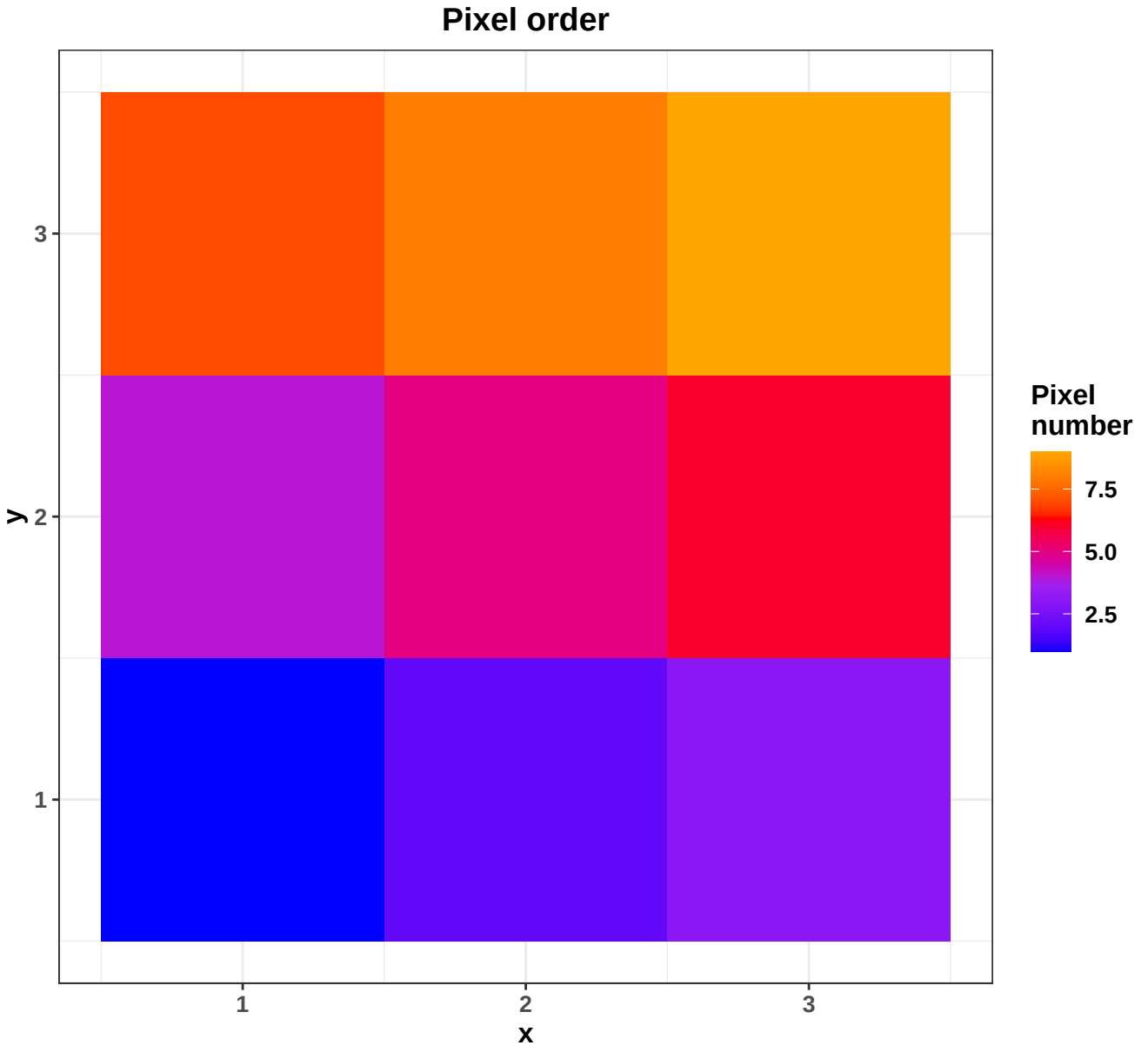
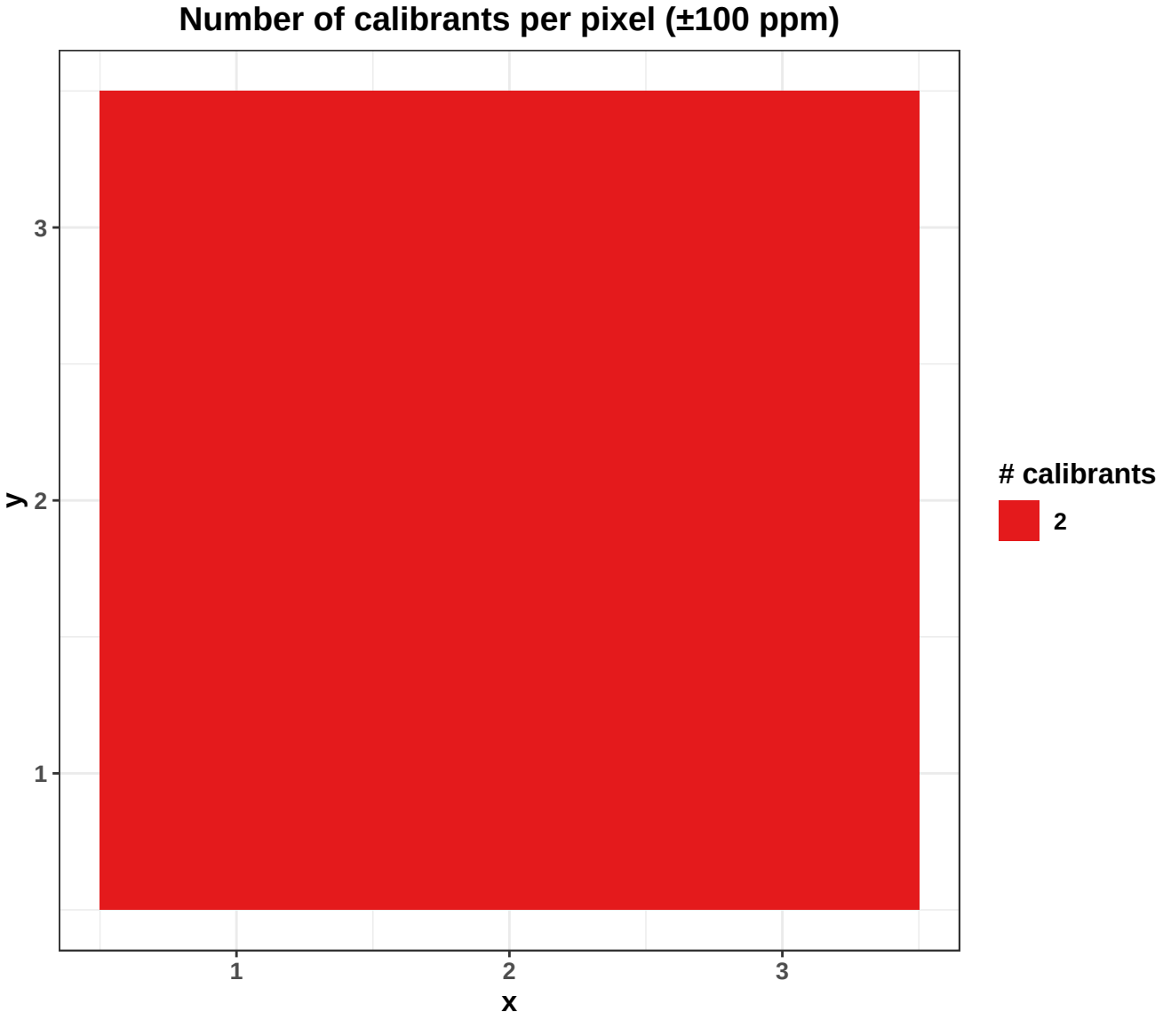
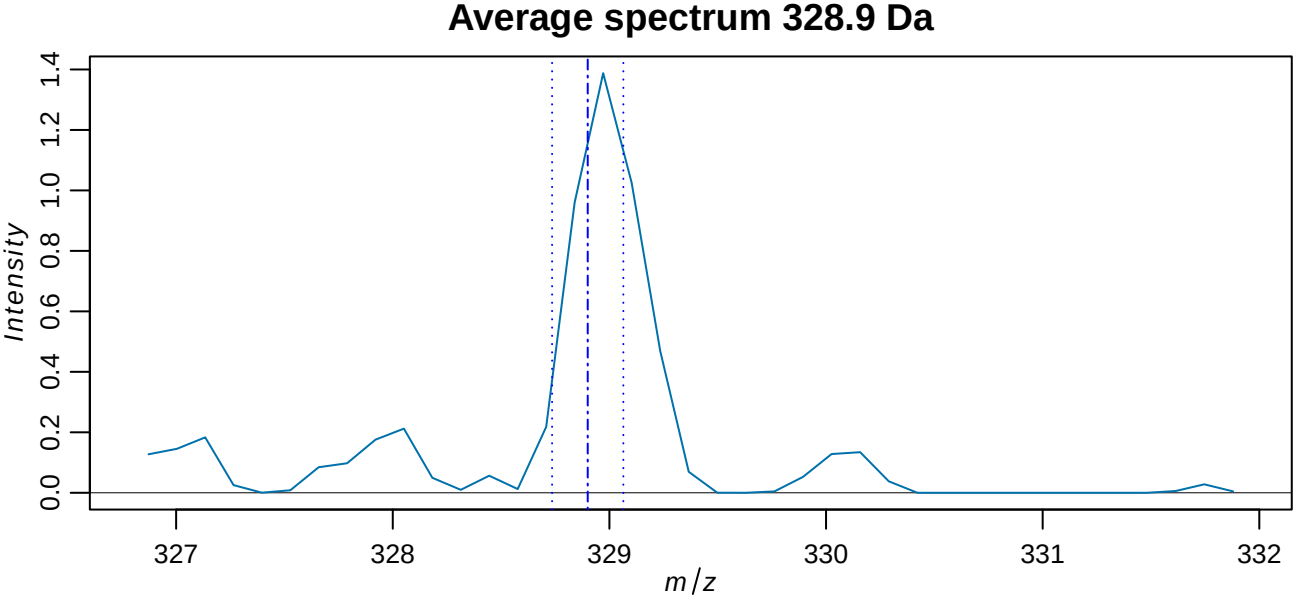
Testfile_imzml

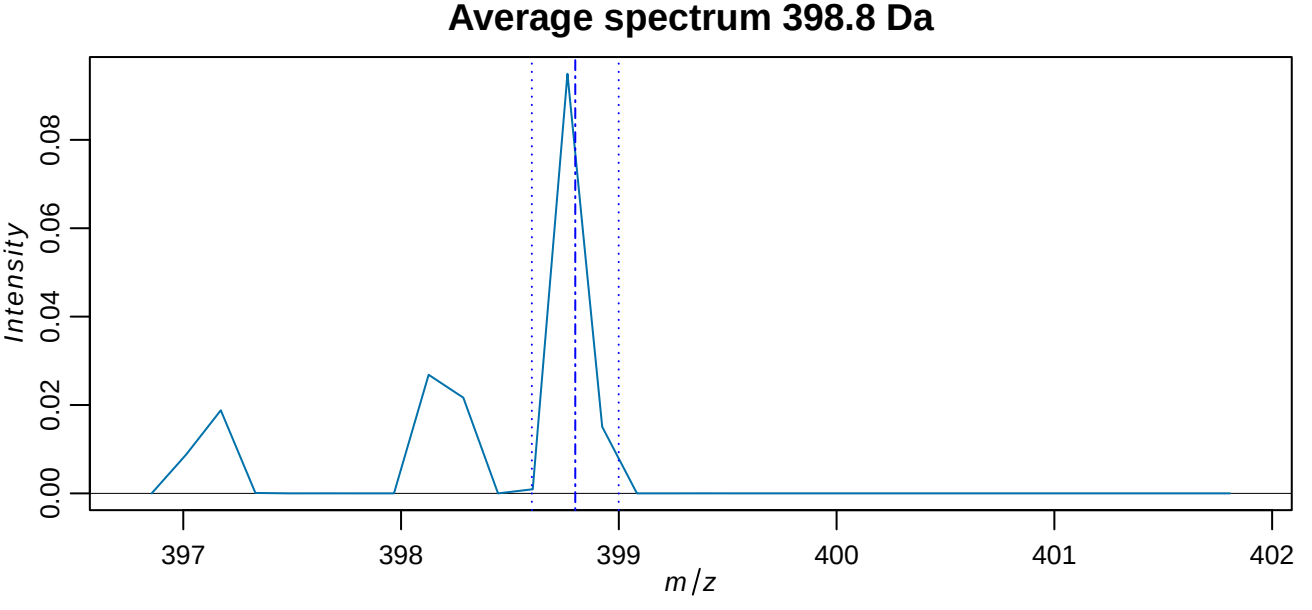
properties	values
Number of m/z features	5199
Range of m/z values	100 − 799.81
Number of pixels	9
Range of x coordinates	1 − 3
Range of y coordinates	1 − 3
Range of intensities	0 − 9.04
Number of NA intensities	0
Number of Inf intensities	0
Number of duplicated coordinates	0
Median of intensities	0
Intensities > 0	40.21 %
Number of empty spectra	0
Median TIC ± sd	125.9 ± 36
Median # peaks per spectrum ± sd	2198 ± 280
maximum m/z window size	0.32
Centroided	FALSE
input m/z (#valid/#input) in inputcalibrantfile1.tabular	3 / 3

