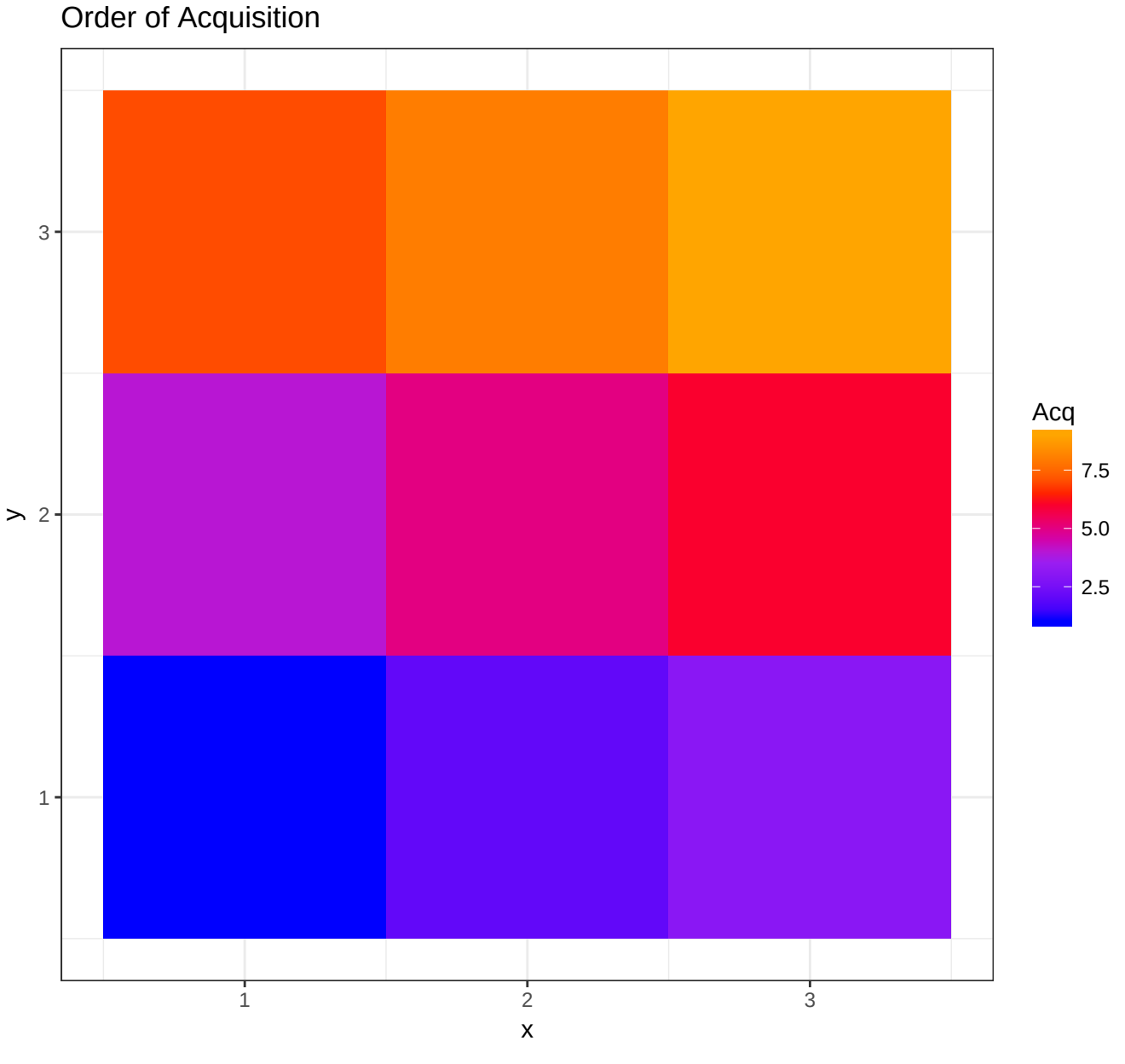
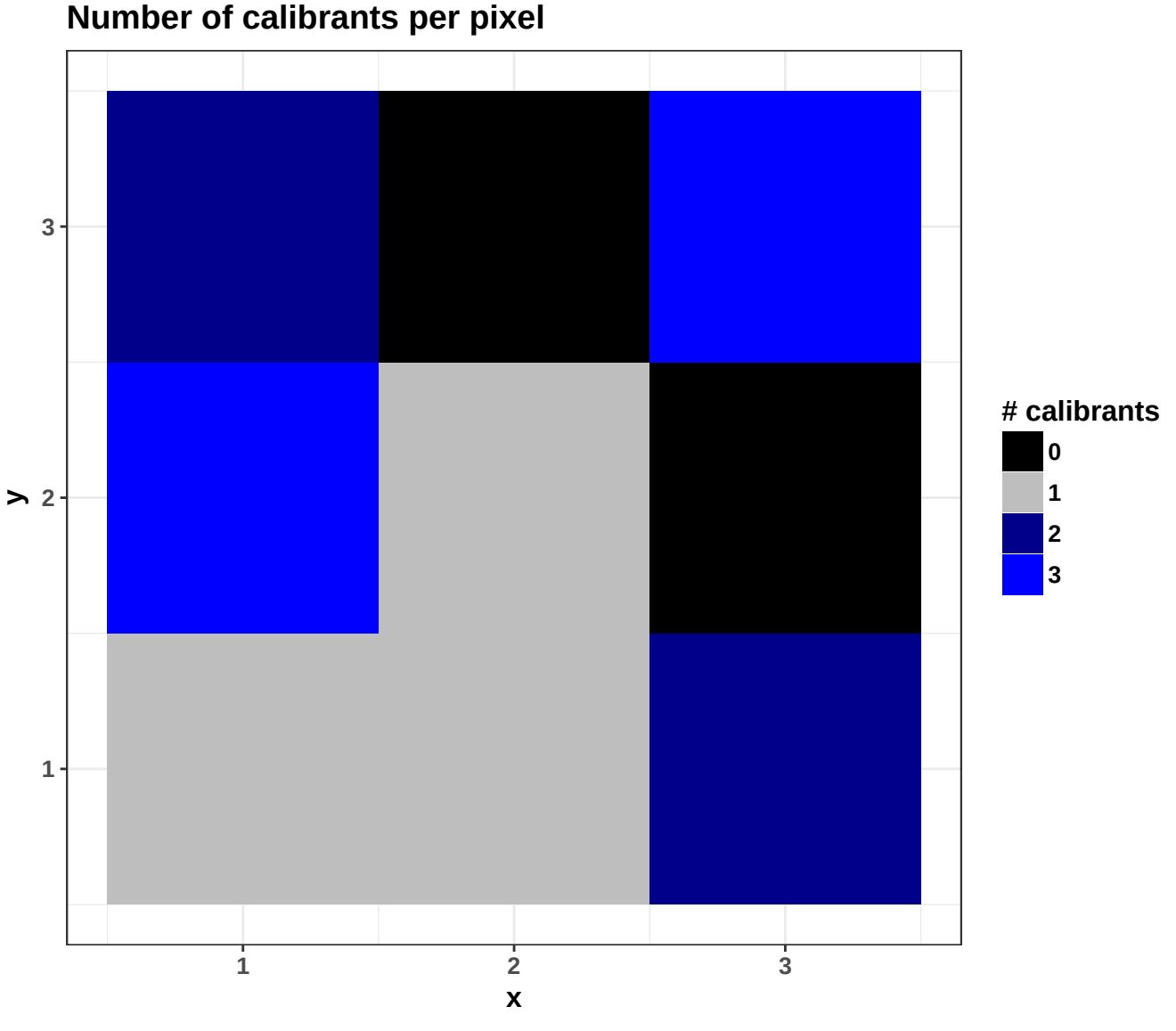
Quality control of MSI data

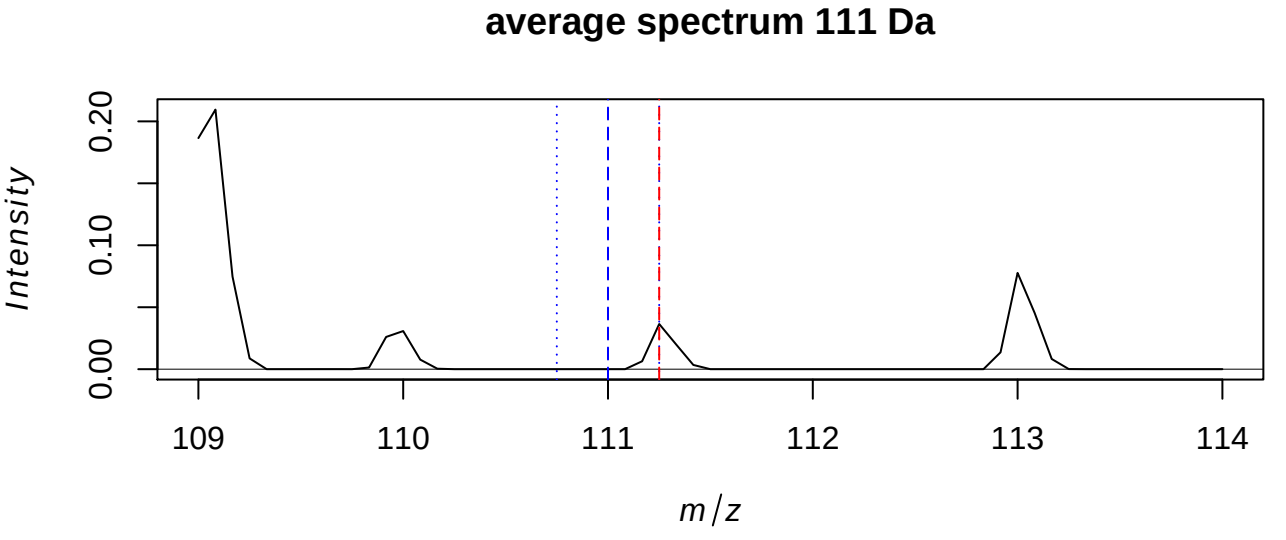
Filename: Testfile_imzml

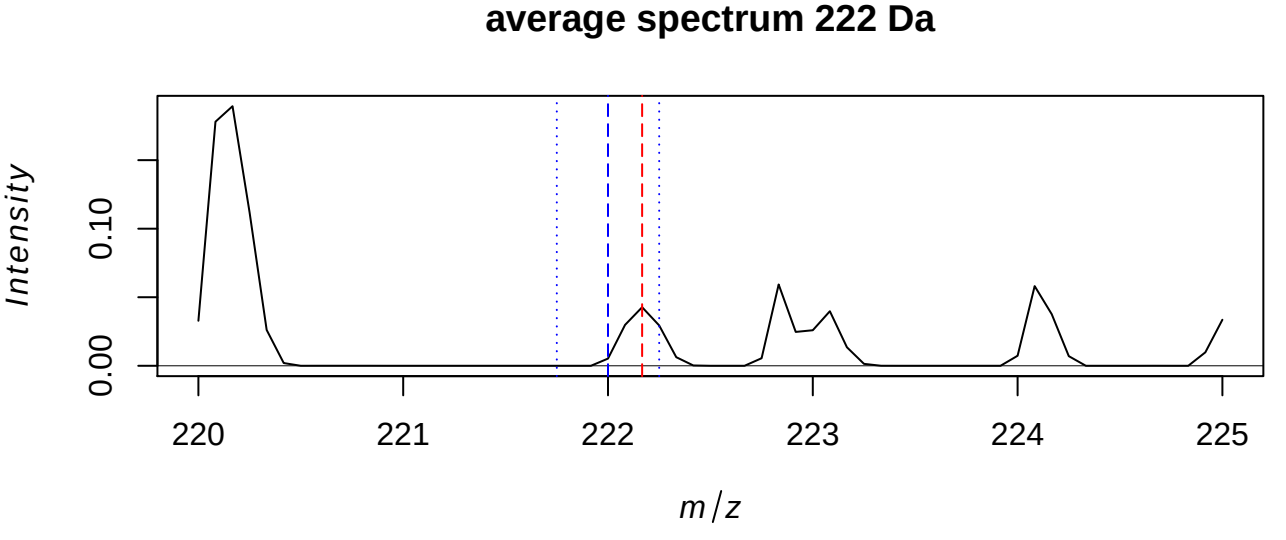
properties	values
Number of mz features	8399
Range of mz values [Da]	100.08 − 799.92
Number of pixels	9
Range of x coordinates	1 − 3
Range of y coordinates	1 − 3
Range of intensities	0 − 9.24
Median of intensities	0
Intensities > 0	30.92 %
Number of zero TICs	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in inputpeptides.csv	3 / 3
# calibrants in inputcalibrantfile1.txt	3 / 3

