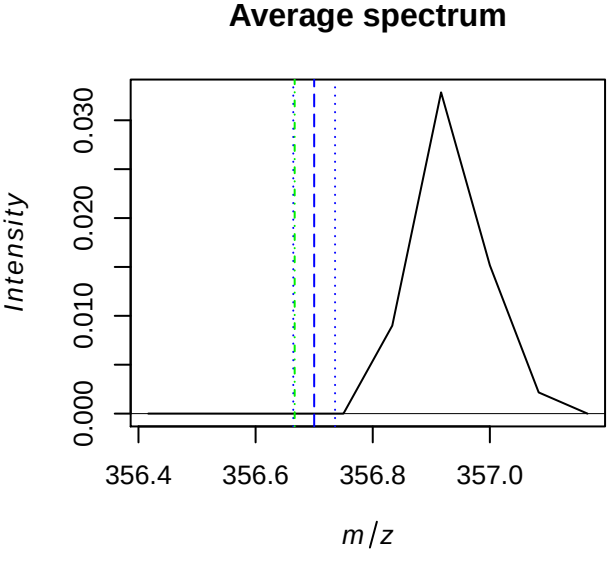


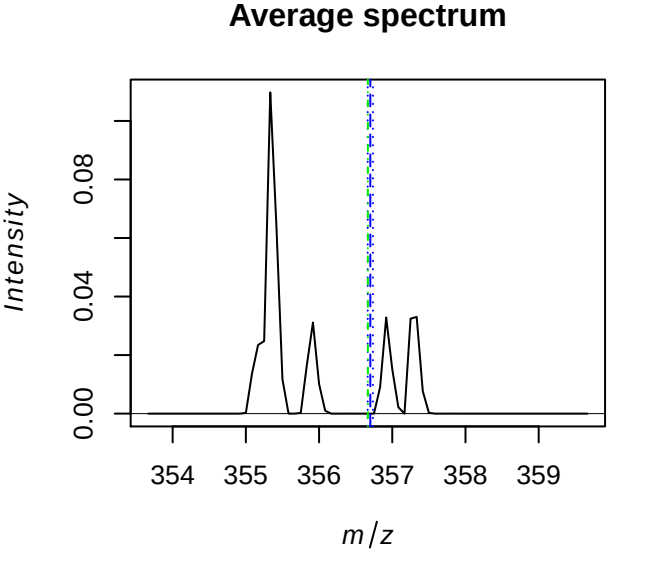

Average spectrum per annotation group
column1
column2
column3
column4
Intensity
0.00
0.05
0.10
0.15
0.20
101.0
101.5
102.0
102.5
103.0
m/z

