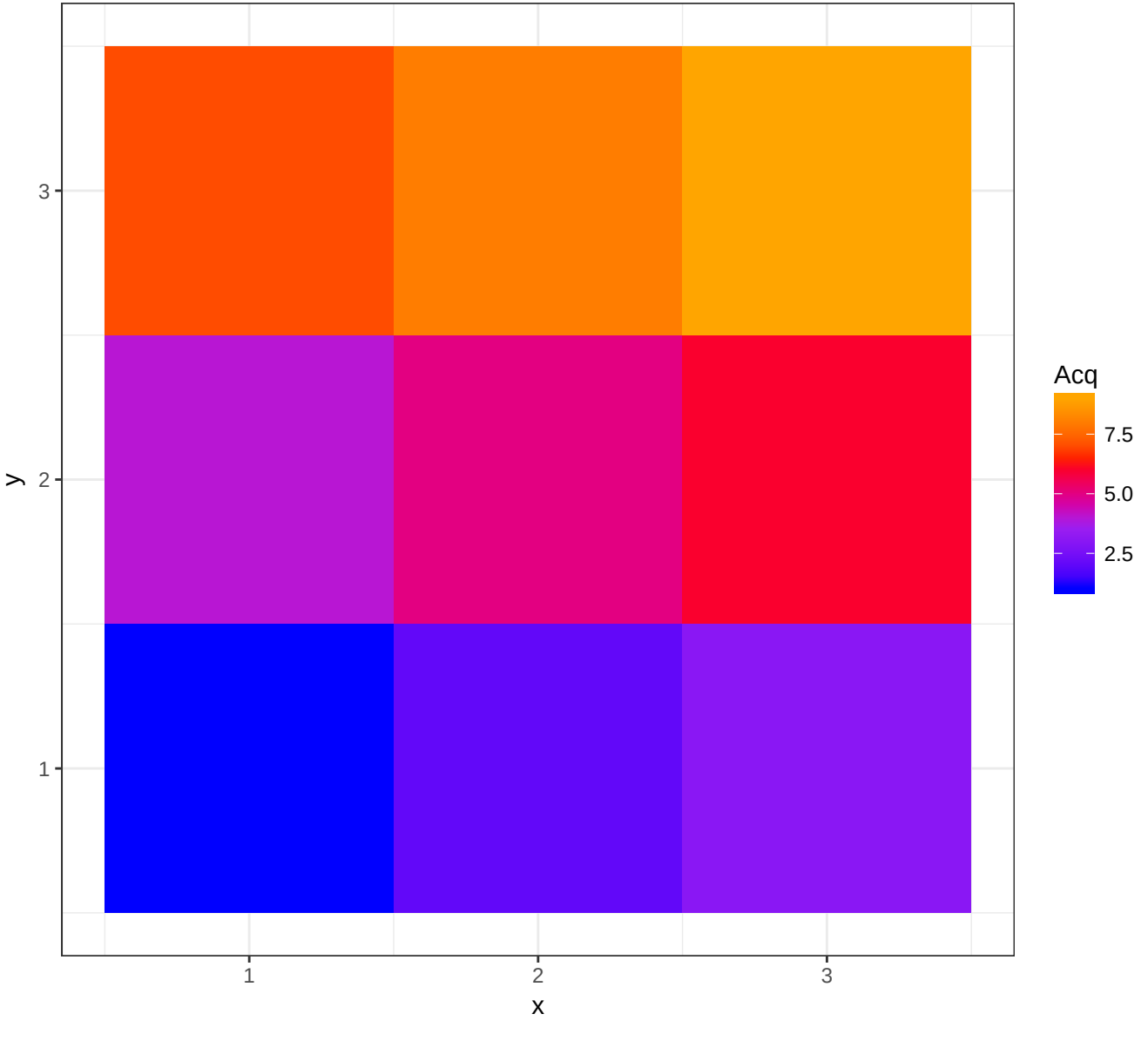
Quality control of MSI data

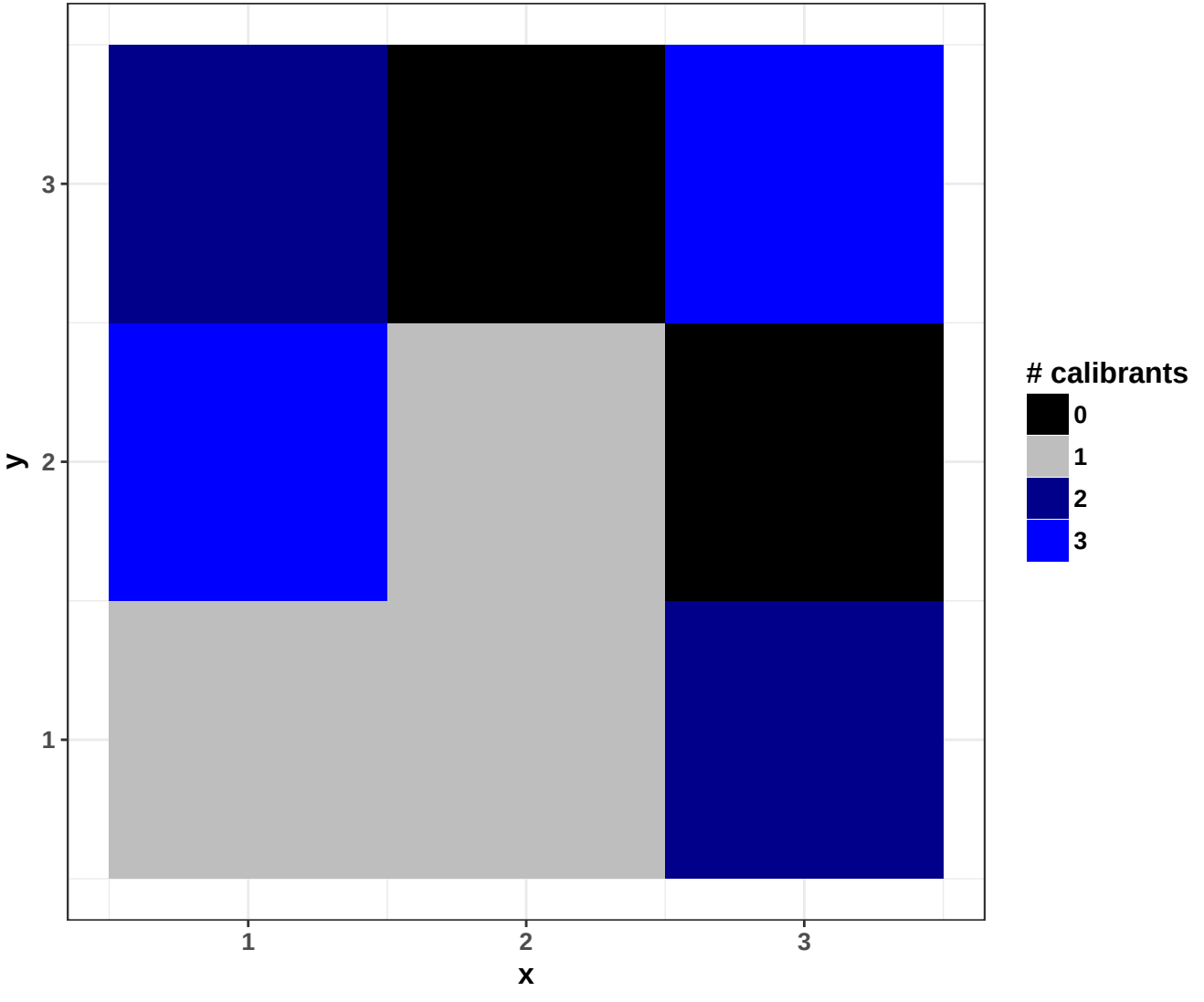
Filename: Testfile_imzml

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

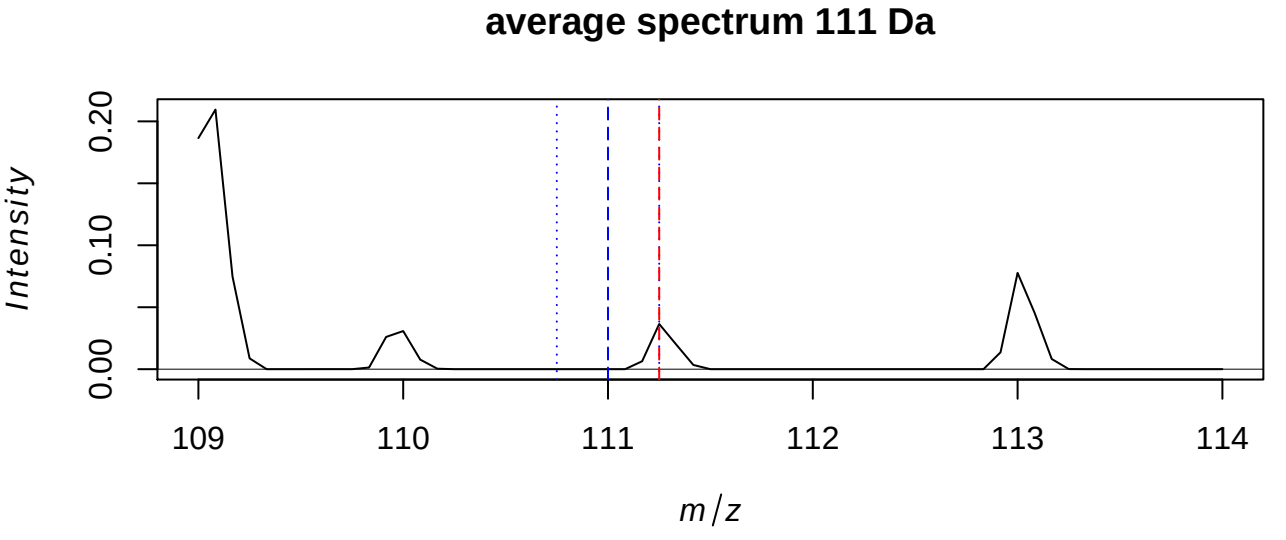
1) Order of Acquisition

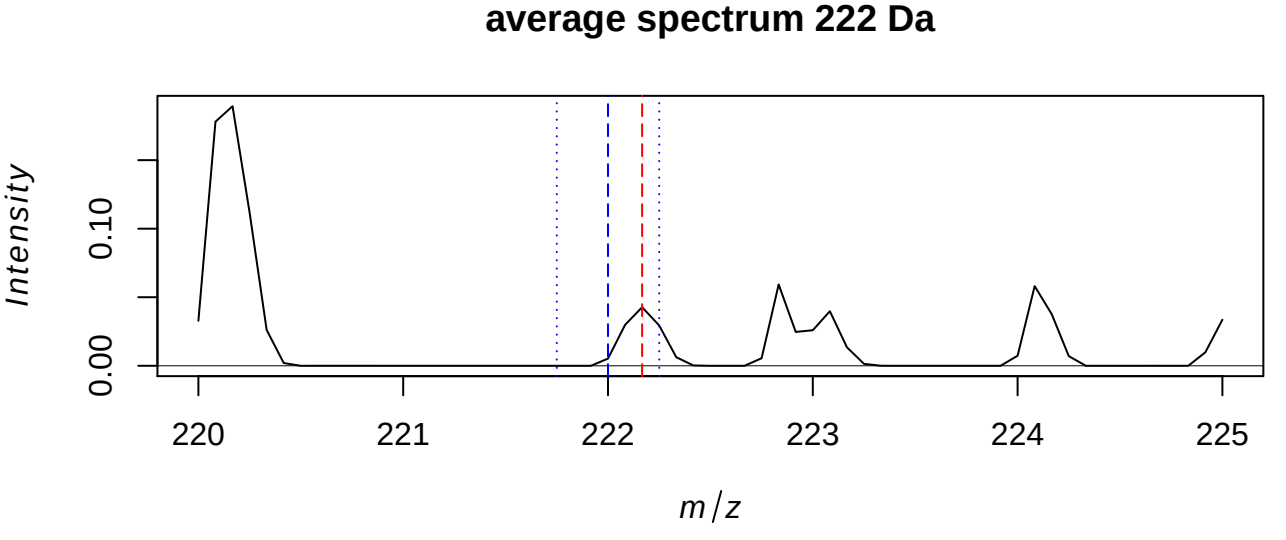