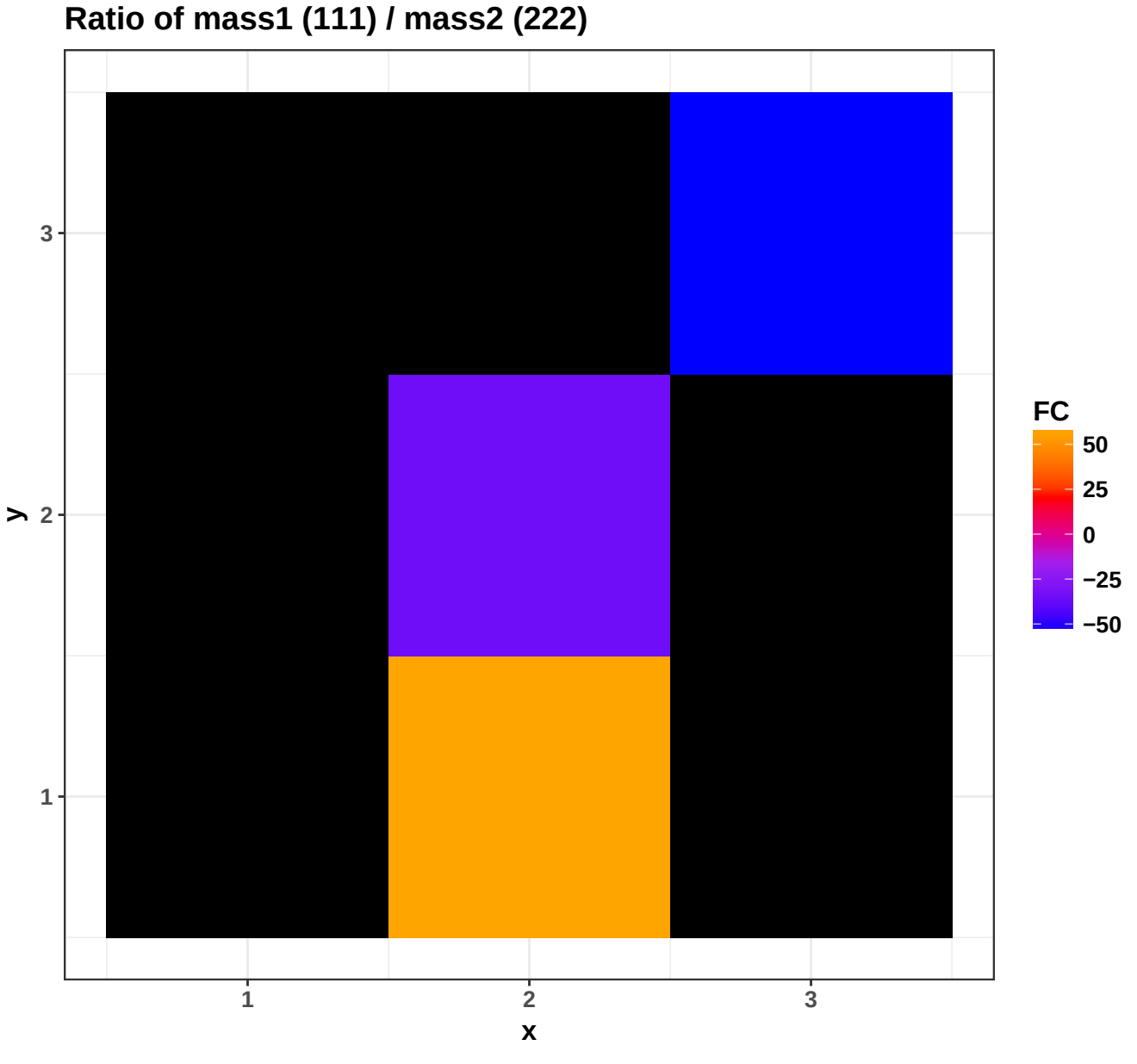

Order of Acquisition
3
2
1
y
1
2
3
x
Acq
7.5
5.0
2.5

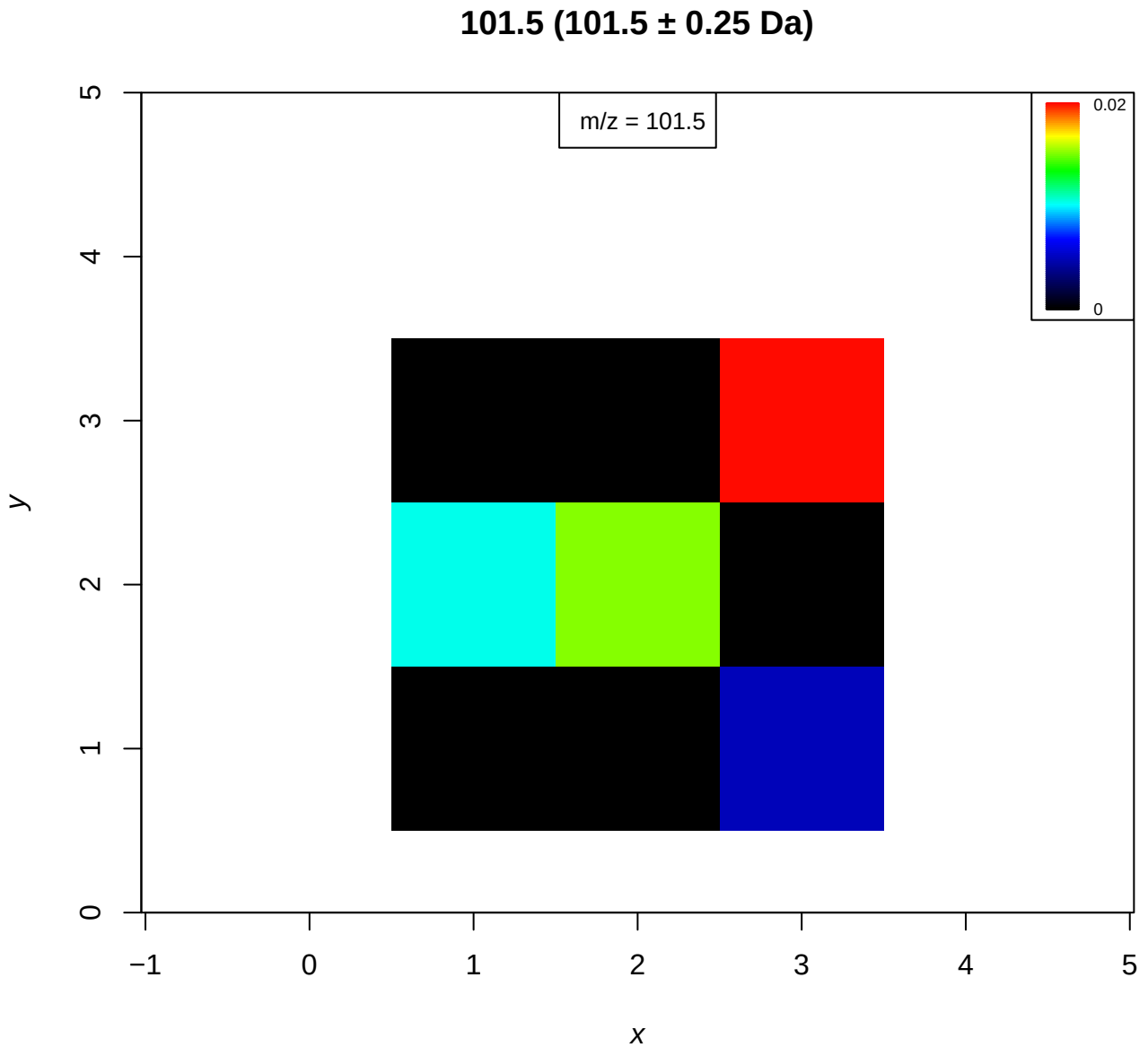

Number of calibrants per pixel
3
2
1
y
1
2
3
x
calibrants
0
1
2
3

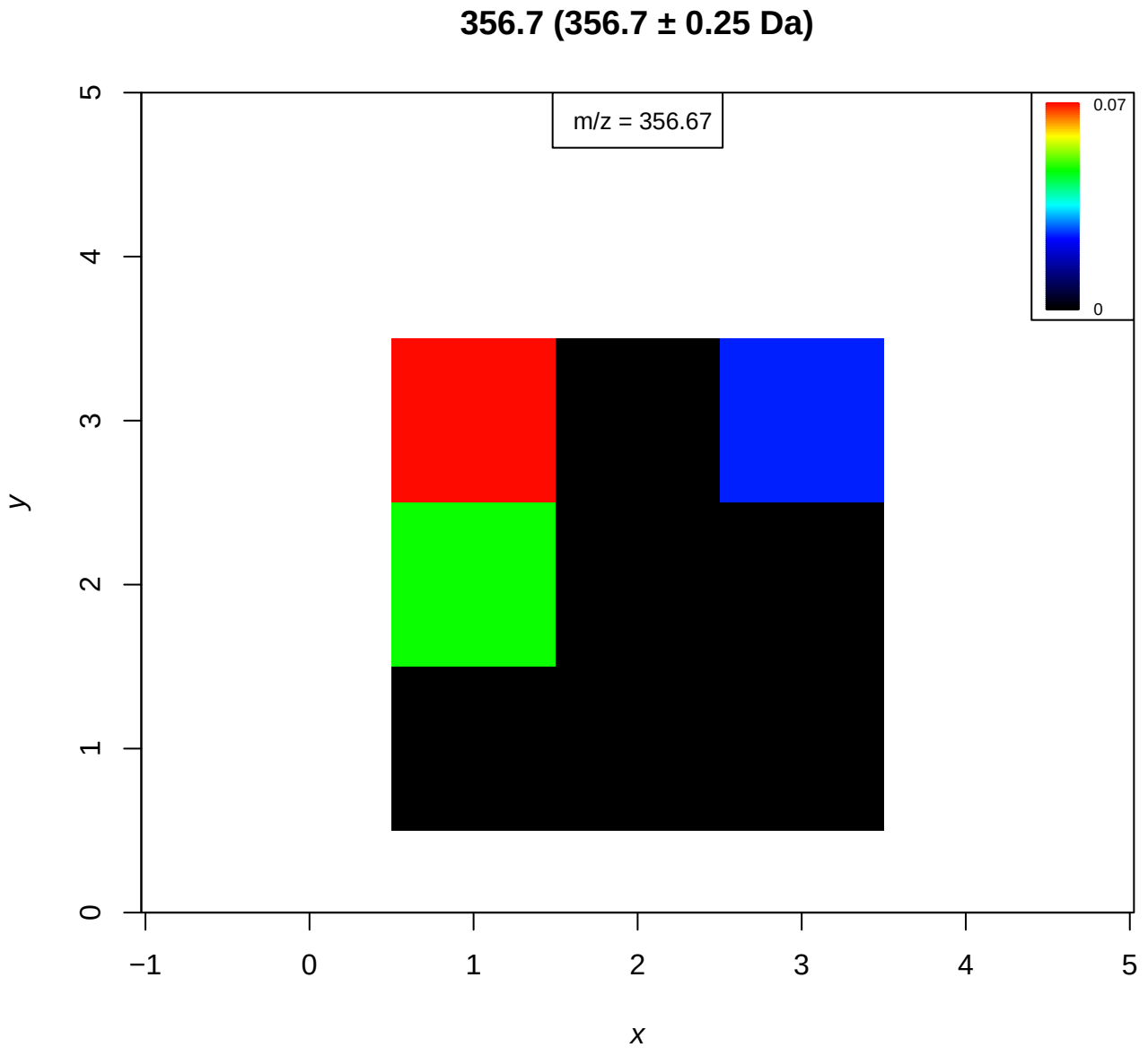
Control of fold change plot

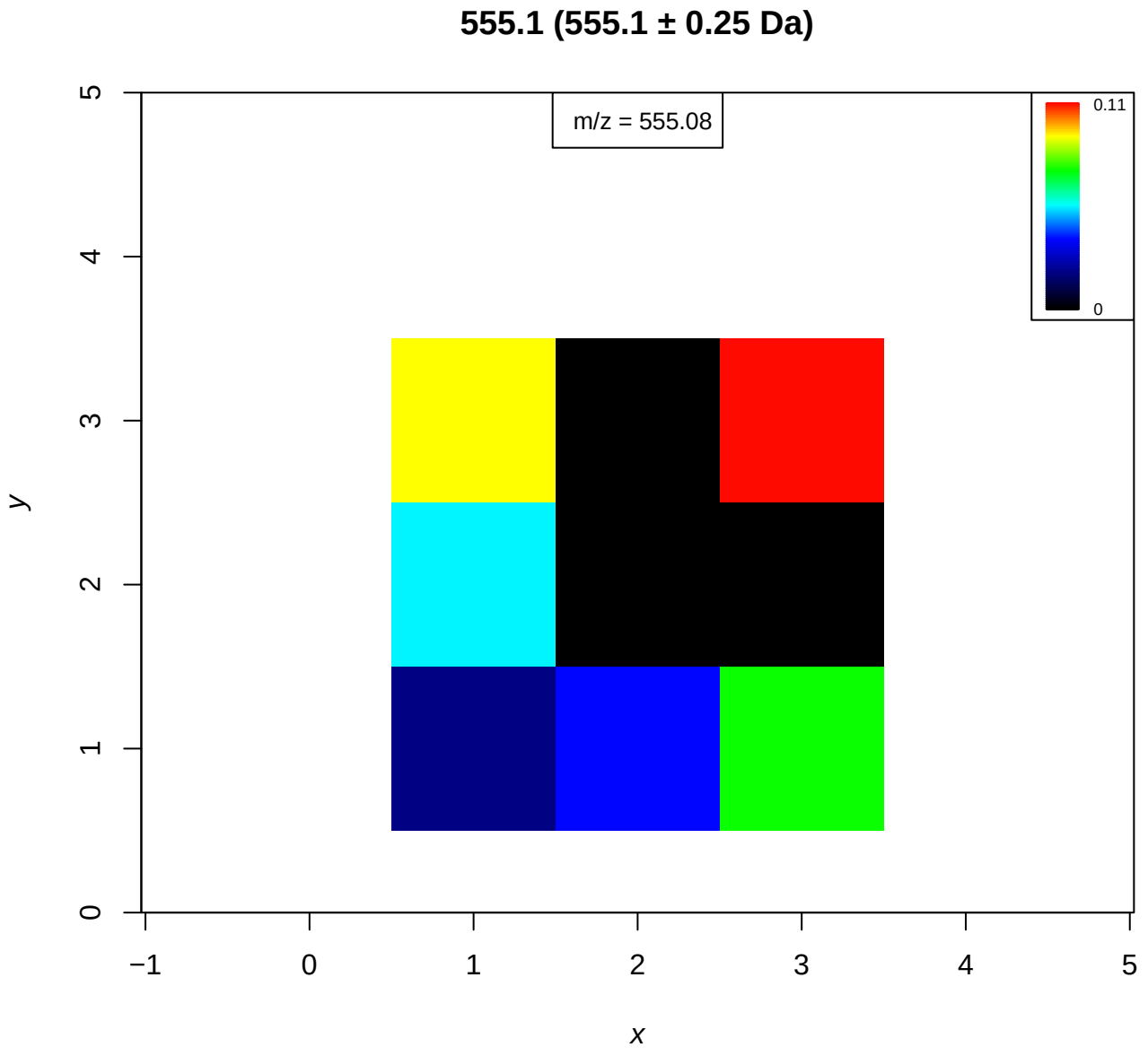


