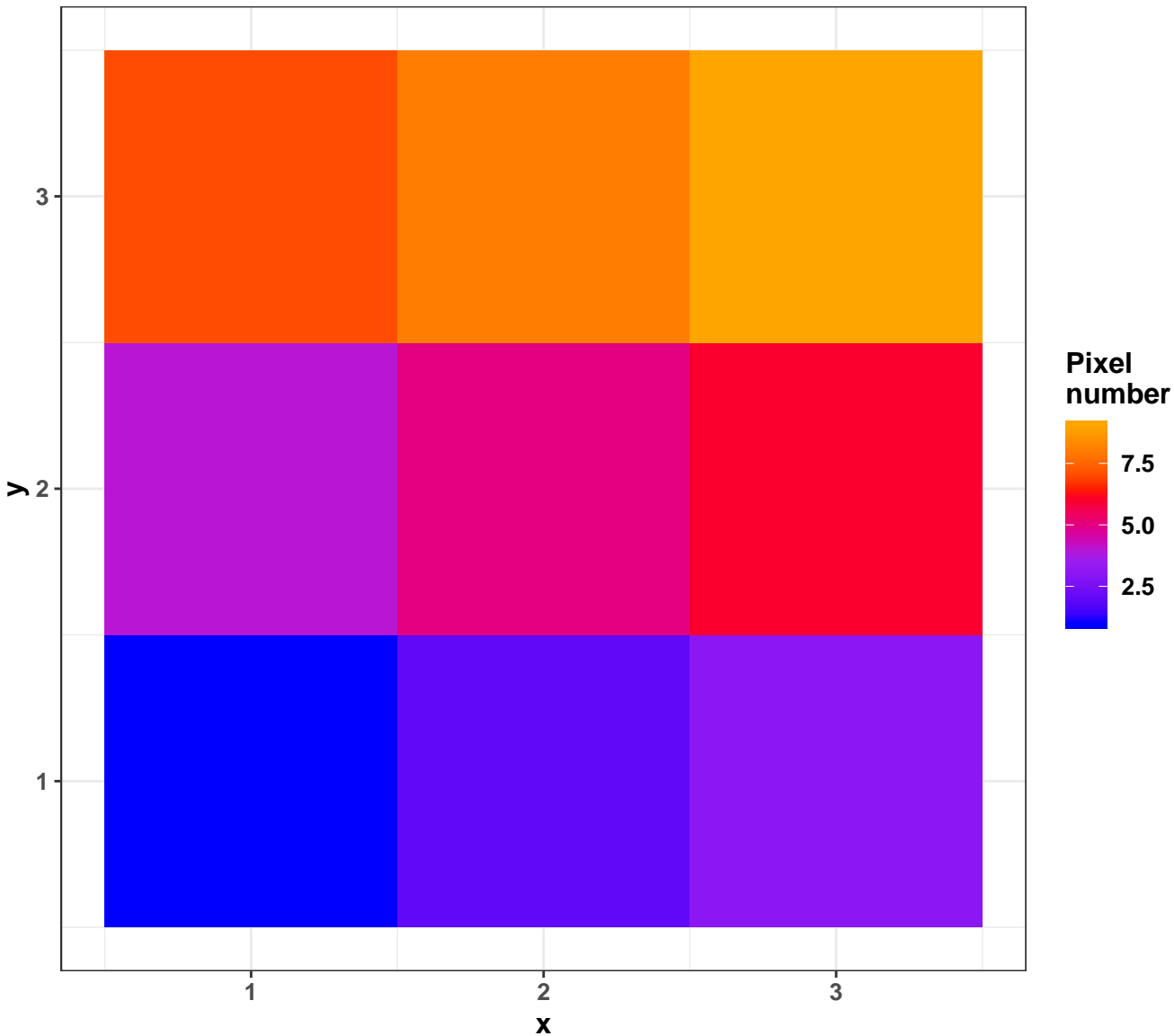


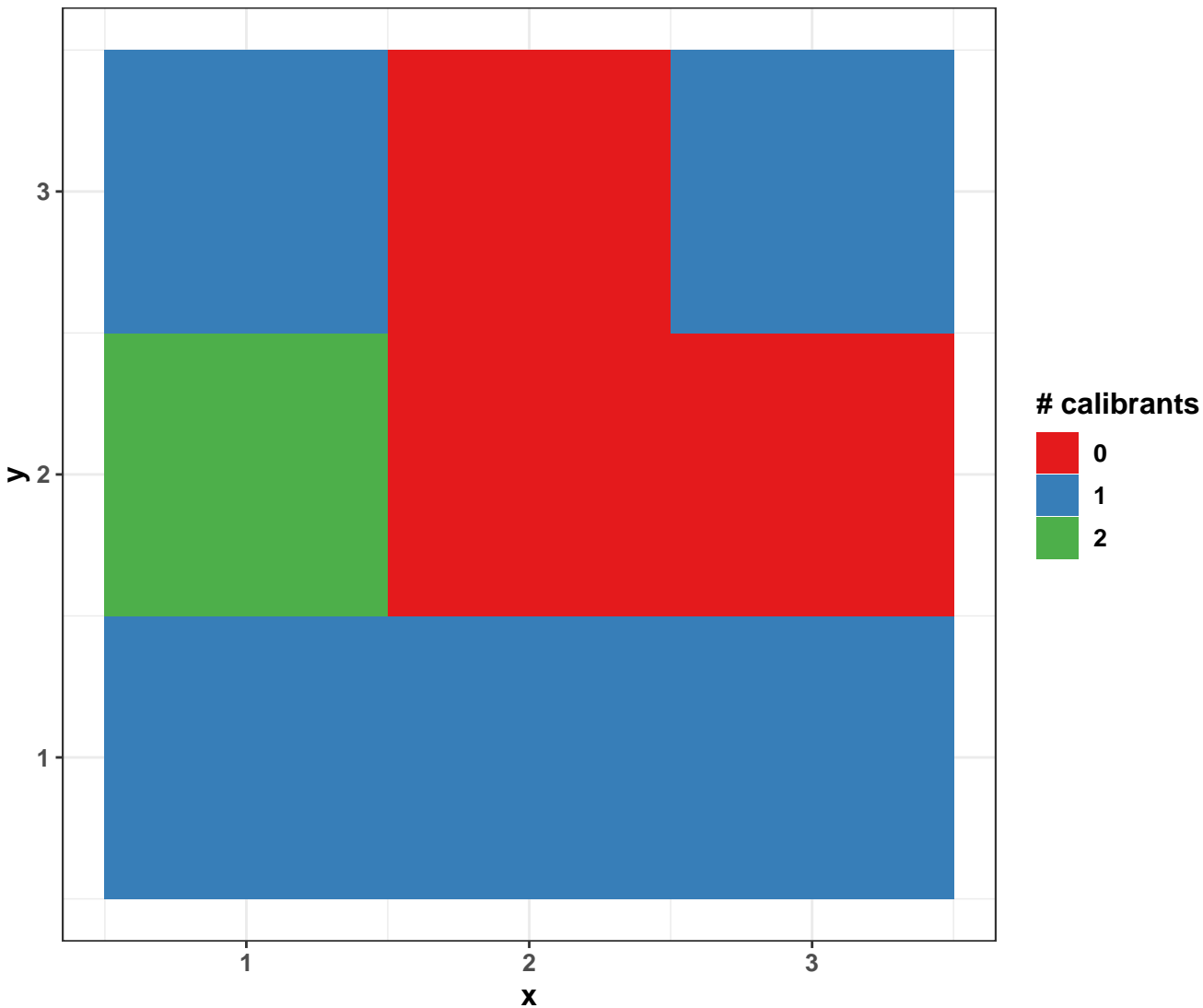
Testfile_imzml

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

Pixel order

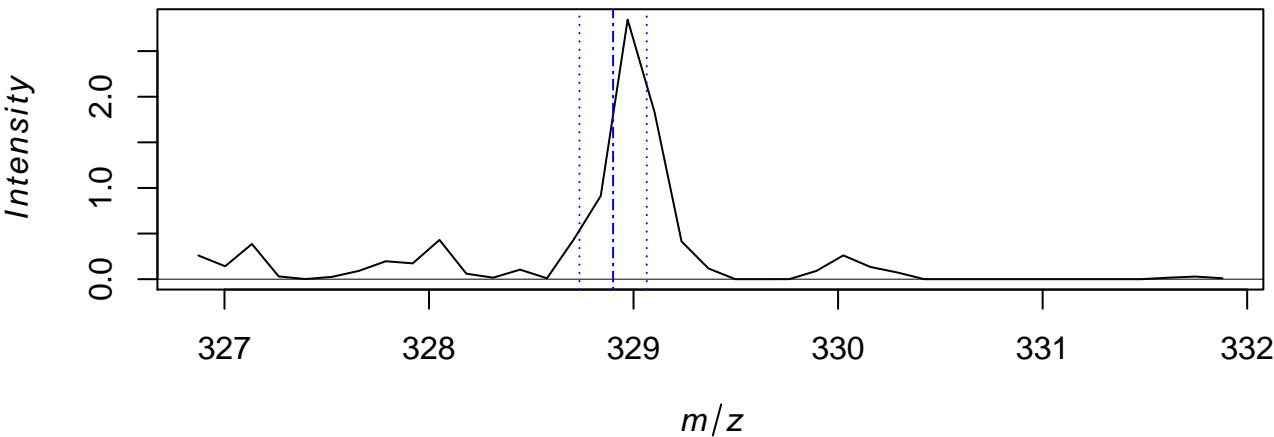


Number of calibrants per pixel (± 100 ppm)

