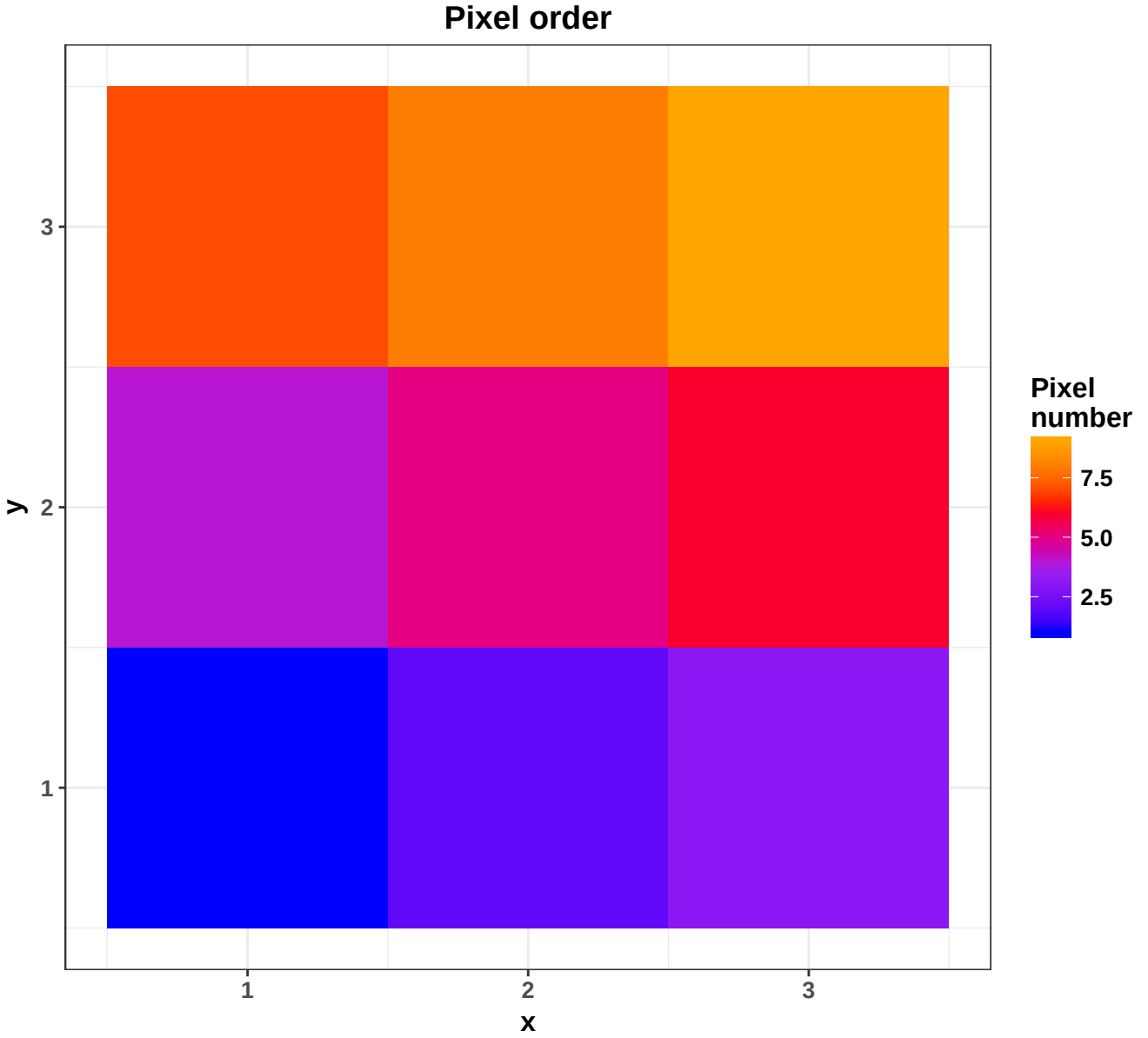
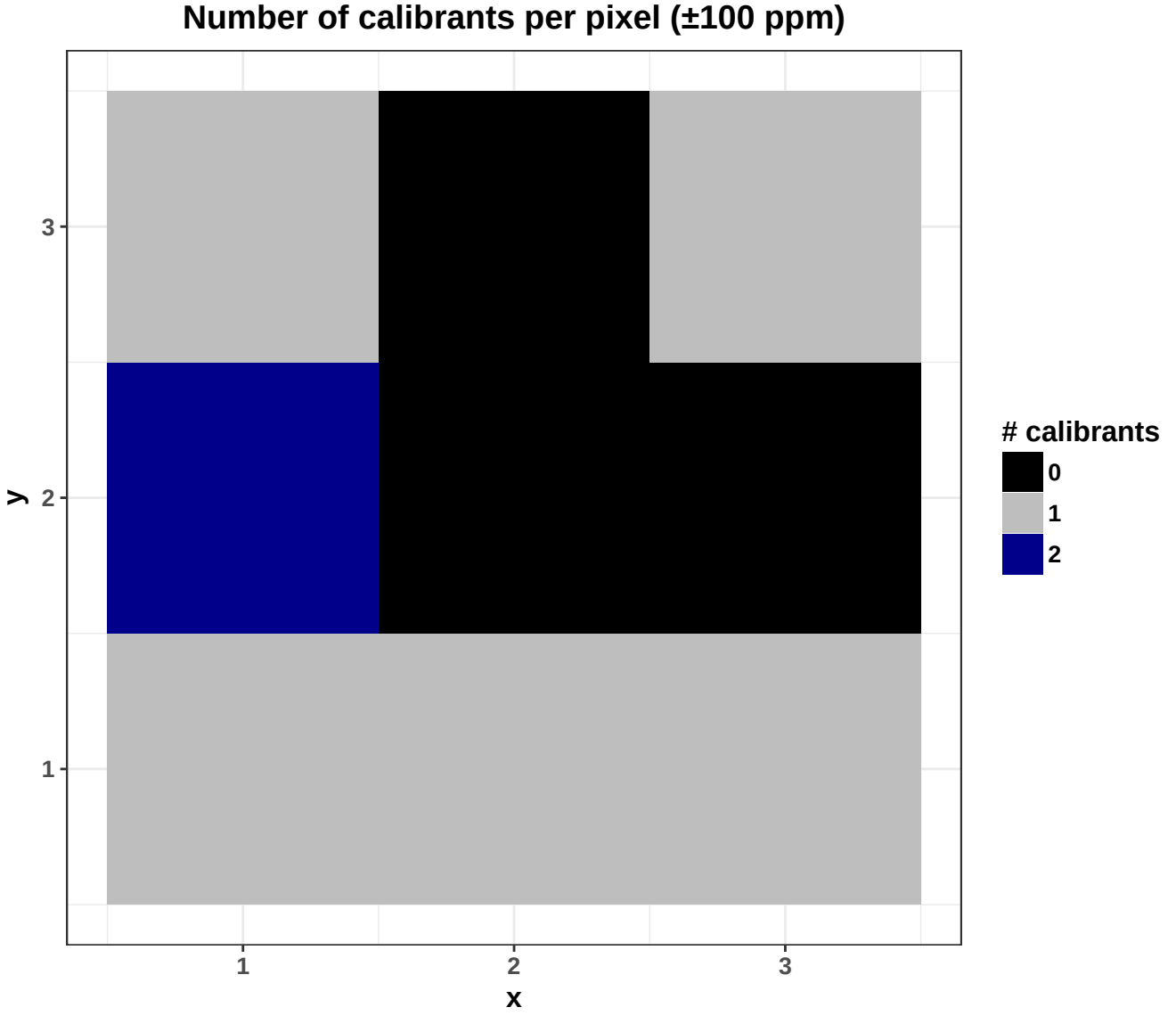
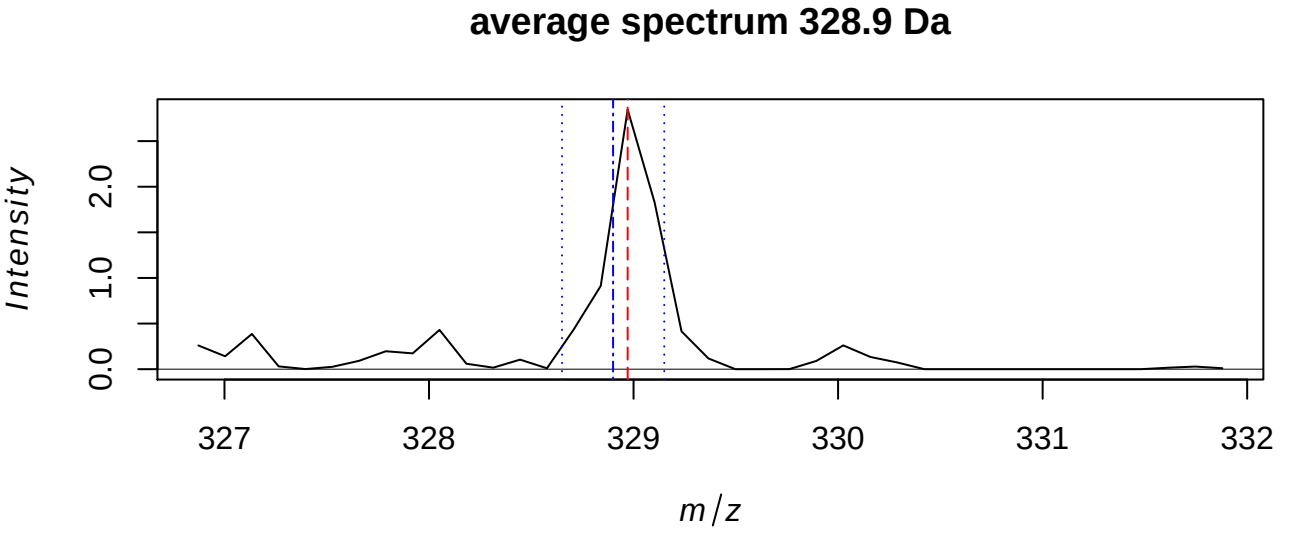
Testfile_imzml

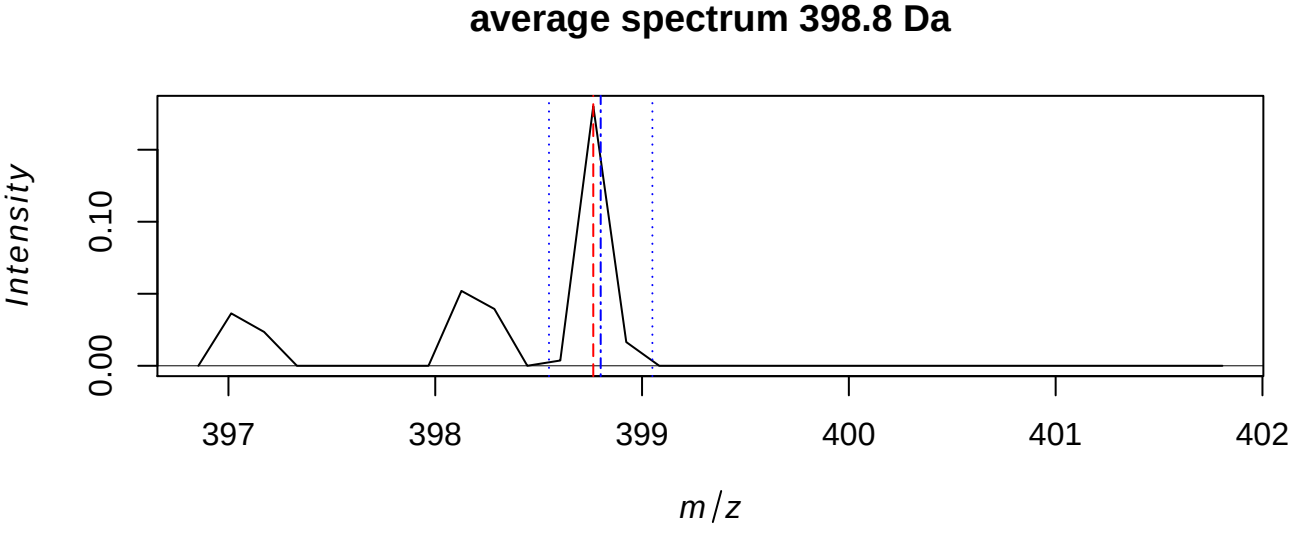
properties	values
Number of m/z features	5199
Range of m/z values	100 − 799.81
Number of pixels	9
Range of x coordinates	1 − 3
Range of y coordinates	1 − 3
Range of intensities	0 − 9.24
Median of intensities	0
Intensities > 0	35.16 %
Number of empty spectra	0
Median TIC	161.81
Median # peaks per spectrum	1961
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.txt	3 / 3

