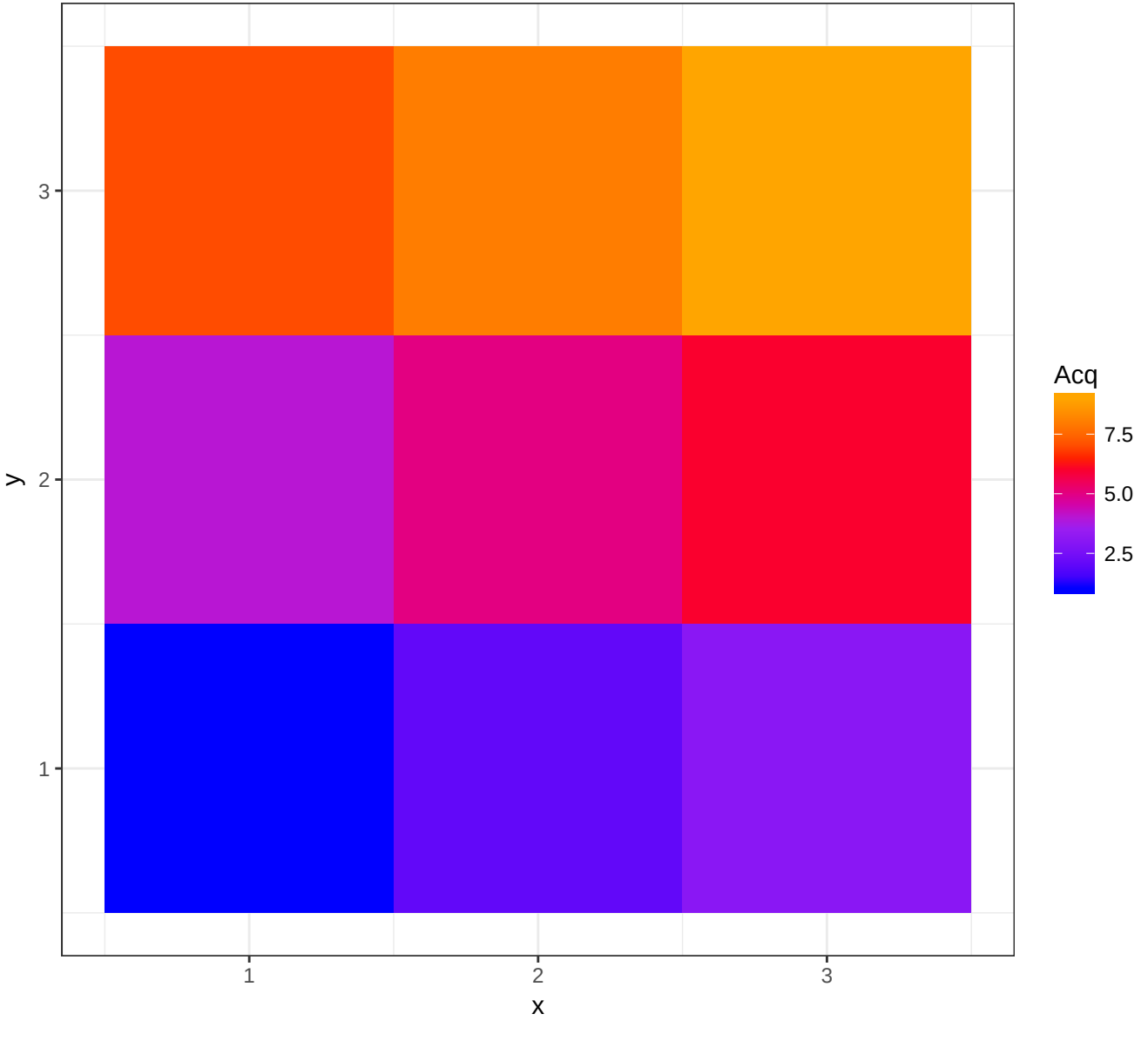
Quality control of MSI data

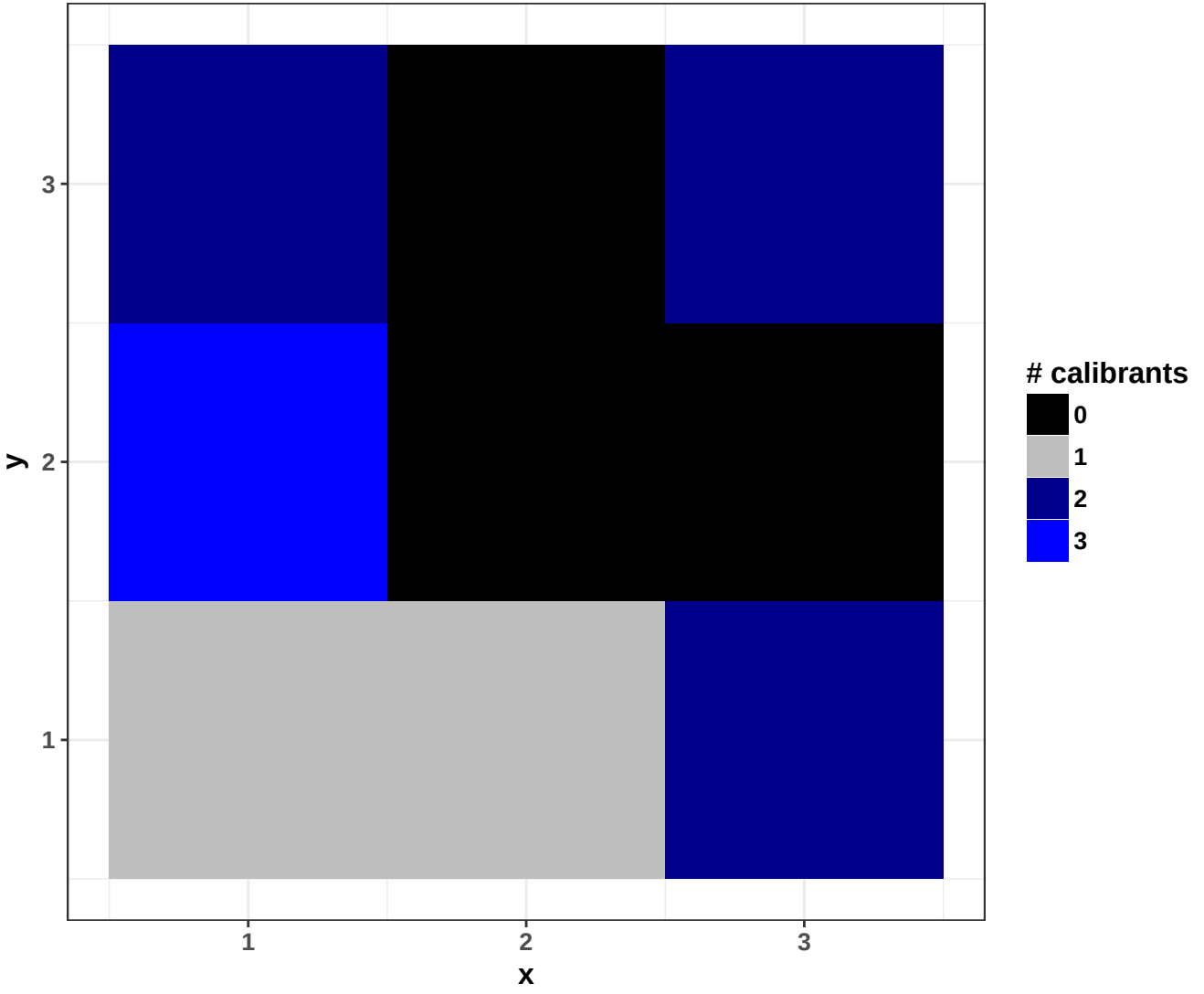
Filename: Testfile_rdata

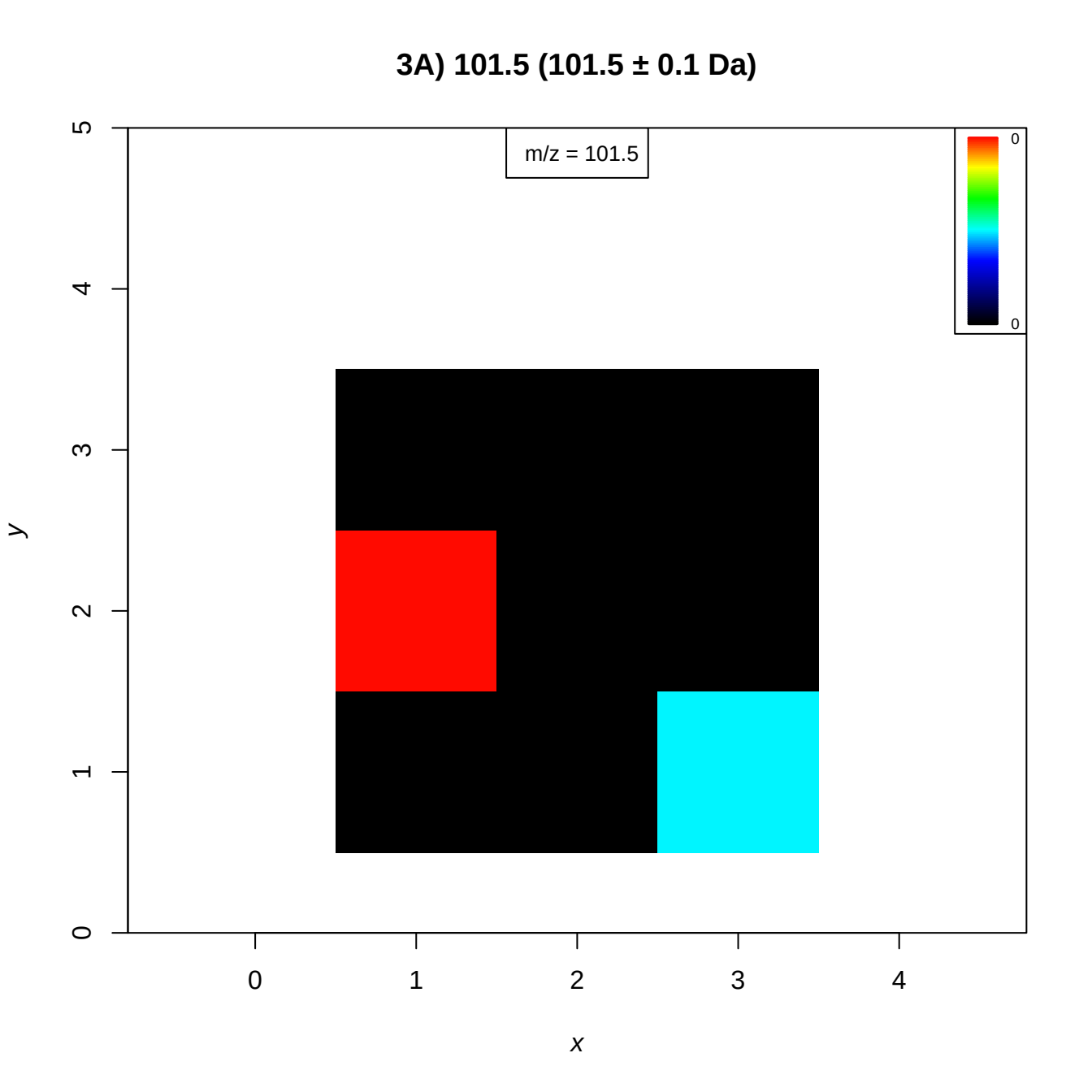
properties	values
Number of mz features	8399
Range of mz values [Da]	100.08 − 799.92
Number of pixels	9
Range of x coordinates	1 − 3
Range of y coordinates	1 − 3
Range of intensities	0 − 318.82
Median of intensities	0
Intensities > 0	30.92 %
Number of zero TICs	0
Preprocessing	
Normalization	tic
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in inputpeptides.csv	2 / 3
# calibrants in inputcalibrantfile1.txt	2 / 3

