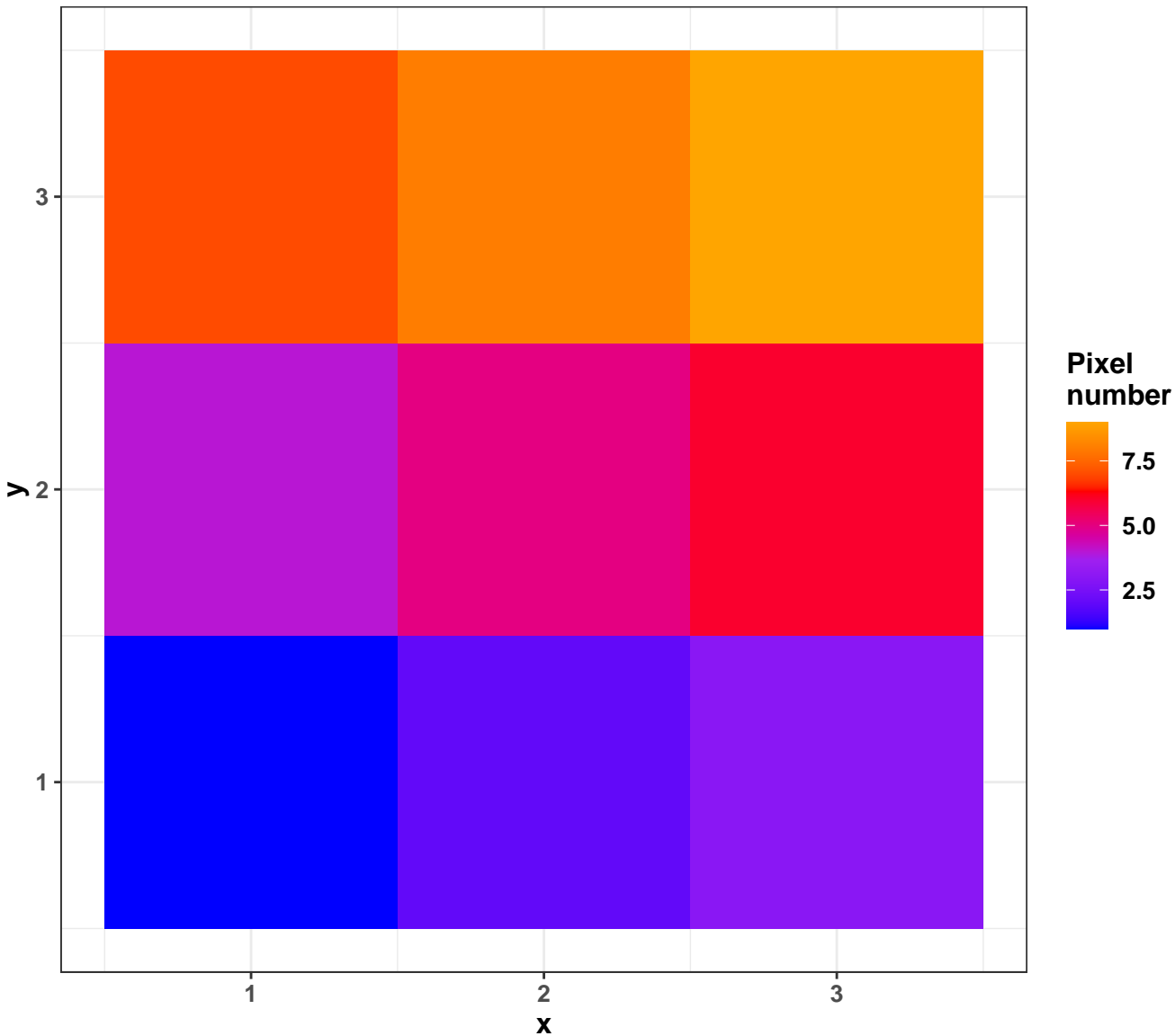


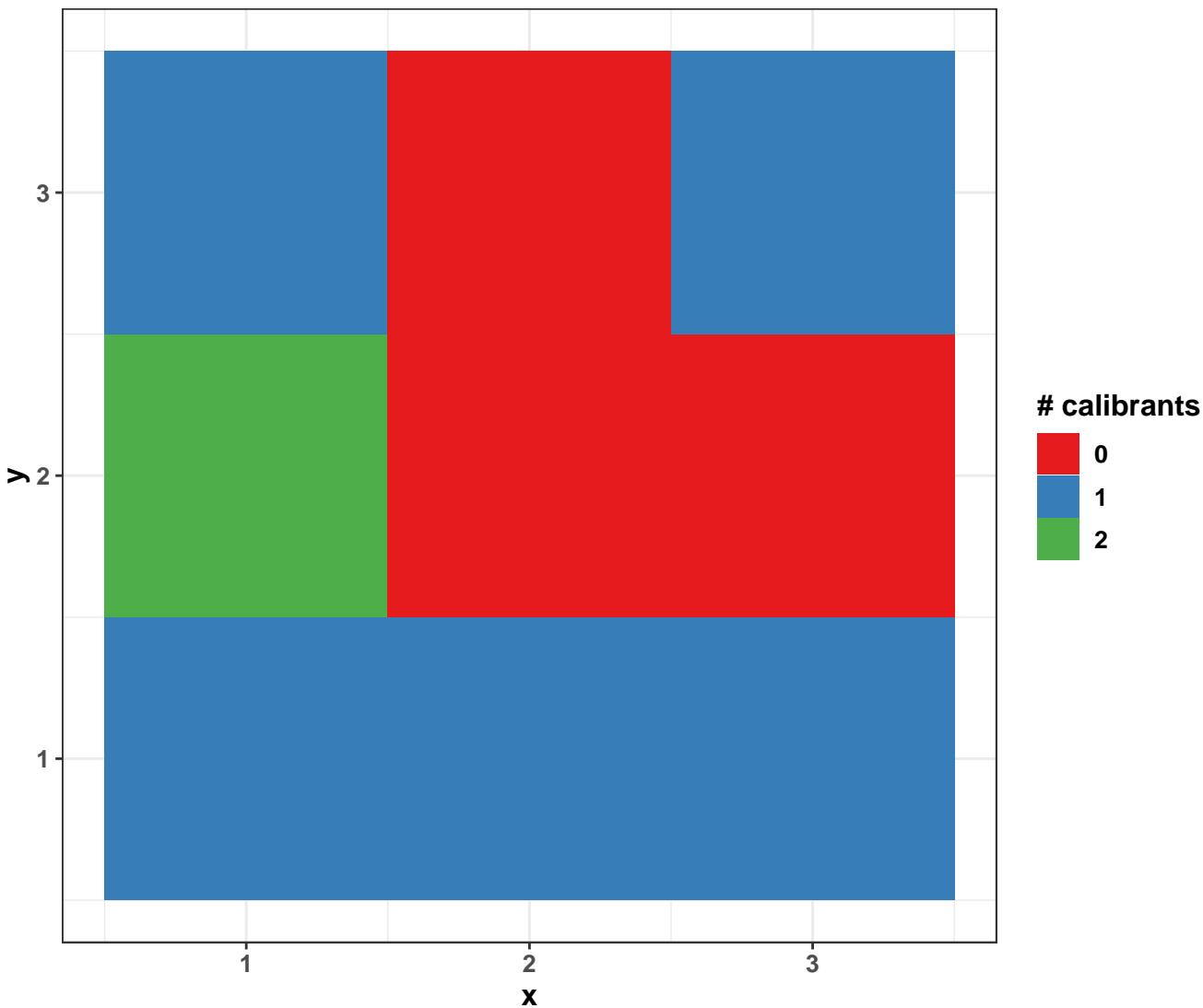
Testfile_imzml

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

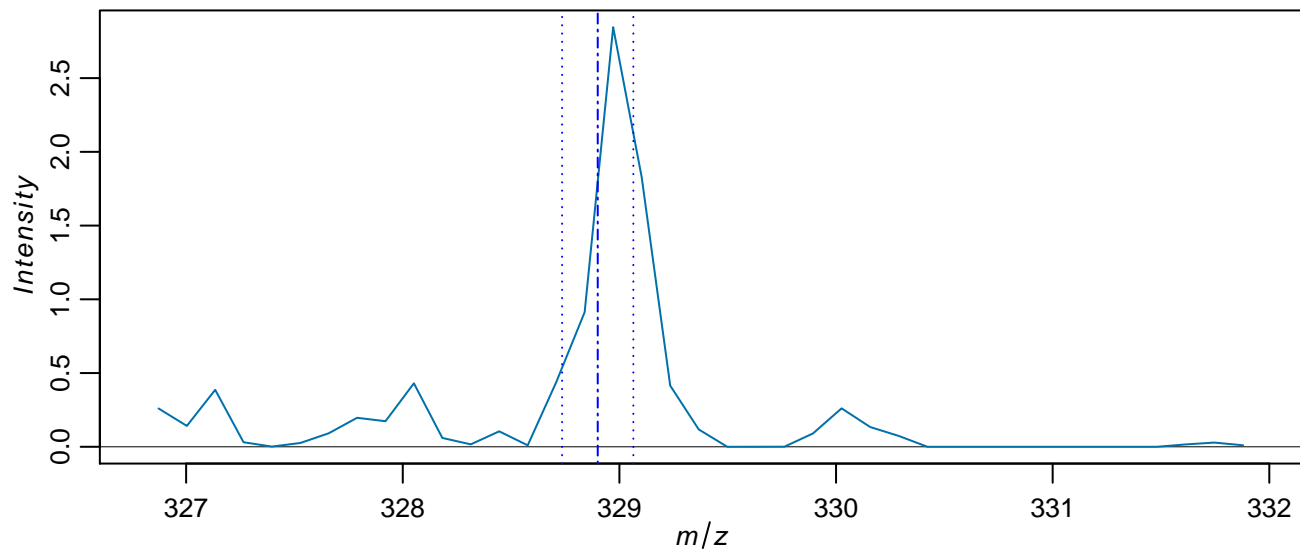


Number of calibrants per pixel (± 100 ppm)