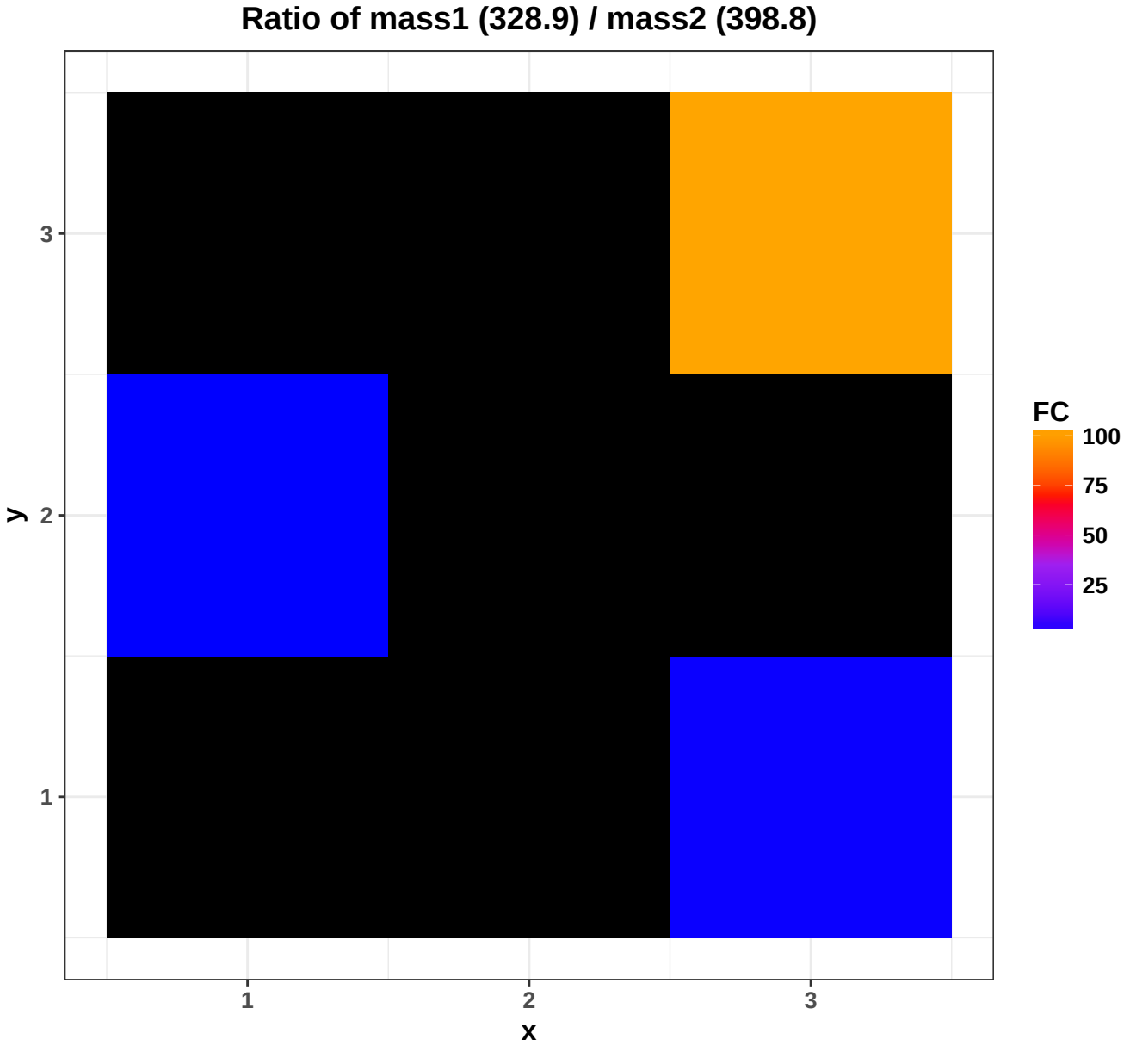

Pixel order
3
2
1
y
1
2
3
x
Pixel number
7.5
5.0
2.5

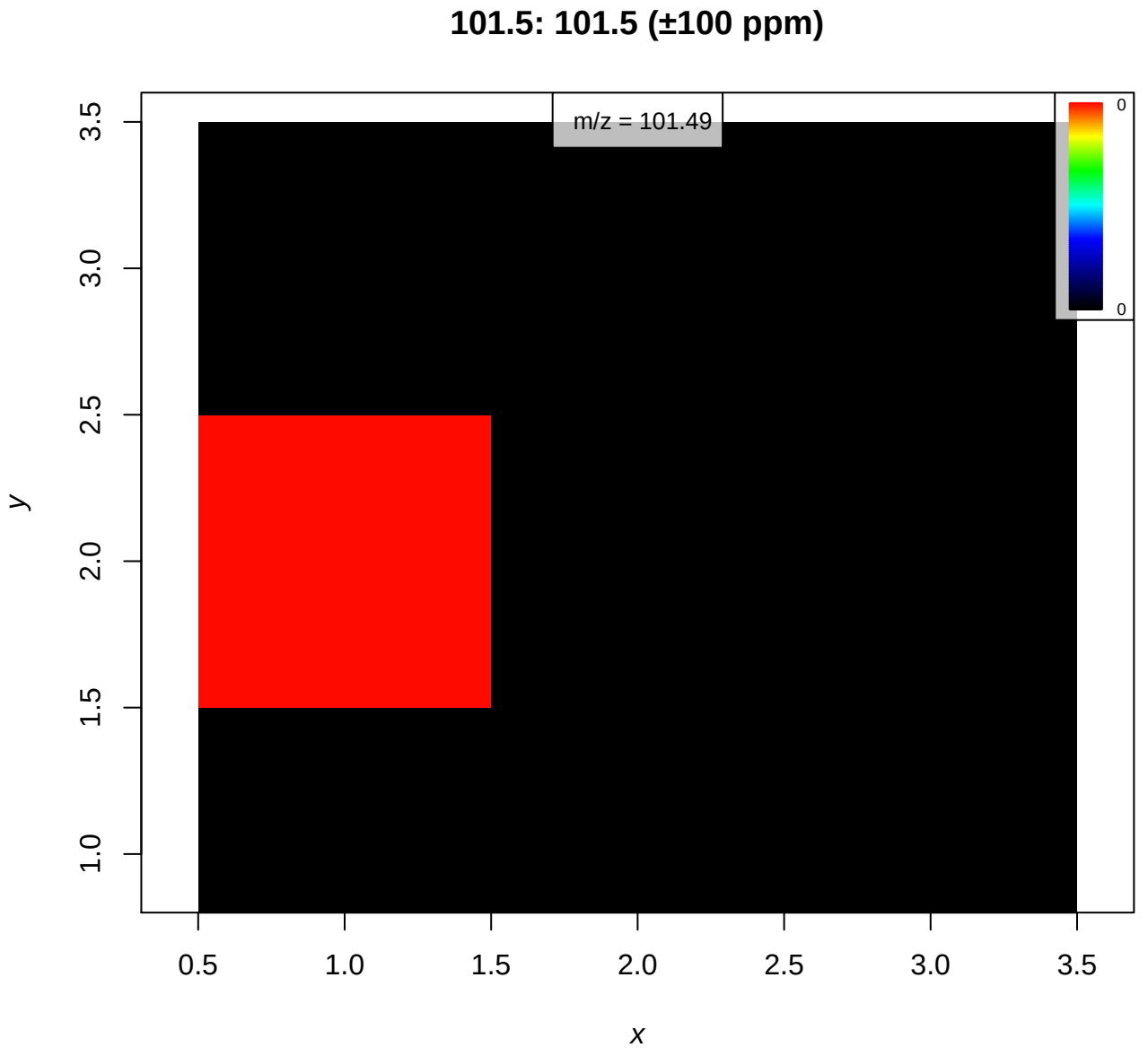

Number of calibrants per pixel (±100 ppm)
3
2
1
y
1
2
3
x
calibrants
0
1
2

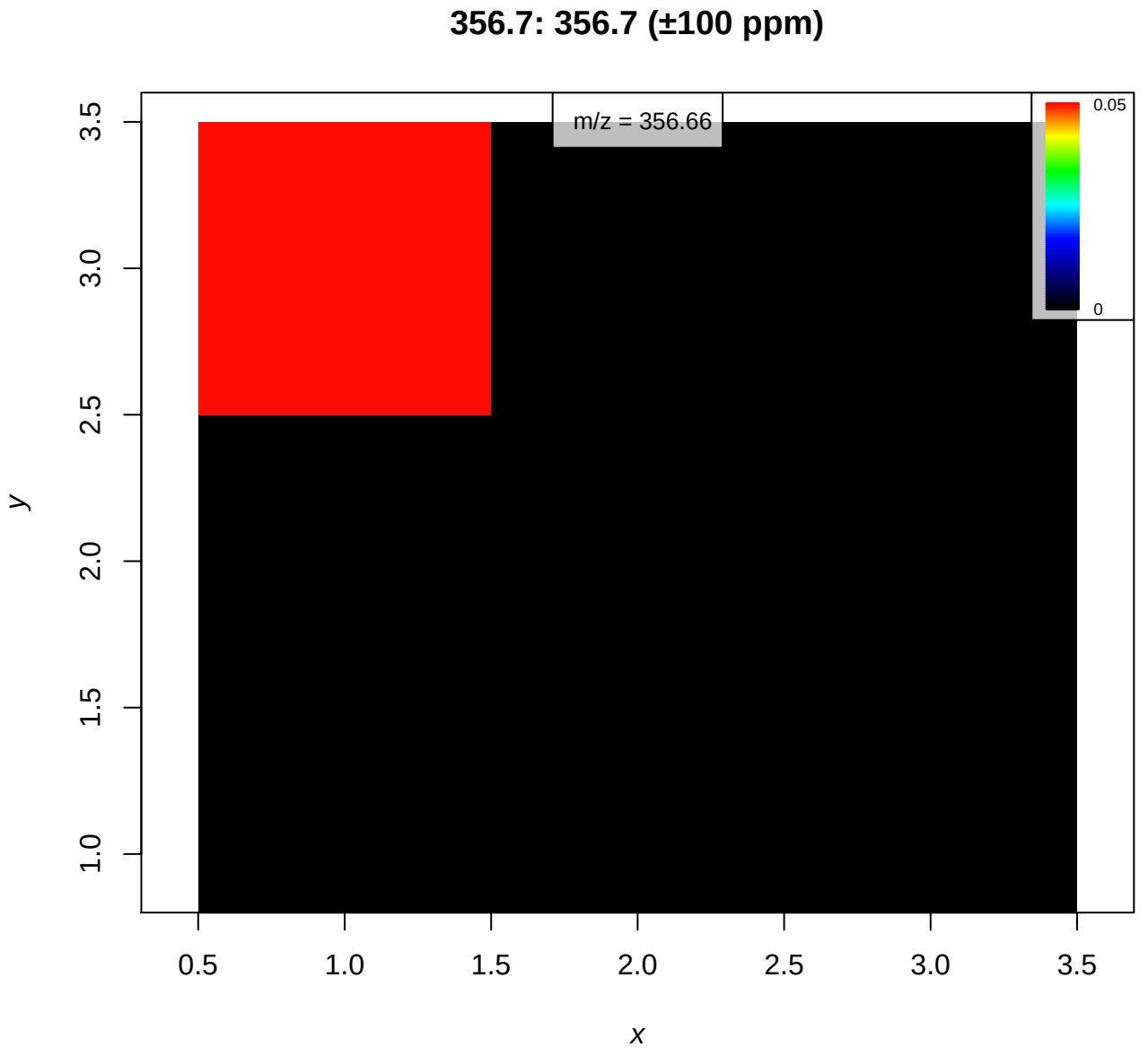
Control of fold change plot

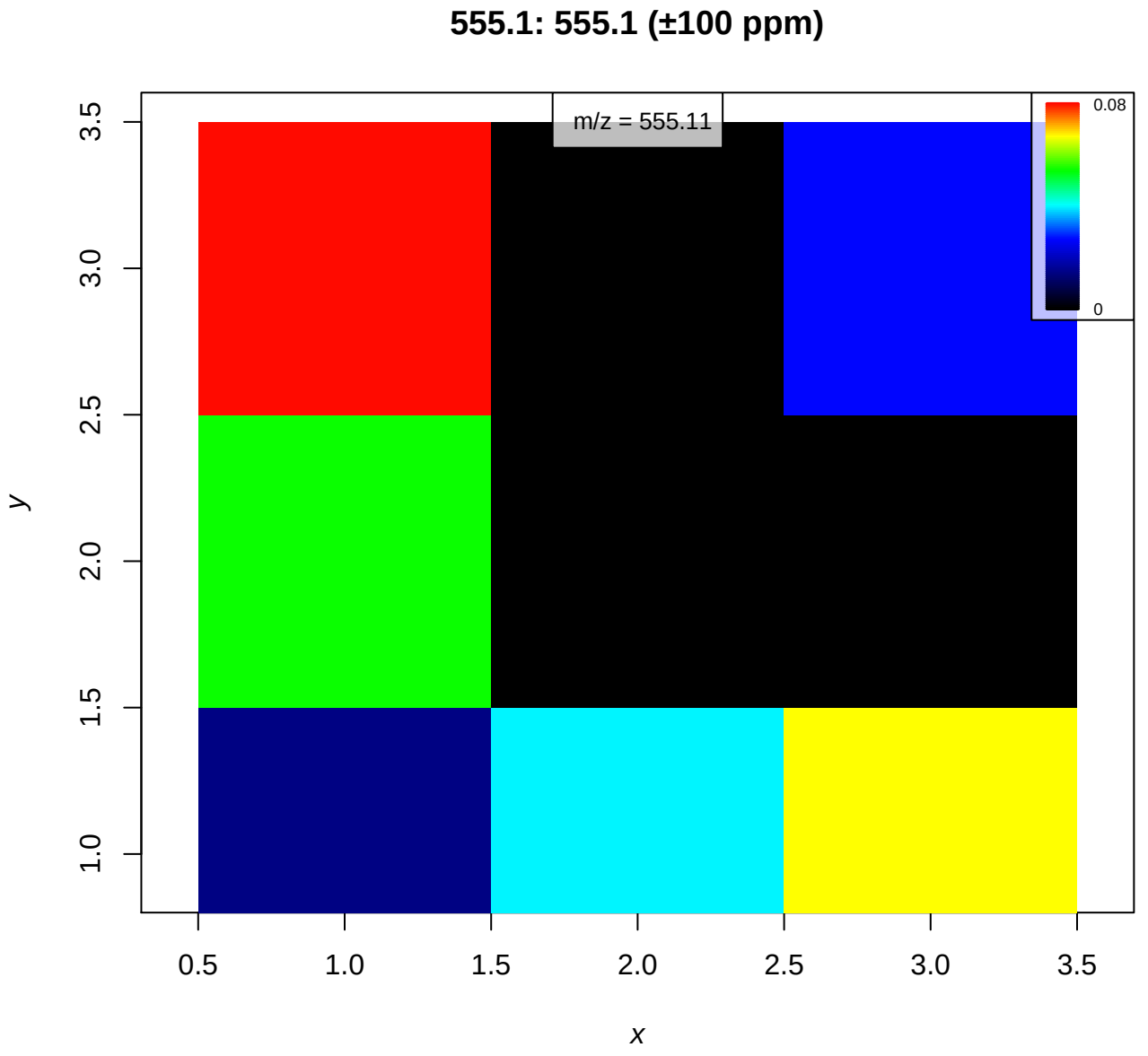