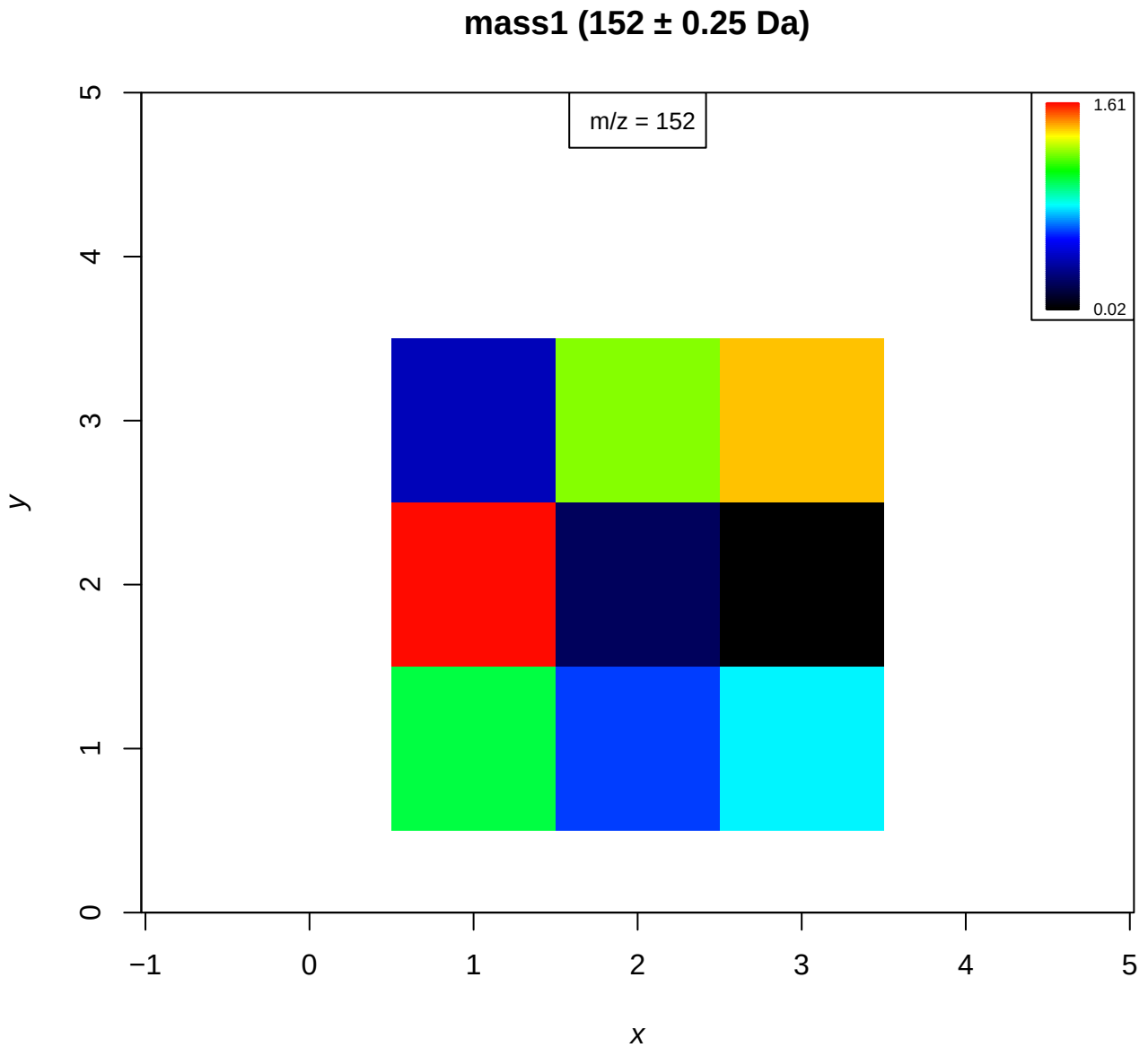


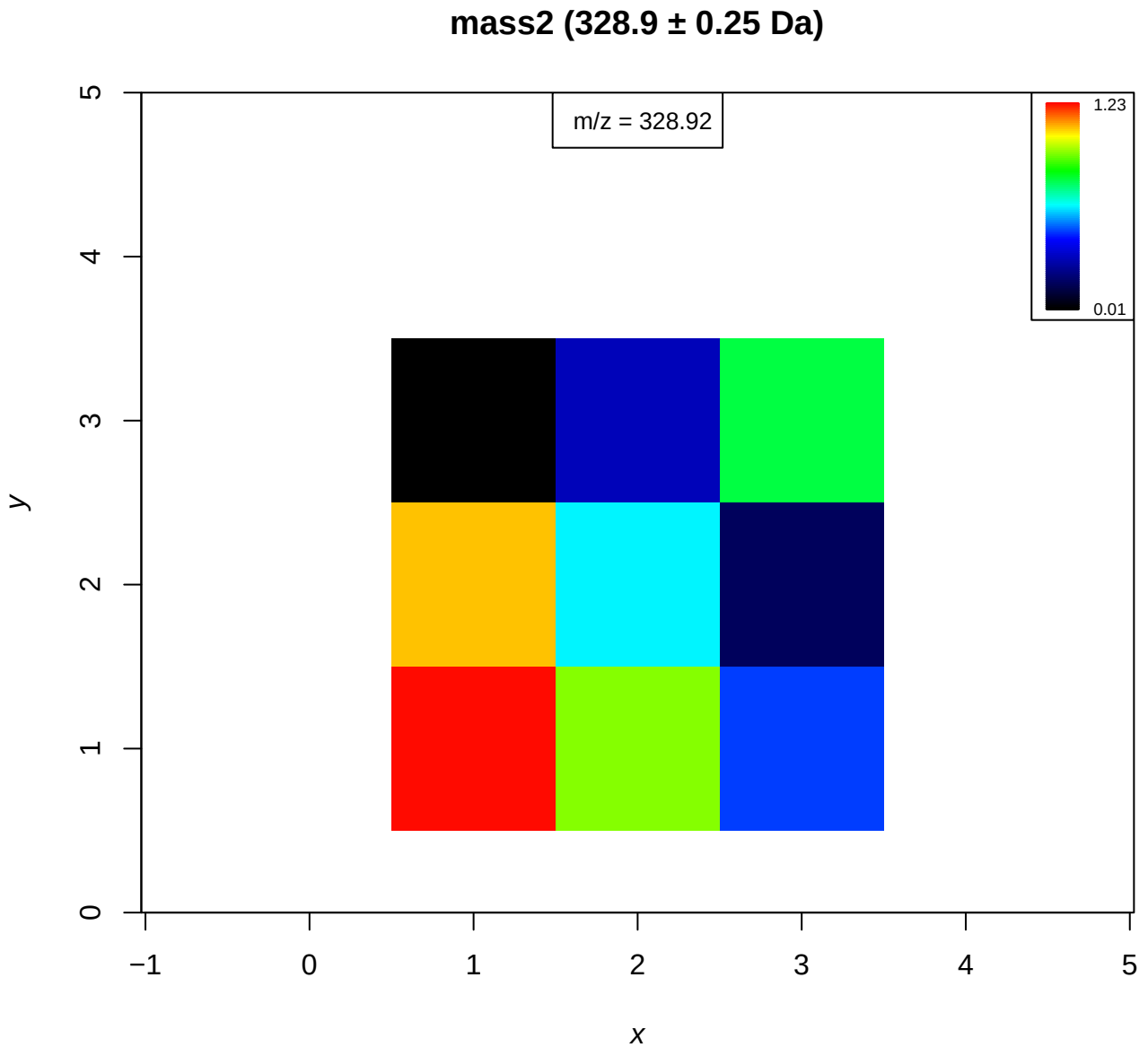

Ratio of mass1 (111) / mass2 (222)
y
3
2
1
x
1
2
3
FC
50
25
0
−25
−50

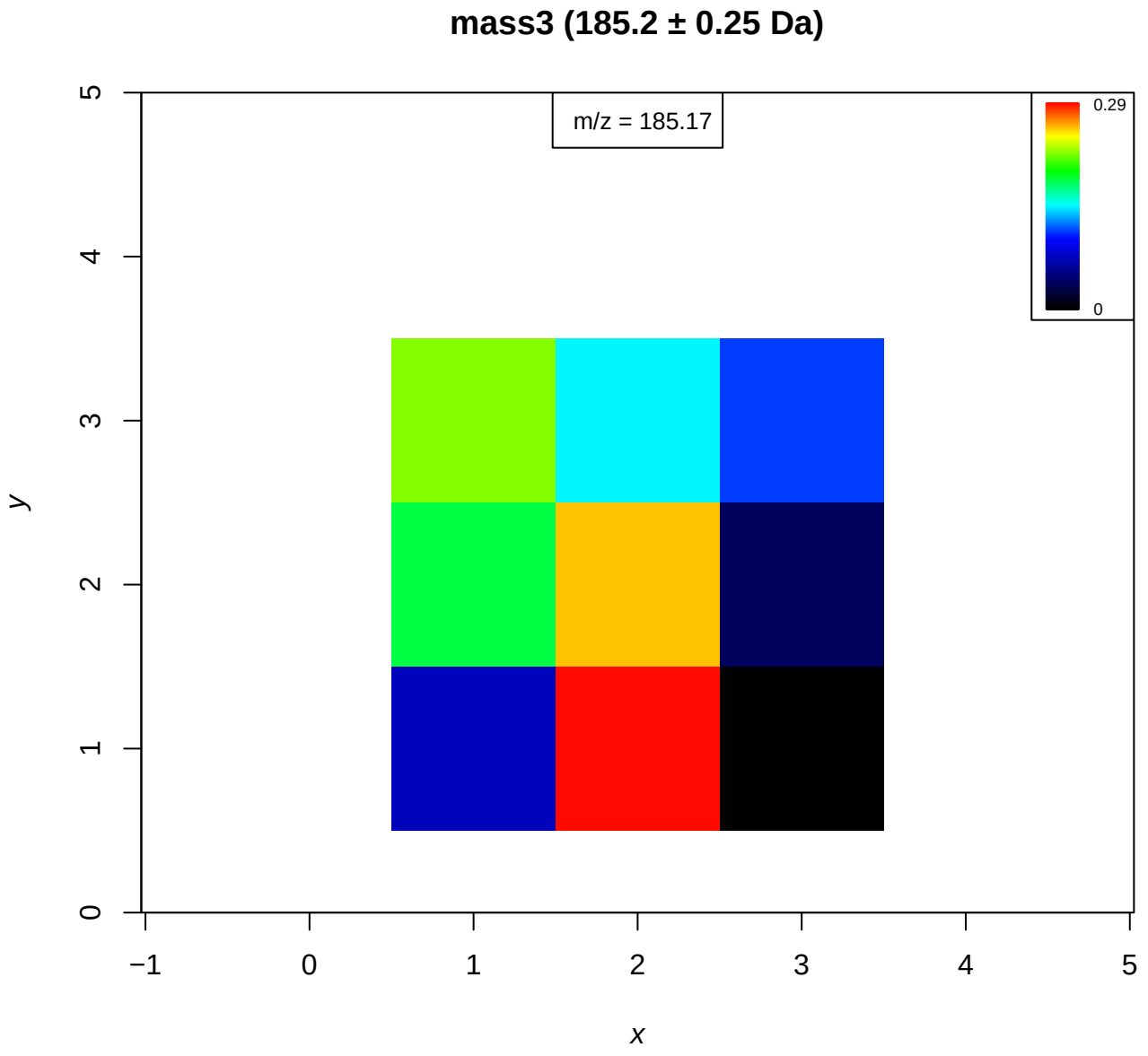

101.5 (101.5 ± 0.25 Da)
m/z = 101.5
0.02
0
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5