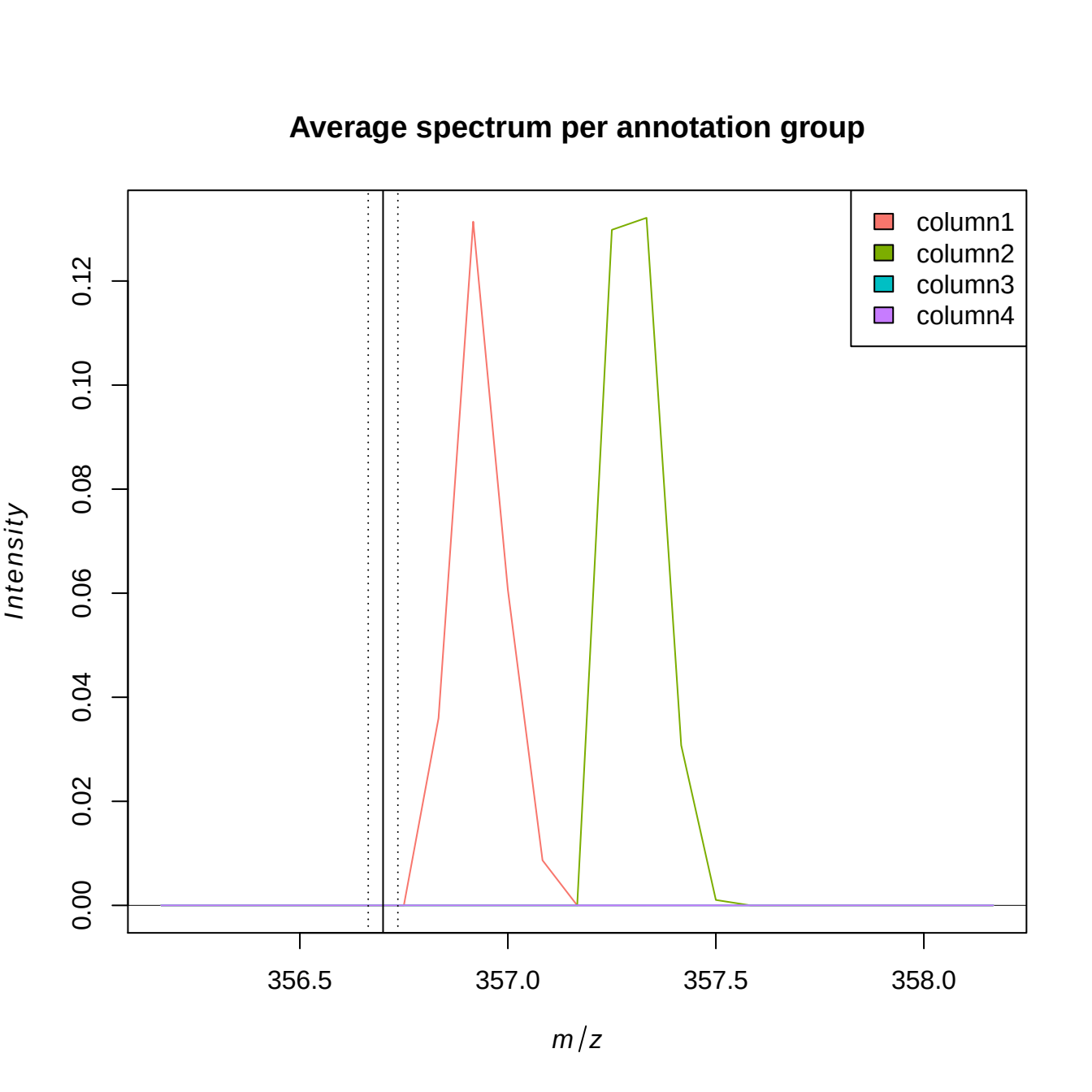
theor. m/z: 356.7 most abundant m/z: NA closest m/z: 356.6667