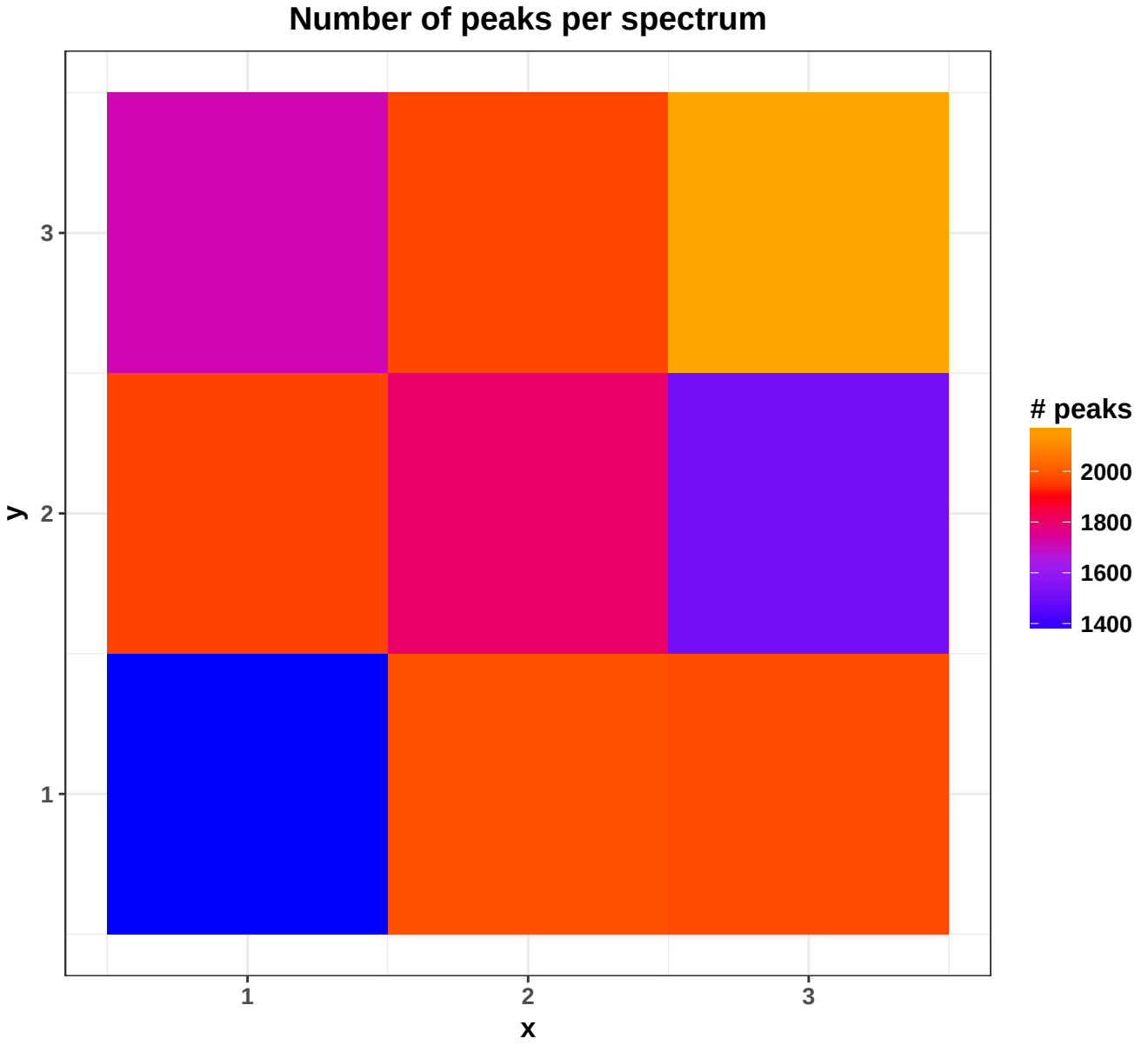


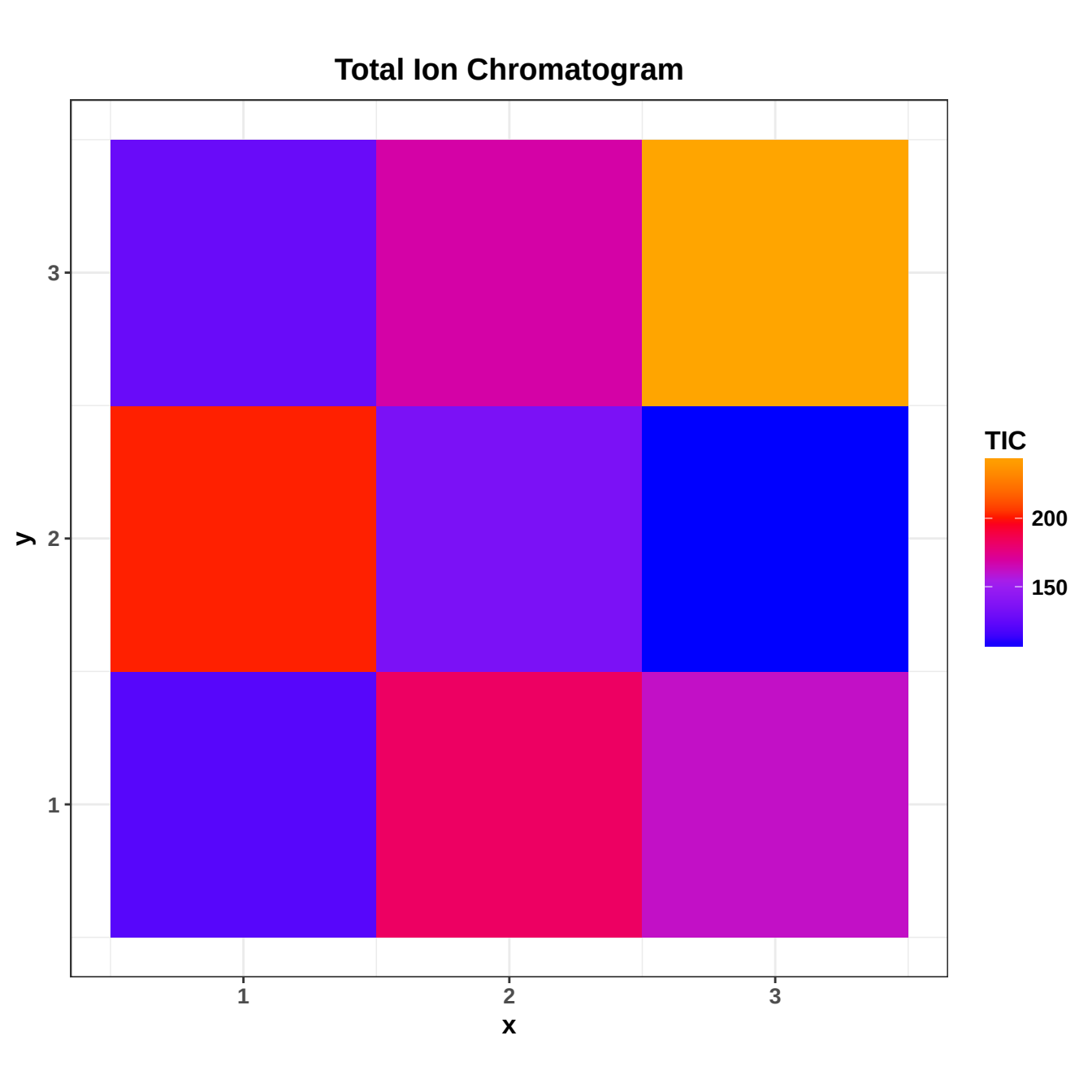

Ratio of mass1 (328.9) / mass2 (398.8)
3
2
1
y
1
2
3
x
FC
100
75
50
25

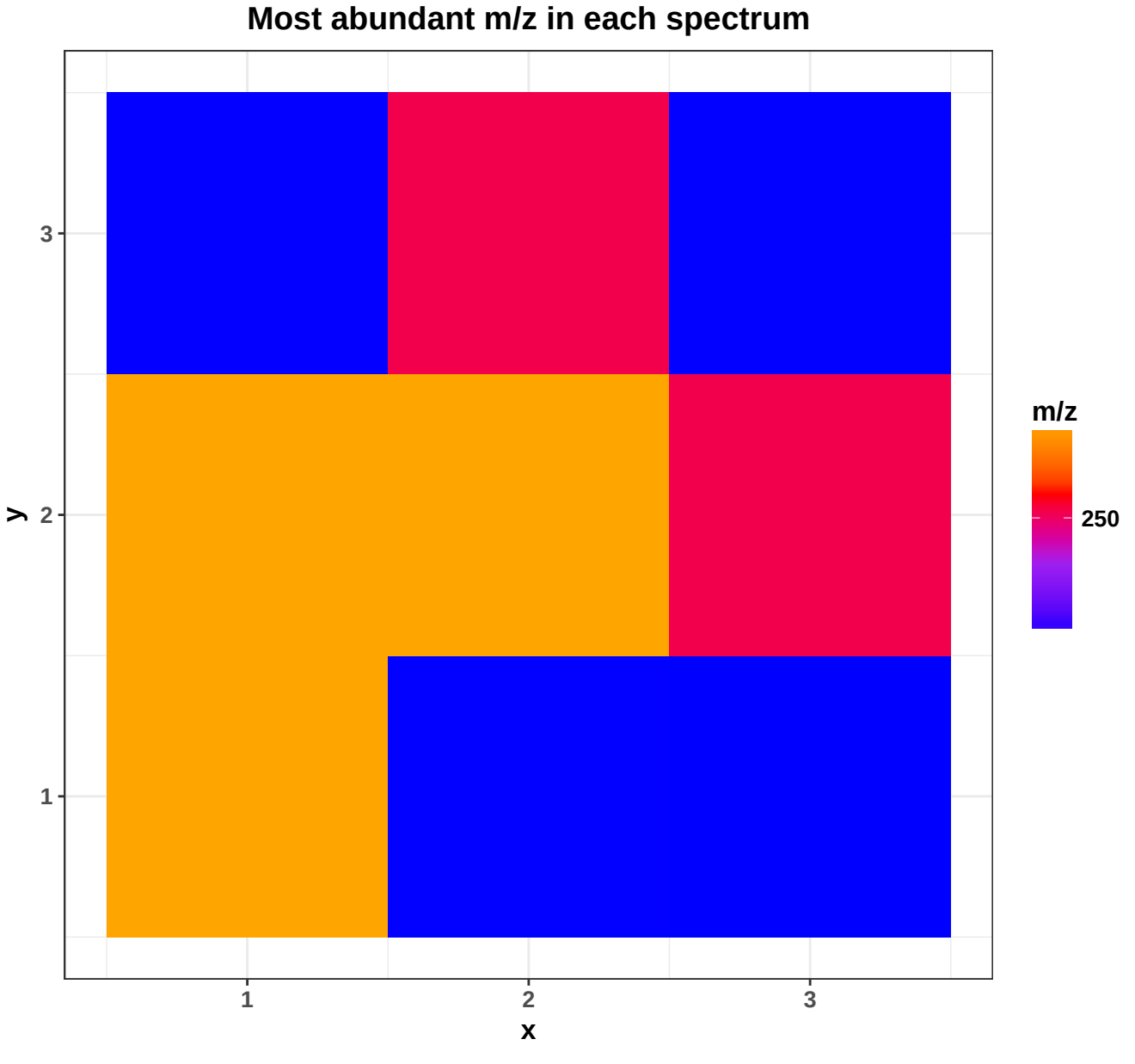

101.5: 101.5 (±100 ppm)
m/z = 101.49
0
0
3.5
3.0
2.5
2.0
1.5
1.0
y
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x