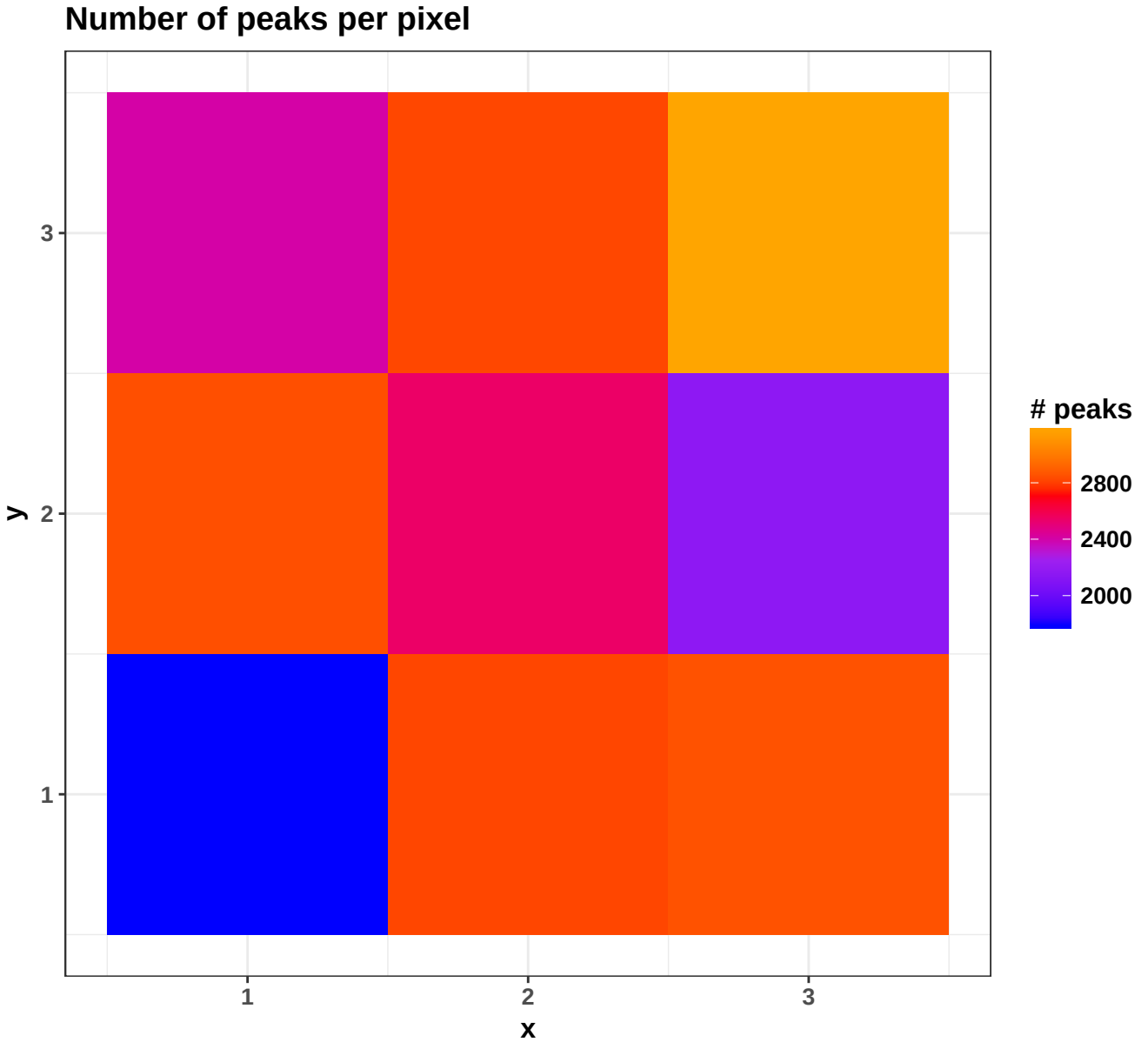

356.7 (356.7 ± 0.25 Da)
m/z = 356.67
0.07
0
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5

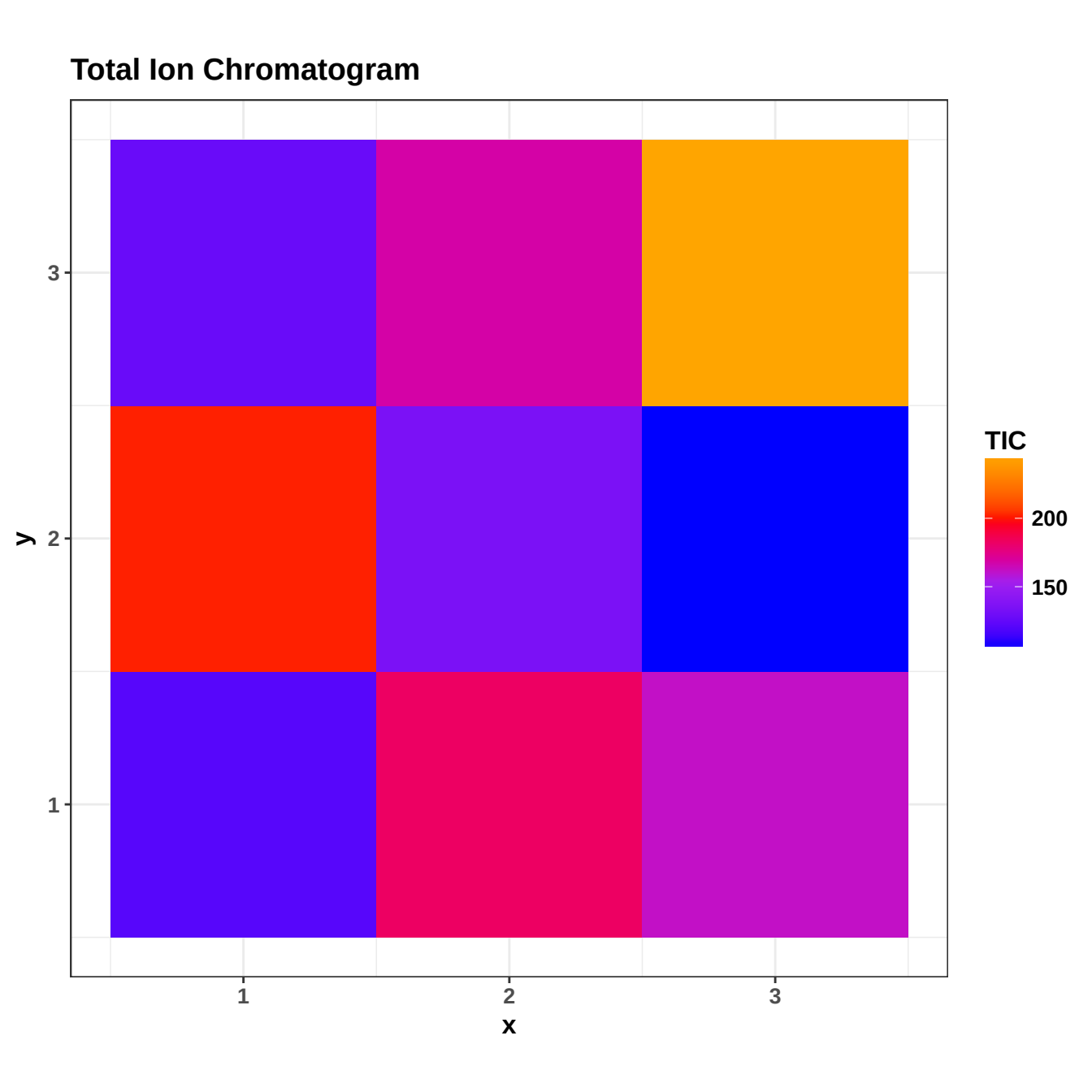

555.1 (555.1 ± 0.25 Da)
m/z = 555.08
0.11
0
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5

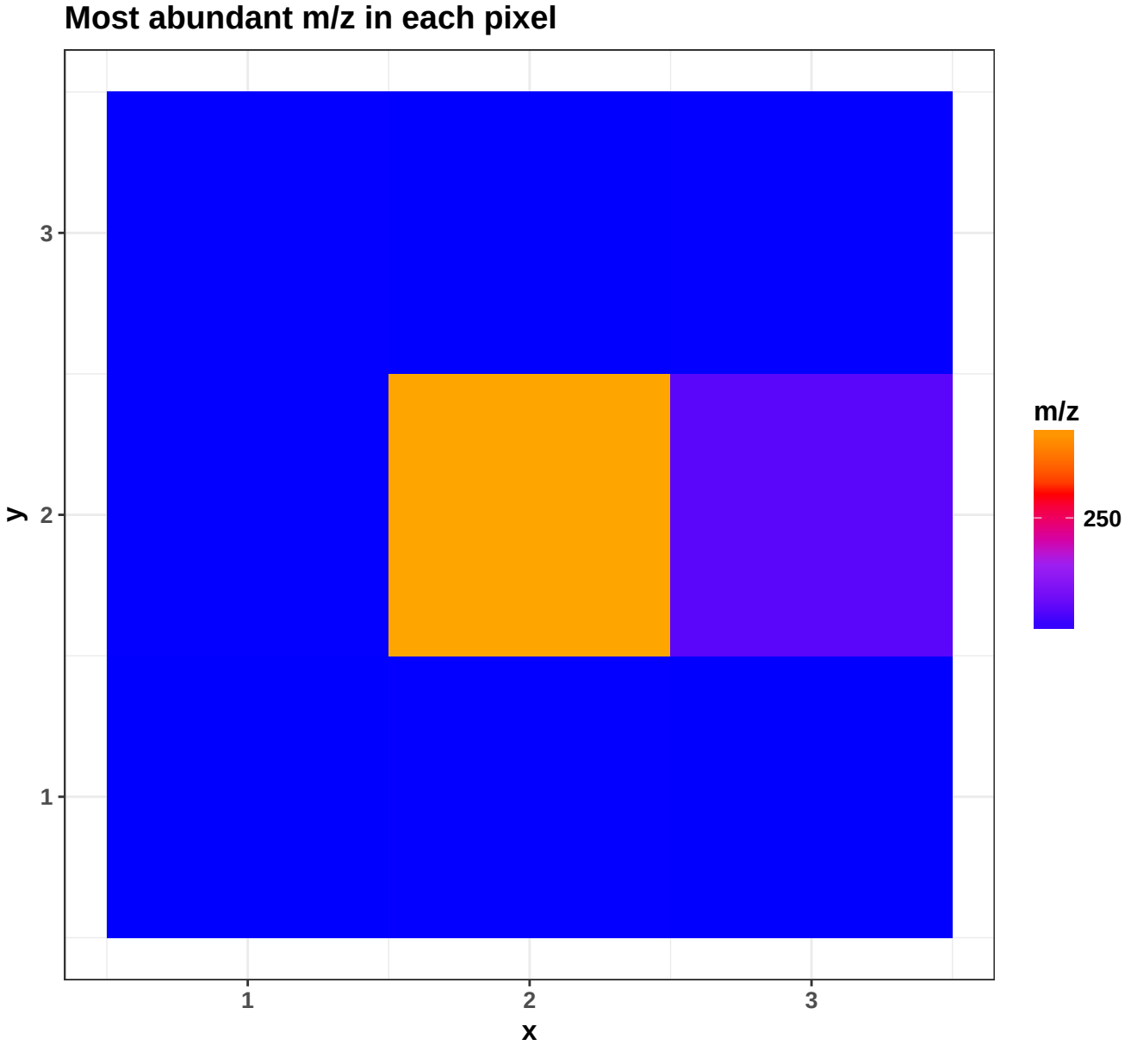

mass1 (152 ± 0.25 Da)
m/z = 152
1.61
0.02
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5

