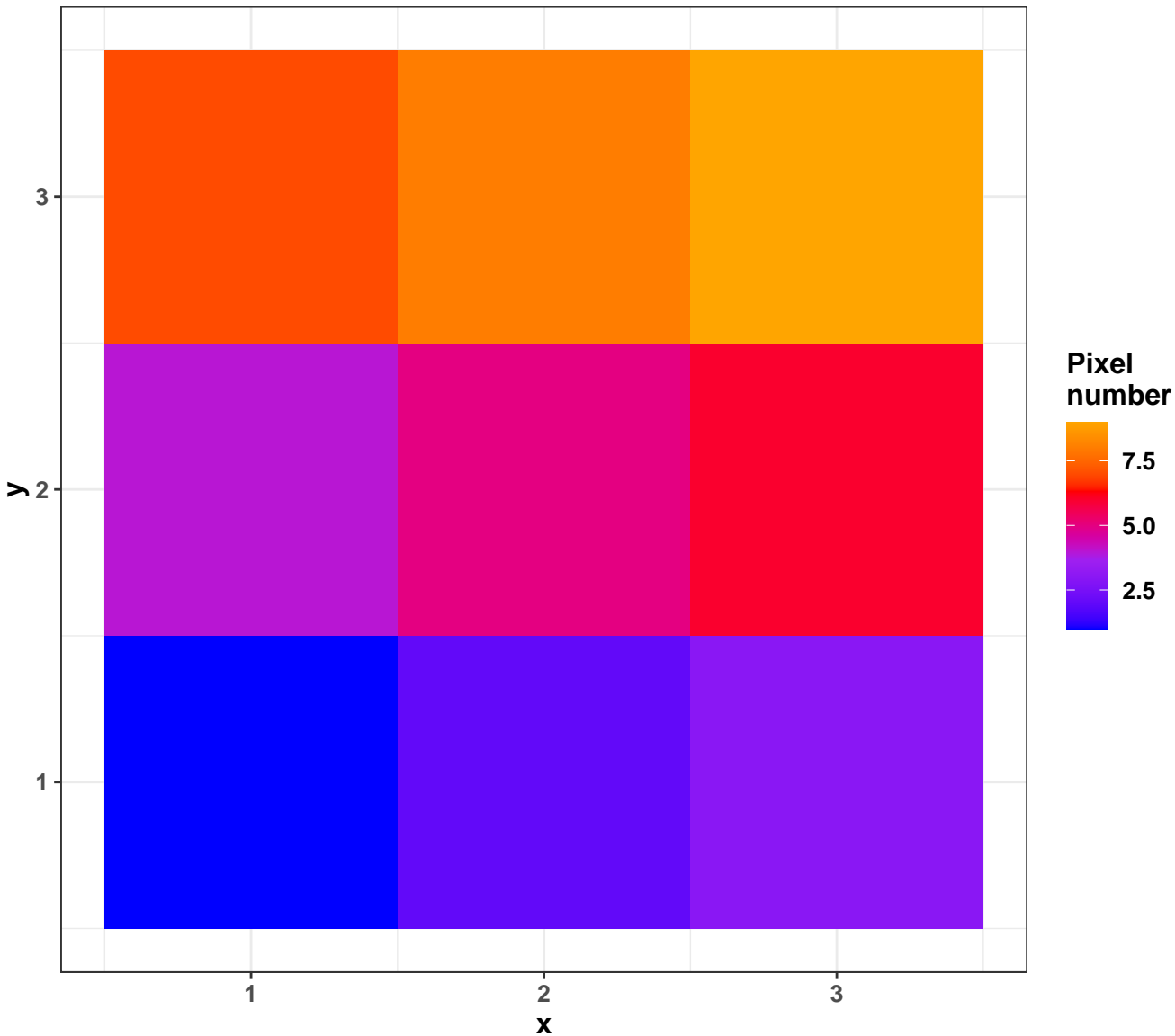


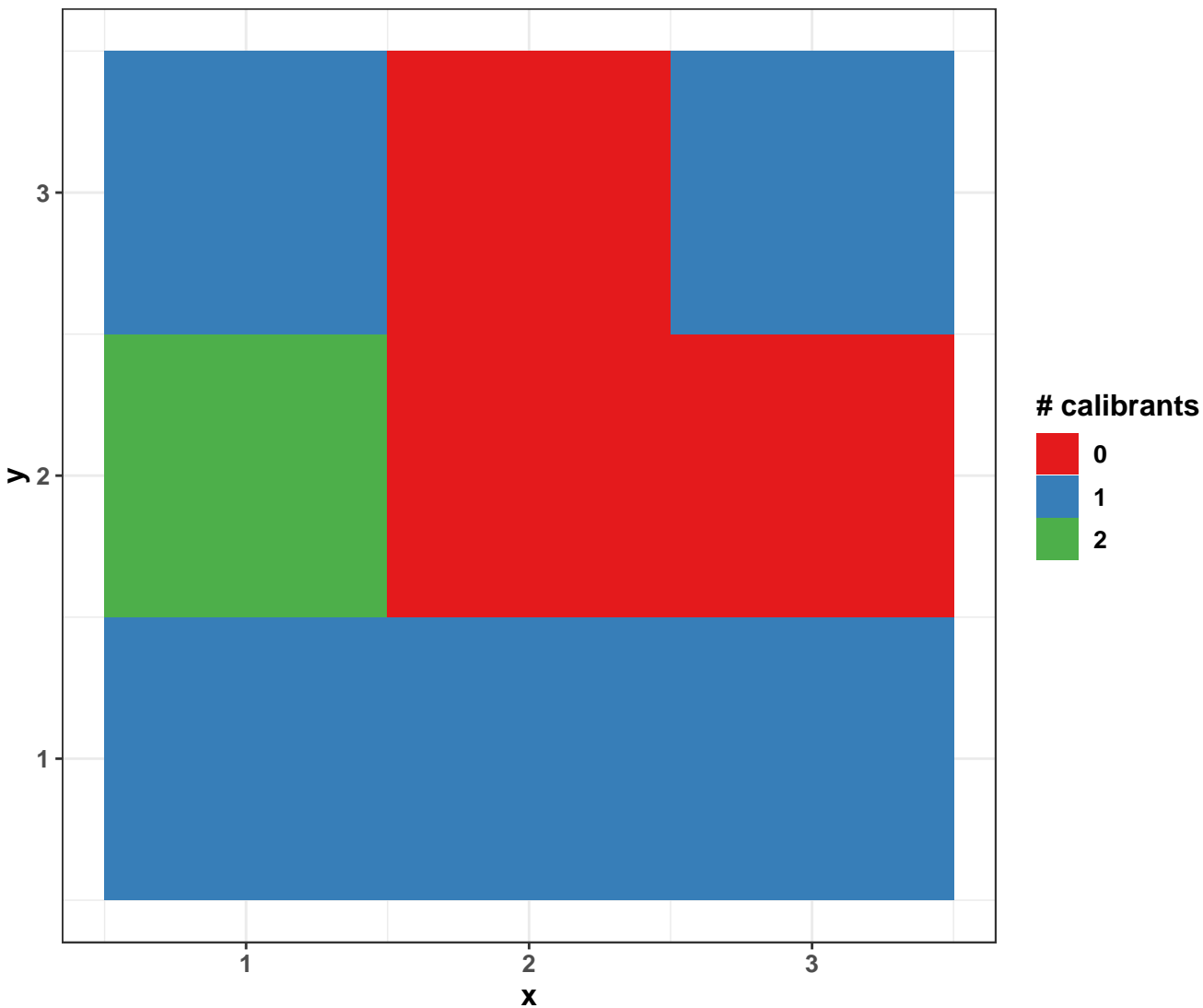
## Testfile\_imzml

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
Number of NA intensities	0
Number of Inf intensities	0
Number of duplicated coordinates	0
Median of intensities	0
Intensities > 0	35.16 %
Number of empty spectra	0
Median TIC ± sd	161.8 ± 43
Median # peaks per spectrum ± sd	1961 ± 260
Centroided	FALSE
input m/z (#valid/#input) in inputcalibrantfile1.tabular	3 / 3

# Pixel order

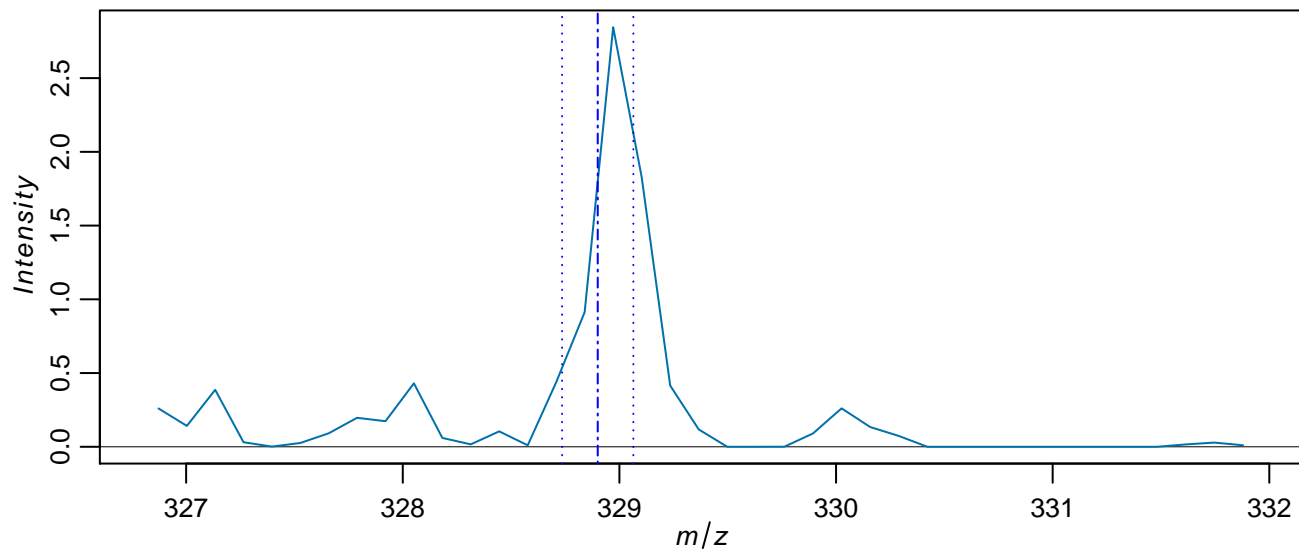


Number of calibrants per pixel ( $\pm 100$  ppm)