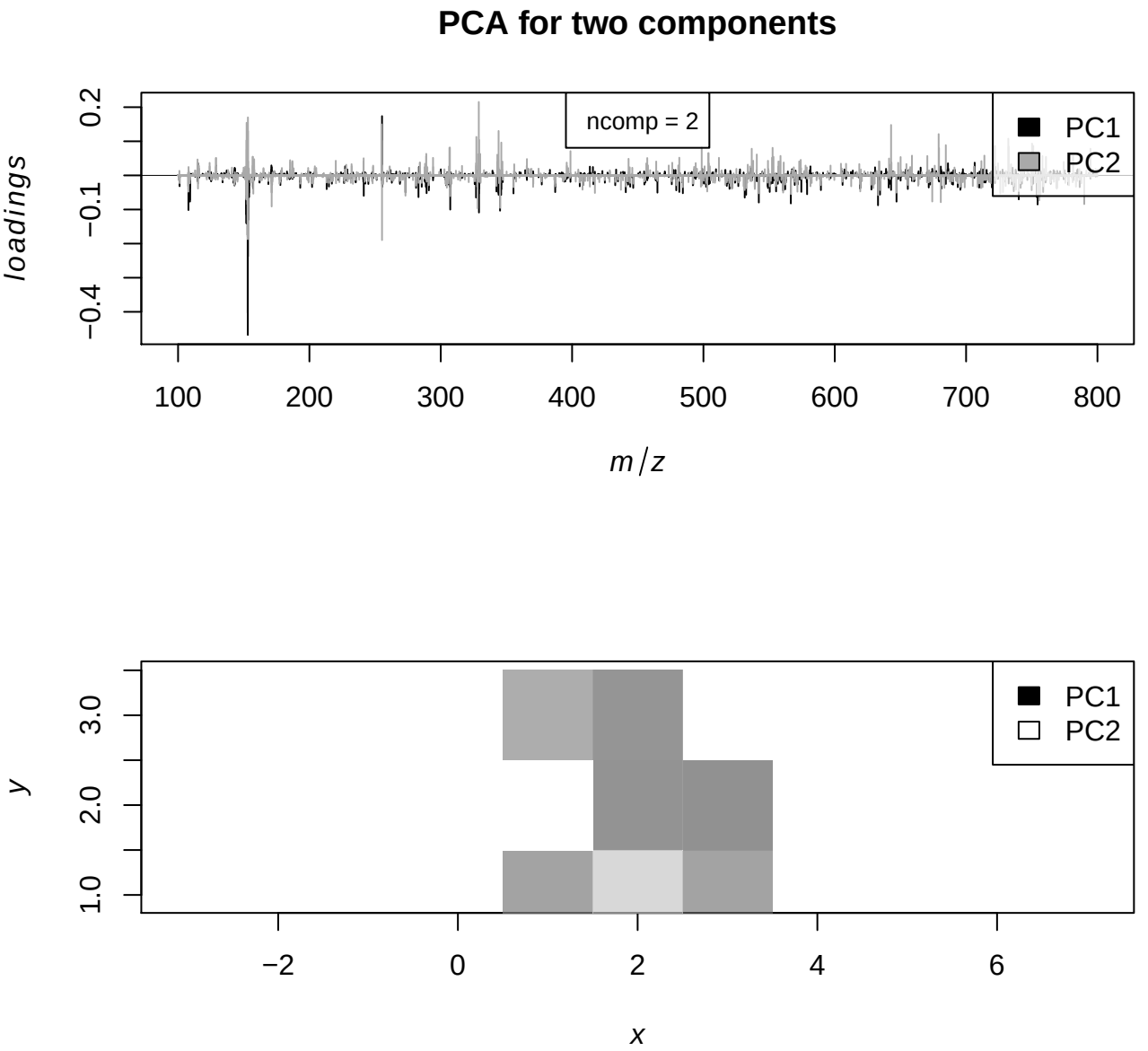

356.7: 356.7 (±100 ppm)
m/z = 356.66
0.05
0
y
x
1.0
1.5
2.0
2.5
3.0
3.5
0.5
1.0
1.5
2.0
2.5
3.0
3.5