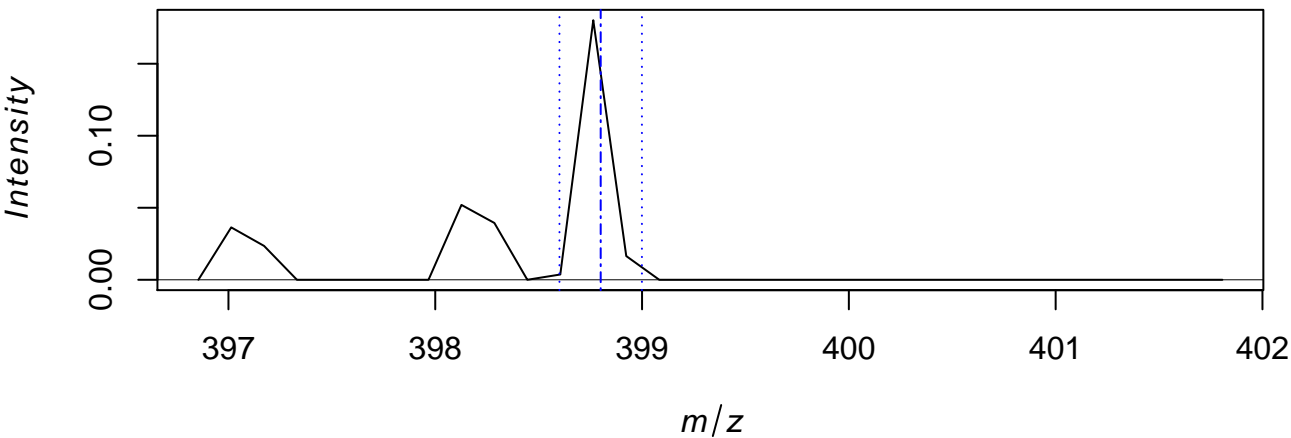


Control of fold change plot

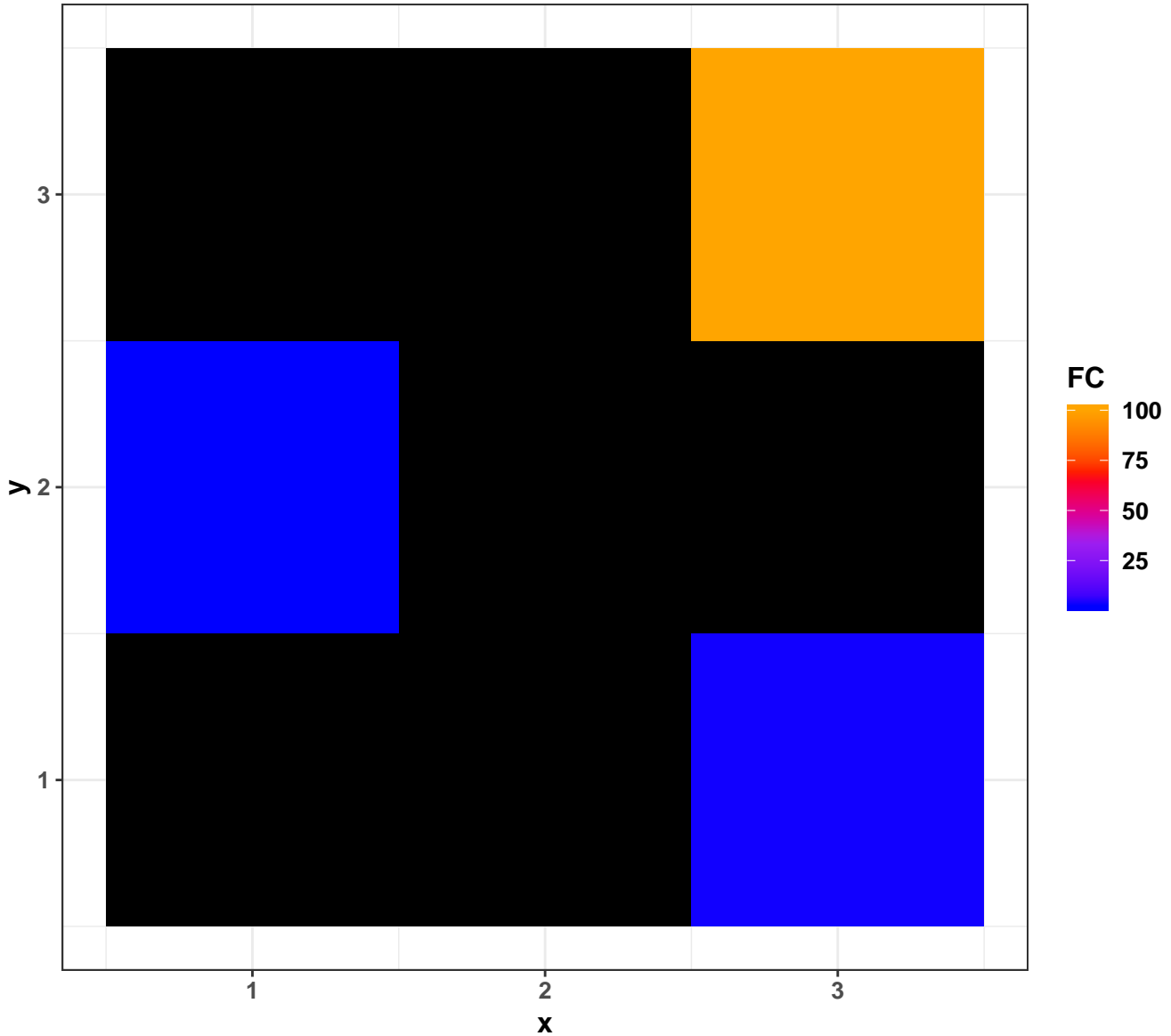
Average spectrum 328.9 Da



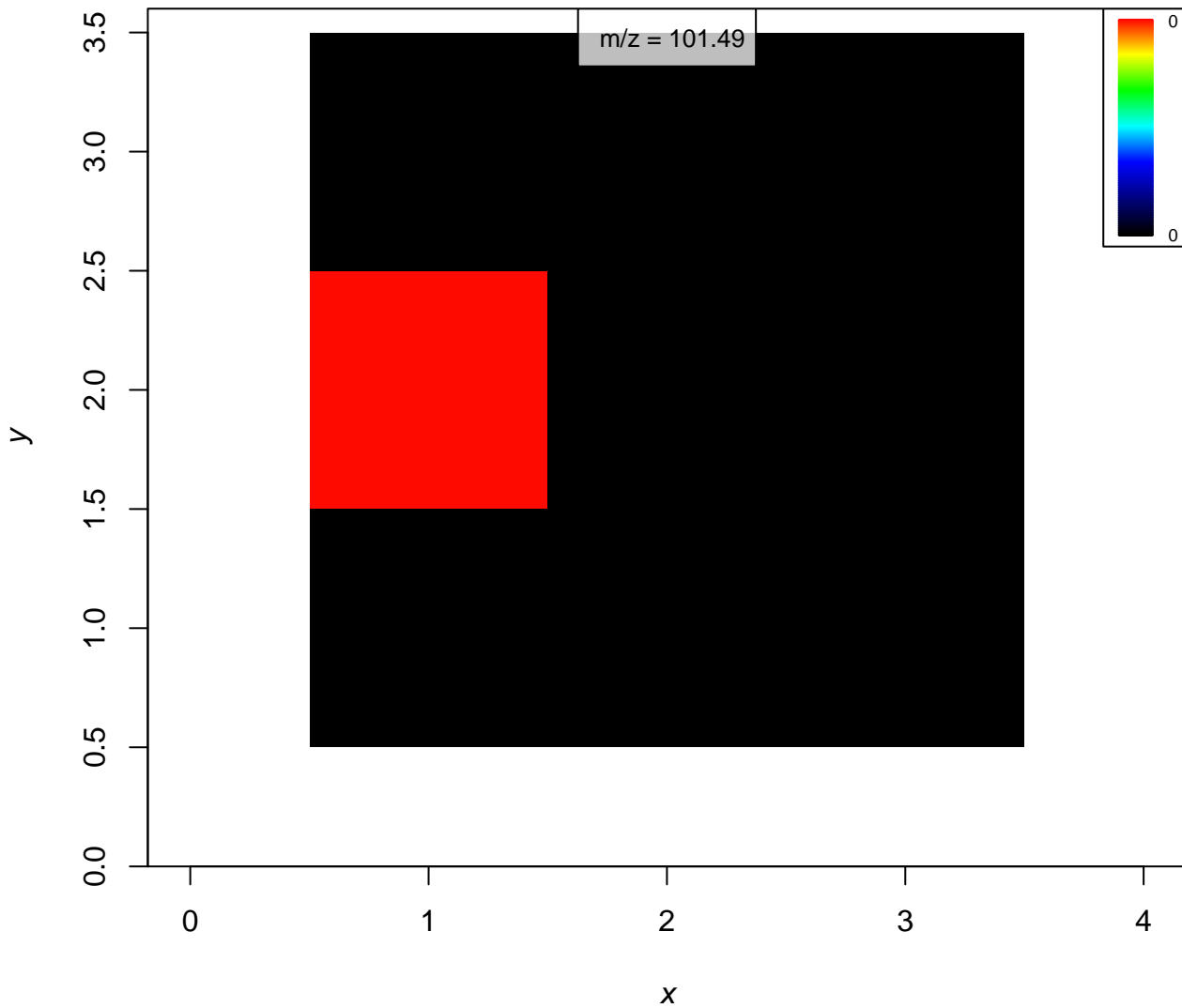
Average spectrum 398.8 Da



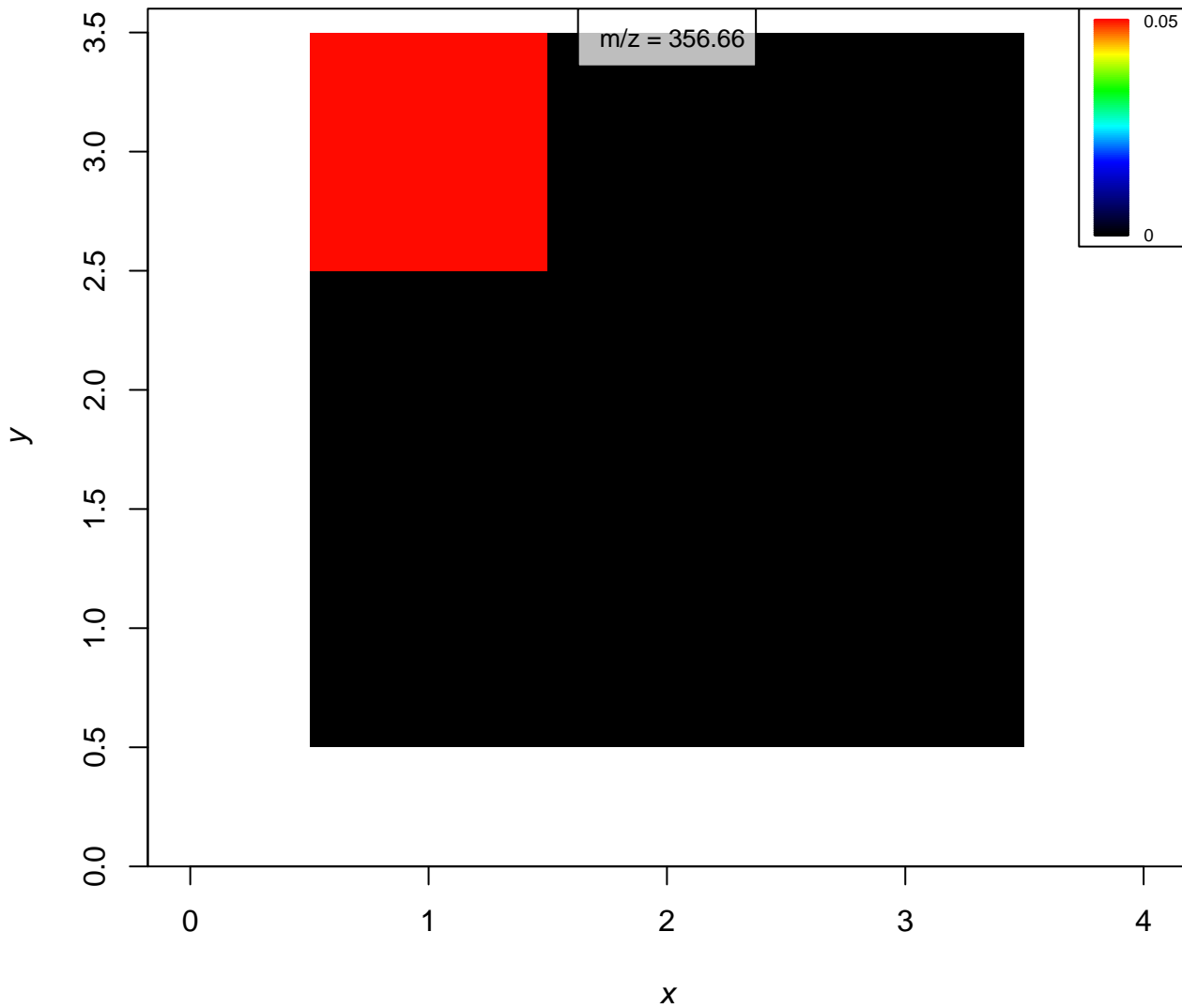
Ratioofmass13289mass23988



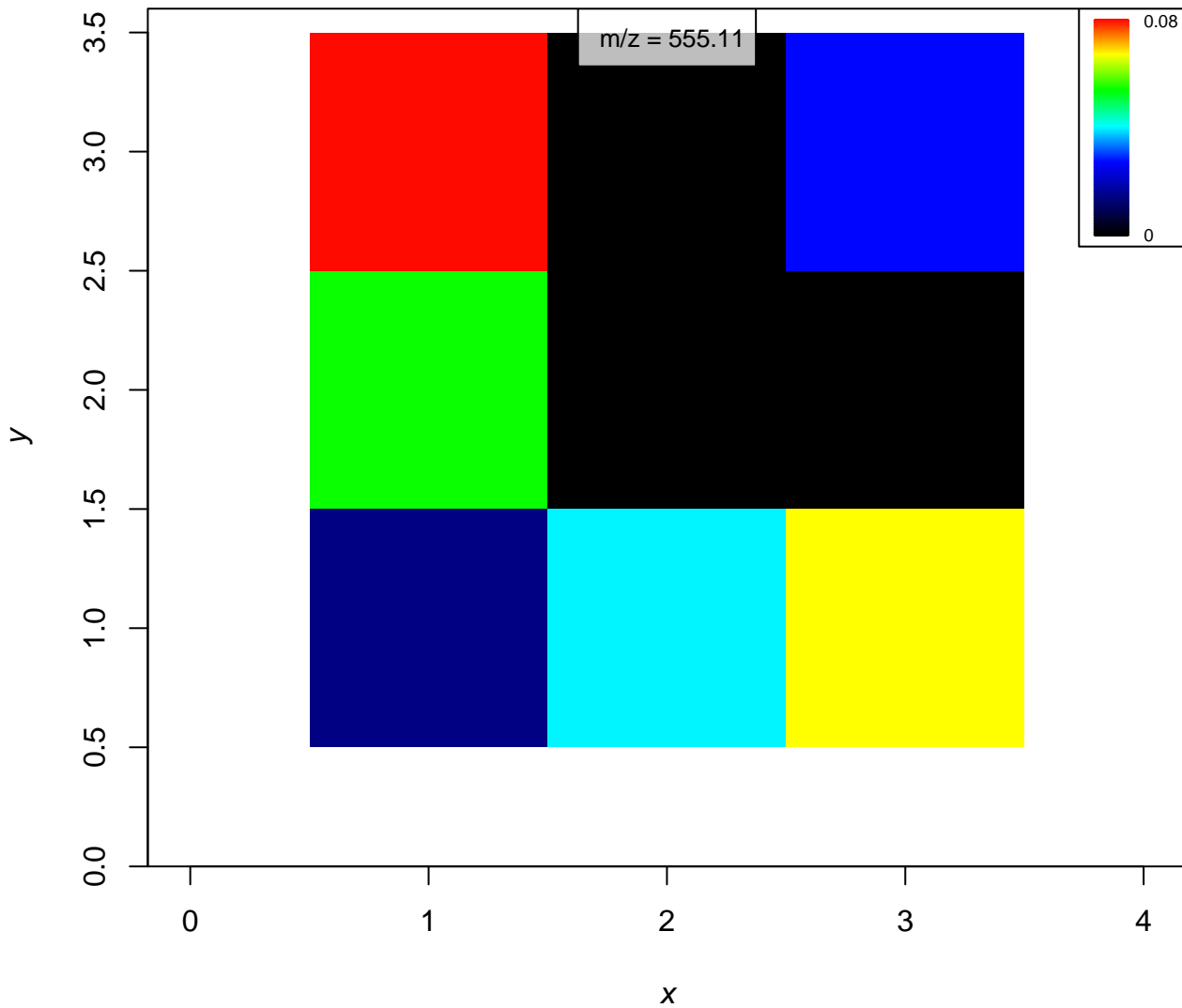
101.5: 101.5 (± 100 ppm)