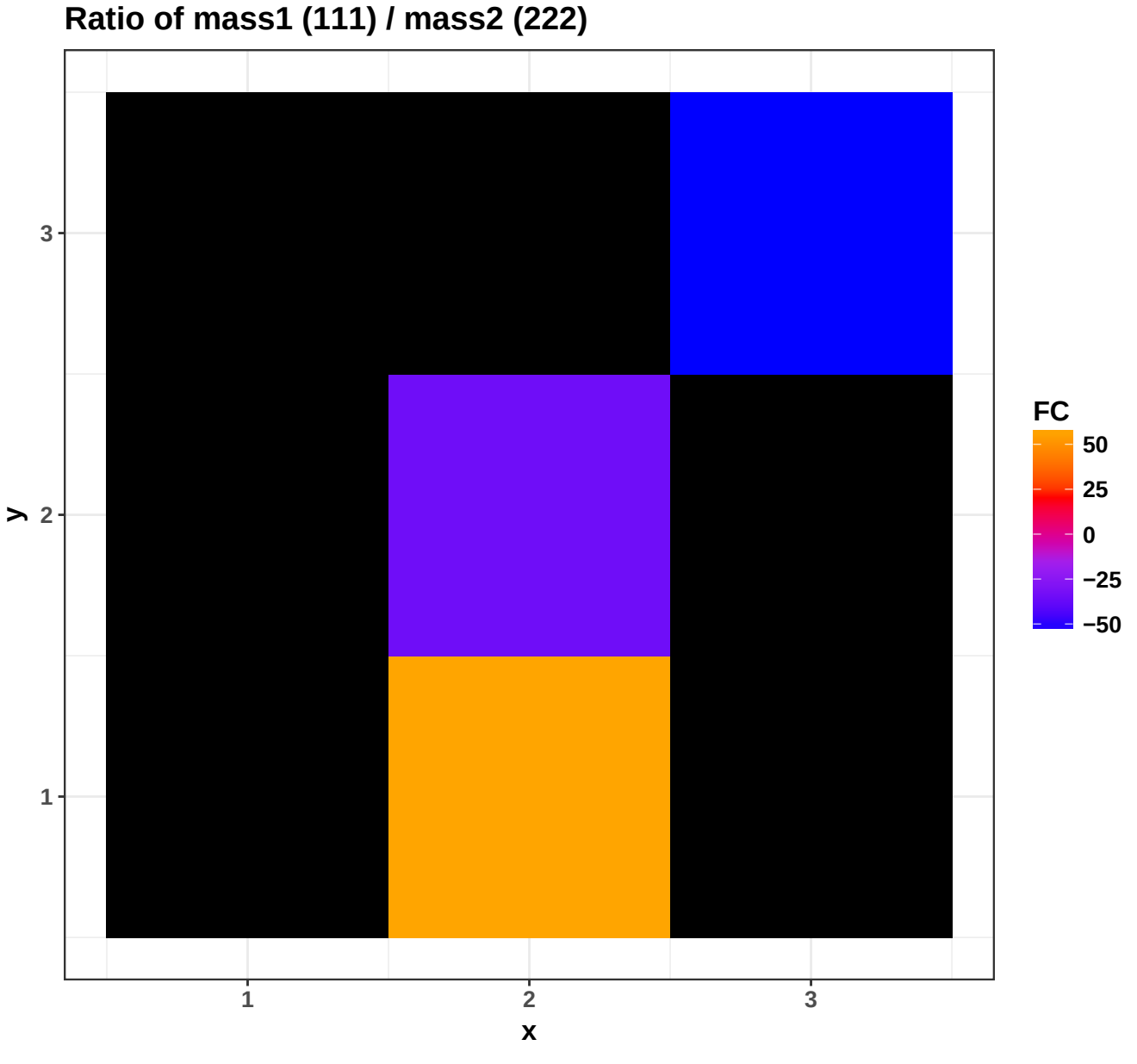
2) Number of calibrants per pixel

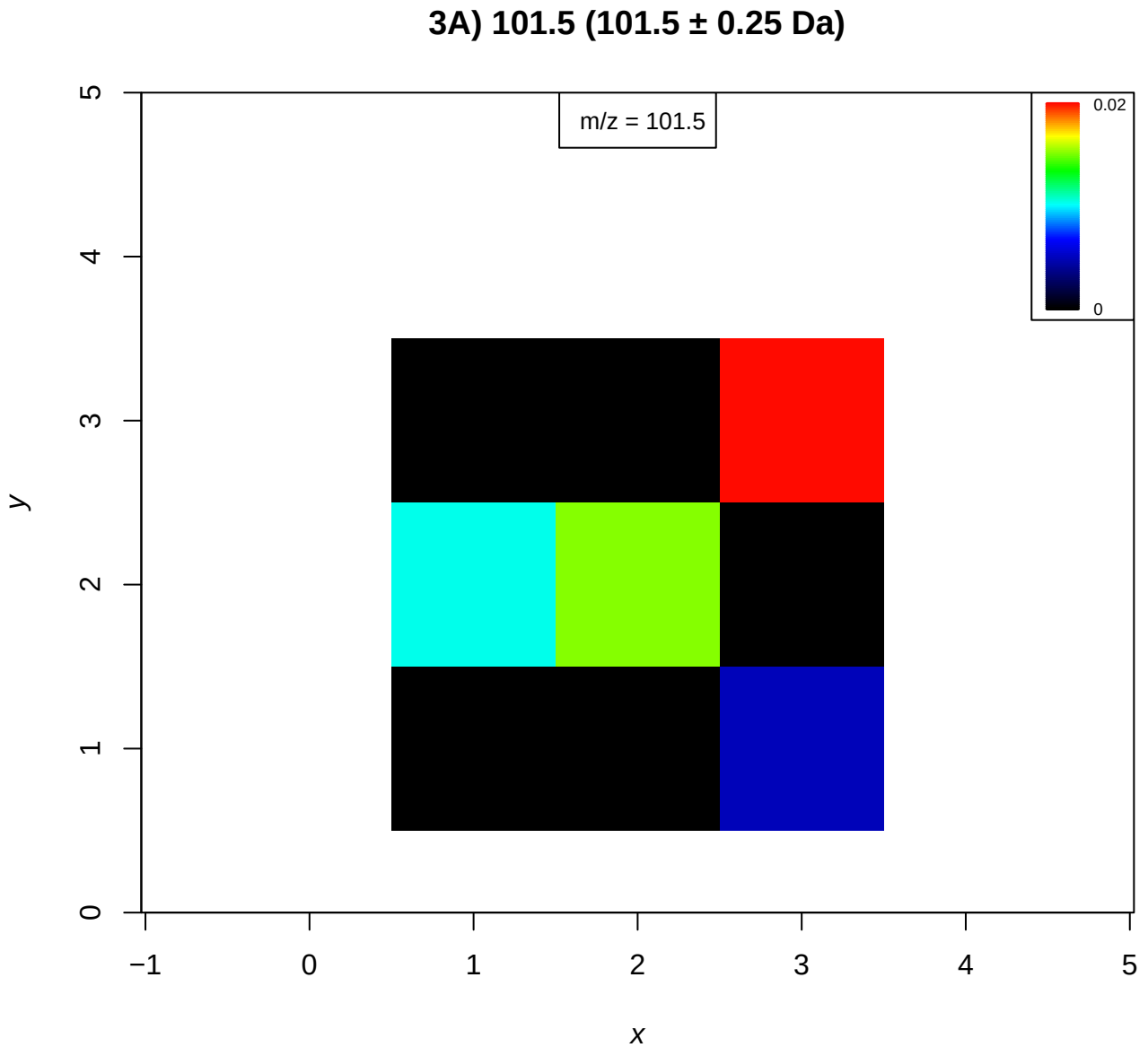


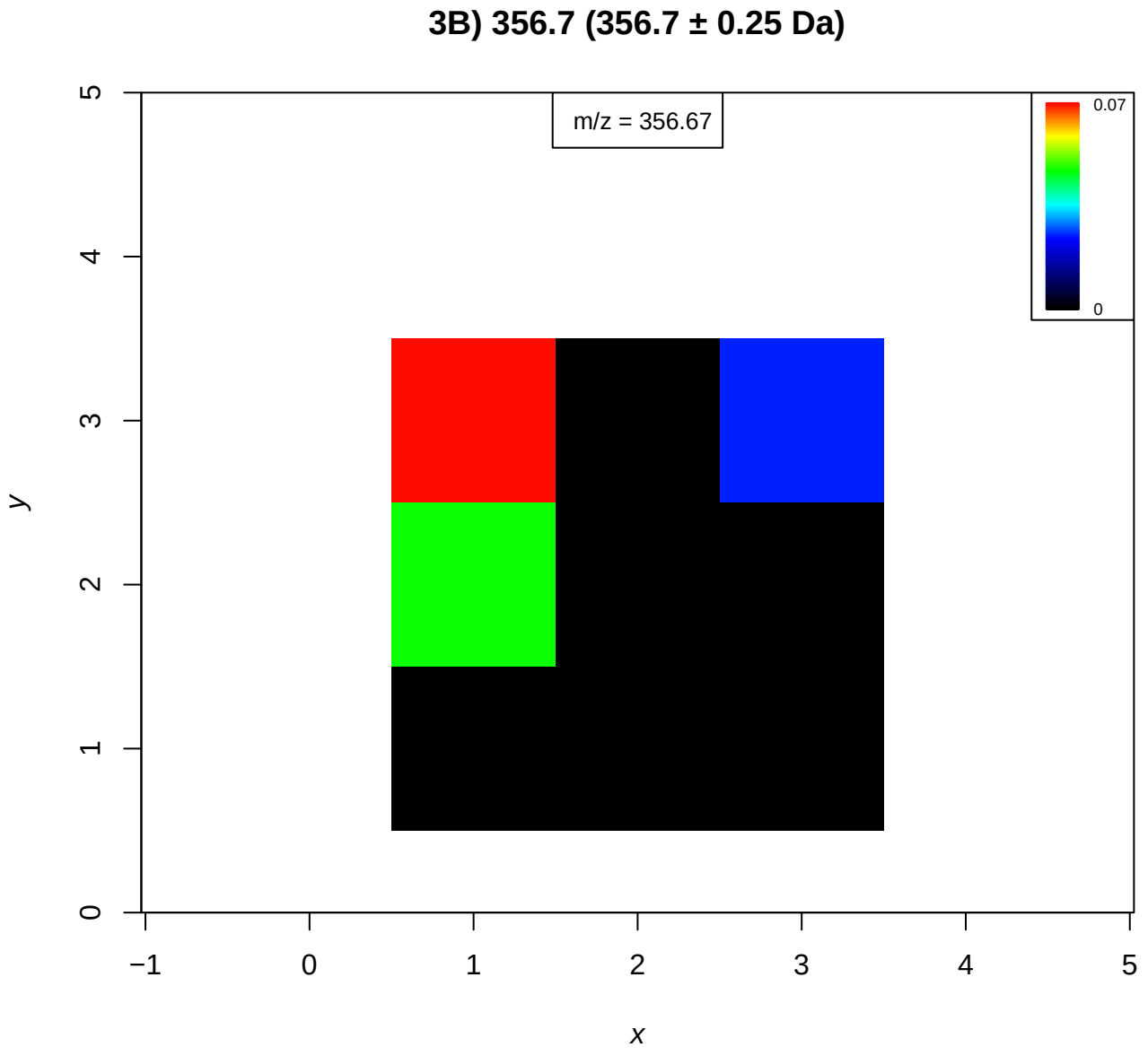
Control of fold change plot

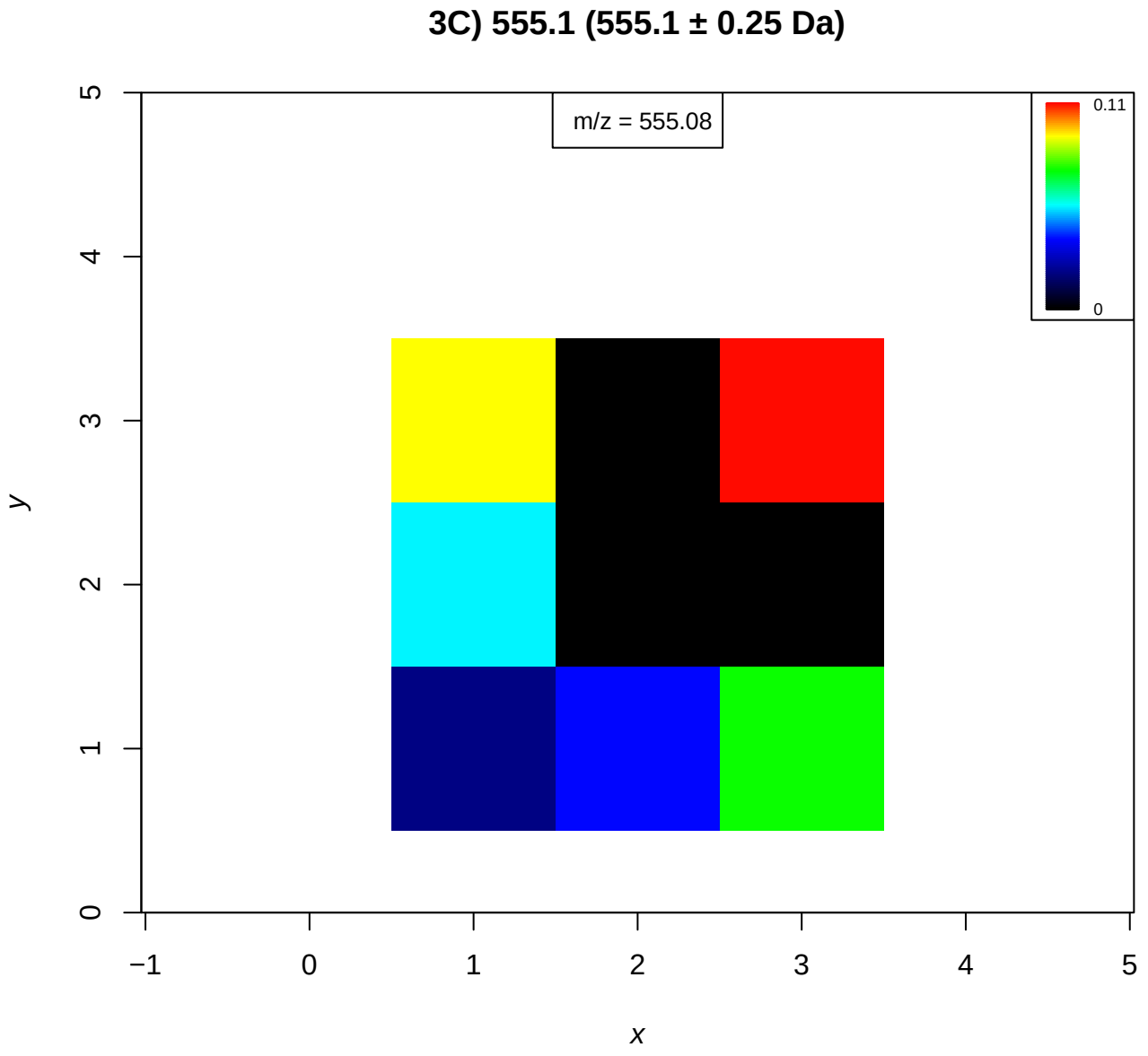


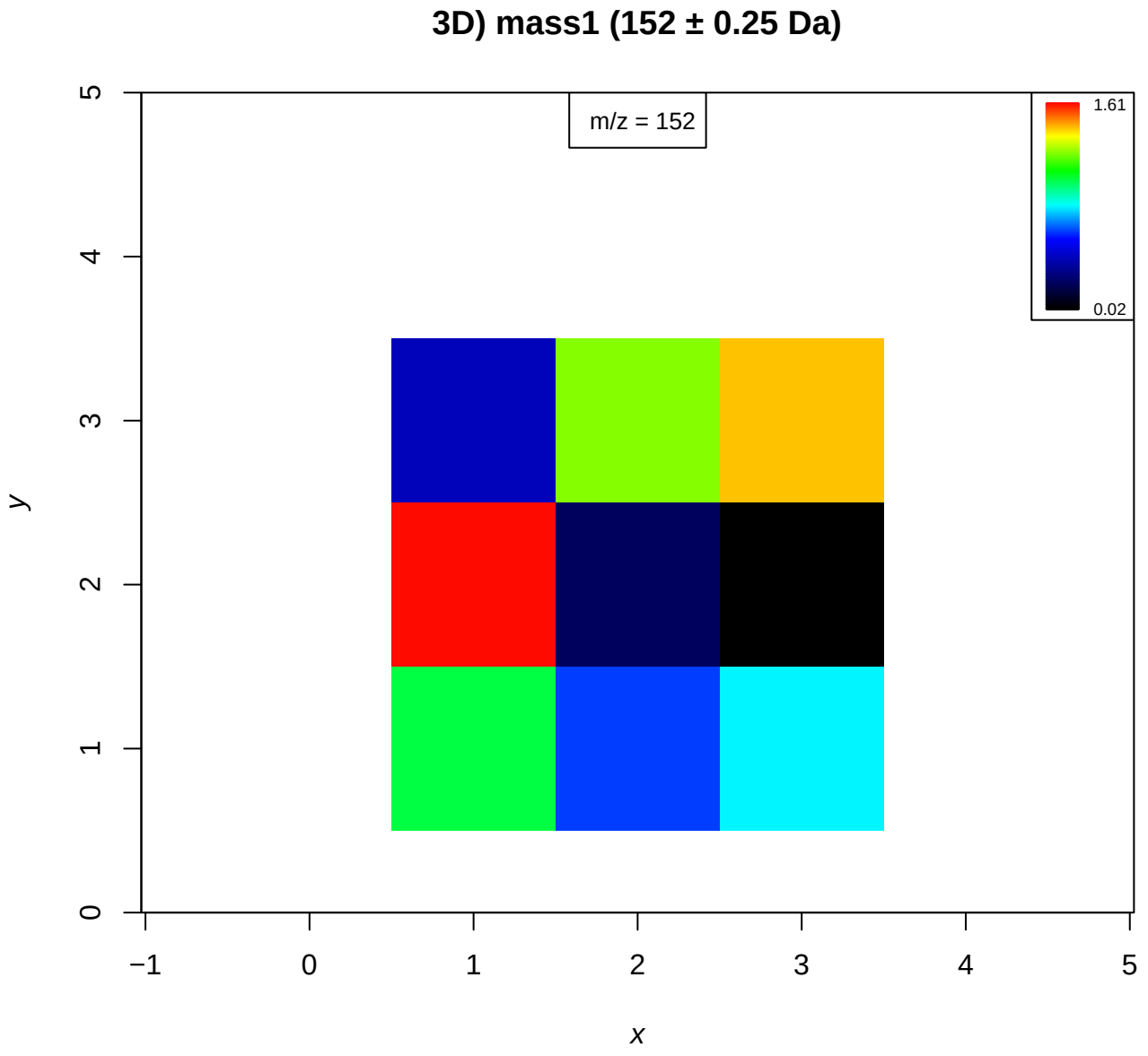