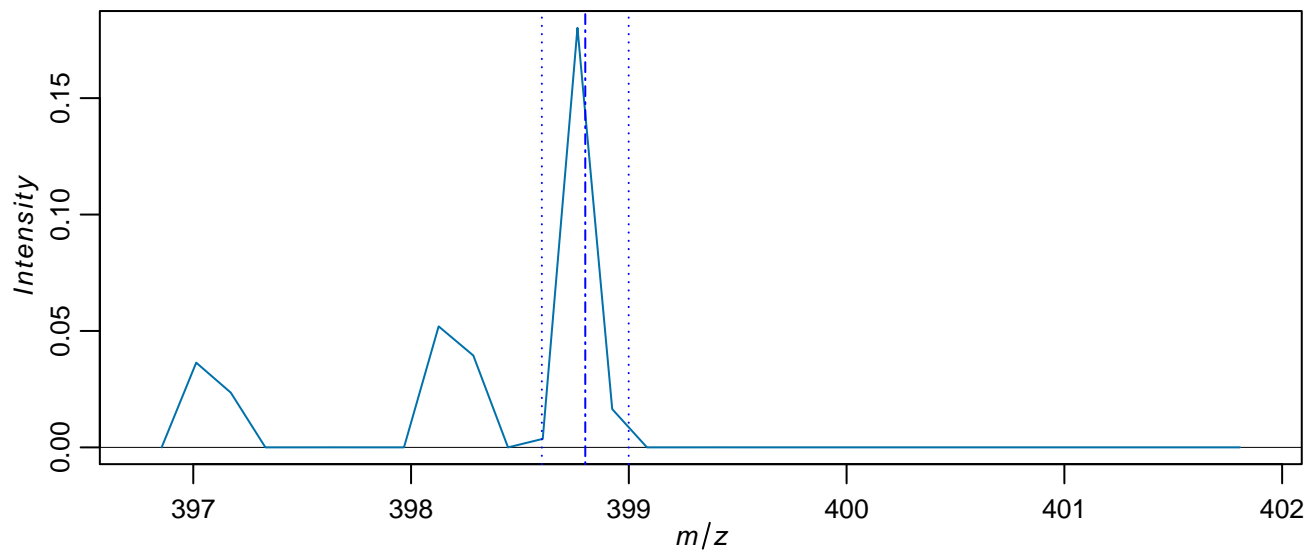


# Control of fold change plot

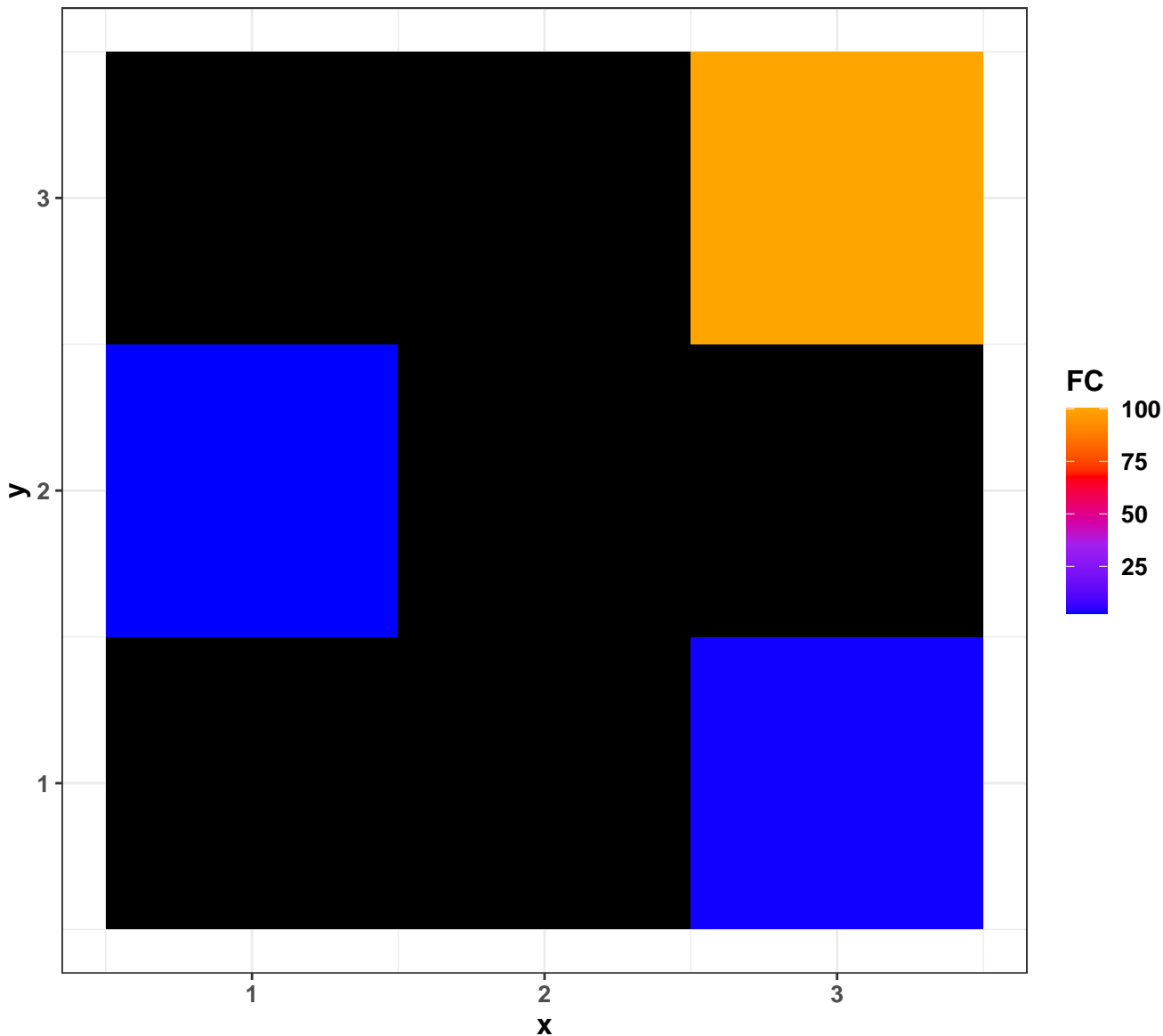
## Average spectrum 328.9 Da



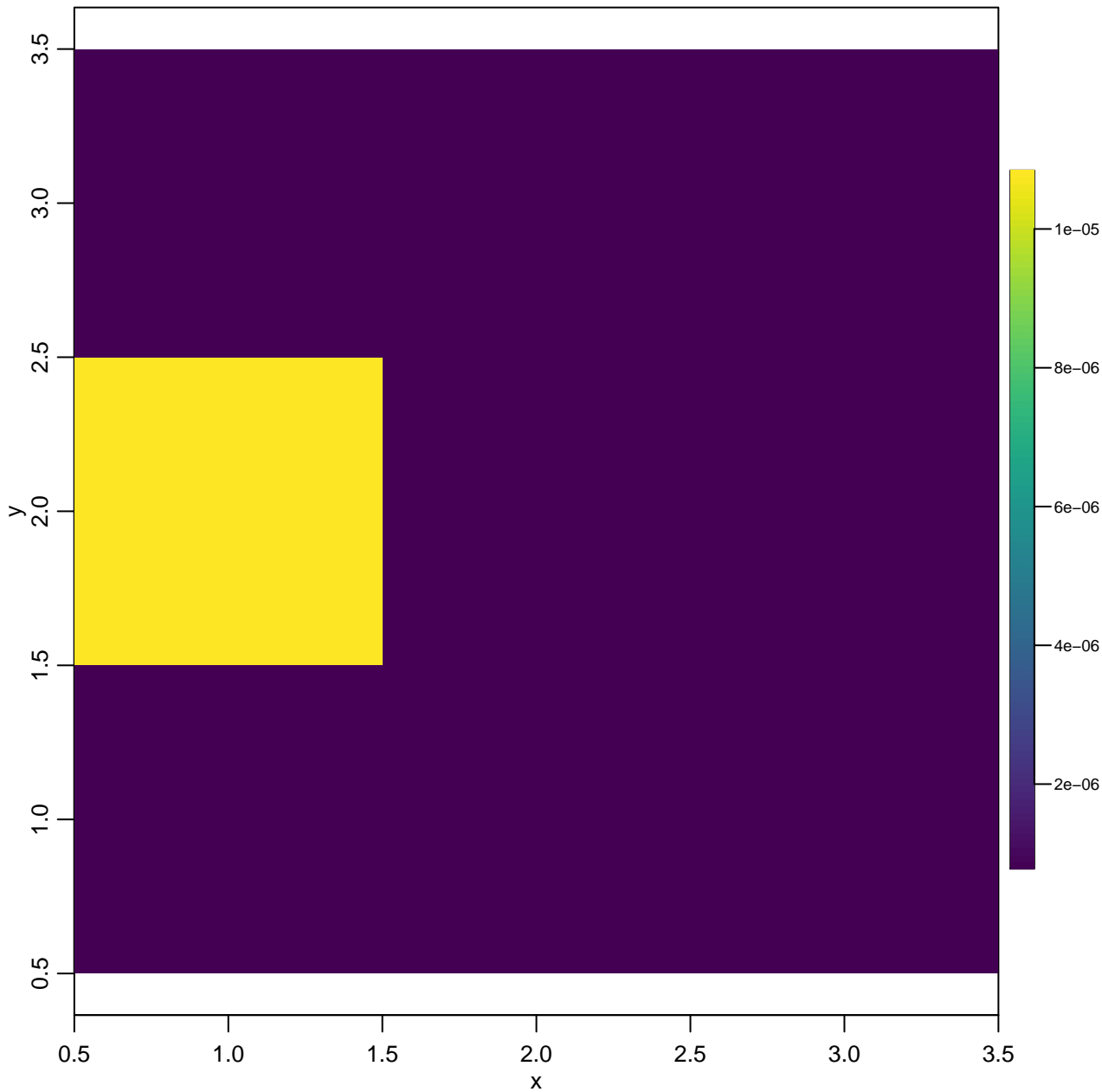
## Average spectrum 398.8 Da



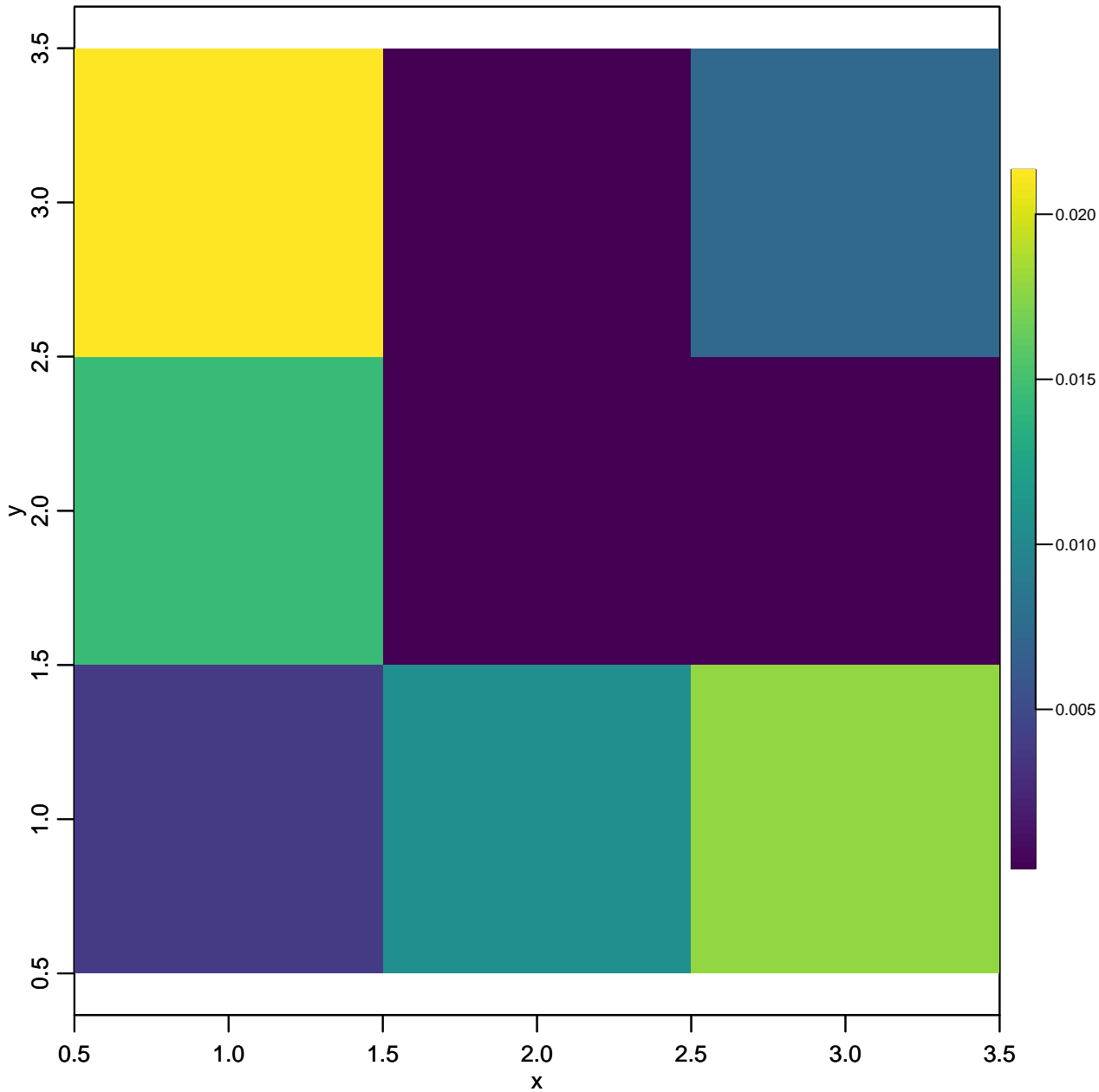
Ratio of mz 3289 and mz 3988



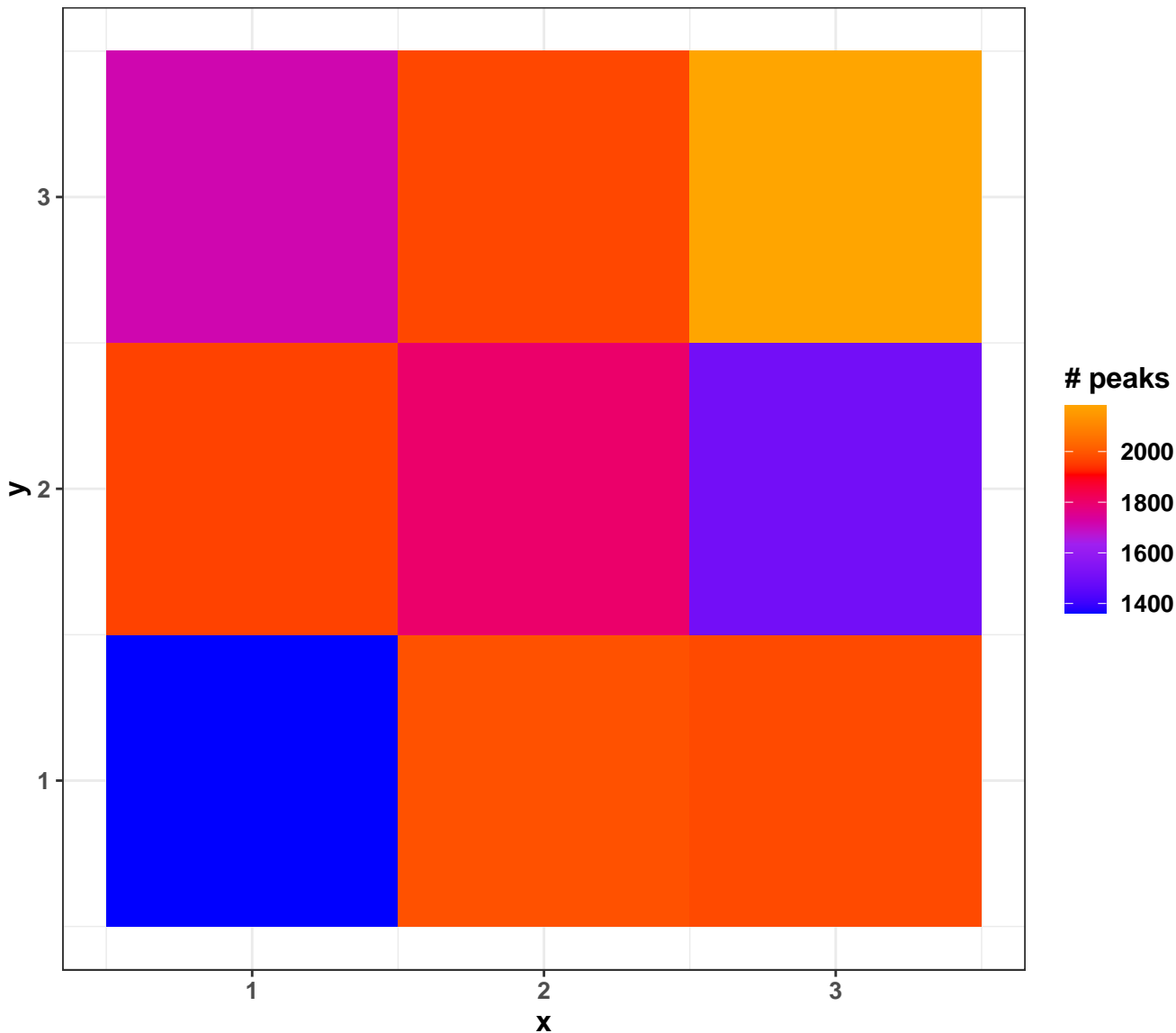
# 101.5: 101.5 ( $\pm 100$ ppm)