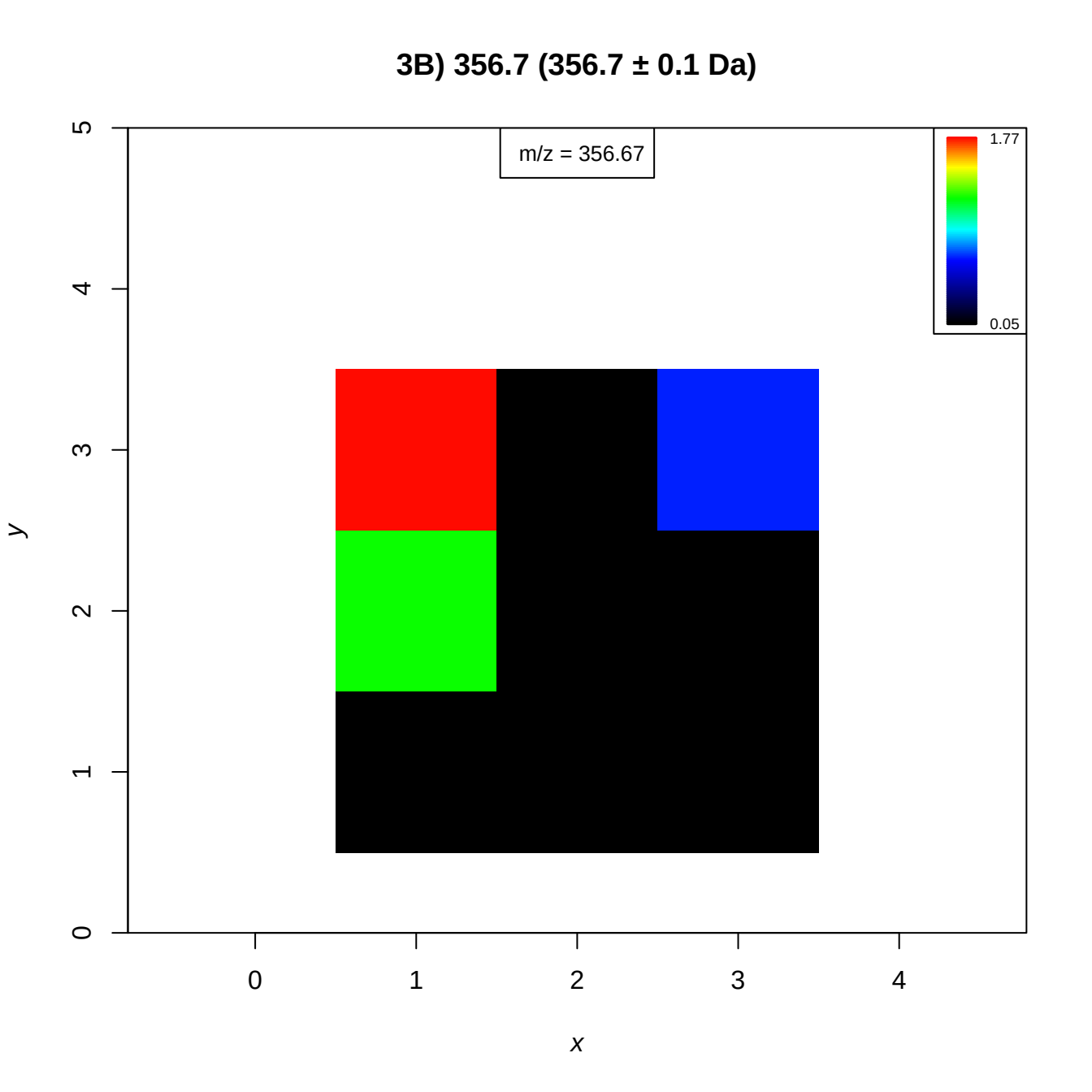
1) Order of Acquisition

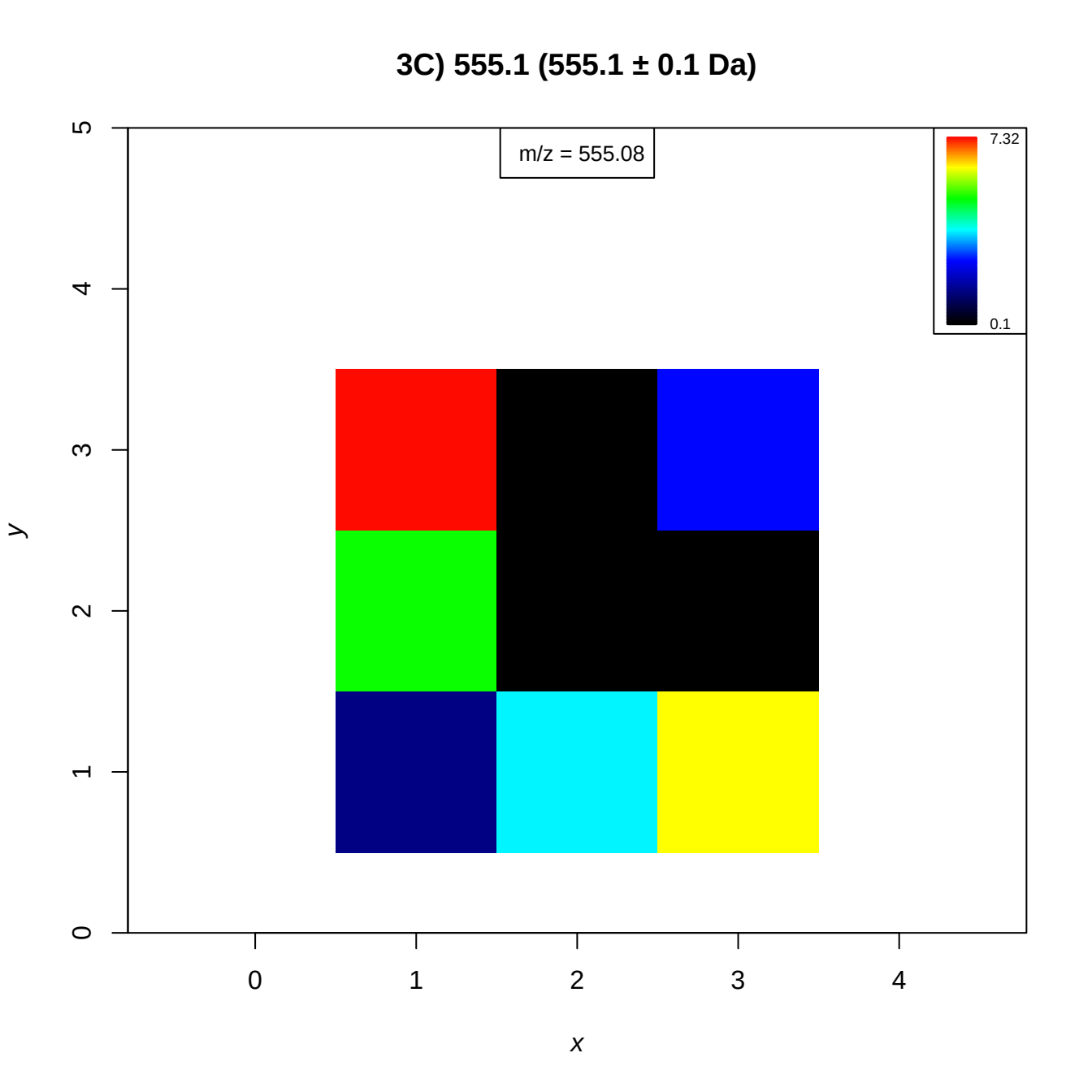


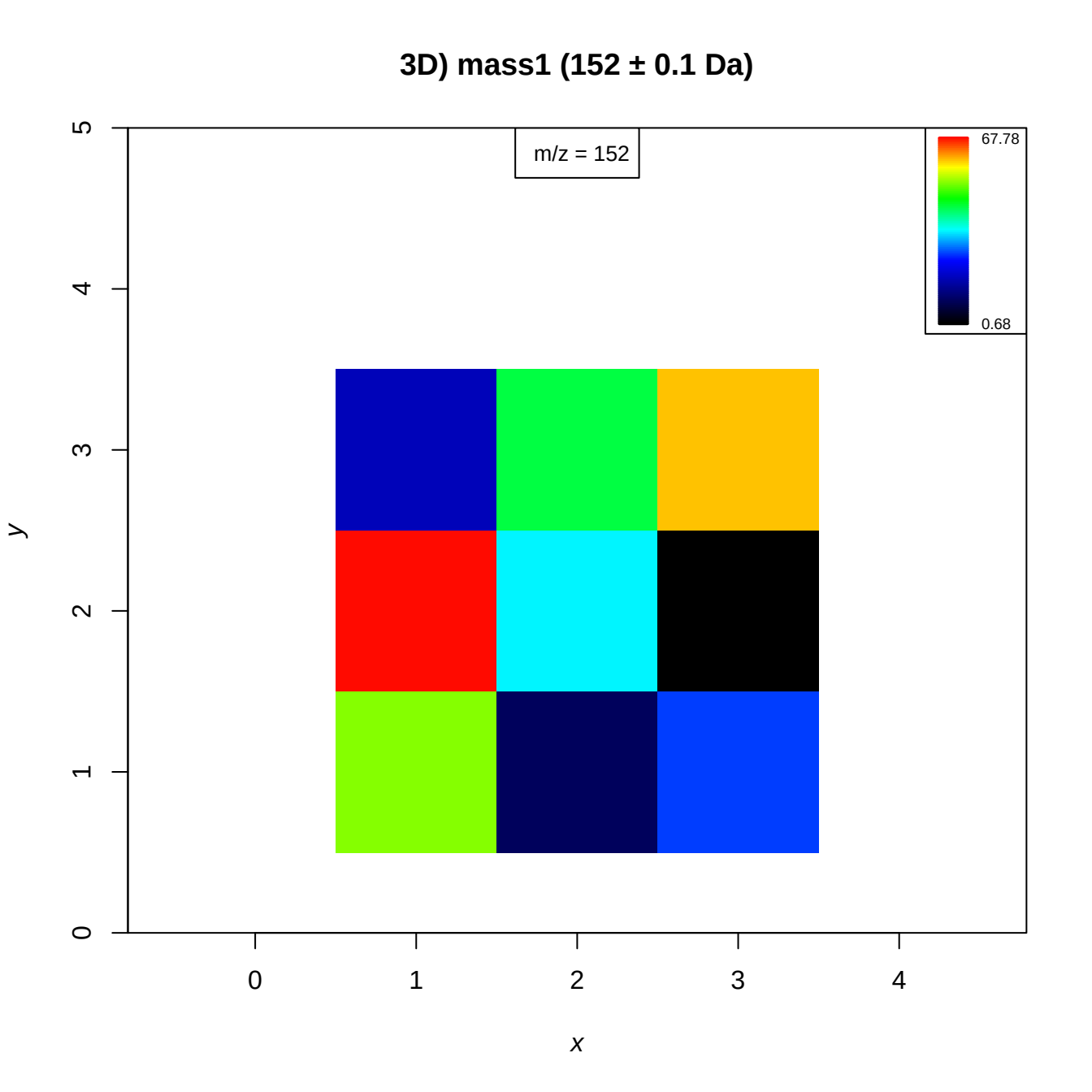
2) Number of calibrants per pixel

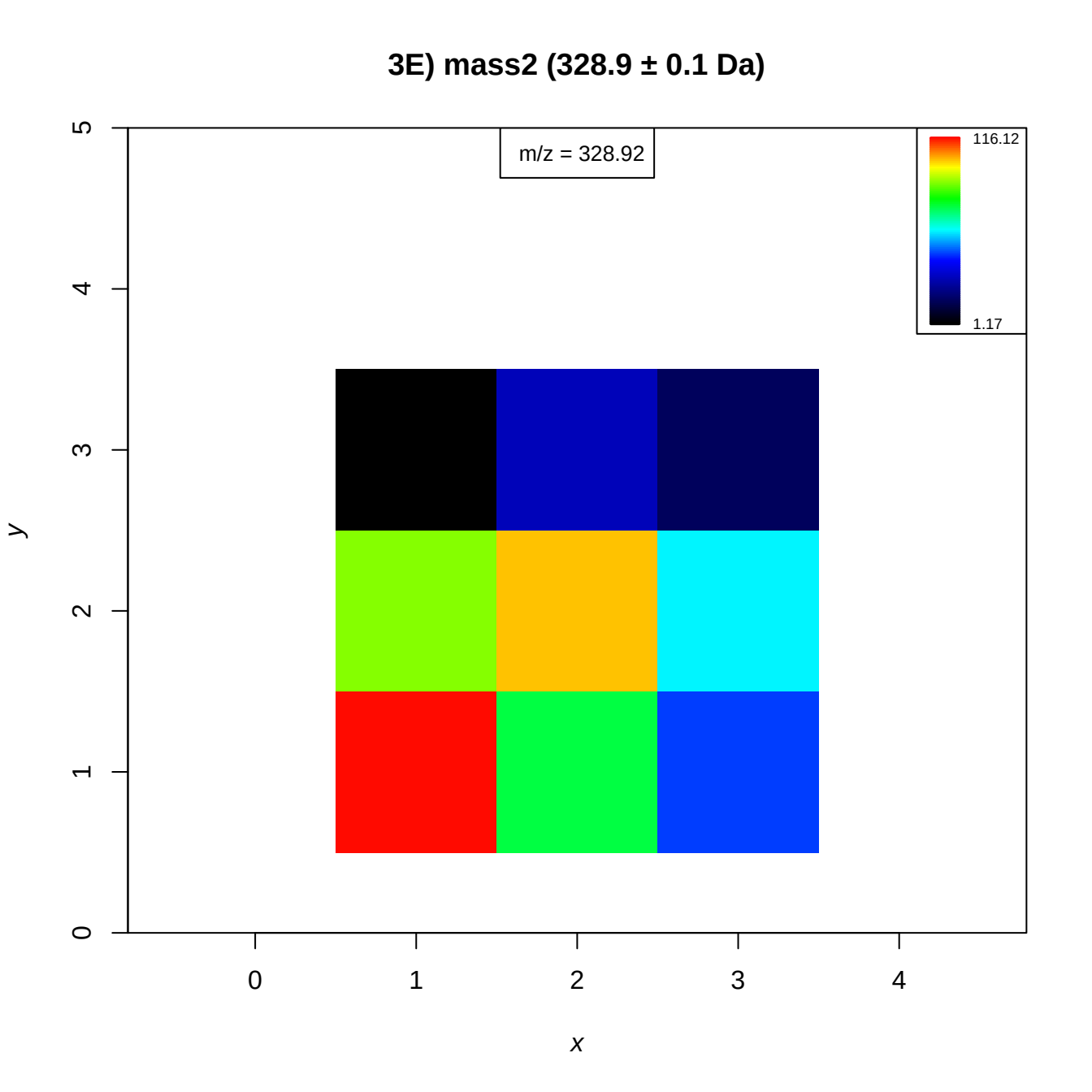


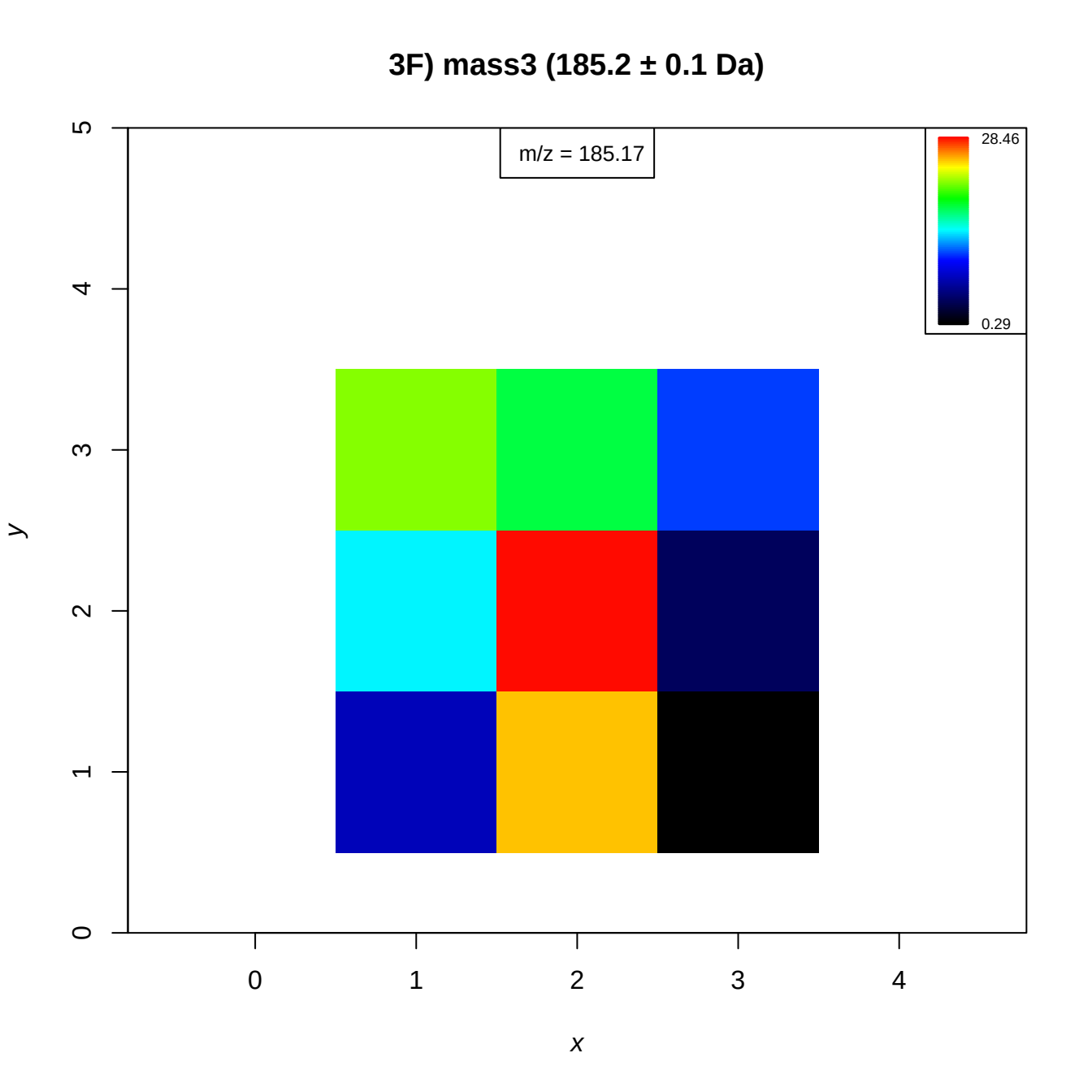

3A) 101.5 (101.5 ± 0.1 Da)
m/z = 101.5
0
0
y
x
0
1
2
3
4
5