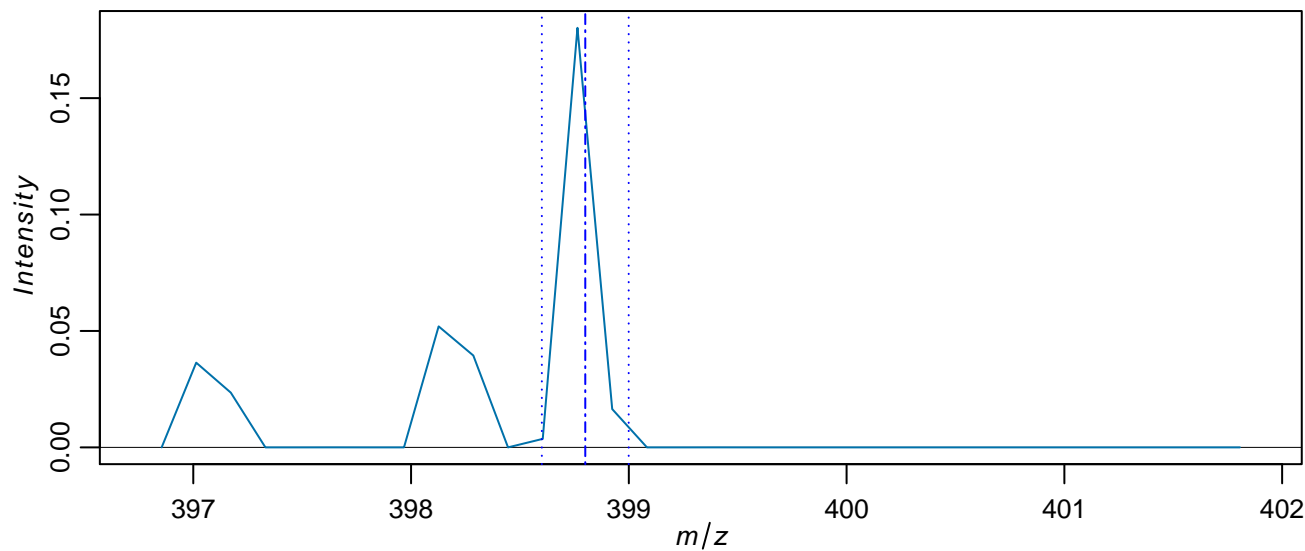


Control of fold change plot

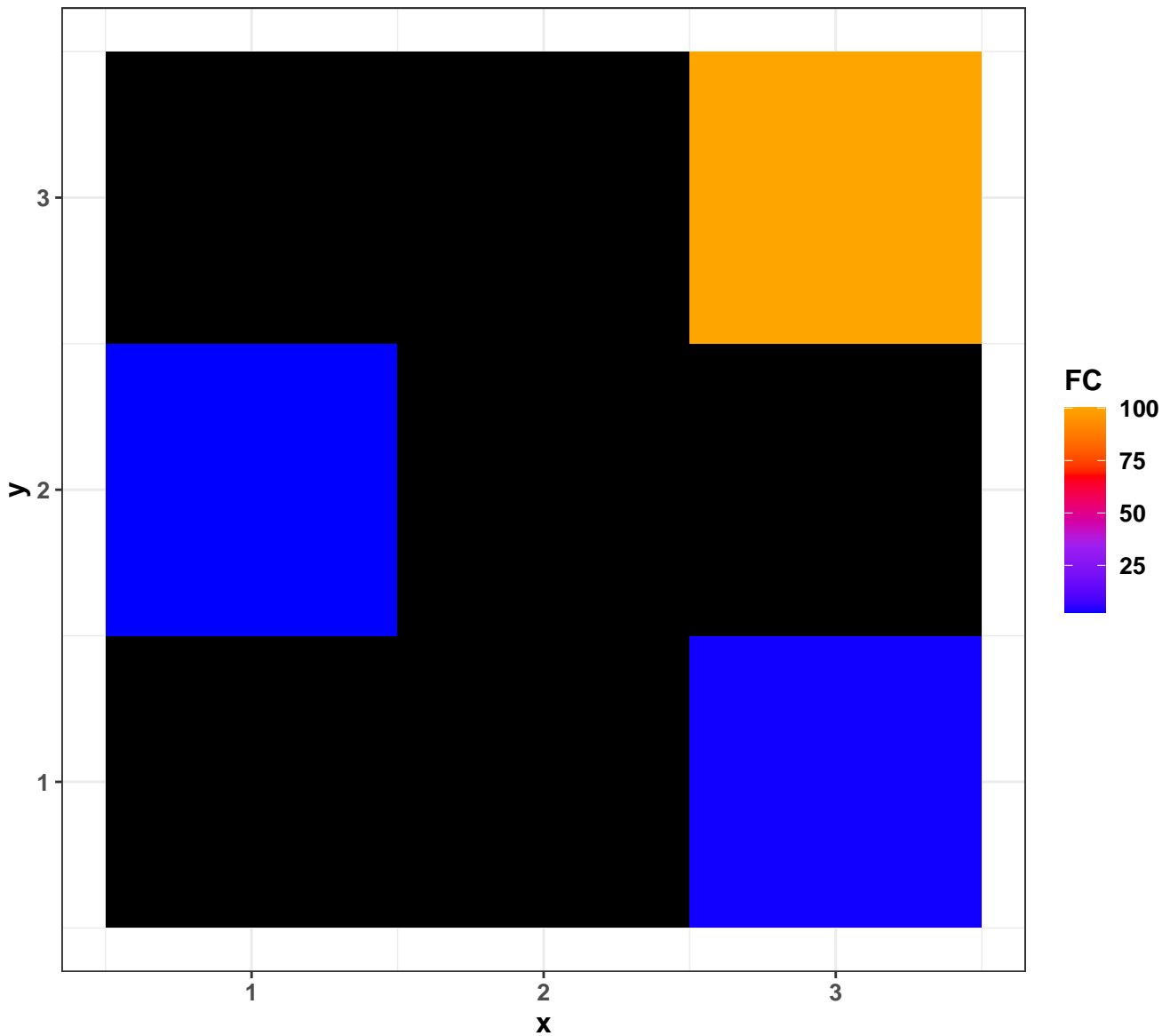
Average spectrum 328.9 Da



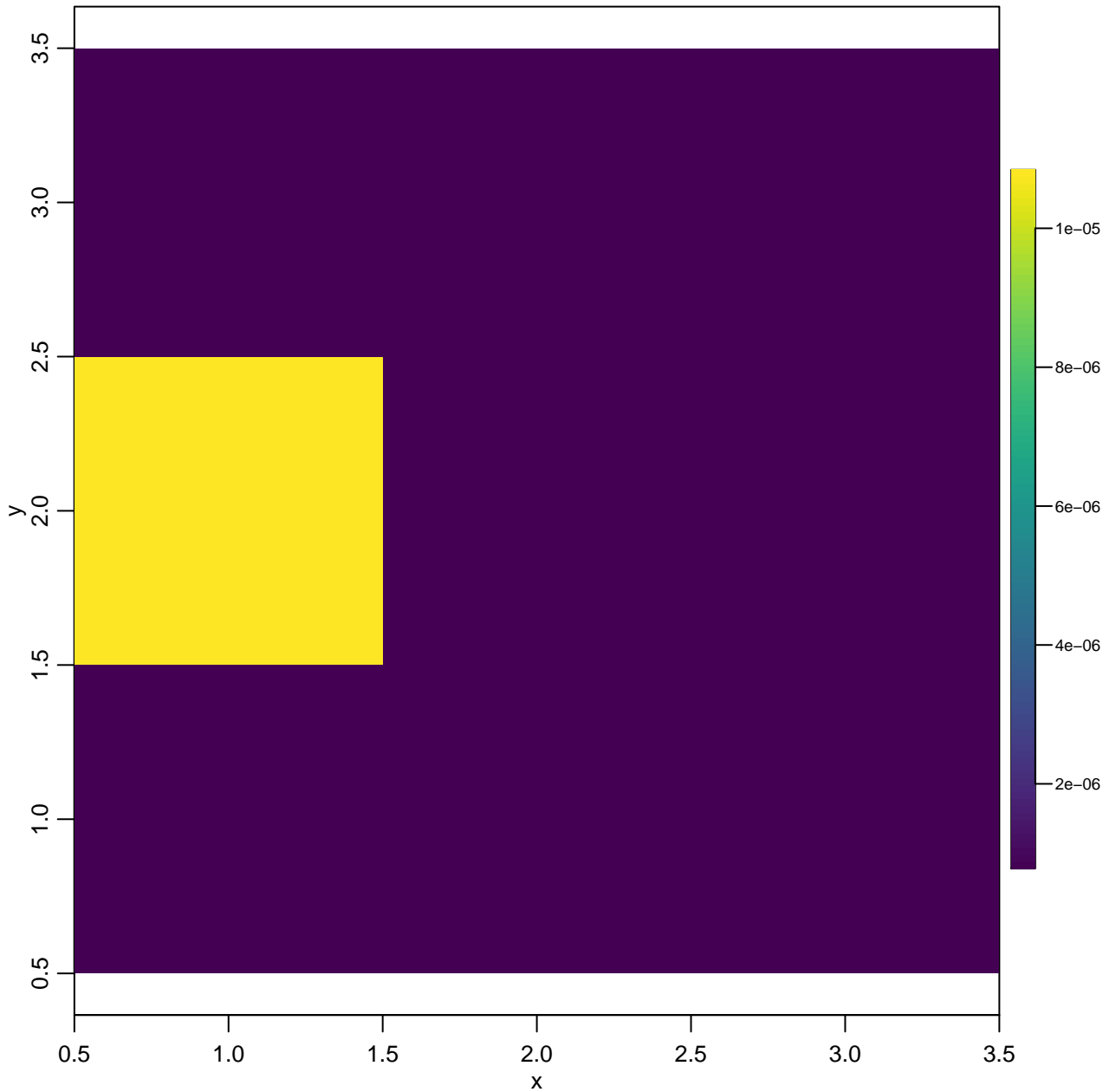
Average spectrum 398.8 Da



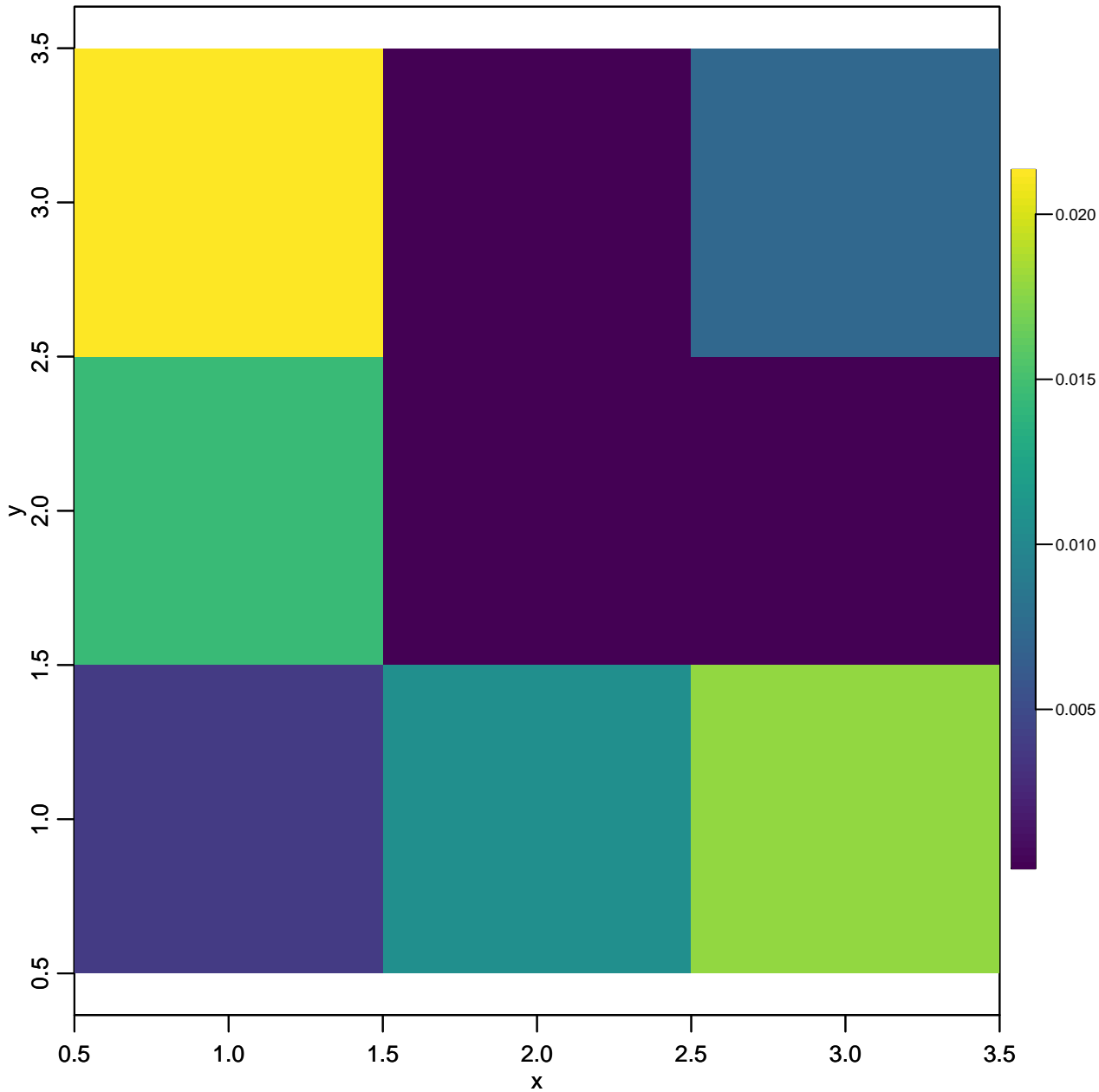
Ratio of mz 3289 and mz 3988



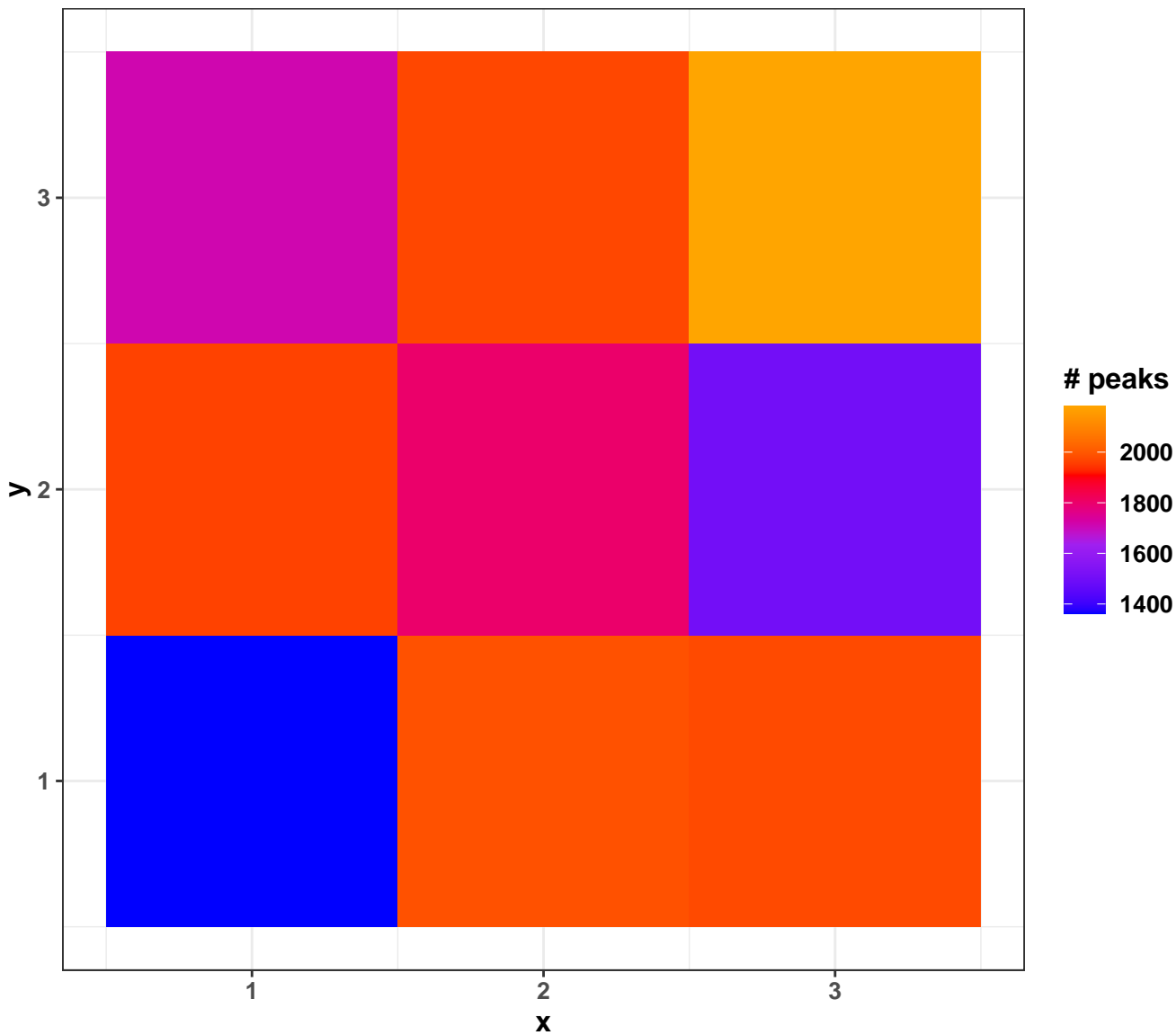
101.5: 101.5 (± 100 ppm)