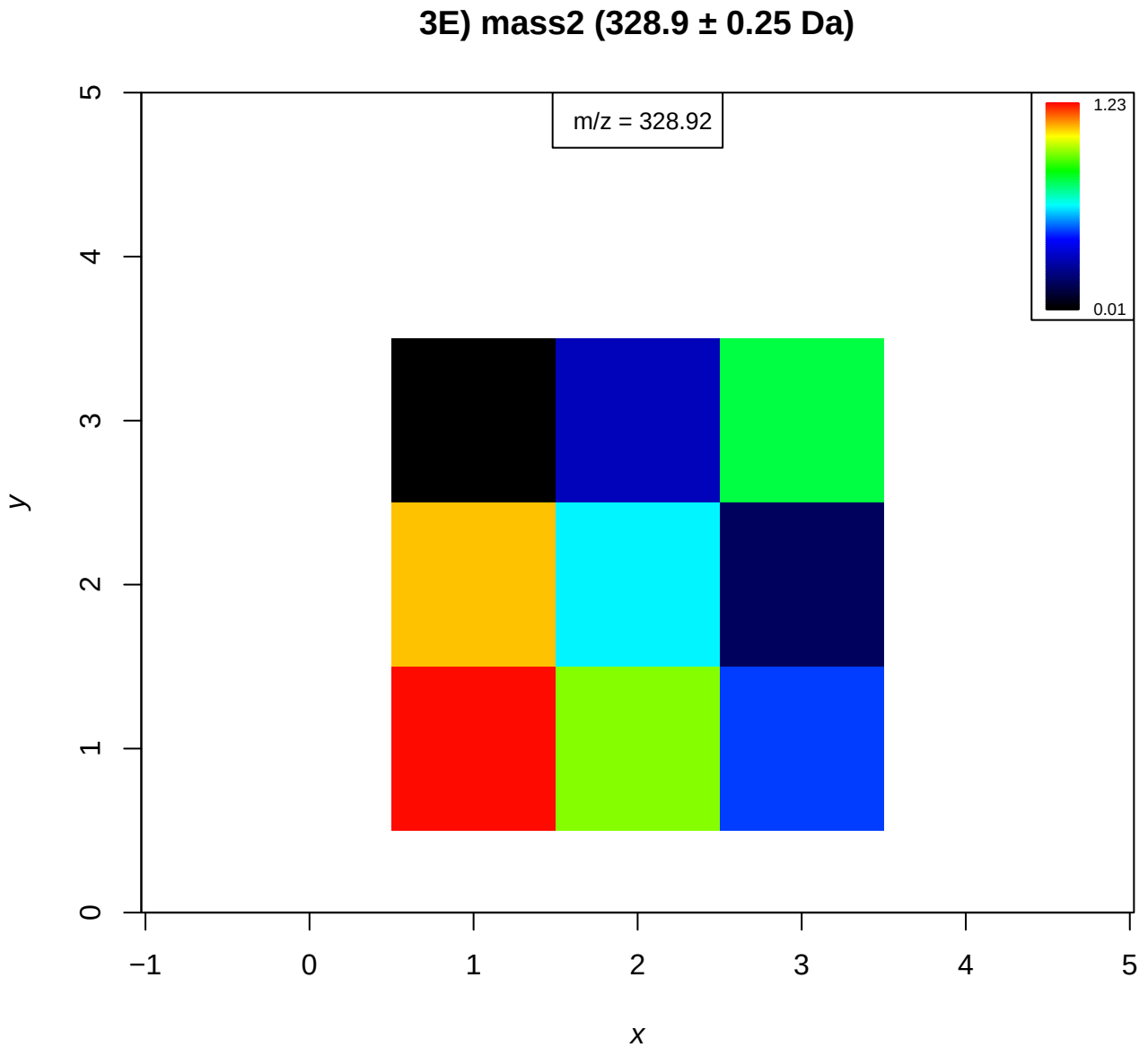

Ratio of mass1 (111) / mass2 (222)
y
3
2
1
x
1
2
3
FC
50
25
0
−25
−50

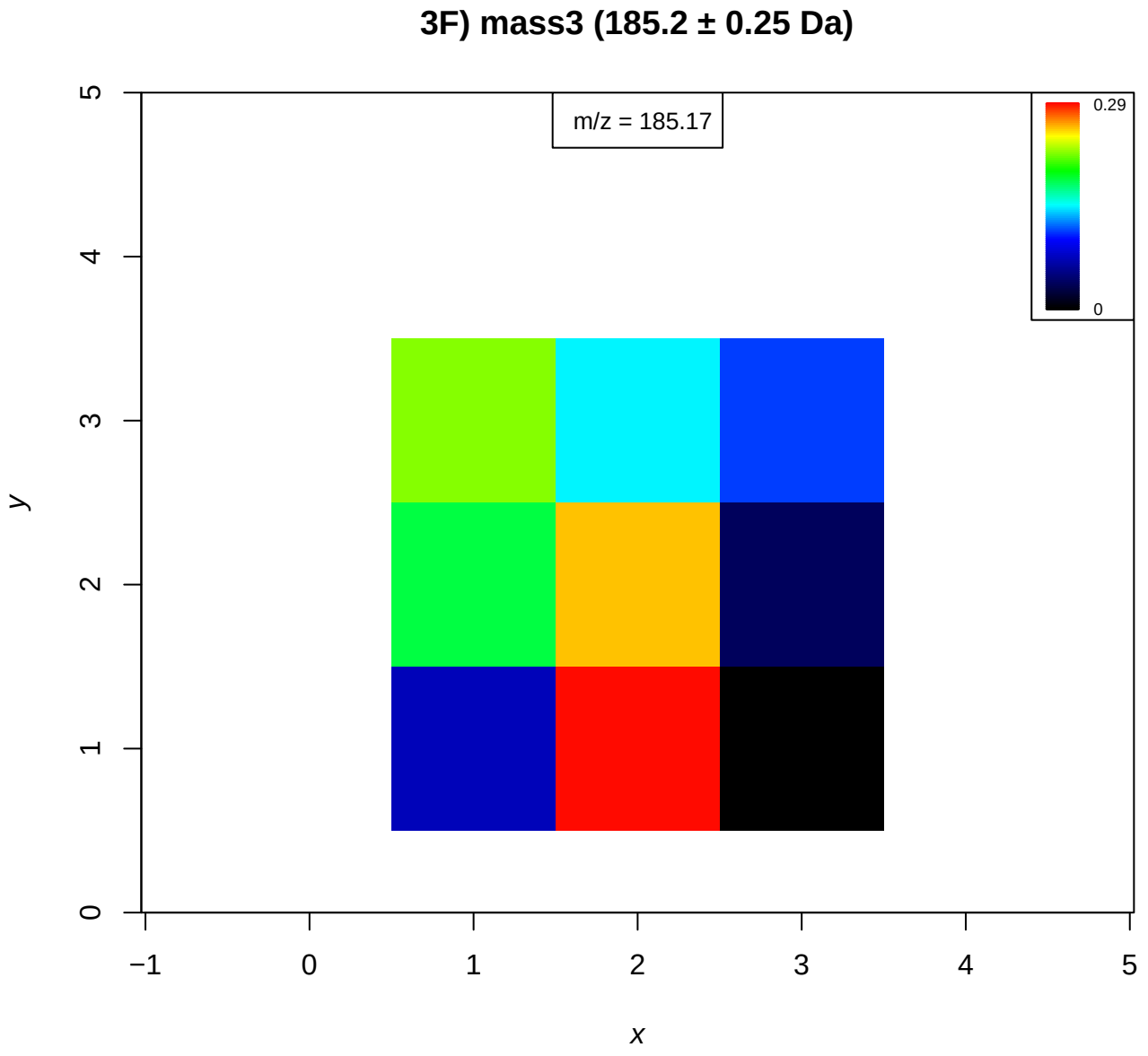

3A) 101.5 (101.5 ± 0.25 Da)
m/z = 101.5
0.02
0
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5

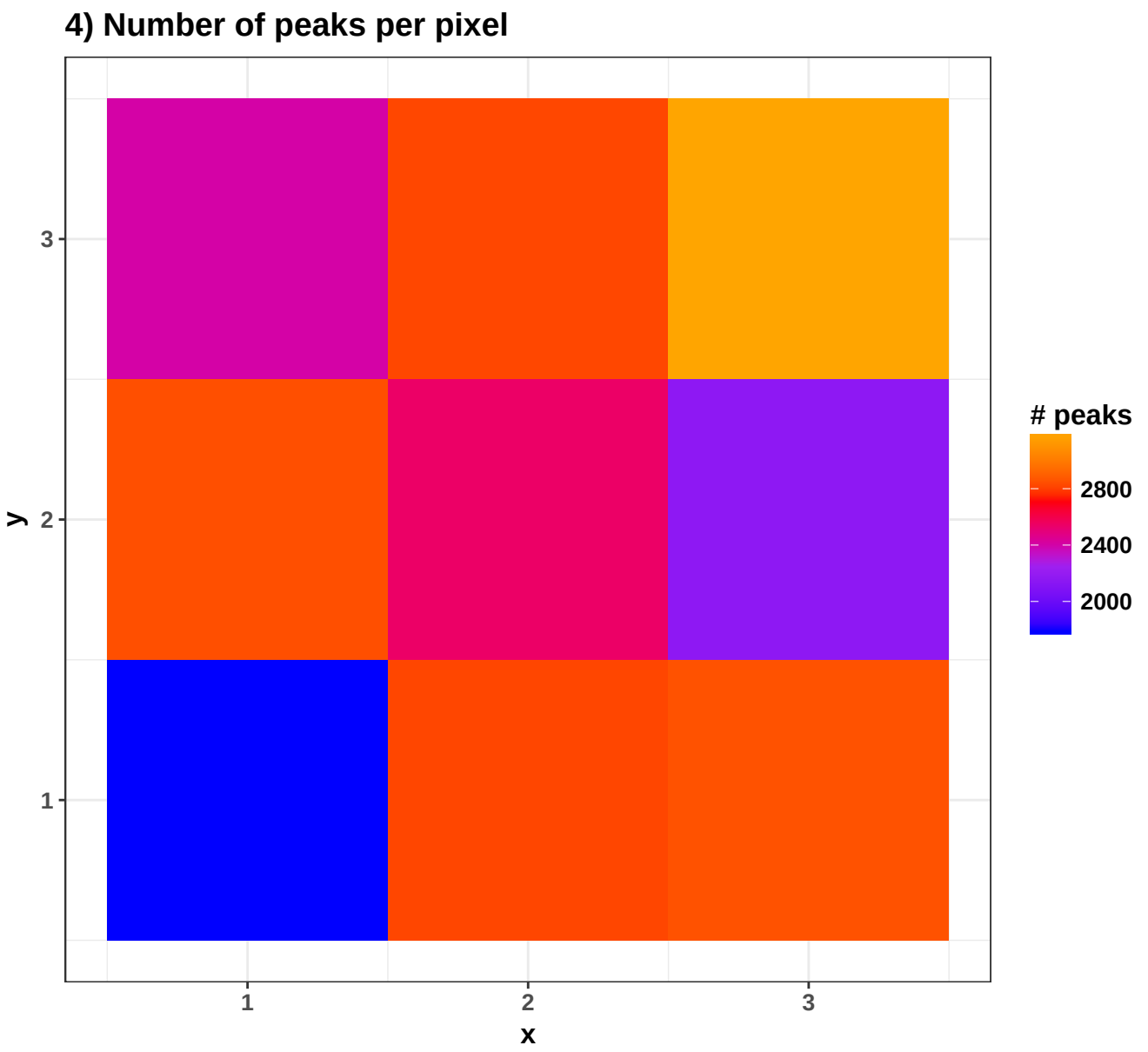