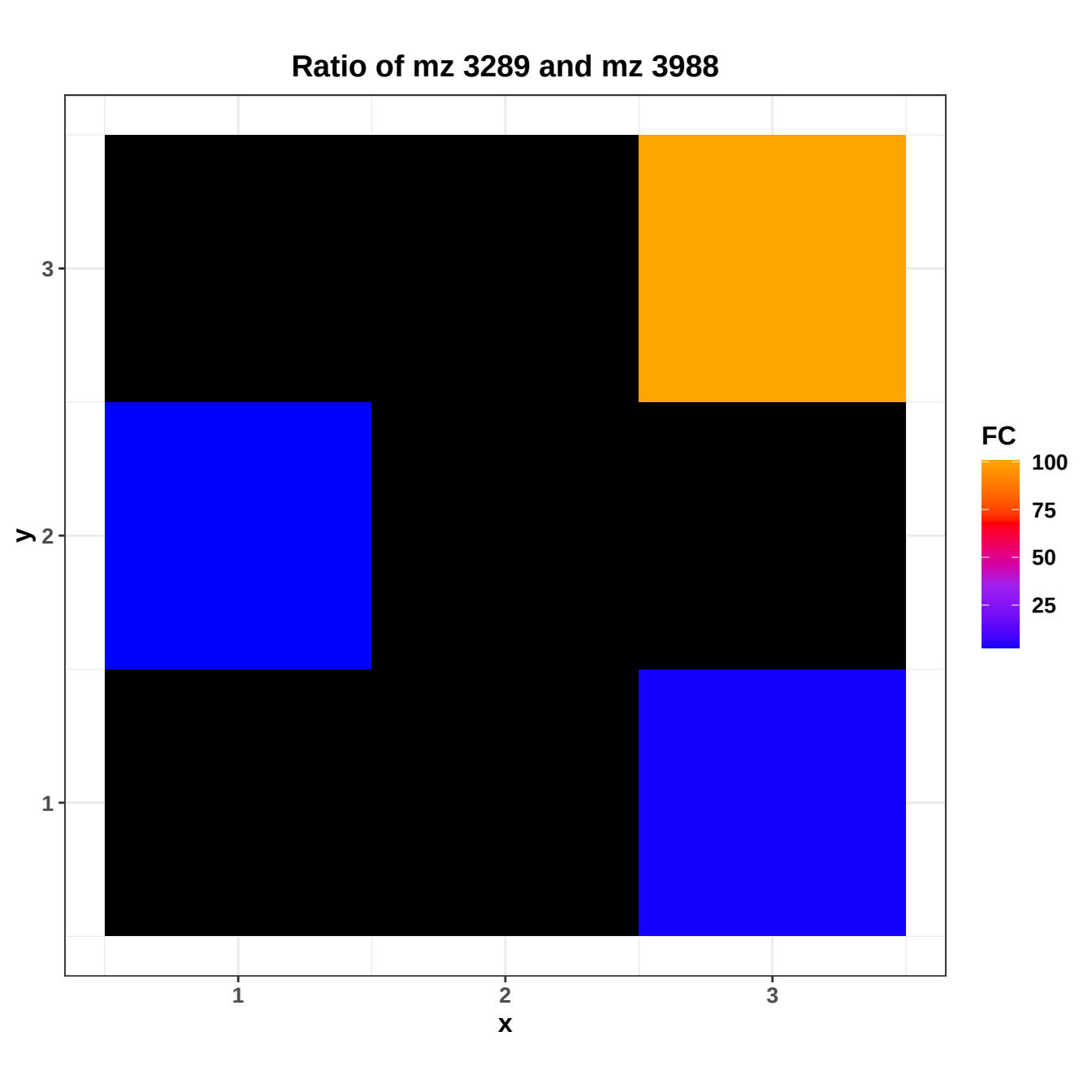

Pixel order
3
2
1
y
1
2
3
x
Pixel number
7.5
5.0
2.5

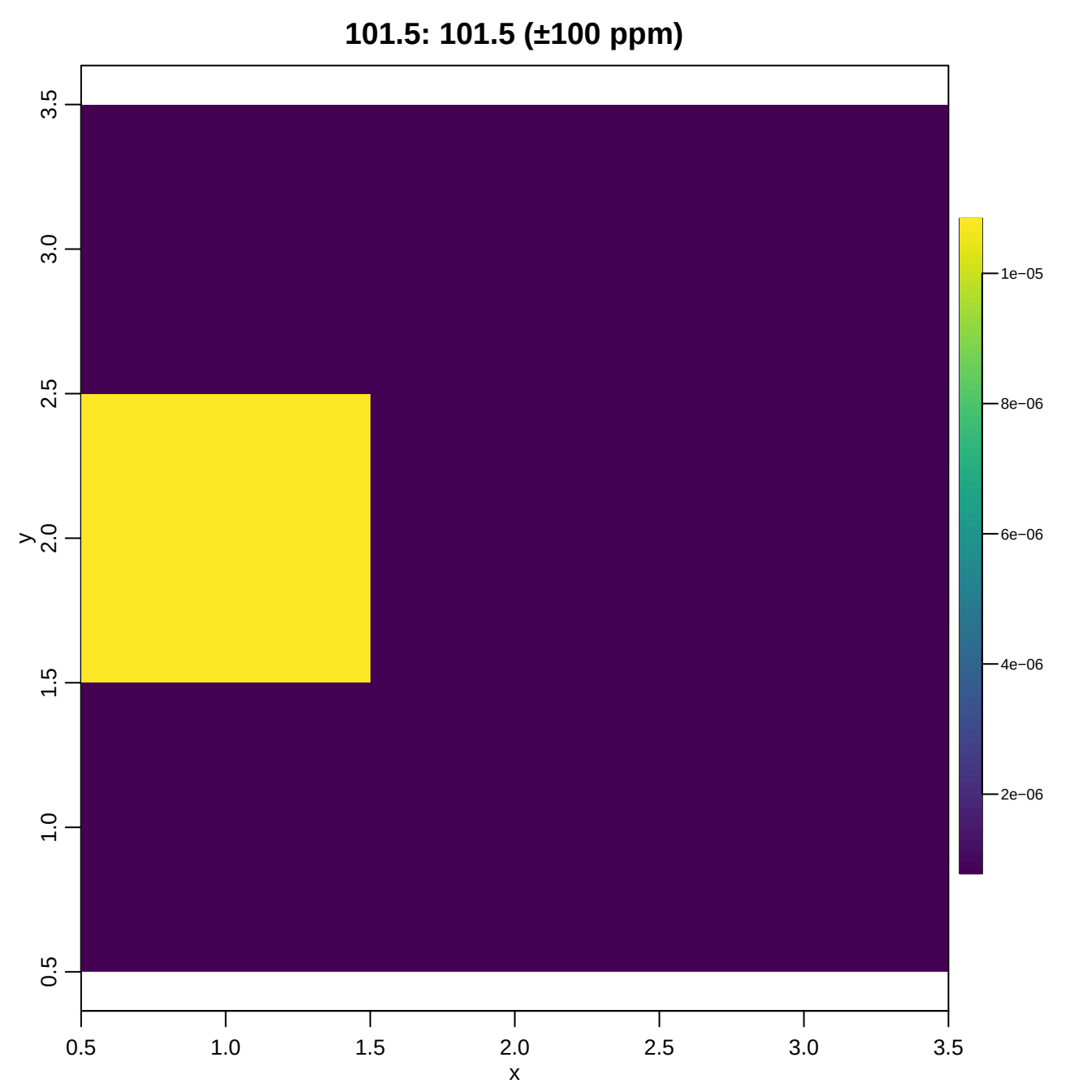

Number of calibrants per pixel (±100 ppm)
3
2
1
y
1
2
3
x
calibrants
2

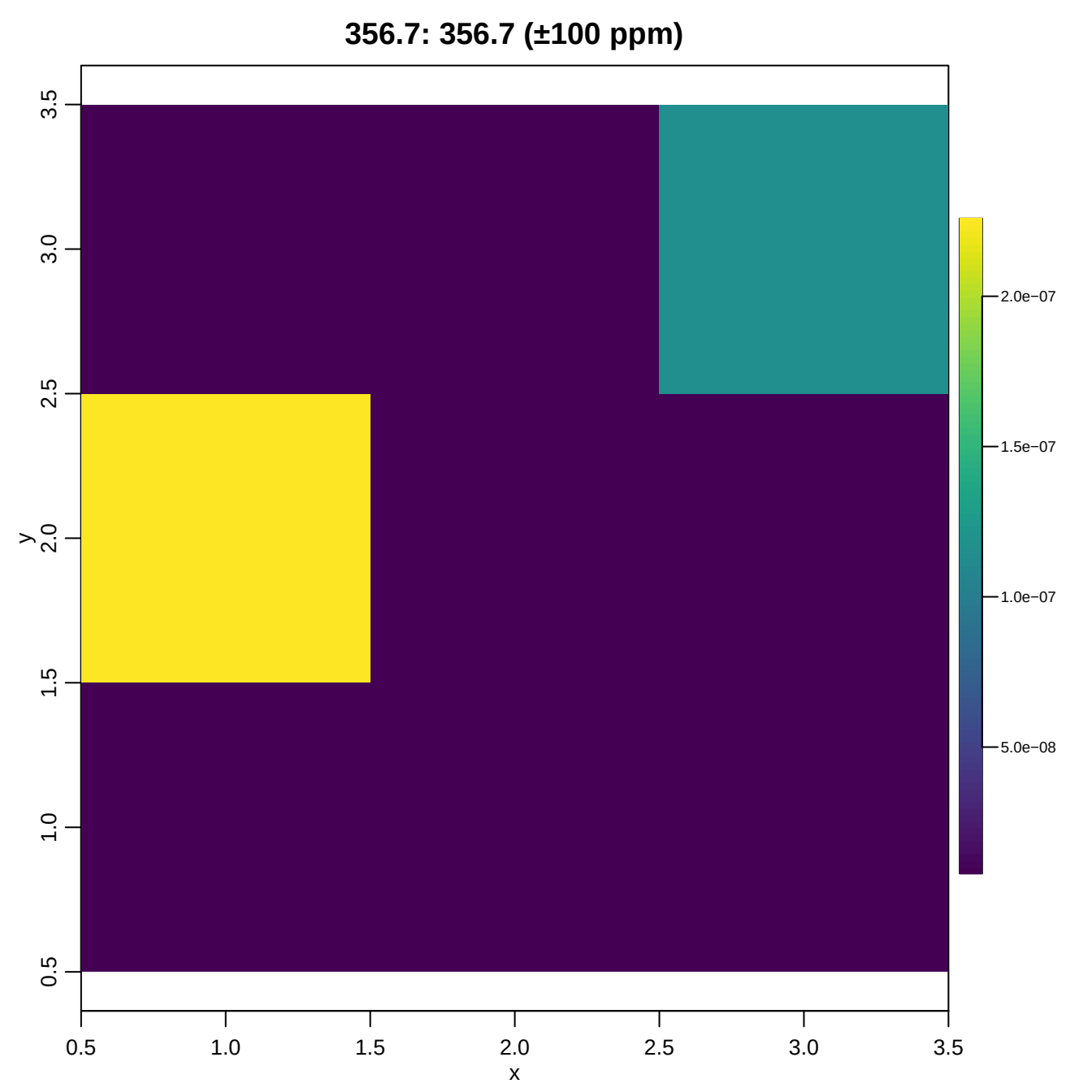
Control of fold change plot

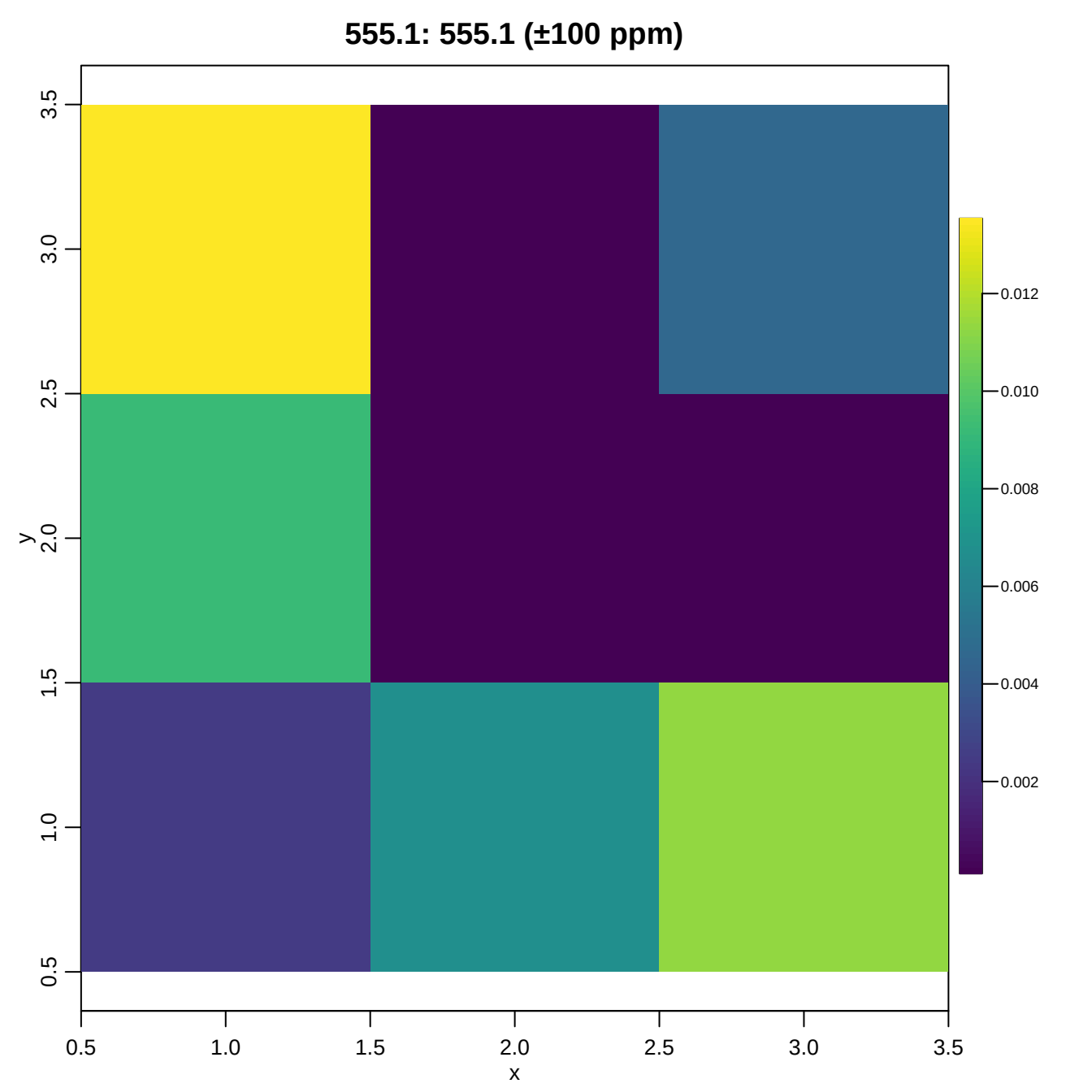


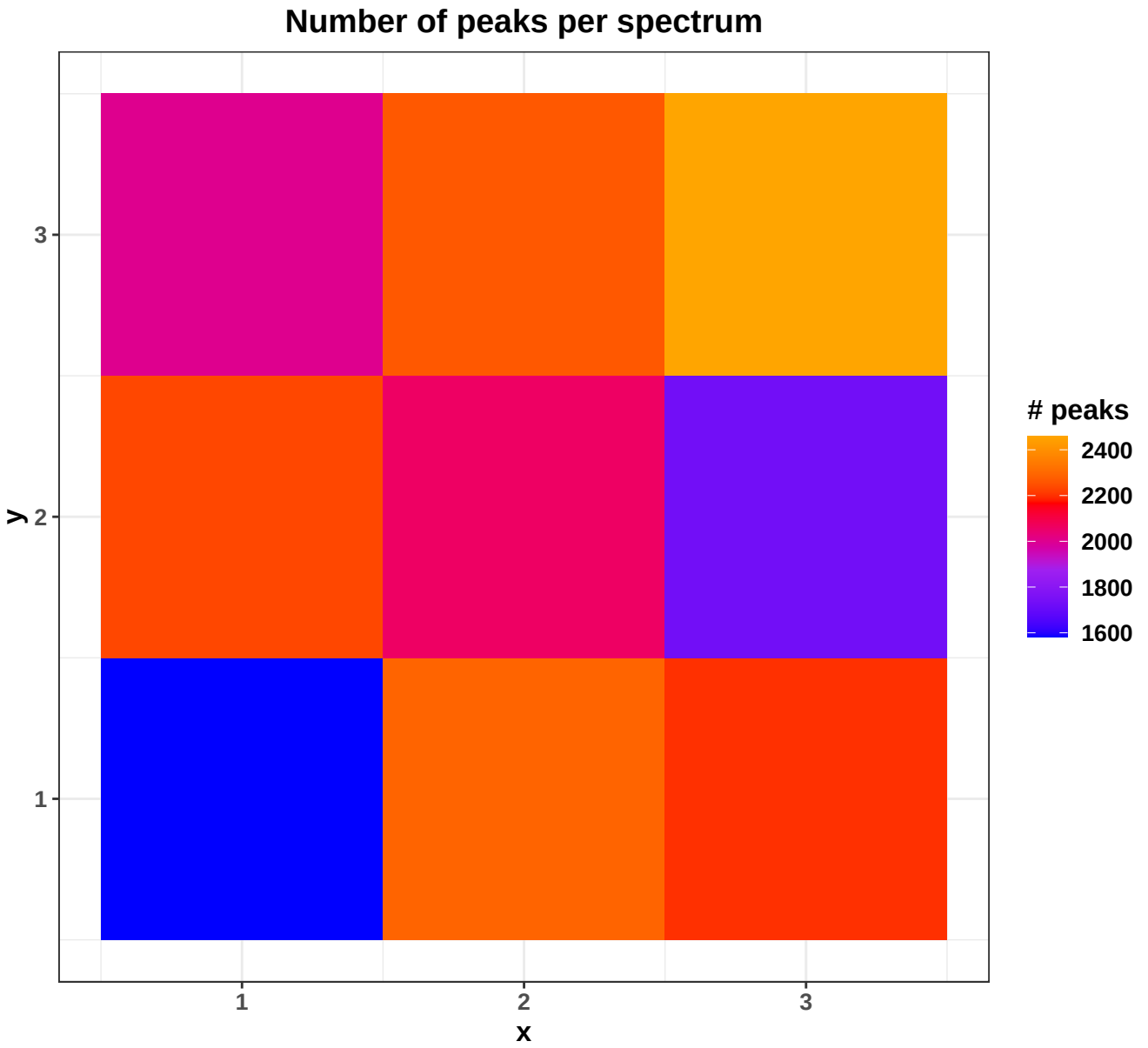


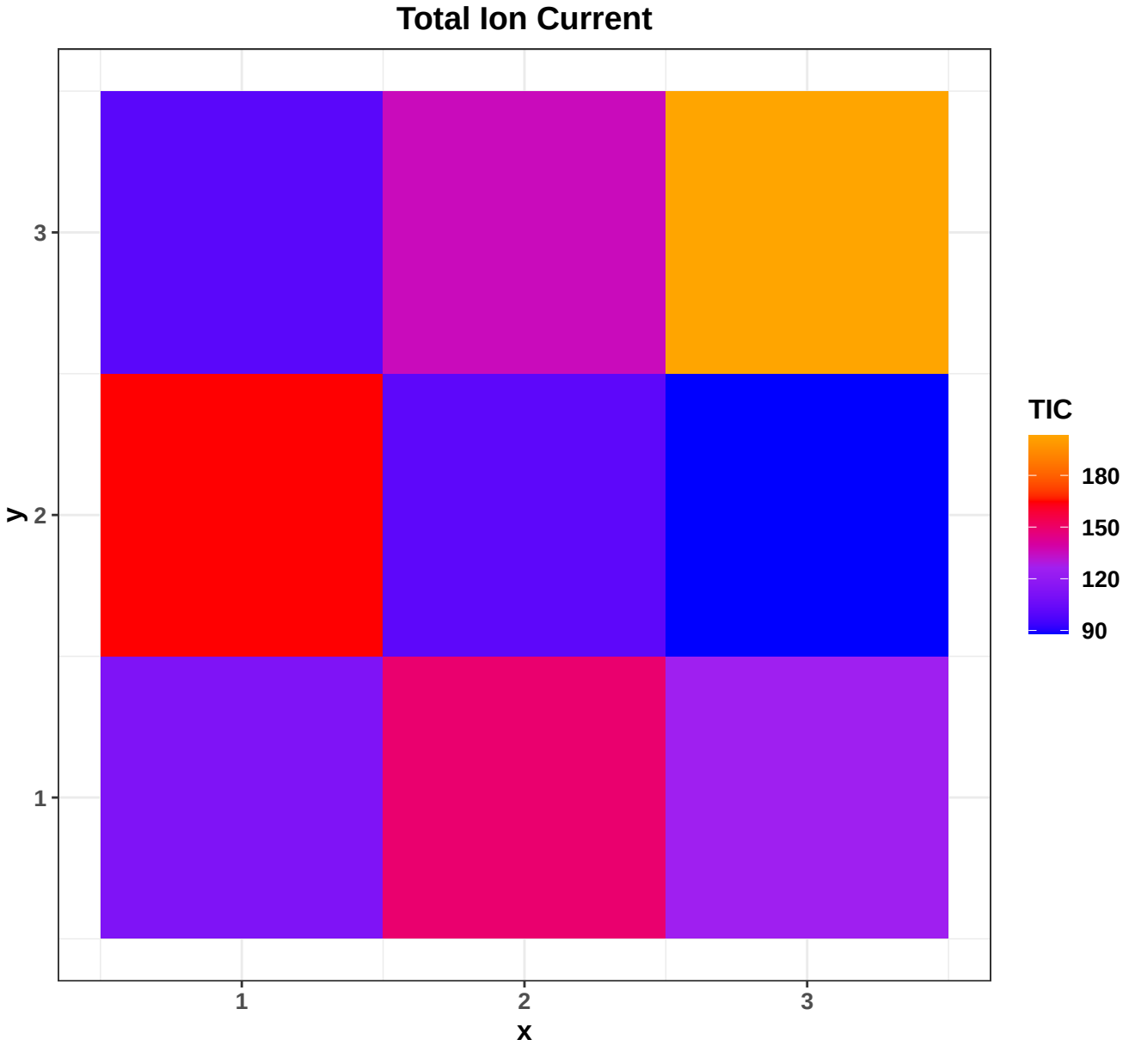

Ratio of mz 3289 and mz 3988
y
3
2
1
x
1
2
3
FC
100
75
50
25