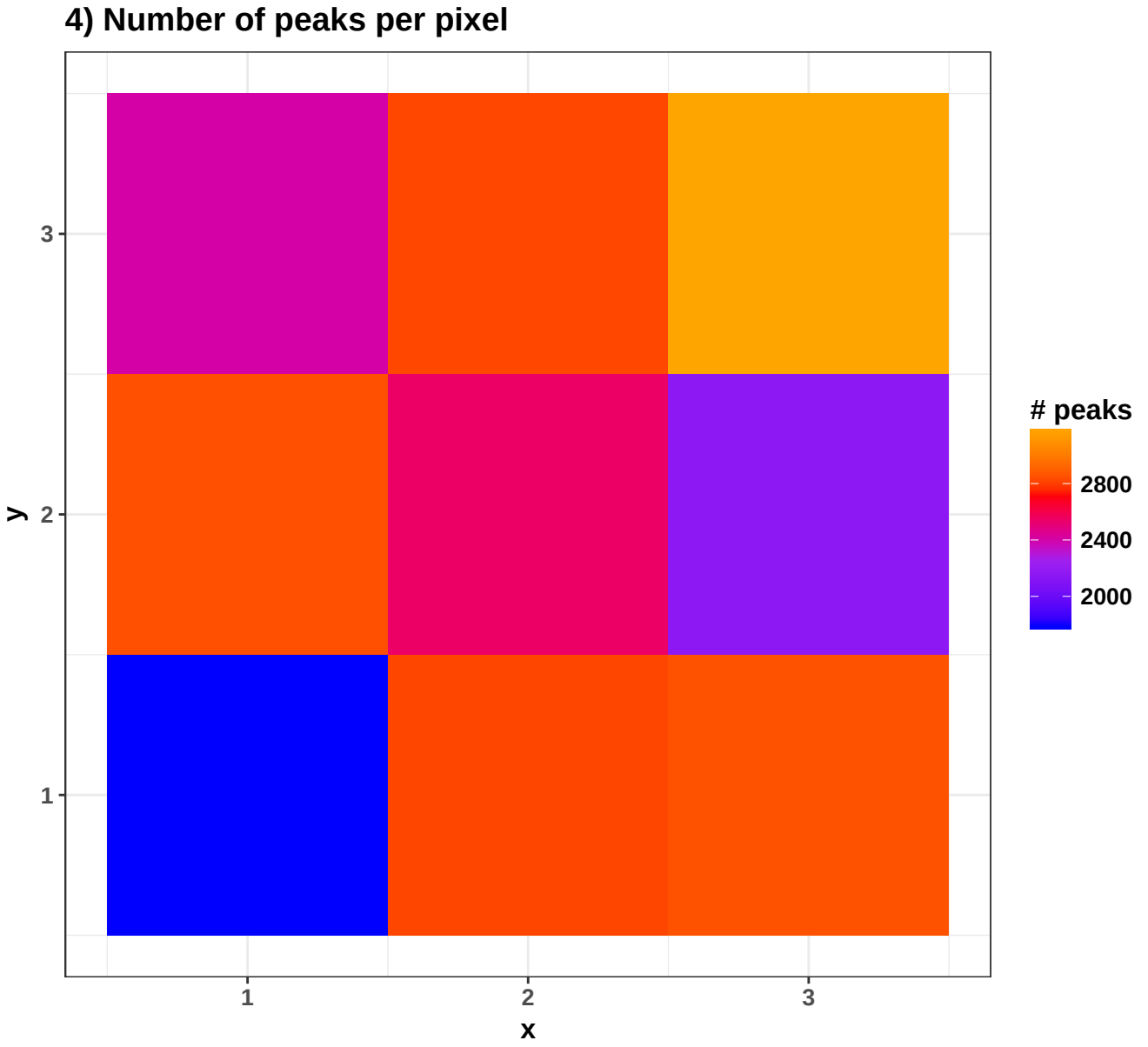

3B) 356.7 (356.7 ± 0.1 Da)
m/z = 356.67
1.77
0.05
y
x
0
1
2
3
4
5


3C) 555.1 (555.1 ± 0.1 Da)
m/z = 555.08
7.32
0.1
y
x
0
1
2
3
4
5

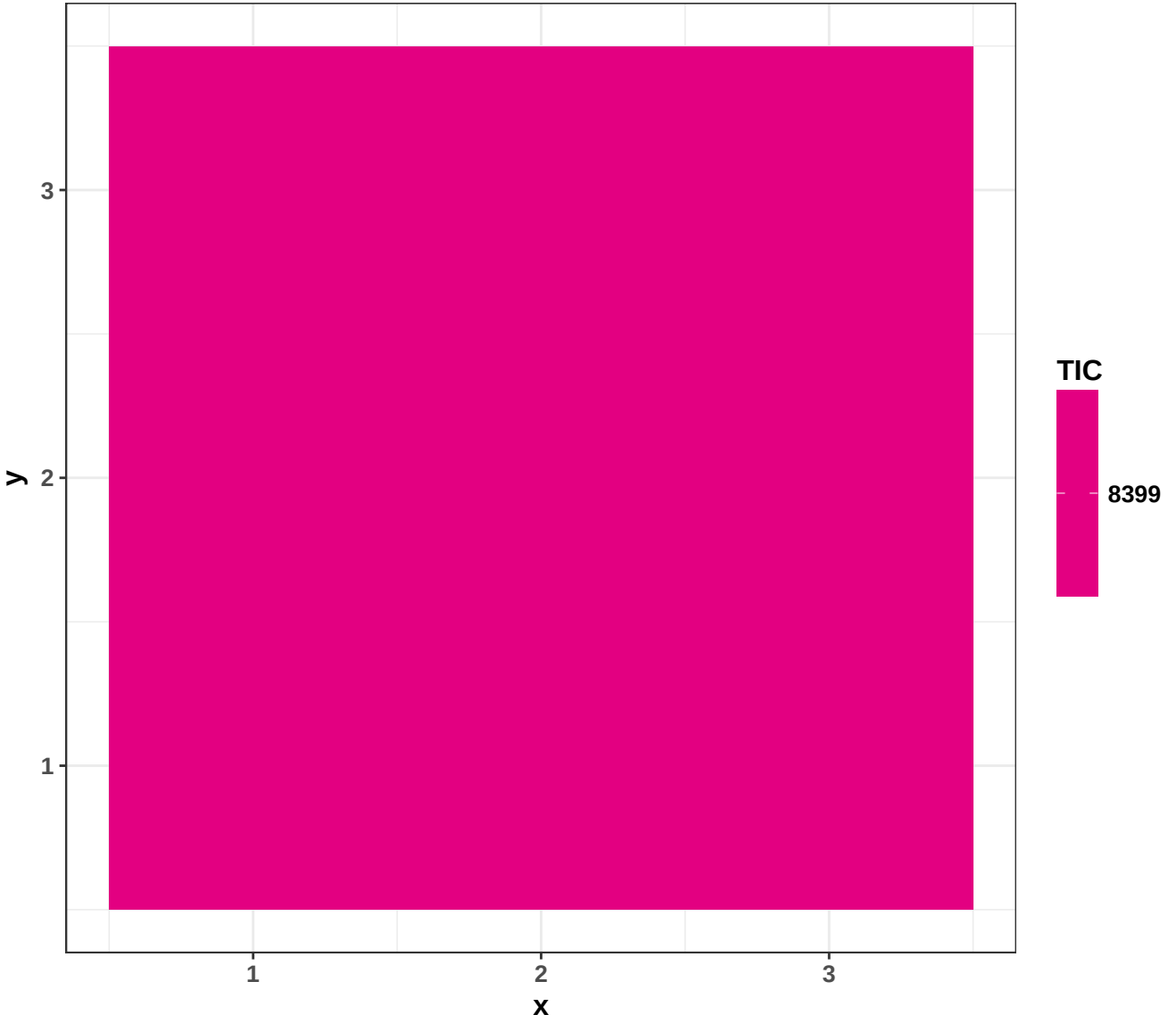

3D) mass1 (152 ± 0.1 Da)
m/z = 152
67.78
0.68
y
x
0
1
2
3
4
5


3E) mass2 (328.9 ± 0.1 Da)
m/z = 328.92
116.12
1.17
y
x
0
1
2
3
4
5