3B) 356.7 (356.7 ± 0.25 Da)
m/z = 356.67
0.07
0
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5


3C) 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

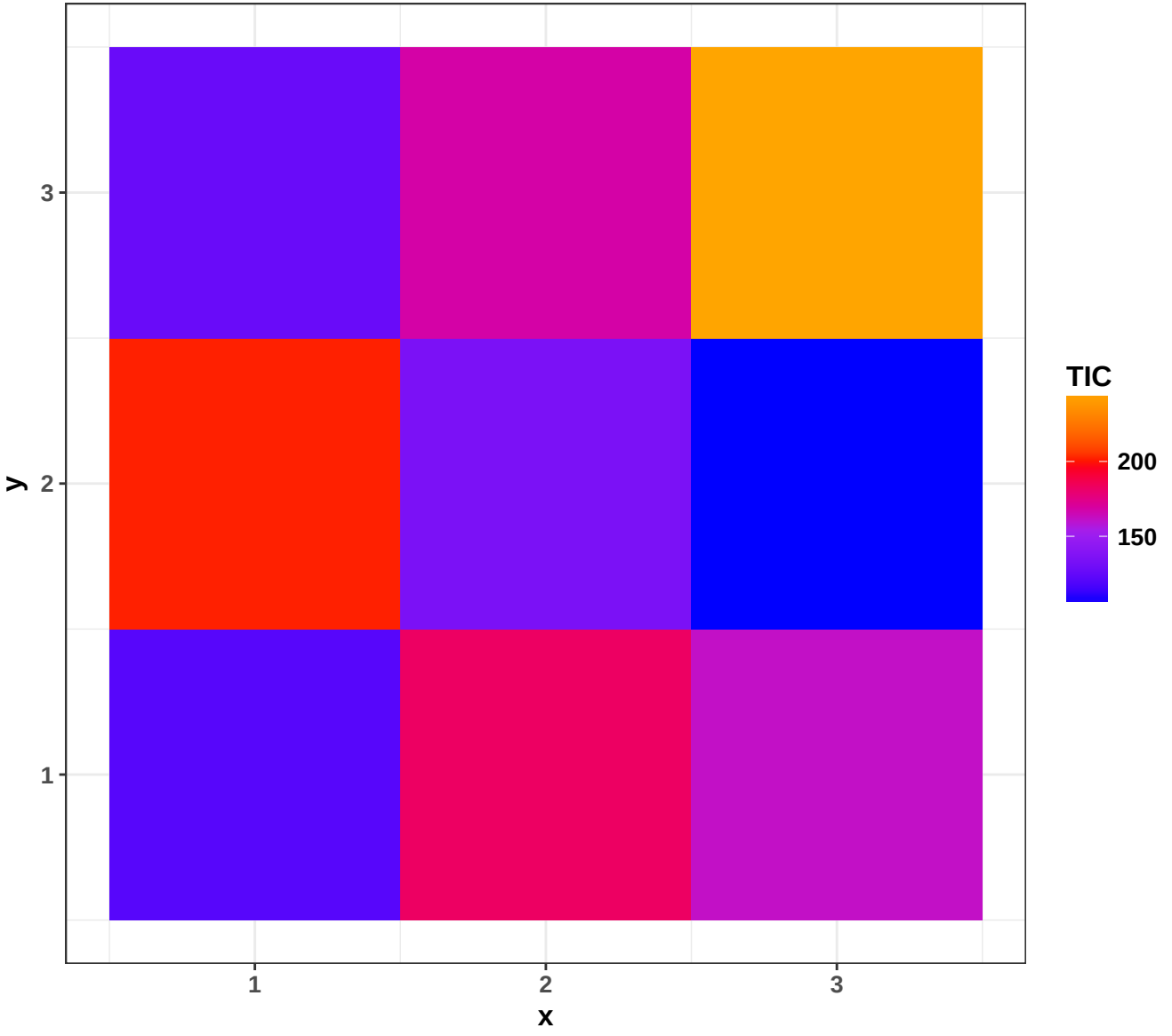

3D) mass1 (152 ± 0.25 Da)
m/z = 152
1.61
0.02
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5