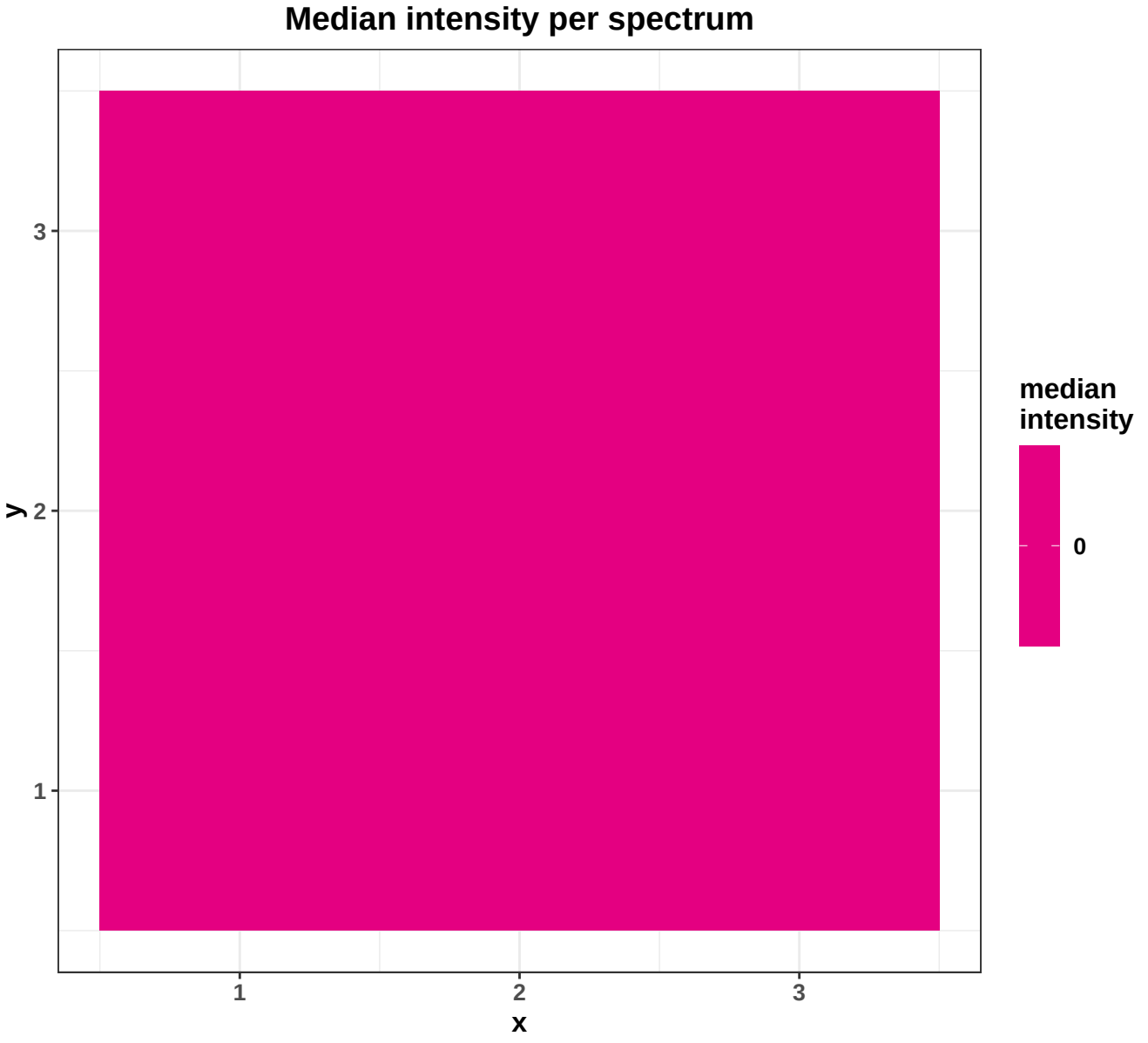

101.5: 101.5 (±100 ppm)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
y
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x
1e−05
8e−06
6e−06
4e−06
2e−06

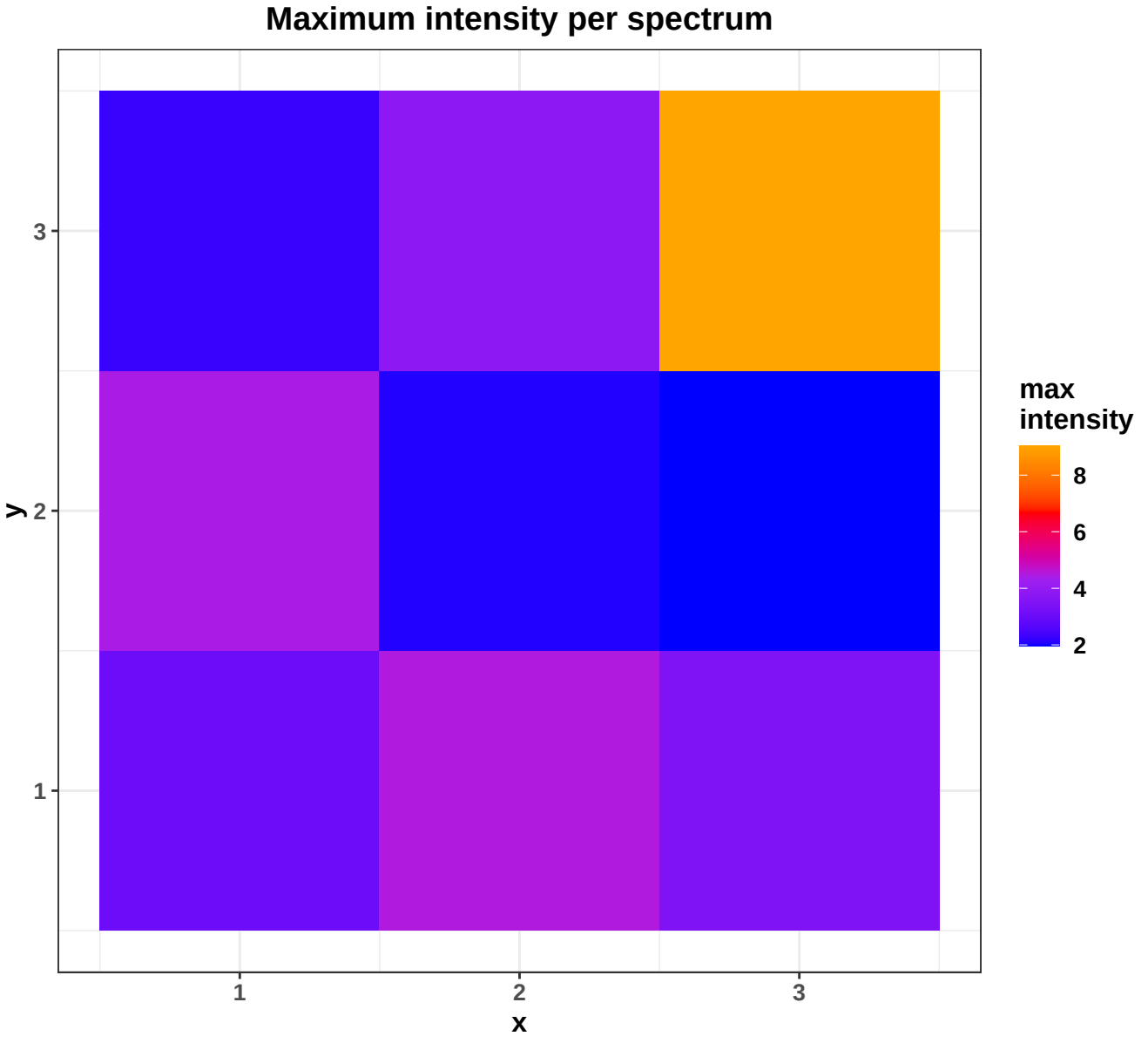

356.7: 356.7 (±100 ppm)
y
x
0.5
1.0
1.5
2.0
2.5
3.0
3.5
2.0e−07
1.5e−07
1.0e−07
5.0e−08

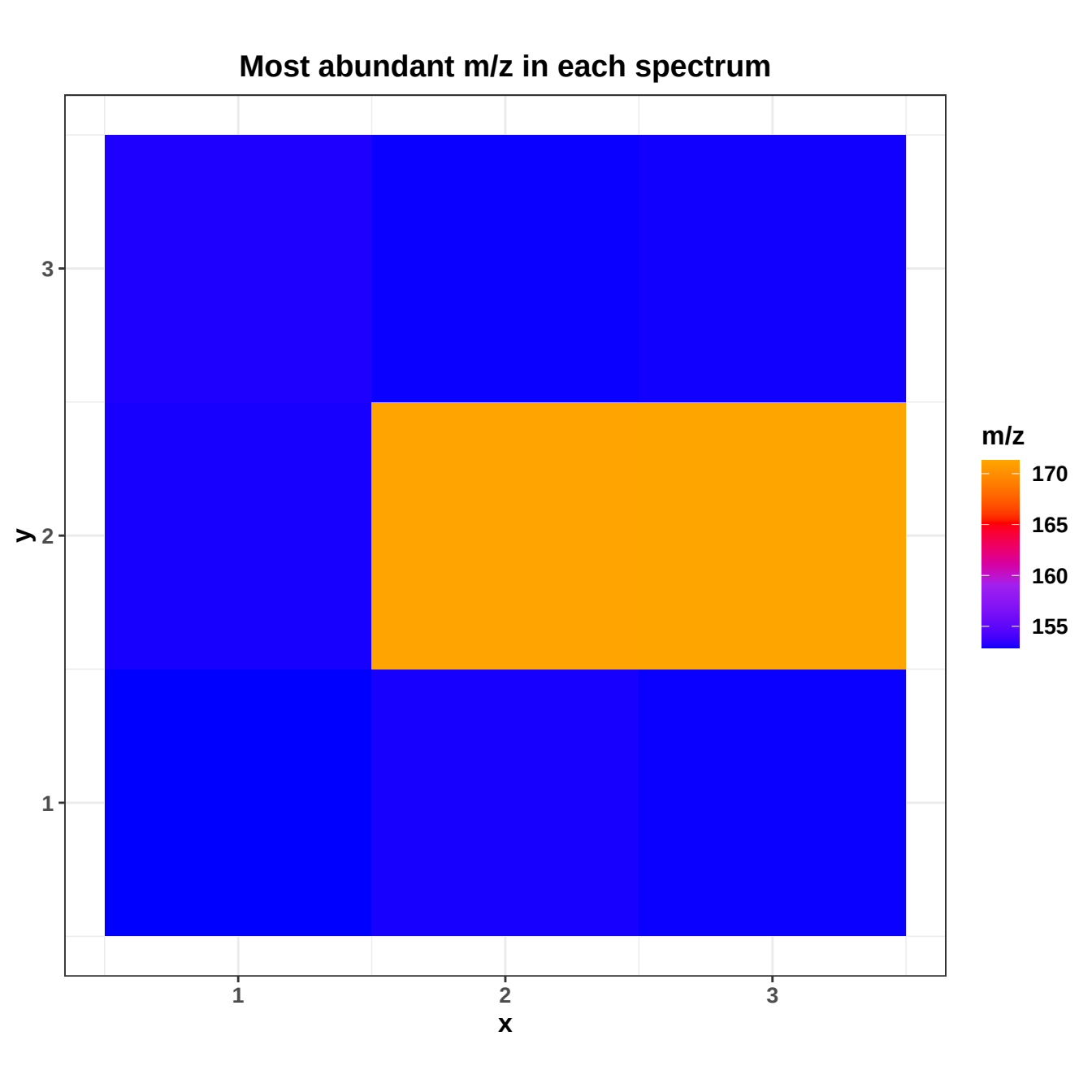

555.1: 555.1 (±100 ppm)
y
x
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0.012
0.010
0.008
0.006
0.004
0.002