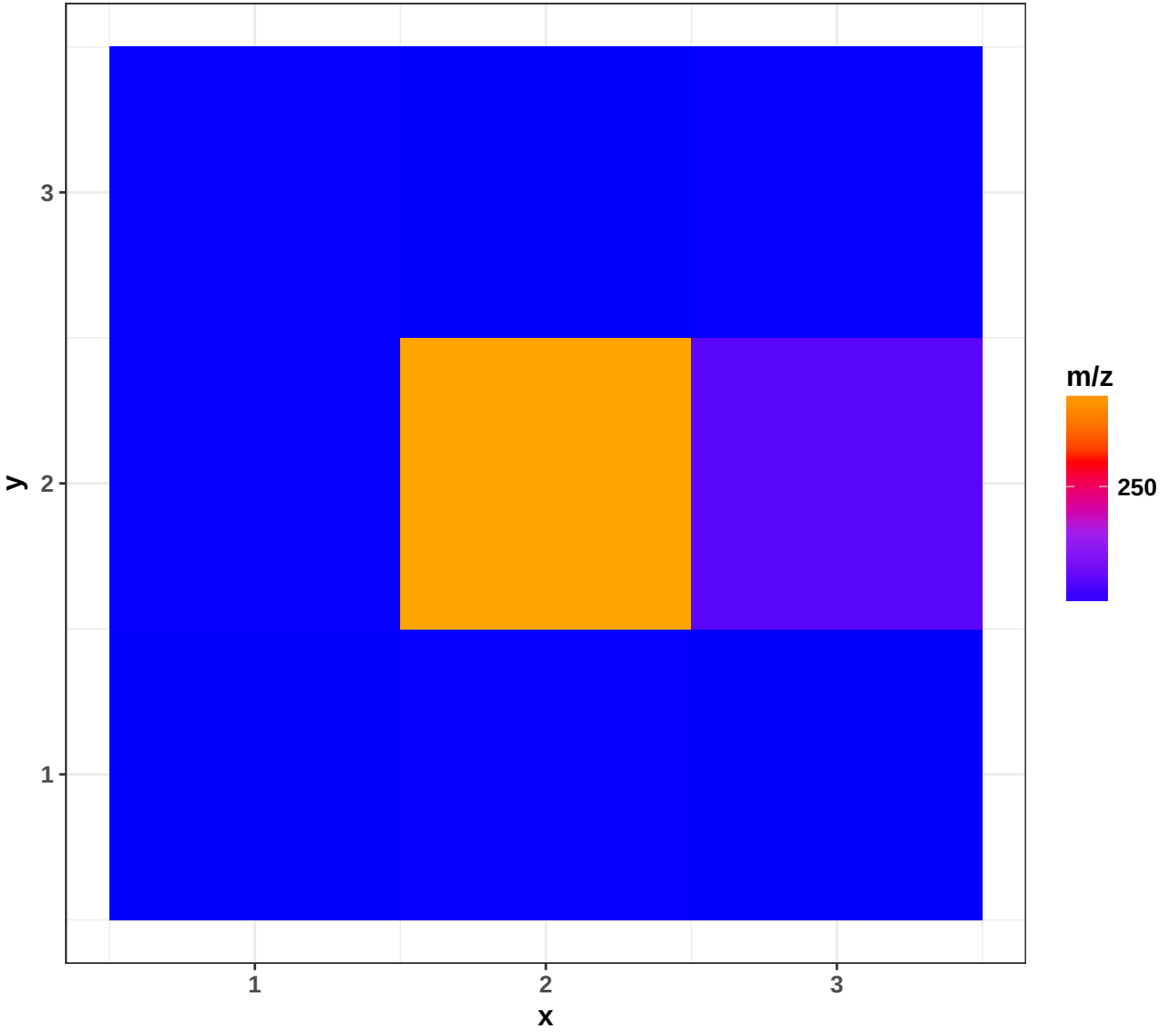

3F) mass3 (185.2 ± 0.1 Da)
m/z = 185.17
28.46
0.29
y
x
0
1
2
3
4
5


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

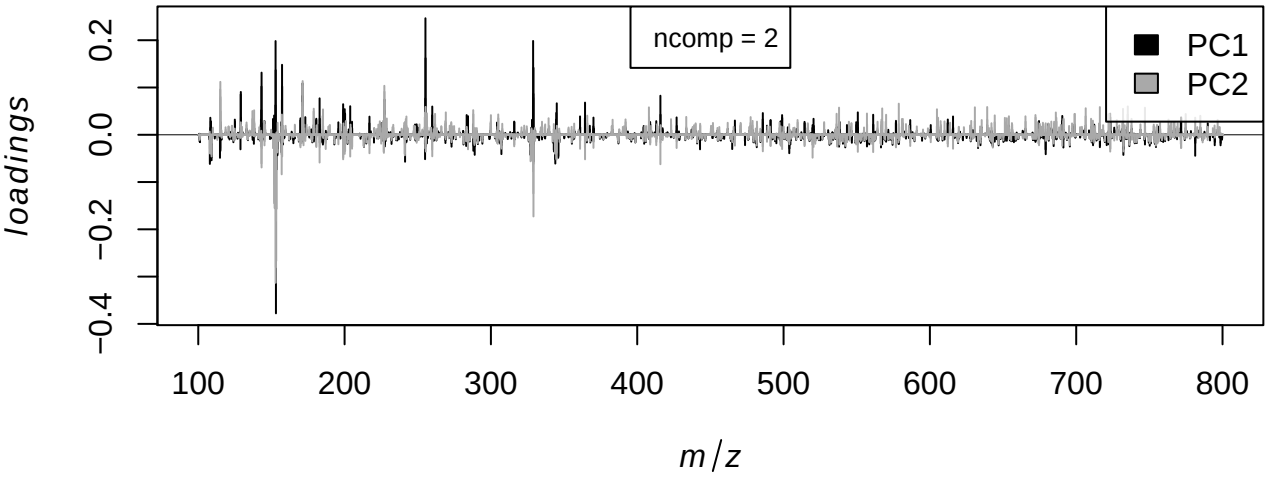
5) Total Ion Chromatogram

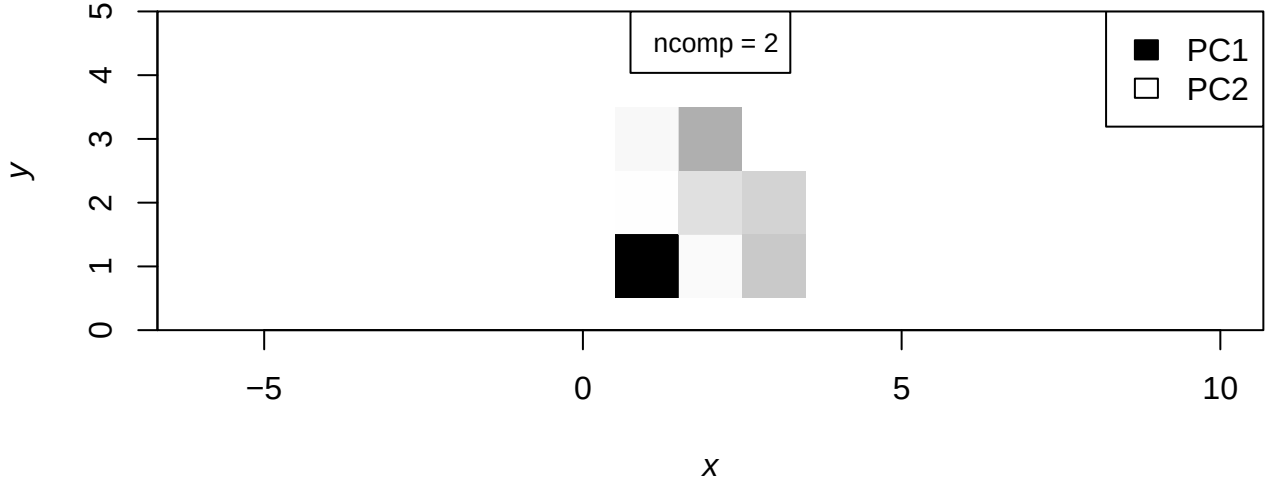


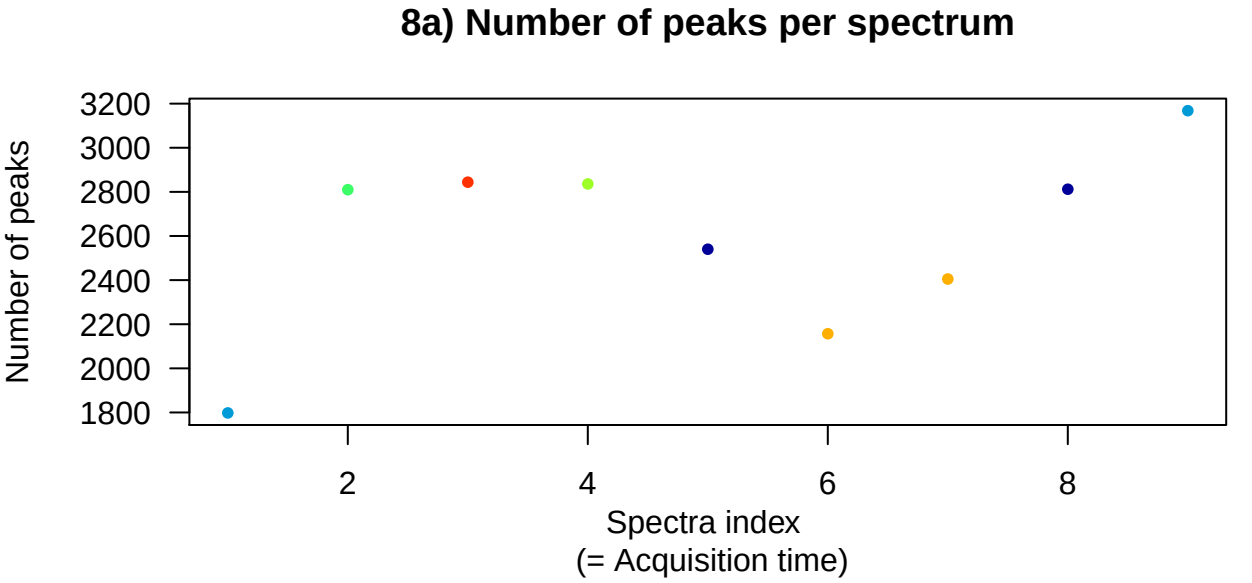
6) Most abundant m/z in each pixel