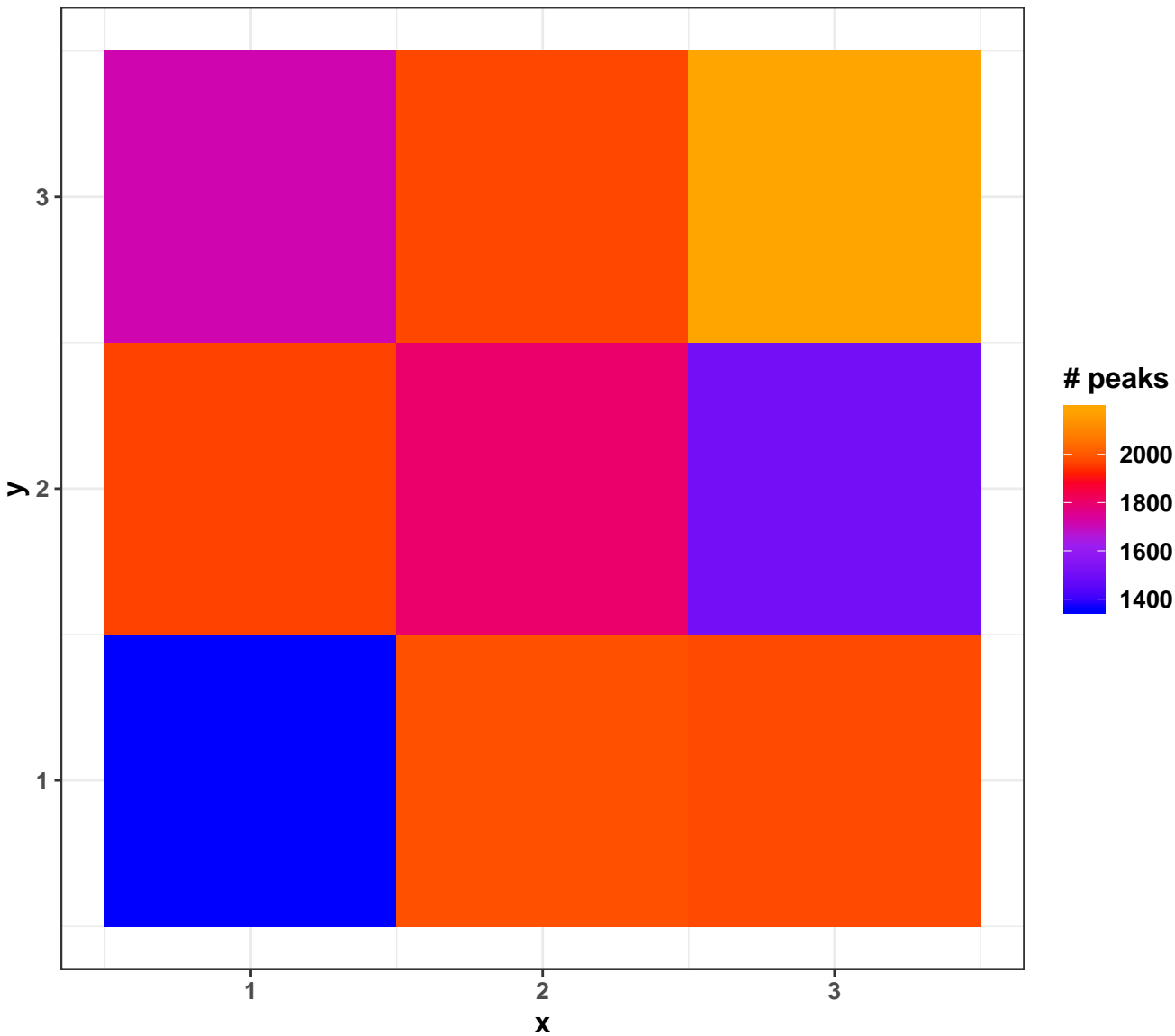
356.7: 356.7 (± 100 ppm)



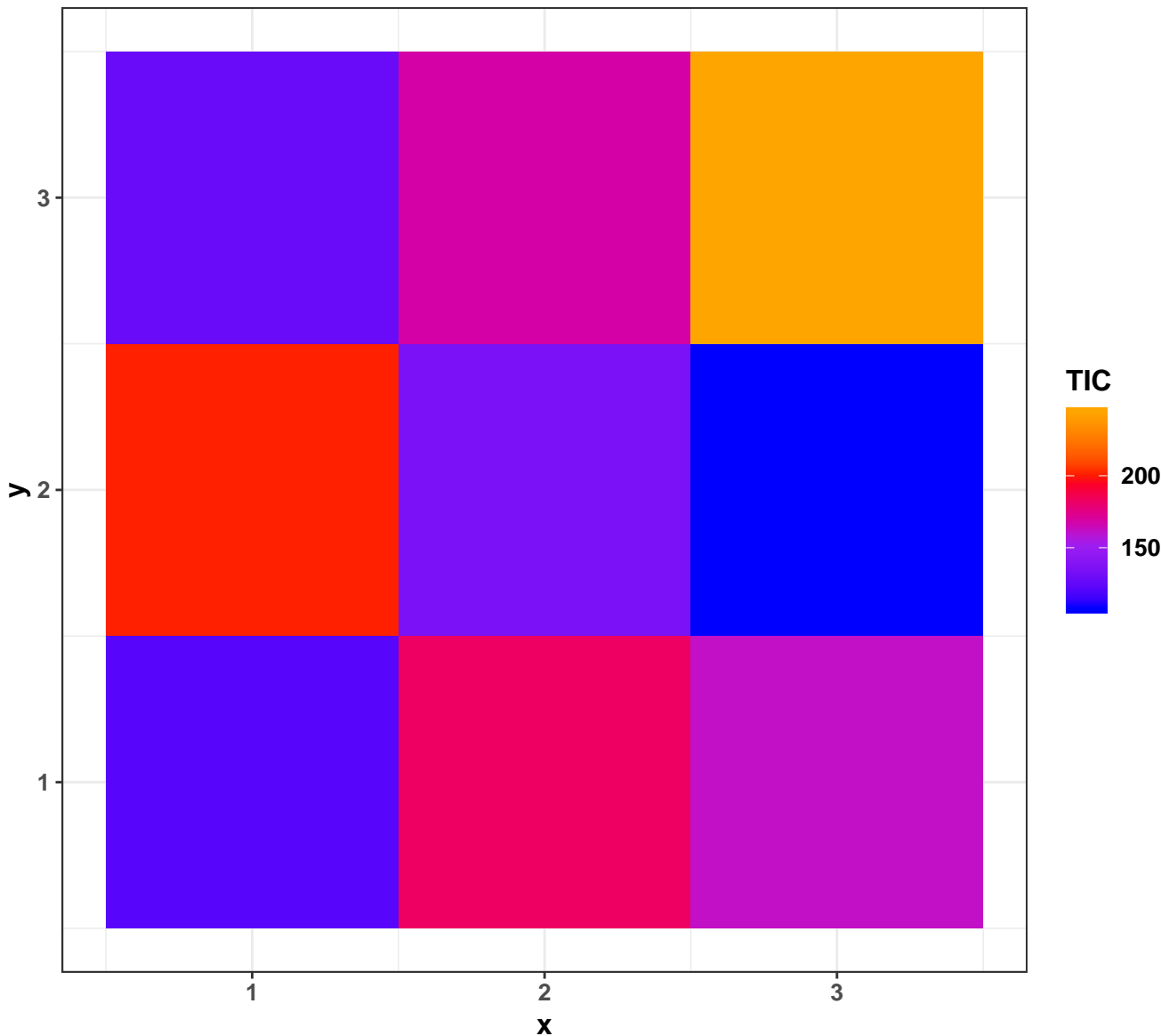
555.1: 555.1 (± 100 ppm)