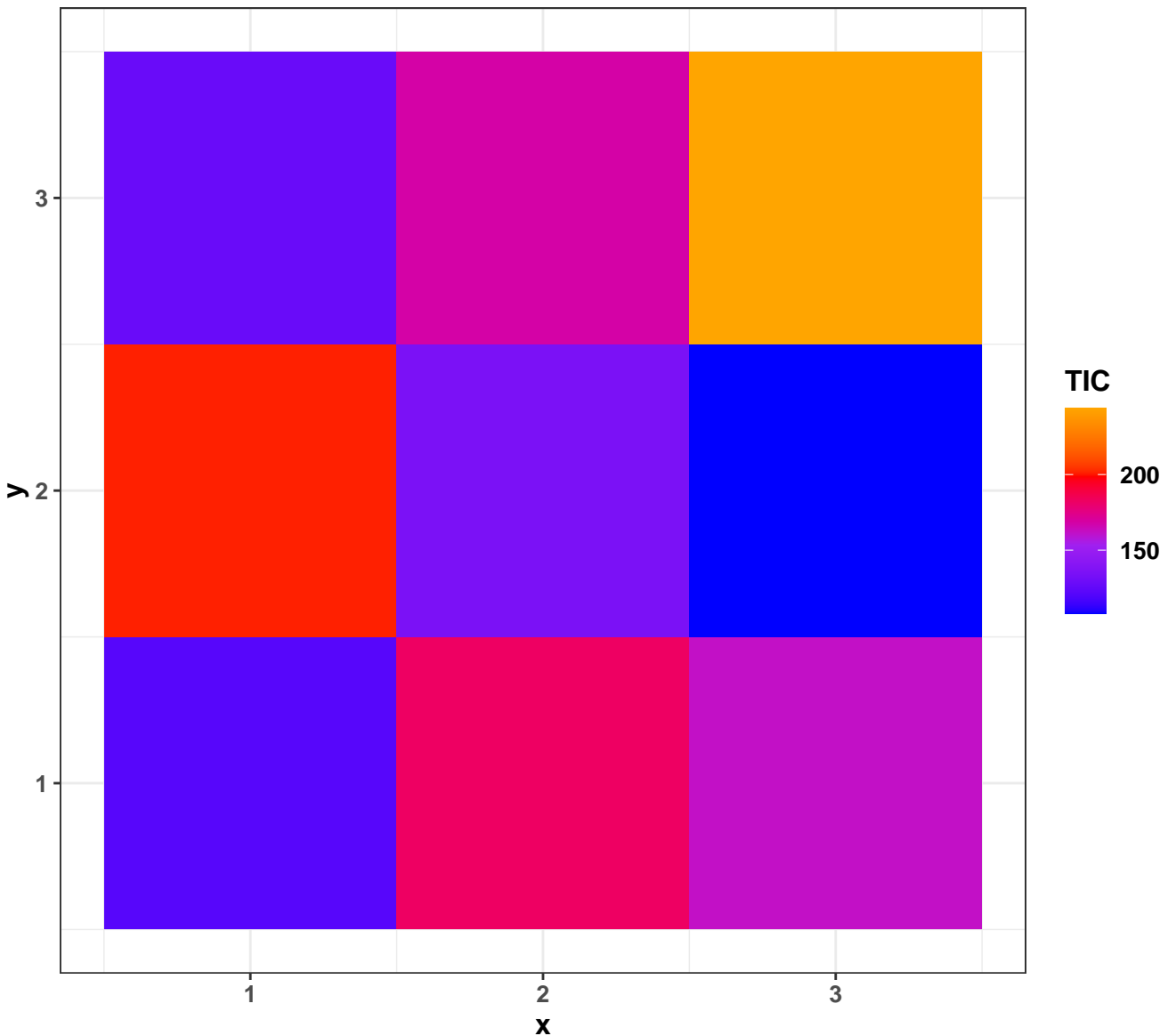
556.7: 556.7 (± 100 ppm)