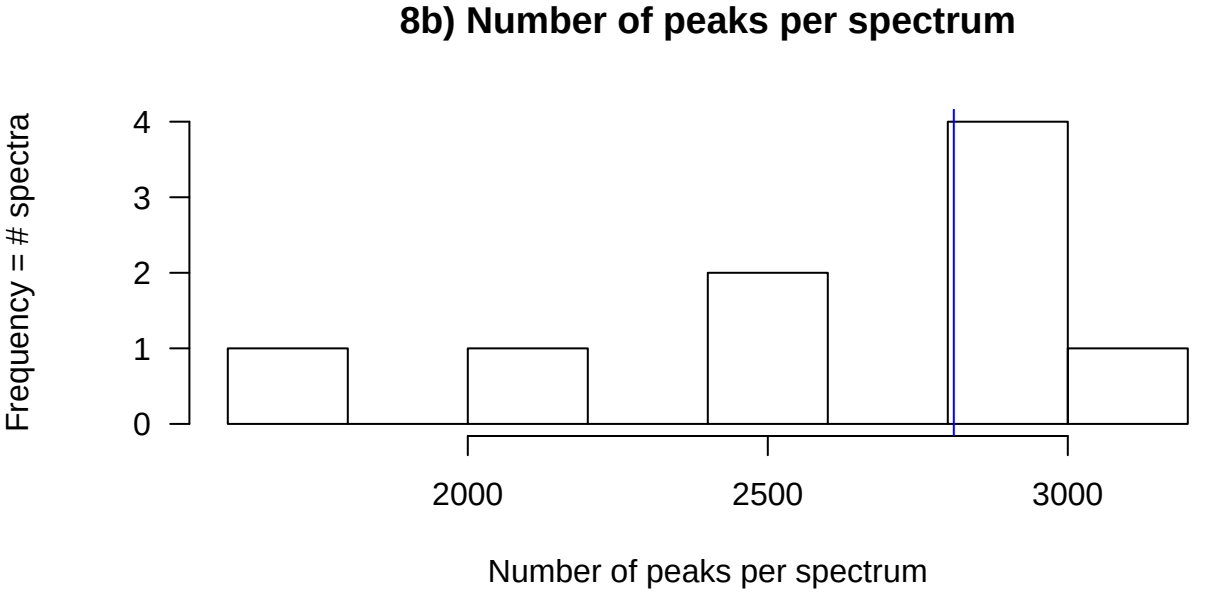


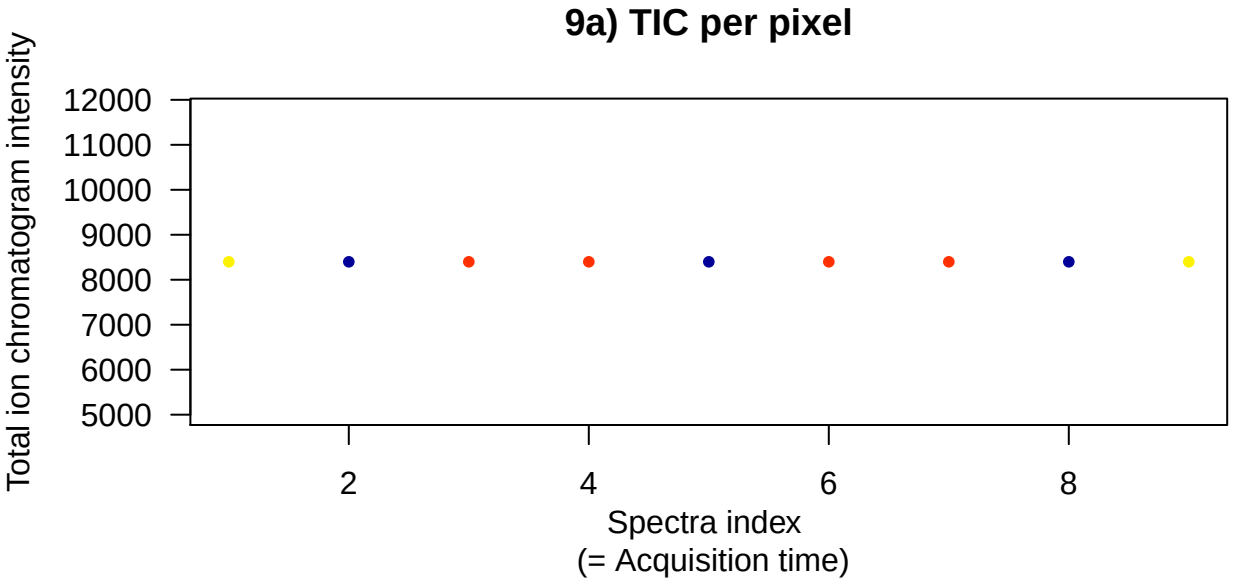
7) PCA for two components

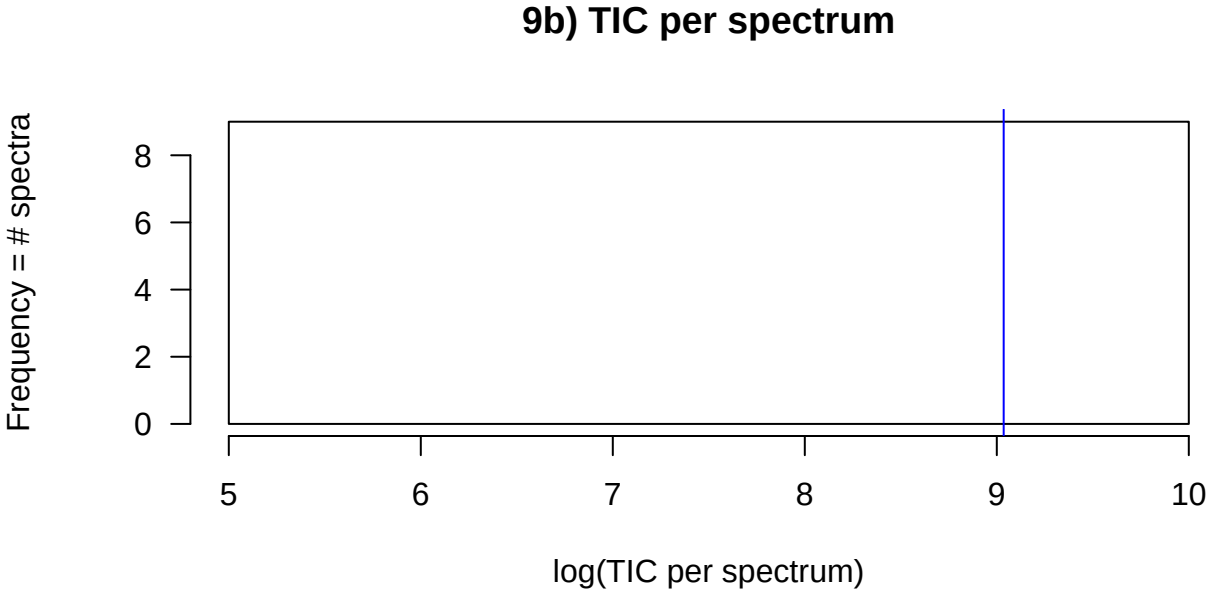




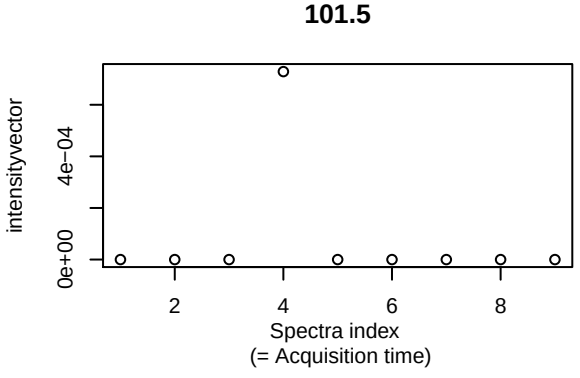

8a) Number of peaks per spectrum
Number of peaks
3200
3000
2800
2600
2400
2200
2000
1800
2
4
6
8
Spectra index
(= Acquisition time)