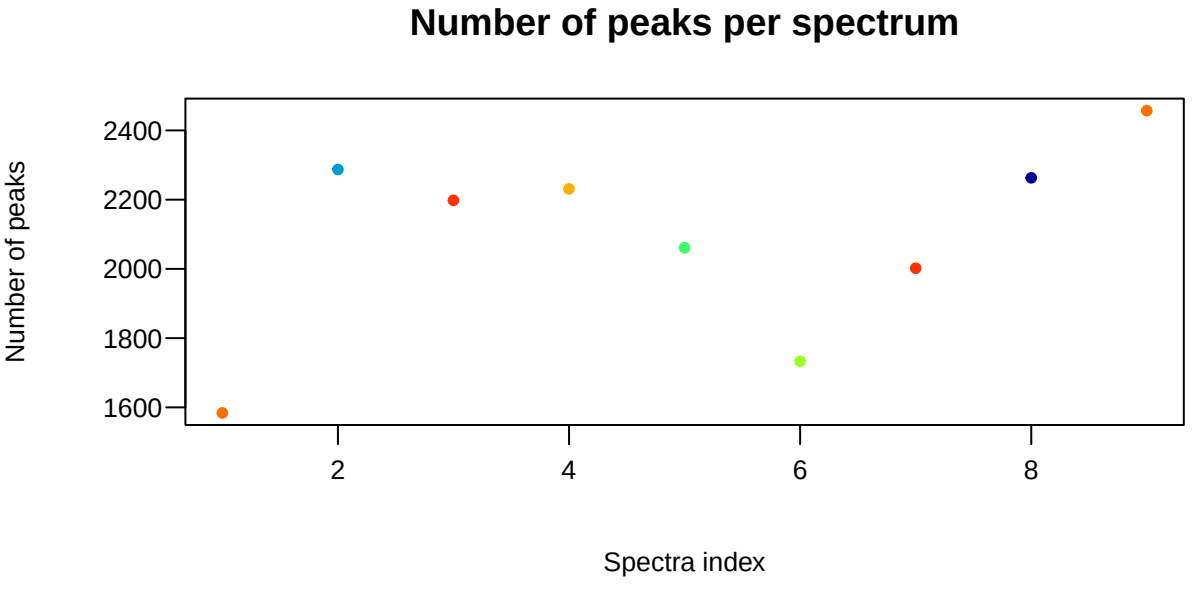

Number of peaks per spectrum
y
3
2
1
x
1
2
3
peaks
2400
2200
2000
1800
1600

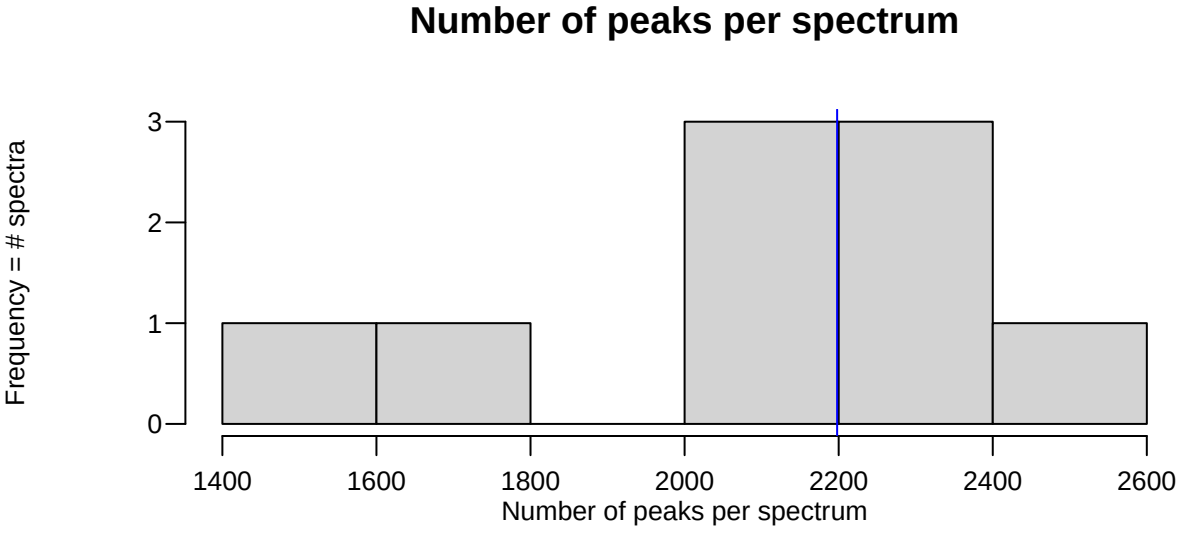

Total Ion Current
y
3
2
1
x
1
2
3
TIC
180
150
120
90

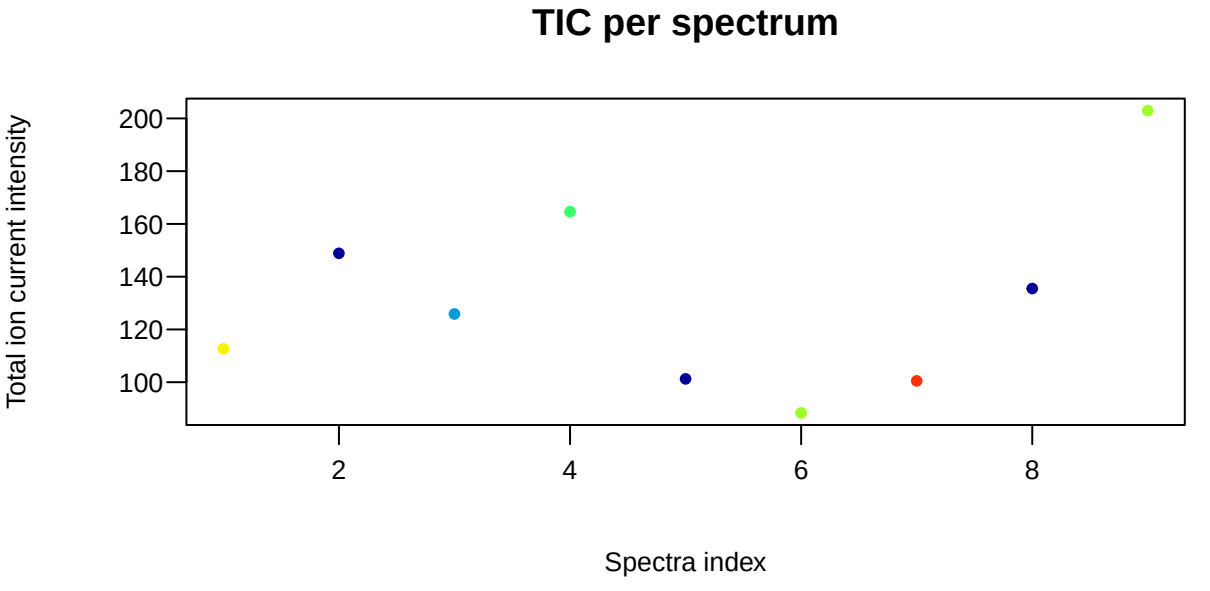

Median intensity per spectrum
3
2
1
y
1
2
3
x
median
intensity
0

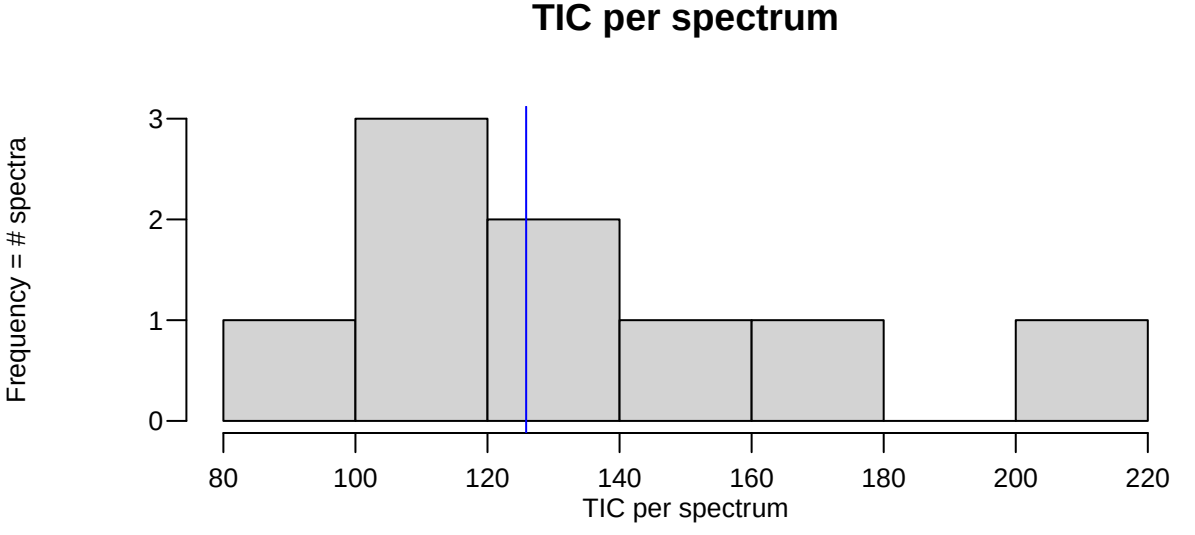

Maximum intensity per spectrum
y
3
2
1
x
1
2
3
max intensity
8
6
4
2

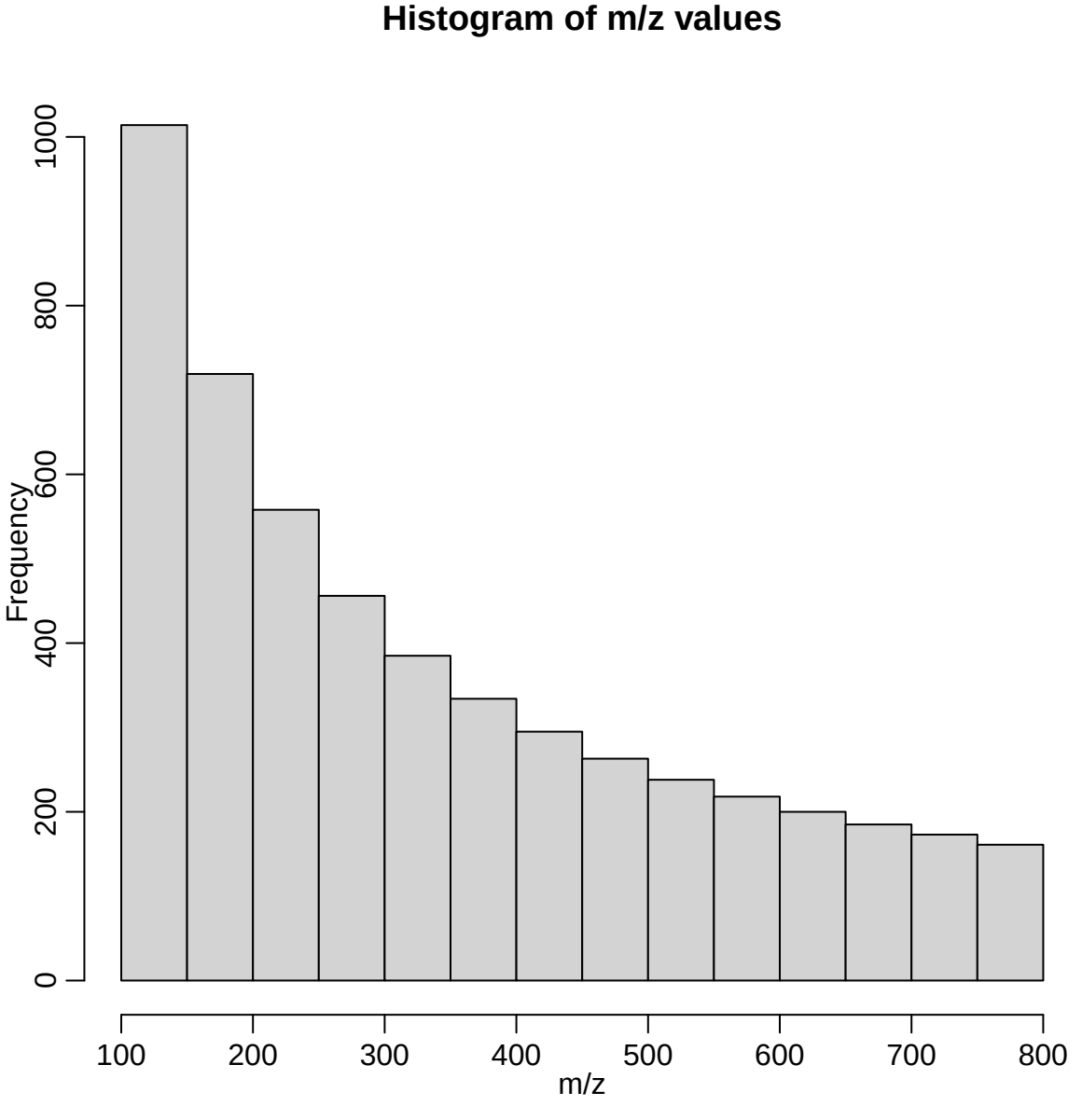

Most abundant m/z in each spectrum
y
3
2
1
x
1
2
3
m/z
170
165
160
155

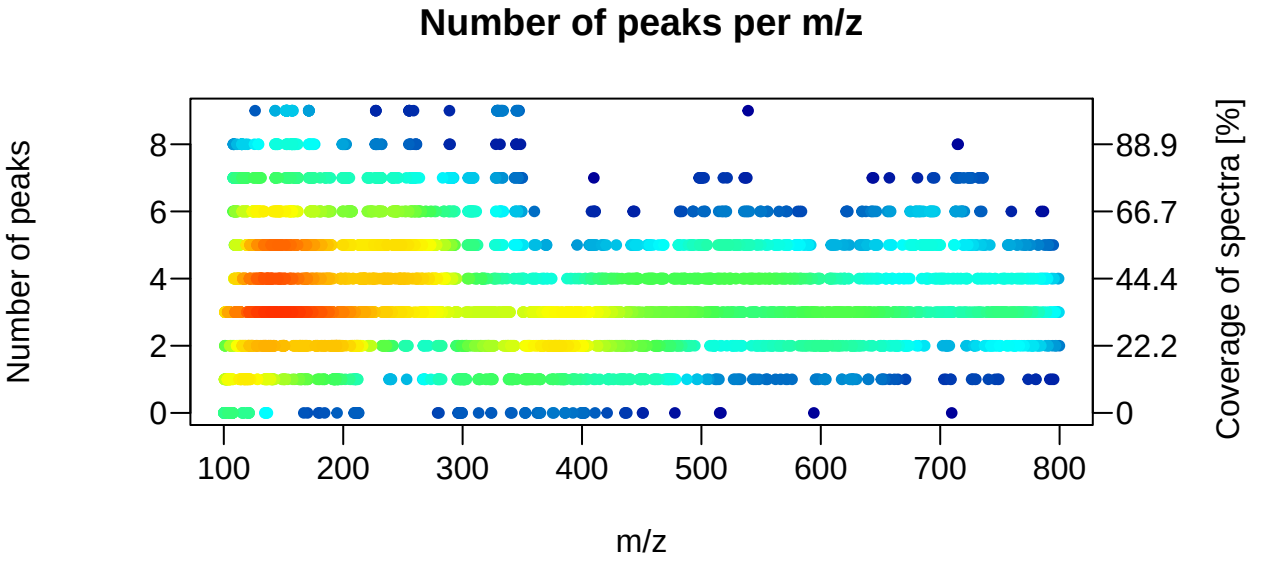

Number of peaks per spectrum
Number of peaks
2400
2200
2000
1800
1600
2
4
6
8
Spectra index