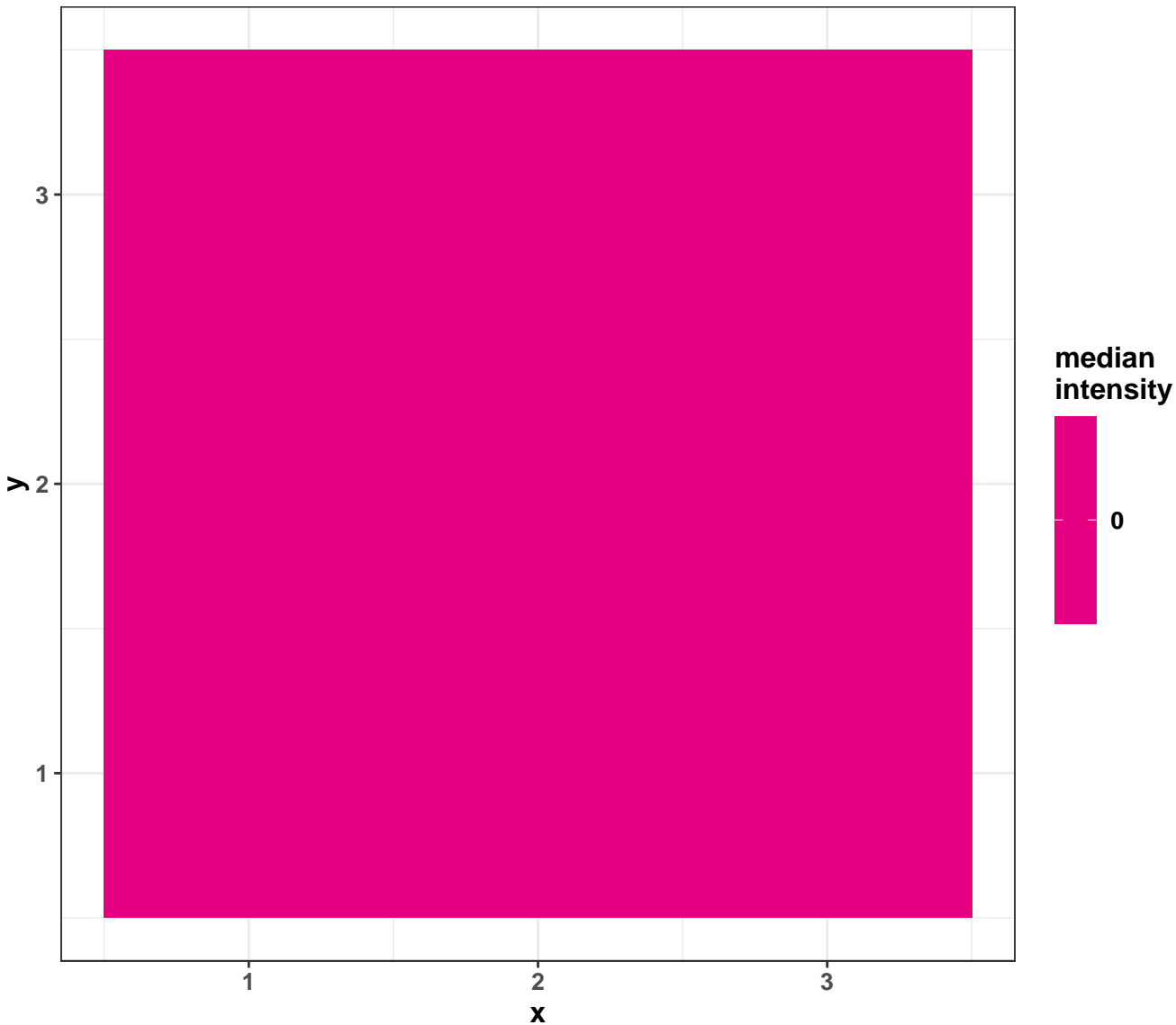
Number of peaks per spectrum



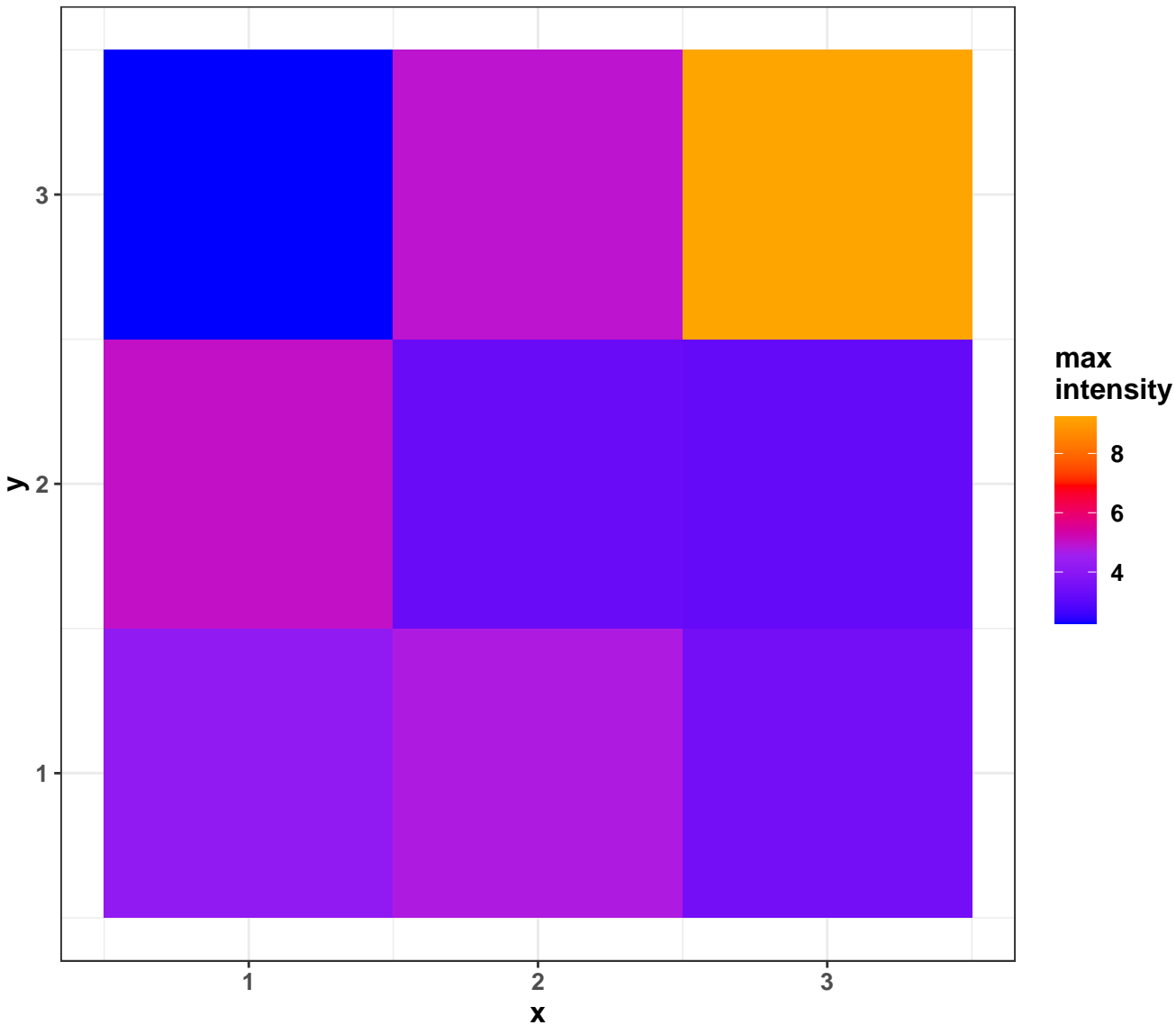
Total Ion Current



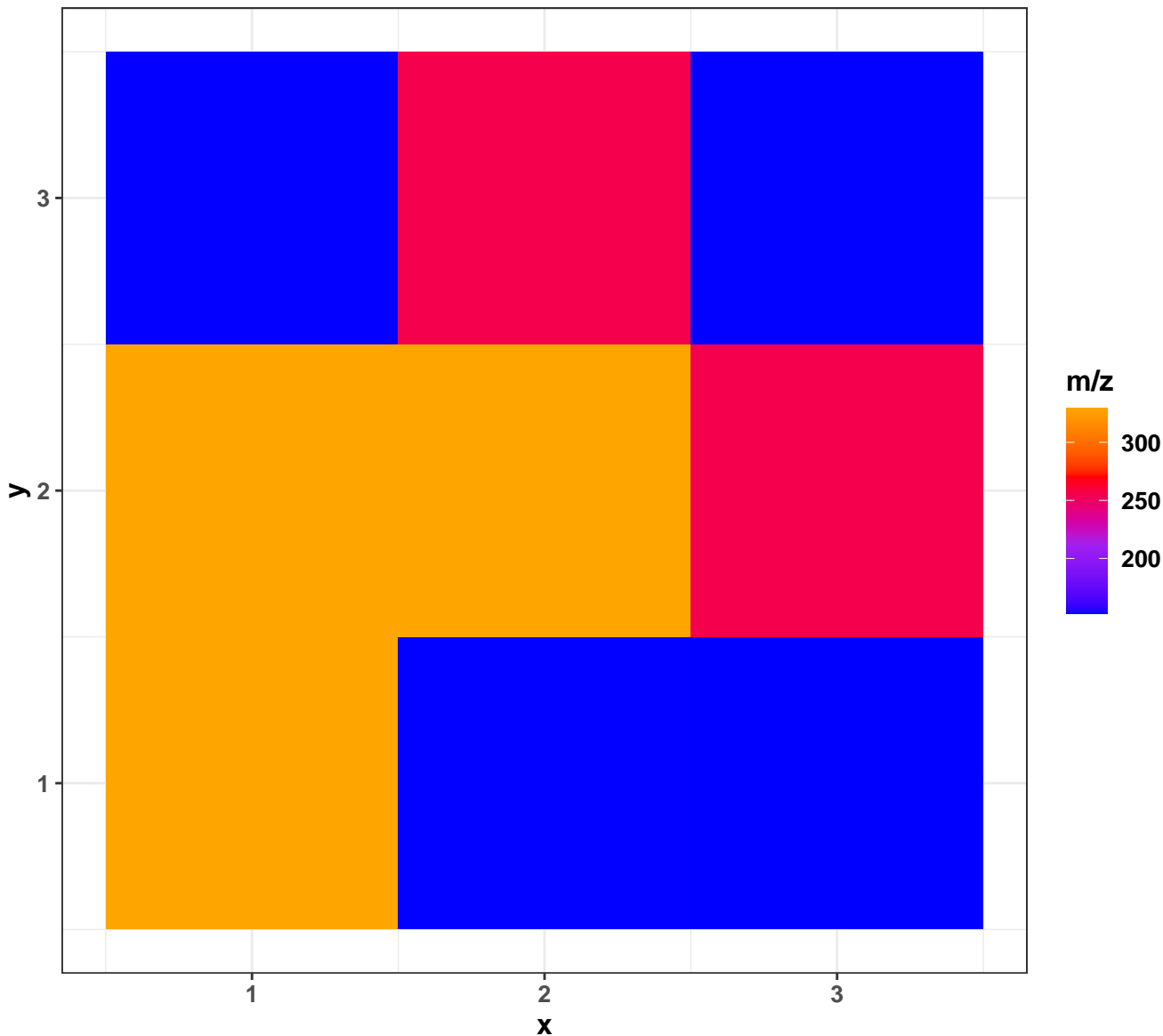
Median intensity per spectrum



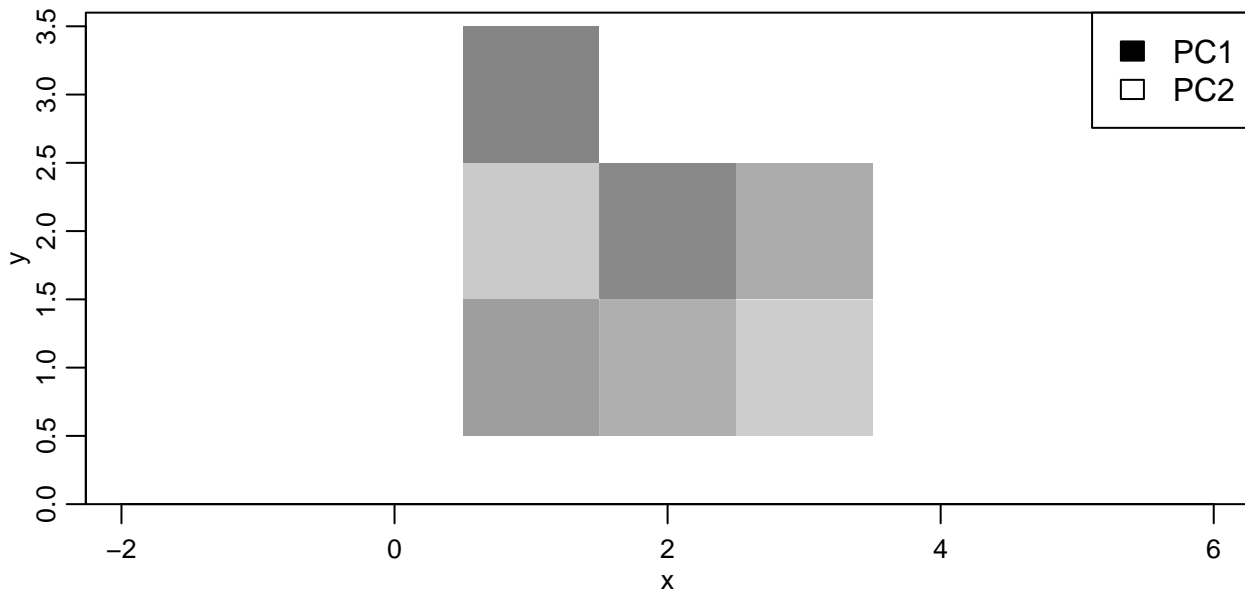
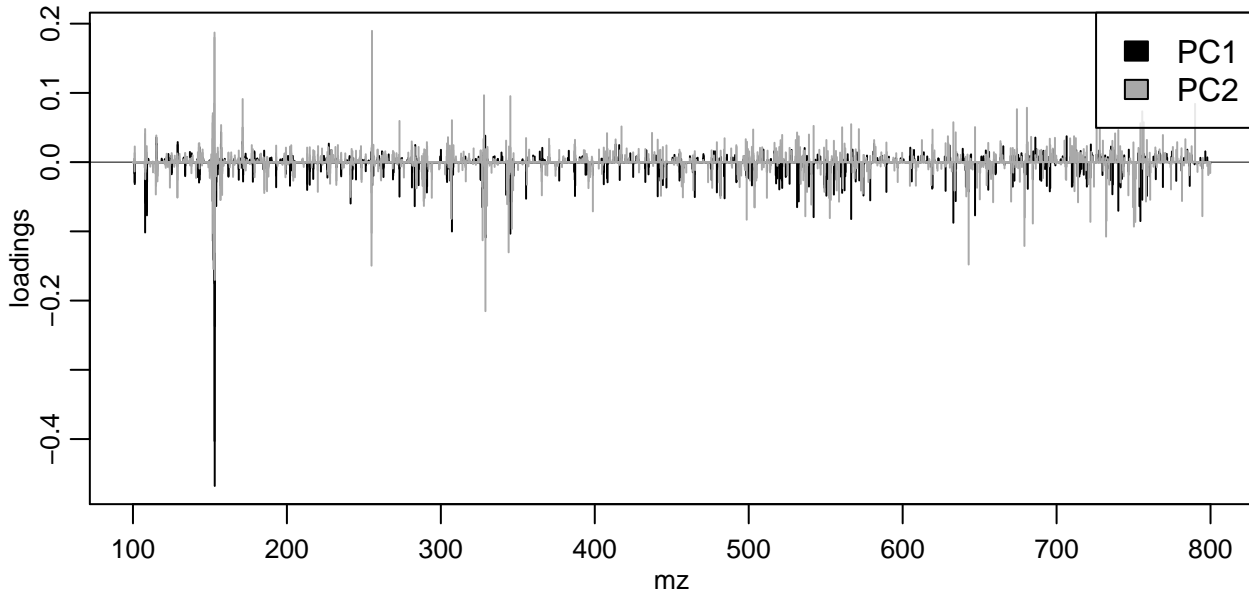
Maximum intensity per spectrum

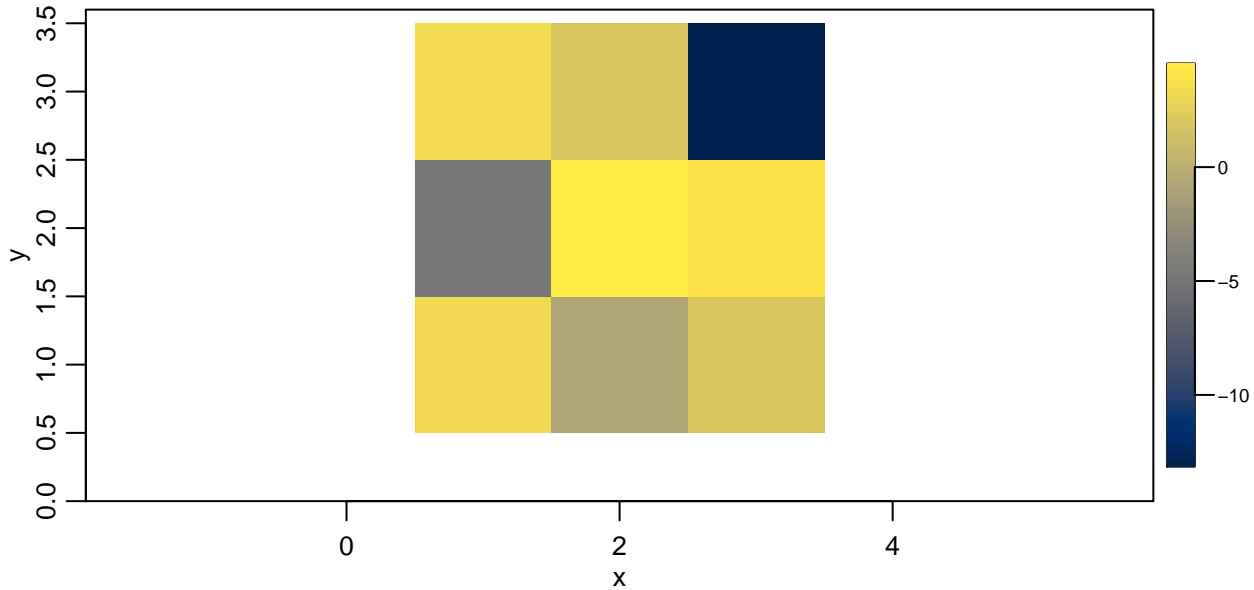
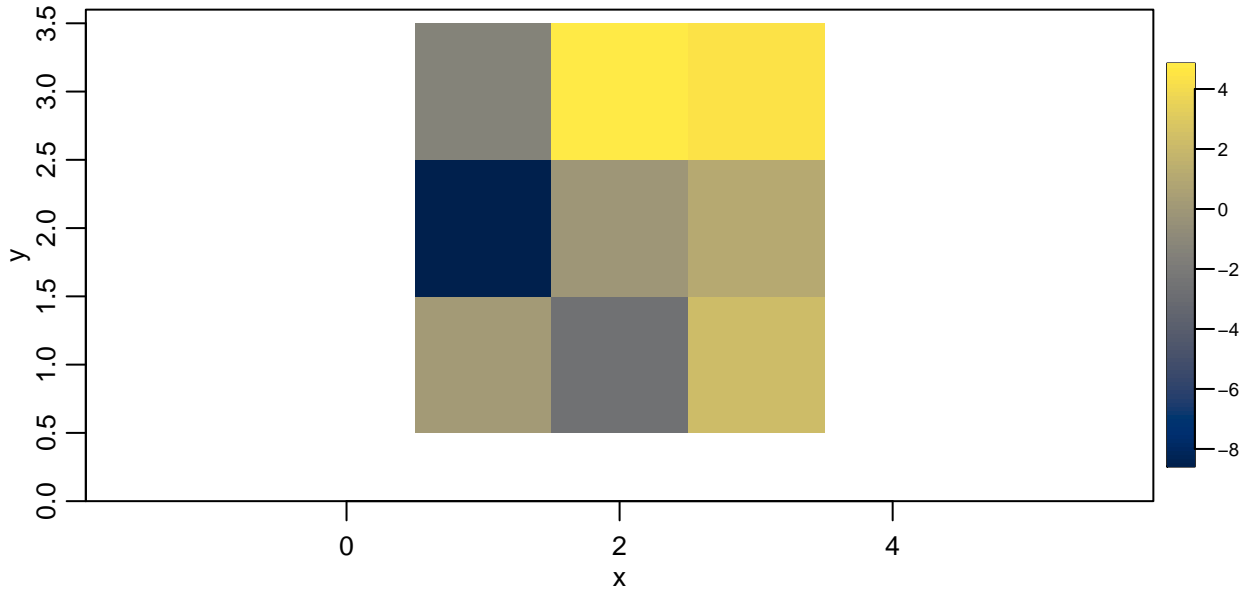