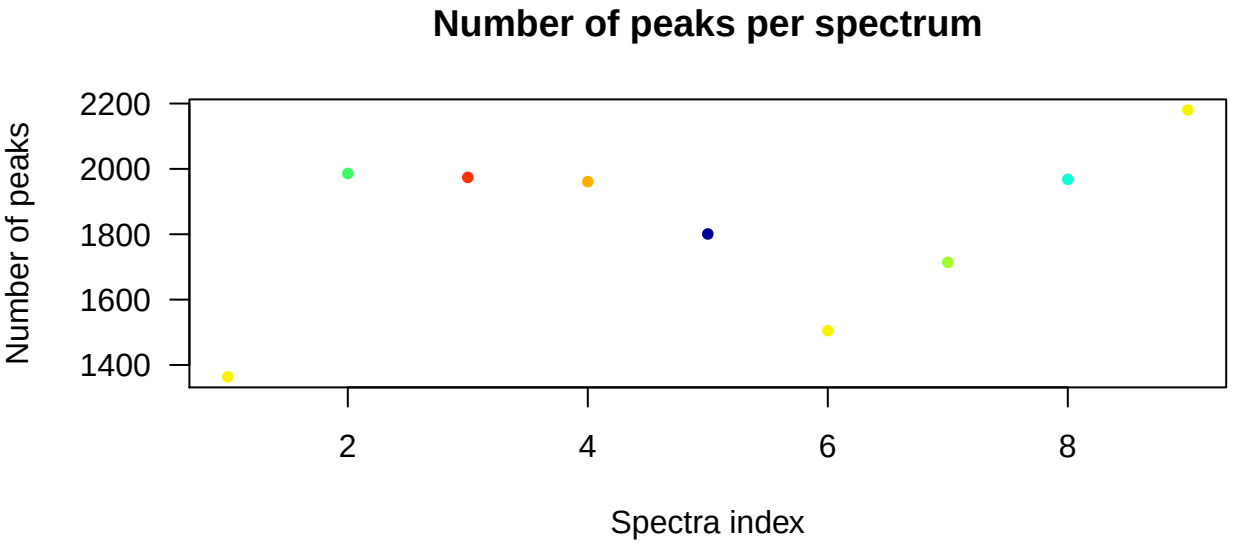

555.1: 555.1 (±100 ppm)
m/z = 555.11
0.08
0
y
x
0.5
1.0
1.5
2.0
2.5
3.0
3.5

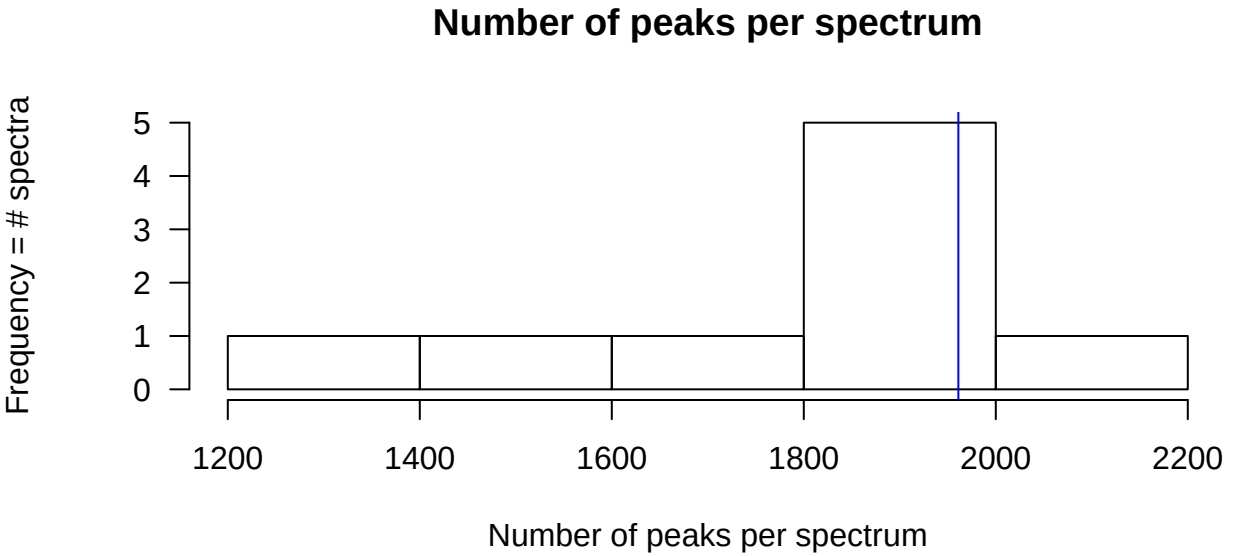

Number of peaks per spectrum
y
3
2
1
x
1
2
3
peaks
2000
1800
1600
1400

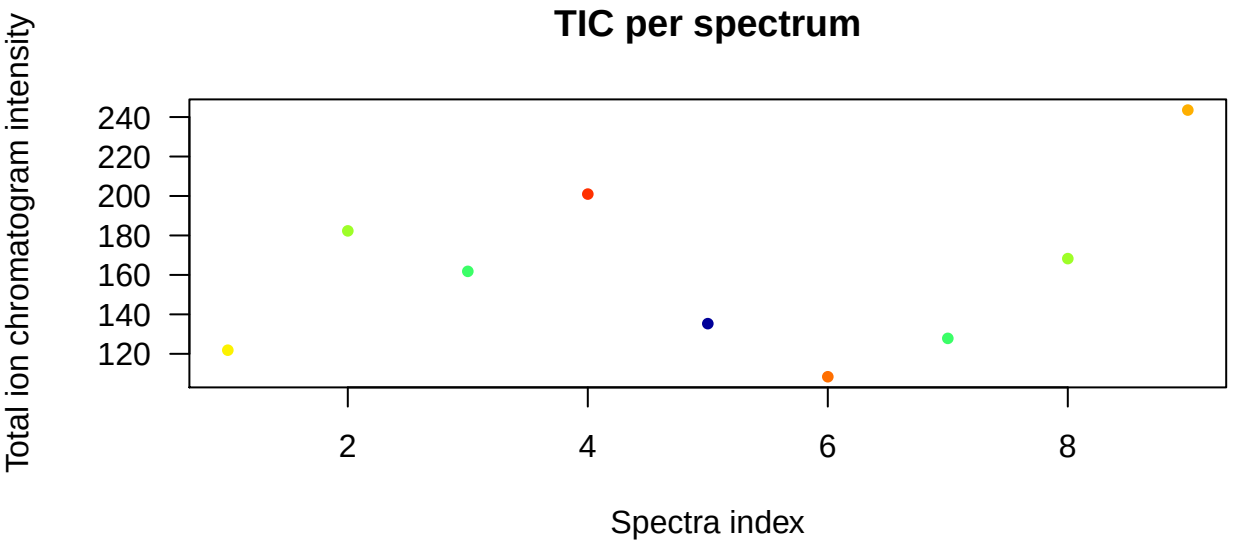

Total Ion Chromatogram
y
3
2
1
x
1
2
3
TIC
200
150

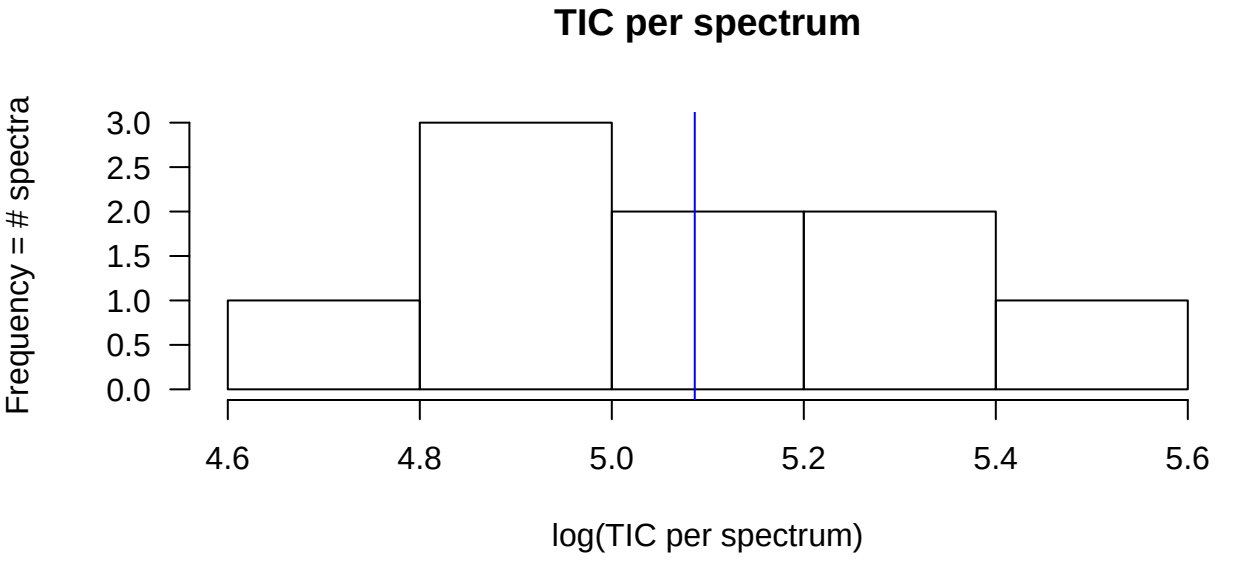

Most abundant m/z in each spectrum
3
2
1
y
1
2
3
x
m/z
250

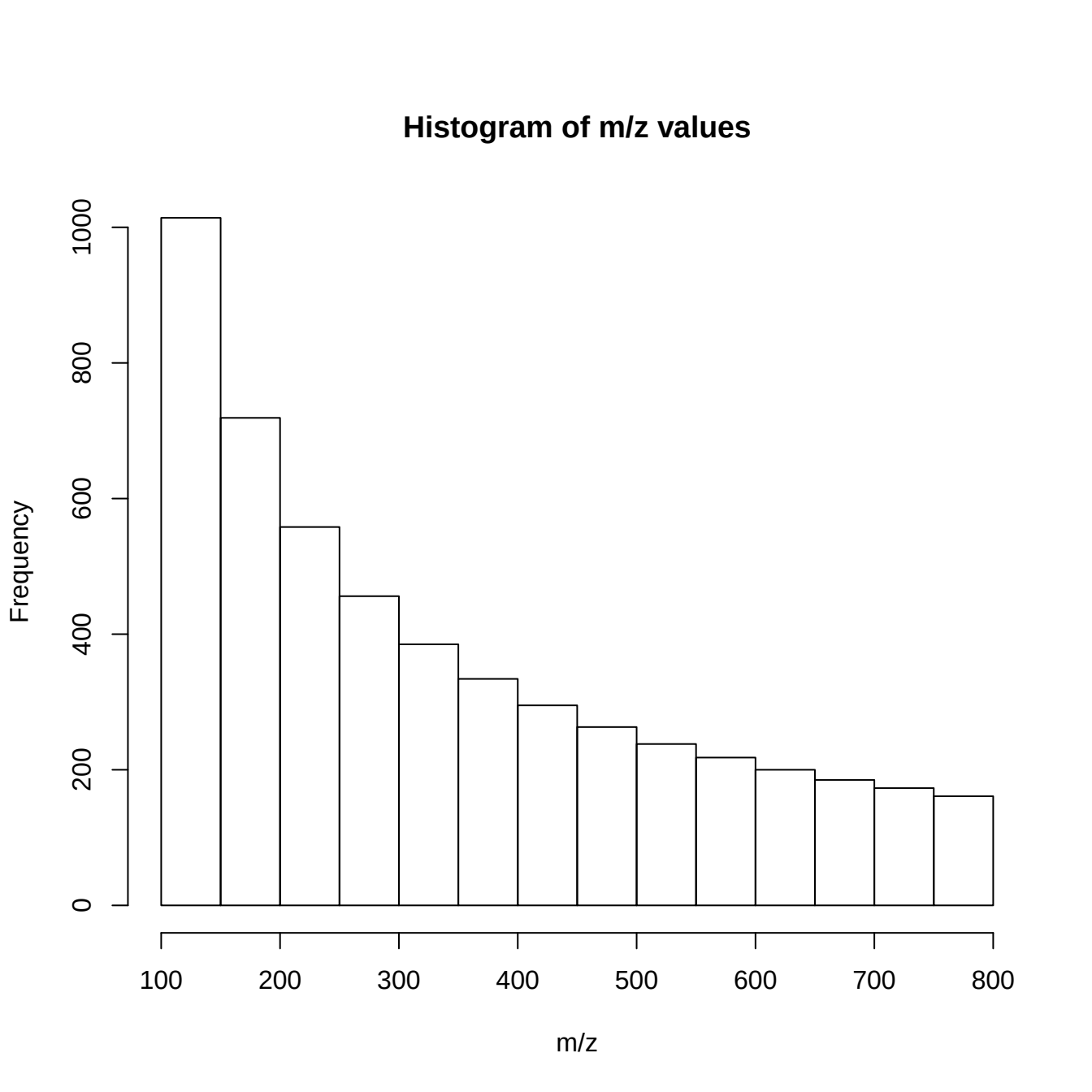

PCA for two components
ncomp = 2
PC1
PC2
loadings
0.2
−0.1
−0.4
100
200
300
400
500
600
700
800
m/z
PC1
PC2
y
3.0
2.0
1.0
−2
0
2
4
6
x

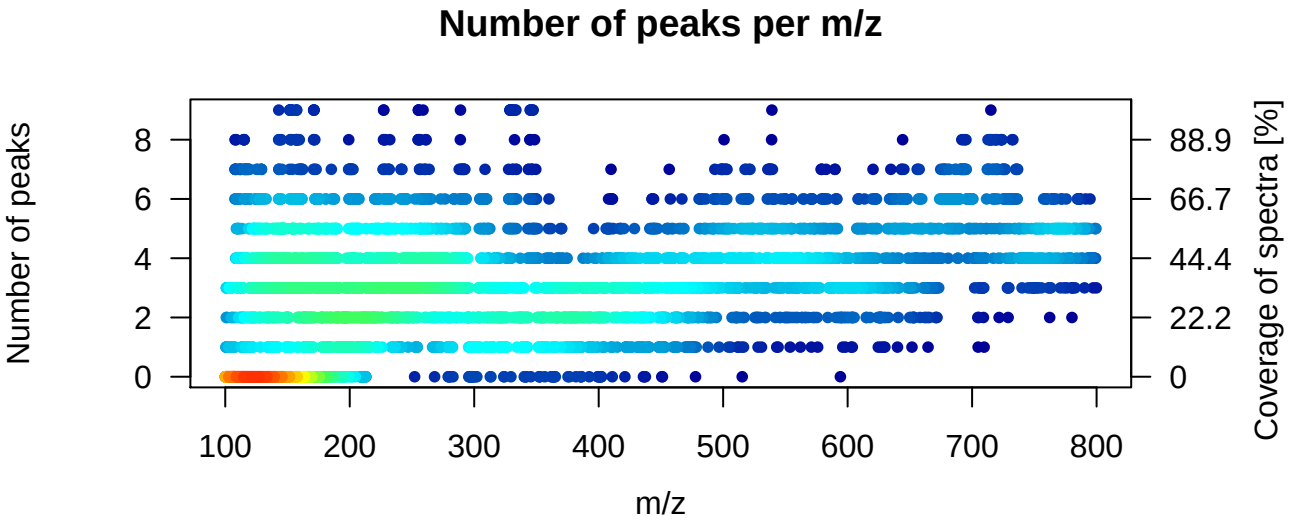

Number of peaks per spectrum
Number of peaks
2200
2000
1800
1600
1400
2
4
6
8
Spectra index

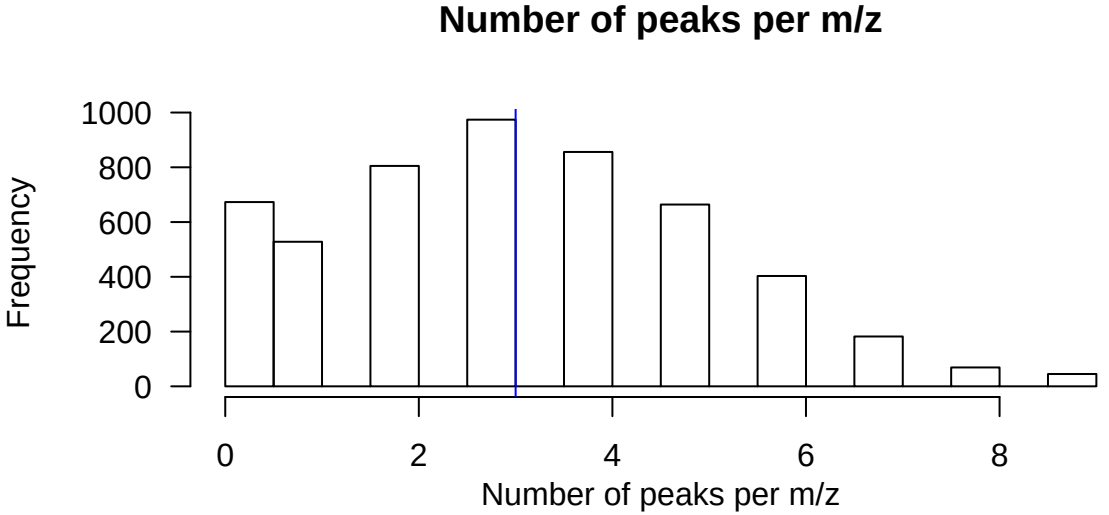

Number of peaks per spectrum
Frequency = # spectra
5
4
3
2
1
0
1200
1400
1600
1800
2000
2200
Number of peaks per spectrum

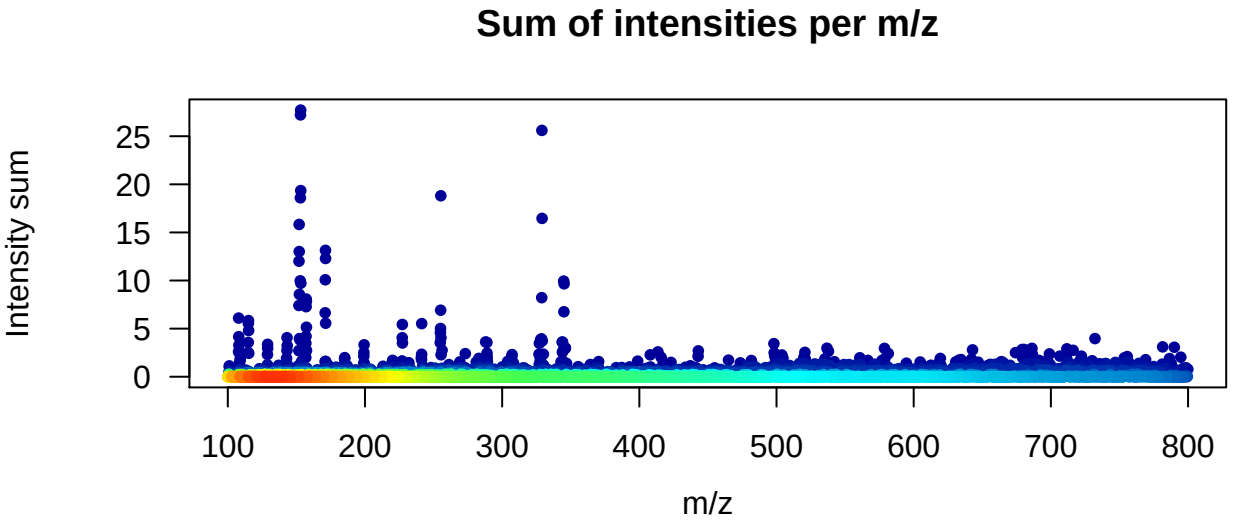

TIC per spectrum
Total ion chromatogram intensity
240
220
200
180
160
140
120
2
4
6
8
Spectra index