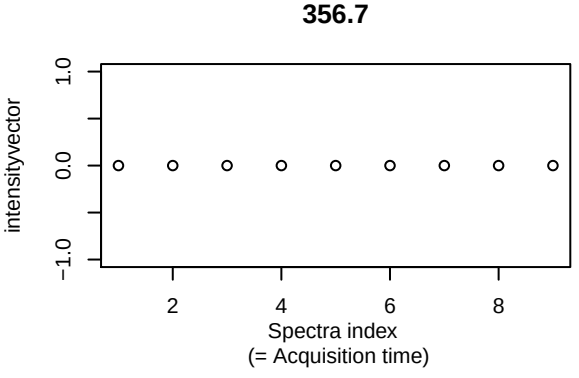

8b) Number of peaks per spectrum
Frequency = # spectra
4
3
2
1
0
2000
2500
3000
Number of peaks per spectrum

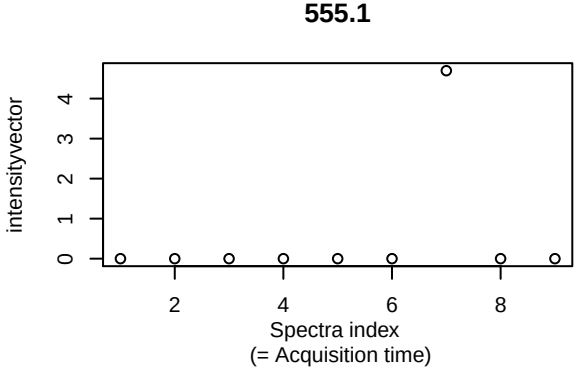

9a) TIC per pixel
Total ion chromatogram intensity
12000
11000
10000
9000
8000
7000
6000
5000
2
4
6
8
Spectra index
(= Acquisition time)

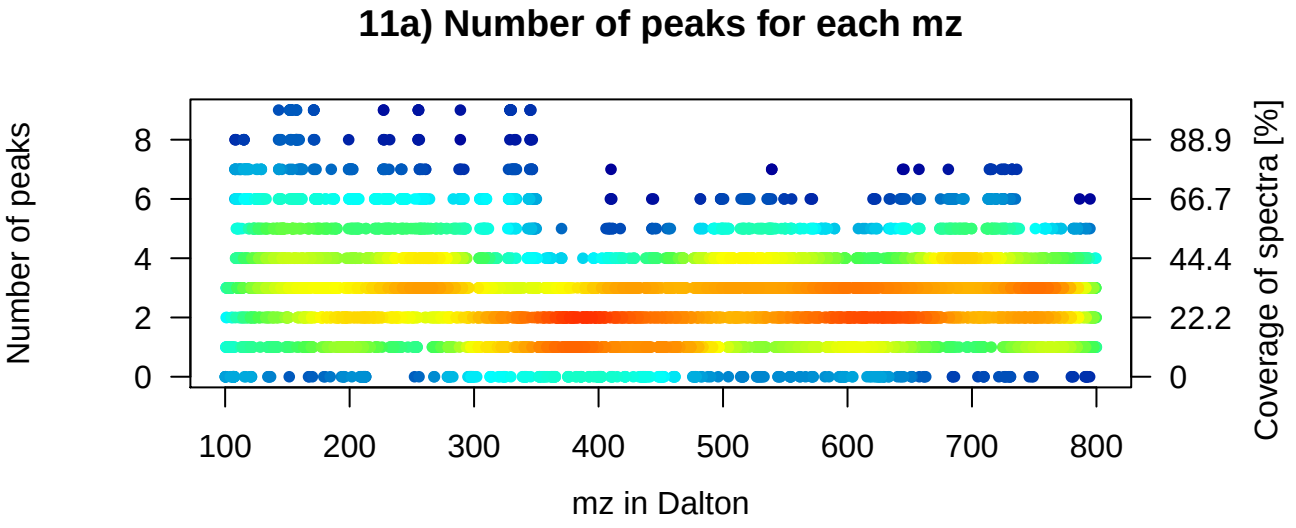

9b) TIC per spectrum
Frequency = # spectra
8
6
4
2
0
5
6
7
8
9
10
log(TIC per spectrum)

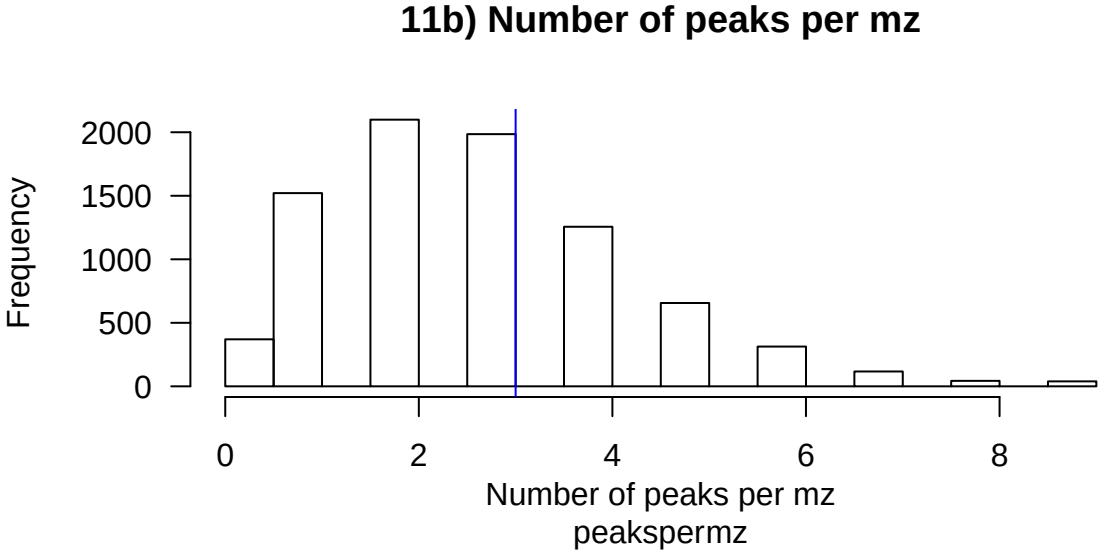
10) intensity of calibrants over acquisition