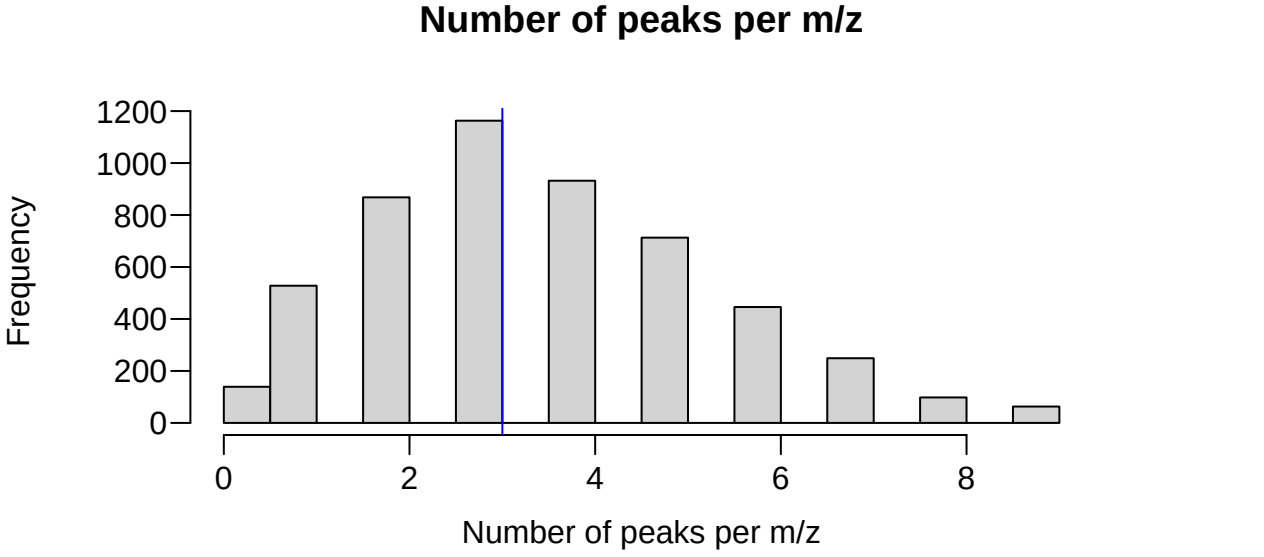

Number of peaks per spectrum
Frequency = # spectra
3
2
1
0
1400
1600
1800
2000
2200
2400
2600
Number of peaks per spectrum

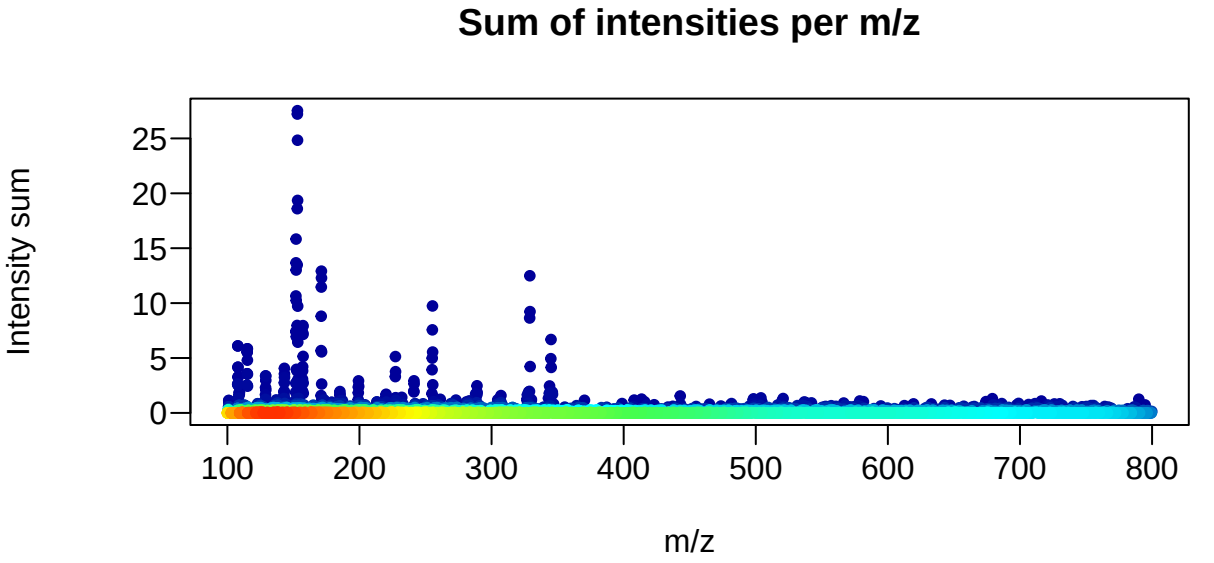

TIC per spectrum
Total ion current intensity
200
180
160
140
120
100
2
4
6
8
Spectra index

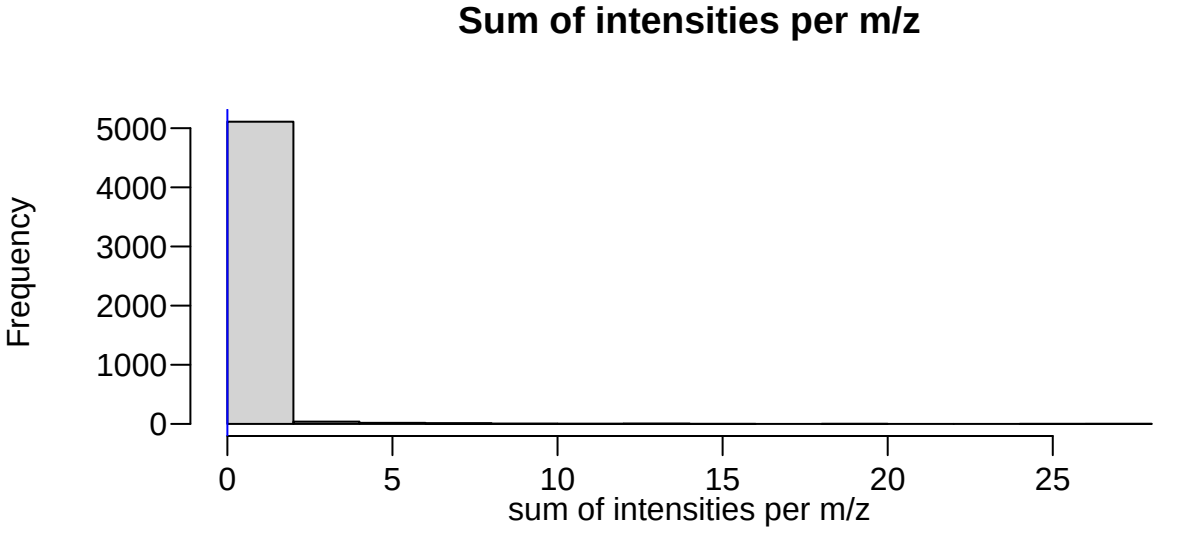

TIC per spectrum
Frequency = # spectra
3
2
1
0
80
100
120
140
160
180
200
220
TIC per spectrum

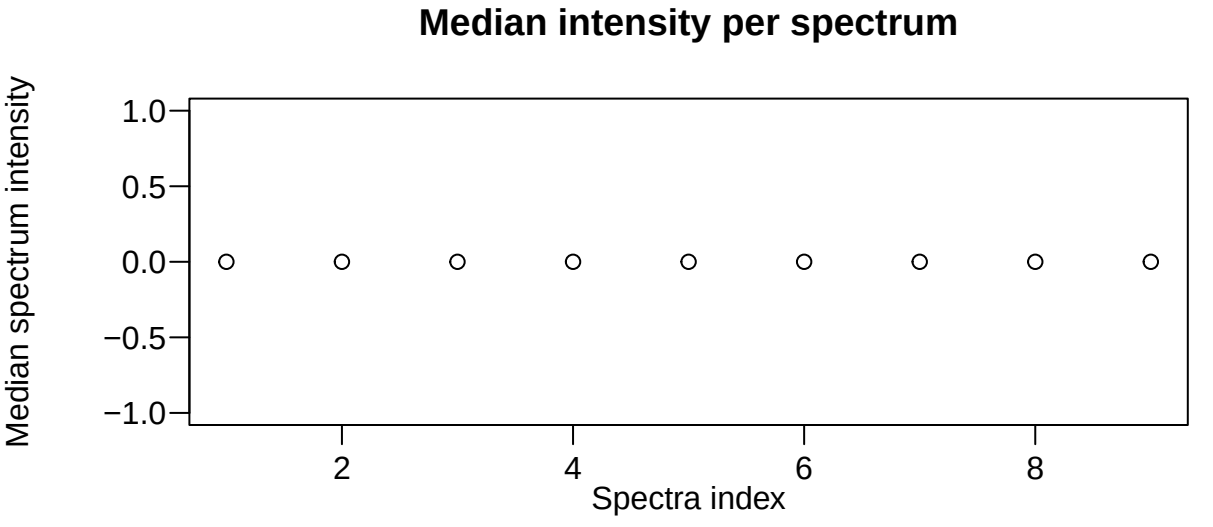

Histogram of m/z values
Frequency
0
200
400
600
800
1000
100
200
300
400
500
600
700
800
m/z

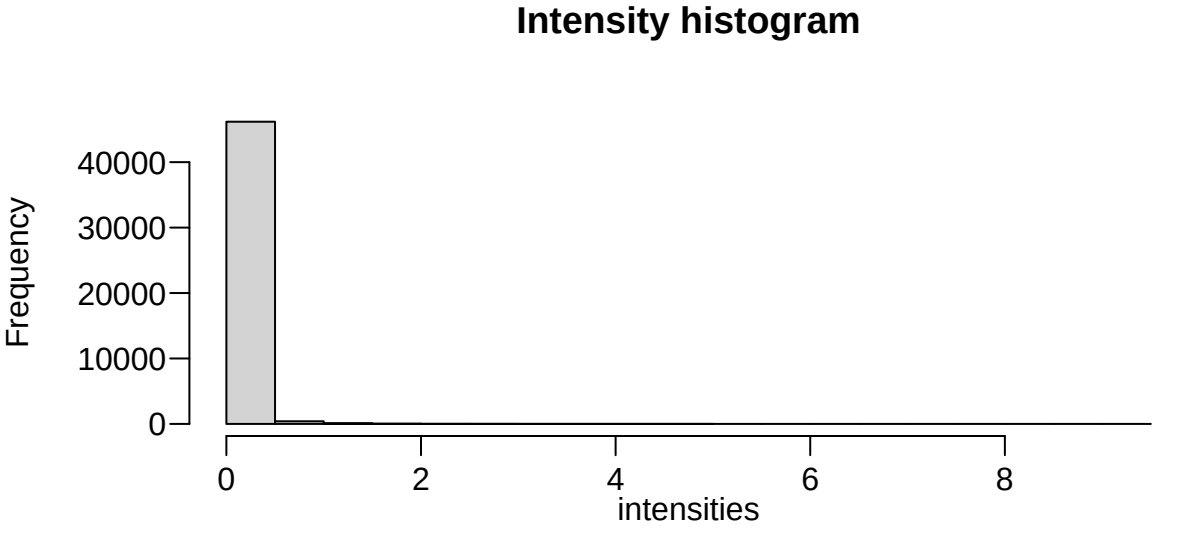

Number of peaks per m/z
Number of peaks
Coverage of spectra [%]
0
2
4
6
8
0
22.2
44.4
66.7
88.9
100
200
300
400
500
600
700
800
m/z

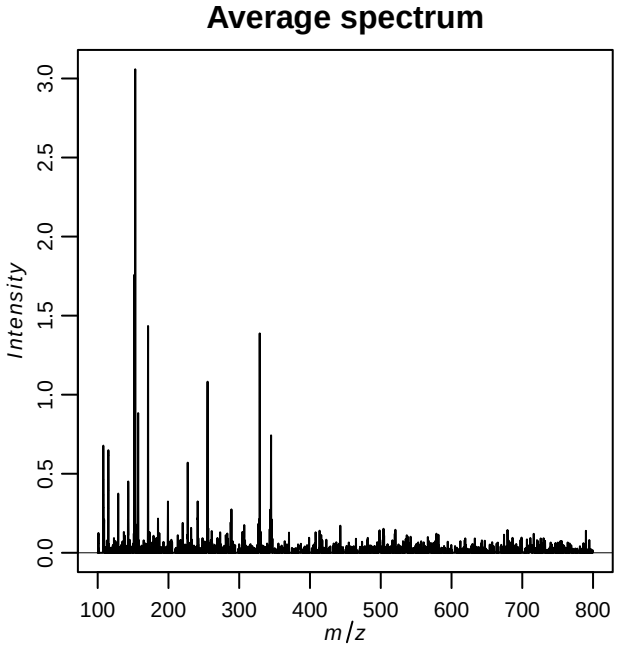

Number of peaks per m/z
Frequency
0
200
400
600
800
1000
1200
0
2
4
6
8
Number of peaks per m/z

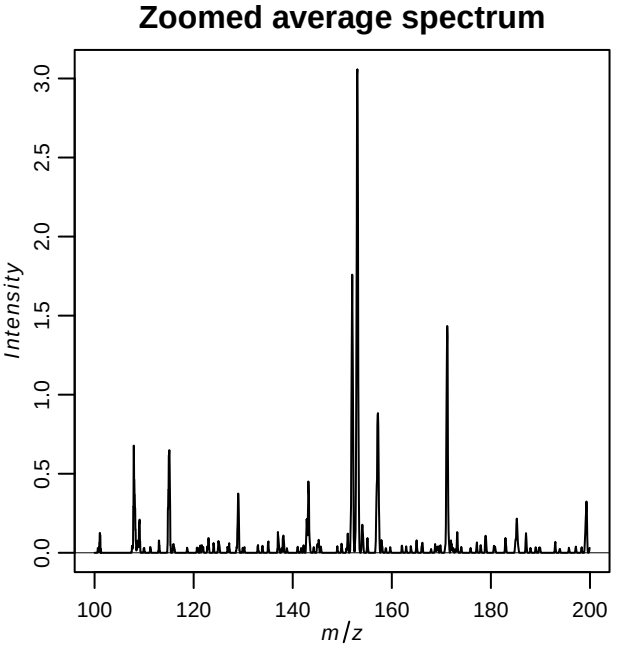

Sum of intensities per m/z
Intensity sum
0
5
10
15
20
25
100
200
300
400
500
600
700
800
m/z