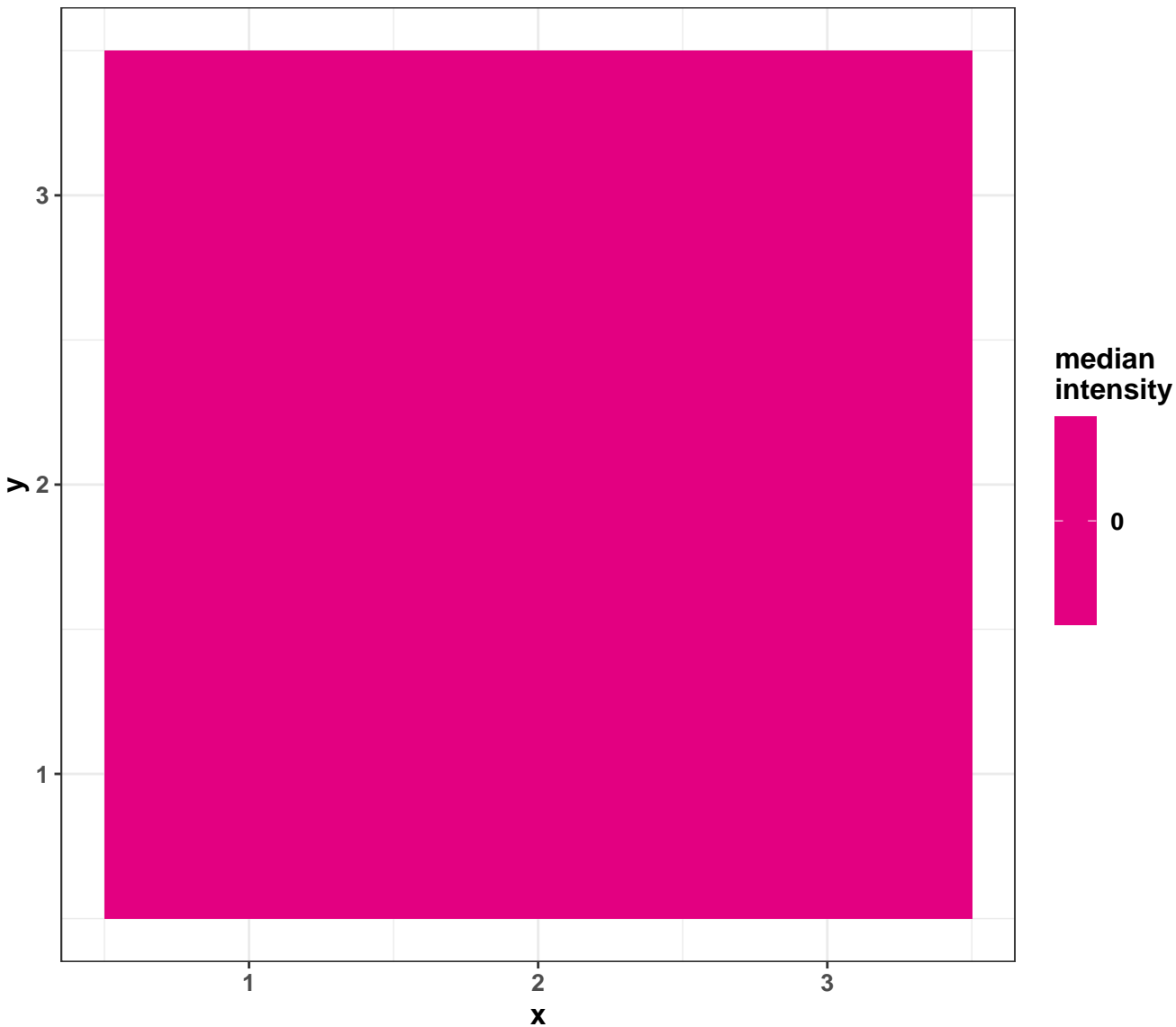
Number of peaks per spectrum



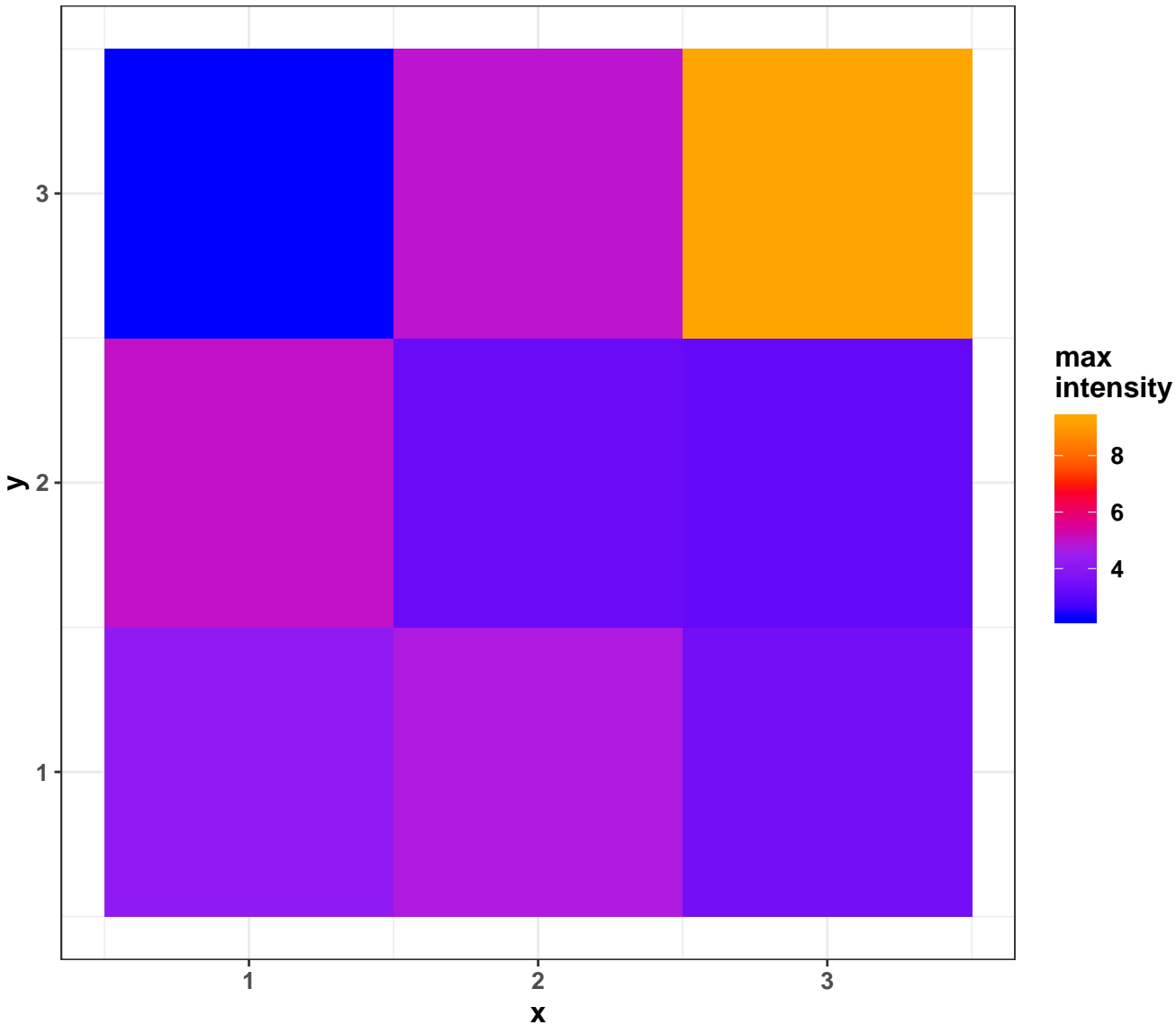
Total Ion Chromatogram



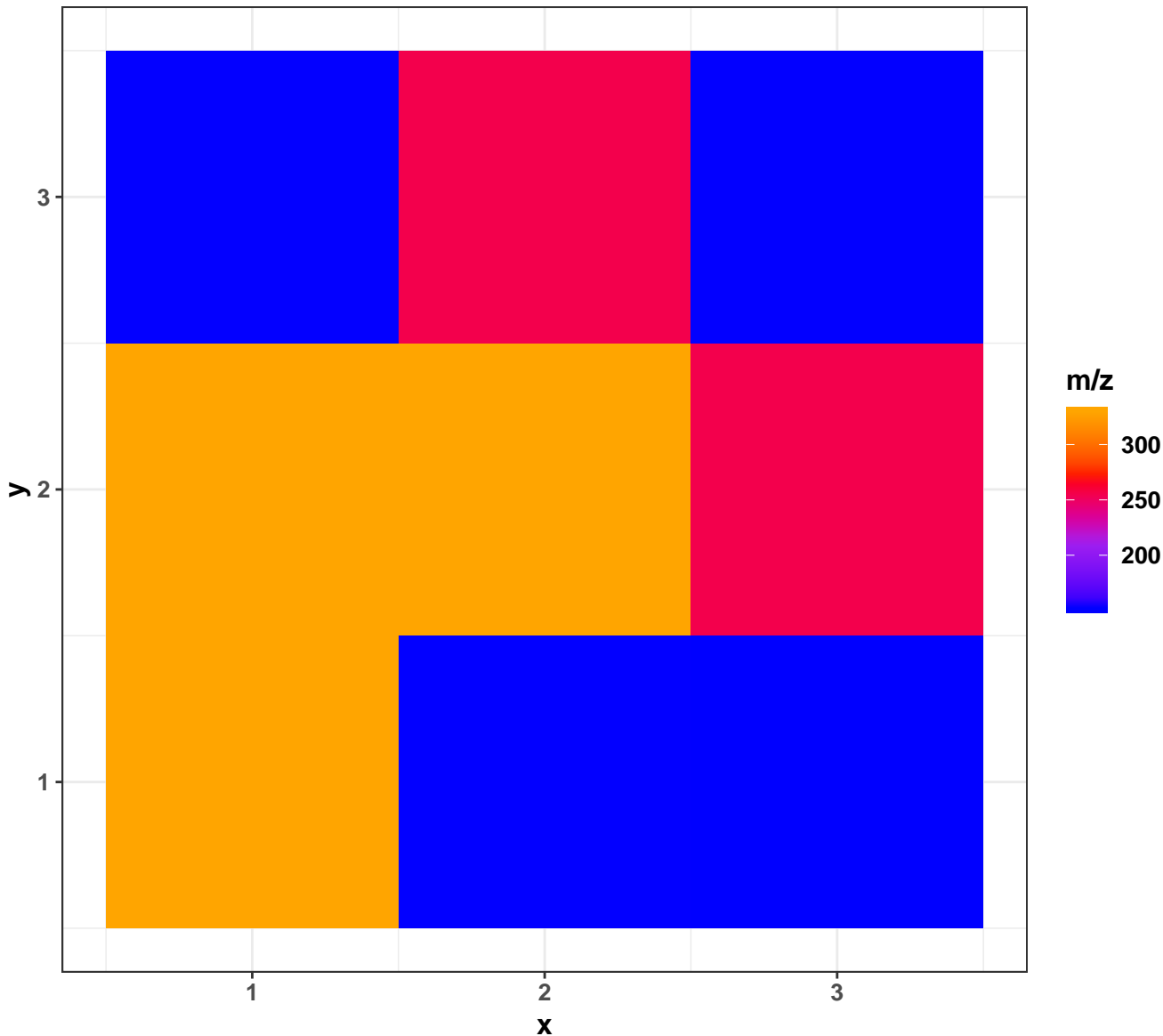
Median intensity per spectrum



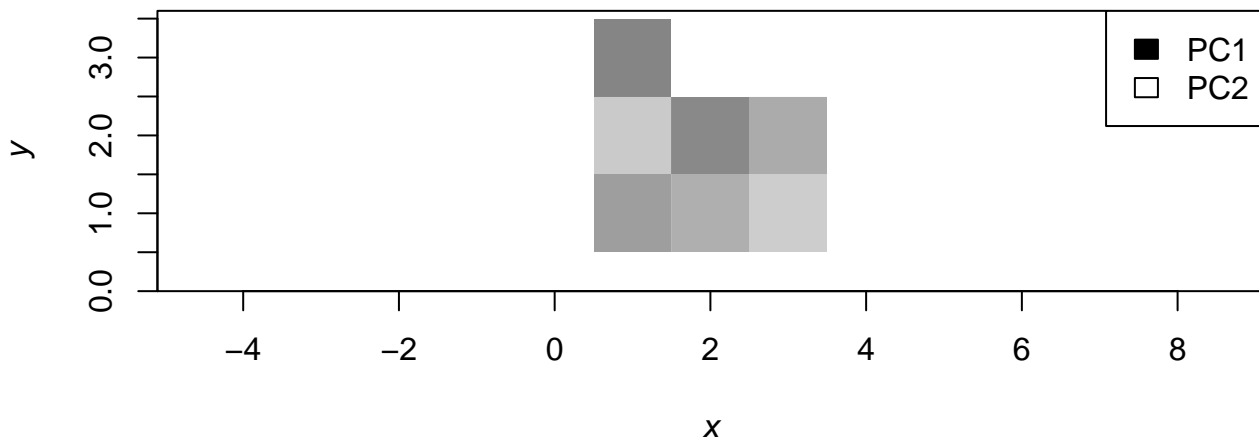
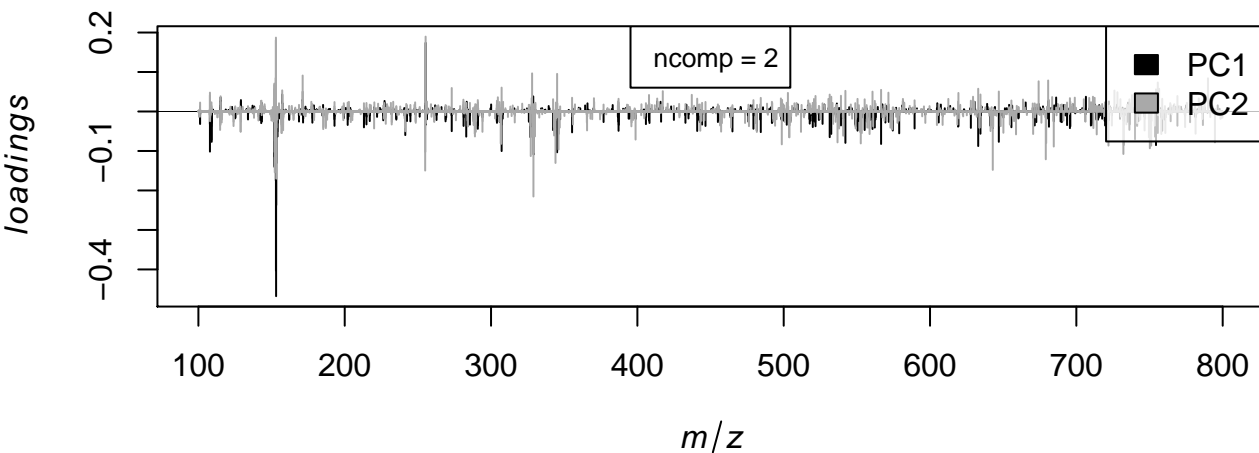
Maximum intensity per spectrum