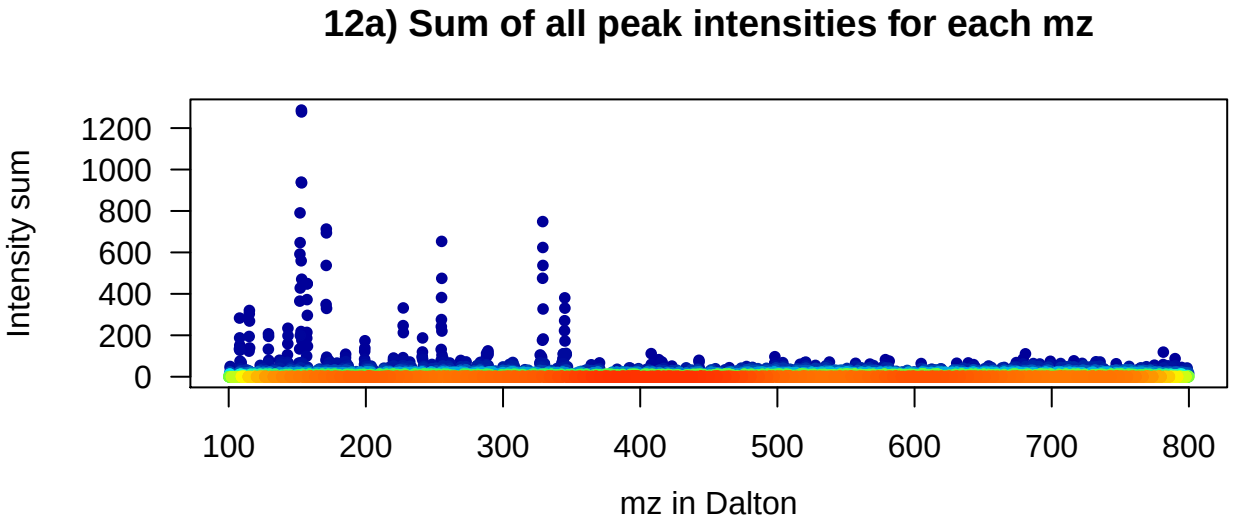


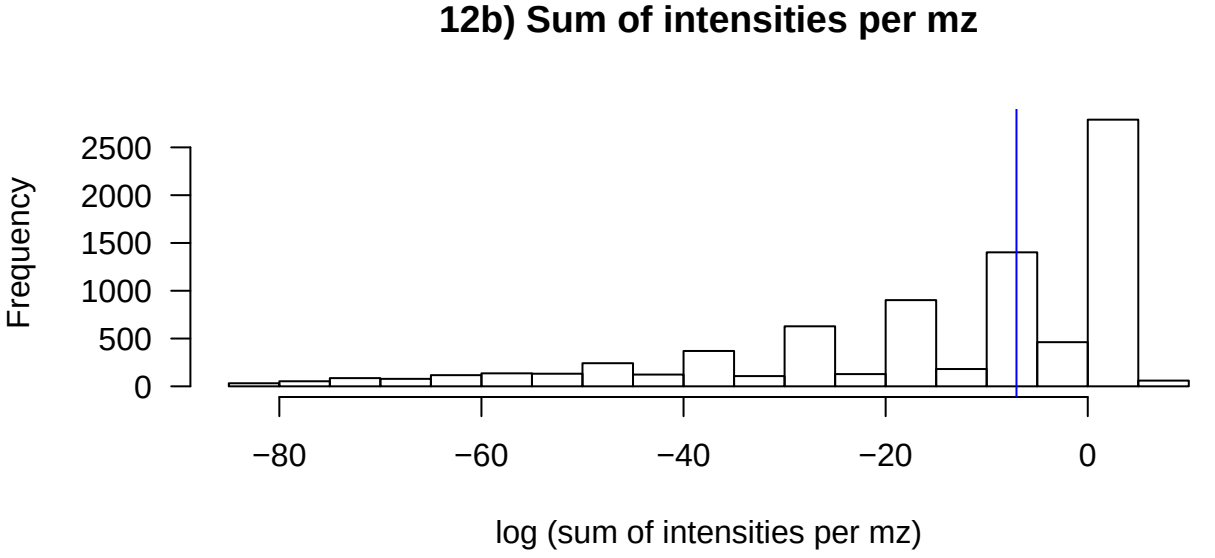


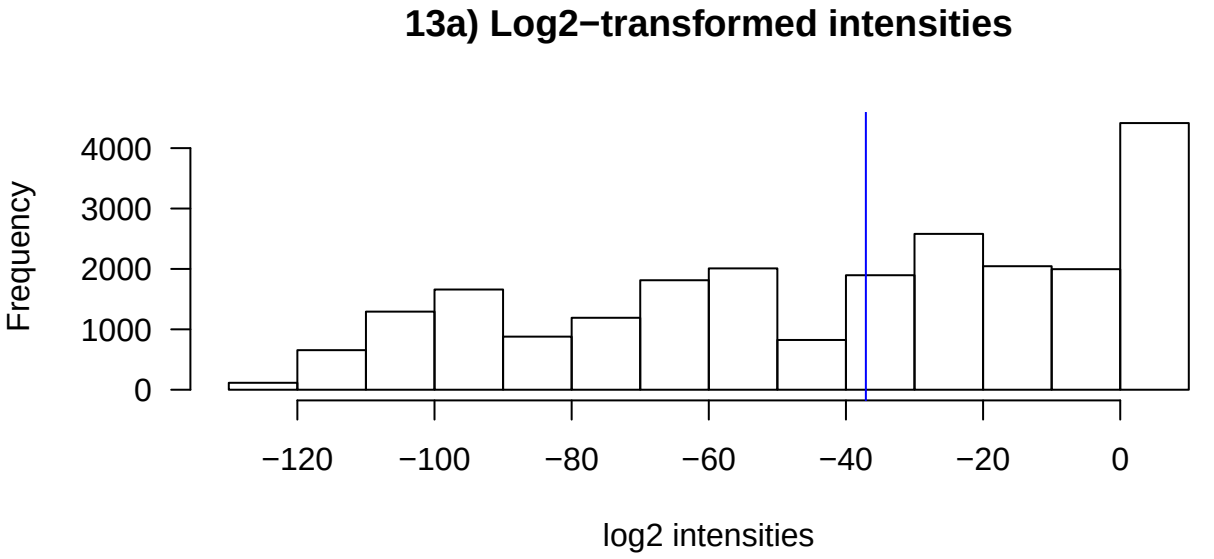


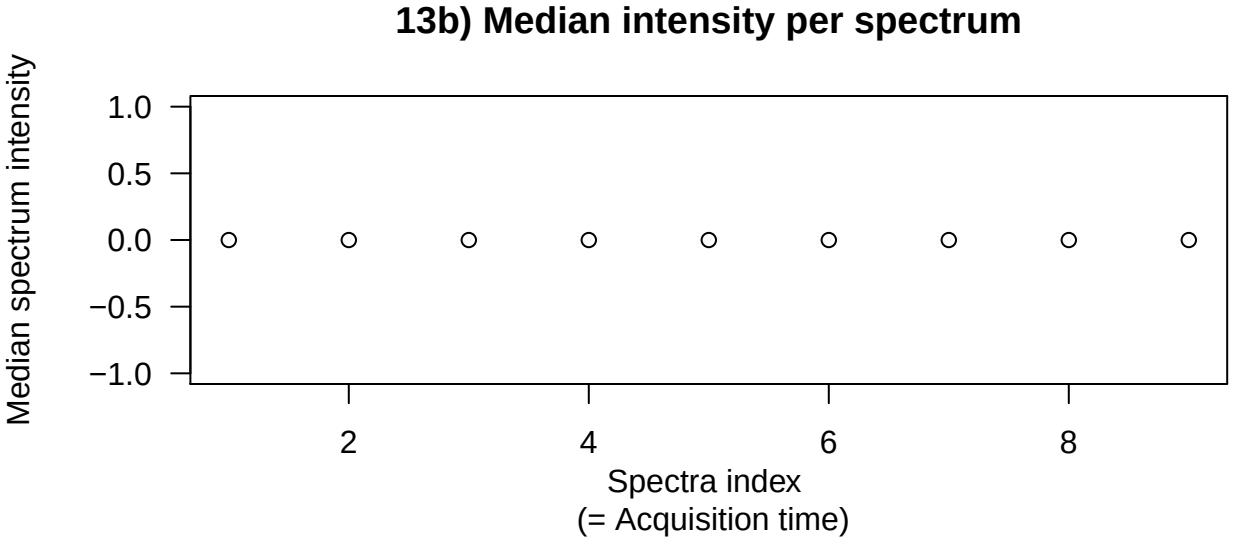

11a) Number of peaks for each mz
Number of peaks
0
2
4
6
8
Coverage of spectra [%]
0
22.2
44.4
66.7
88.9
100
200
300
400
500
600
700
800
mz in Dalton

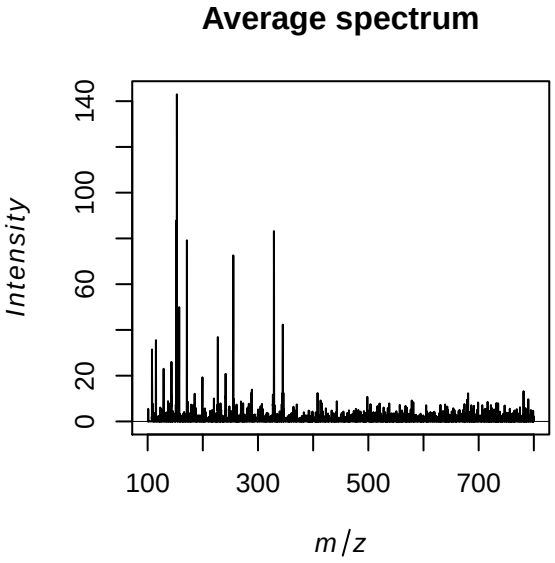

11b) Number of peaks per mz
Frequency
0
500
1000
1500
2000
0
2
4
6
8
Number of peaks per mz
peakspermz

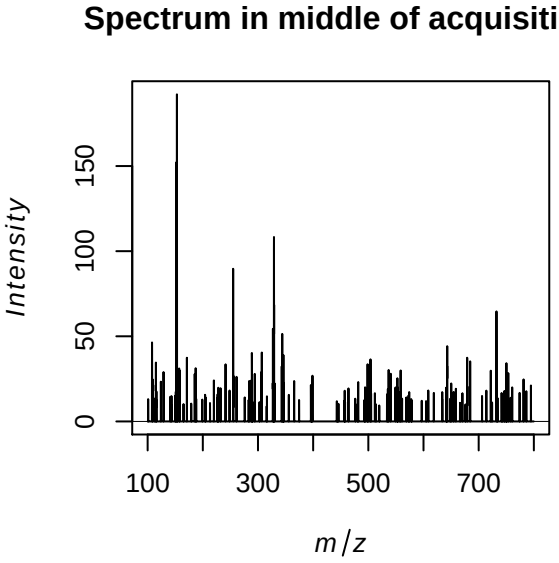

12a) Sum of all peak intensities for each mz
Intensity sum
1200
1000
800
600
400
200
0
100
200
300
400
500
600
700
800
mz in Dalton

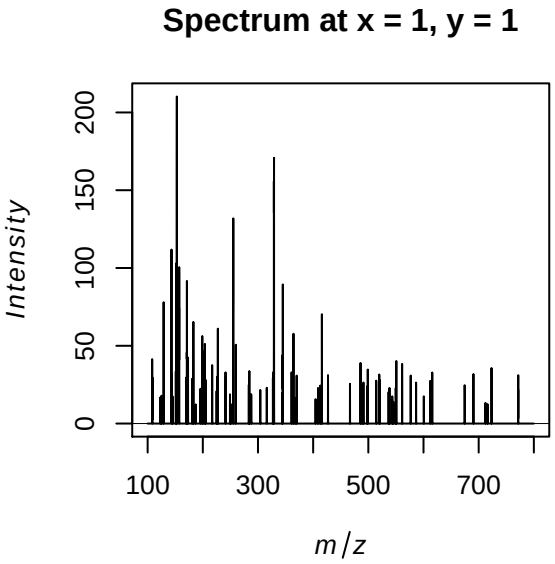

12b) Sum of intensities per mz
Frequency
2500
2000
1500
1000
500
0
−80
−60
−40
−20
0
log (sum of intensities per mz)

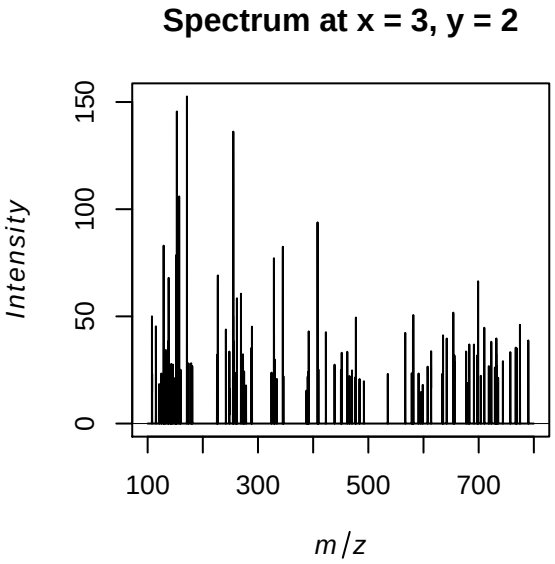

13a) Log2−transformed intensities
Frequency
4000
3000
2000
1000
0
−120
−100
−80
−60
−40
−20
0
log2 intensities