3E) 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

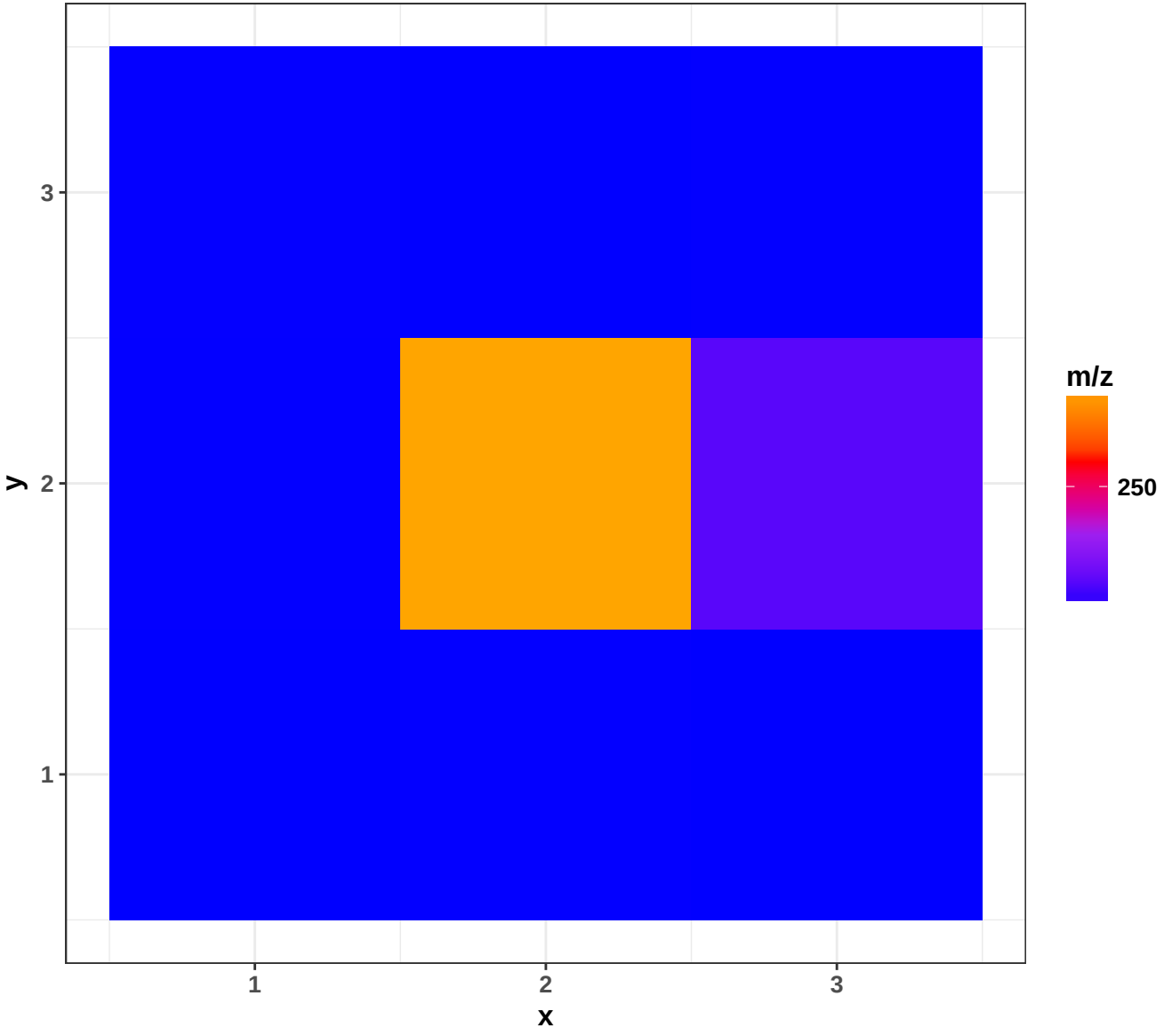

3F) mass3 (185.2 ± 0.25 Da)
m/z = 185.17
0.29
0
y
x
0
1
2
3
4
5
−1
0
1
2
3
4
5


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

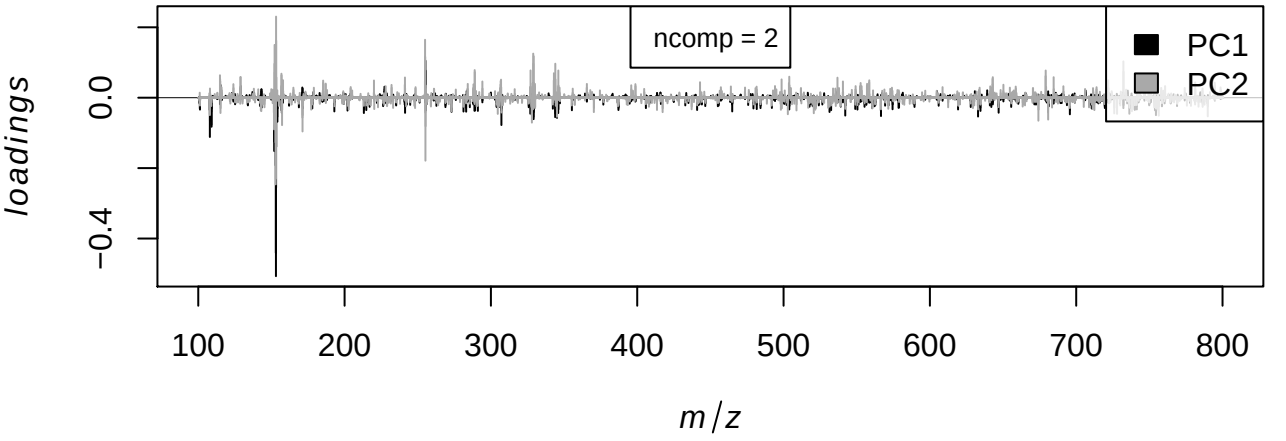
5) Total Ion Chromatogram

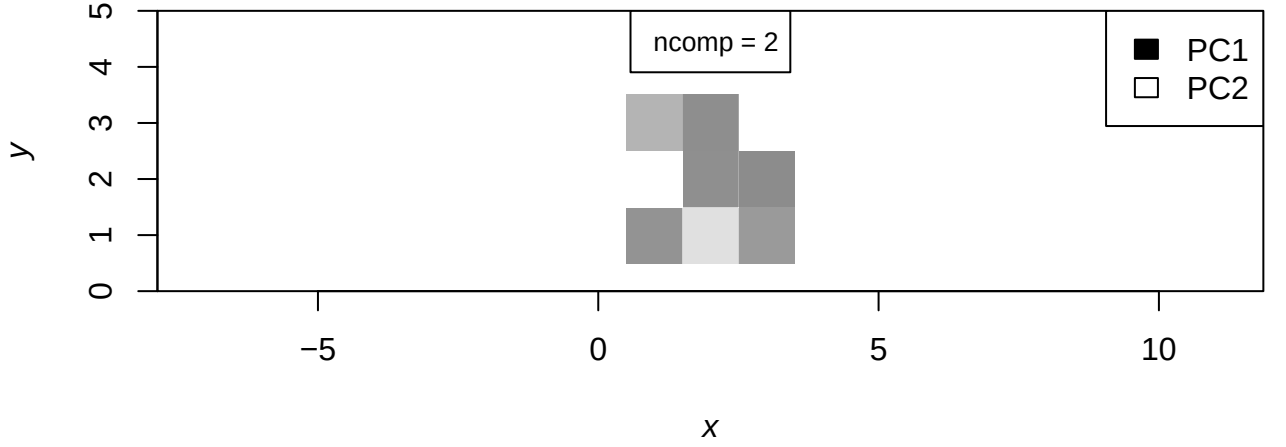


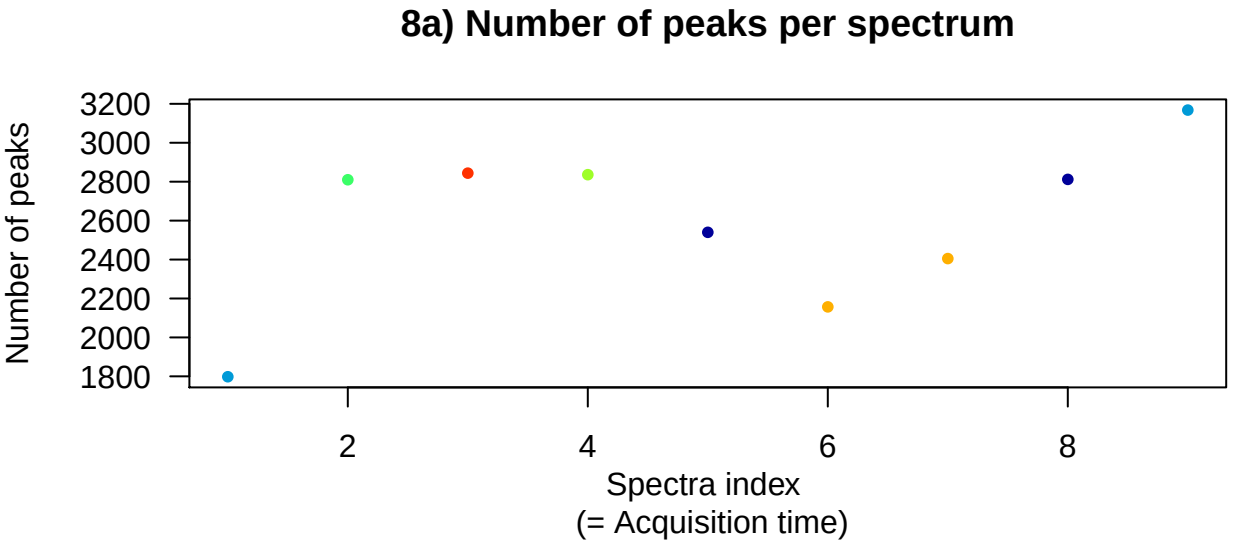
6) Most abundant m/z in each pixel

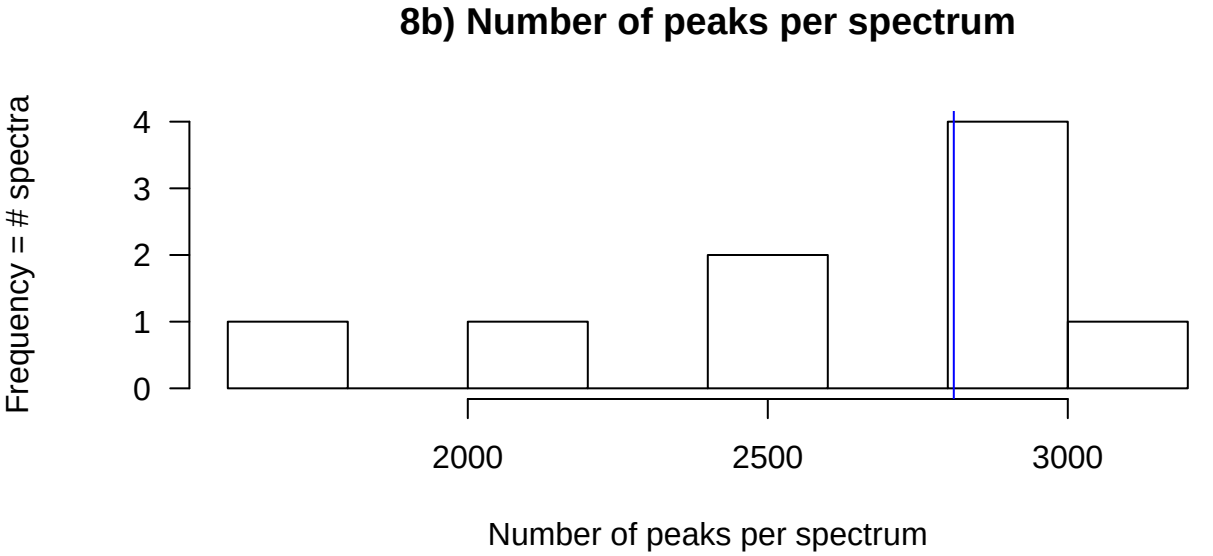


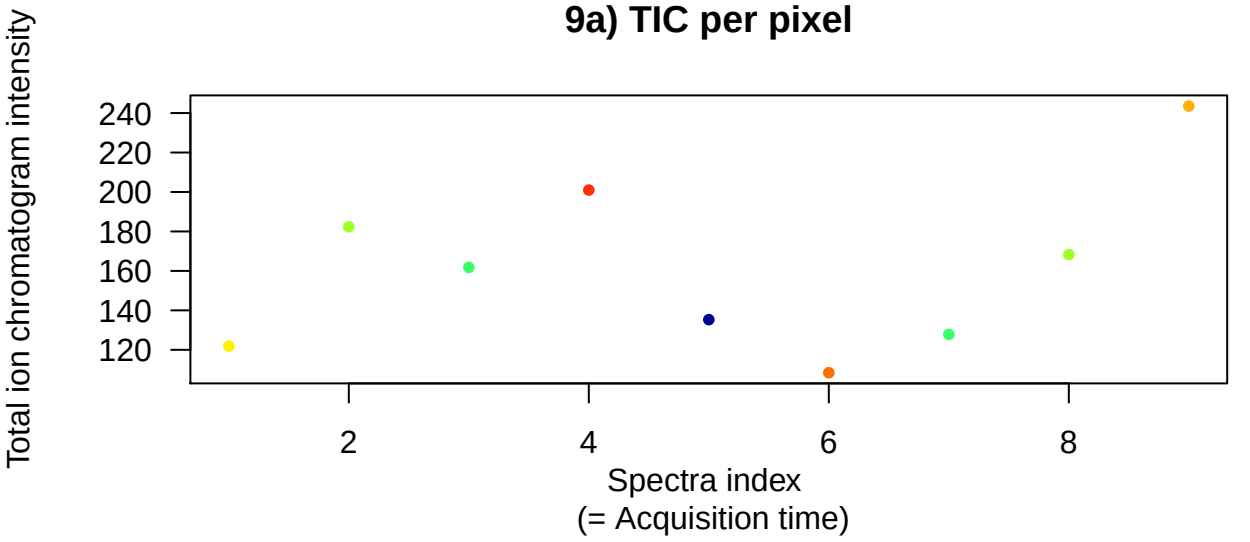
7) PCA for two components

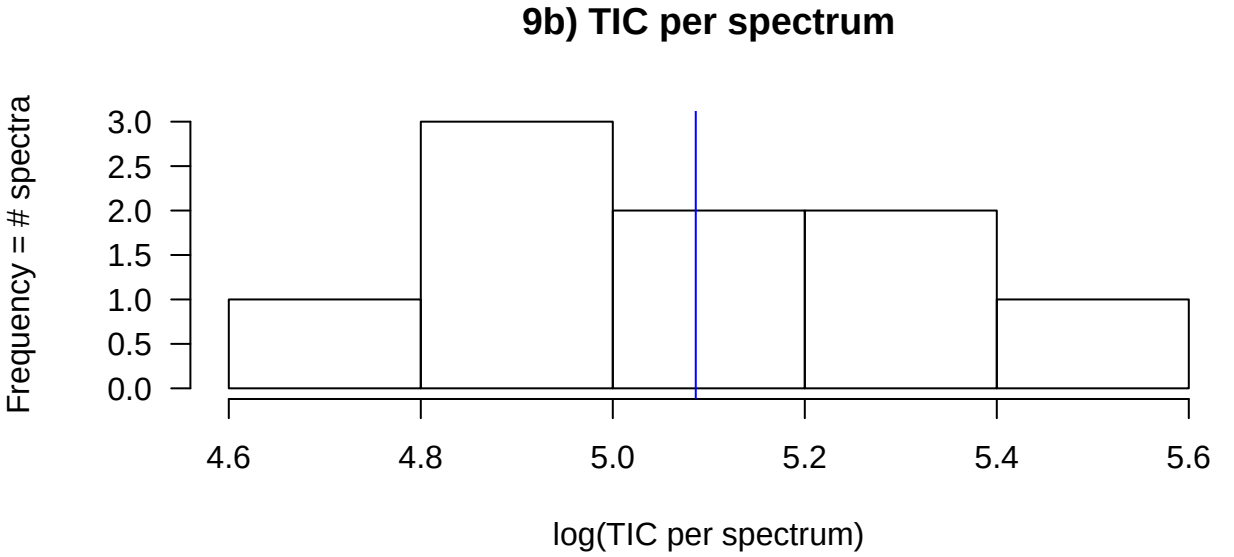




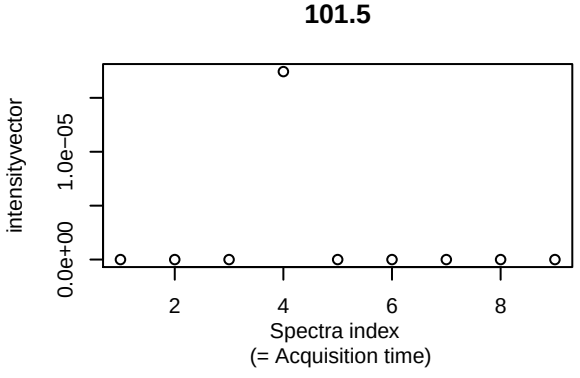

8a) Number of peaks per spectrum
Number of peaks