Most abundant m/z in each spectrum

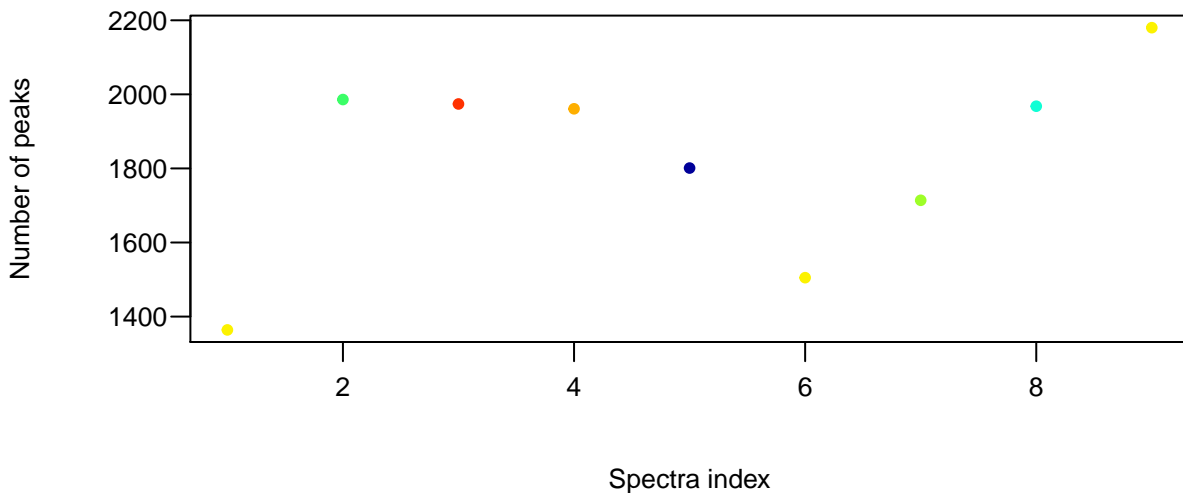


PCA for two components

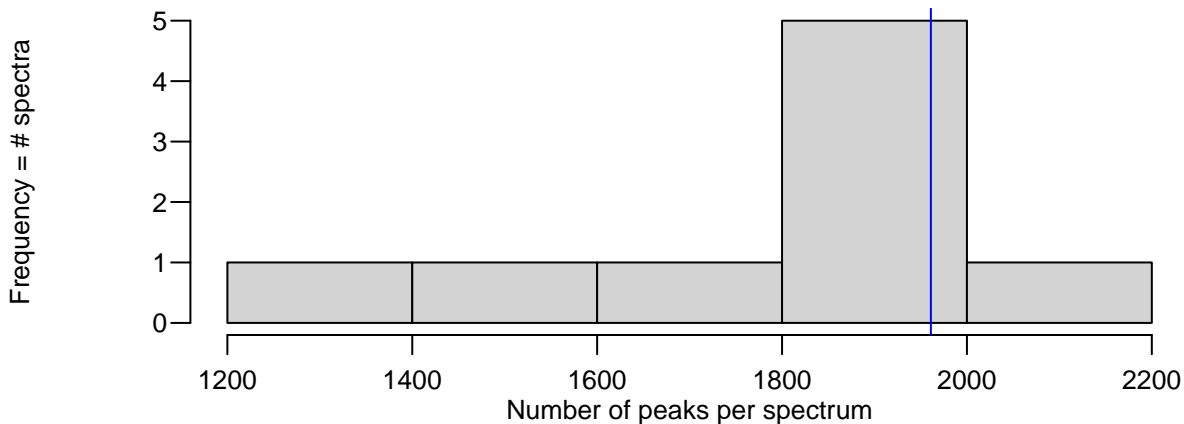


PC1**PC2**

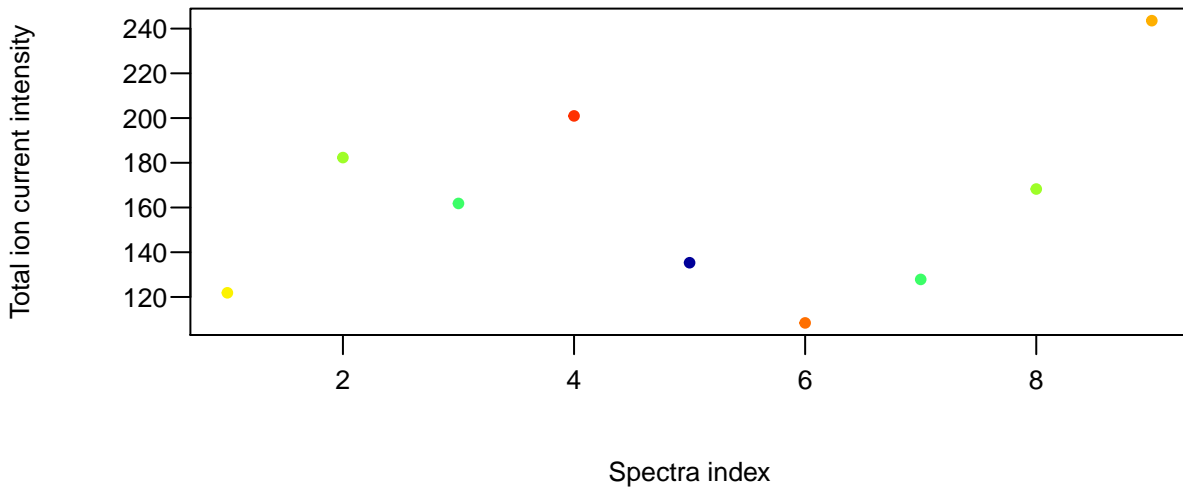
Number of peaks per spectrum



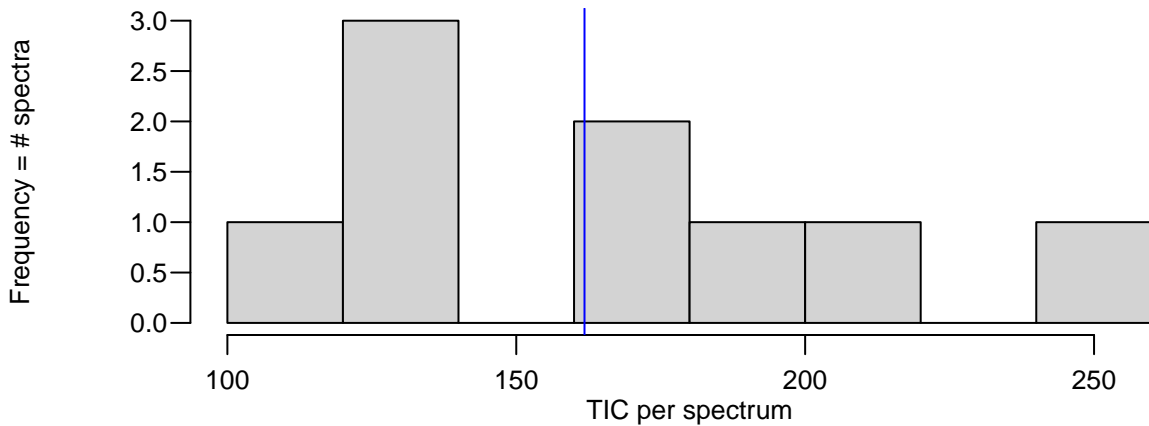
Number of peaks per spectrum



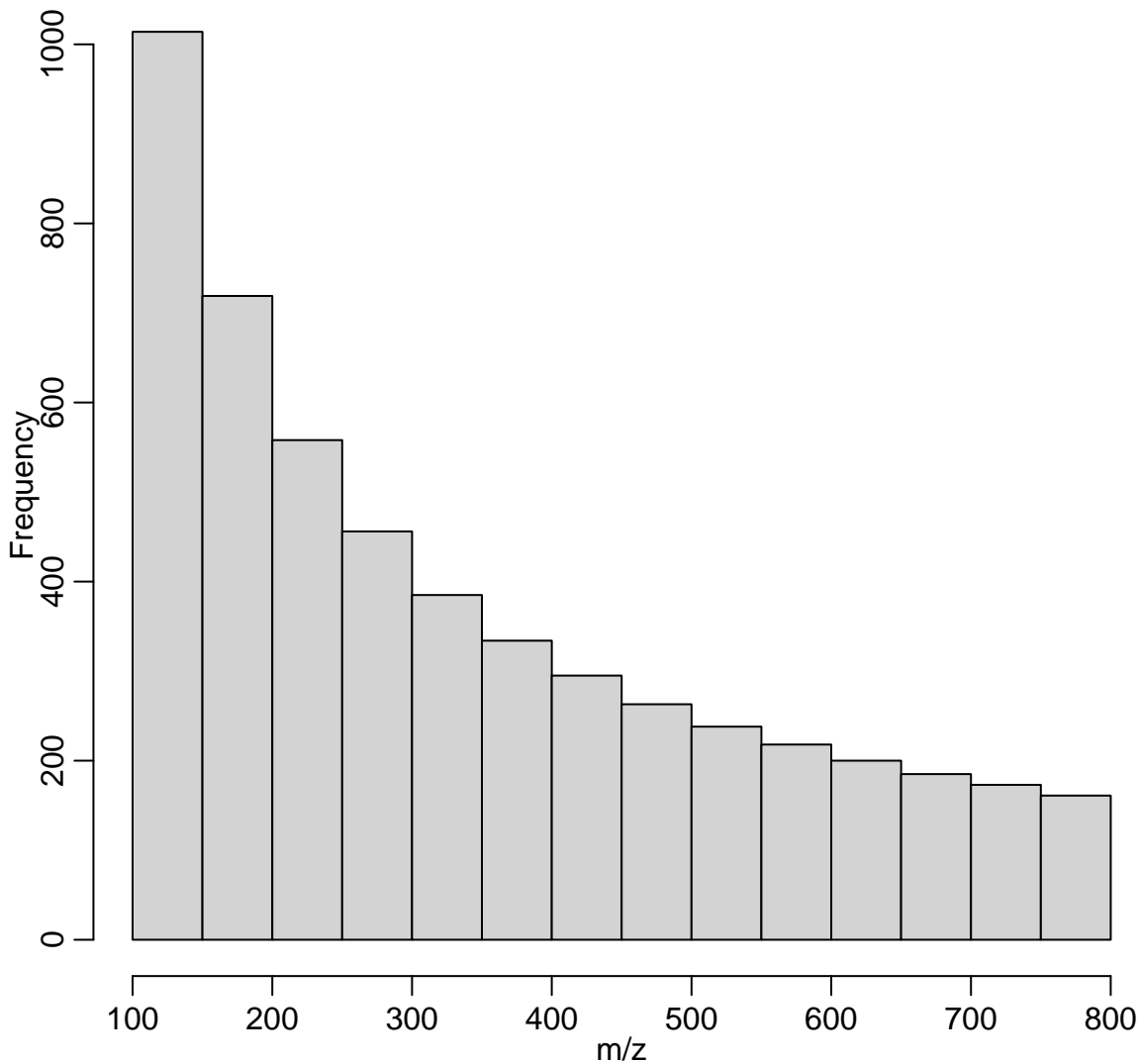
TIC per spectrum



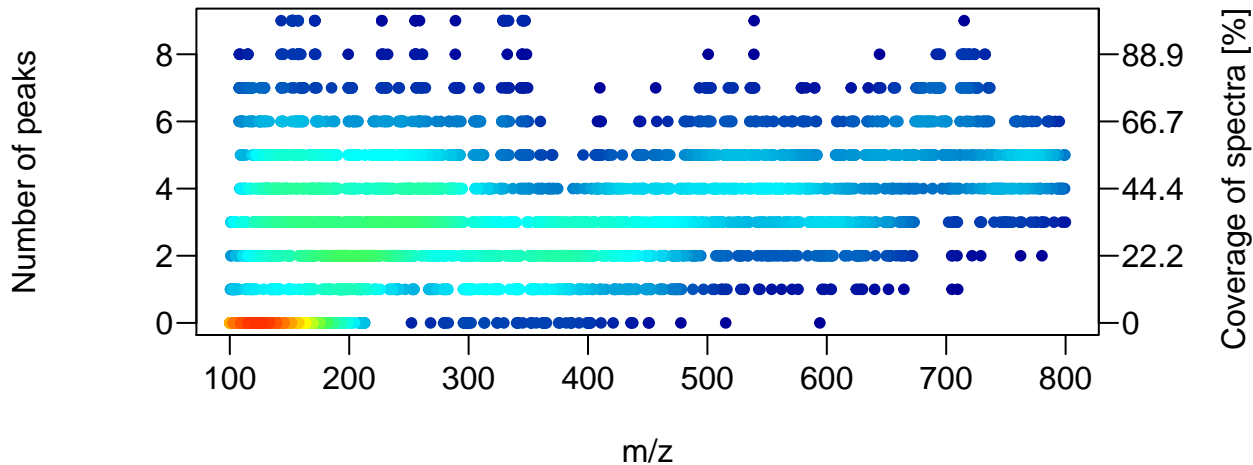
TIC per spectrum



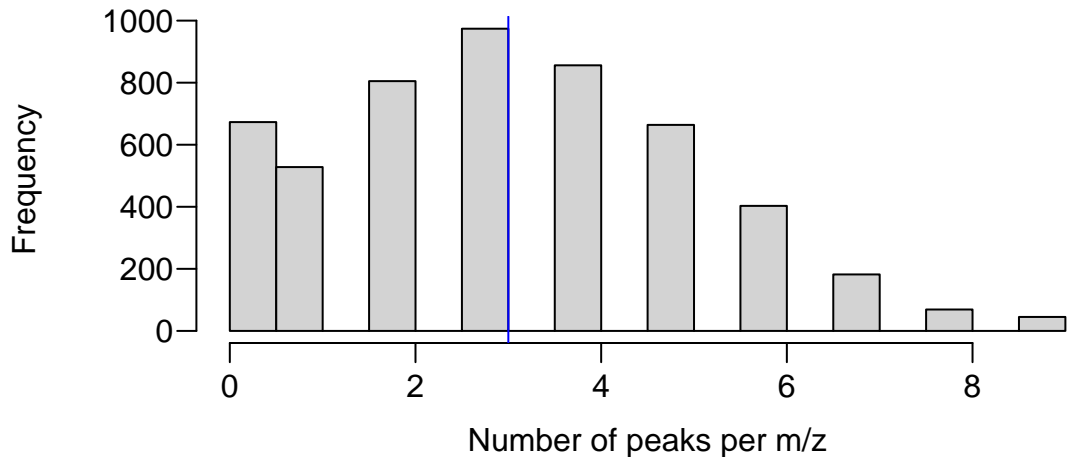
Histogram of m/z values



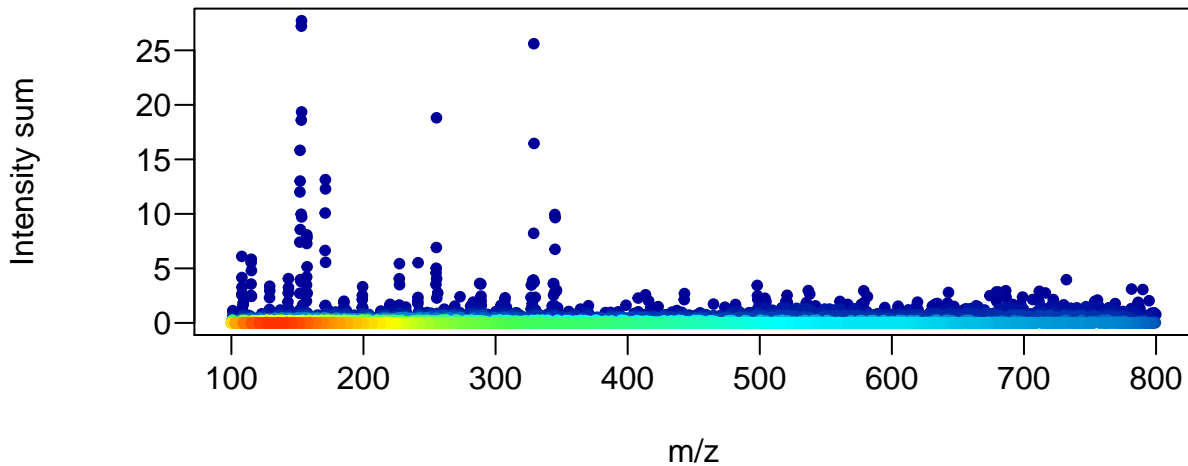
Number of peaks per m/z



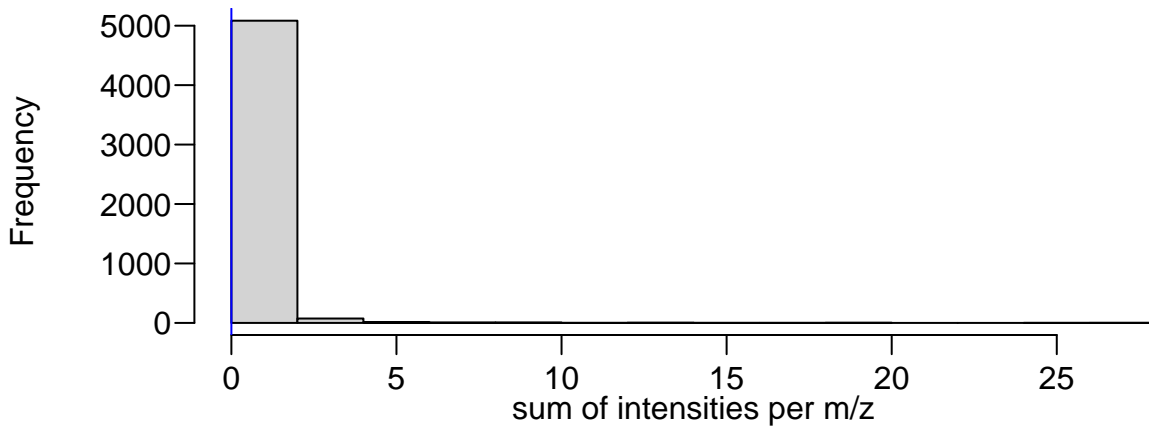