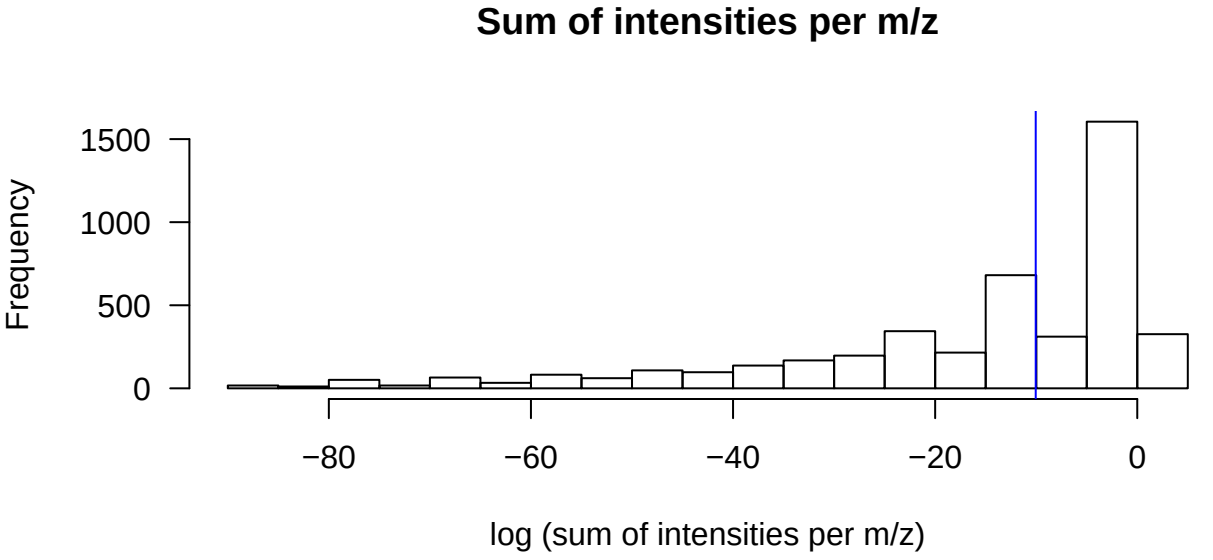

TIC per spectrum
Frequency = # spectra
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.6
4.8
5.0
5.2
5.4
5.6
log(TIC per spectrum)

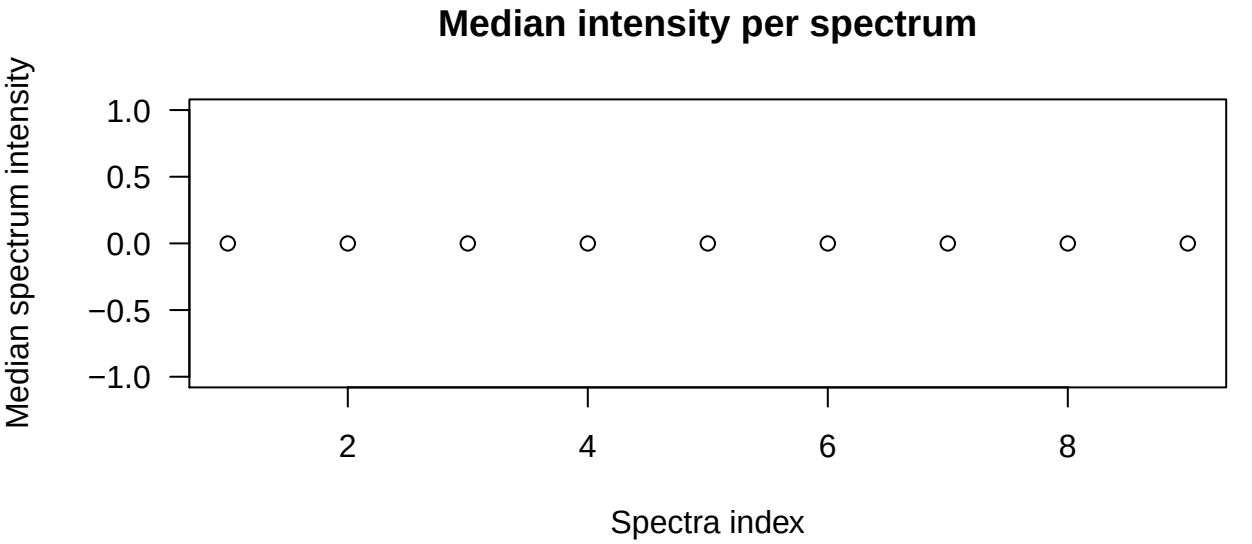

Histogram of m/z values
Frequency
0
200
400
600
800
1000
100
200
300
400
500
600
700
800
m/z

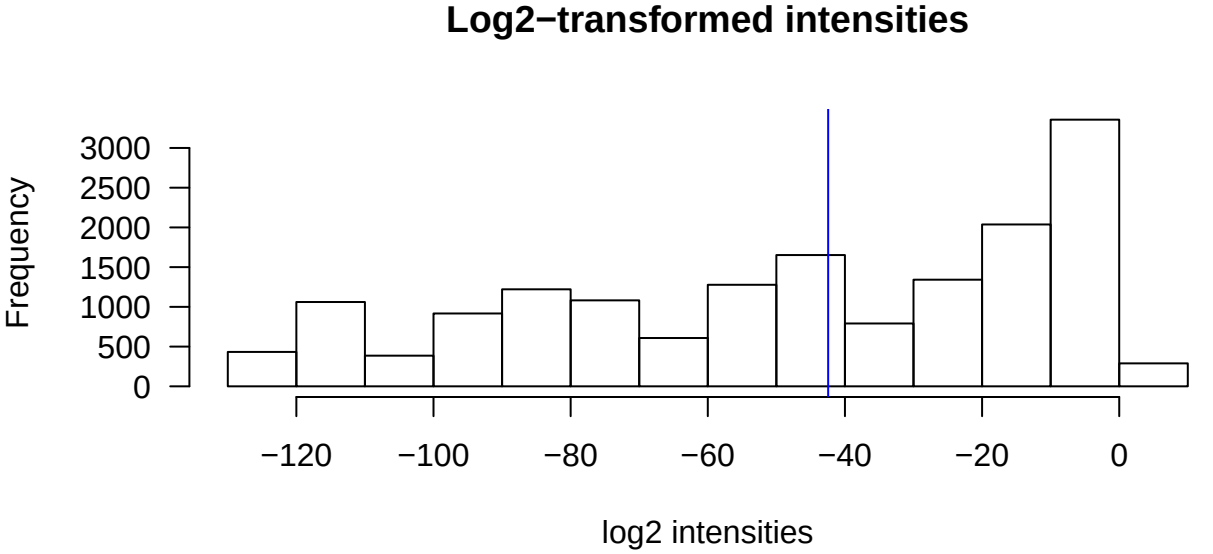

Number of peaks per m/z
Number of peaks
Coverage of spectra [%]
m/z
0
2
4
6
8
22.2
44.4
66.7
88.9
100
200
300
400
500
600
700
800

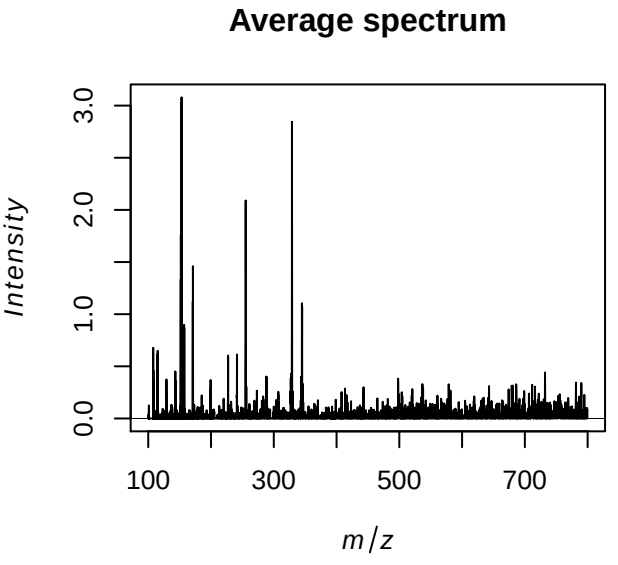

Number of peaks per m/z
Frequency
Number of peaks per m/z
0
200
400
600
800
1000
0
2
4
6
8

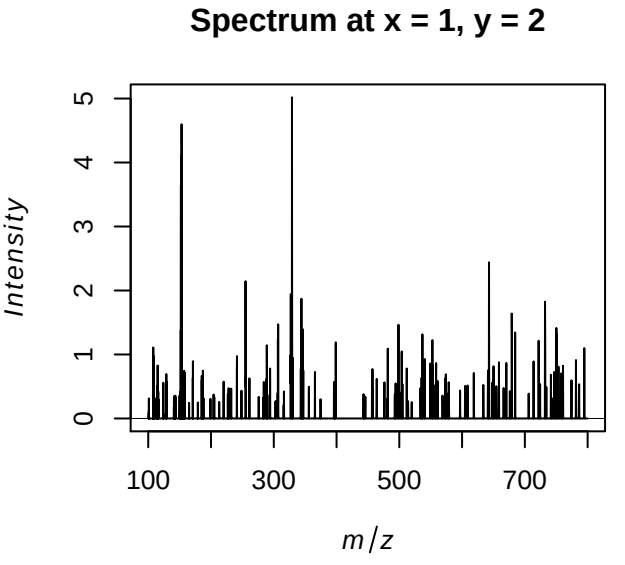

Sum of intensities per m/z
Intensity sum
0
5
10
15
20
25
100
200
300
400
500
600
700
800
m/z

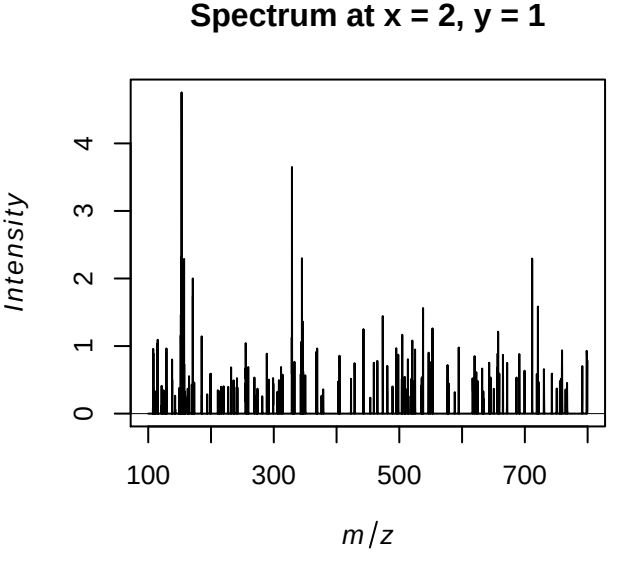

Sum of intensities per m/z
Frequency
0
500
1000
1500
−80
−60
−40
−20
0
log (sum of intensities per m/z)

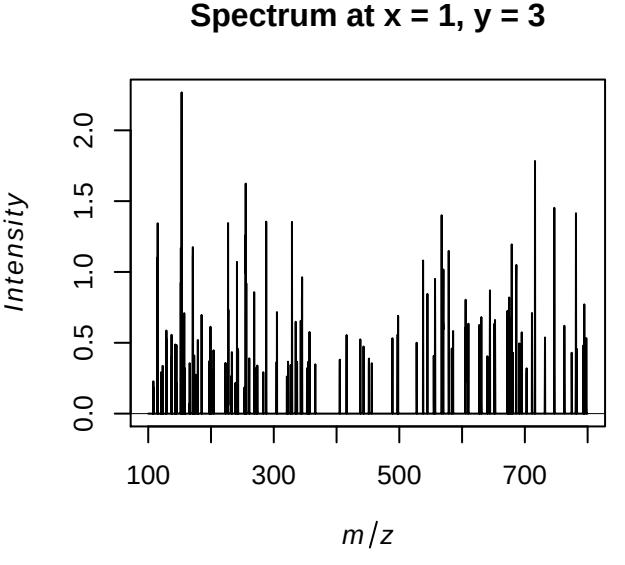

Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
Spectra index


Log2−transformed intensities
Frequency
3000
2500
2000
1500
1000
500
0
−120
−100
−80
−60
−40
−20
0
log2 intensities