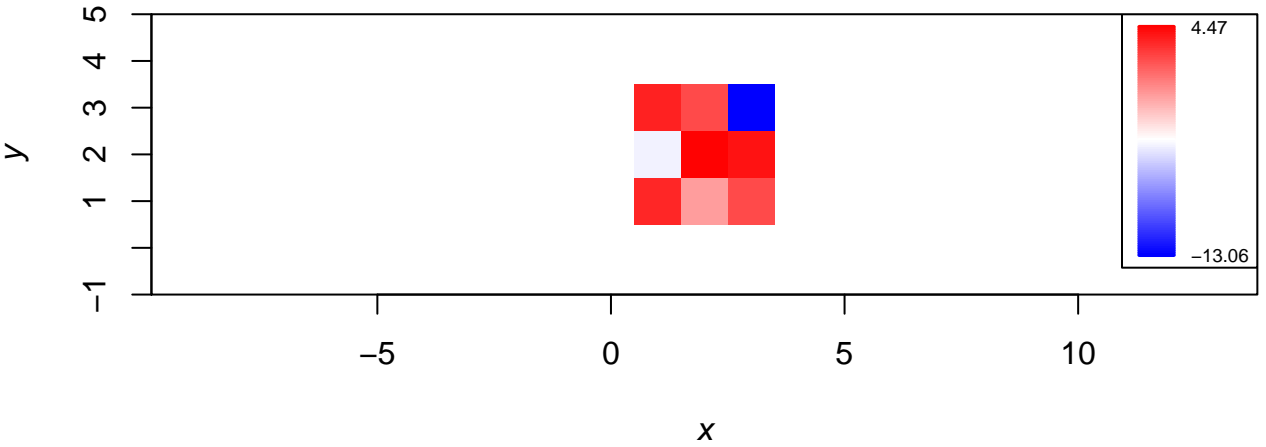
Most abundant m/z in each spectrum



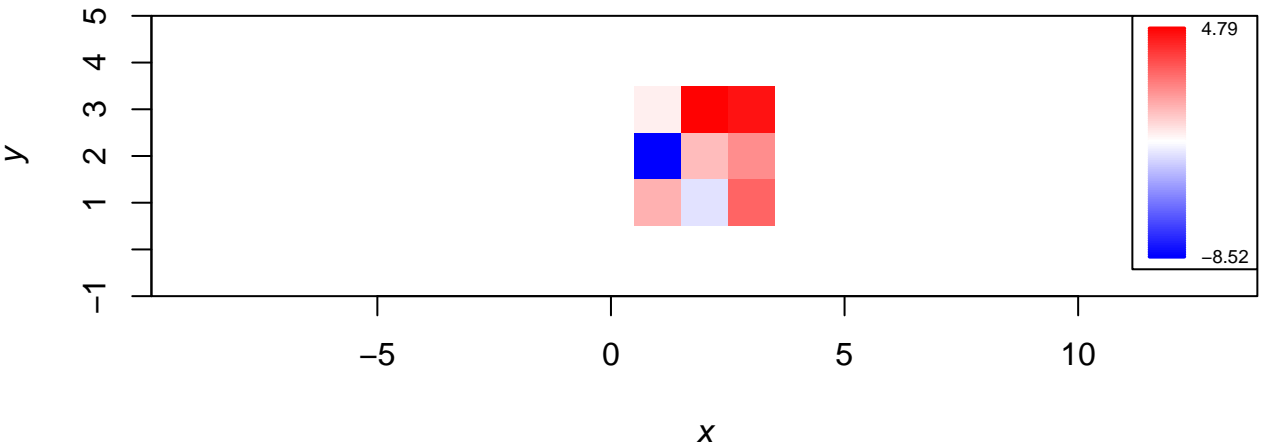
PCA for two components



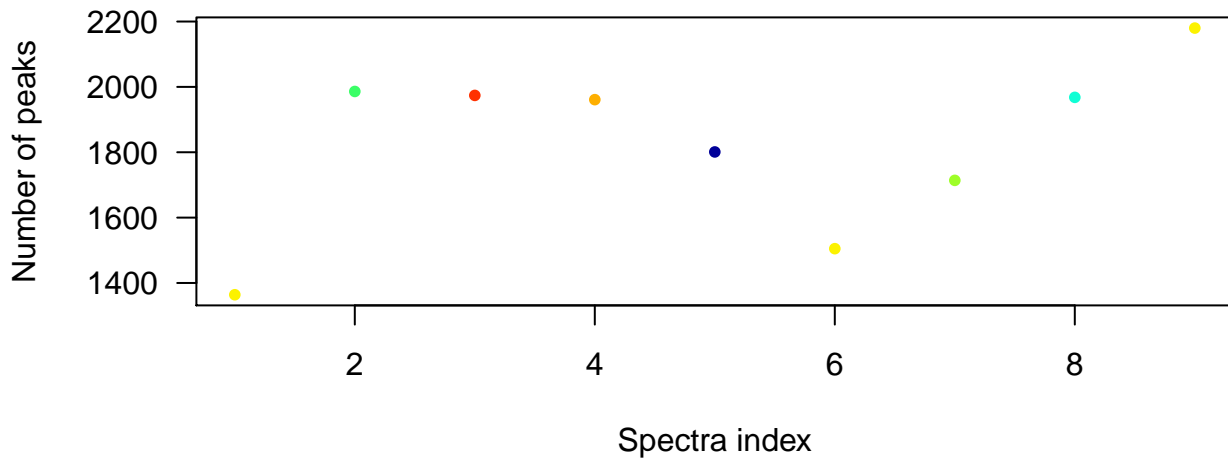
PC1



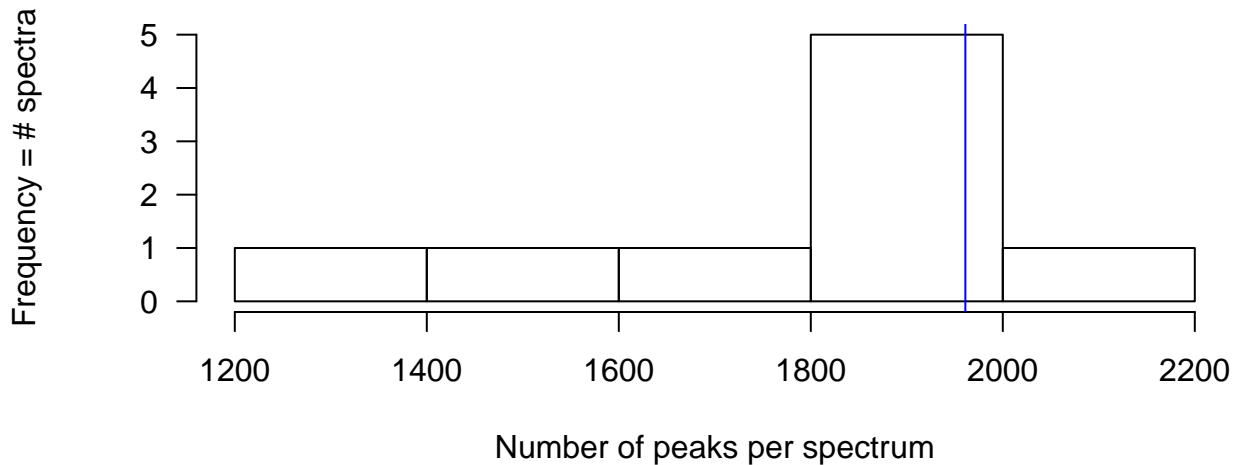
PC2



Number of peaks per spectrum

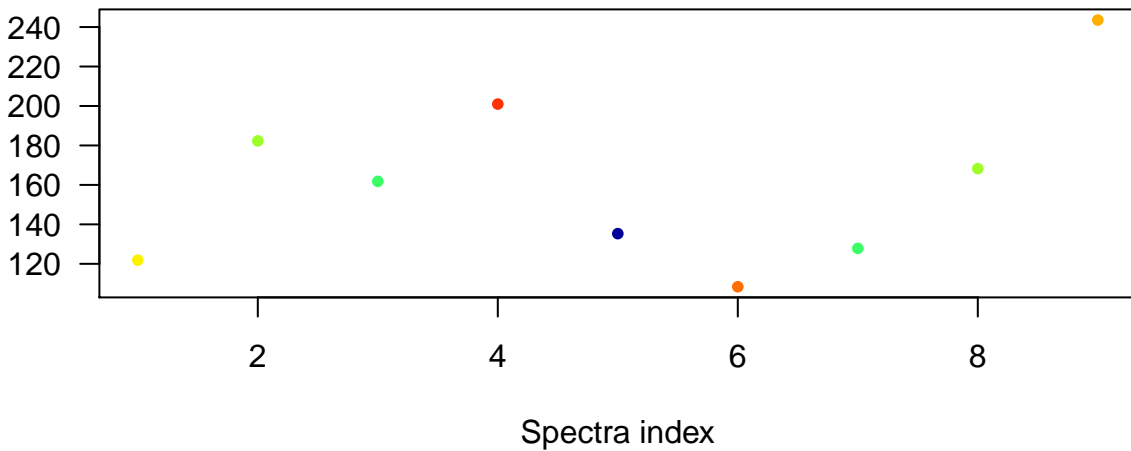


Number of peaks per spectrum



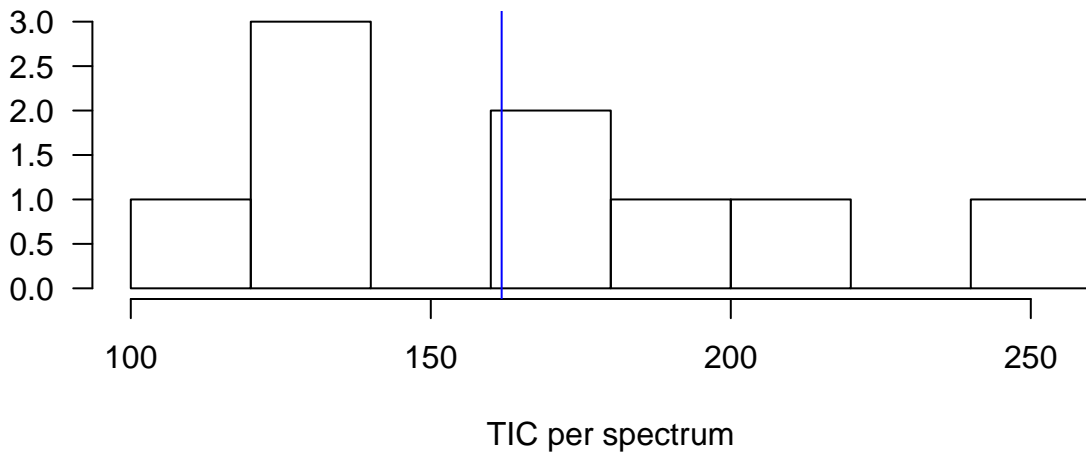
Total ion chromatogram intensity

TIC per spectrum

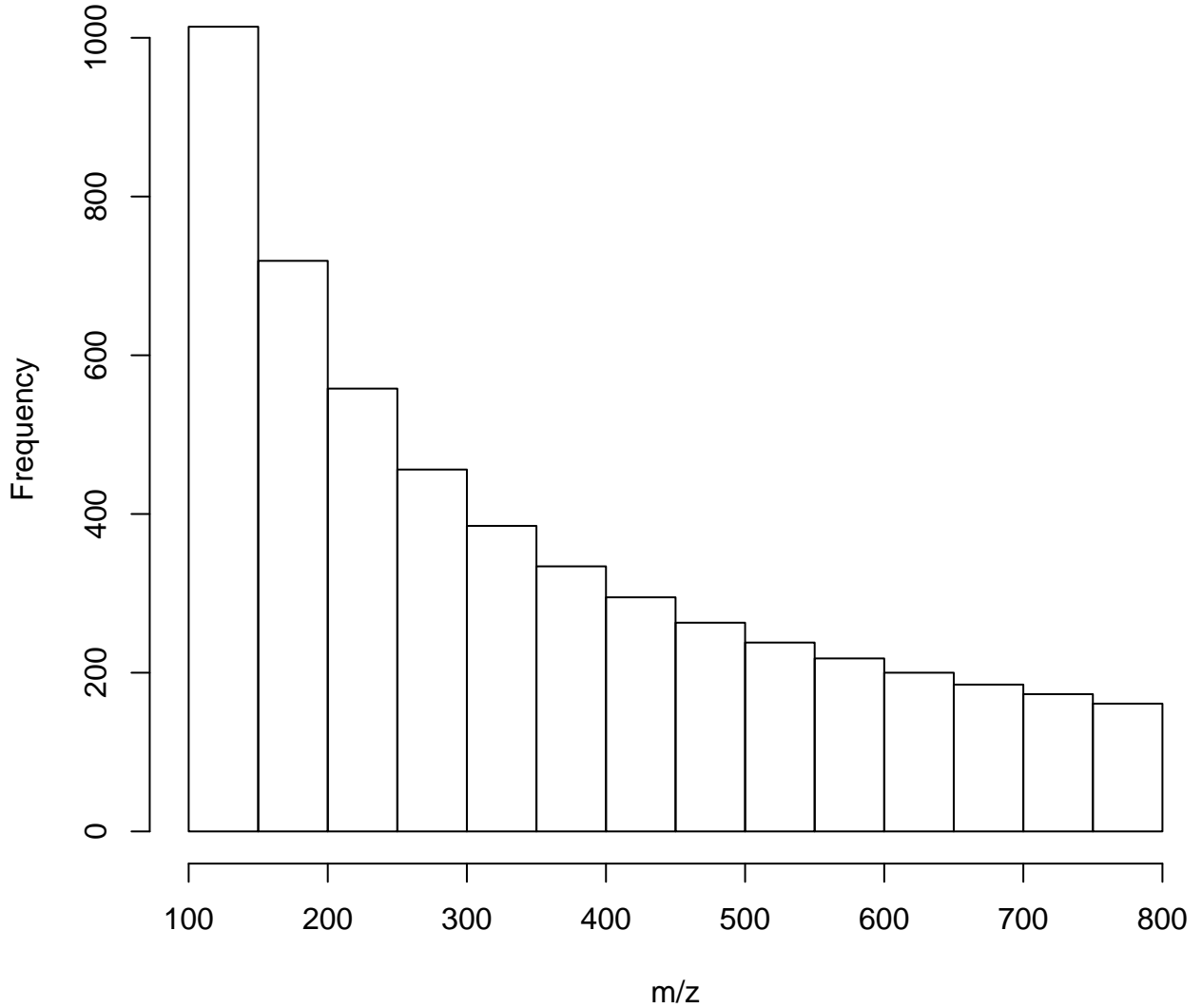


Frequency = # spectra

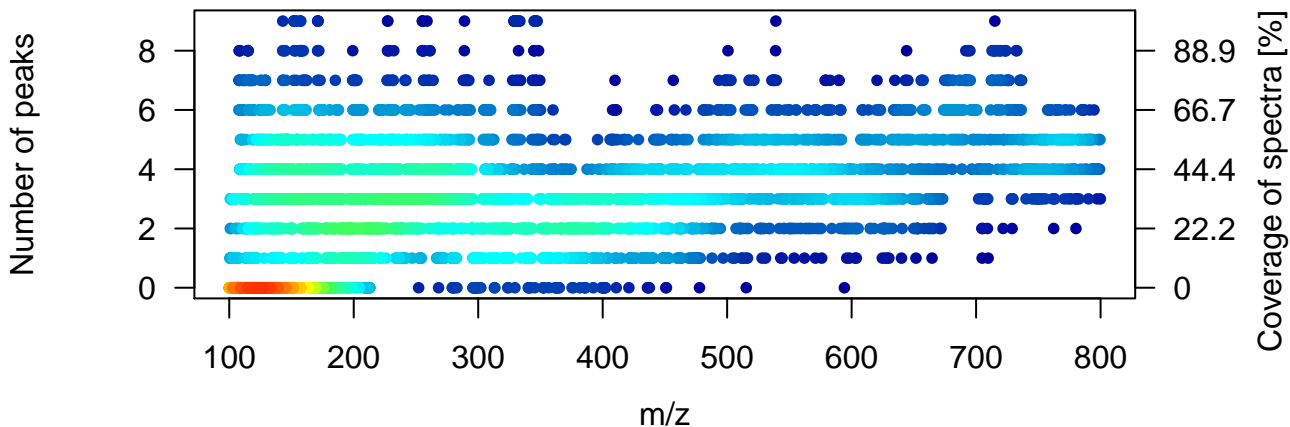
TIC per spectrum



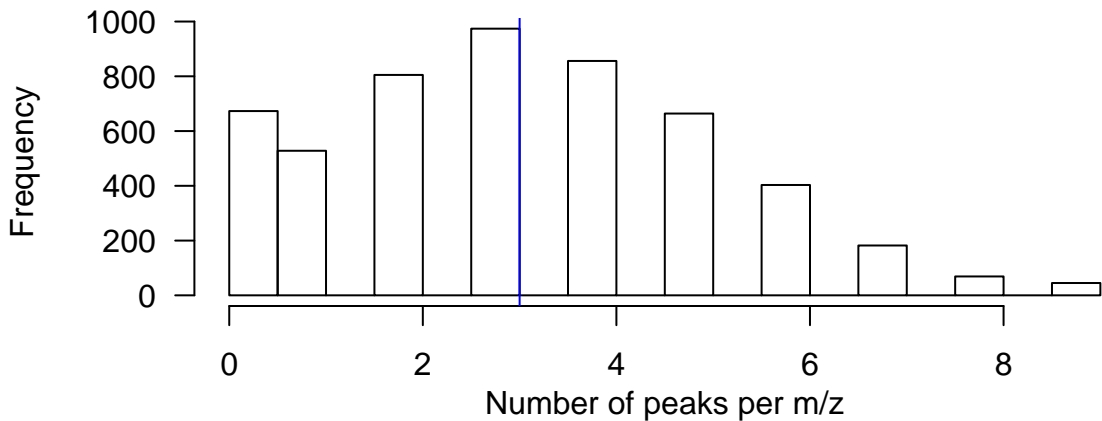
Histogram of m/z values



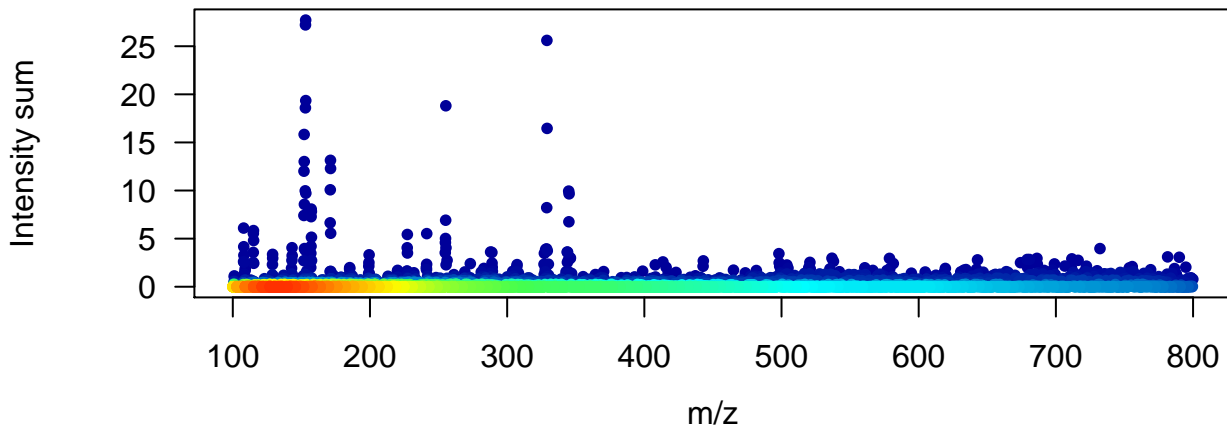
Number of peaks per m/z