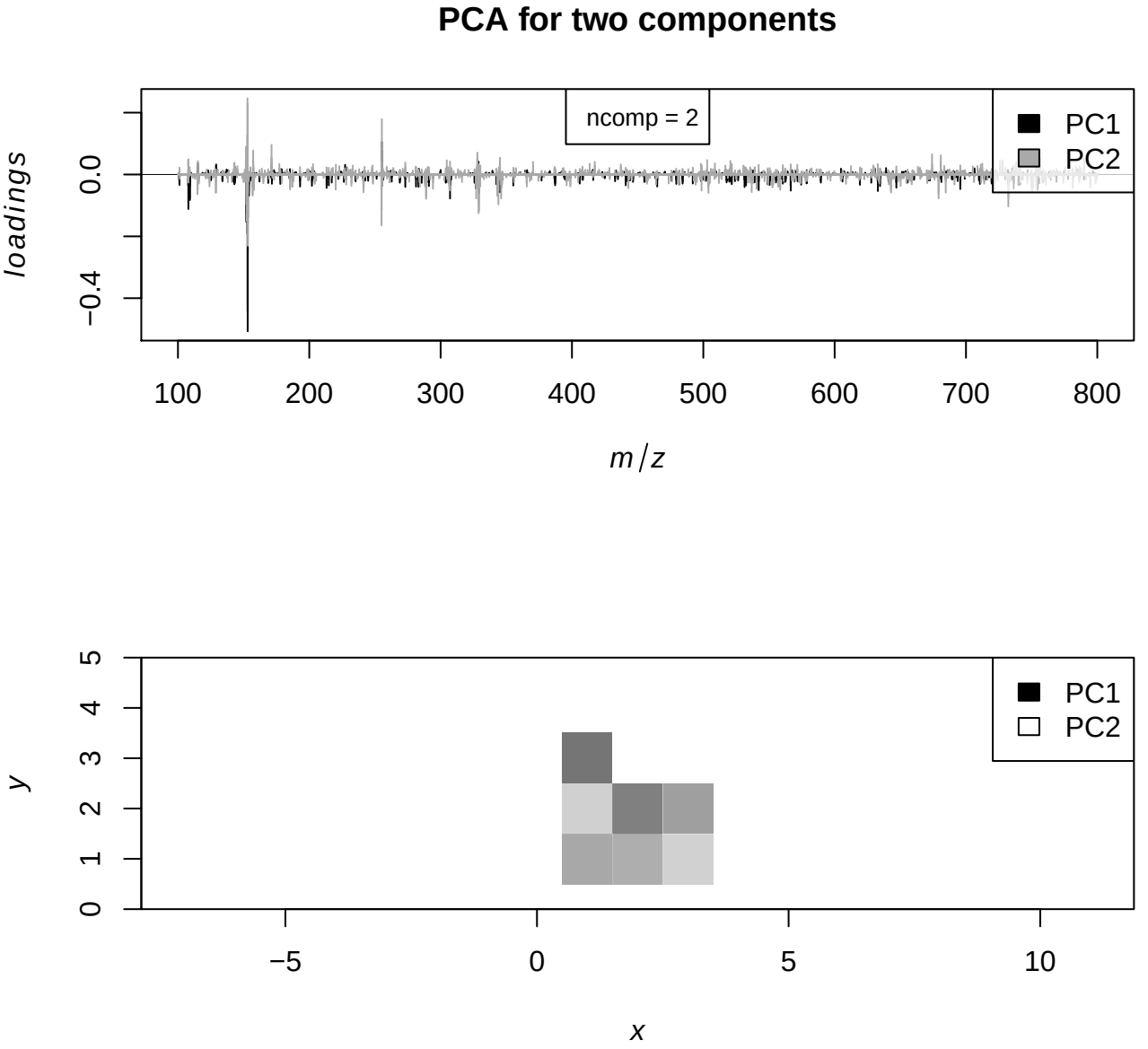

mass2 (328.9 ± 0.25 Da)
m/z = 328.92
1.23
0.01
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5