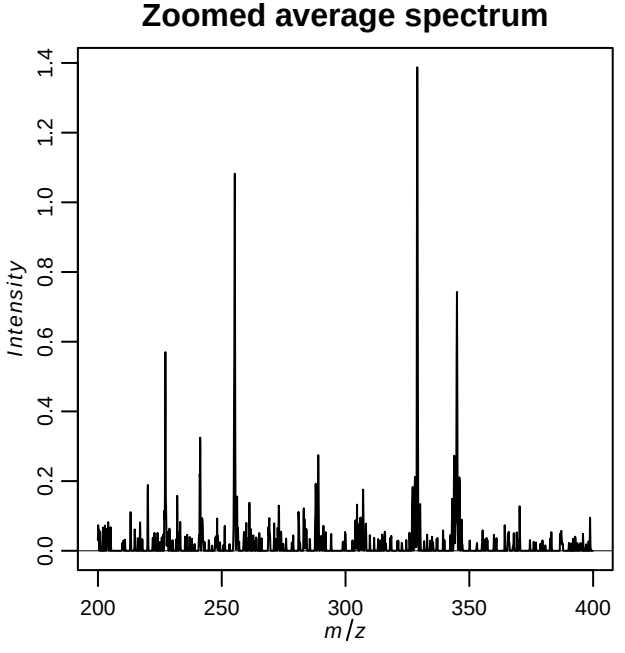

Sum of intensities per m/z
Frequency
0
1000
2000
3000
4000
5000
0
5
10
15
20
25
sum of intensities per m/z

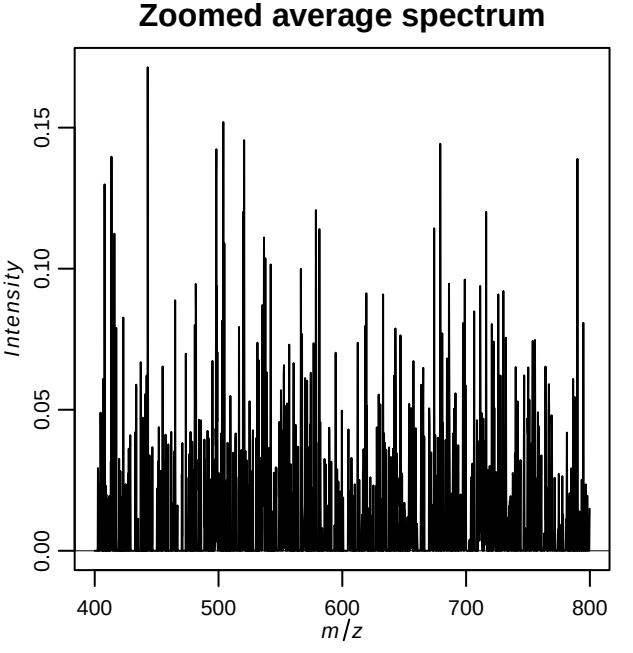

Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
Spectra index

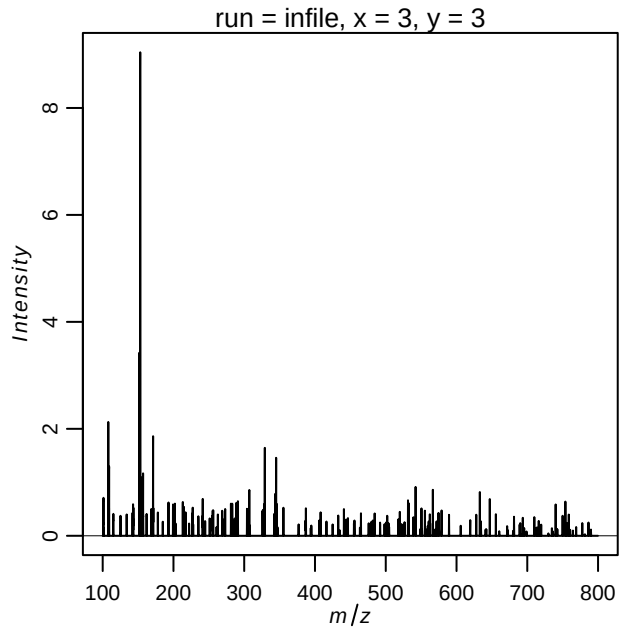

Intensity histogram
Frequency
40000
30000
20000
10000
0
0
2
4
6
8
intensities

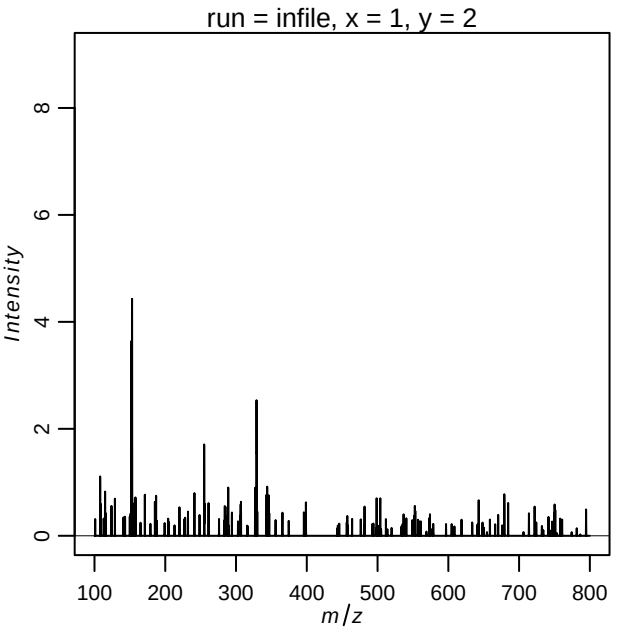

Average spectrum
Intensity
0.0
0.5
1.0
1.5
2.0
2.5
3.0
100
200
300
400
500
600
700
800
m/z

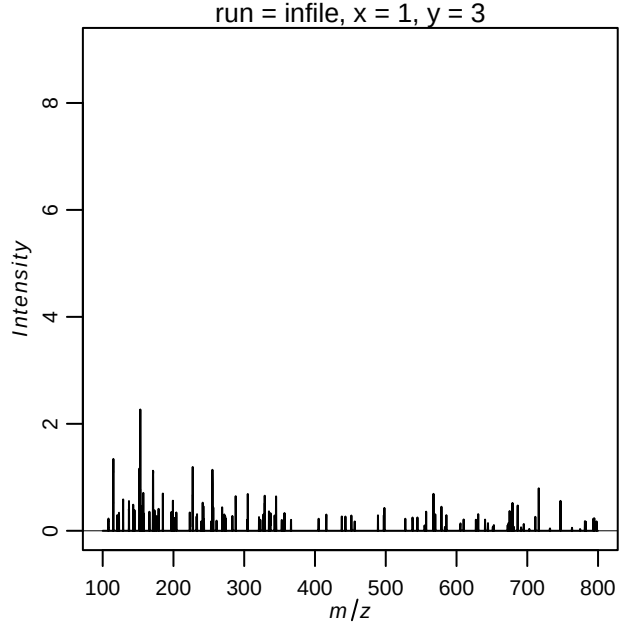

Zoomed average spectrum
Intensity
0.0
0.5
1.0
1.5
2.0
2.5
3.0
100
120
140
160
180
200
m/z

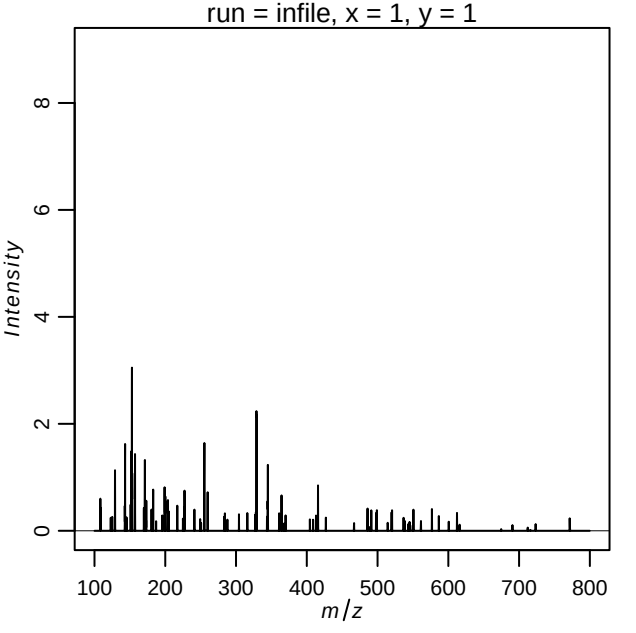

Zoomed average spectrum
Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
250
300
350
400
m/z


Zoomed average spectrum
Intensity
0.00
0.05
0.10
0.15
400
500
600
700
800
m/z

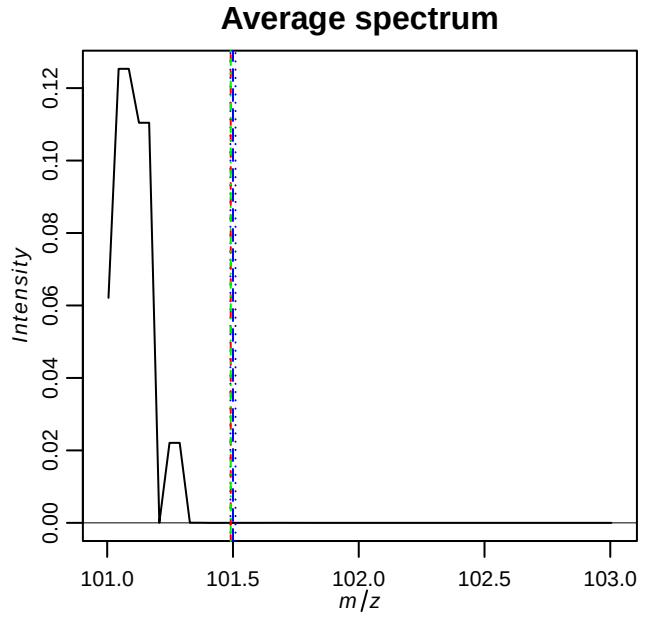

run = infile, x = 3, y = 3
Intensity
0
2
4
6
8
100
200
300
400
500
600
700
800
m/z

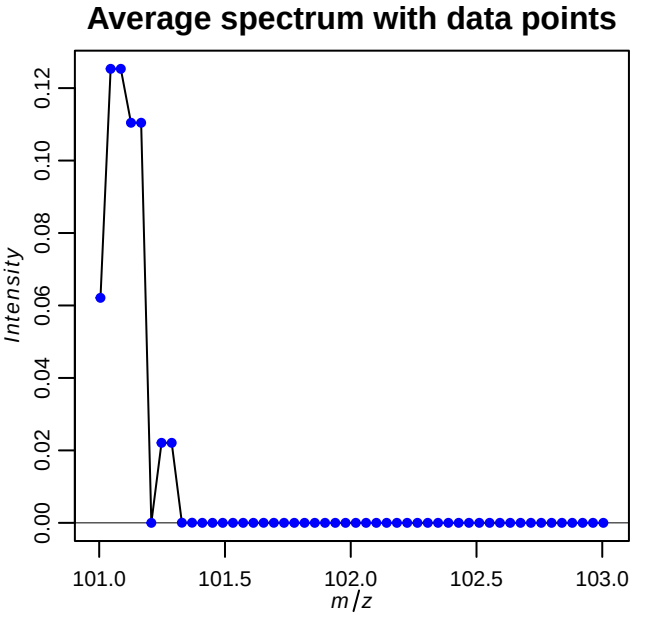

run = infile, x = 1, y = 2
Intensity
0
2
4
6
8
100
200
300
400
500
600
700
800
m/z

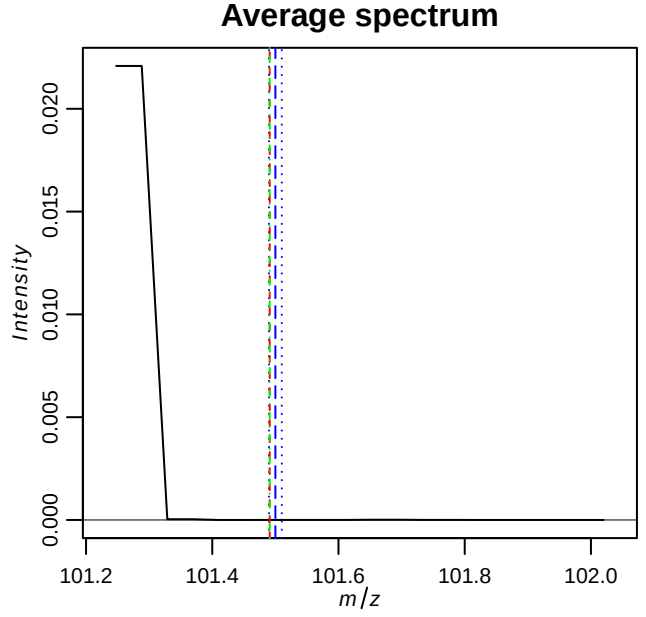

run = infile, x = 1, y = 3
Intensity
0
2
4
6
8
100
200
300
400
500
600
700
800
m/z

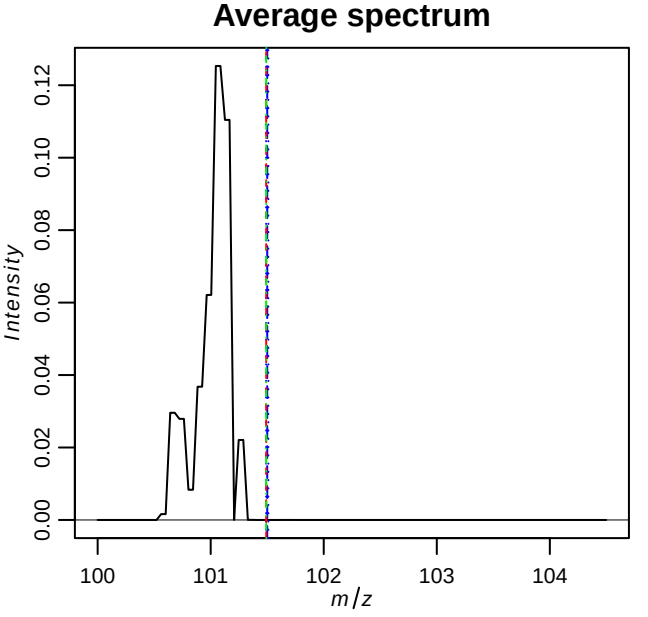

run = infile, x = 1, y = 1
Intensity
0
2
4
6
8
100
200
300
400
500
600
700
800
m/z