3200
3000
2800
2600
2400
2200
2000
1800
2
4
6
8
Spectra index
(= Acquisition time)

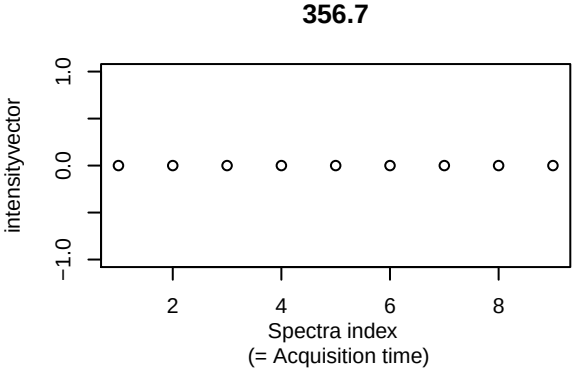

8b) Number of peaks per spectrum
Frequency = # spectra
4
3
2
1
0
2000
2500
3000
Number of peaks per spectrum

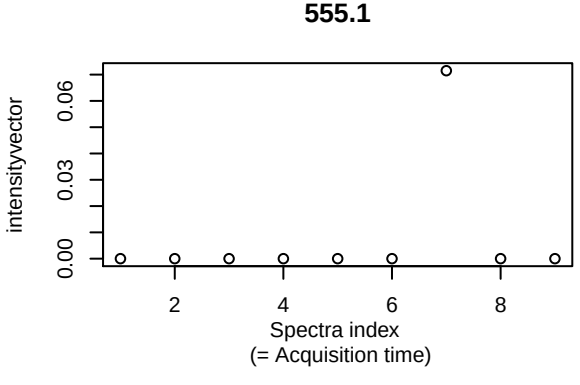

9a) TIC per pixel
Total ion chromatogram intensity
240
220
200
180
160
140
120
2
4
6
8
Spectra index
(= Acquisition time)

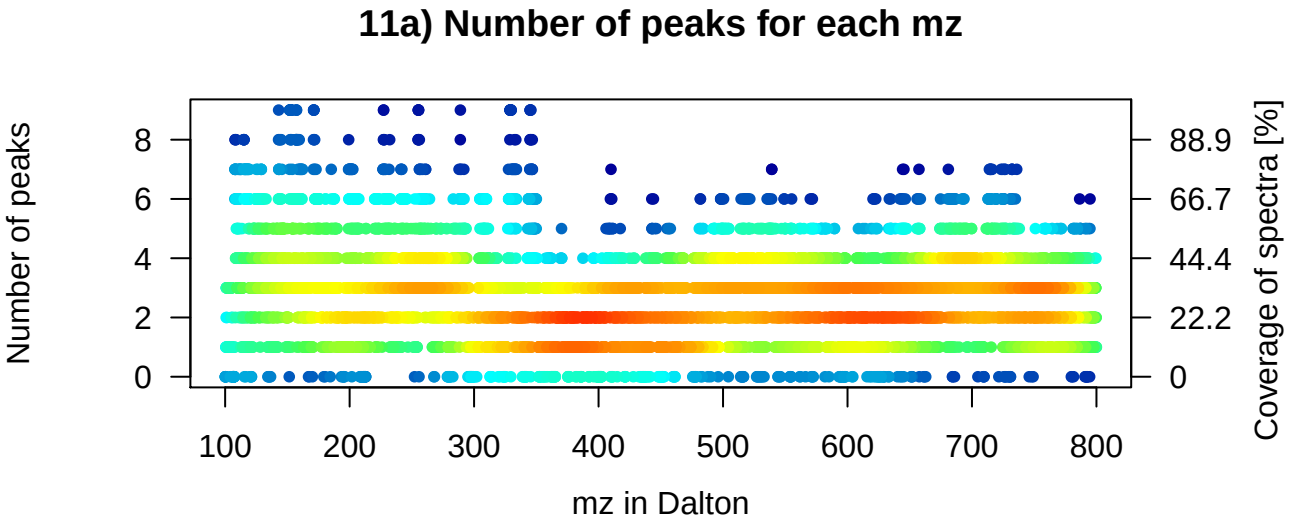

9b) TIC per spectrum
Frequency = # spectra
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.6
4.8
5.0
5.2
5.4
5.6
log(TIC per spectrum)

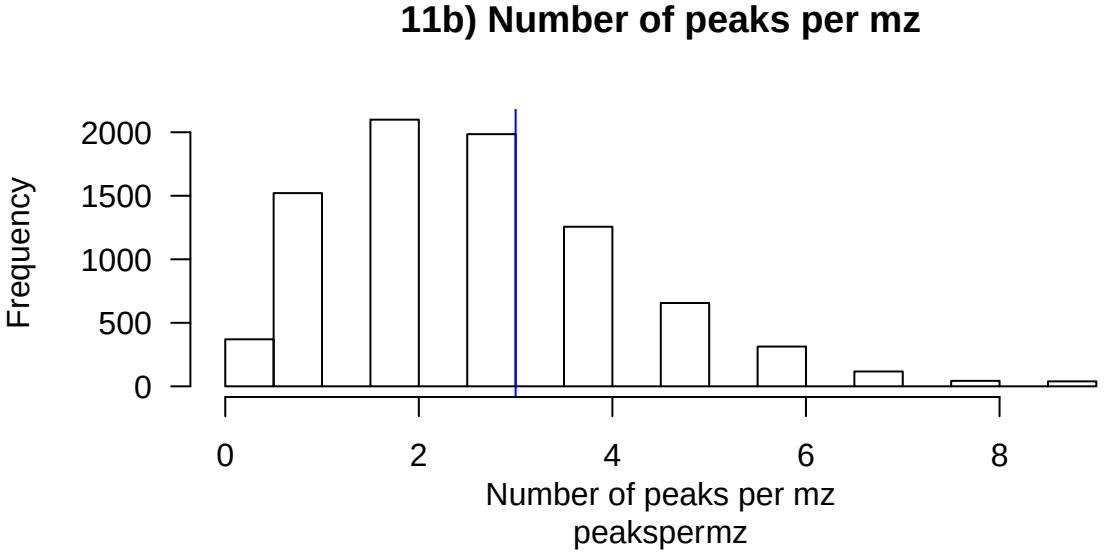
10) intensity of calibrants over acquisition