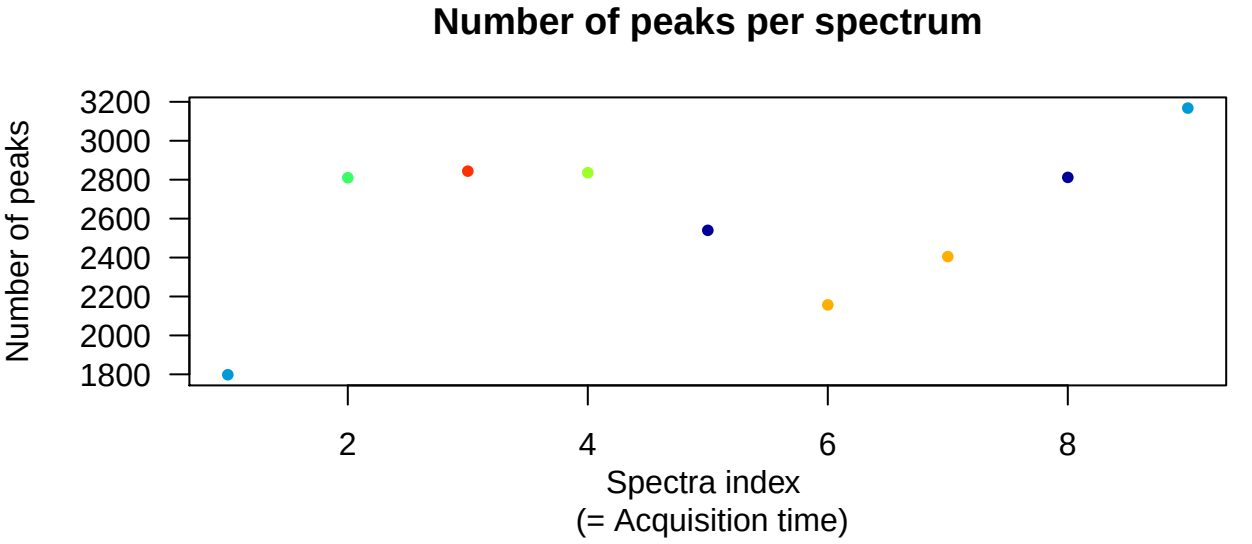

mass3 (185.2 ± 0.25 Da)
m/z = 185.17
0.29
0
y
x
5
4
3
2
1
0
−1
0
1
2
3
4
5

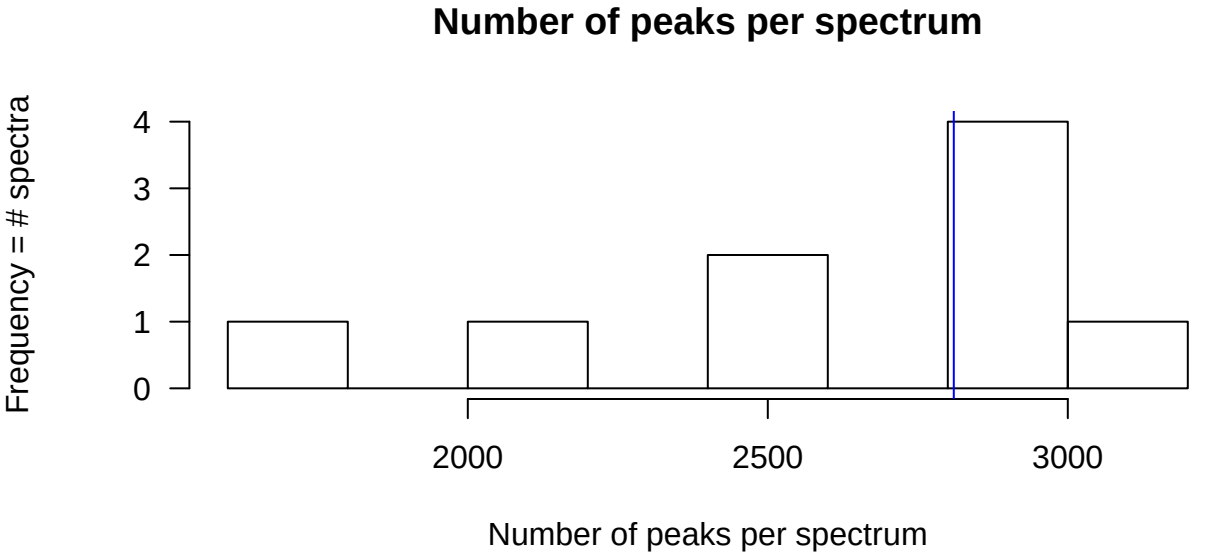

Number of peaks per pixel
3
2
1
y
1
2
3
x
peaks
2800
2400
2000

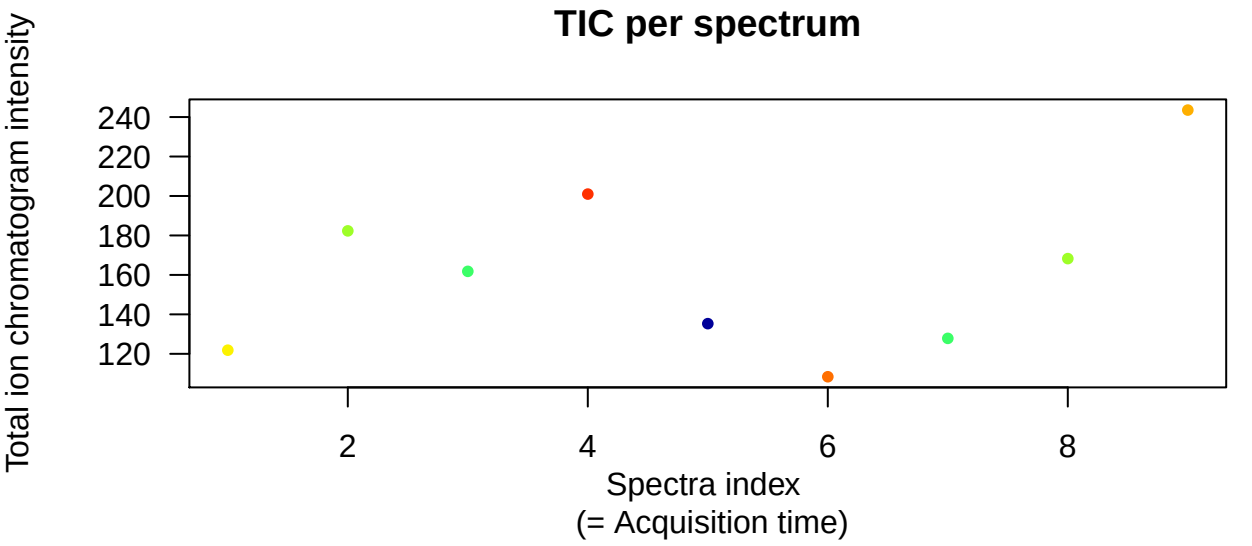

Total Ion Chromatogram
y
3
2
1
x
1
2
3
TIC
200
150

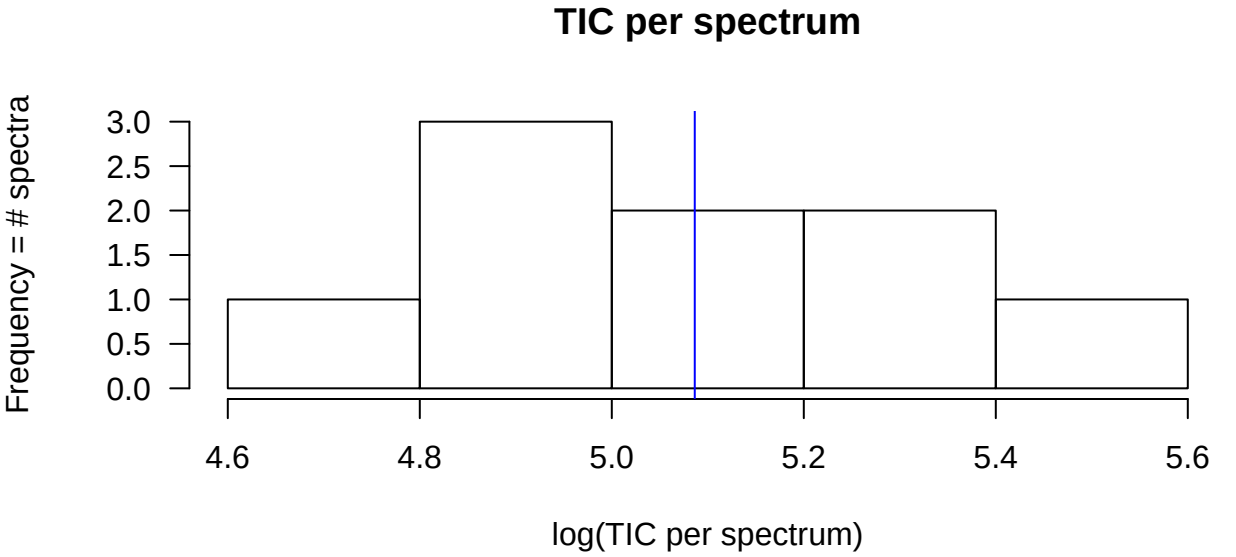

Most abundant m/z in each pixel
3
2
1
y
1
2
3
x
m/z
250

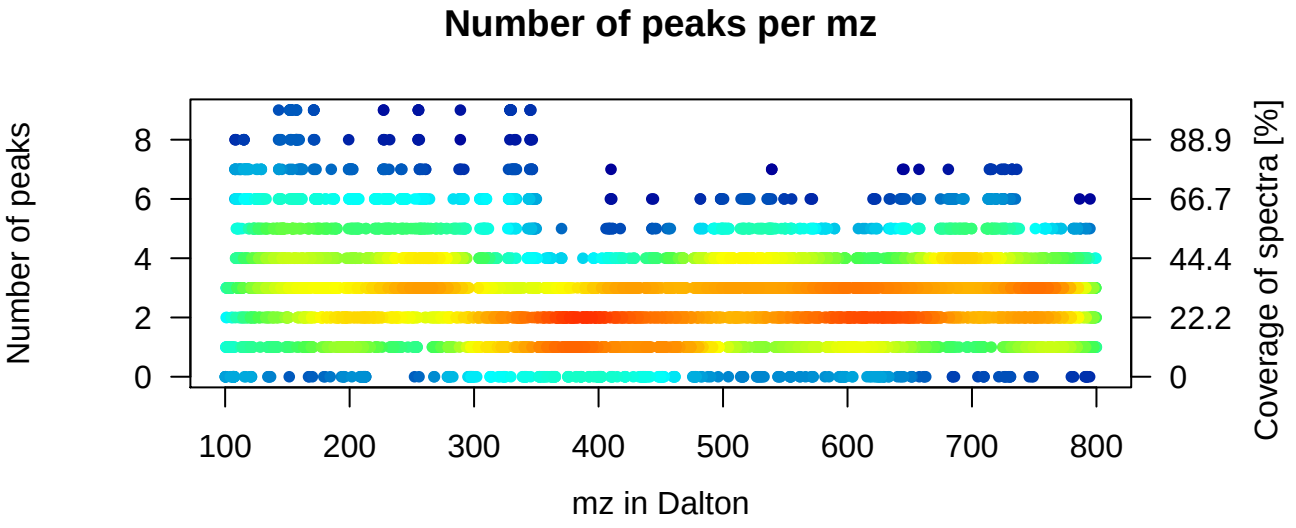

PCA for two components
ncomp = 2
PC1
PC2
loadings
0.0
−0.4
100
200
300
400
500
600
700
800
m/z
PC1
PC2
y
0
1
2
3
4
5
−5
0
5
10
x

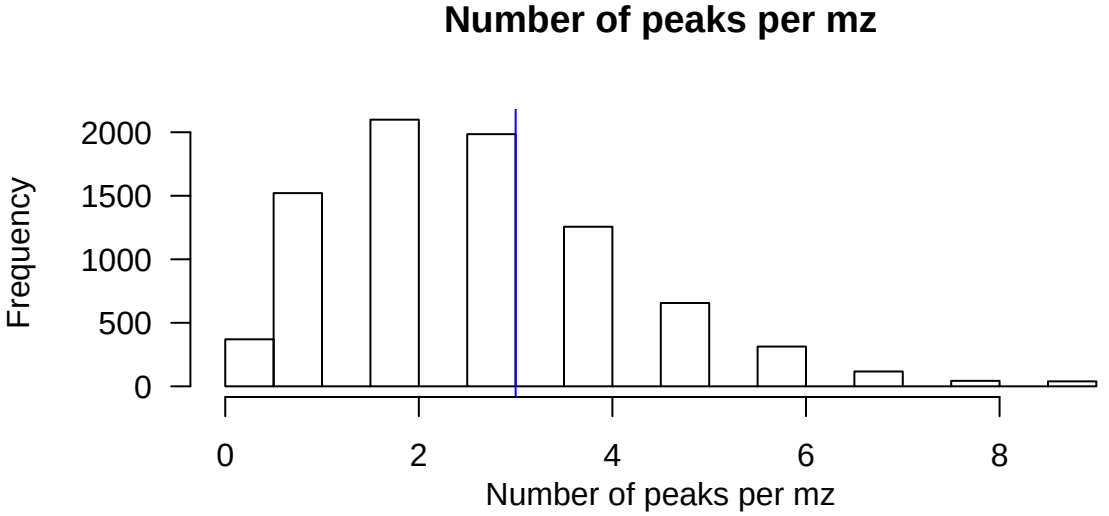

Number of peaks per spectrum
Number of peaks
3200
3000
2800
2600
2400
2200
2000
1800
2
4
6
8
Spectra index
(= Acquisition time)

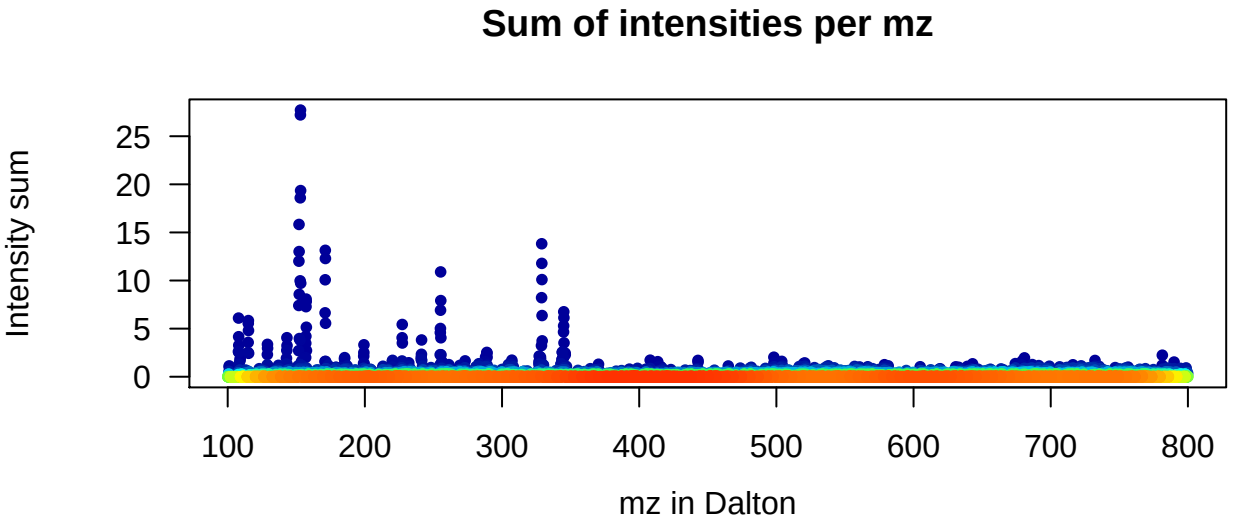

Number of peaks per spectrum
Frequency = # spectra
4
3
2
1
0
2000
2500
3000
Number of peaks per spectrum

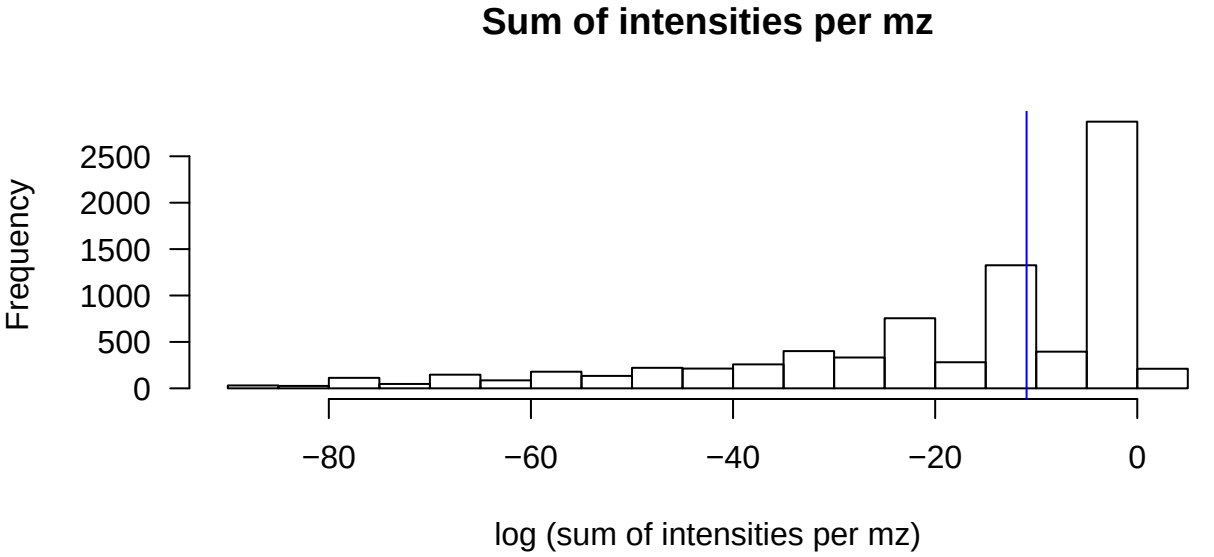

TIC per spectrum
Total ion chromatogram intensity
240
220
200
180
160
140
120
2
4
6
8
Spectra index
(= Acquisition time)

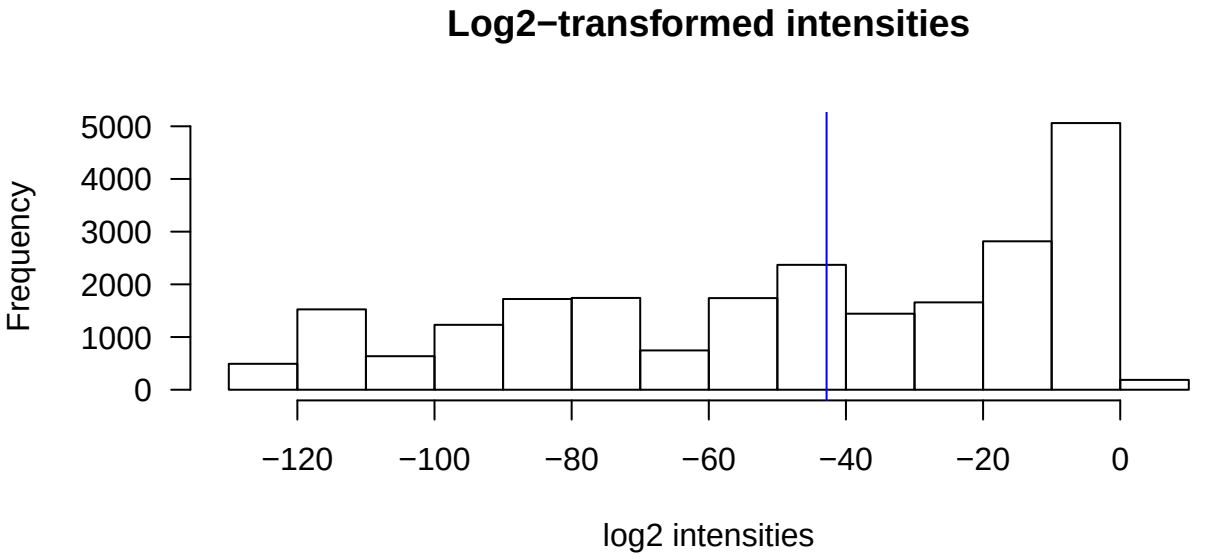

TIC per spectrum
Frequency = # spectra
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.6
4.8
5.0
5.2
5.4
5.6
log(TIC per spectrum)

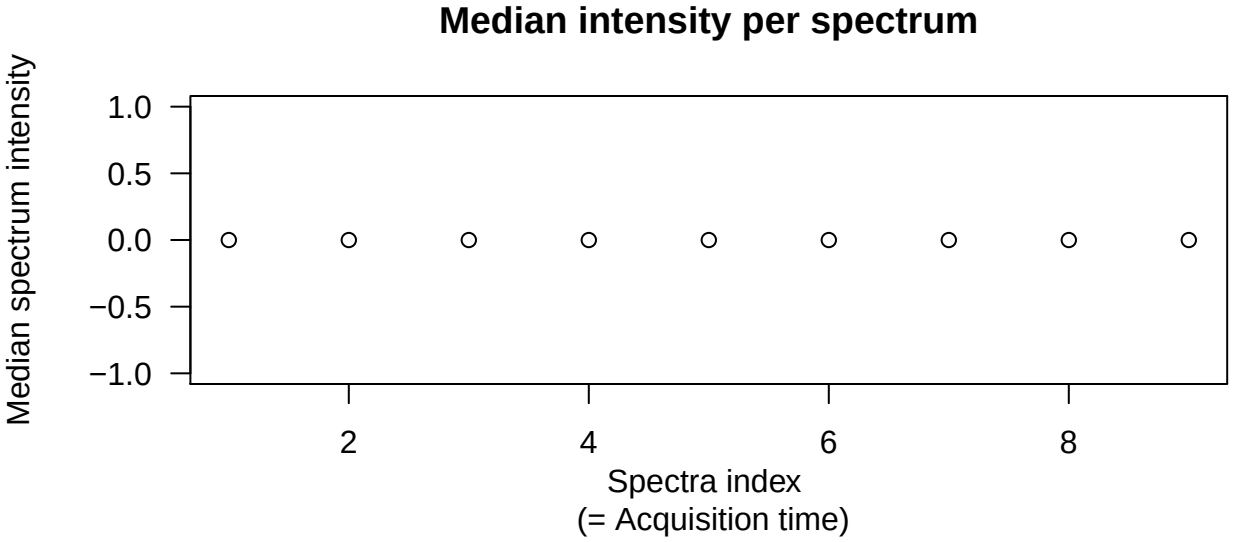

Number of peaks per mz
Number of peaks
0
2
4
6
8
Coverage of spectra [%]
0
22.2
44.4
66.7
88.9
100
200
300
400
500
600
700
800
mz in Dalton