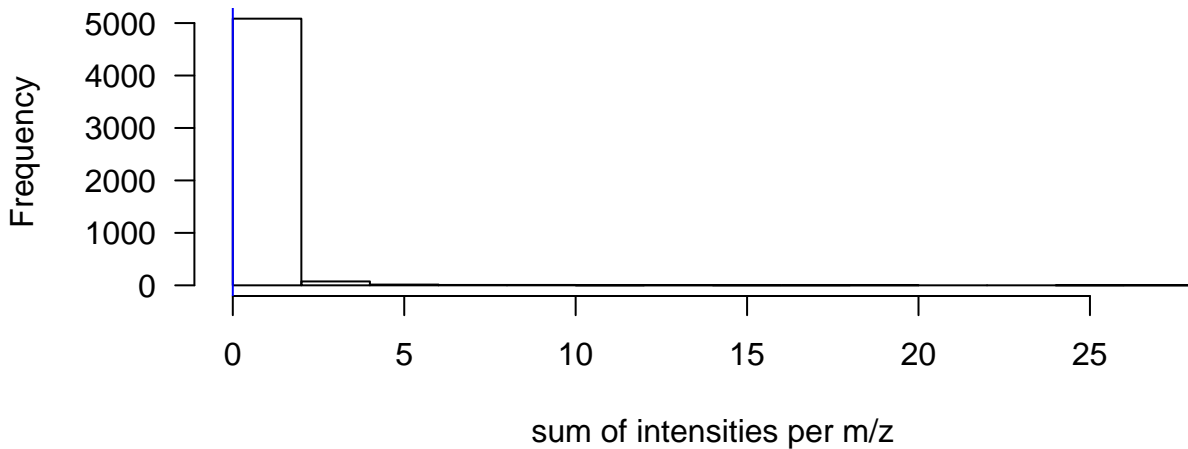
Number of peaks per m/z



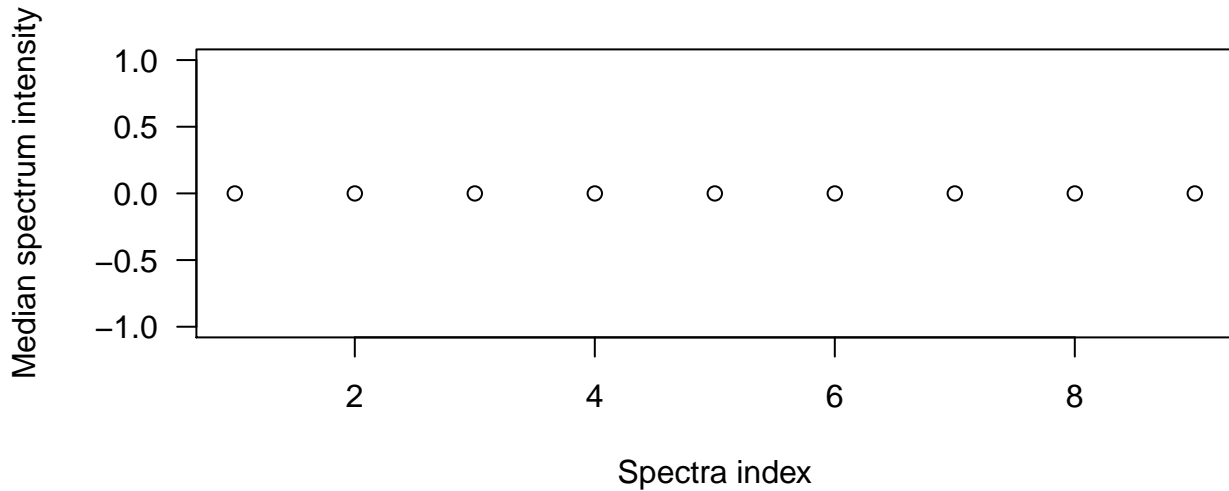
Sum of intensities per m/z



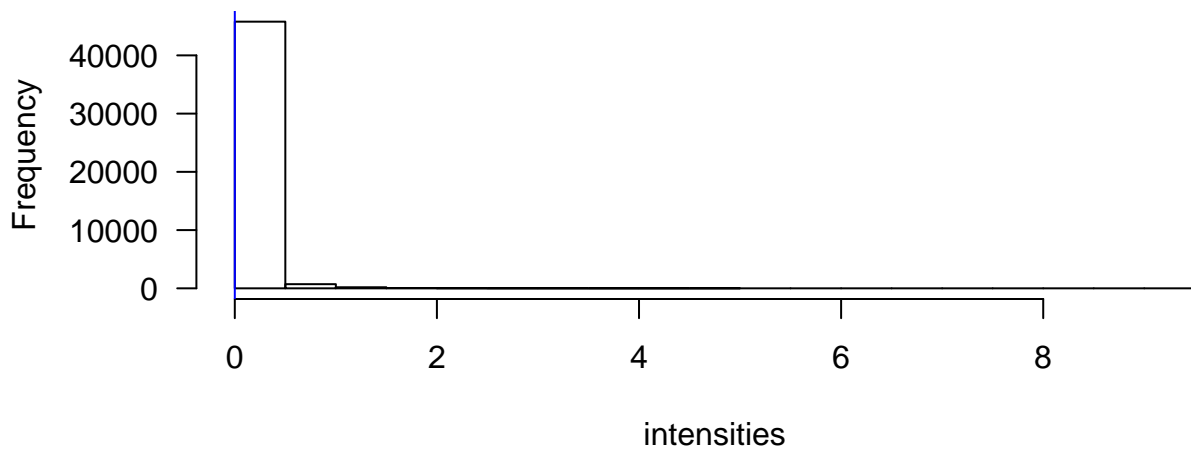
Sum of intensities per m/z



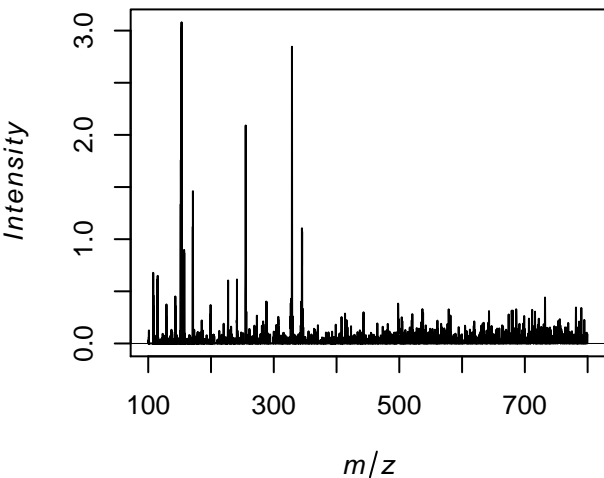
Median intensity per spectrum



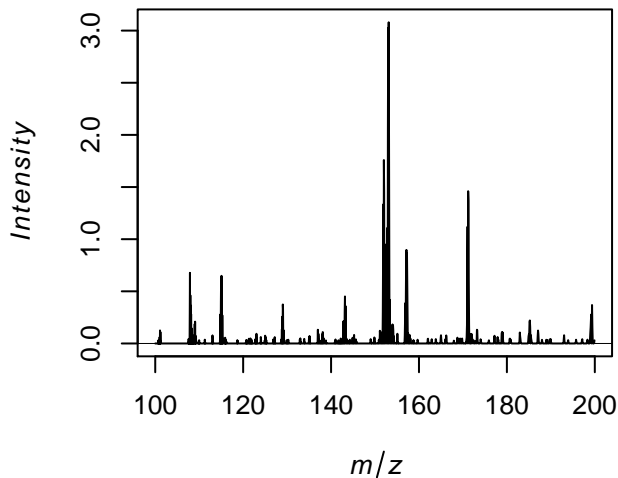
Intensity histogram



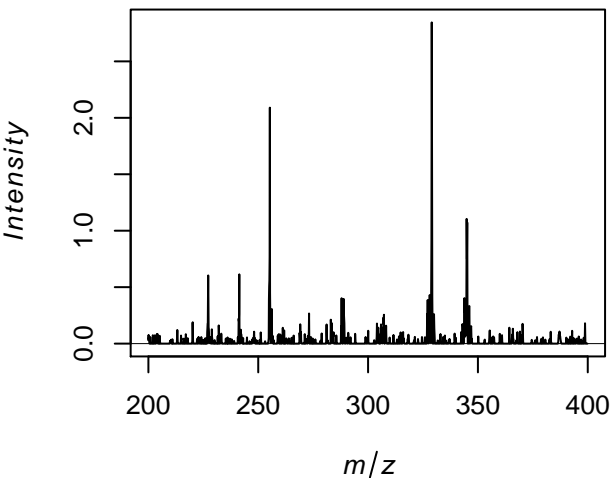
Average spectrum



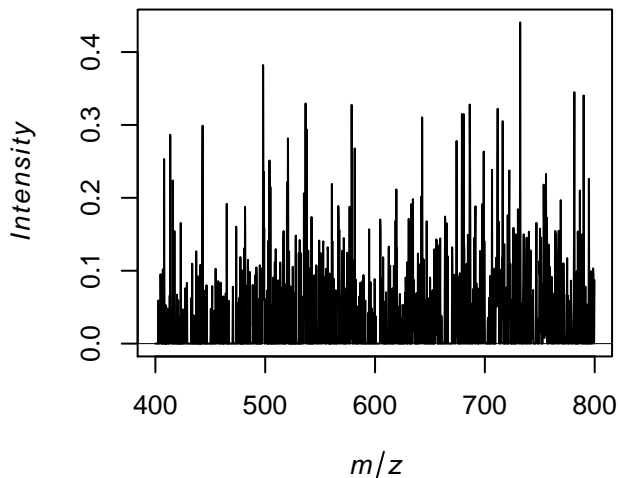
Zoomed average spectrum



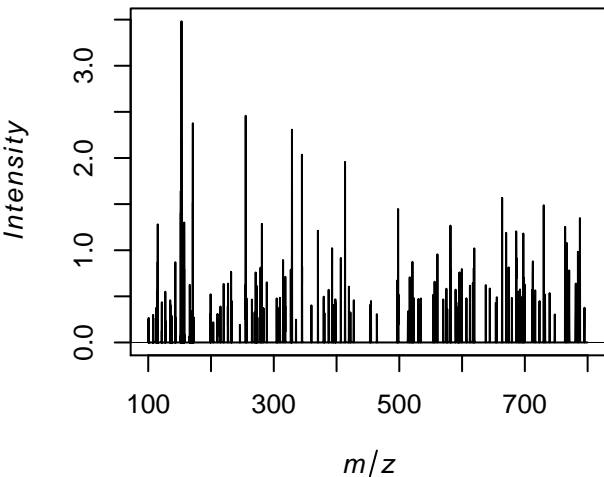
Zoomed average spectrum



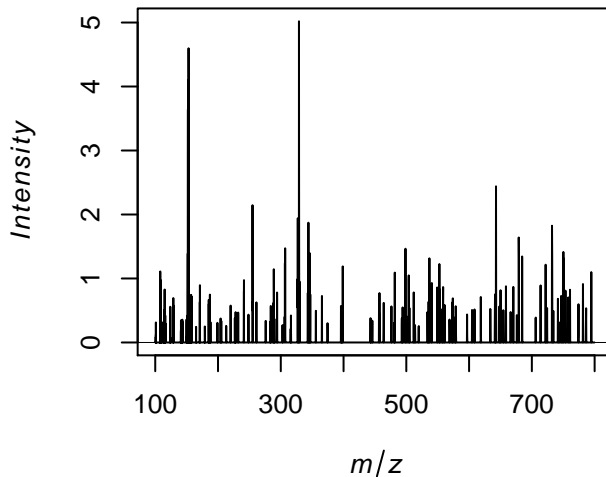
Zoomed average spectrum



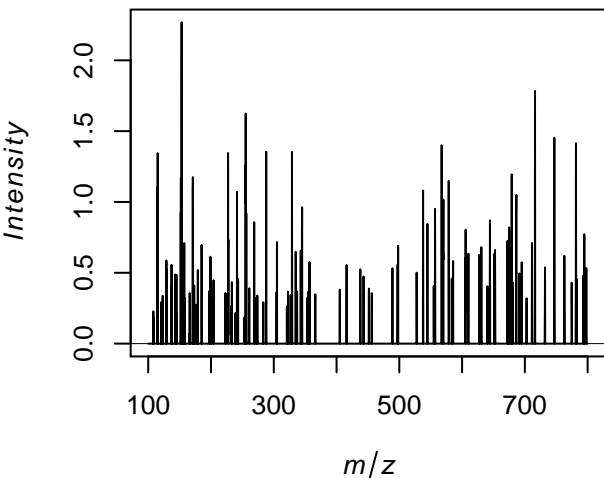
Spectrum at x = 3, y = 1



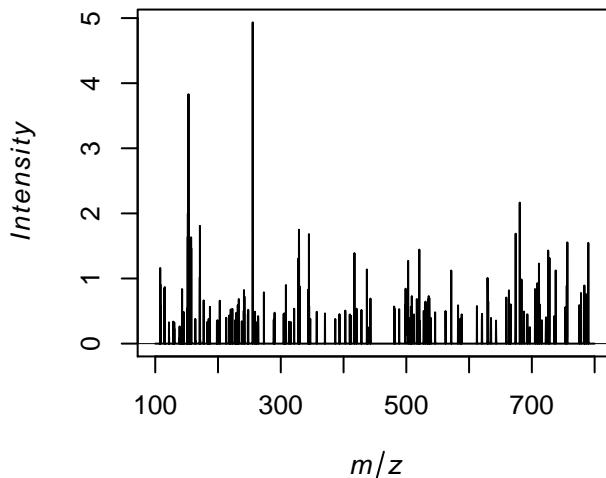
Spectrum at x = 1, y = 2