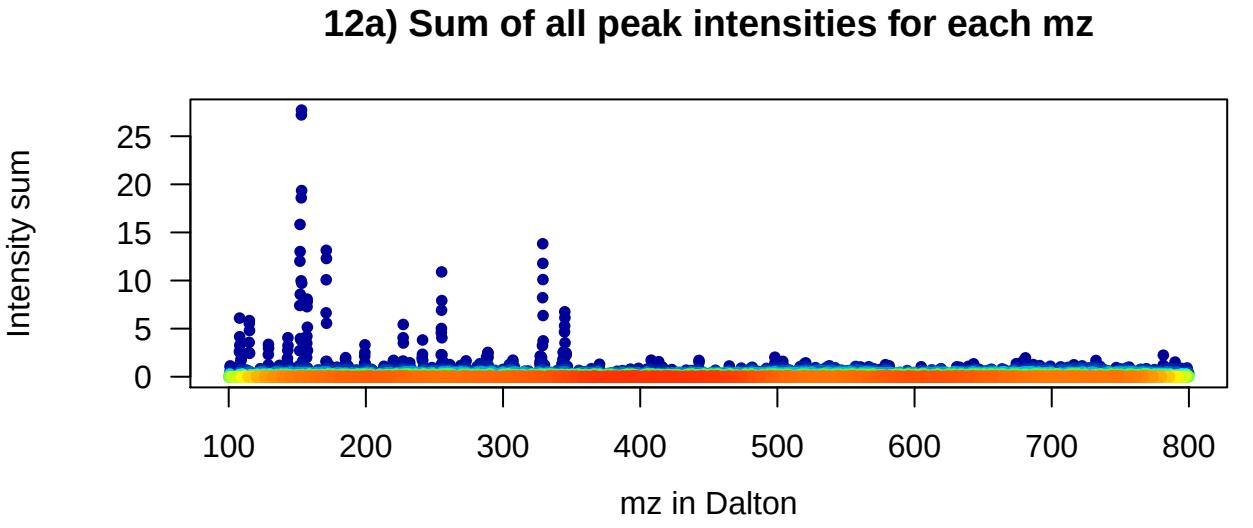


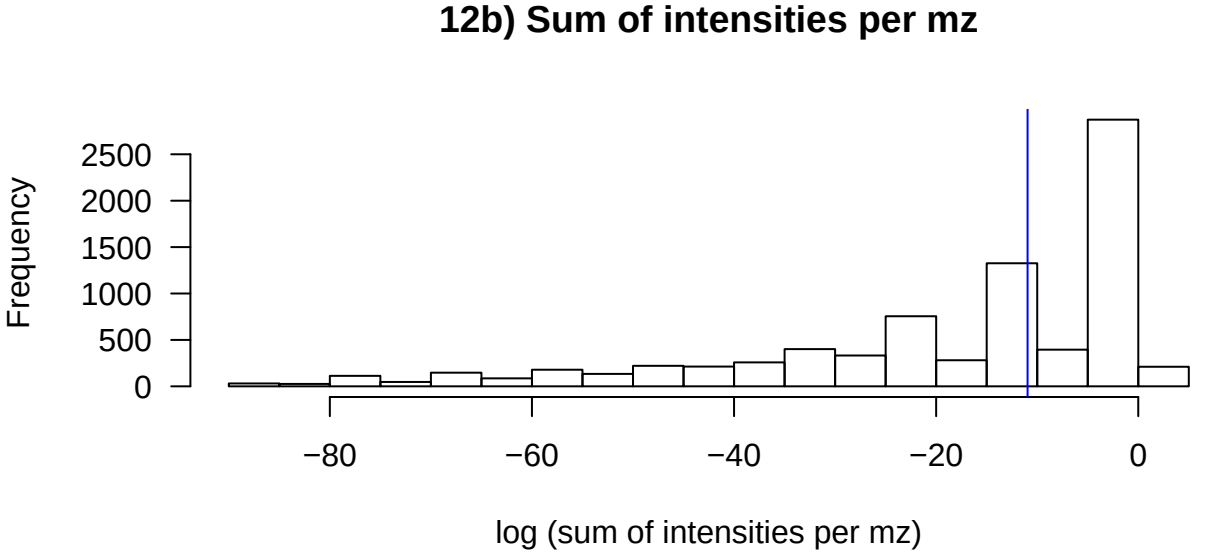


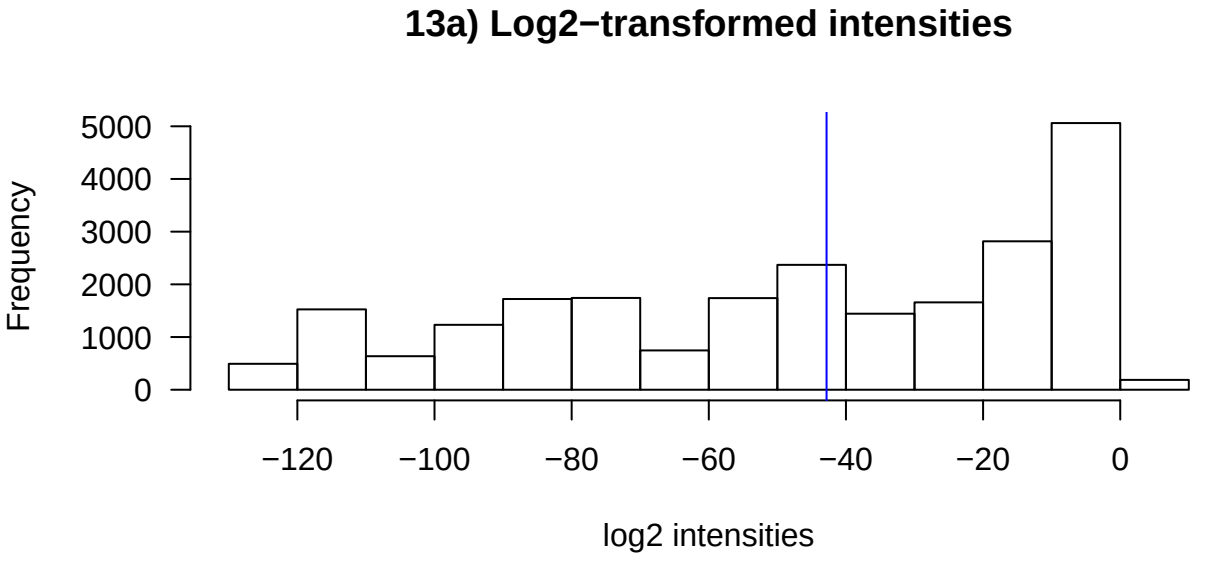


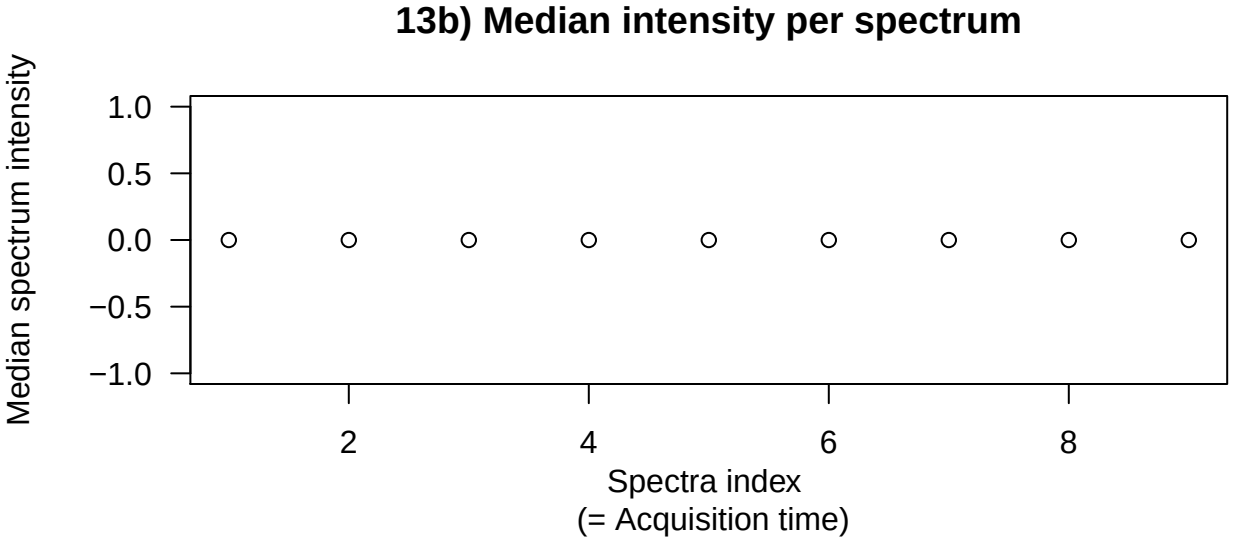

11a) Number of peaks for each mz
Number of peaks
0
2
4
6
8
Coverage of spectra [%]
0
22.2
44.4
66.7
88.9
100
200
300
400
500
600
700
800
mz in Dalton

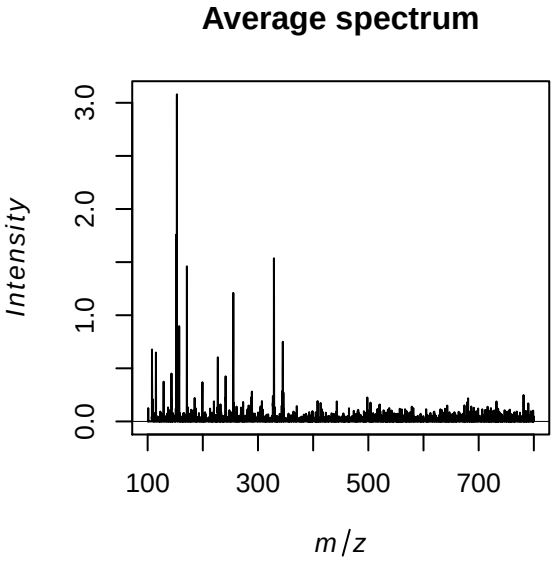

11b) Number of peaks per mz
Frequency
0
500
1000
1500
2000
0
2
4
6
8
Number of peaks per mz
peakspermz

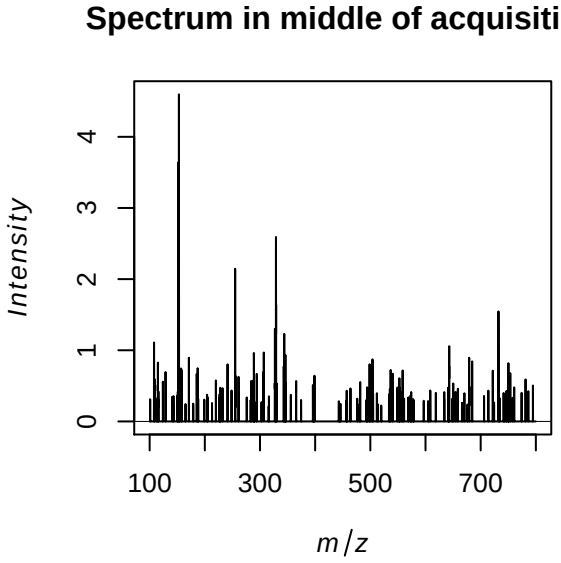

12a) Sum of all peak intensities for each mz
Intensity sum
0
5
10
15
20
25
100
200
300
400
500
600
700
800
mz in Dalton

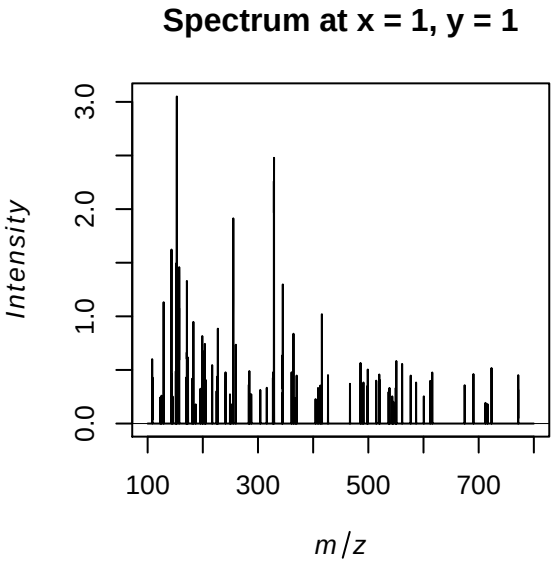

12b) Sum of intensities per mz
Frequency
0
500
1000
1500
2000
2500
−80
−60
−40
−20
0
log (sum of intensities per mz)

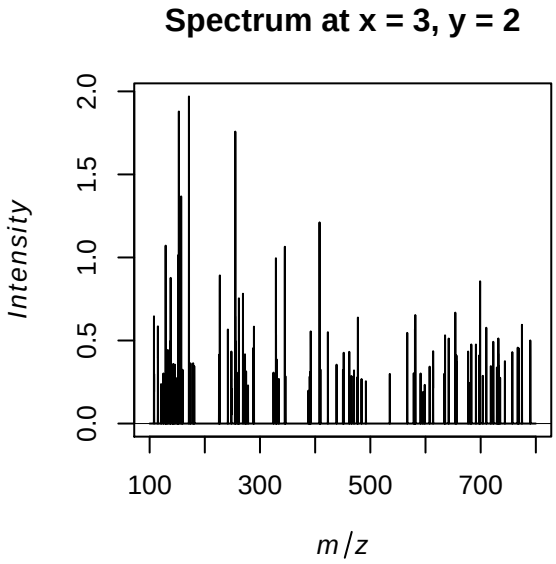

13a) Log2−transformed intensities
Frequency
5000
4000
3000
2000
1000
0
−120
−100
−80
−60
−40
−20
0
log2 intensities