# 556.7: 556.7 ( $\pm 100$ ppm)

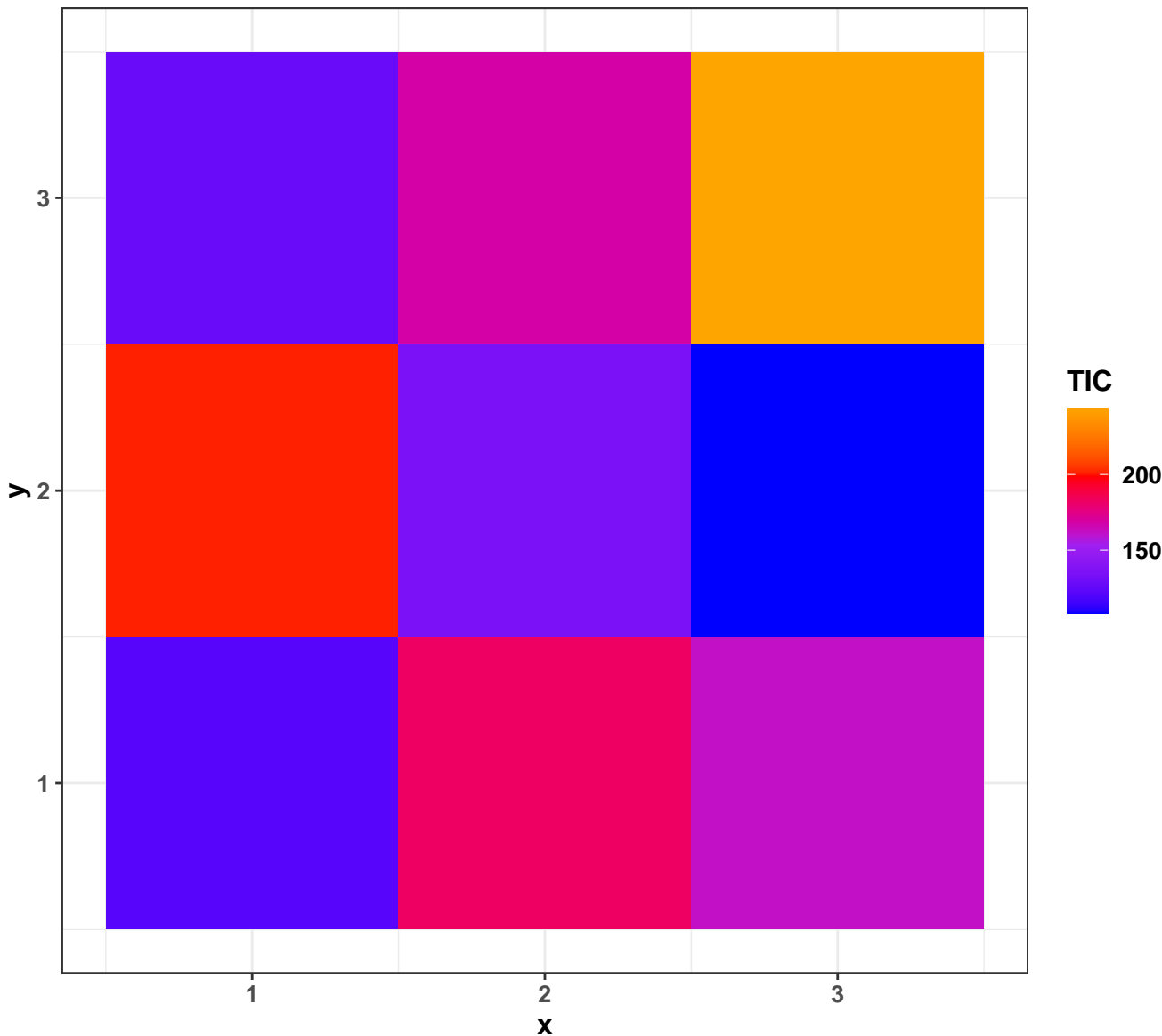


# Number of peaks per spectrum

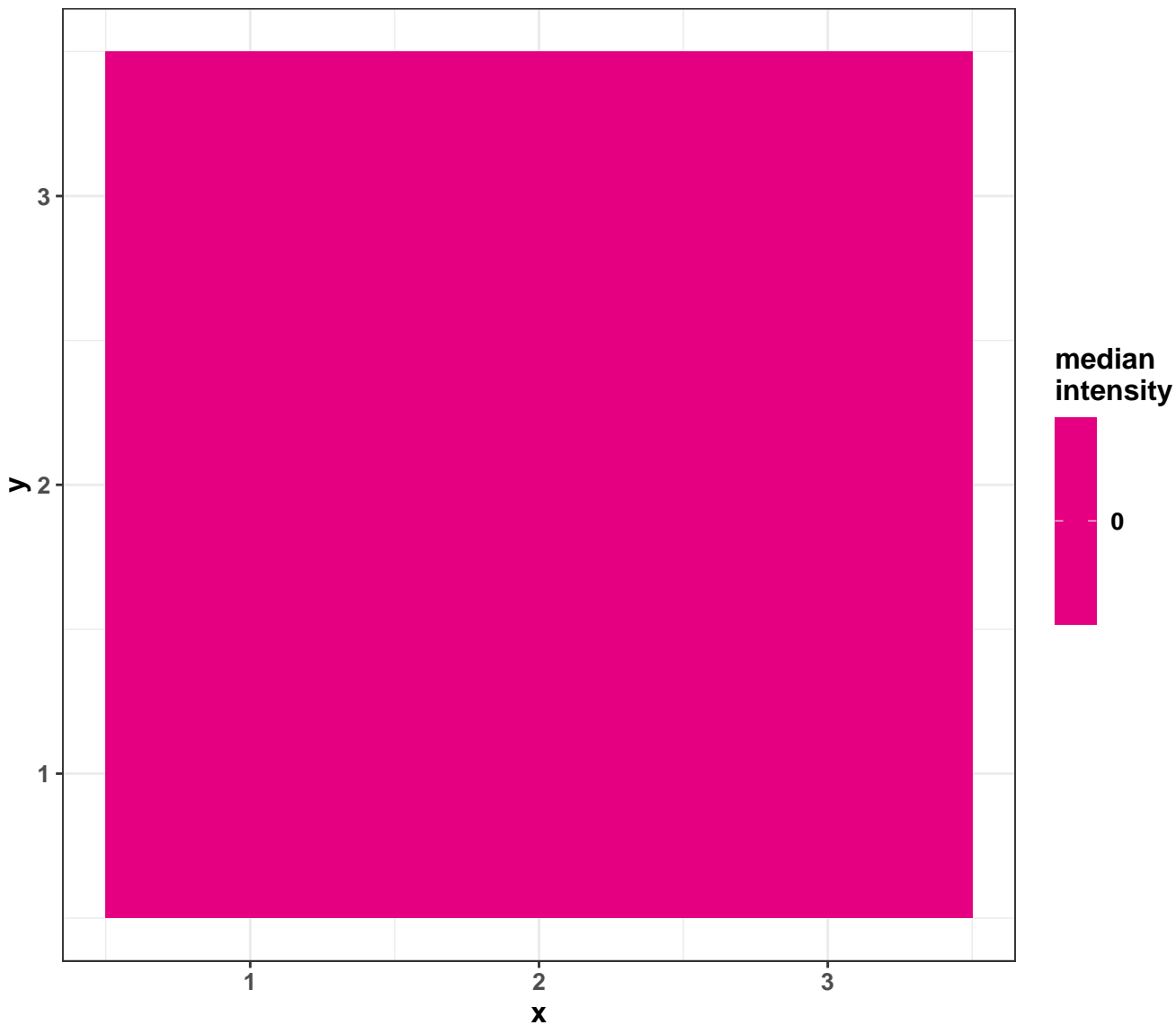




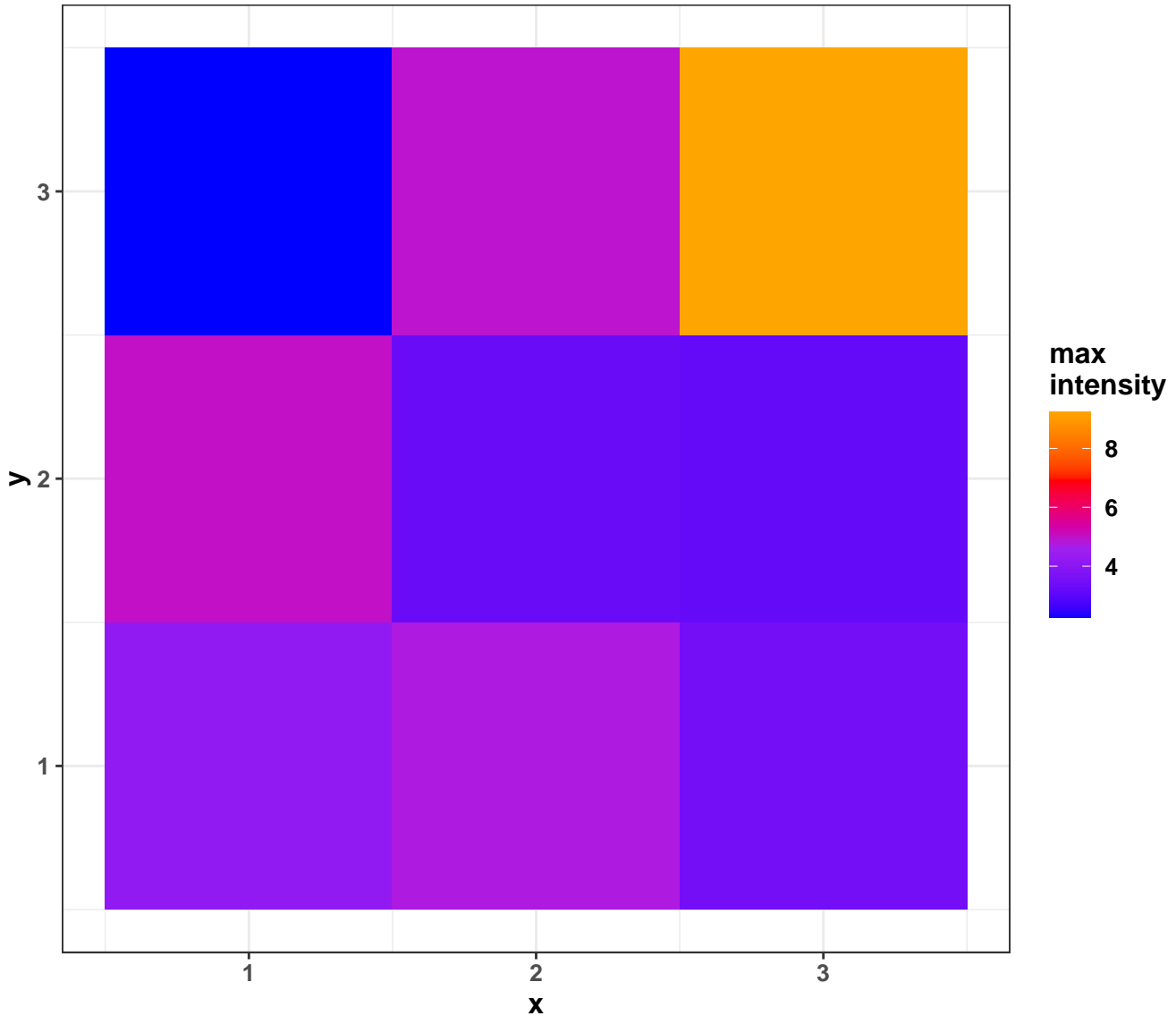
# Total Ion Current



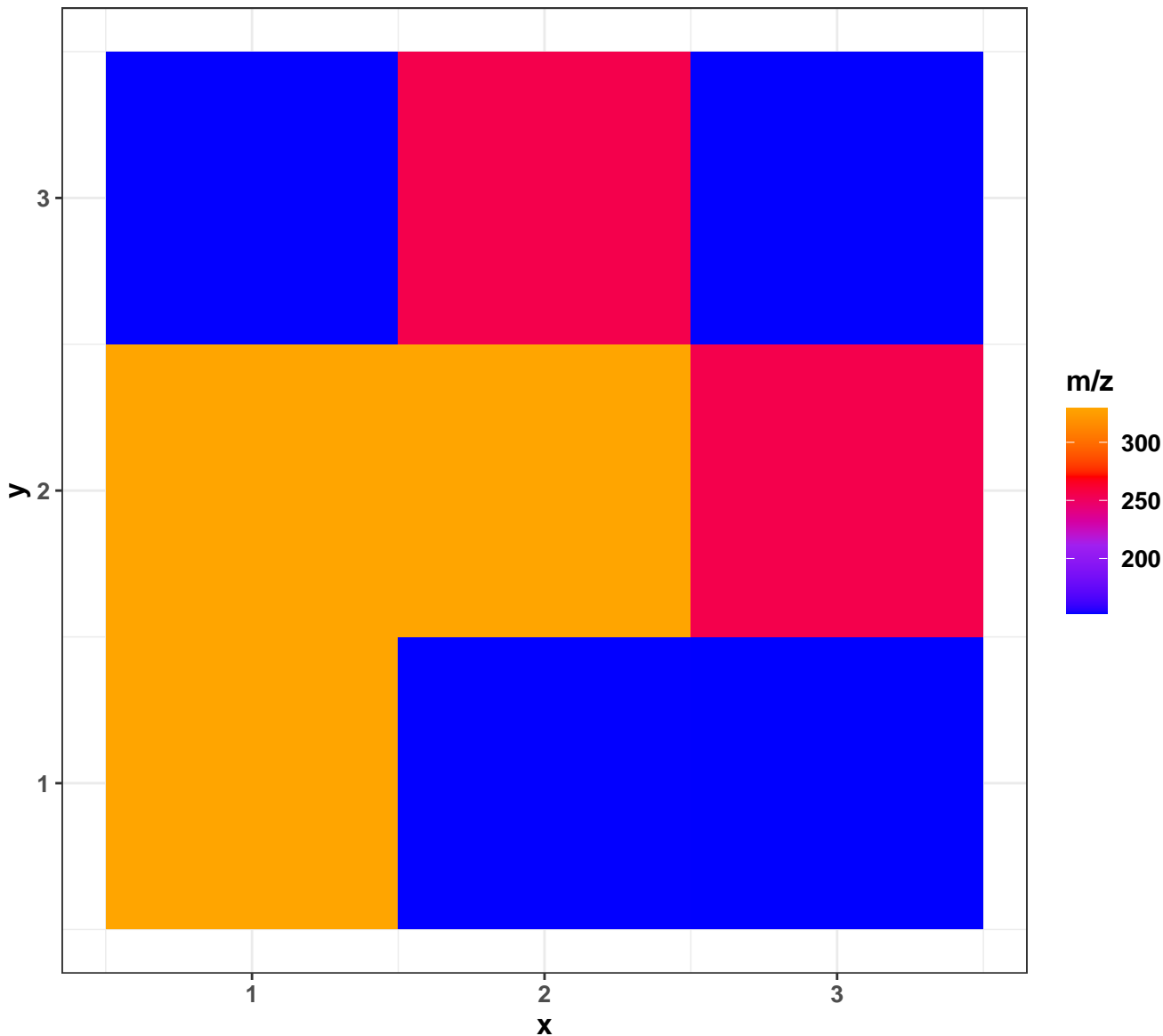