Spectrum at x = 1, y = 3



Spectrum at x = 2, y = 3

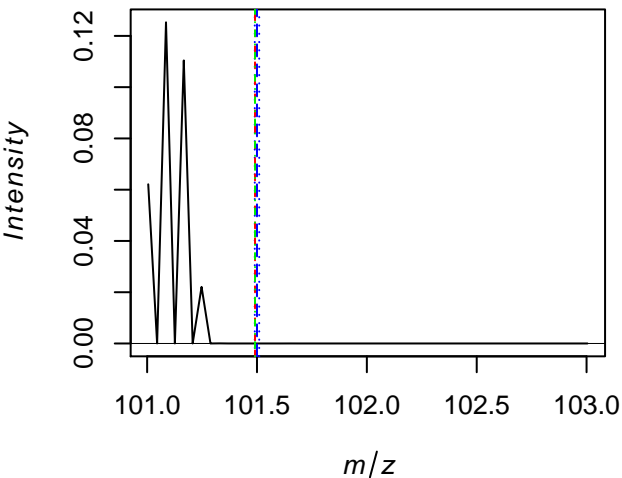


theor. m/z: 101.5

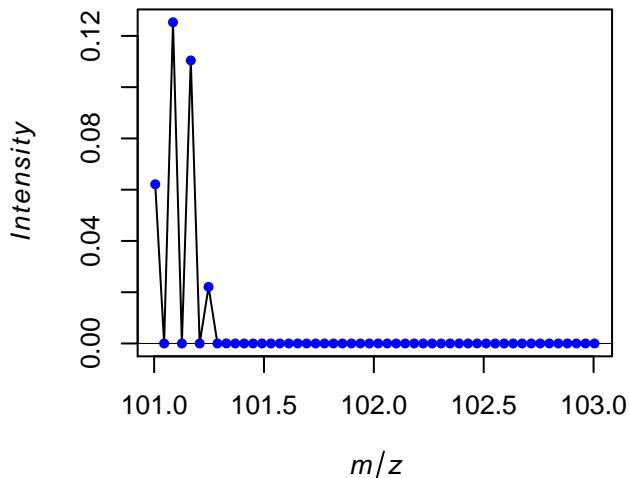
most abundant m/z: 101.491

closest m/z: 101.491

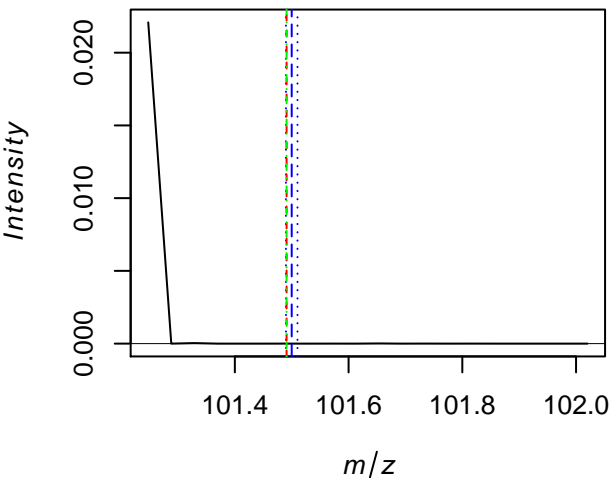
Average spectrum



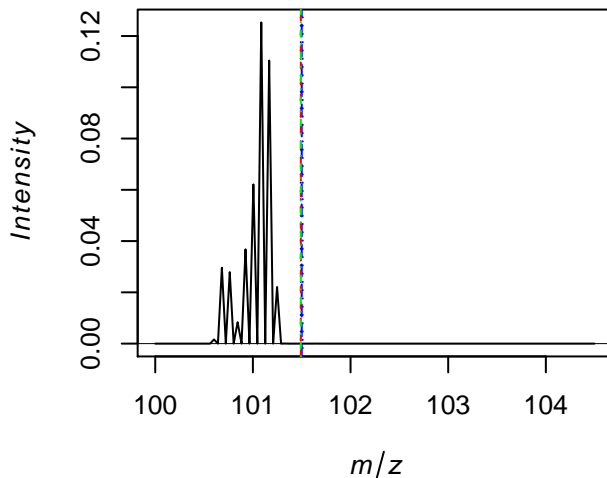
Average spectrum with data points



Average spectrum



Average spectrum

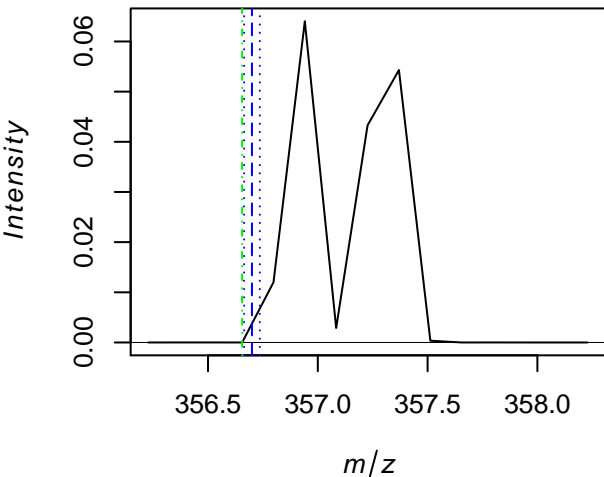


theor. m/z: 356.7

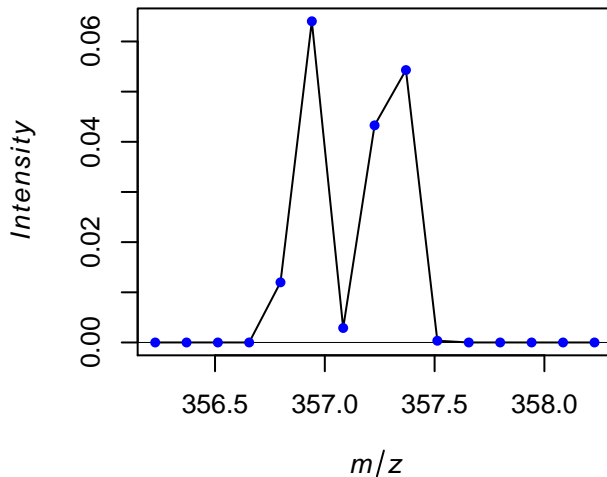
most abundant m/z: NA

closest m/z: 356.6555

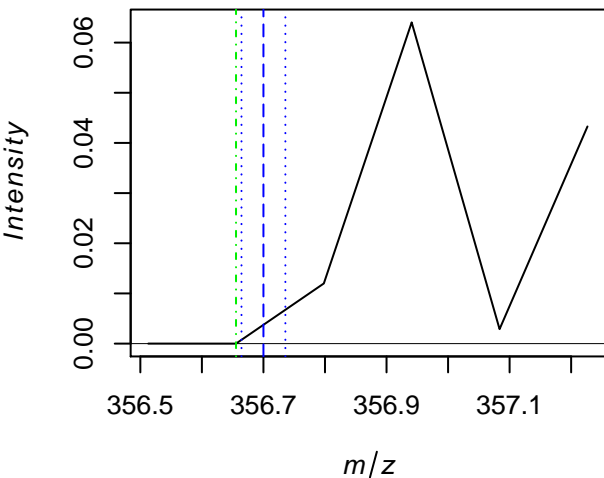
Average spectrum



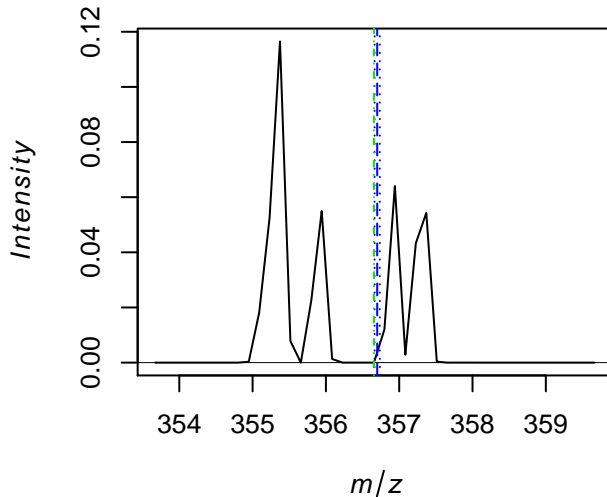
Average spectrum with data points



Average spectrum



Average spectrum