Number of peaks per m/z



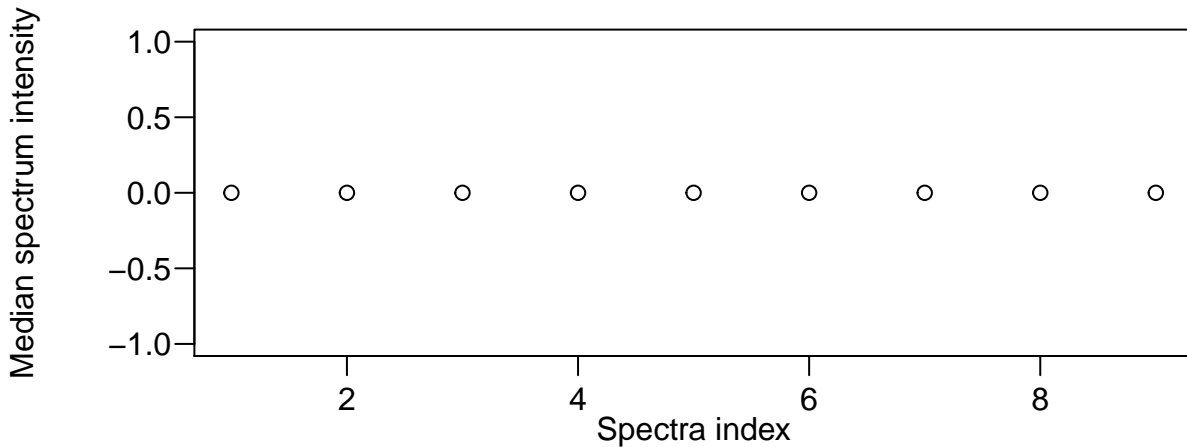
Sum of intensities per m/z



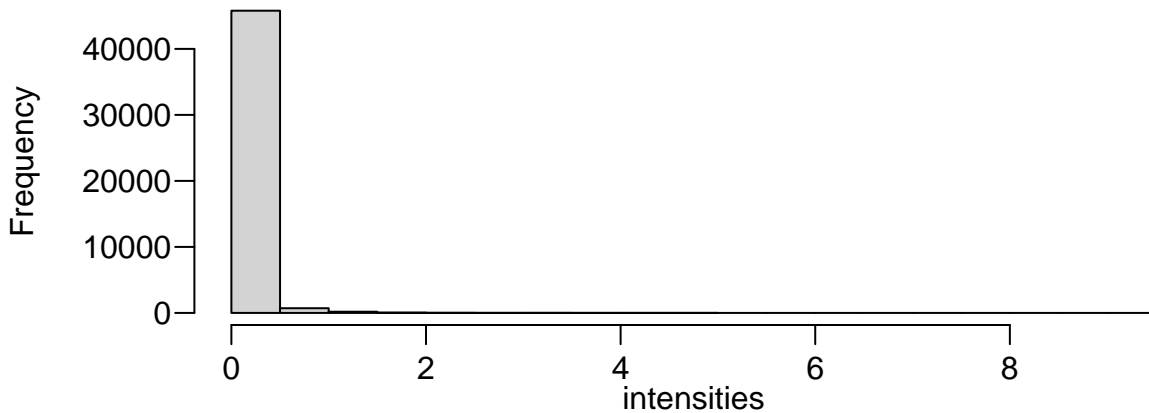
Sum of intensities per m/z

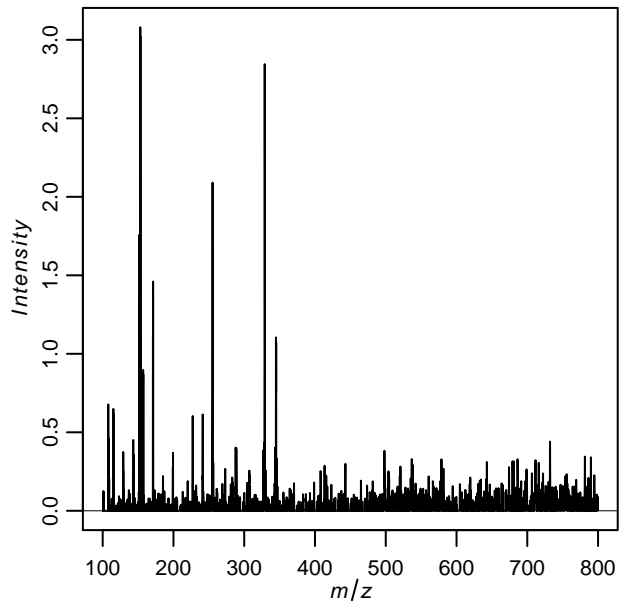
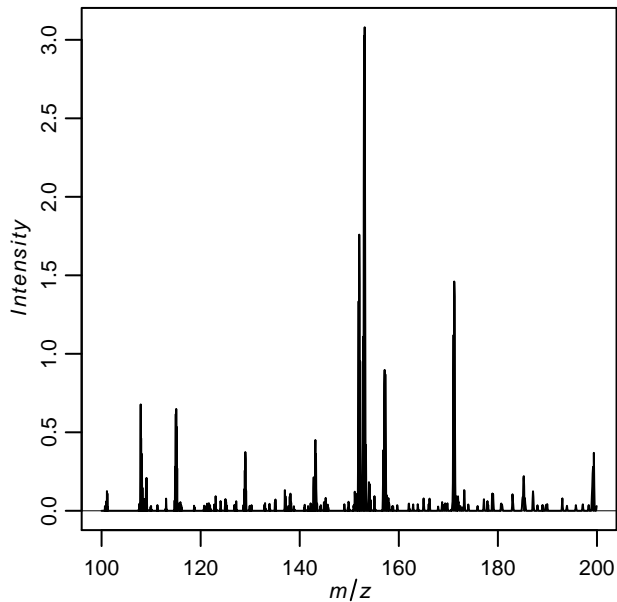
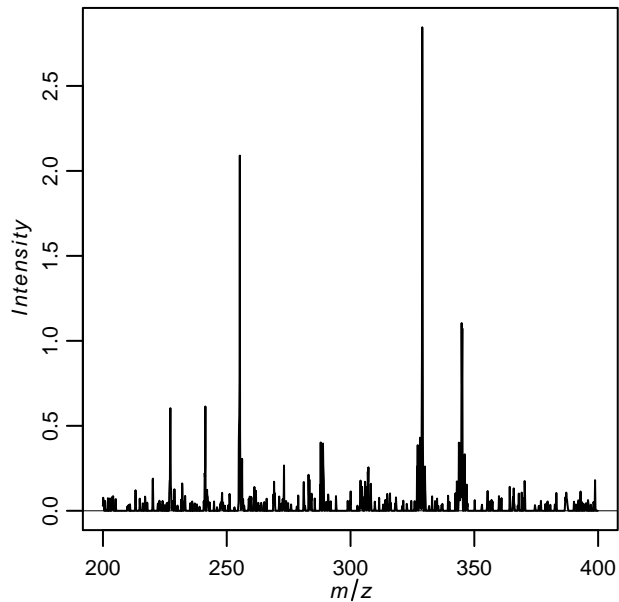
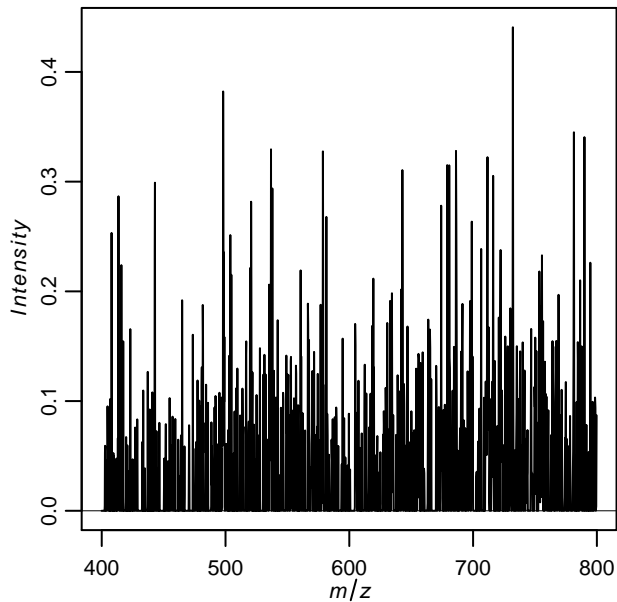


Median intensity per spectrum

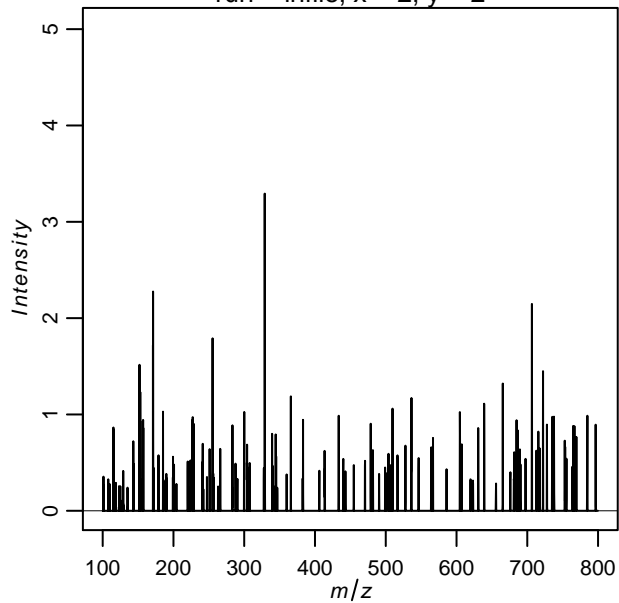


Intensity histogram

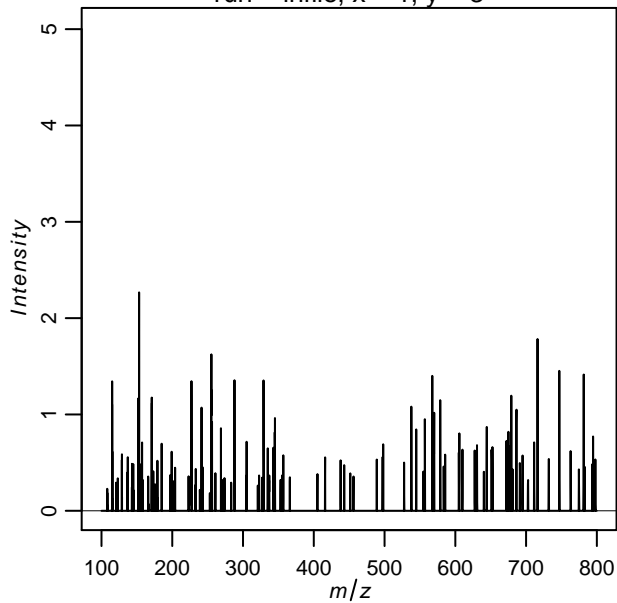


Average spectrum**Zoomed average spectrum****Zoomed average spectrum****Zoomed average spectrum**