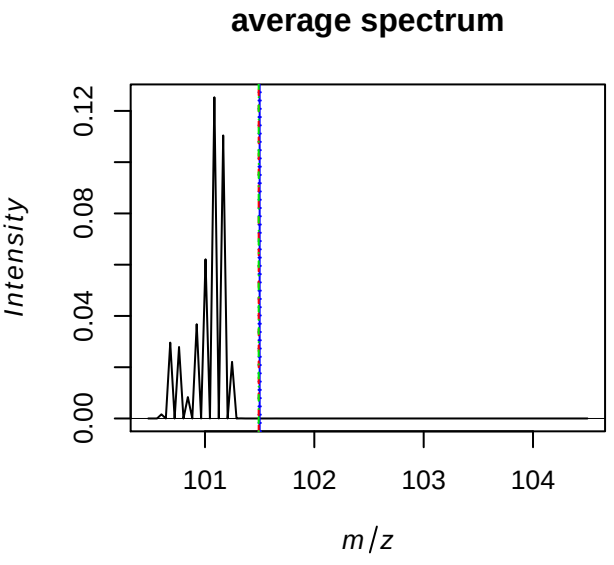

Average spectrum
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z

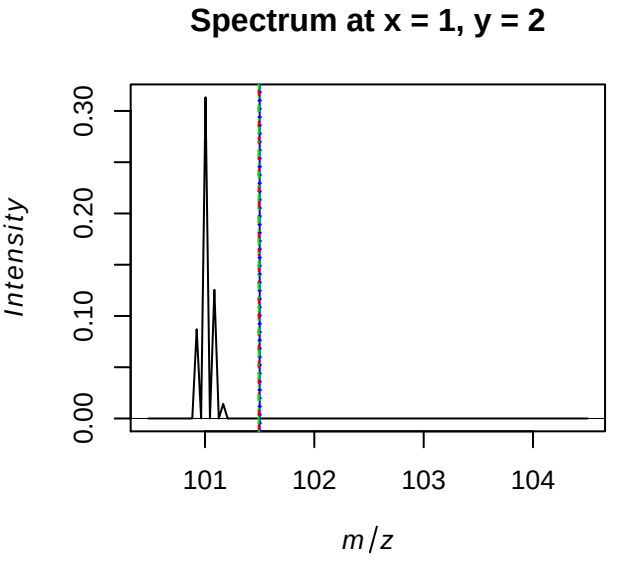

Spectrum at x = 1, y = 2
Intensity
0
1
2
3
4
5
100
300
500
700
m/z

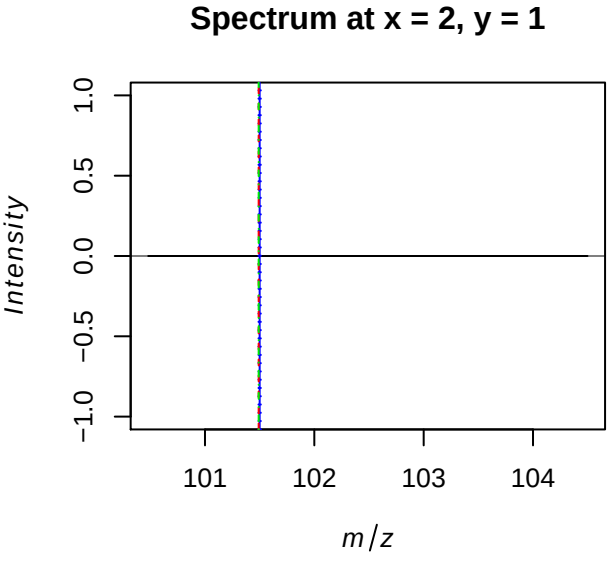

Spectrum at x = 2, y = 1
Intensity
0
1
2
3
4
100
300
500
700
m/z

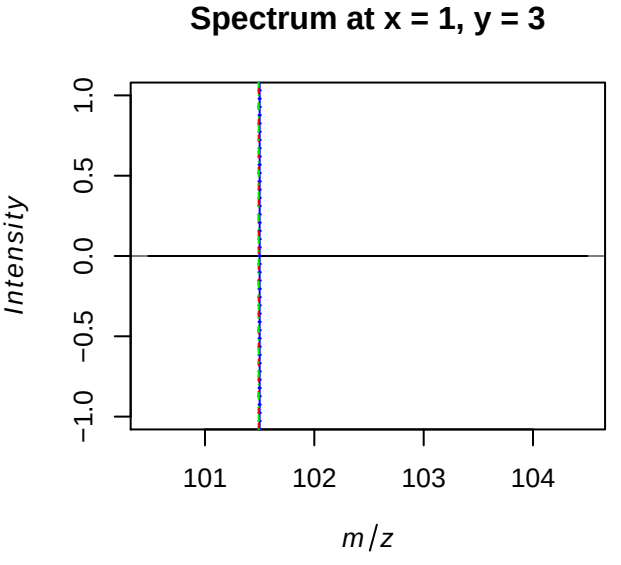

Spectrum at x = 1, y = 3
Intensity
0.0
0.5
1.0
1.5
2.0
100
300
500
700
m/z

theor. m/z: 101.5 most abundant m/z: 101.491 closest m/z: 101.491

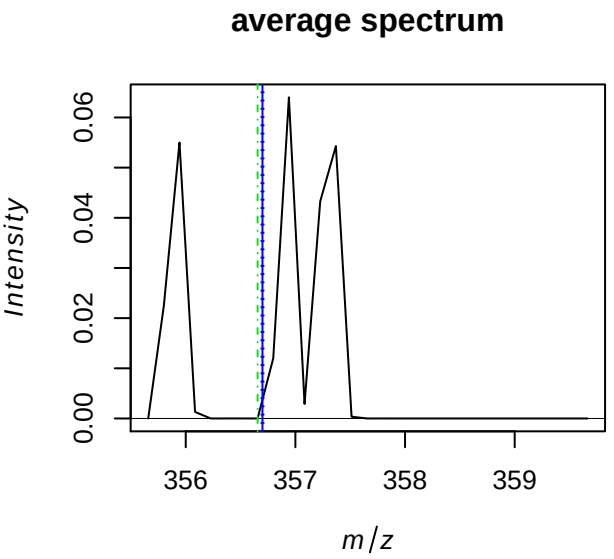


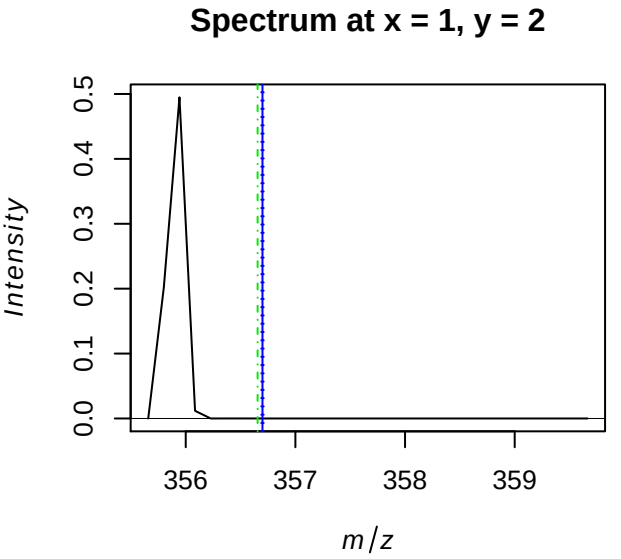


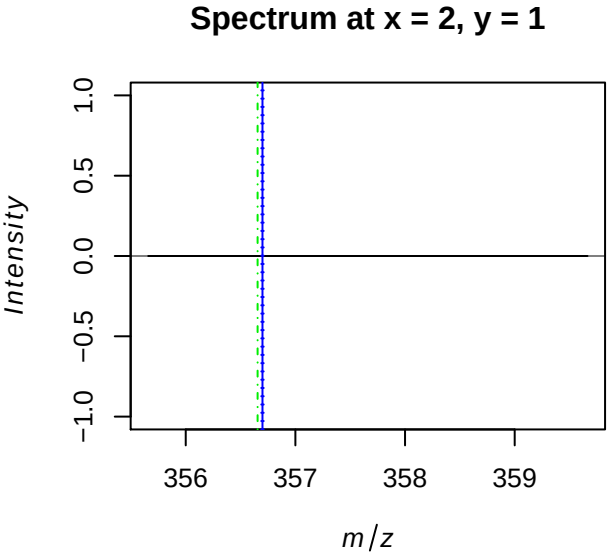


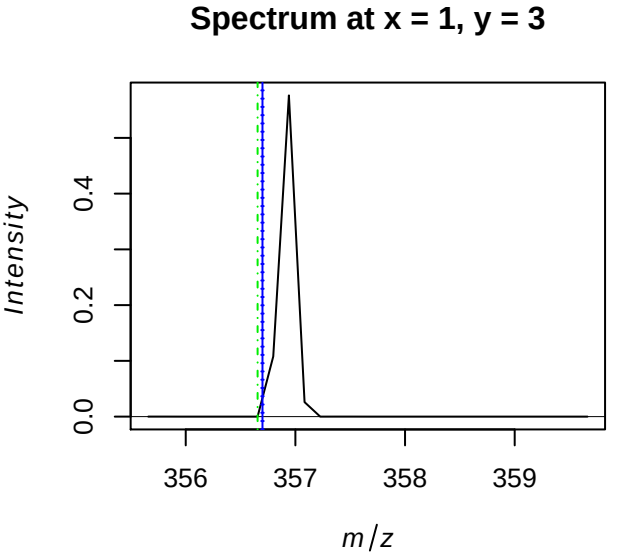


theor. m/z: 101.5 most abundant m/z: NA closest m/z: 356.6555