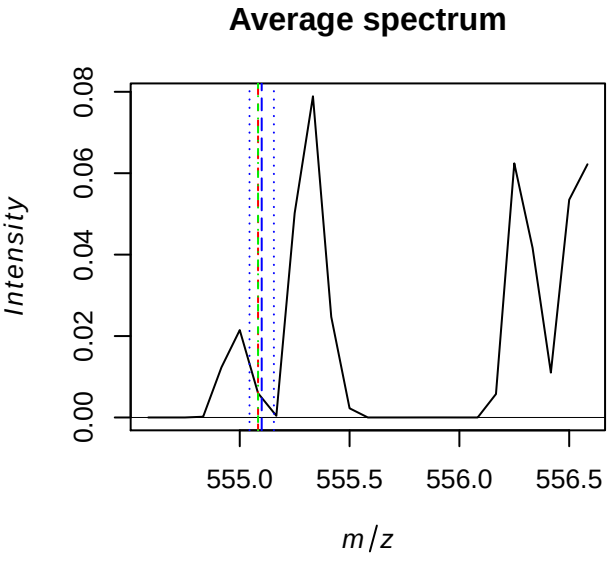


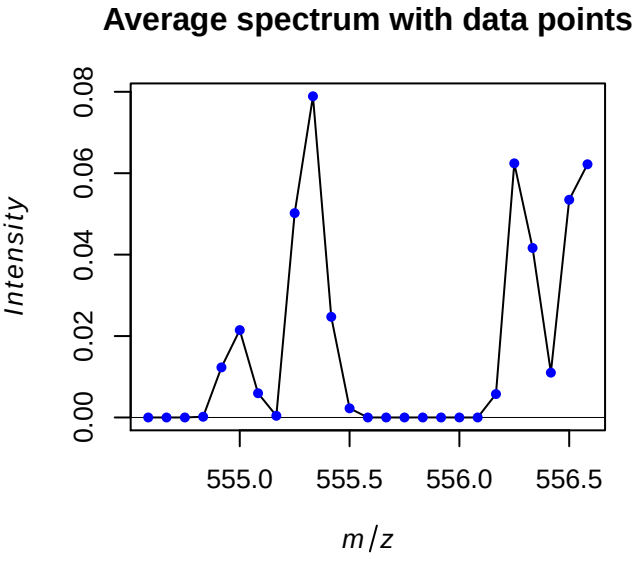


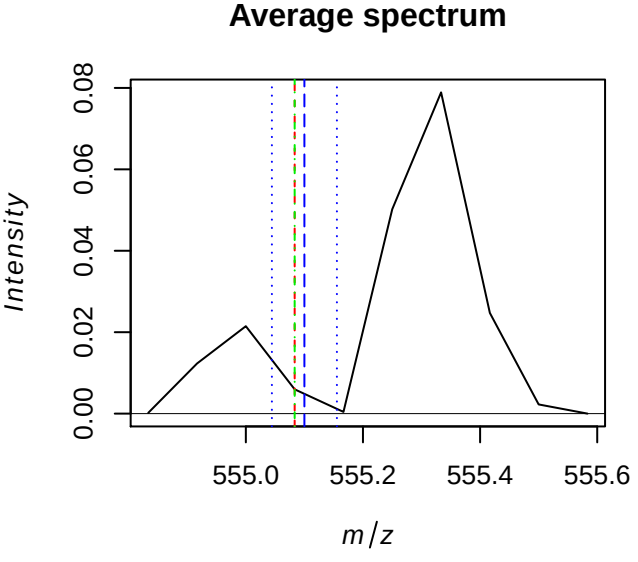


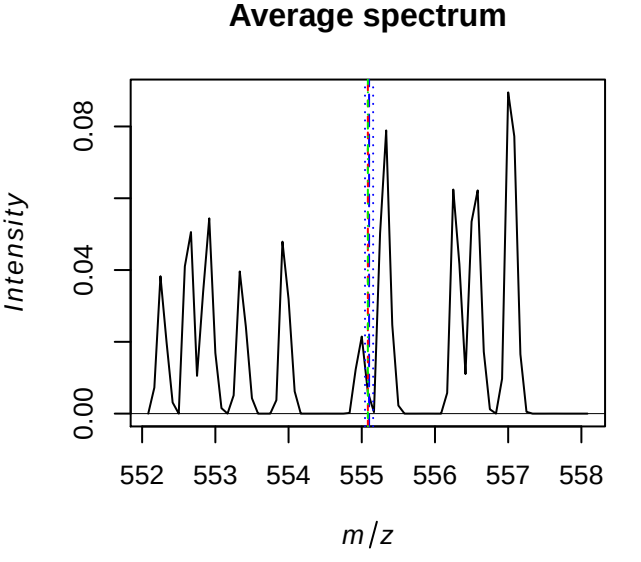

Average spectrum per annotation group
column1
column2
column3
column4
Intensity
0.00
0.02
0.04
0.06
0.08
0.10
0.12
356.5
357.0
357.5
358.0
m/z