# Median intensity per spectrum



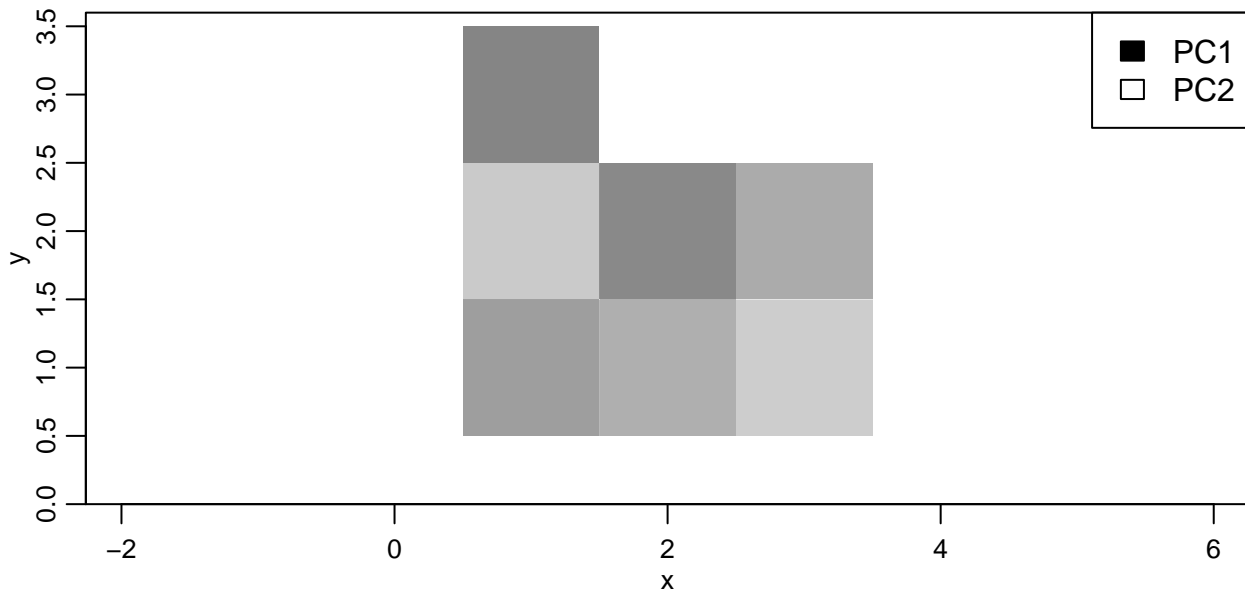
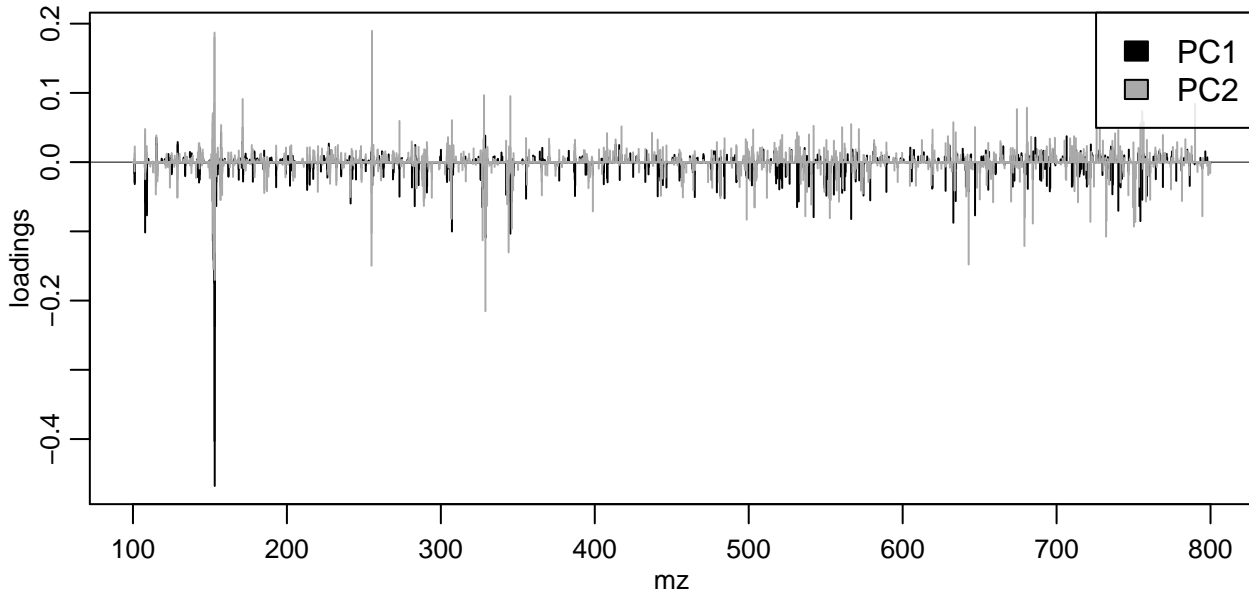
# Maximum intensity per spectrum

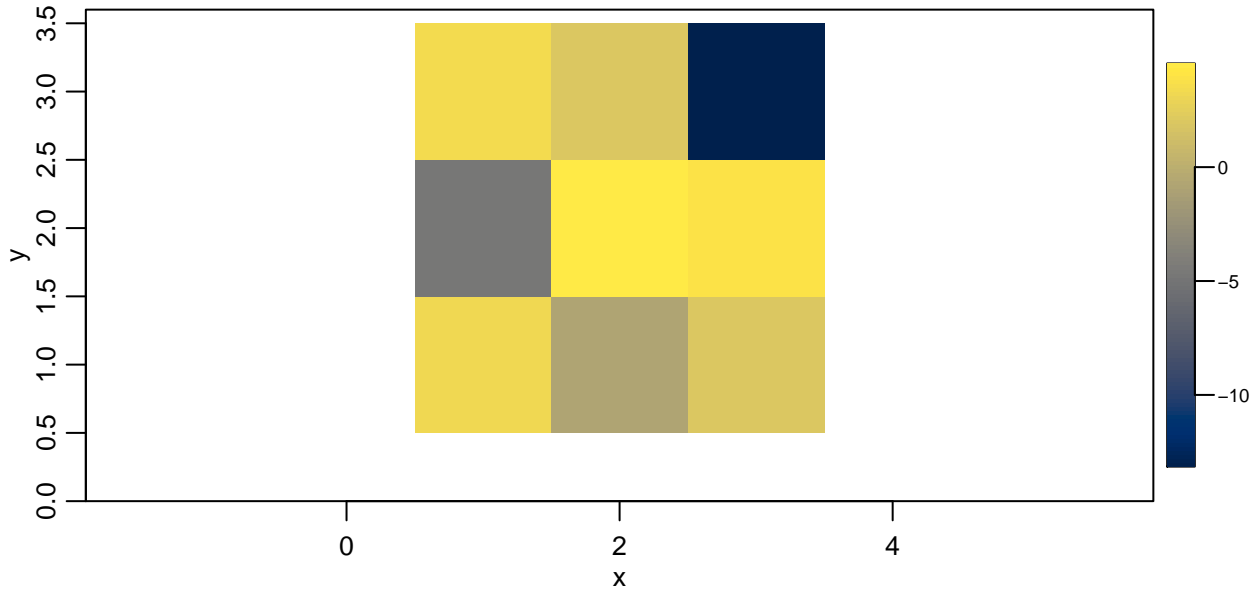
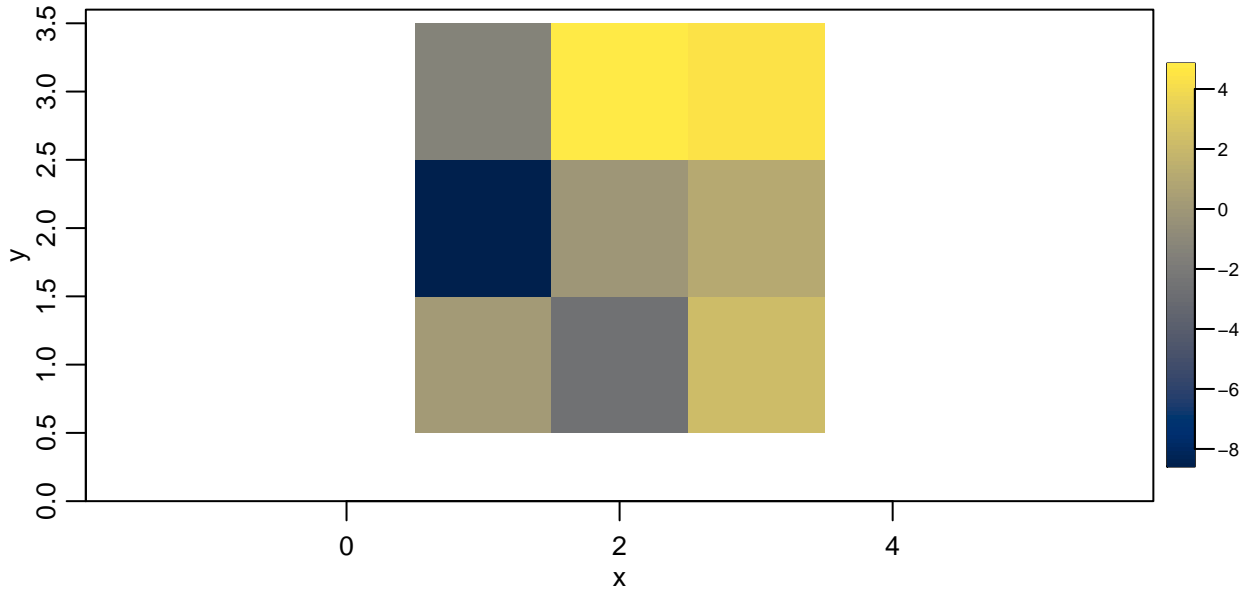