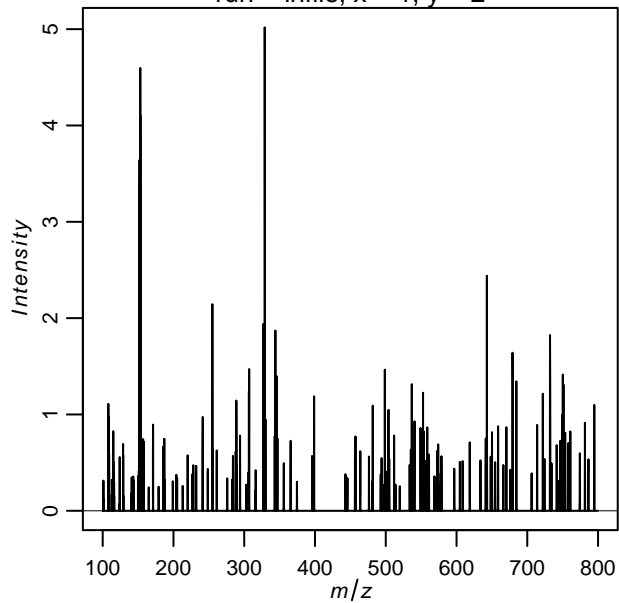
run = infile, x = 2, y = 2



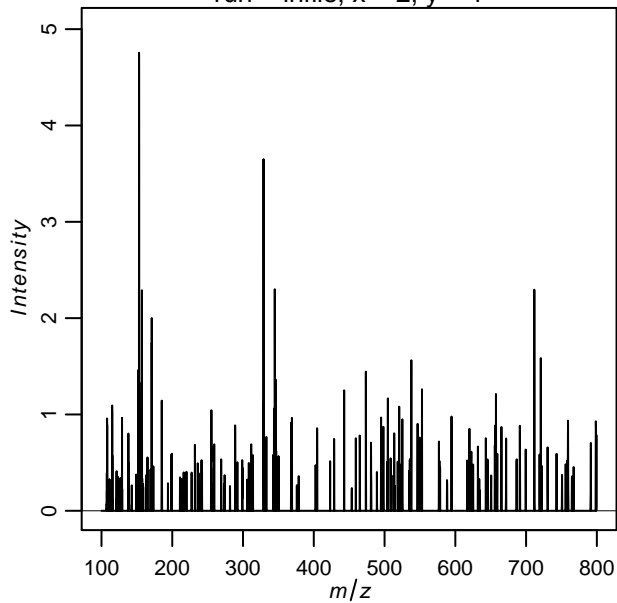
run = infile, x = 1, y = 3



run = infile, x = 1, y = 2



run = infile, x = 2, y = 1

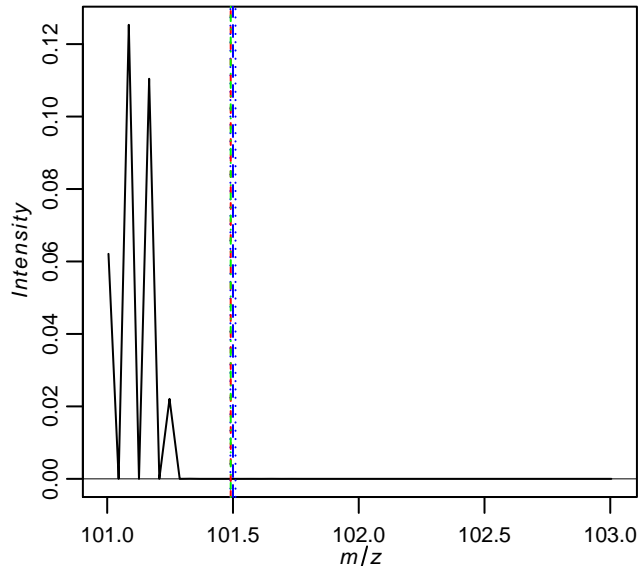


theor. m/z: 101.5

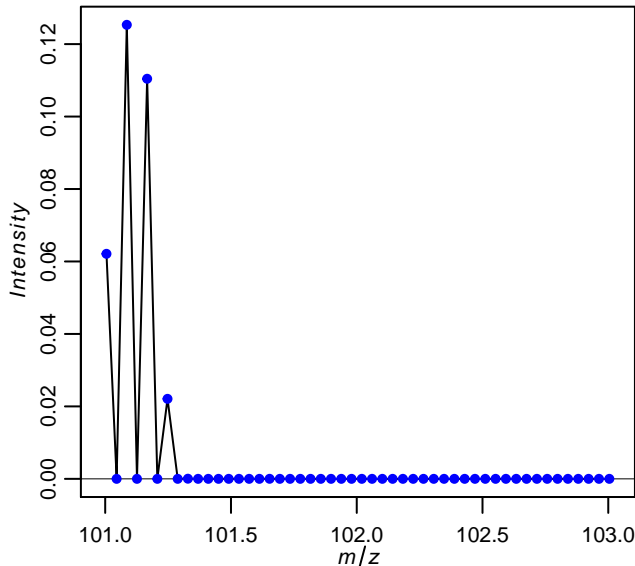
most abundant m/z: 101.491

closest m/z: 101.491

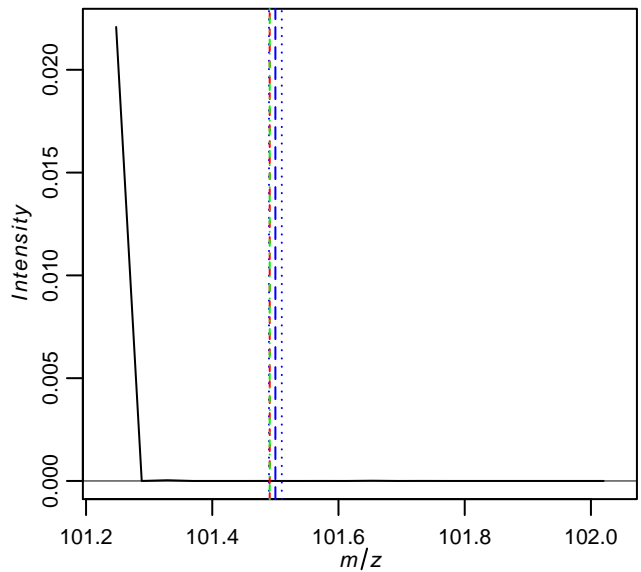
Average spectrum



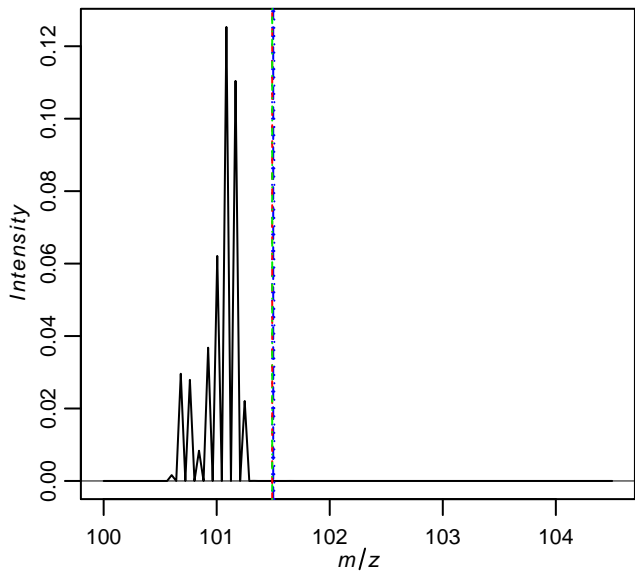
Average spectrum with data points



Average spectrum



Average spectrum

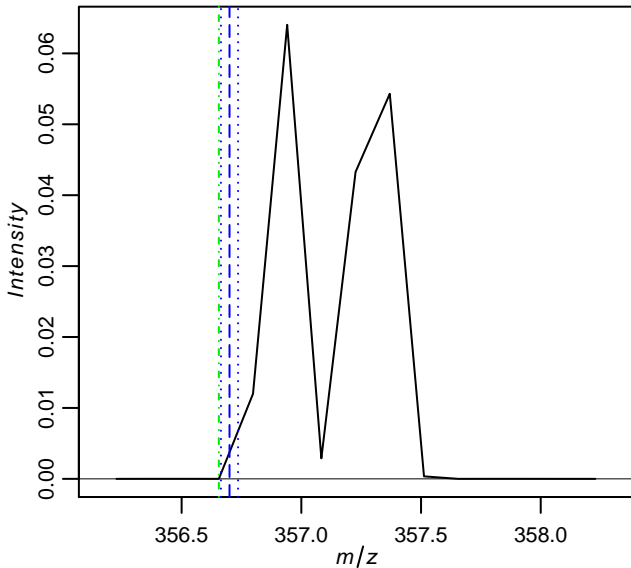


theor. m/z: 356.7

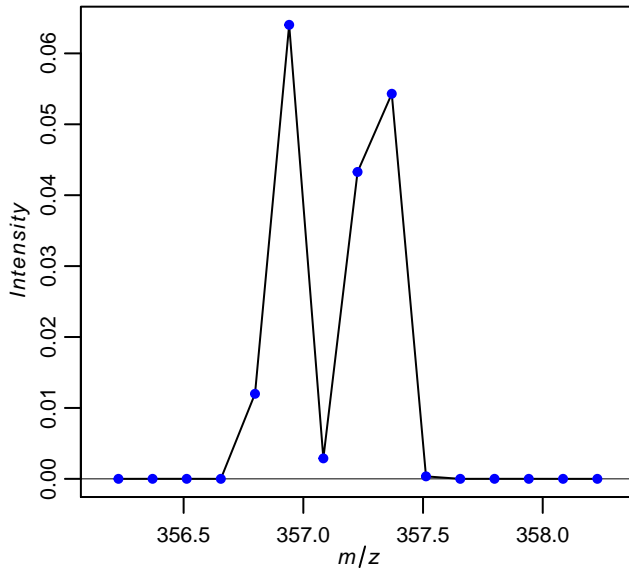
most abundant m/z: NA

closest m/z: 356.6555

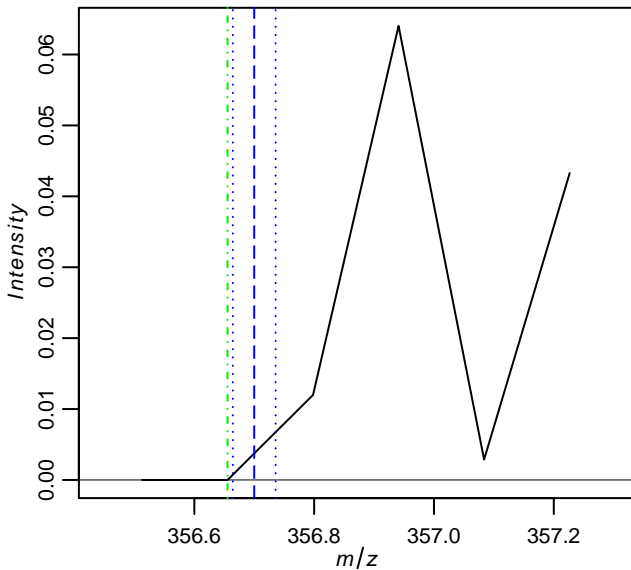
Average spectrum



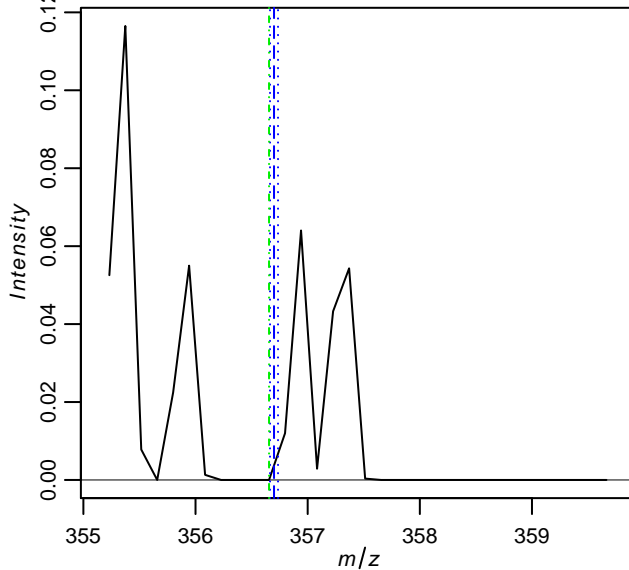
Average spectrum with data points



Average spectrum



Average spectrum