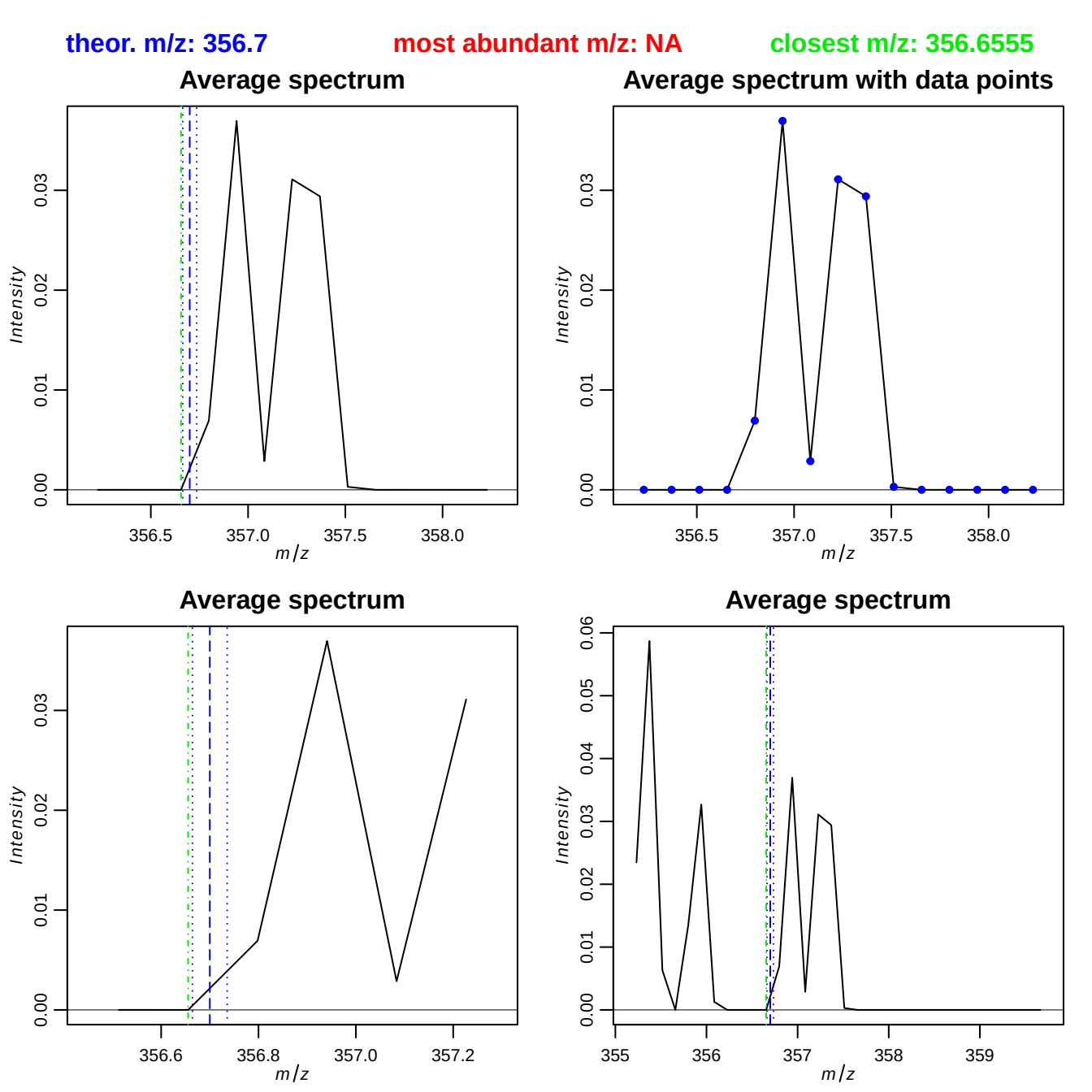
theor. m/z: 101.5 most abundant m/z: 101.491 closest m/z: 101.491