# Most abundant m/z in each spectrum

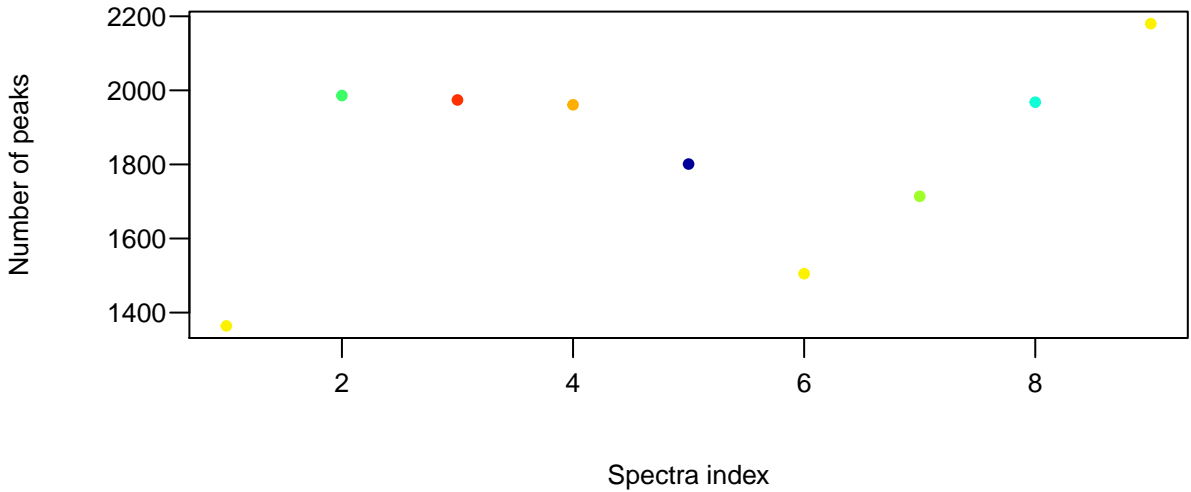


# PCA for two components

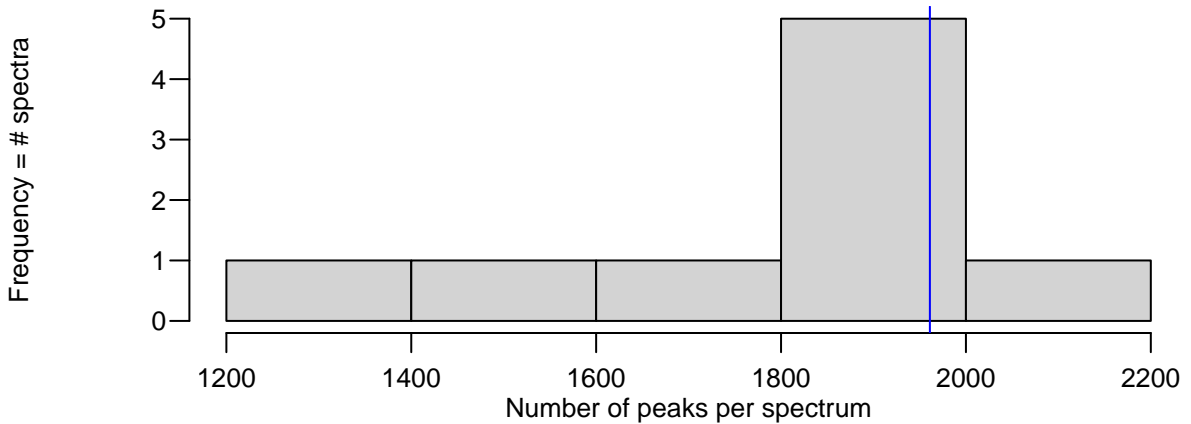


**PC1****PC2**

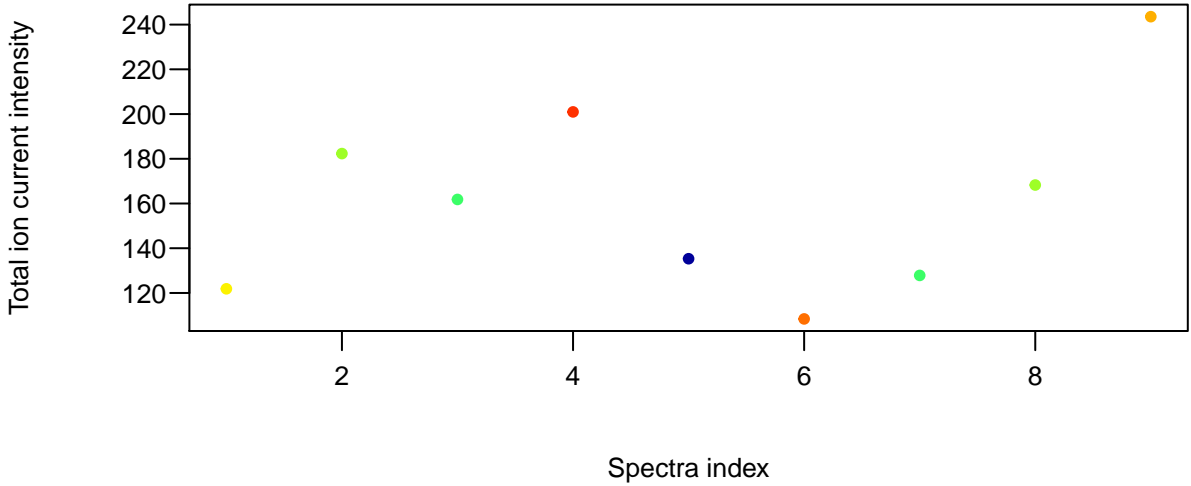
## Number of peaks per spectrum



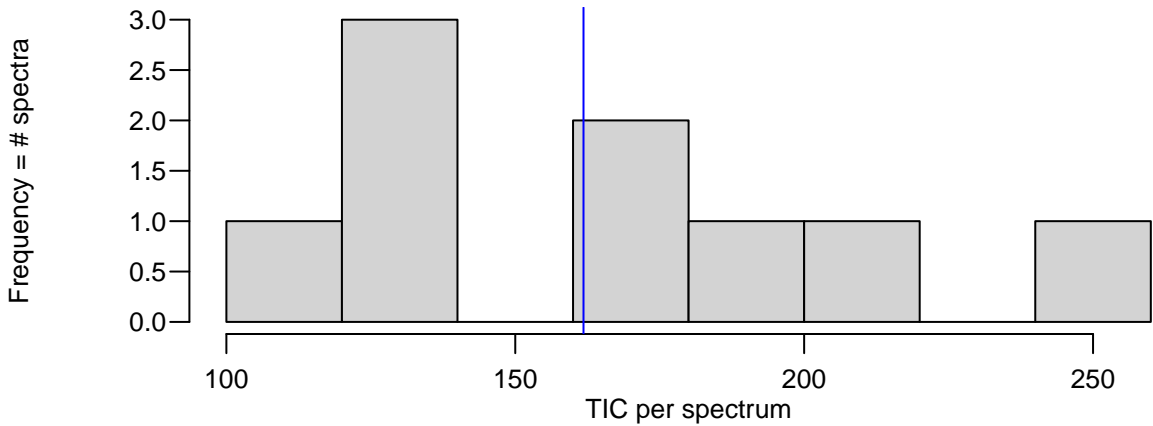
## Number of peaks per spectrum



## TIC per spectrum

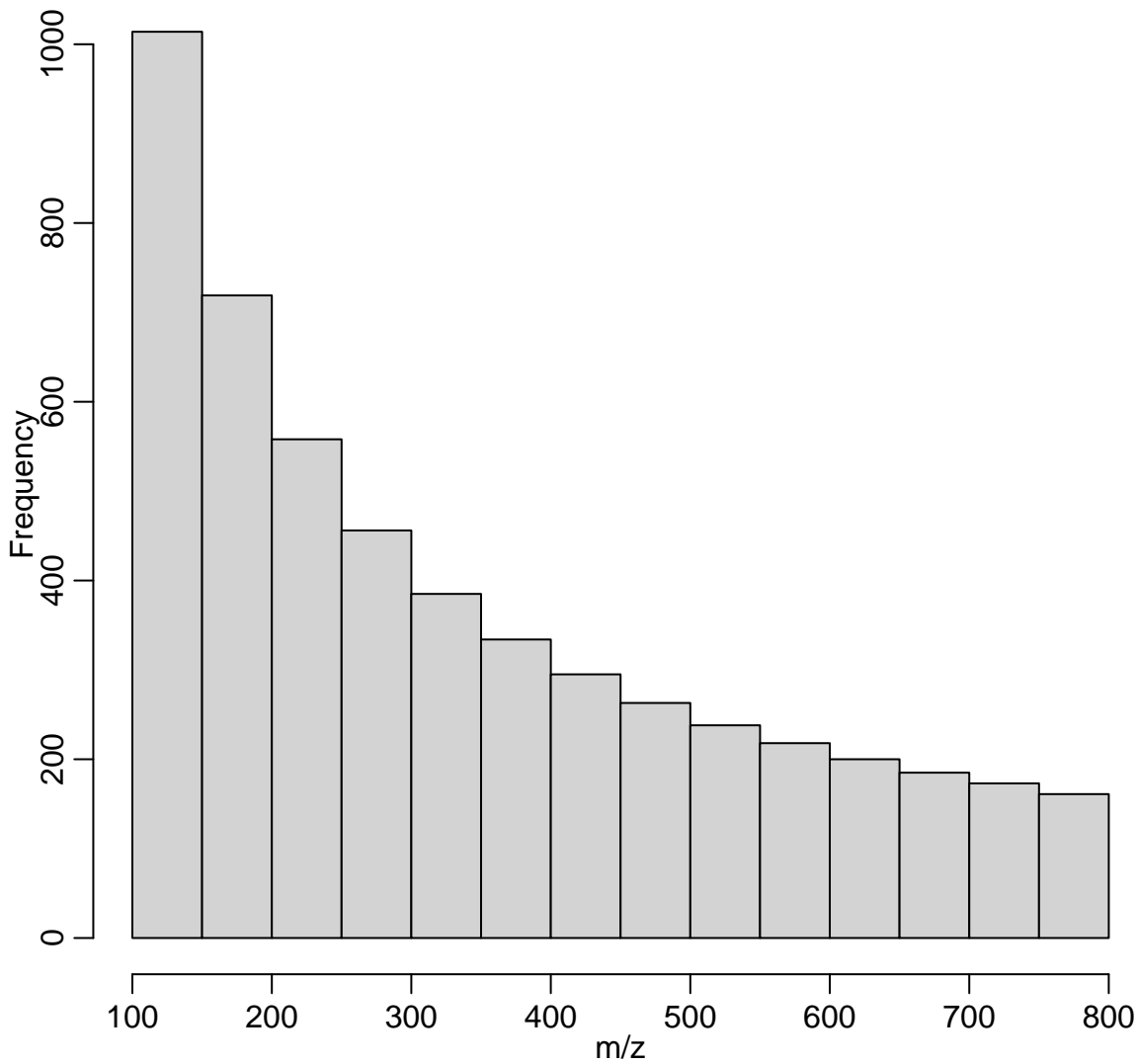


## TIC per spectrum

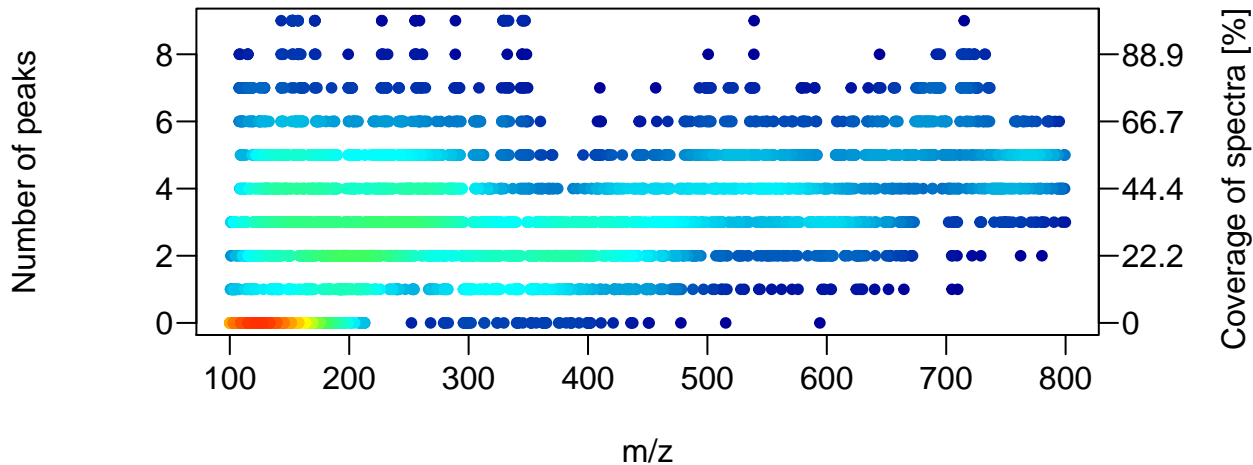




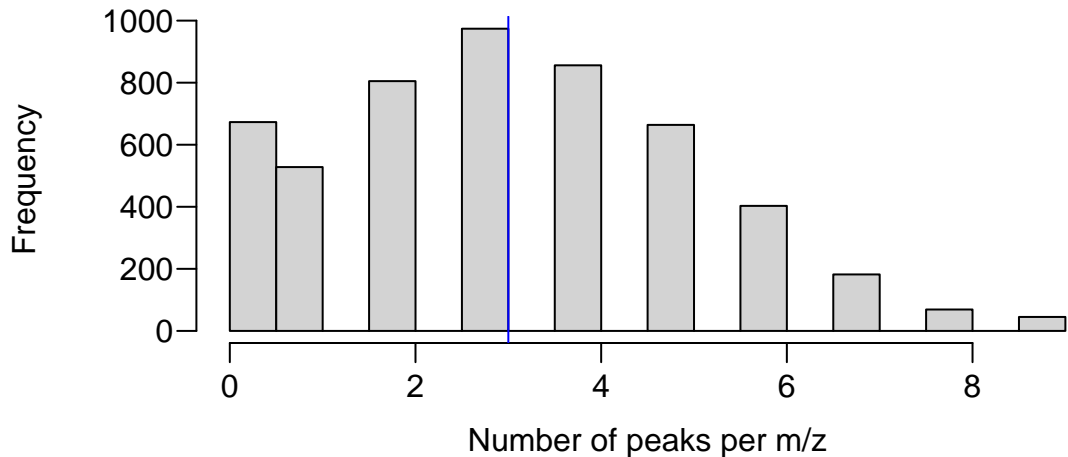