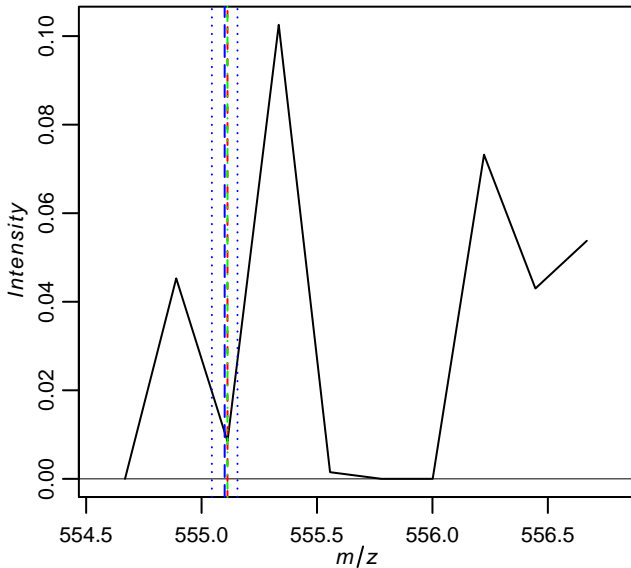


theor. m/z: 555.1

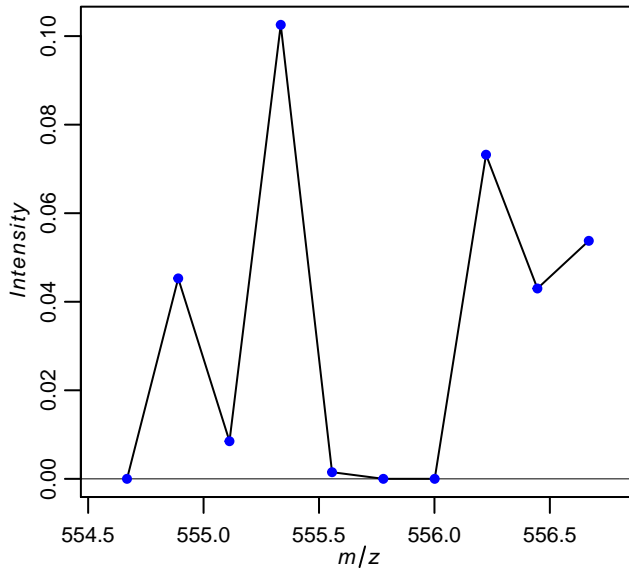
most abundant m/z: 555.122

closest m/z: 555.122

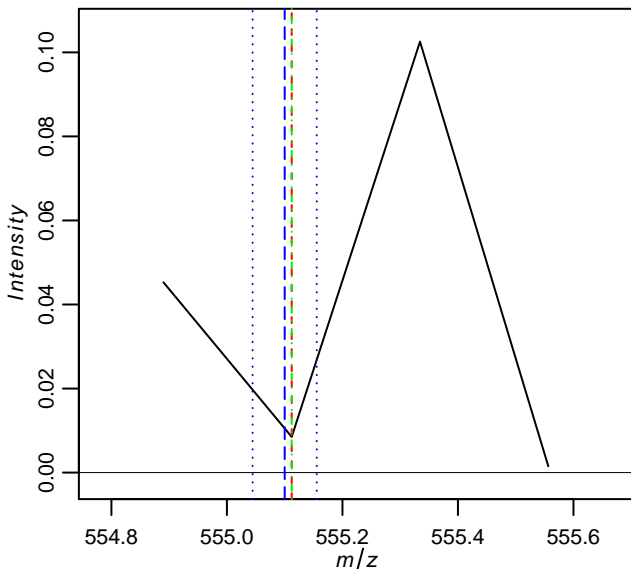
Average spectrum



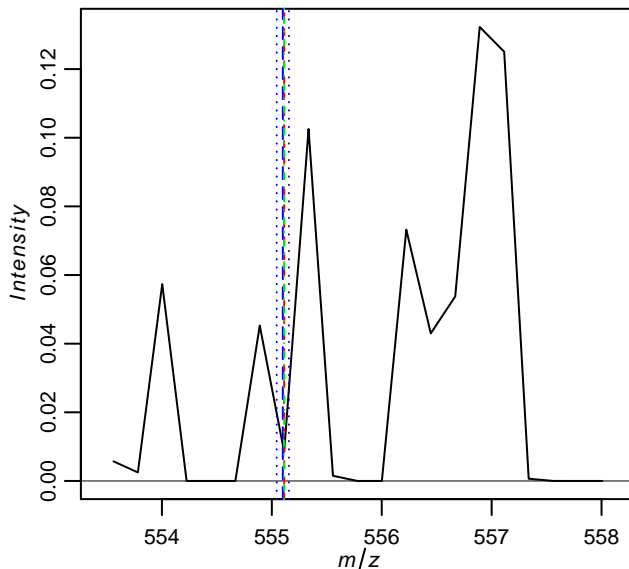
Average spectrum with data points



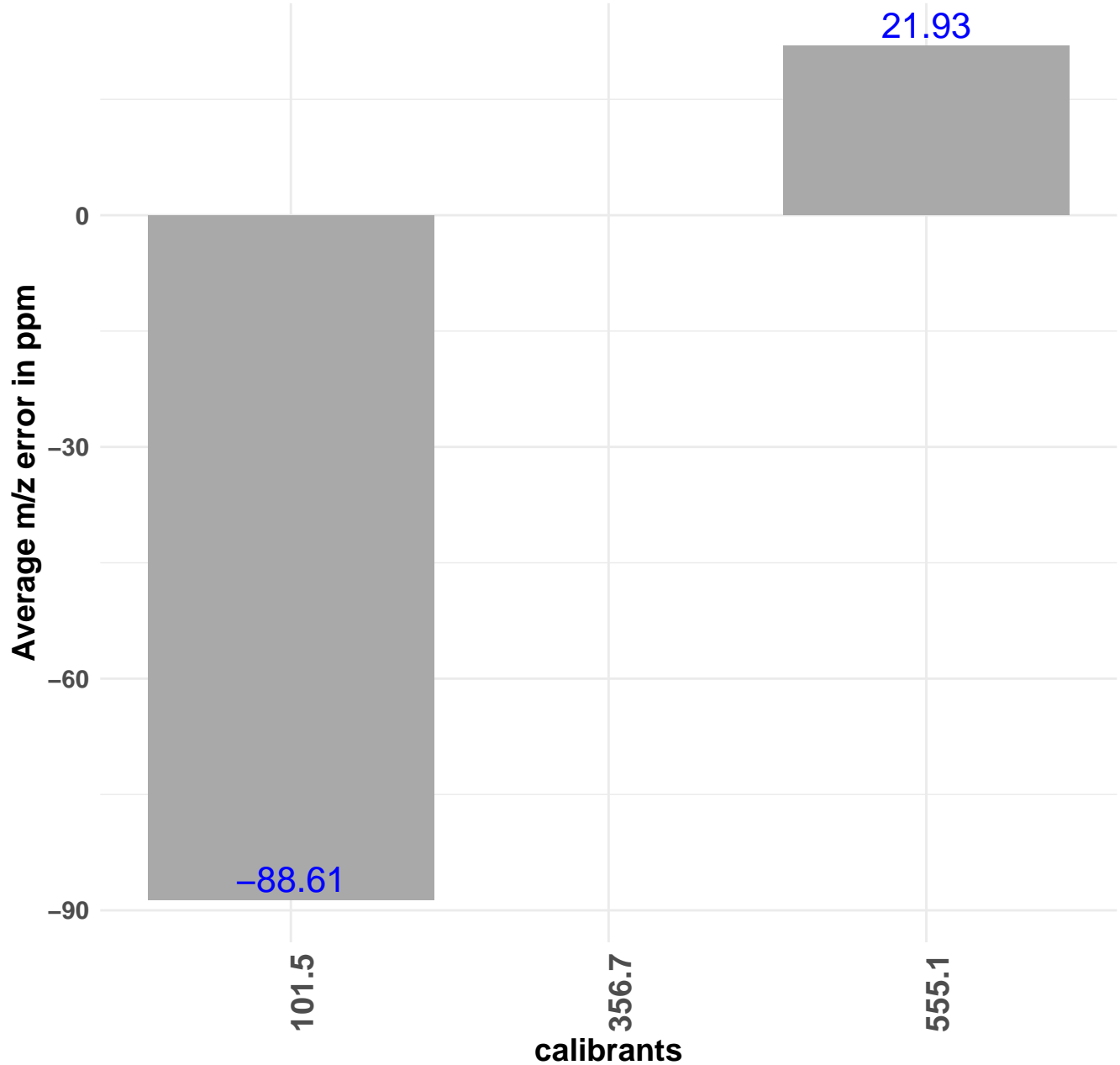
Average spectrum



Average spectrum

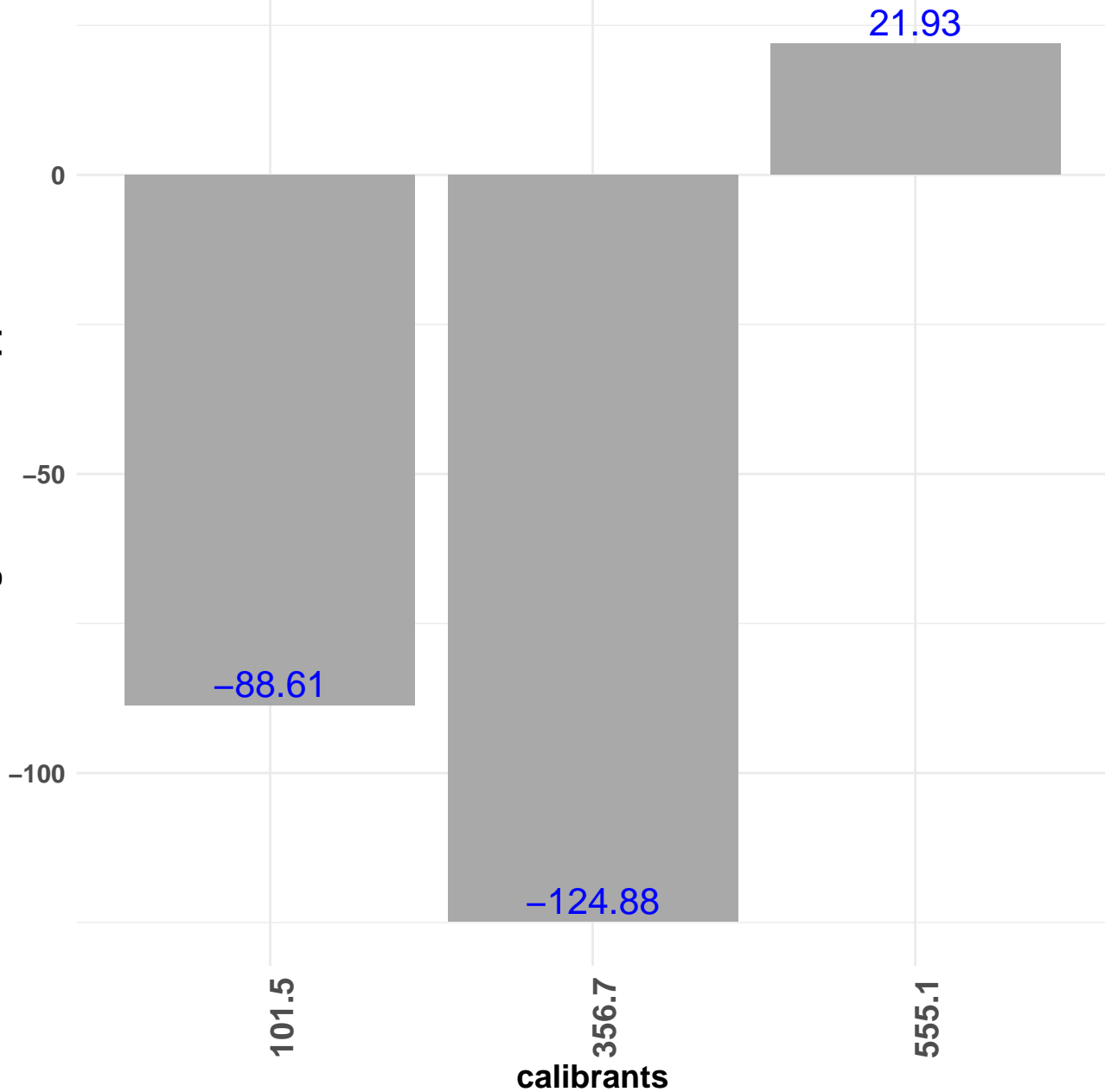


Average m/z error (max. average intensity vs. theor. calibrant m/z)

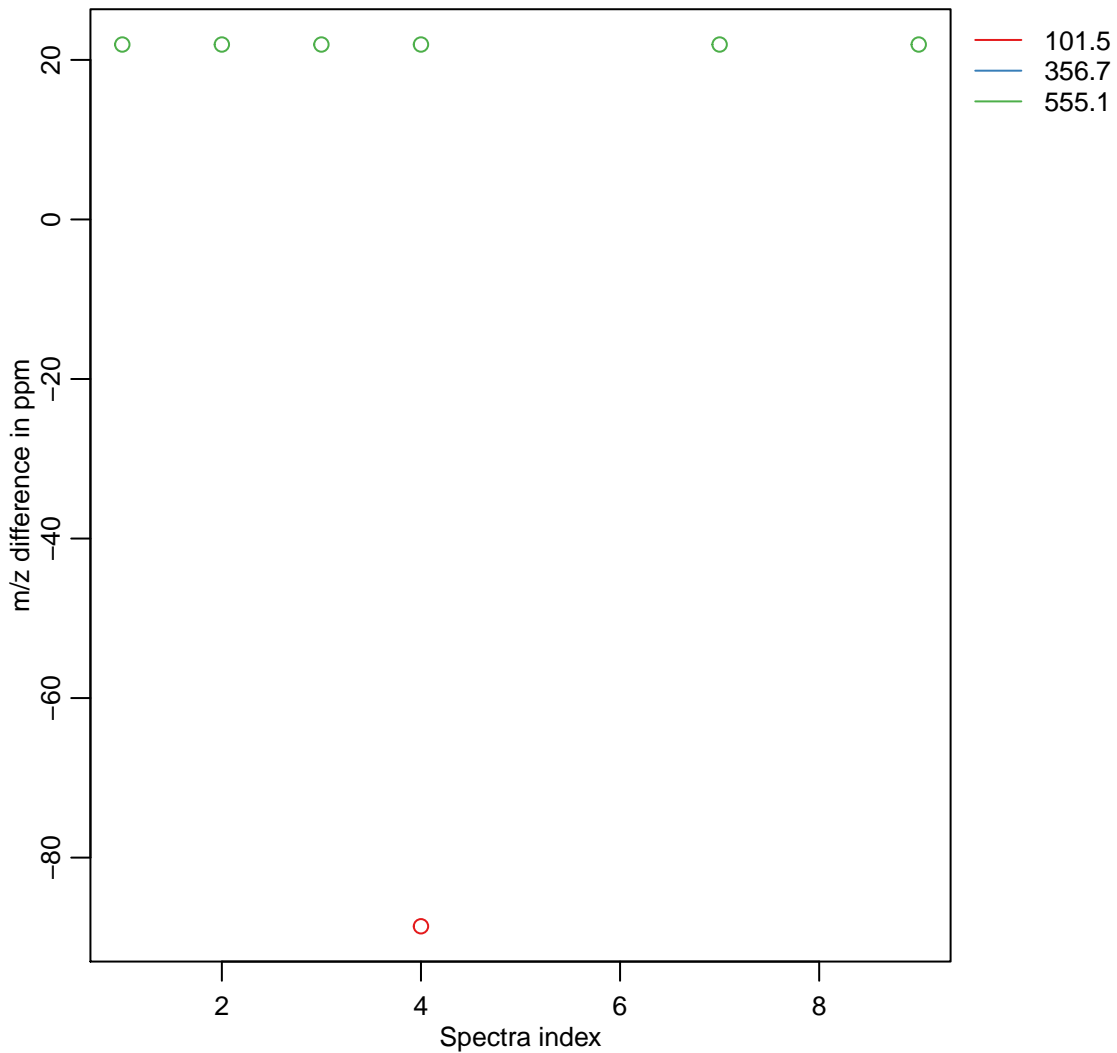


Average m/z error (closest measured m/z vs. theor. calibrant m/z)

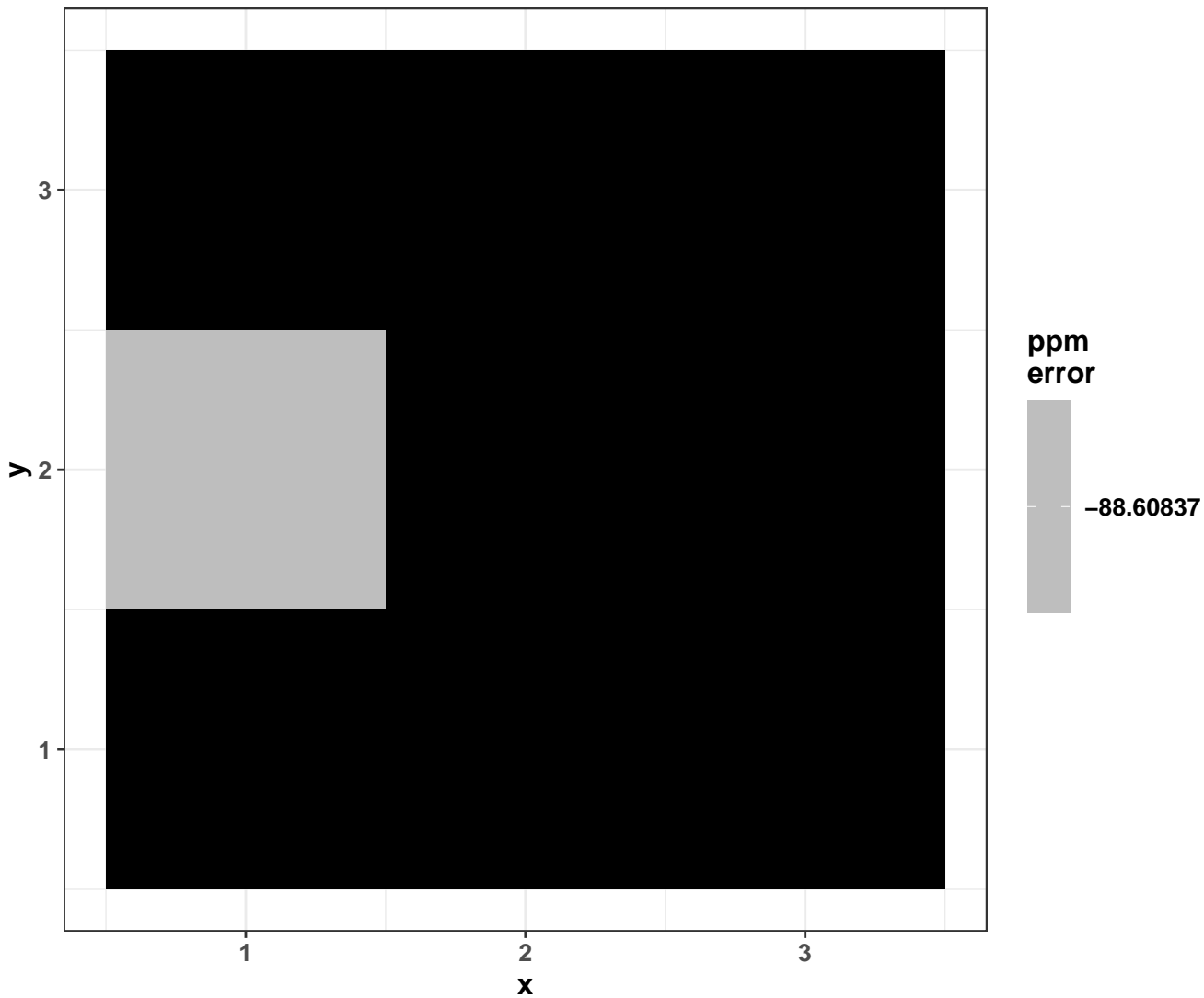
Average m/z error in ppm



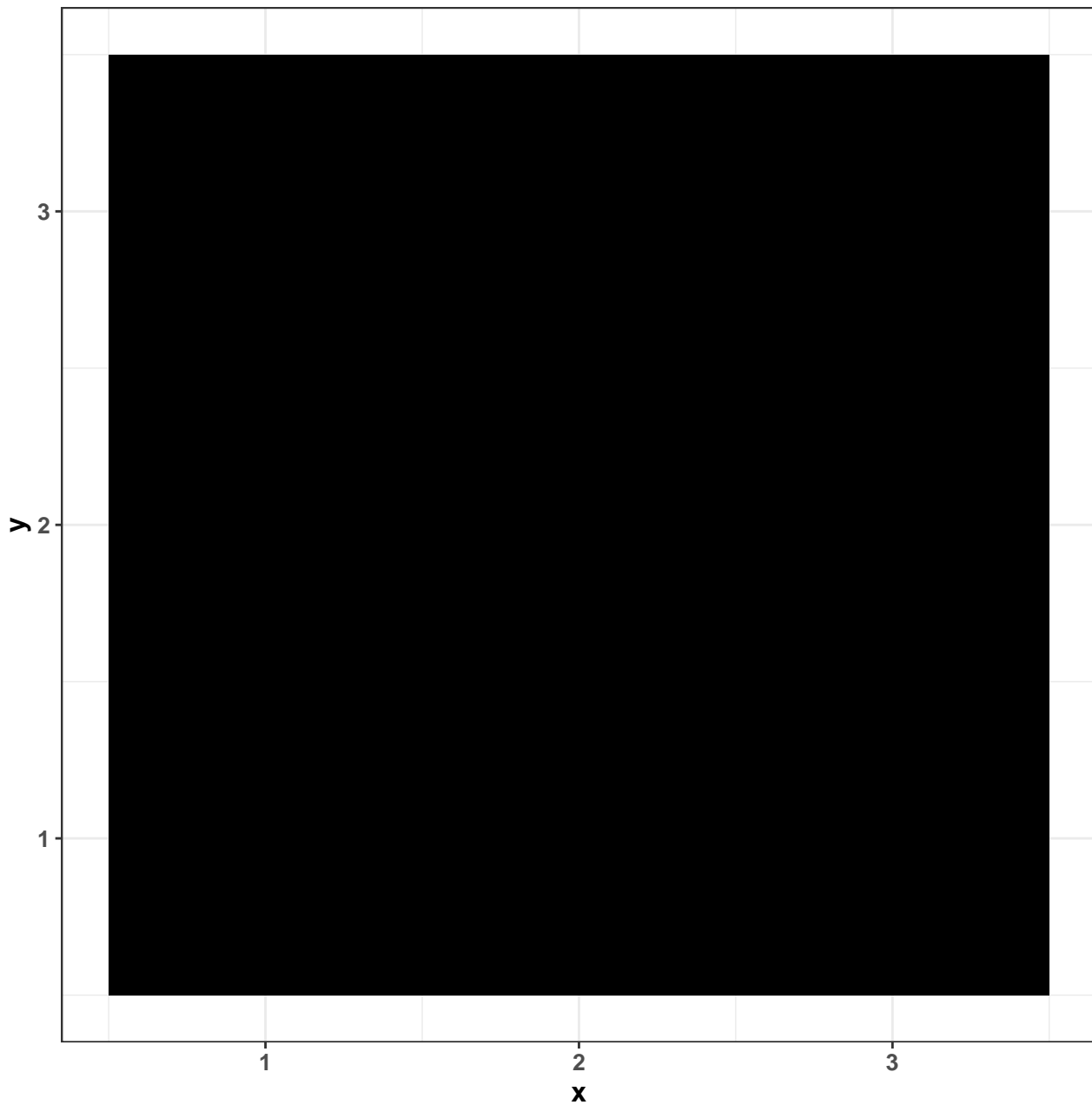
Difference m/z with max. average intensity vs. theor. m/z (per spectrum)



m/z accuracy for 101.5



m/z accuracy for 356.7



m/z accuracy for 555.1