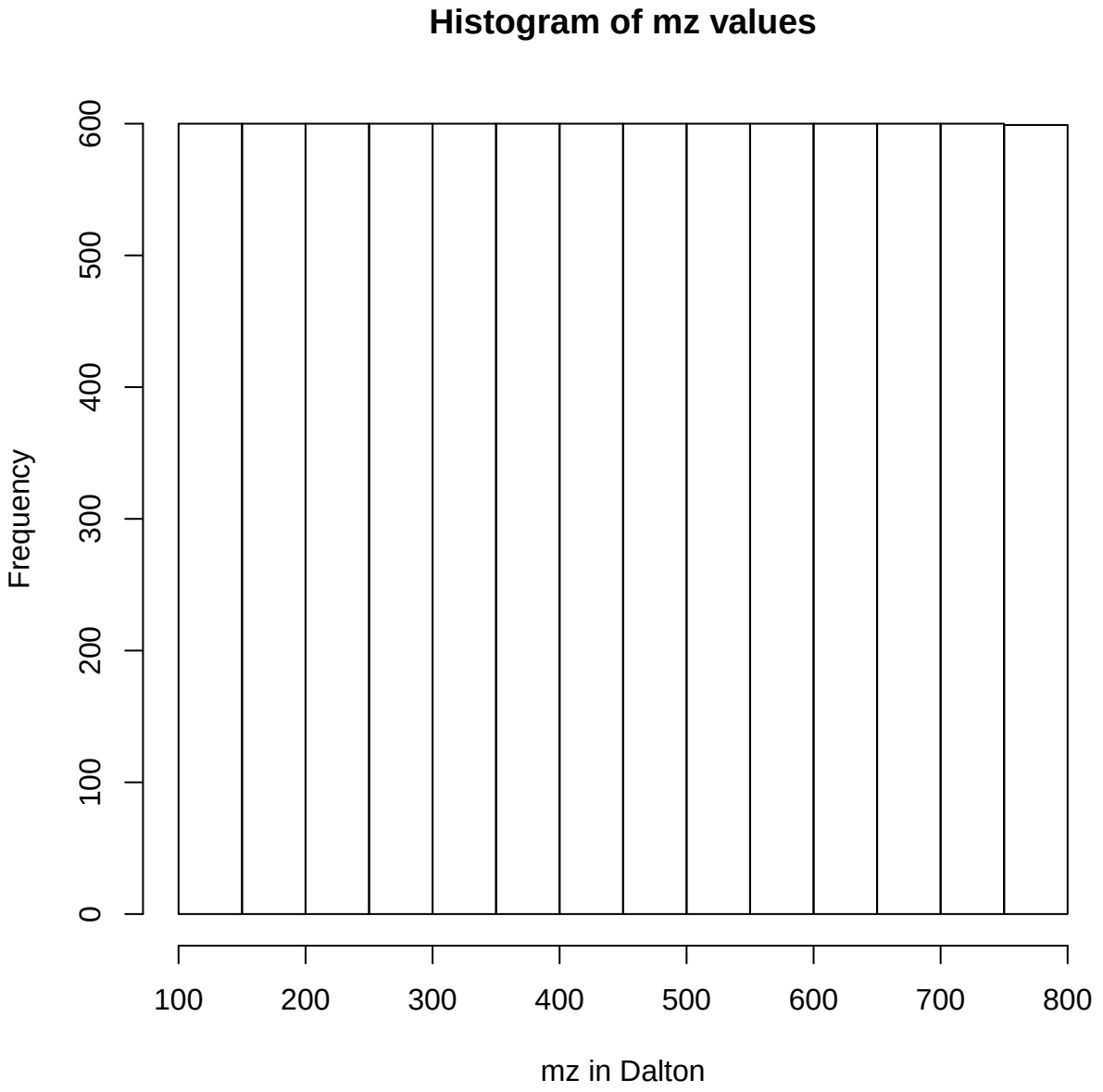

Number of peaks per mz
Frequency
0
500
1000
1500
2000
0
2
4
6
8
Number of peaks per mz

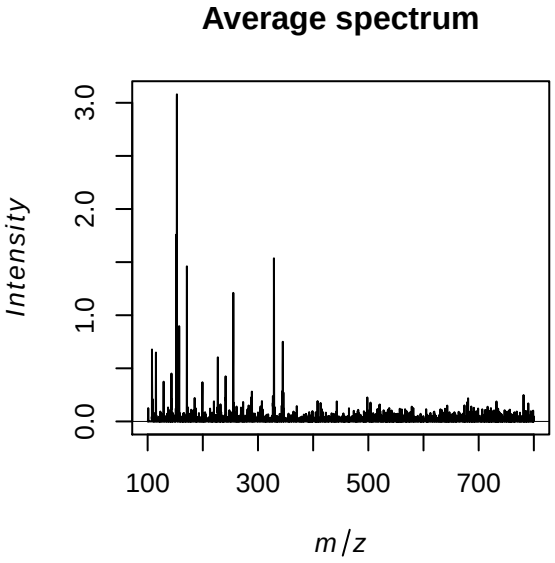

Sum of intensities per mz
Intensity sum
0
5
10
15
20
25
100
200
300
400
500
600
700
800
mz in Dalton

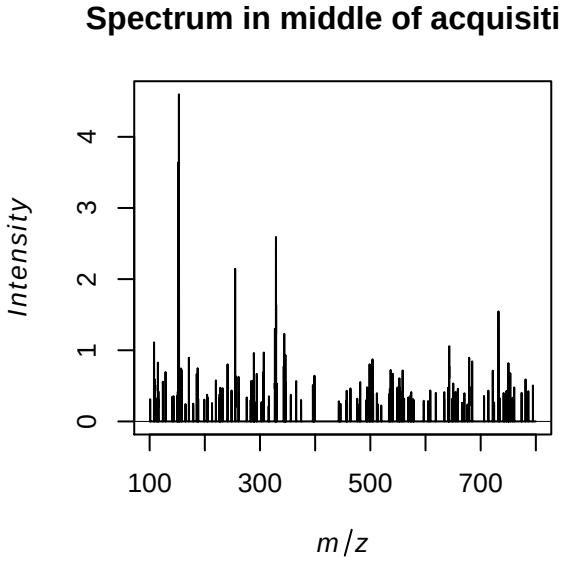

Sum of intensities per mz
Frequency
0
500
1000
1500
2000
2500
−80
−60
−40
−20
0
log (sum of intensities per mz)

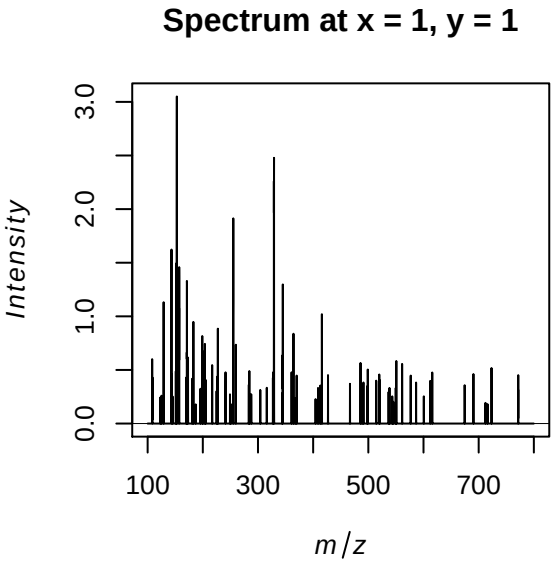

Log2−transformed intensities
Frequency
5000
4000
3000
2000
1000
0
−120
−100
−80
−60
−40
−20
0
log2 intensities

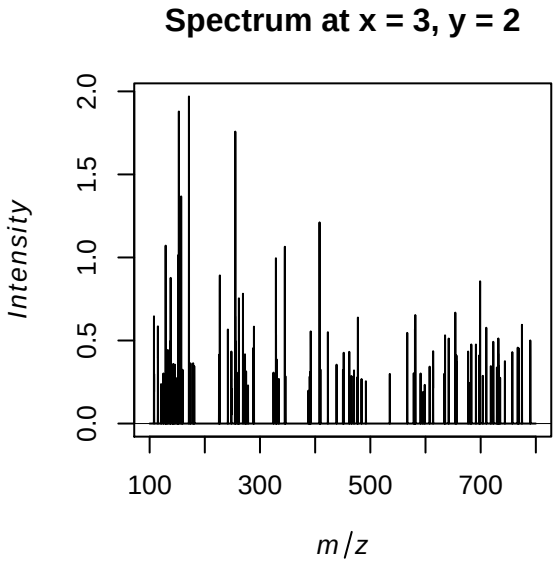

Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
Spectra index
(= Acquisition time)

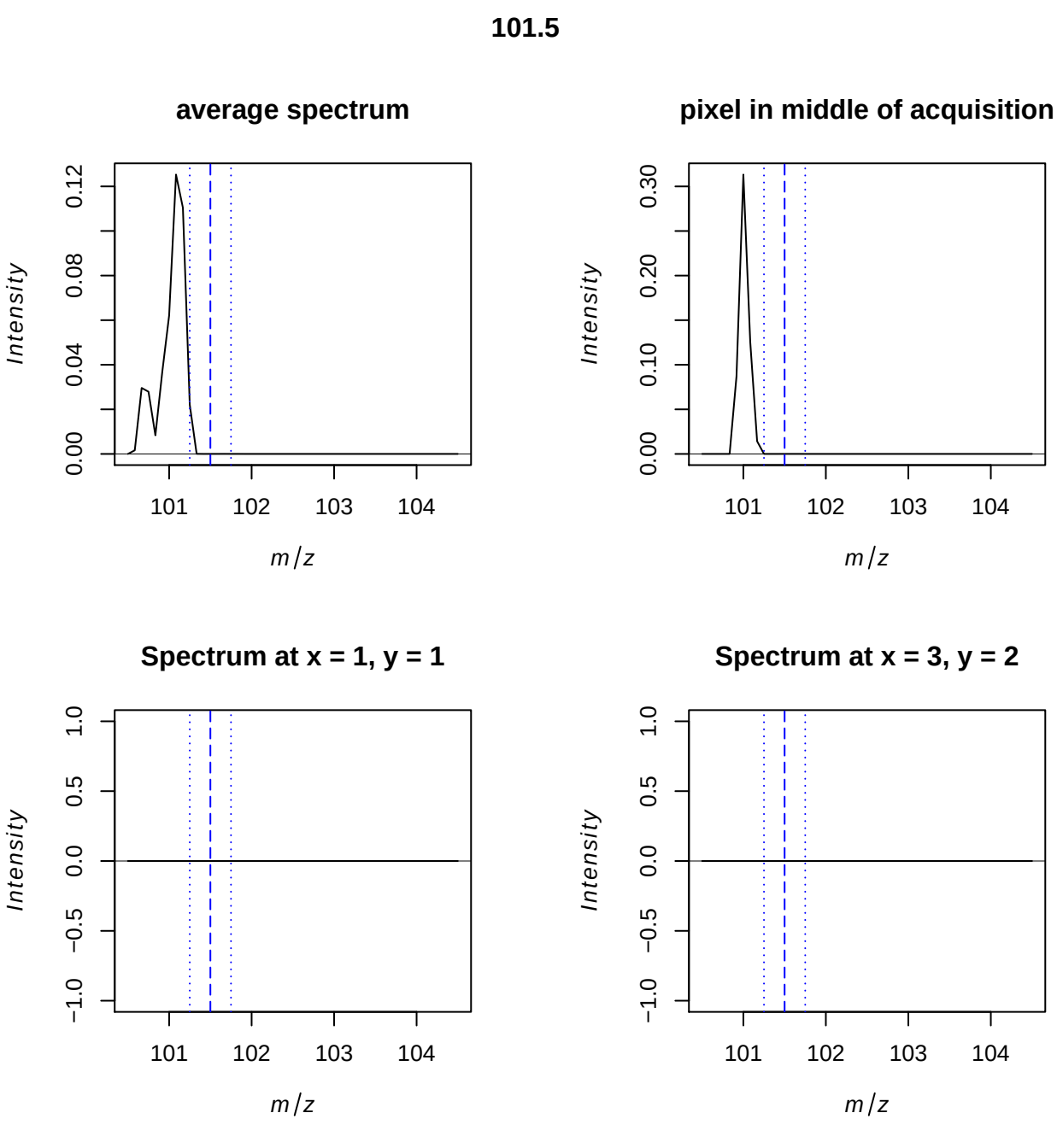

Histogram of mz values
Frequency
0
100
200
300
400
500
600
100
200
300
400
500
600
700
800
mz in Dalton