# Histogram of m/z values



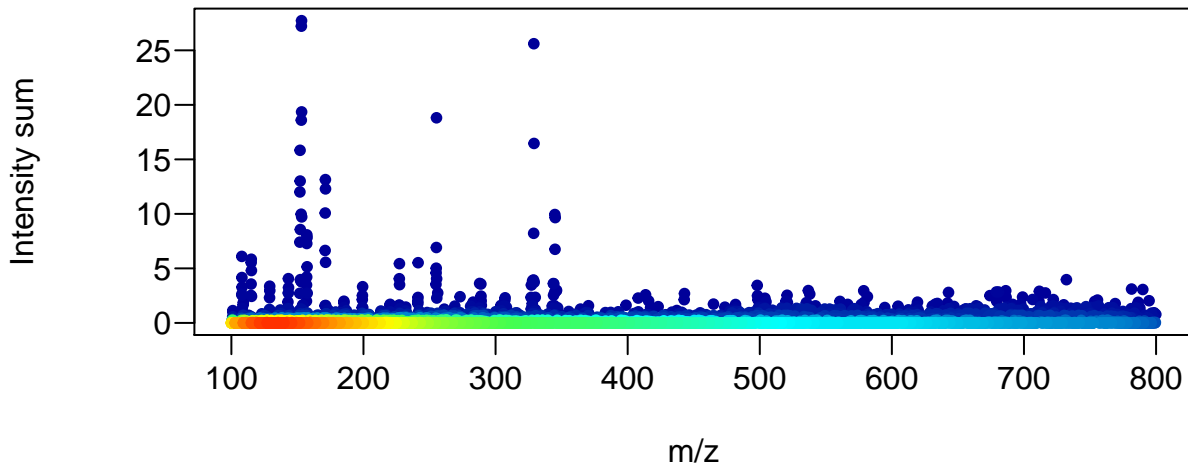
### Number of peaks per m/z



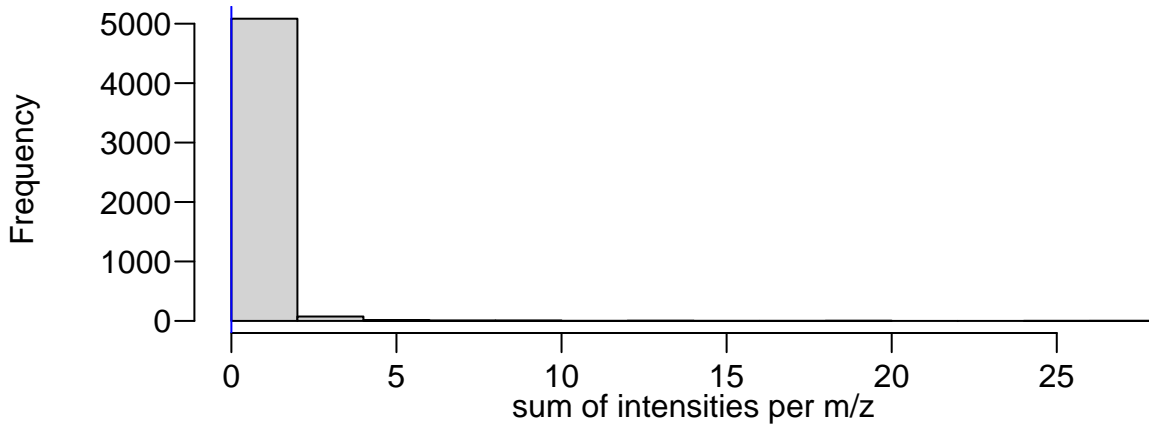
### Number of peaks per m/z



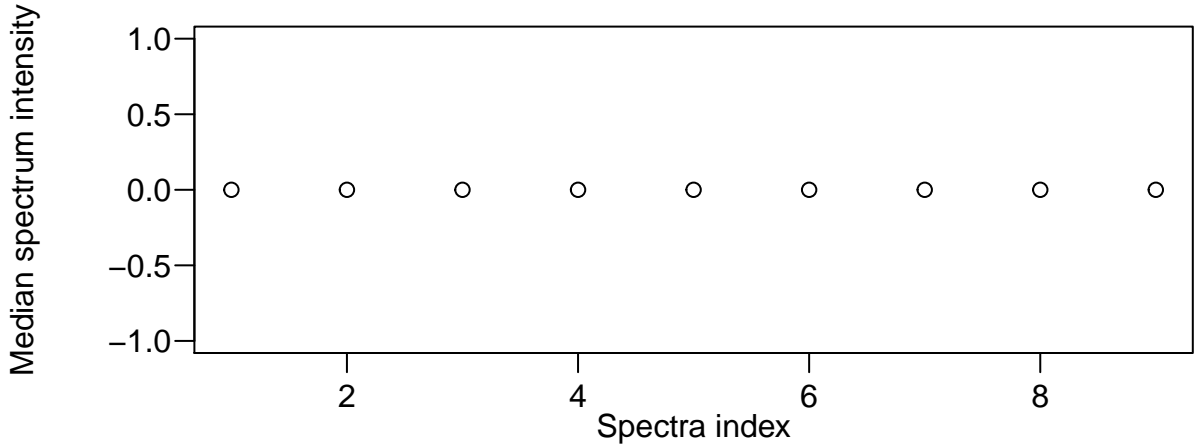
### Sum of intensities per m/z



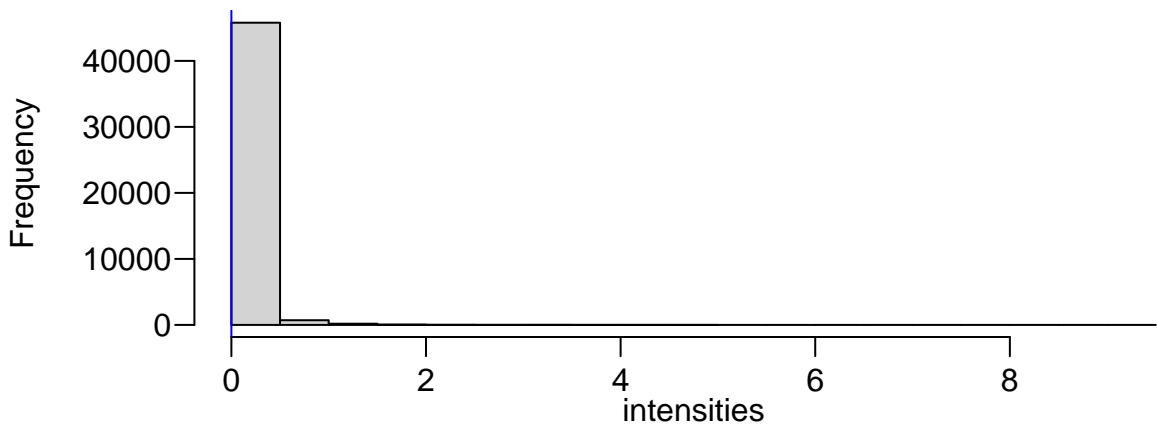
### Sum of intensities per m/z

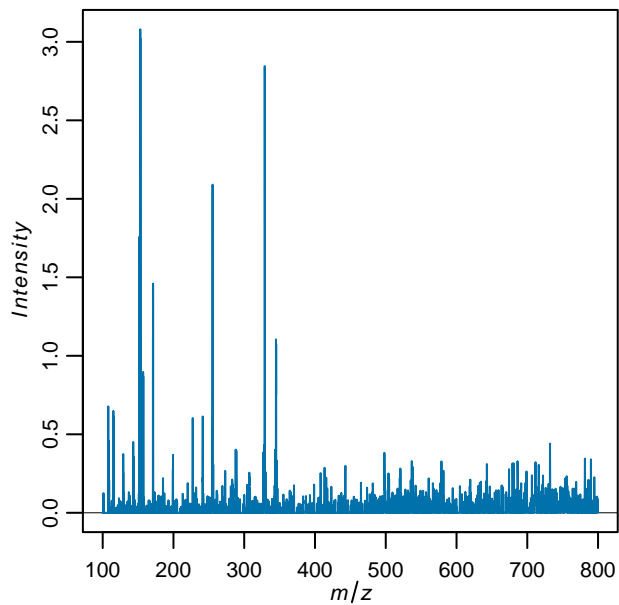
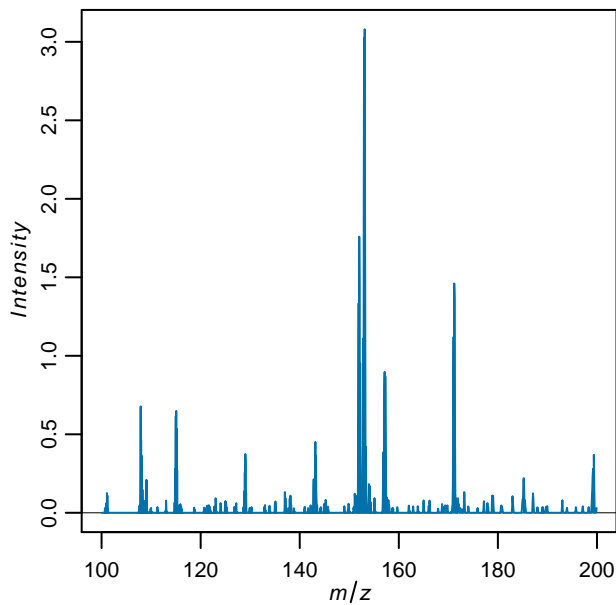
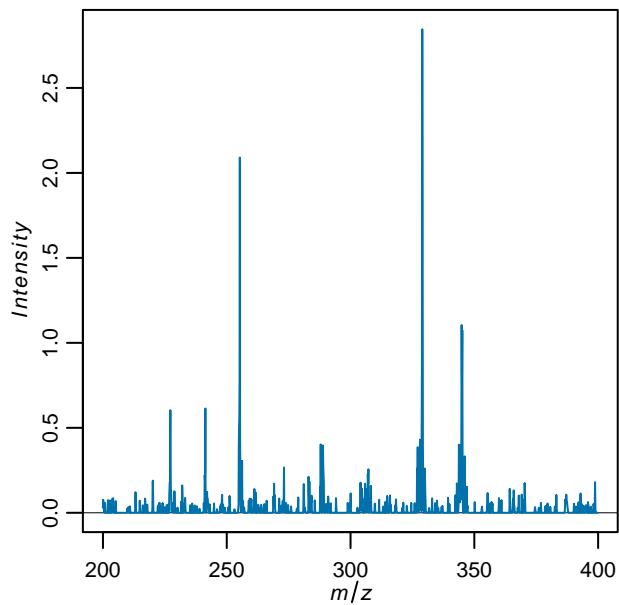
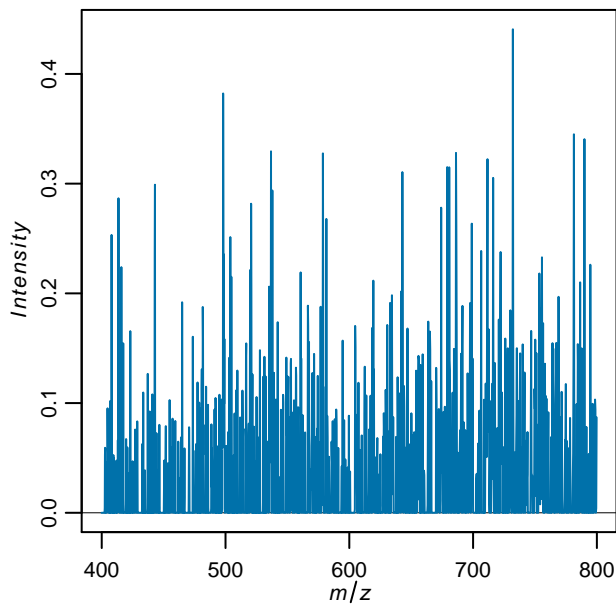