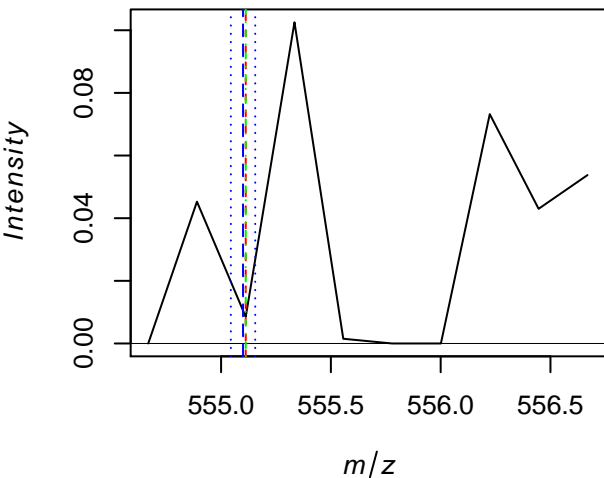


theor. m/z: 555.1

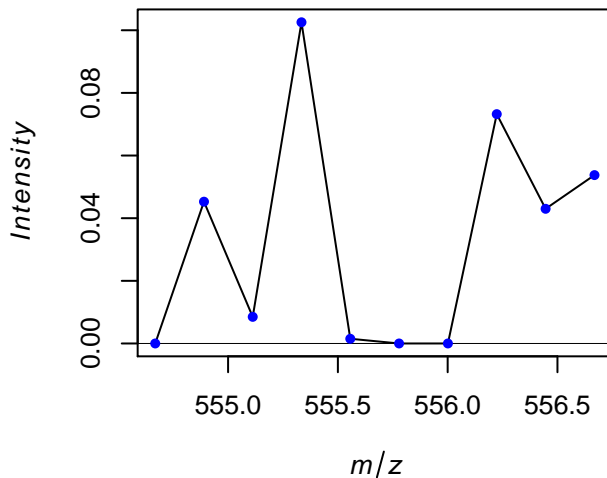
most abundant m/z: 555.122

closest m/z: 555.122

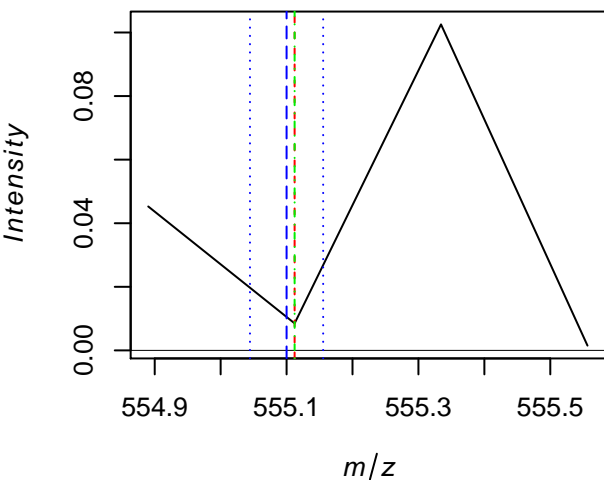
Average spectrum



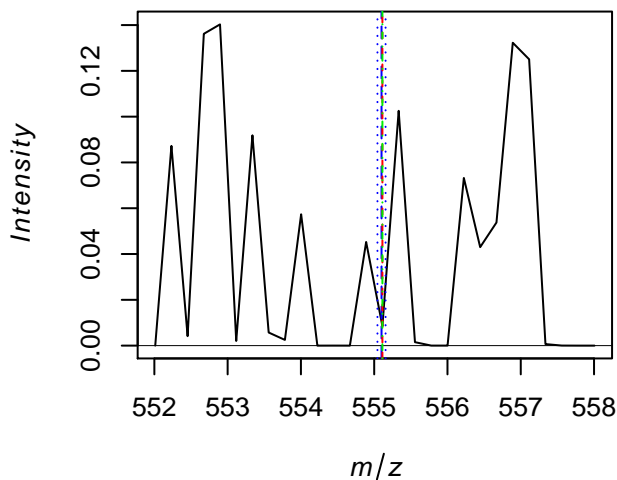
Average spectrum with data points



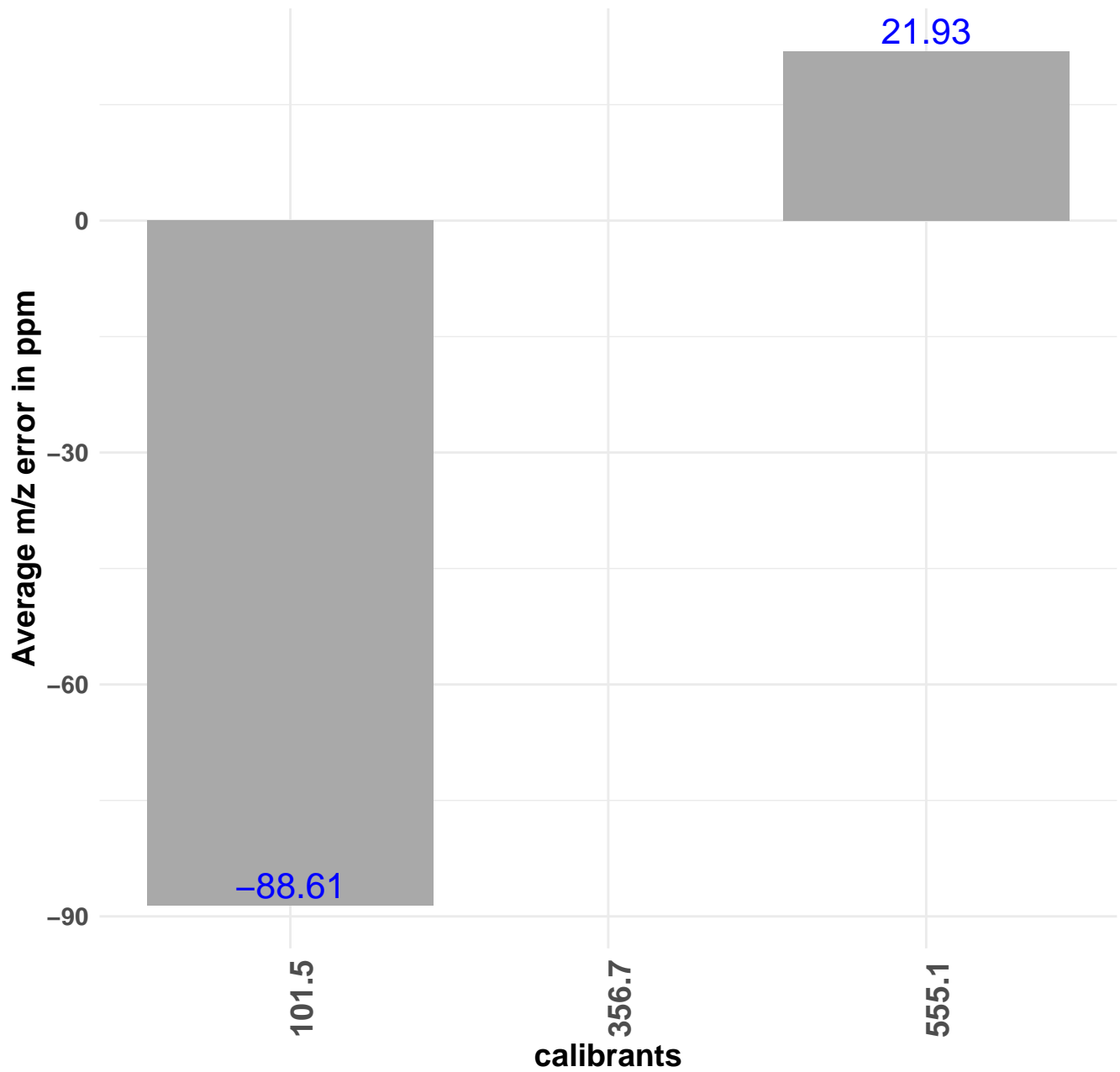
Average spectrum



Average spectrum

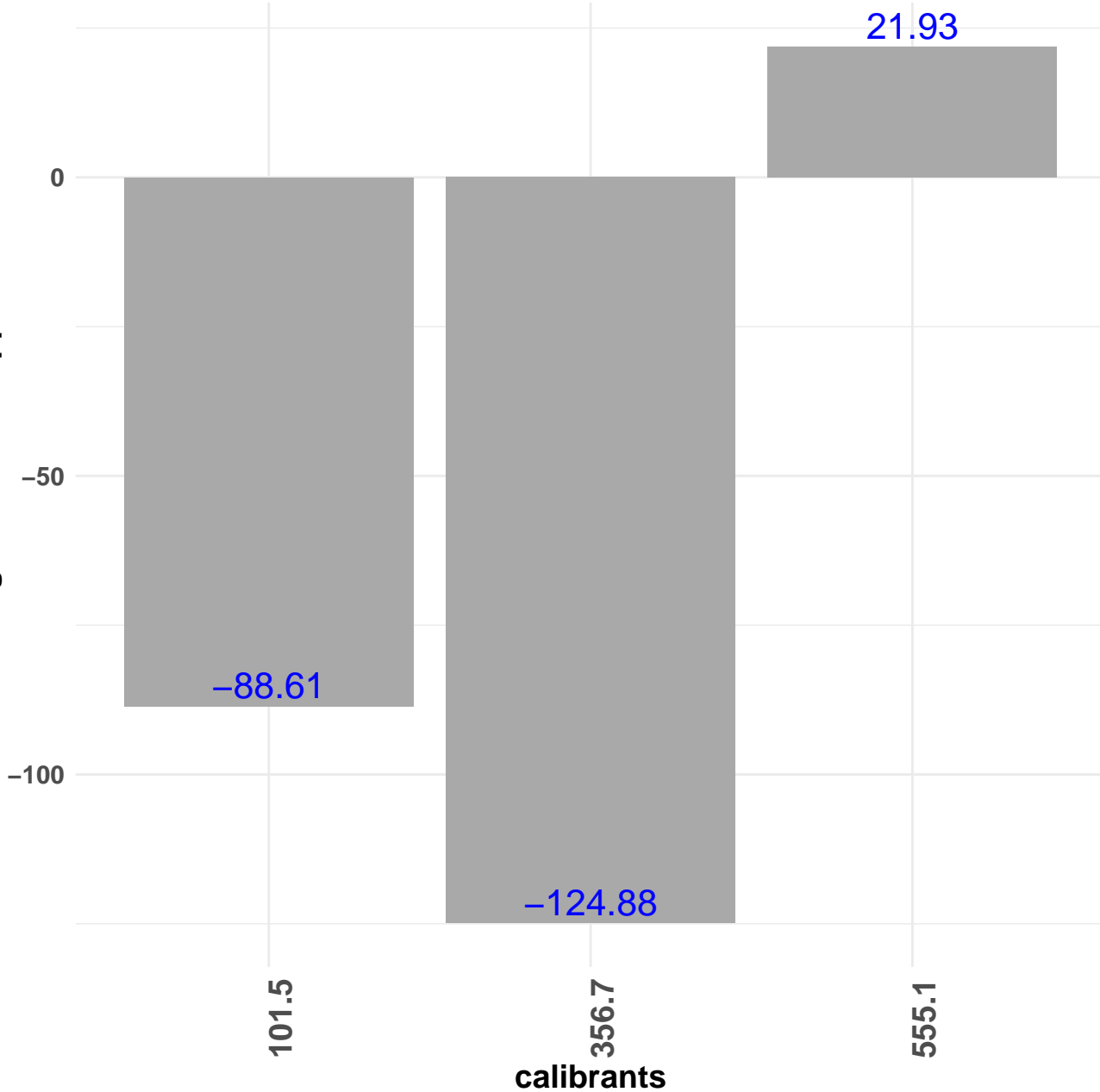


Average m/z error (max. average intensity vs. theor. calibrant m/z)

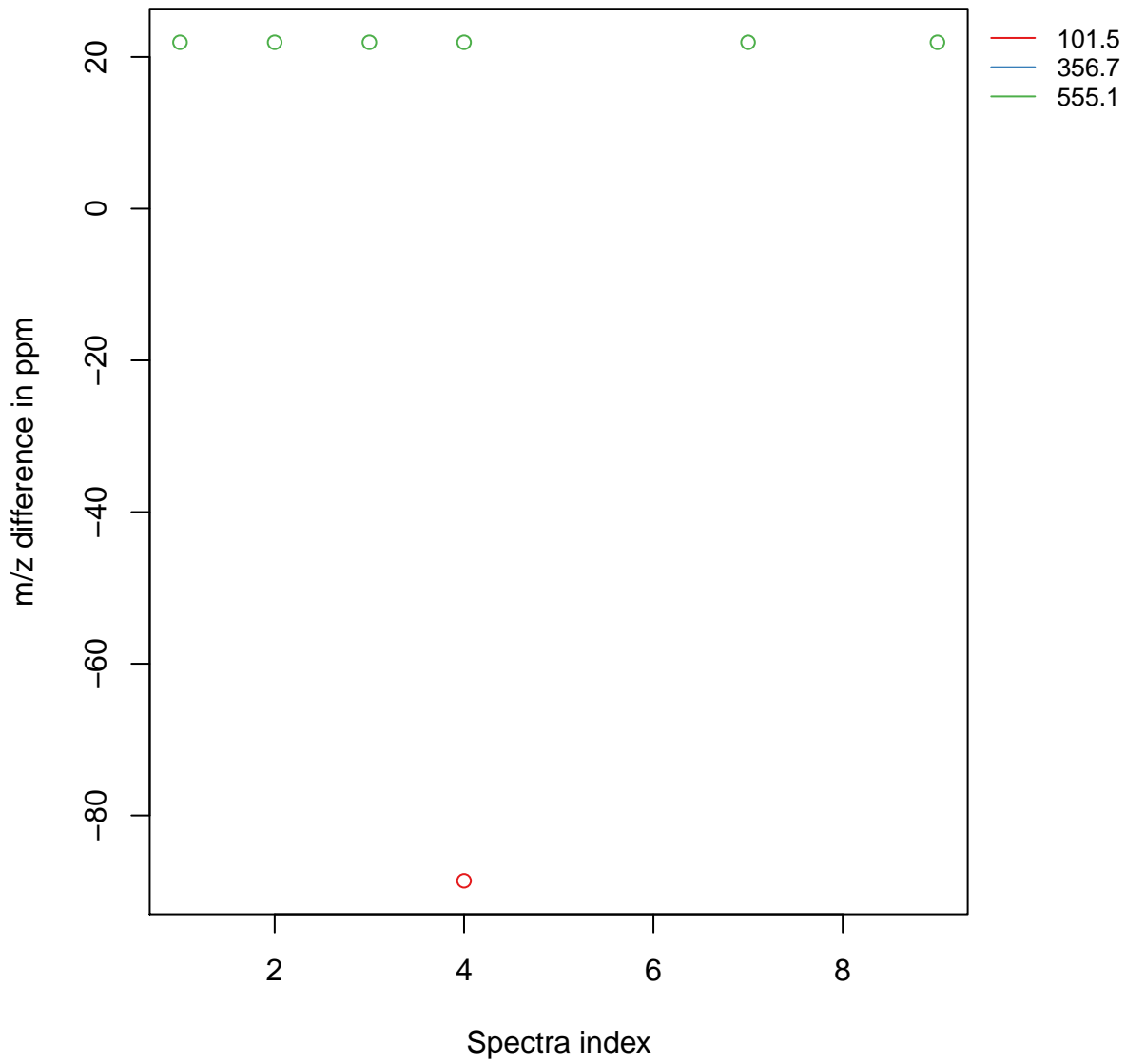


Average m/z error (closest measured m/z vs. theor. calibrant m/z)

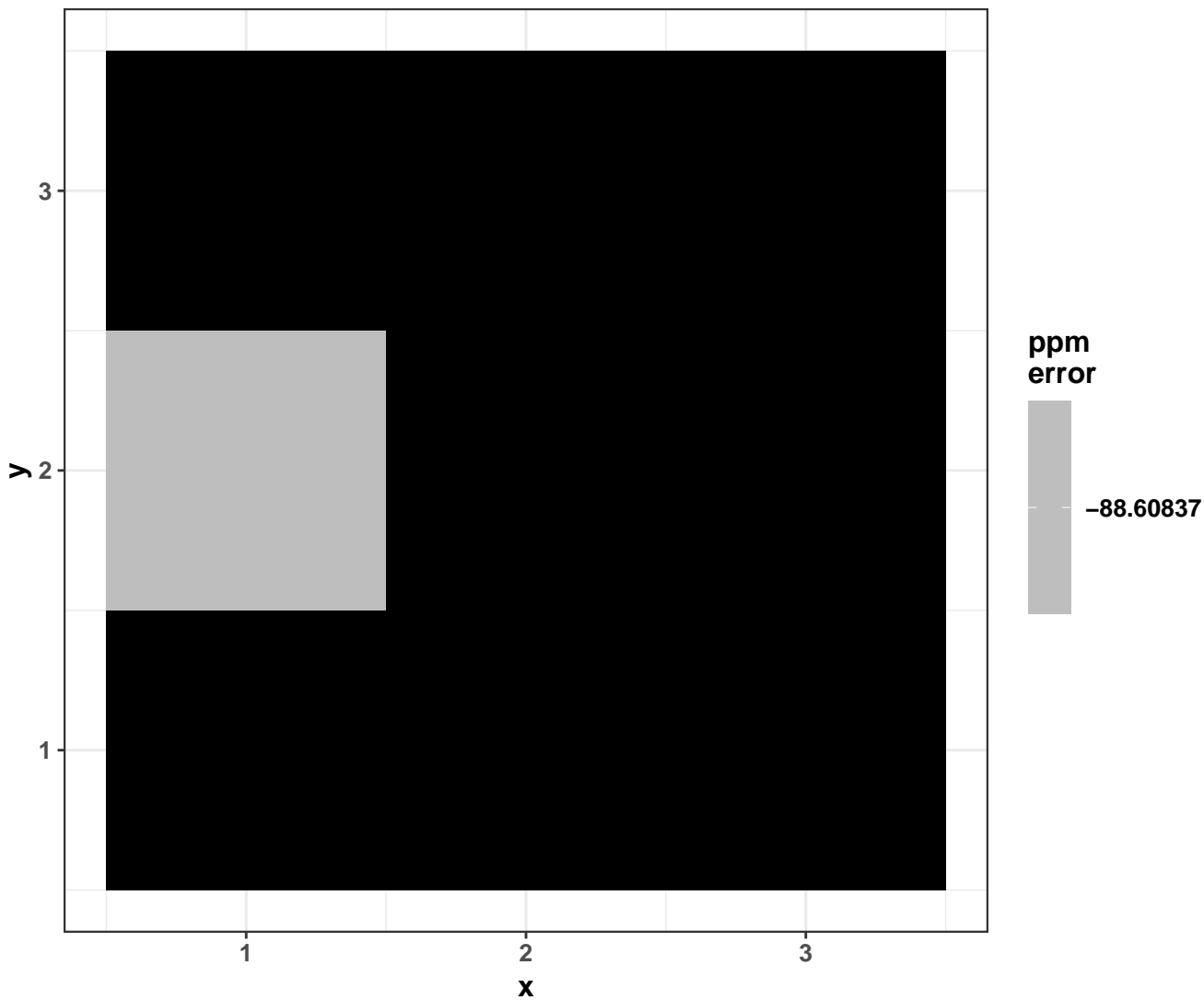
Average m/z error in ppm



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