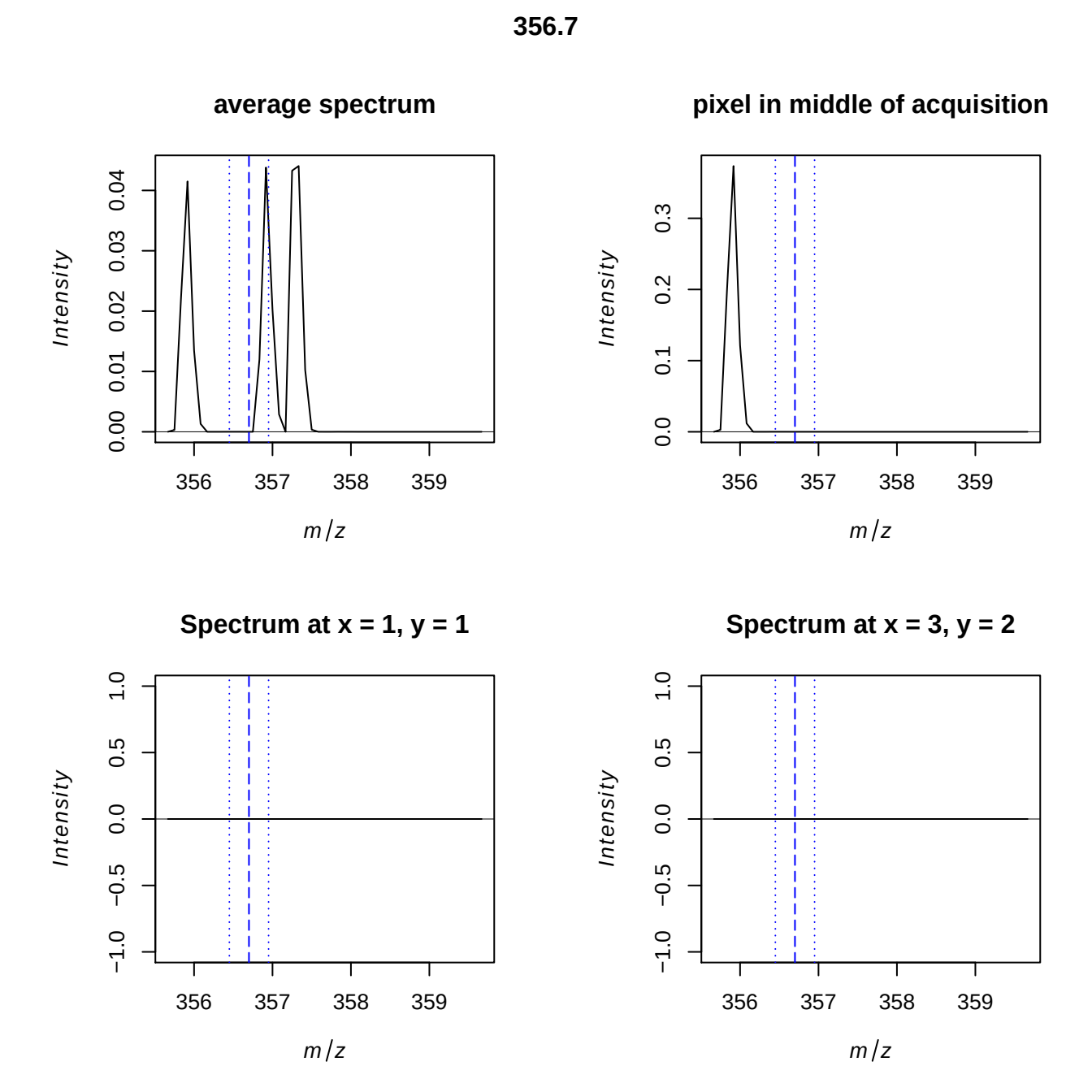

Average spectrum
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z


Spectrum in middle of acquisition
Intensity
0
1
2
3
4
100
300
500
700
m/z

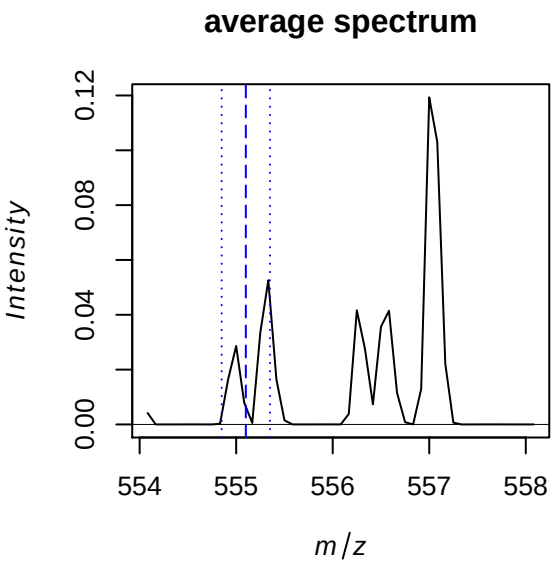

Spectrum at x = 1, y = 1
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z

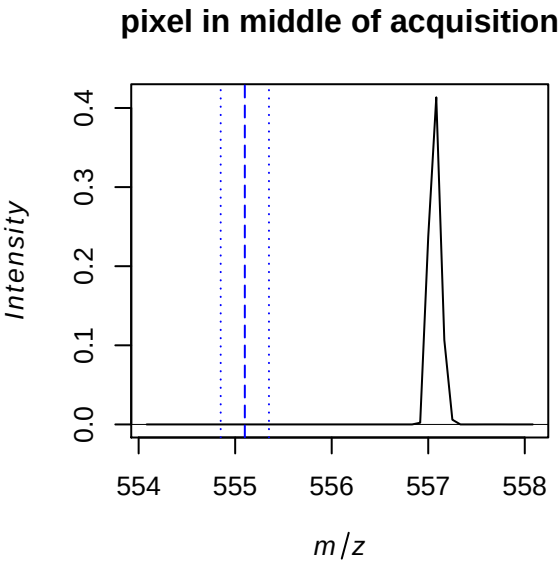

Spectrum at x = 3, y = 2
Intensity
0.0
0.5
1.0
1.5
2.0
100
300
500
700
m/z

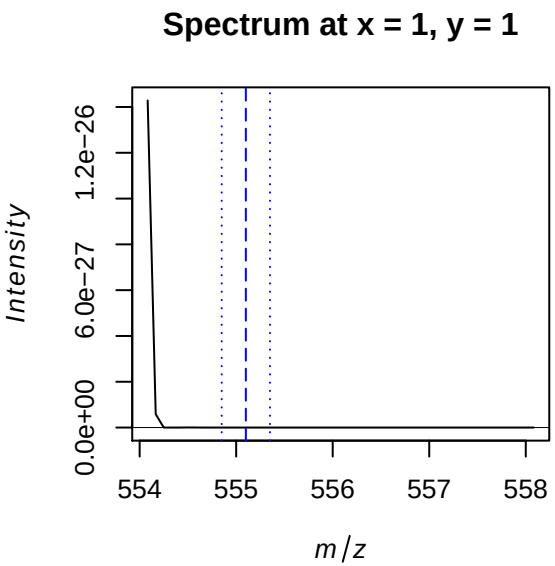

101.5
average spectrum
pixel in middle of acquisition
Spectrum at x = 1, y = 1
Spectrum at x = 3, y = 2
Intensity
m/z
0.00
0.04
0.08
0.12
0.10
0.20
0.30
−1.0
−0.5
0.0
0.5
1.0
101
102
103
104

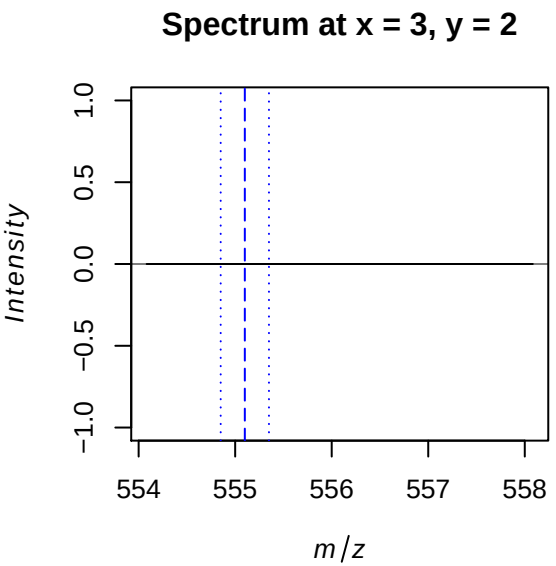

356.7
average spectrum
pixel in middle of acquisition
Spectrum at x = 1, y = 1
Spectrum at x = 3, y = 2
Intensity
m/z
0.00
0.01
0.02
0.03
0.04
0.0
0.1
0.2
0.3
−1.0
−0.5
0.0
0.5
1.0
356
357
358
359

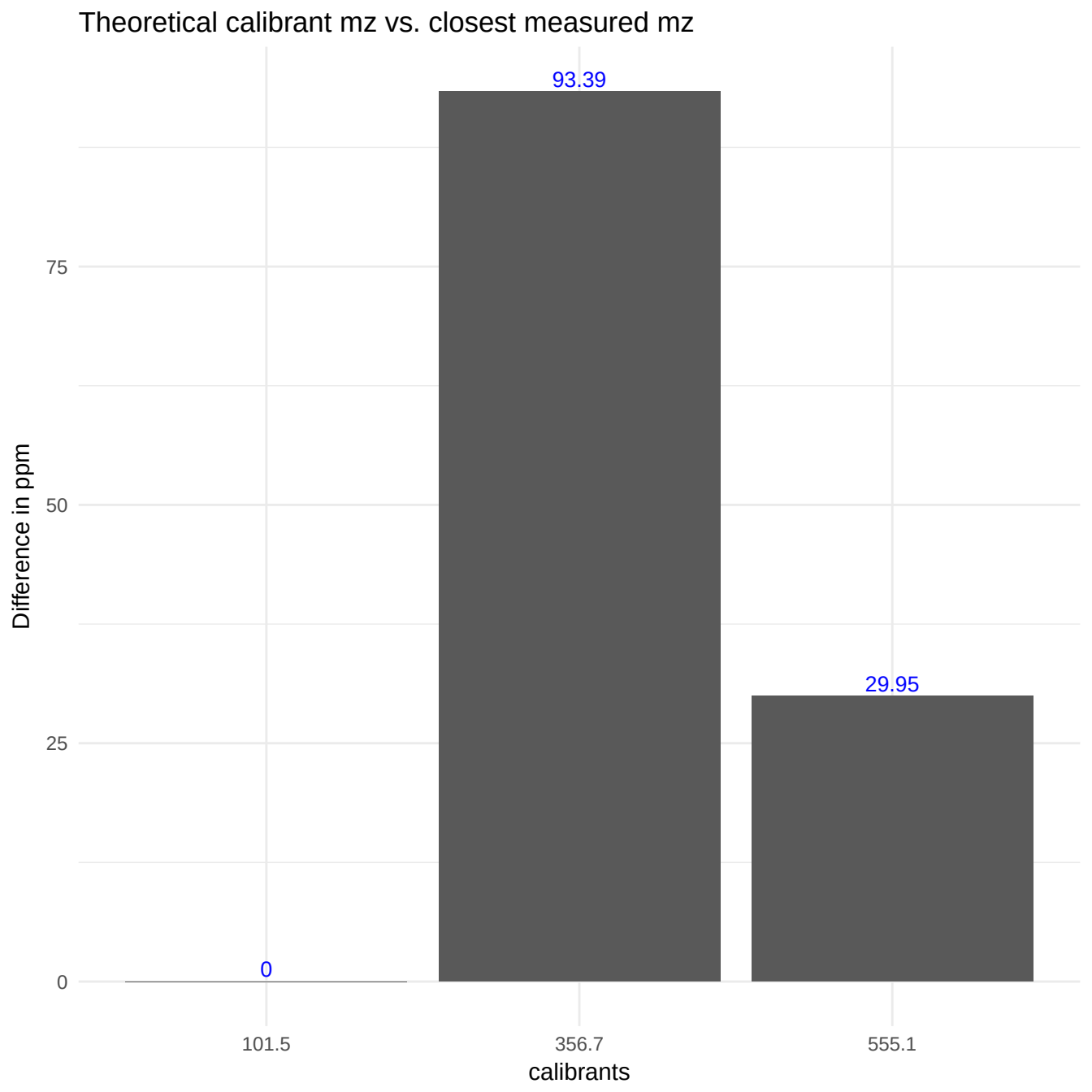
555.1


average spectrum
Intensity
0.00
0.04
0.08
0.12
554
555
556
557
558
m/z


pixel in middle of acquisition
Intensity
0.0
0.1
0.2
0.3
0.4
554
555
556
557
558
m/z


Spectrum at x = 1, y = 1
Intensity
0.0e+00
6.0e−27
1.2e−26
554
555
556
557
558
m/z


Spectrum at x = 3, y = 2
Intensity
−1.0
−0.5
0.0
0.5
1.0
554
555
556
557
558
m/z


Theoretical calibrant mz vs. closest measured mz
93.39
29.95
0
75
50
25
0
Difference in ppm
101.5
356.7
555.1
calibrants