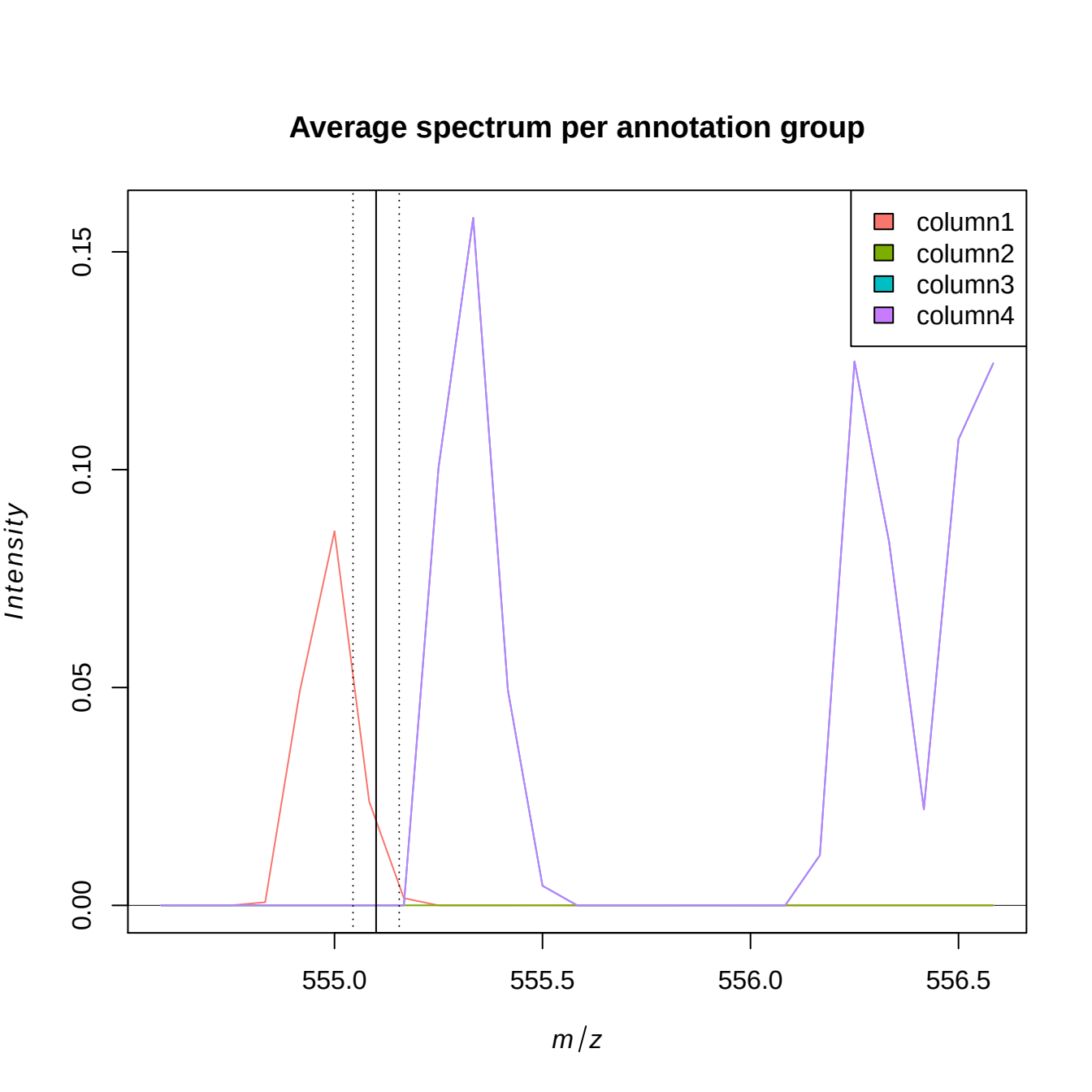
theor. m/z: 555.1 most abundant m/z: 555.0834 closest m/z: 555.0834