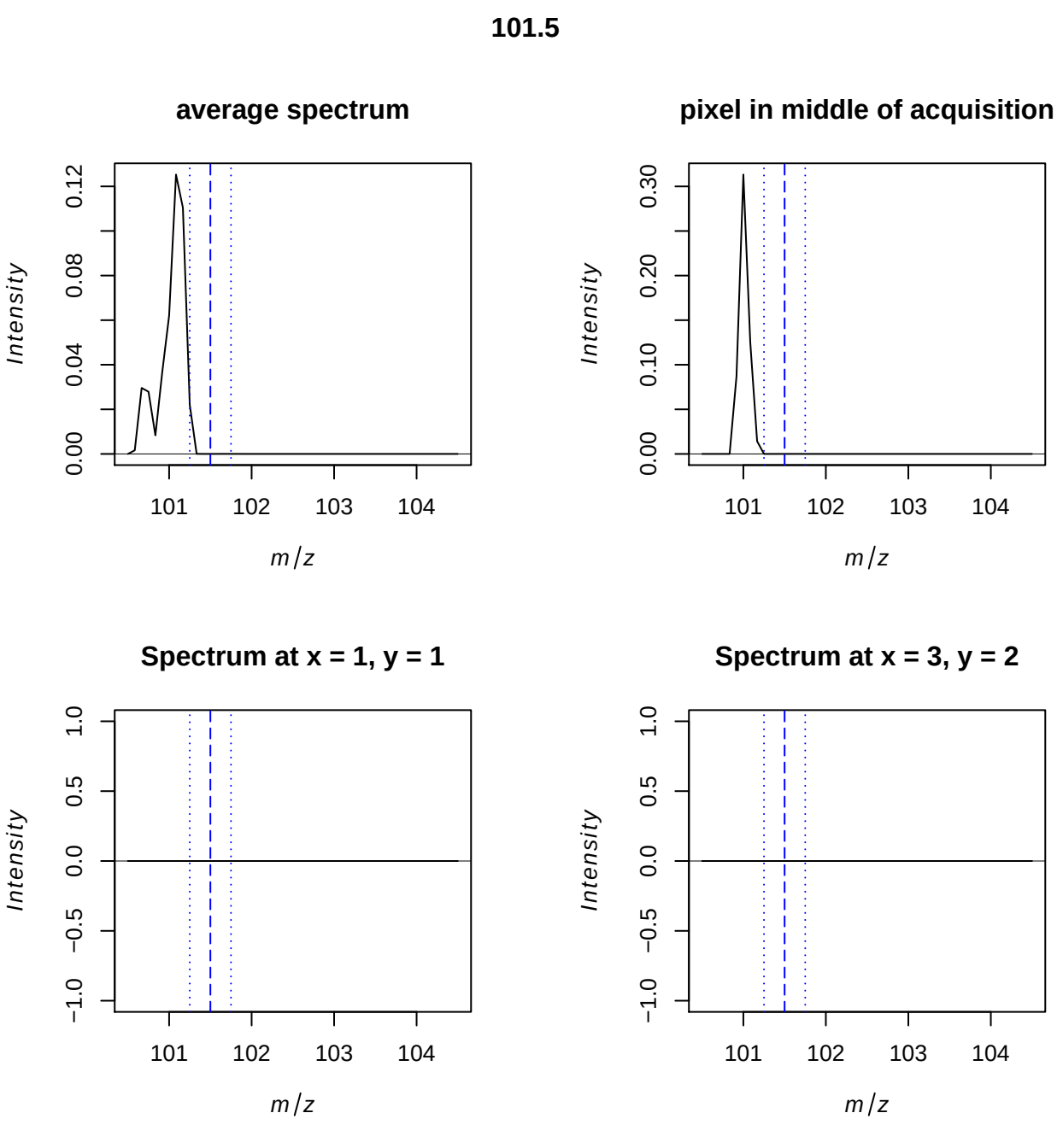

13b) Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
Spectra index
(= Acquisition time)

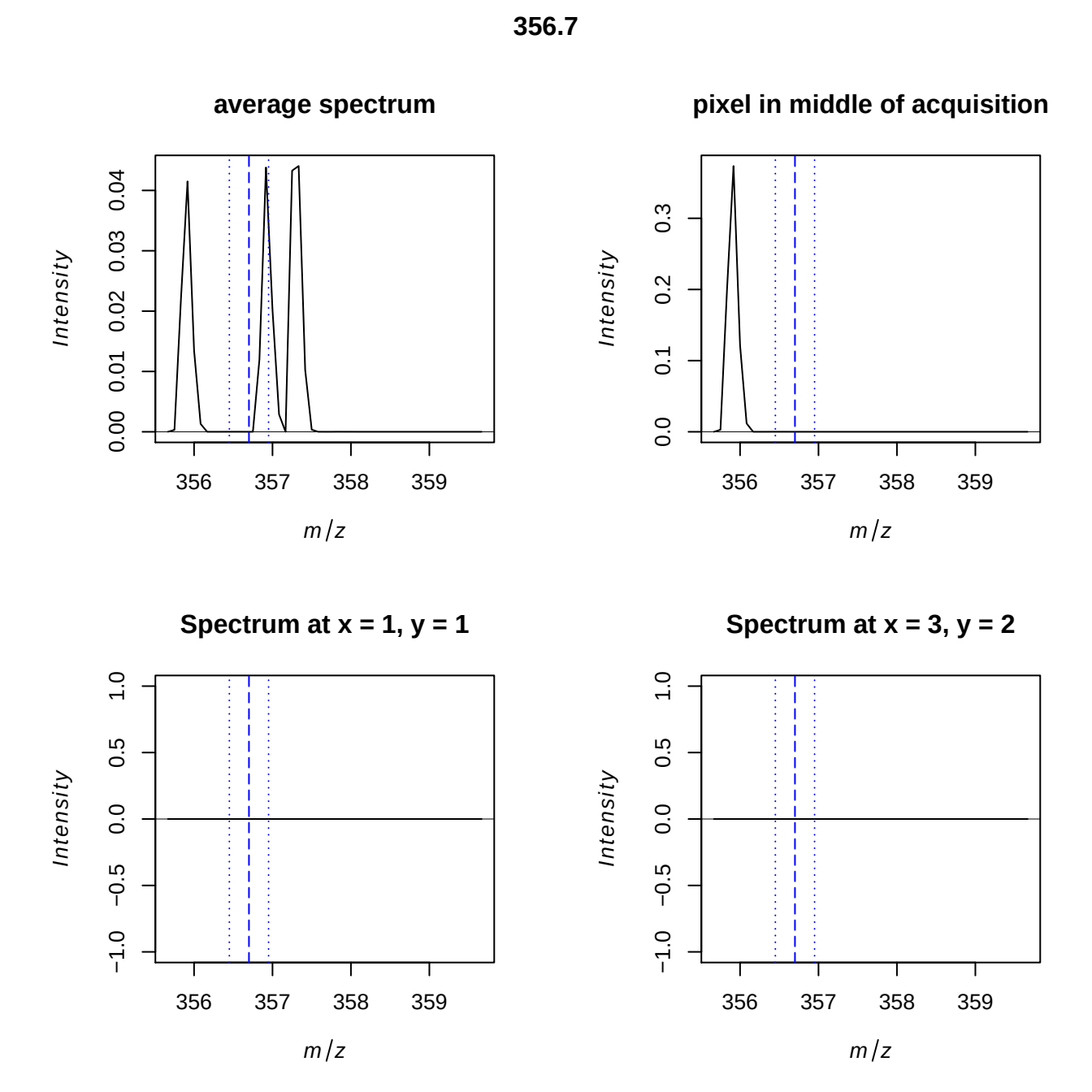

Average spectrum
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z


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

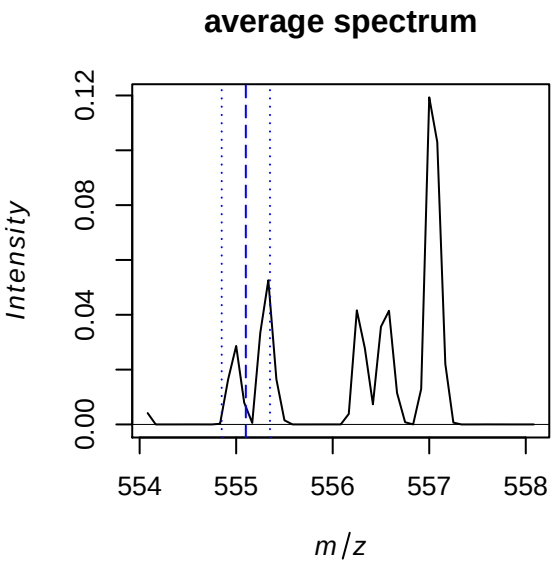

Spectrum at x = 1, y = 1
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z

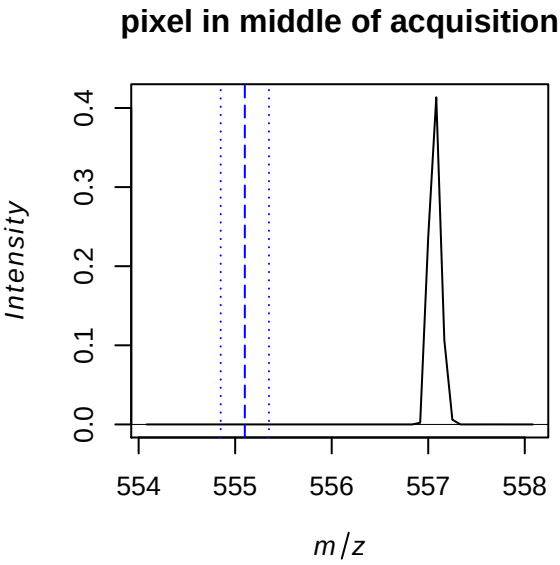

Spectrum at x = 3, y = 2
Intensity
0.0
0.5
1.0
1.5
2.0
100
300
500
700
m/z

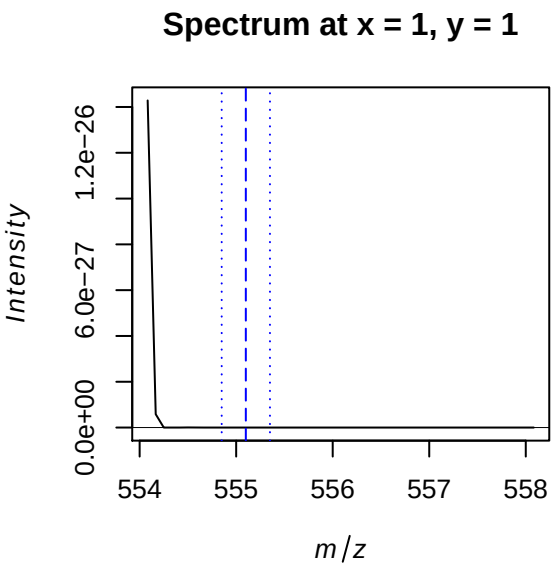

101.5
average spectrum
pixel in middle of acquisition
Spectrum at x = 1, y = 1
Spectrum at x = 3, y = 2
Intensity
m/z
0.00
0.04
0.08
0.12
0.10
0.20
0.30
−1.0
−0.5
0.0
0.5
1.0
101
102
103
104

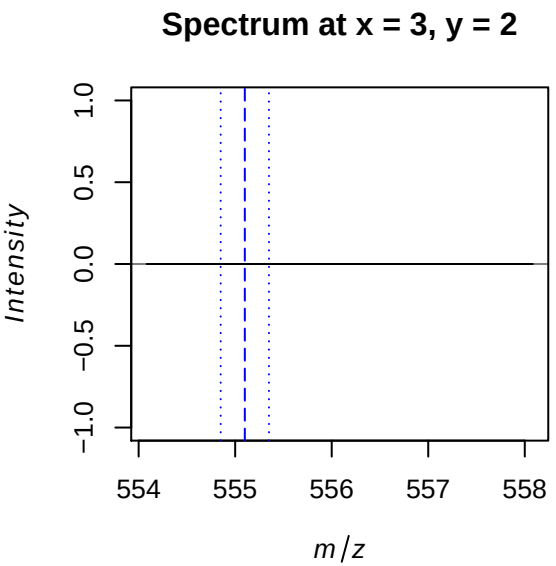

356.7
average spectrum
pixel in middle of acquisition
Spectrum at x = 1, y = 1
Spectrum at x = 3, y = 2
Intensity
m/z
0.00
0.01
0.02
0.03
0.04
0.0
0.1
0.2
0.3
−1.0
−0.5
0.0
0.5
1.0
356
357
358
359

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