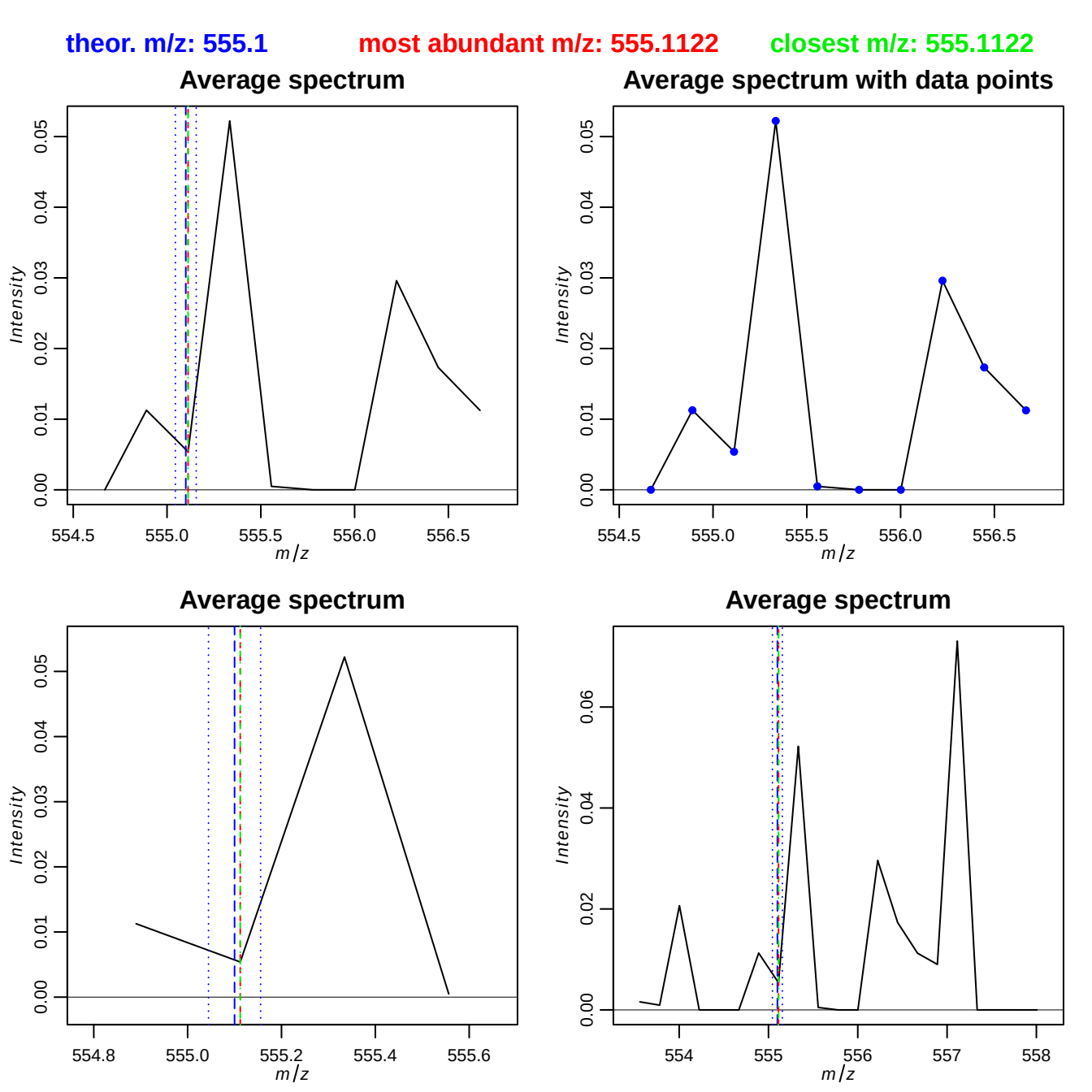


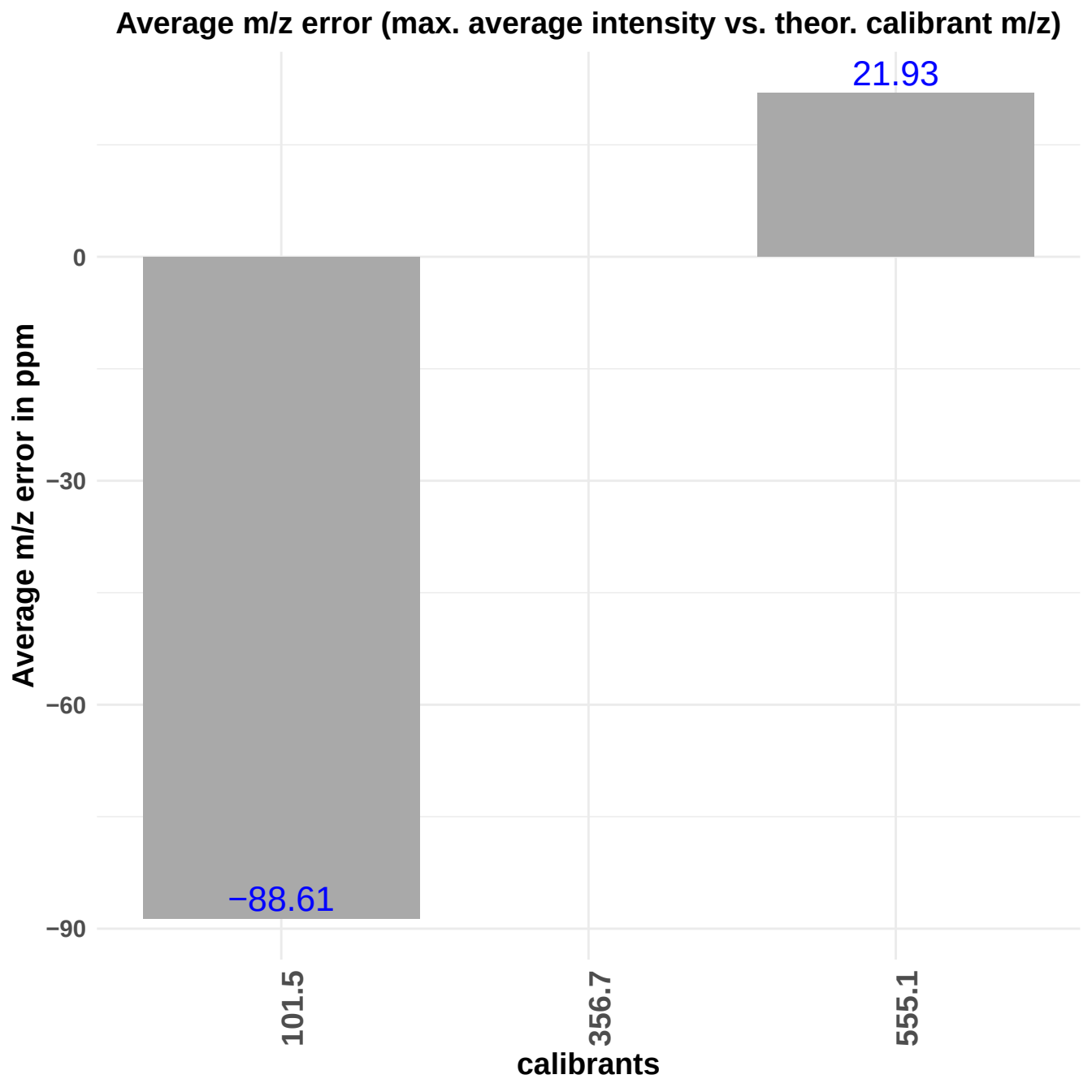


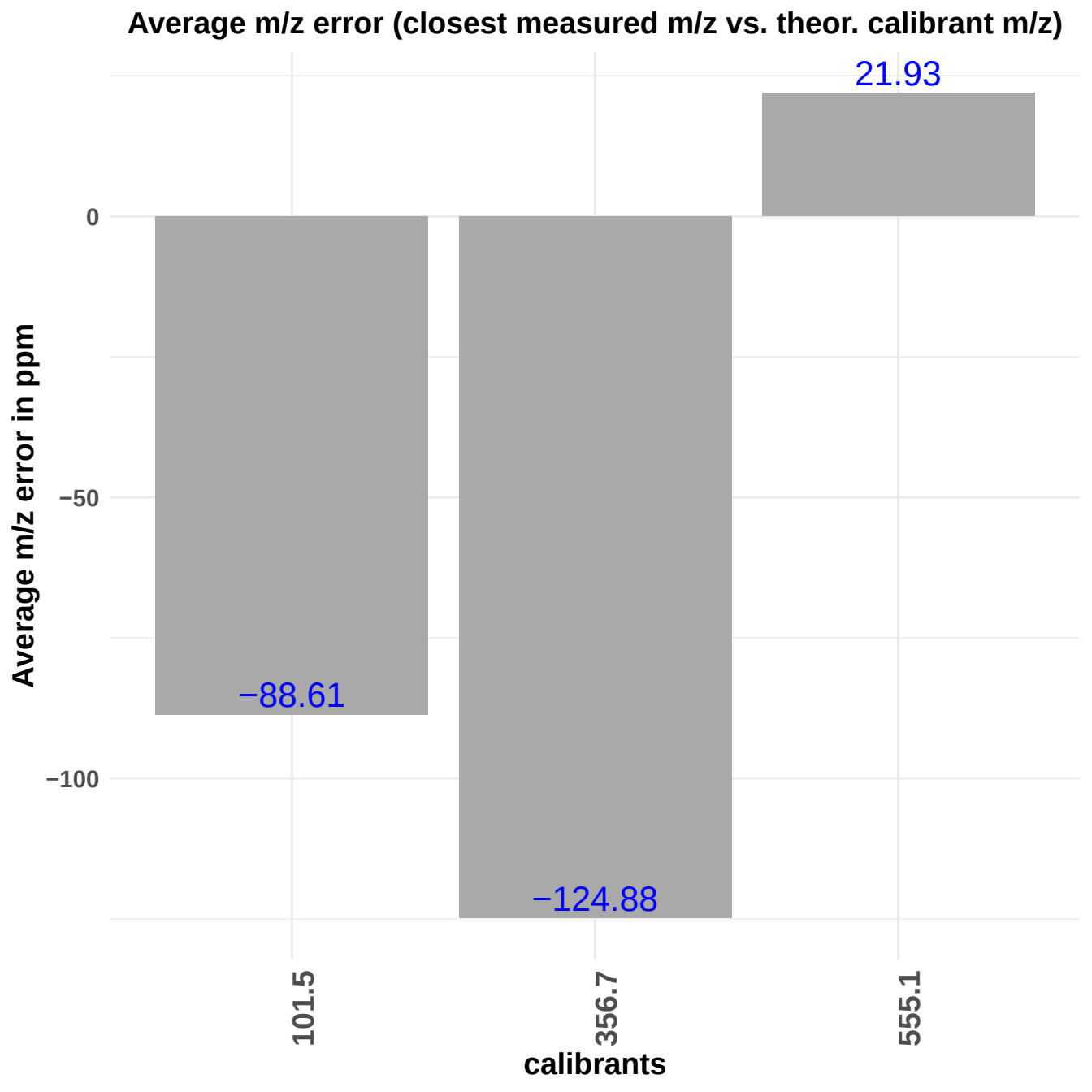


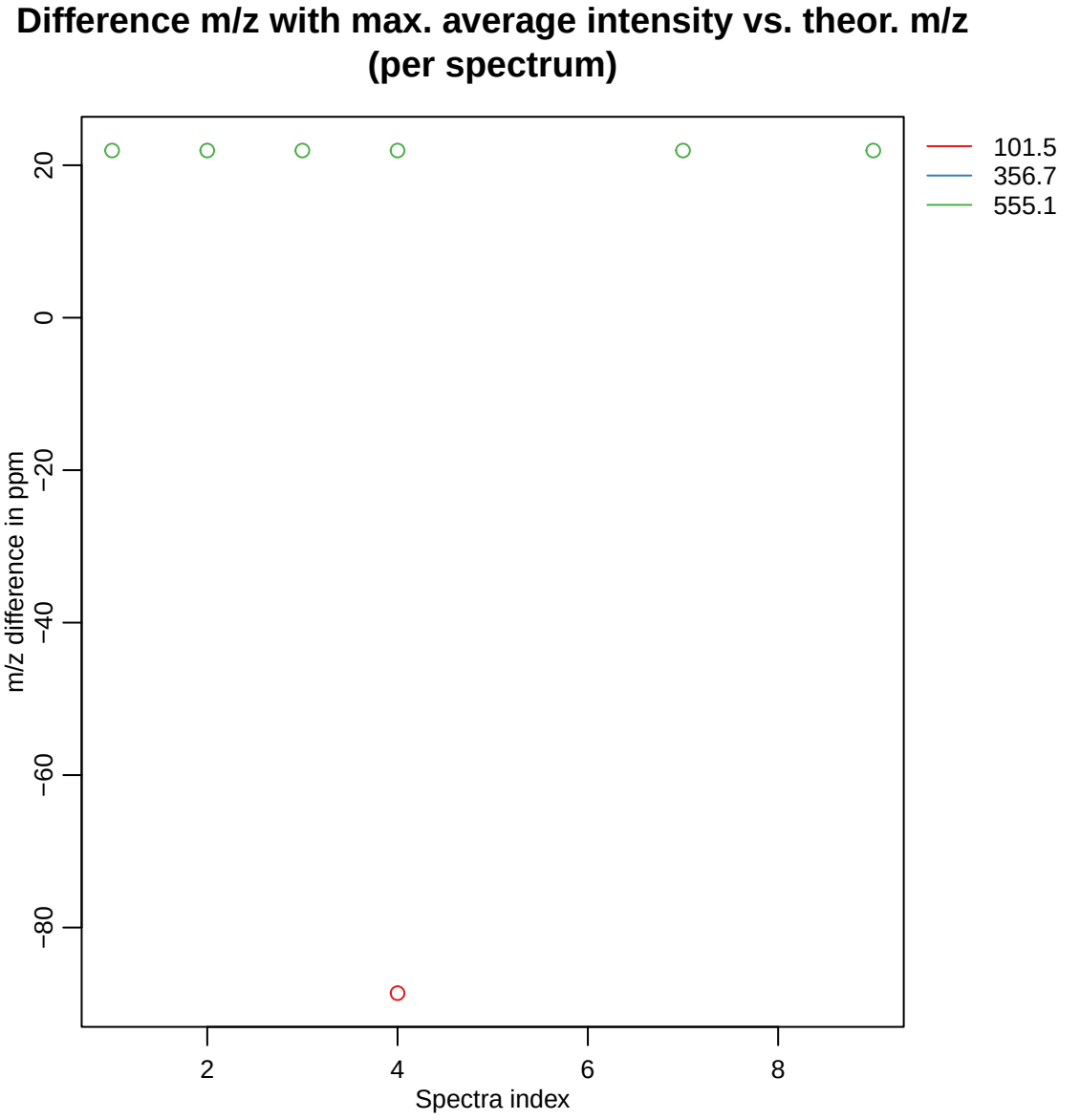


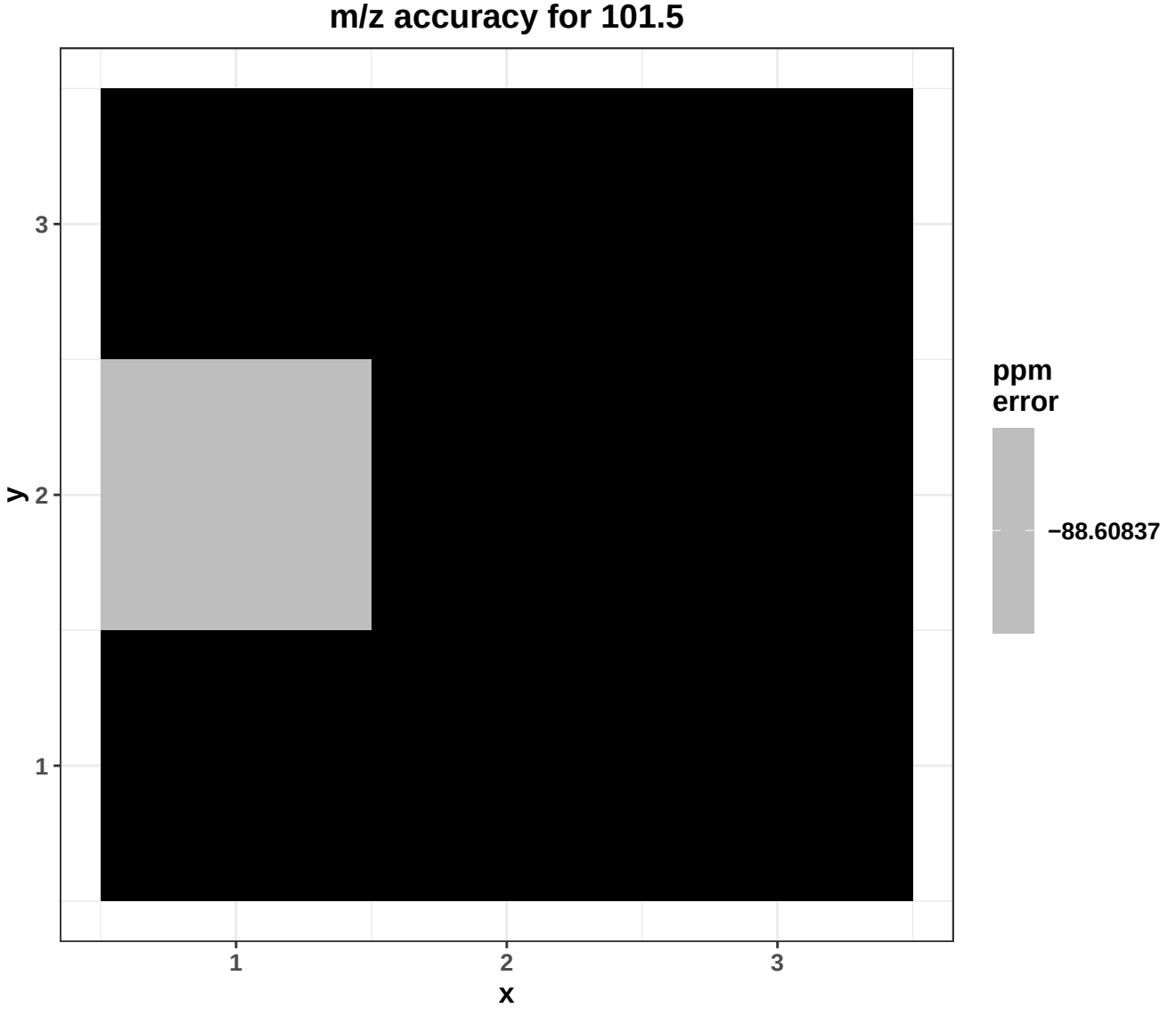

theor. m/z: 356.7
most abundant m/z: NA
closest m/z: 356.6555
Average spectrum
Intensity
m/z
Average spectrum with data points
Intensity
m/z
Average spectrum
Intensity
m/z
Average spectrum
Intensity
m/z

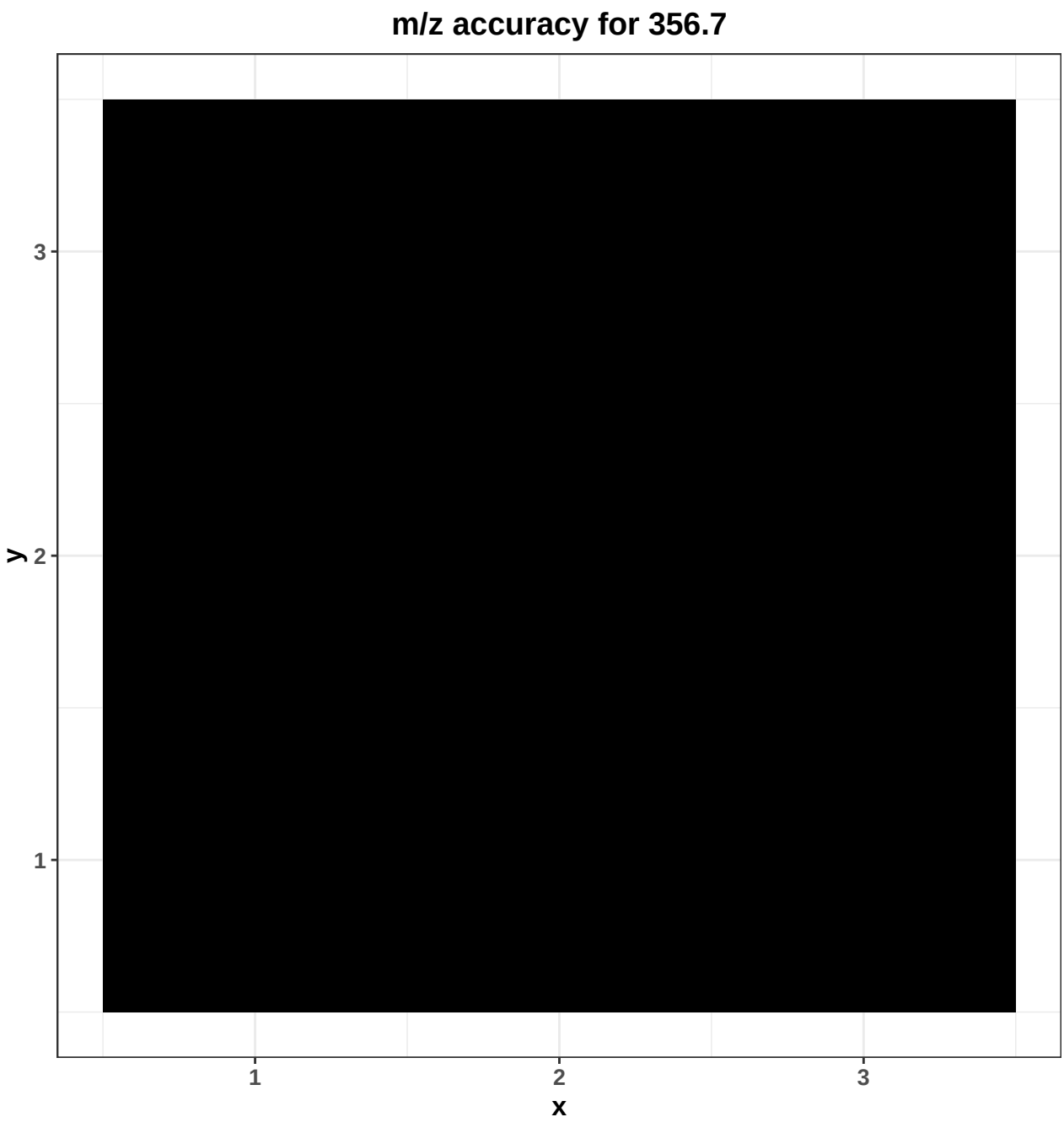

theor. m/z: 555.1
most abundant m/z: 555.1122
closest m/z: 555.1122
Average spectrum
Intensity
m/z
Average spectrum with data points
Intensity
m/z
Average spectrum
Intensity
m/z
Average spectrum
Intensity
m/z

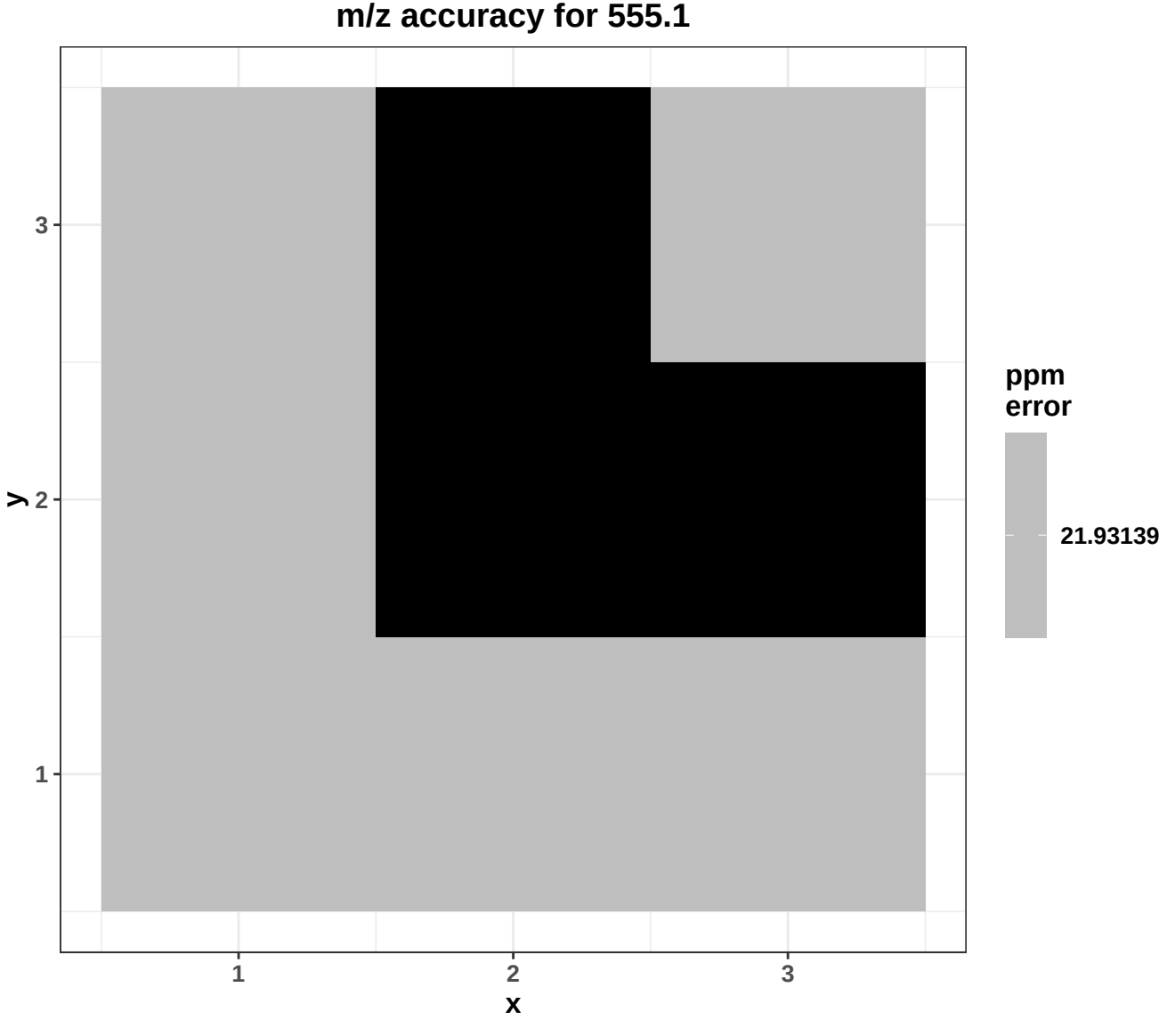

Average m/z error (max. average intensity vs. theor. calibrant m/z)
21.93
−88.61
0
−30
−60
−90
Average m/z error in ppm
101.5
356.7
555.1
calibrants


Average m/z error (closest measured m/z vs. theor. calibrant m/z)
21.93
0
−50
−100
Average m/z error in ppm
−88.61
−124.88
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


m/z accuracy for 101.5
3
2
1
y
1
2
3
x
ppm
error
−88.60837


m/z accuracy for 356.7
y
3
2
1
1
2
3
x


m/z accuracy for 555.1
3
2
1
y
1
2
3
x
ppm
error
21.93139