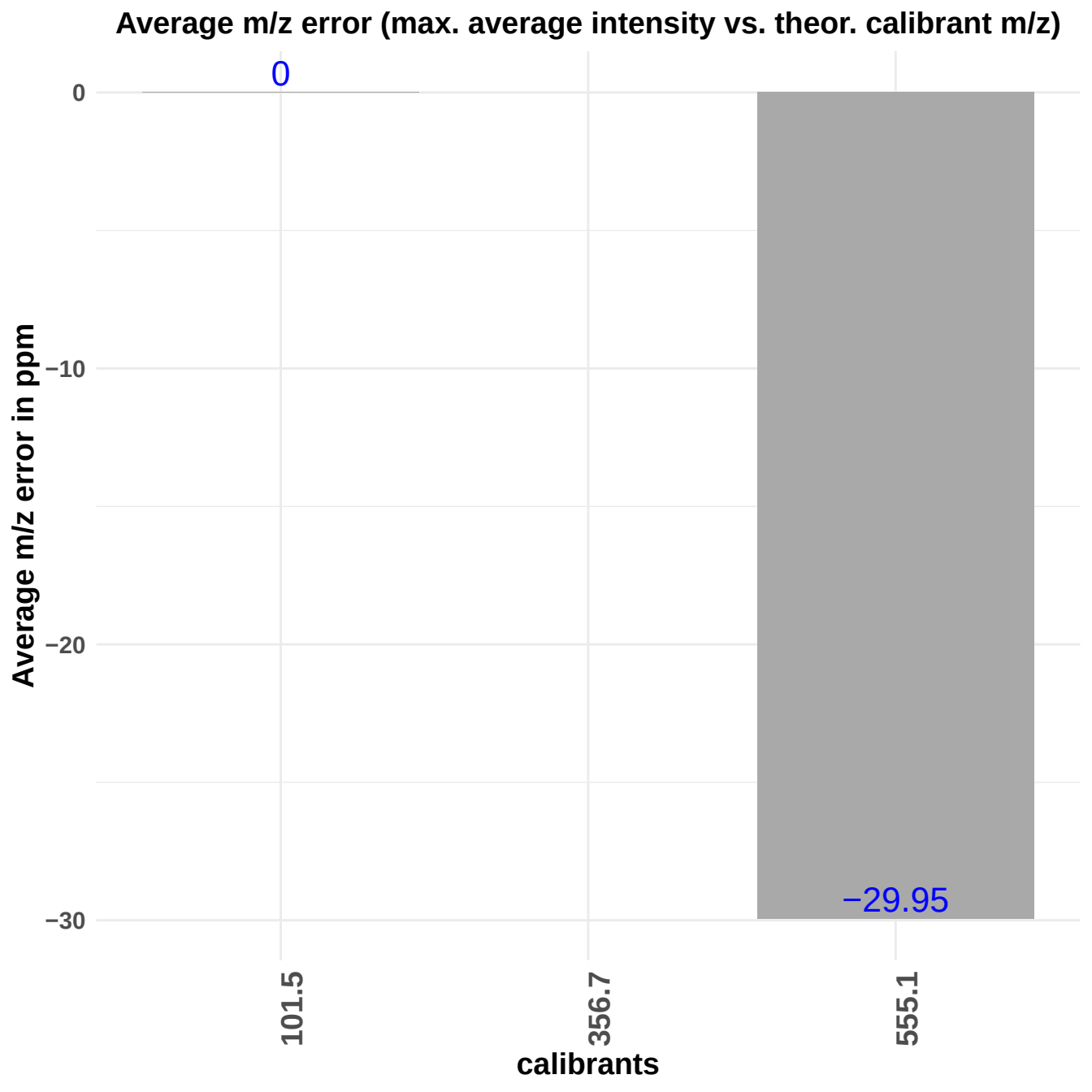


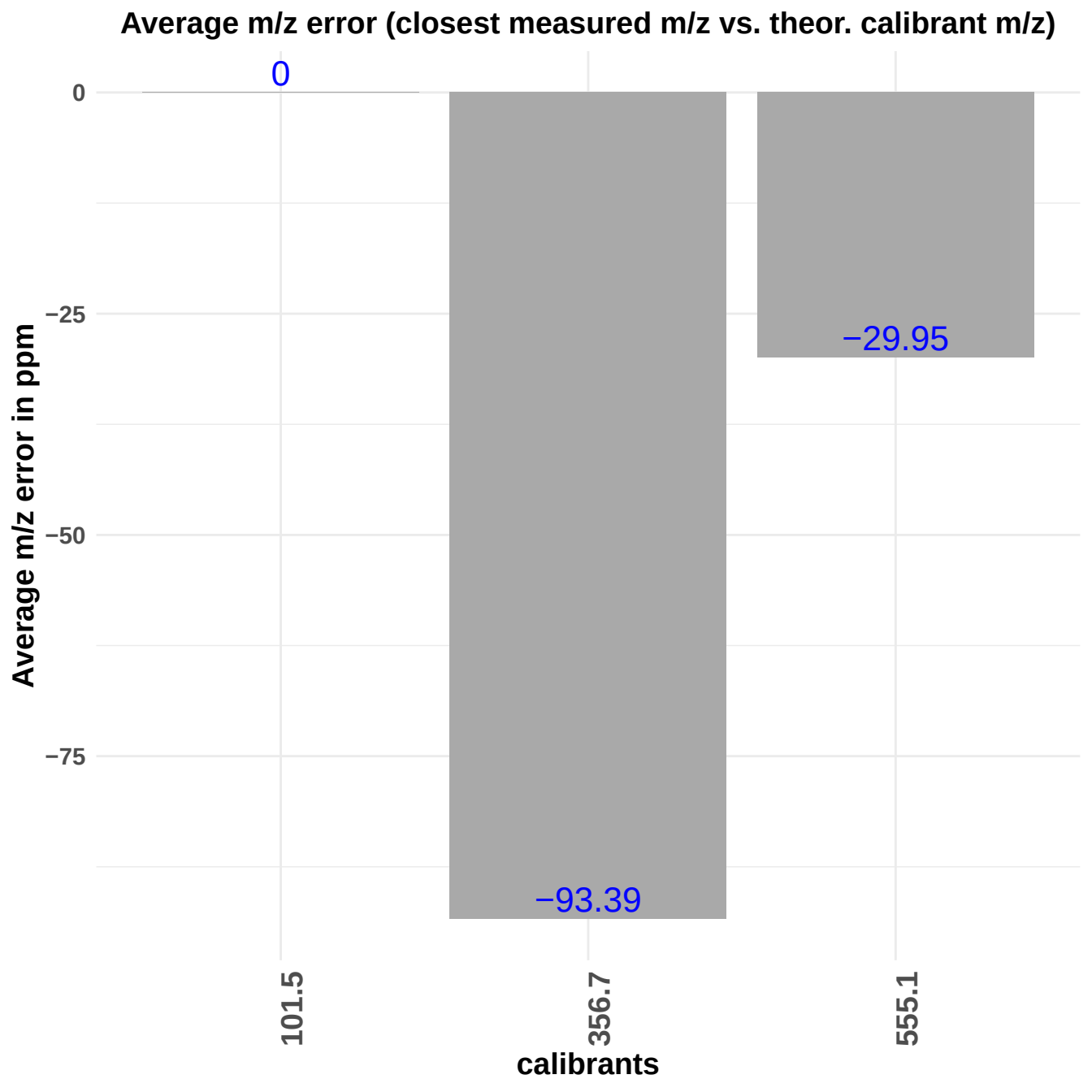


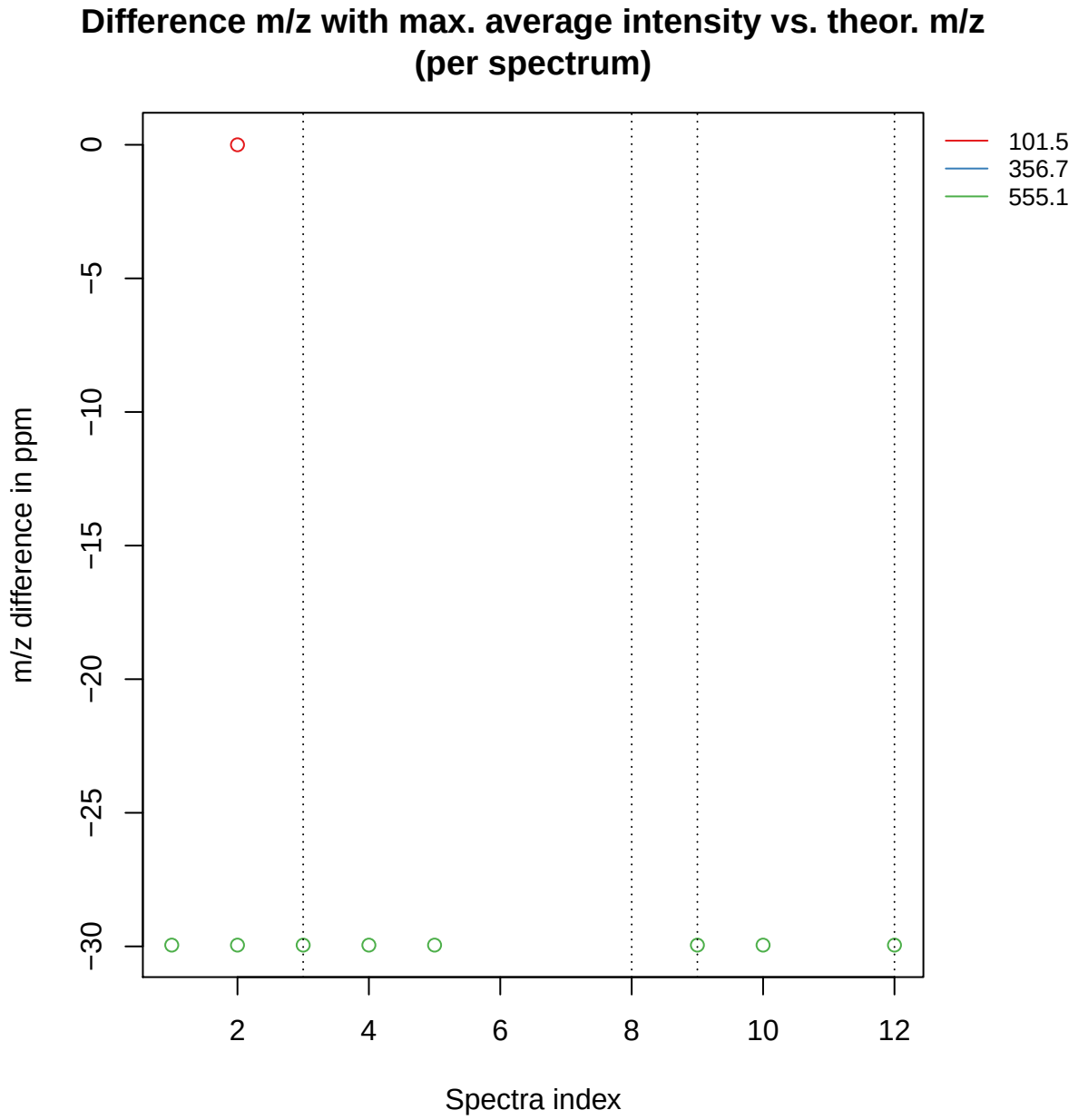





Average spectrum per annotation group
column1
column2
column3
column4
0.00
0.05
0.10
0.15
Intensity
555.0
555.5
556.0
556.5
m/z


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


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


Difference m/z with max. average intensity vs. theor. m/z
(per spectrum)
m/z difference in ppm
0
−5
−10
−15
−20
−25
−30
2
4
6
8
10
12
Spectra index
101.5
356.7
555.1