## Median intensity per spectrum

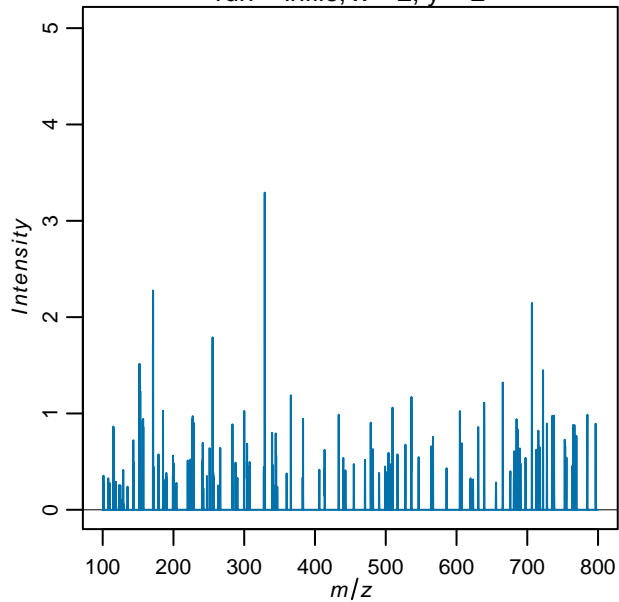


## Intensity histogram

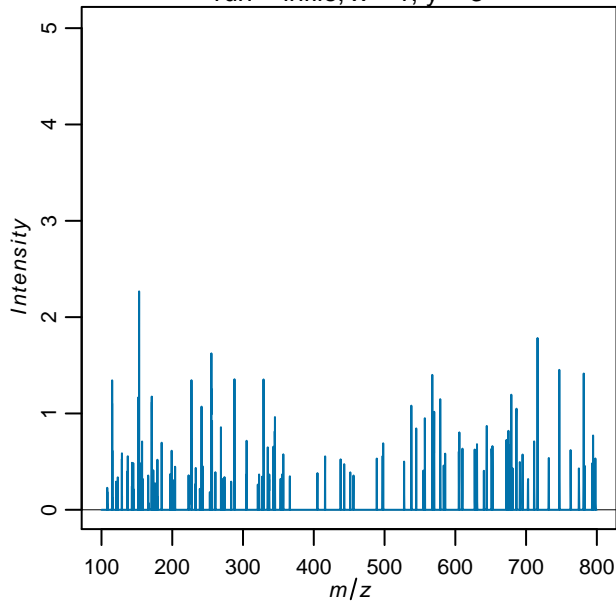


**Average spectrum****Zoomed average spectrum****Zoomed average spectrum****Zoomed average spectrum**

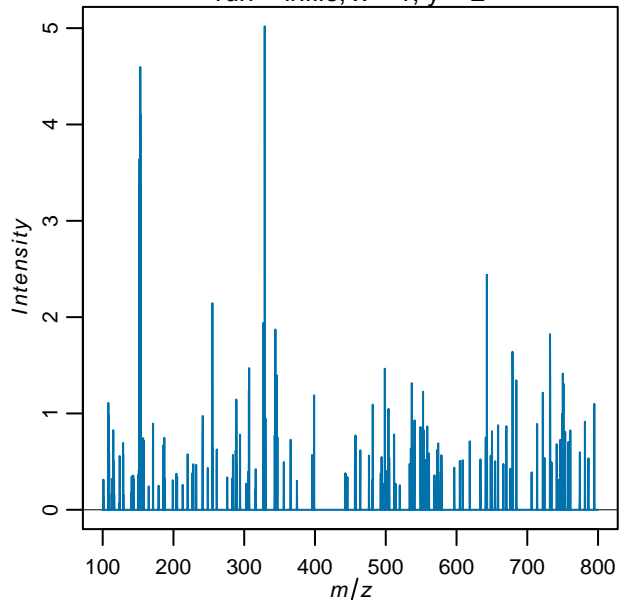
run = infile, x = 2, y = 2



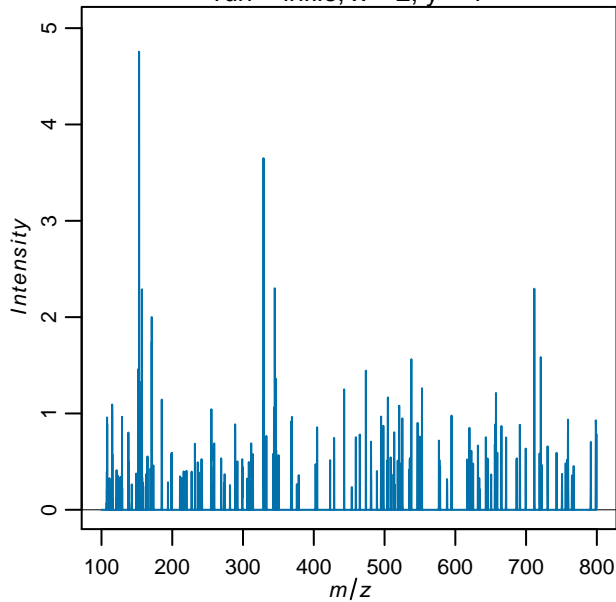
run = infile, x = 1, y = 3



run = infile, x = 1, y = 2



run = infile, x = 2, y = 1

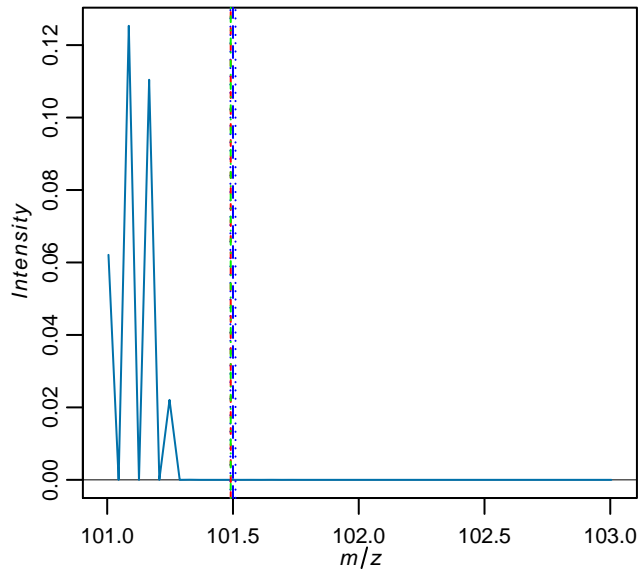


theor. m/z: 101.5

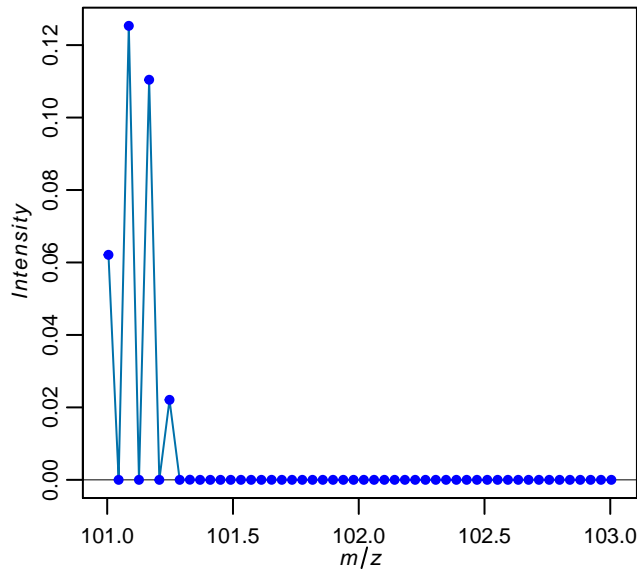
most abundant m/z: 101.491

closest m/z: 101.491

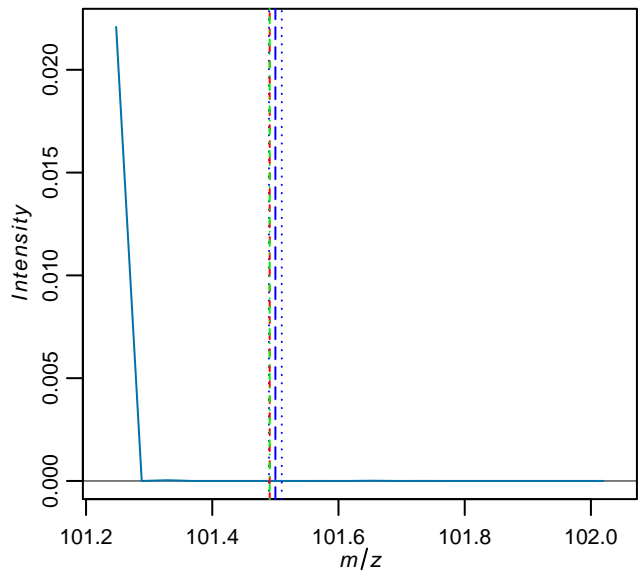
Average spectrum



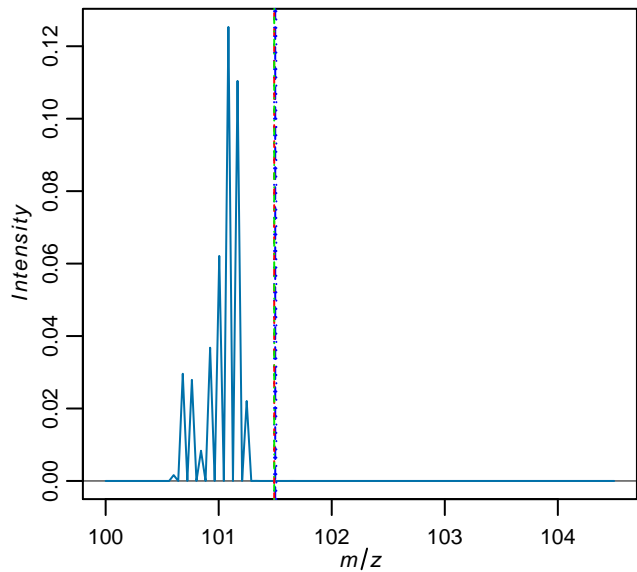
Average spectrum with data points



Average spectrum



Average spectrum

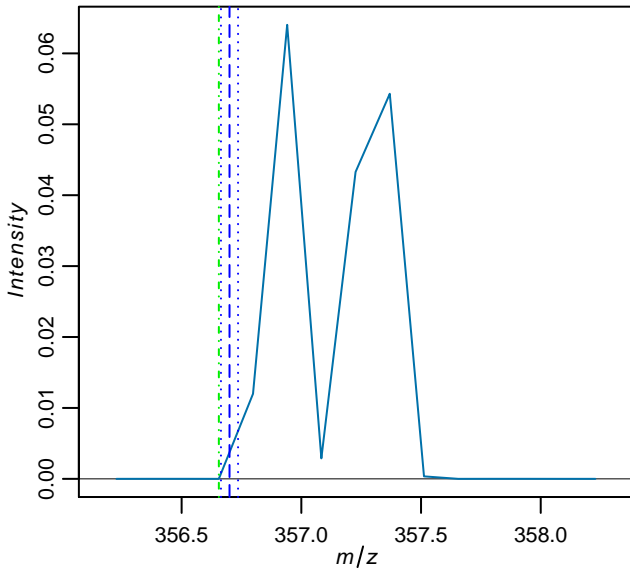


theor. m/z: 356.7

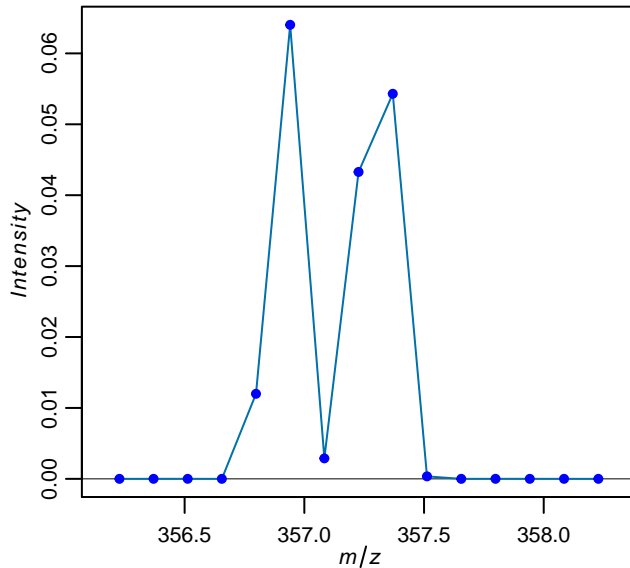
most abundant m/z: NA

closest m/z: 356.6555

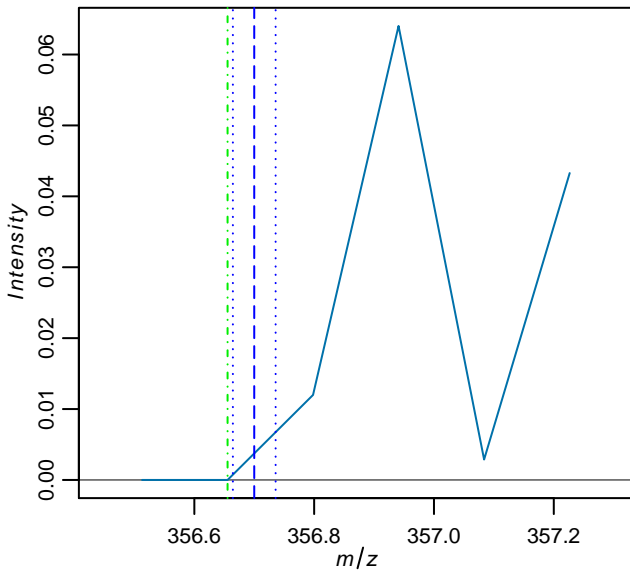
Average spectrum