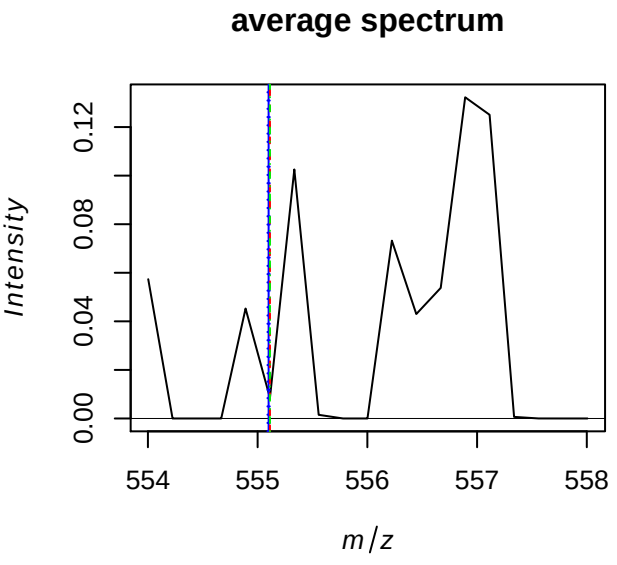


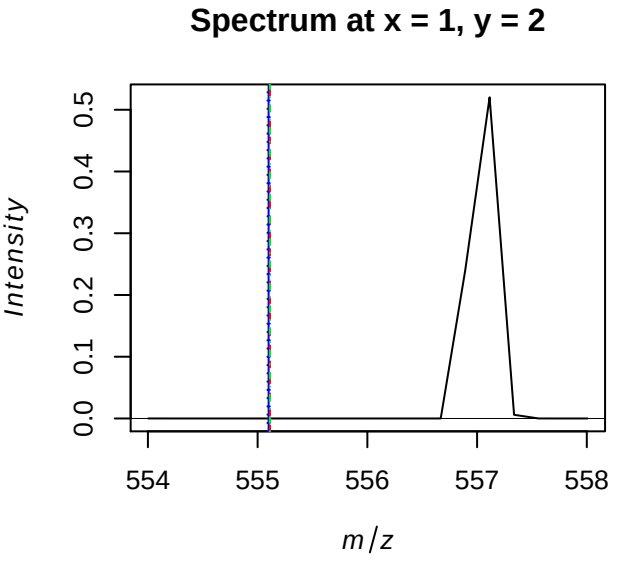


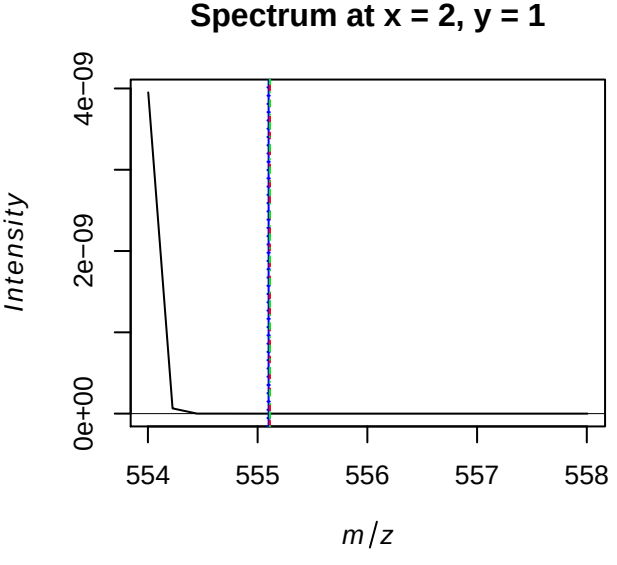


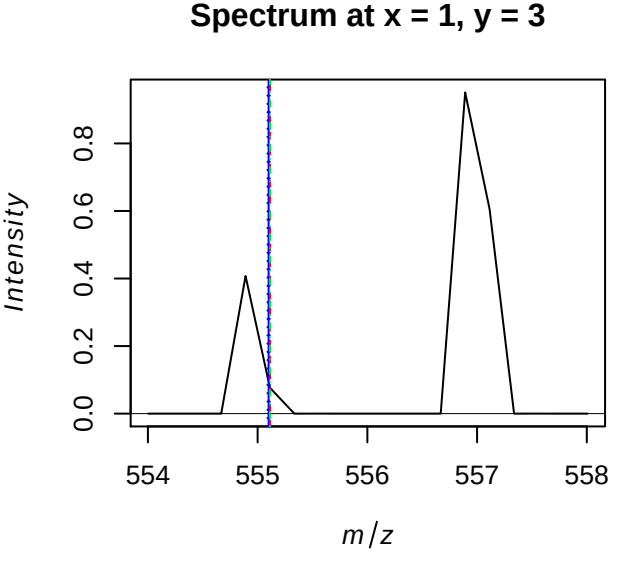


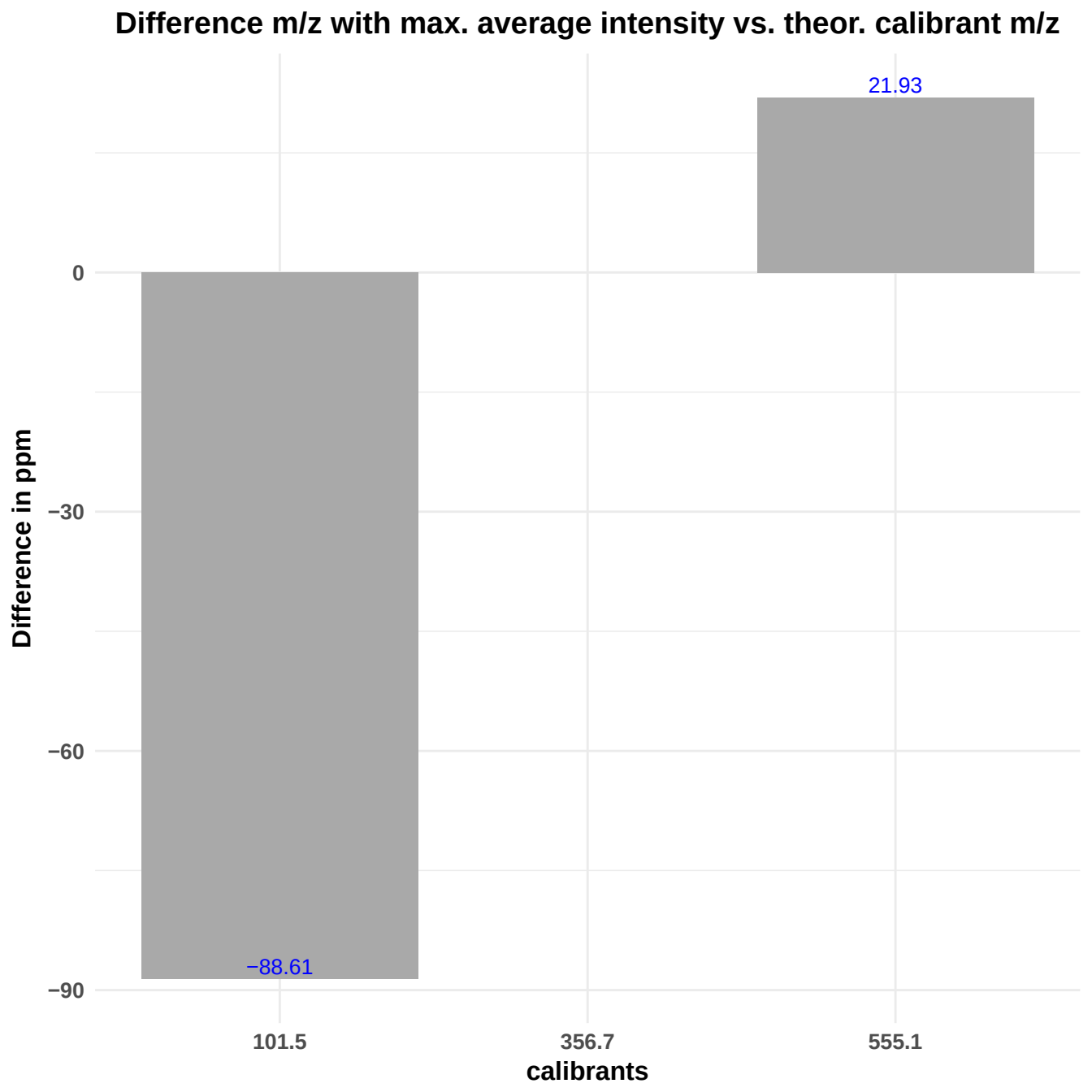
theor. m/z: 101.5 most abundant m/z: 555.1122 closest m/z: 555.1122

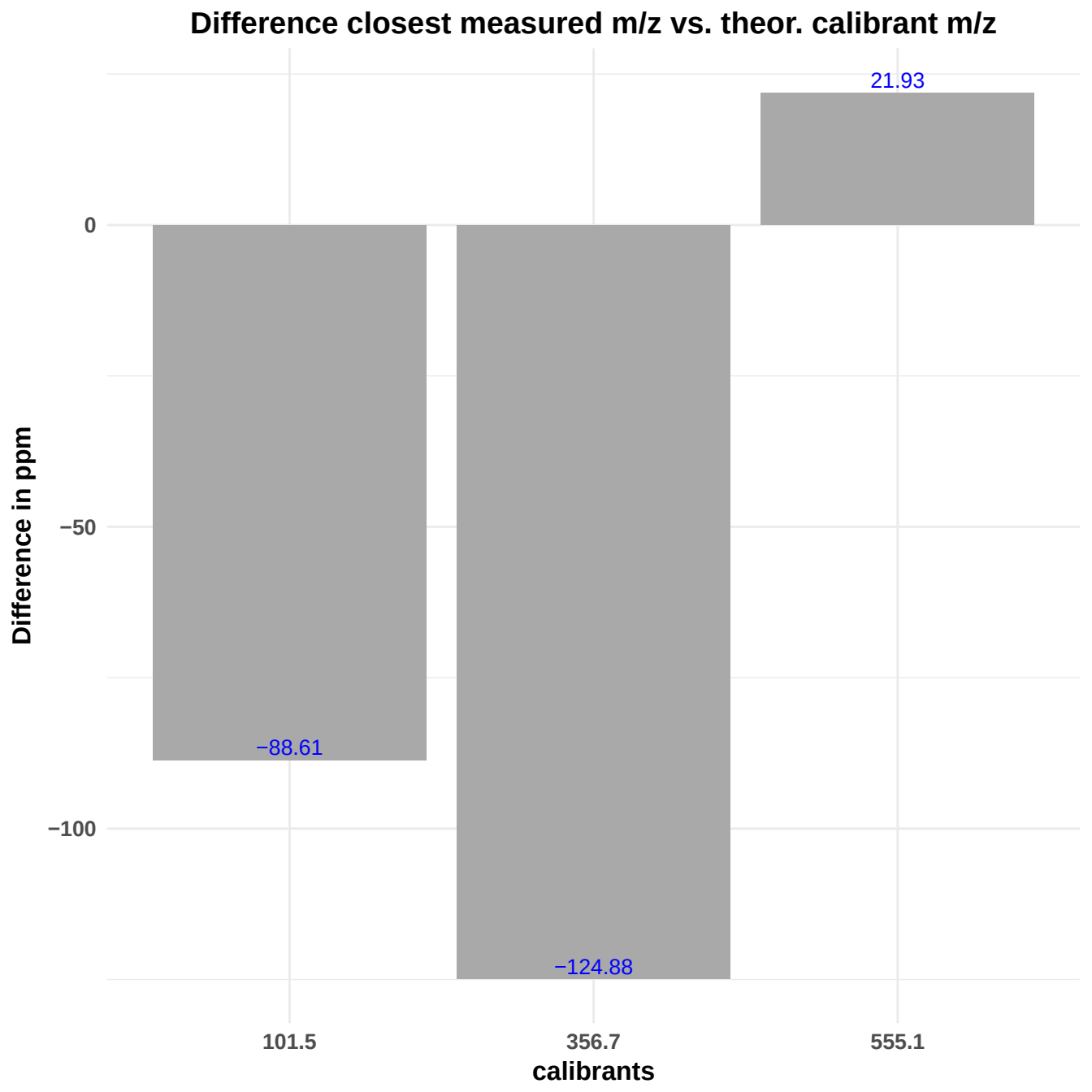


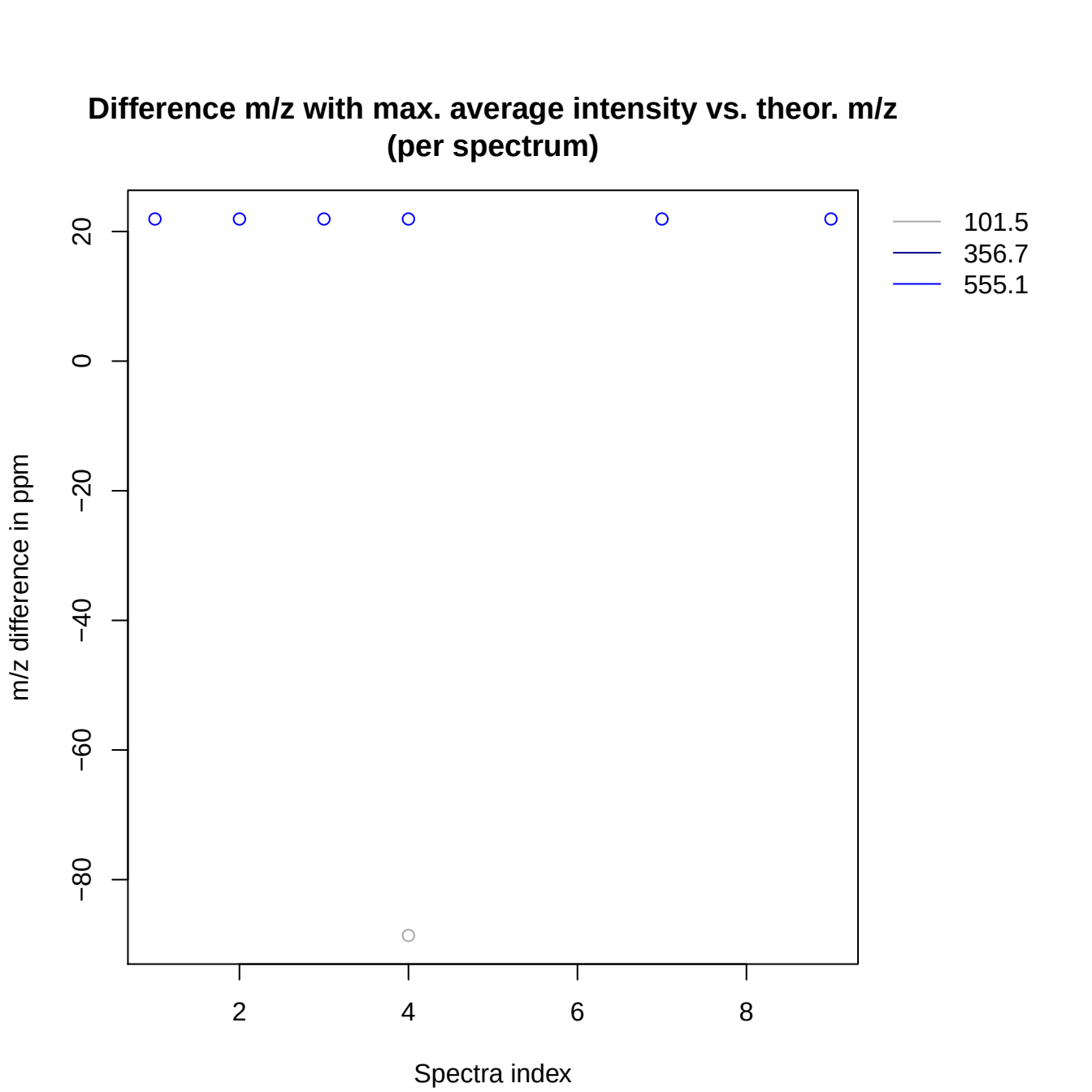







Difference m/z with max. average intensity vs. theor. calibrant m/z
21.93
0
−30
−60
−90
Difference in ppm
−88.61
101.5
356.7
555.1
calibrants


Difference closest measured m/z vs. theor. calibrant m/z
21.93
0
−50
−100
−88.61
−124.88
Difference 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
20
0
−20
−40
−60
−80
2
4
6
8
Spectra index
101.5
356.7
555.1