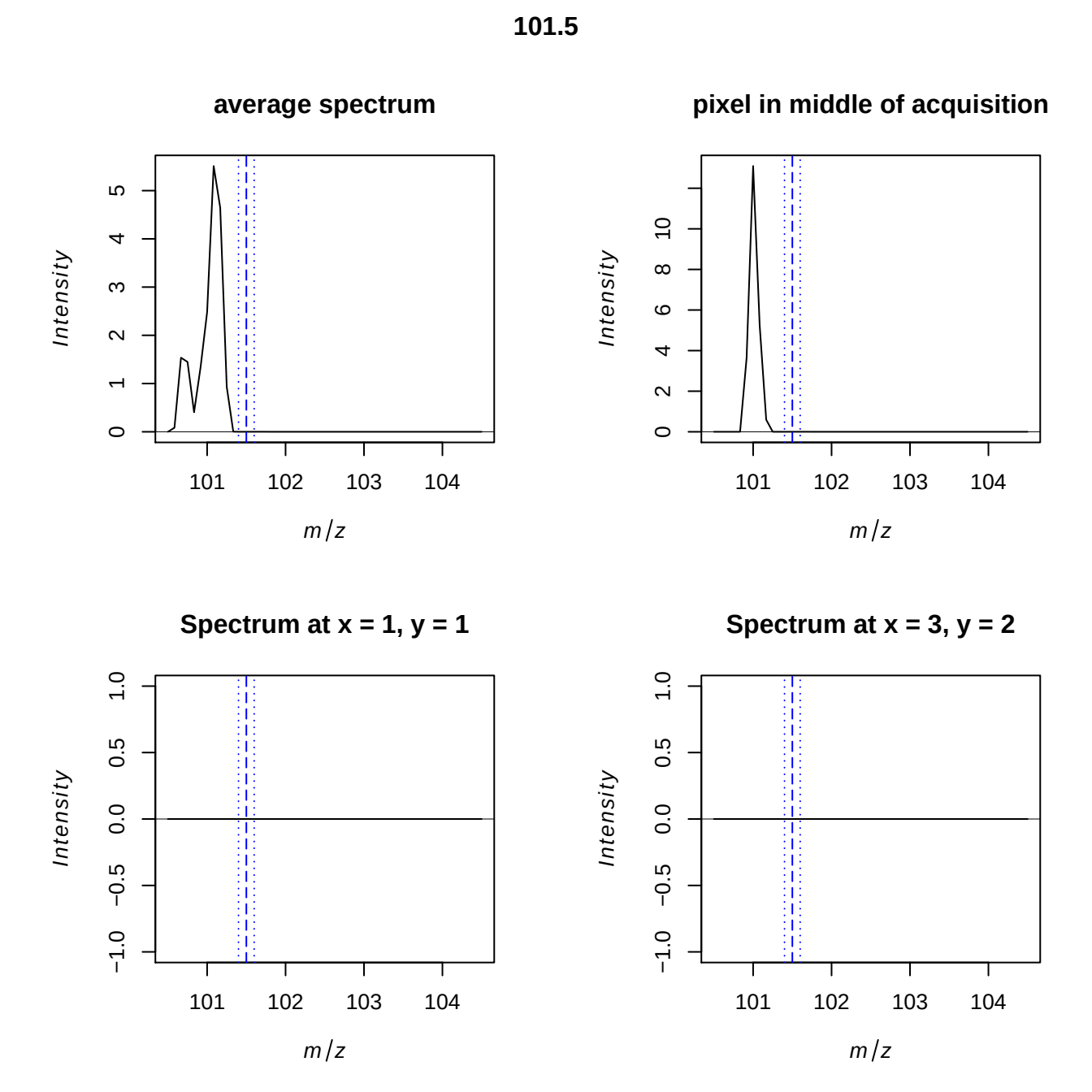

13b) Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
Spectra index
(= Acquisition time)

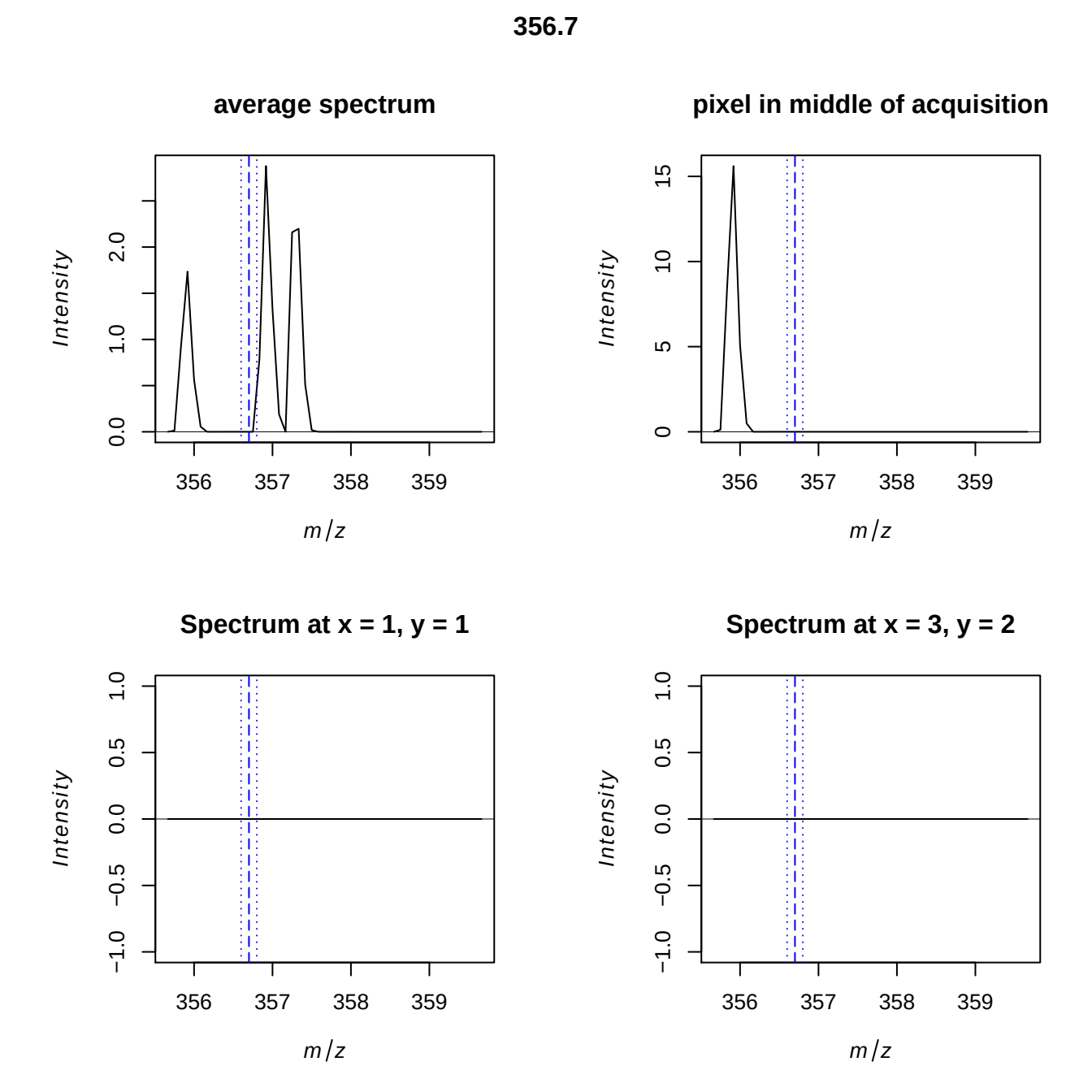

Average spectrum
Intensity
0
20
60
100
140
100
300
500
700
m/z


Spectrum in middle of acquisition
Intensity
0
50
100
150
100
300
500
700
m/z

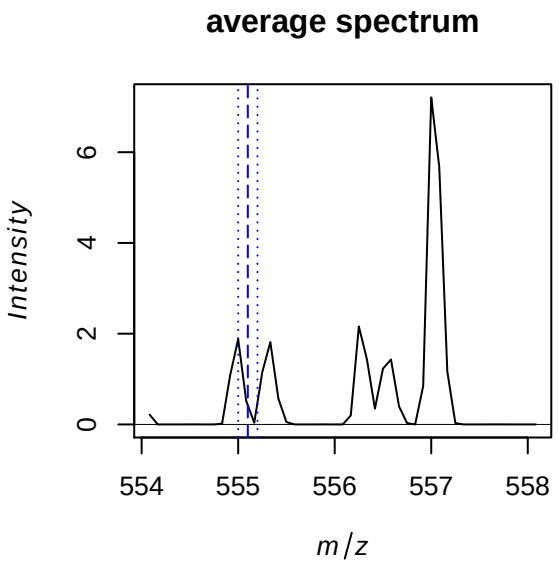

Spectrum at x = 1, y = 1
Intensity
0
50
100
150
200
100
300
500
700
m/z

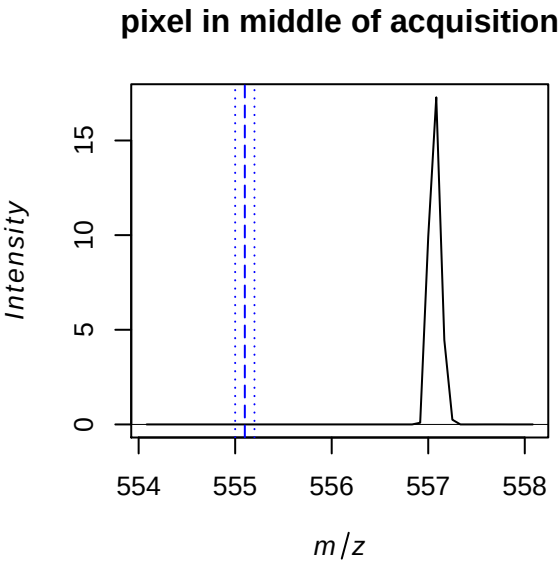

Spectrum at x = 3, y = 2
Intensity
0
50
100
150
100
300
500
700
m/z

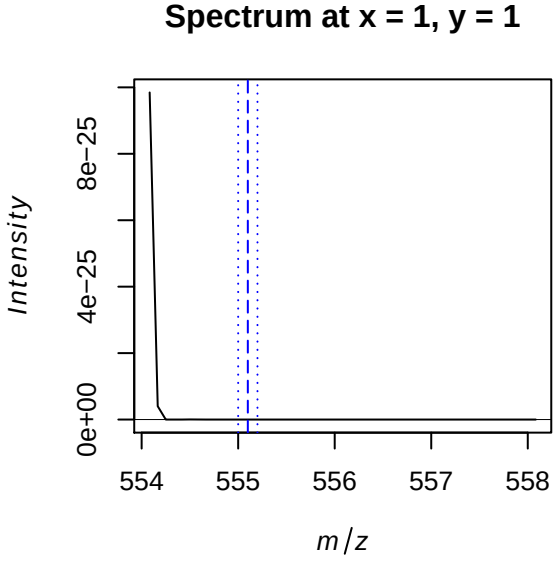

101.5
average spectrum
pixel in middle of acquisition
Spectrum at x = 1, y = 1
Spectrum at x = 3, y = 2
Intensity
m/z
0
1
2
3
4
5
6
8
10
−1.0
−0.5
0.0
0.5
1.0
101
102
103
104

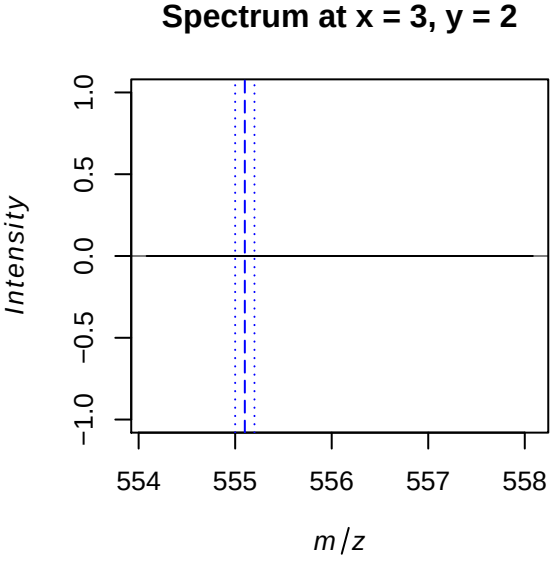

356.7
average spectrum
pixel in middle of acquisition
Spectrum at x = 1, y = 1
Spectrum at x = 3, y = 2
Intensity
m/z
0.0
1.0
2.0
0
5
10
15
−1.0
−0.5
0.5
356
357
358
359

555.1


average spectrum
Intensity
0
2
4
6
554
555
556
557
558
m/z


pixel in middle of acquisition
Intensity
0
5
10
15
554
555
556
557
558
m/z


Spectrum at x = 1, y = 1
Intensity
0e+00
4e−25
8e−25
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