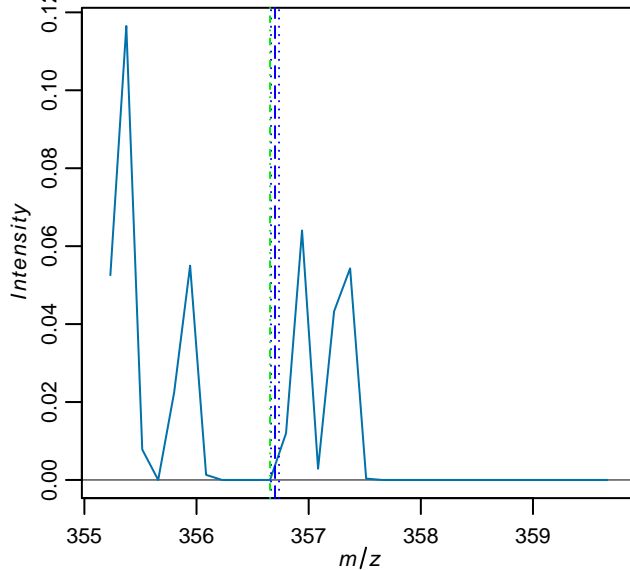
Average spectrum with data points



Average spectrum



Average spectrum



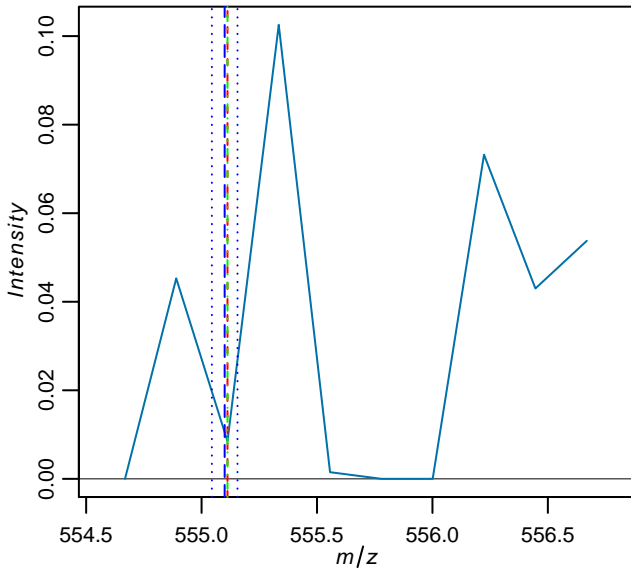


theor. m/z: 555.1

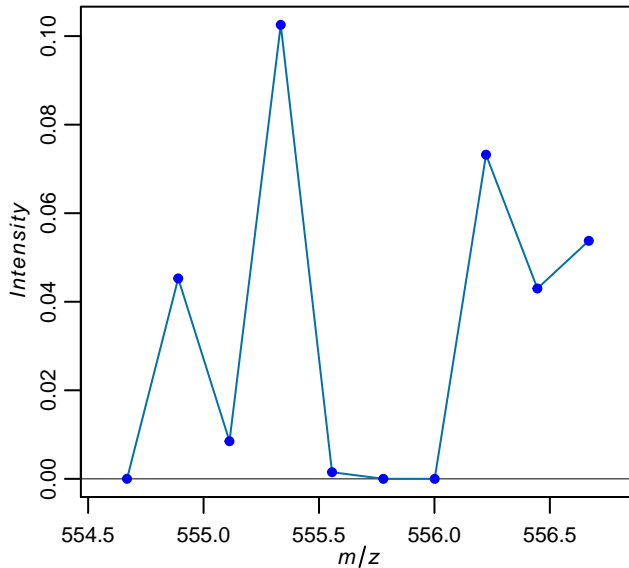
most abundant m/z: 555.122

closest m/z: 555.122

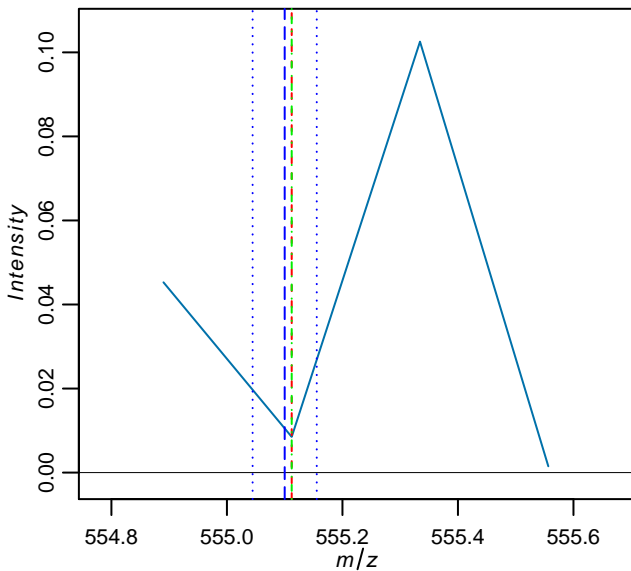
Average spectrum



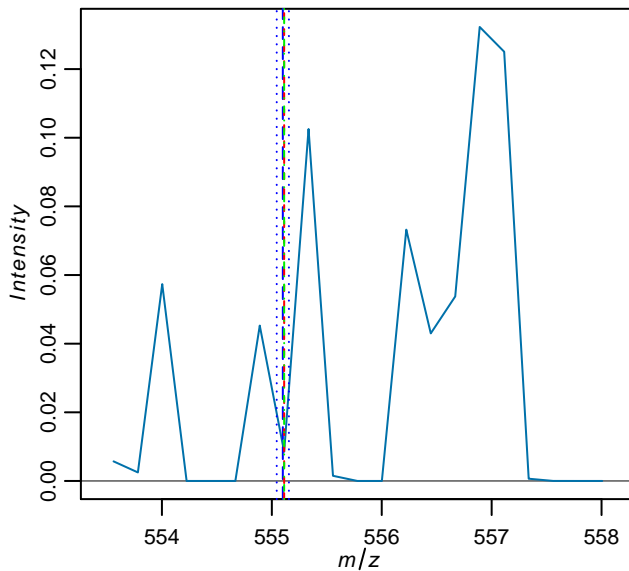
Average spectrum with data points



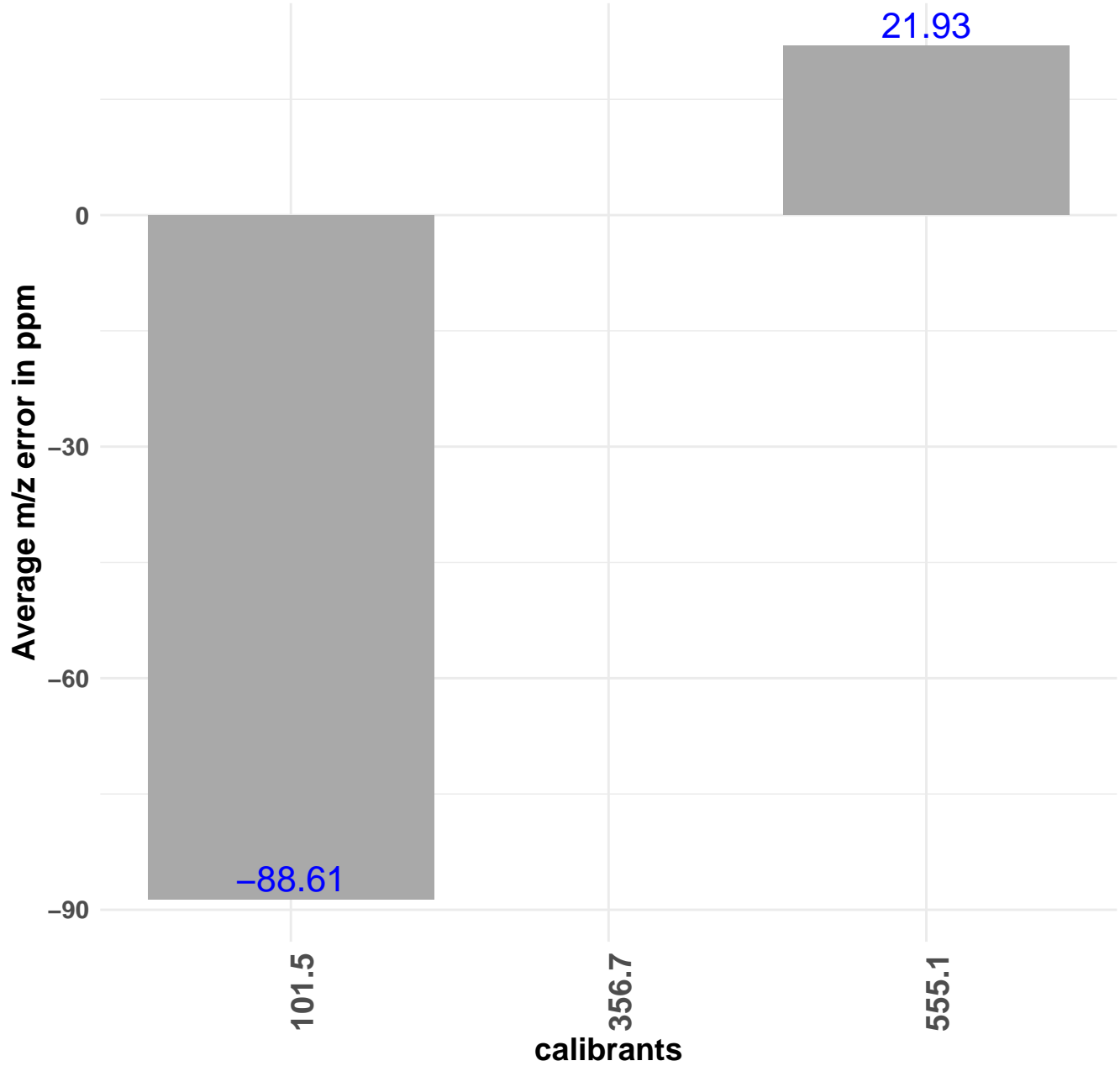
Average spectrum



Average spectrum

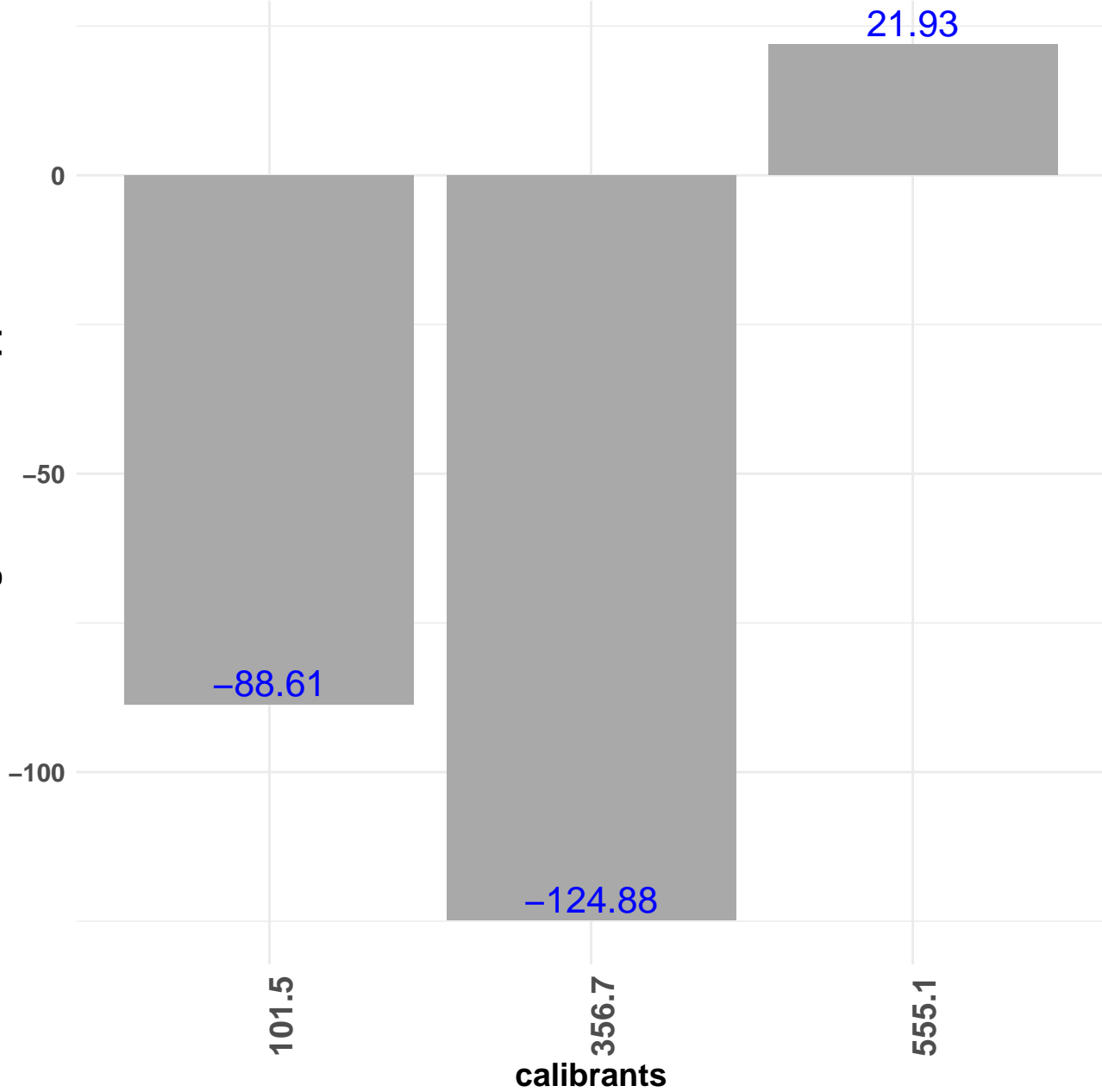


# Average m/z error (max. average intensity vs. theor. calibrant m/z)

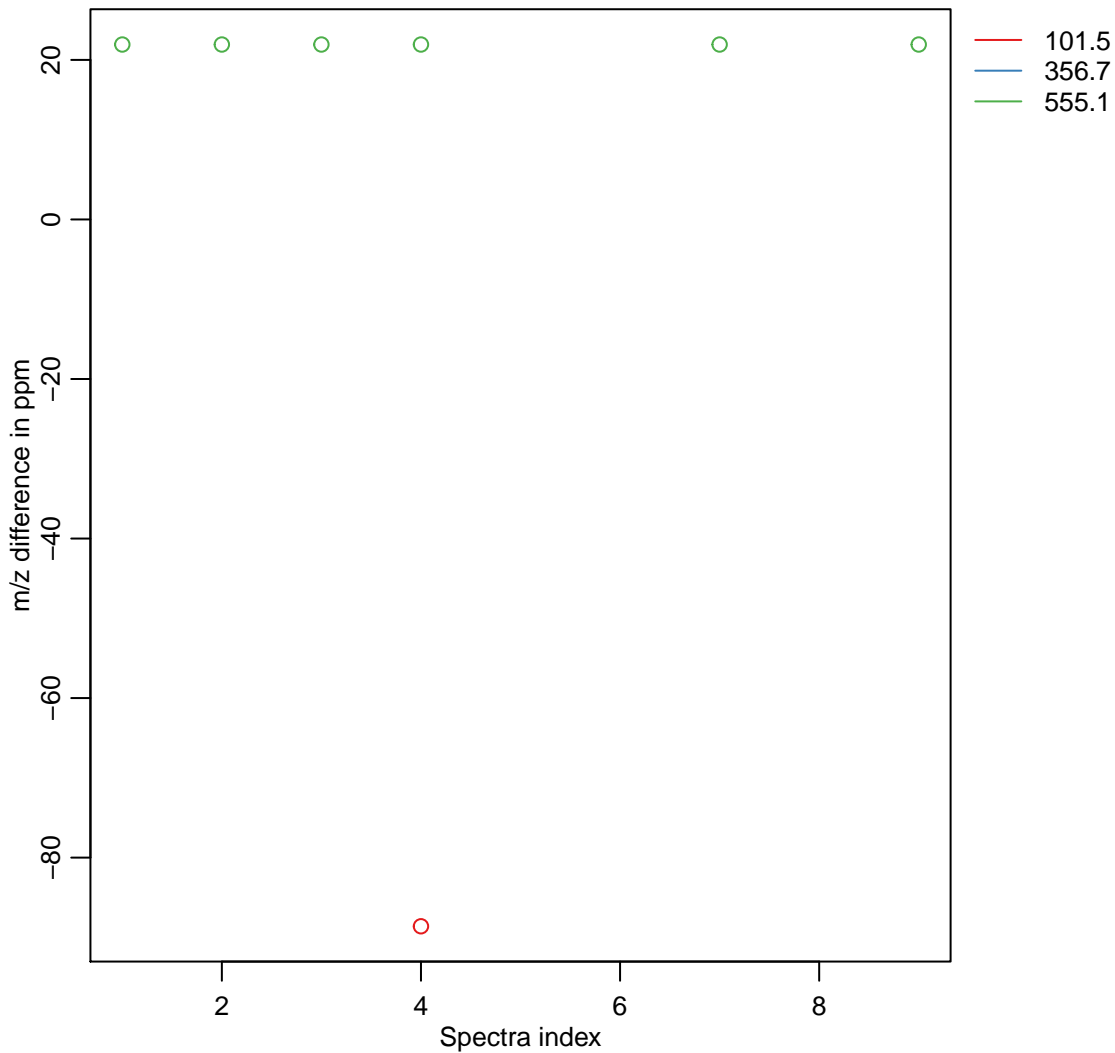


# Average m/z error (closest measured m/z vs. theor. calibrant m/z)

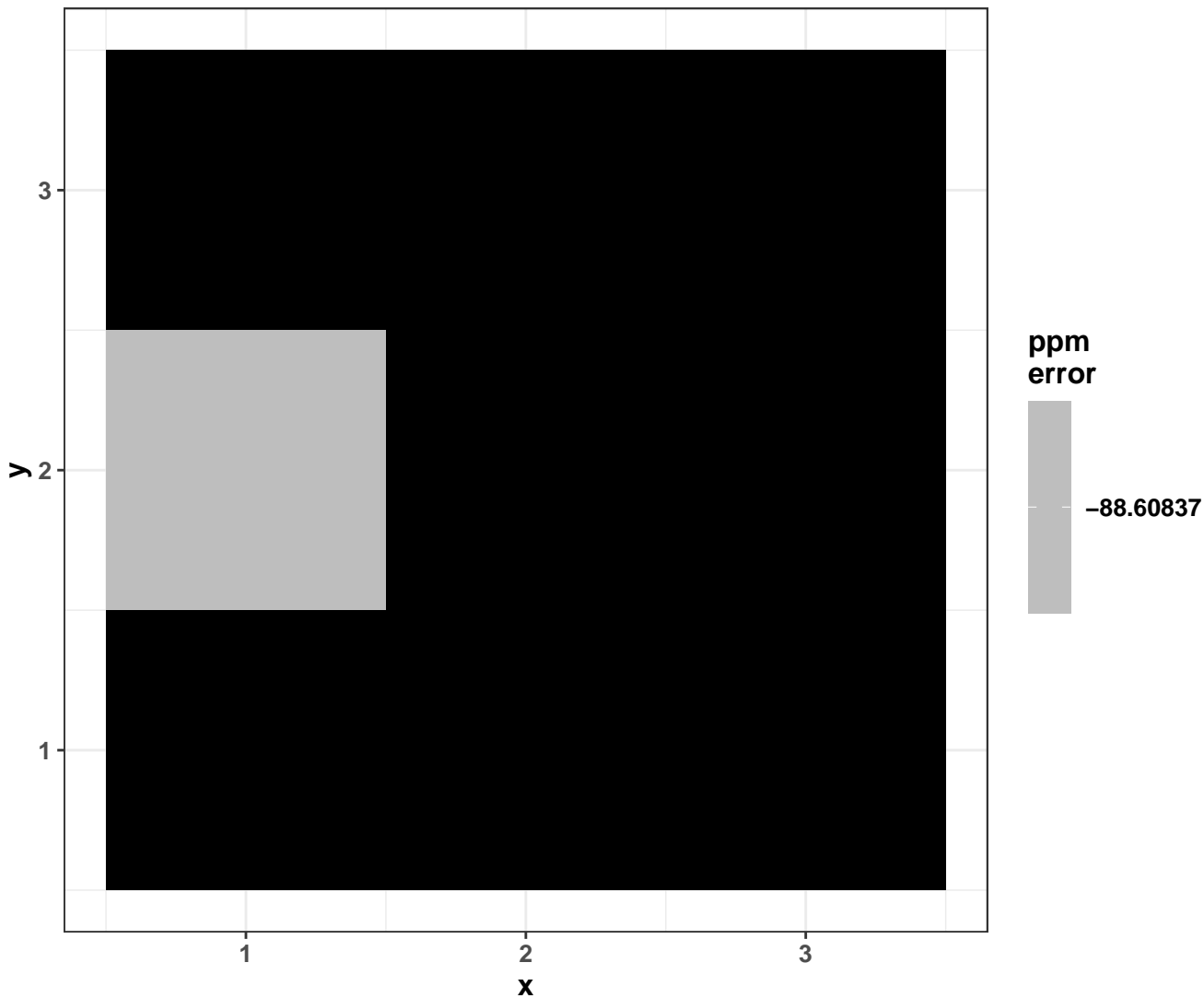
Average m/z error in ppm



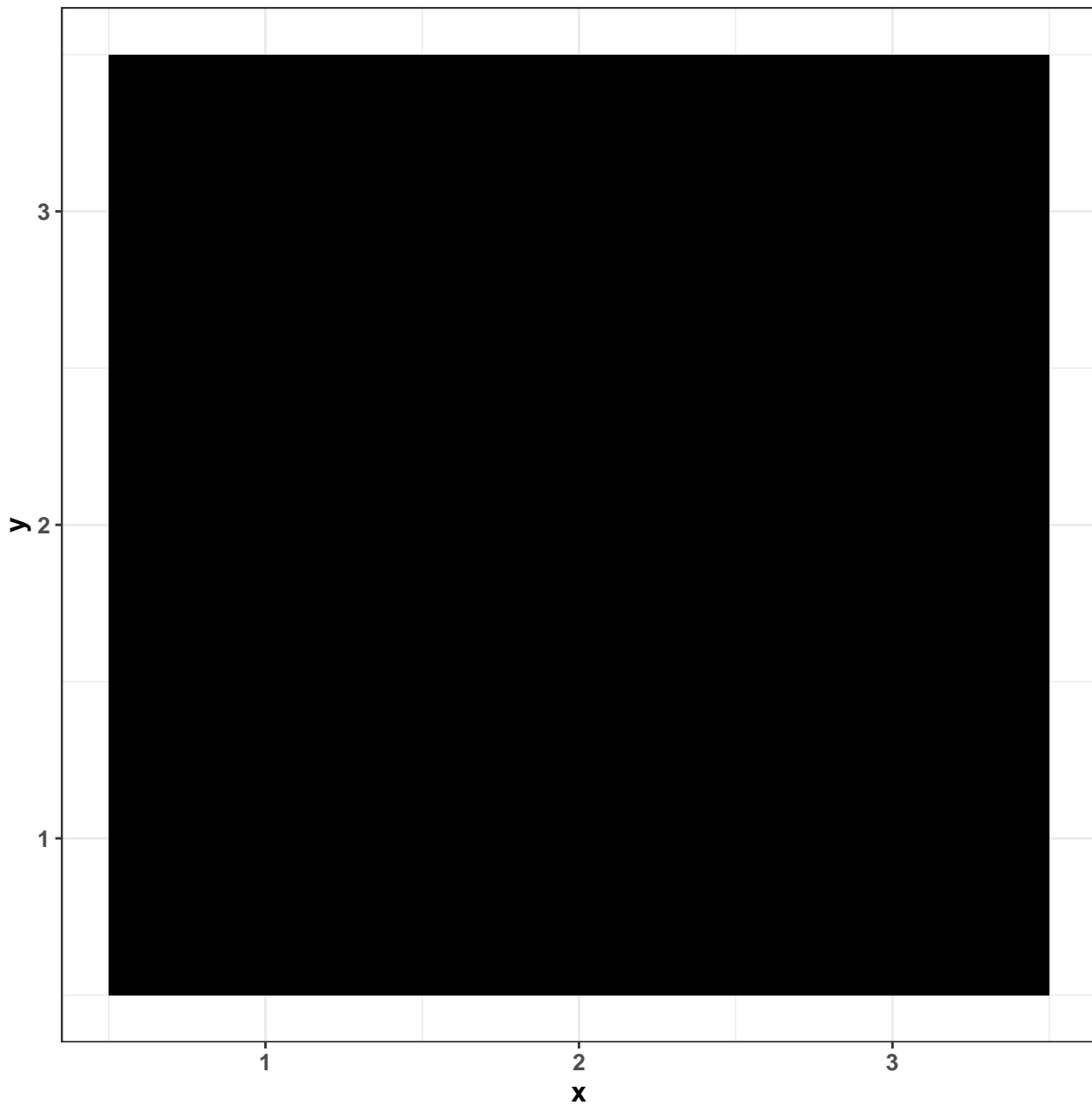
## Difference m/z with max. average intensity vs. theor. m/z (per spectrum)



# m/z accuracy for 101.5



# m/z accuracy for 356.7



# m/z accuracy for 555.1

