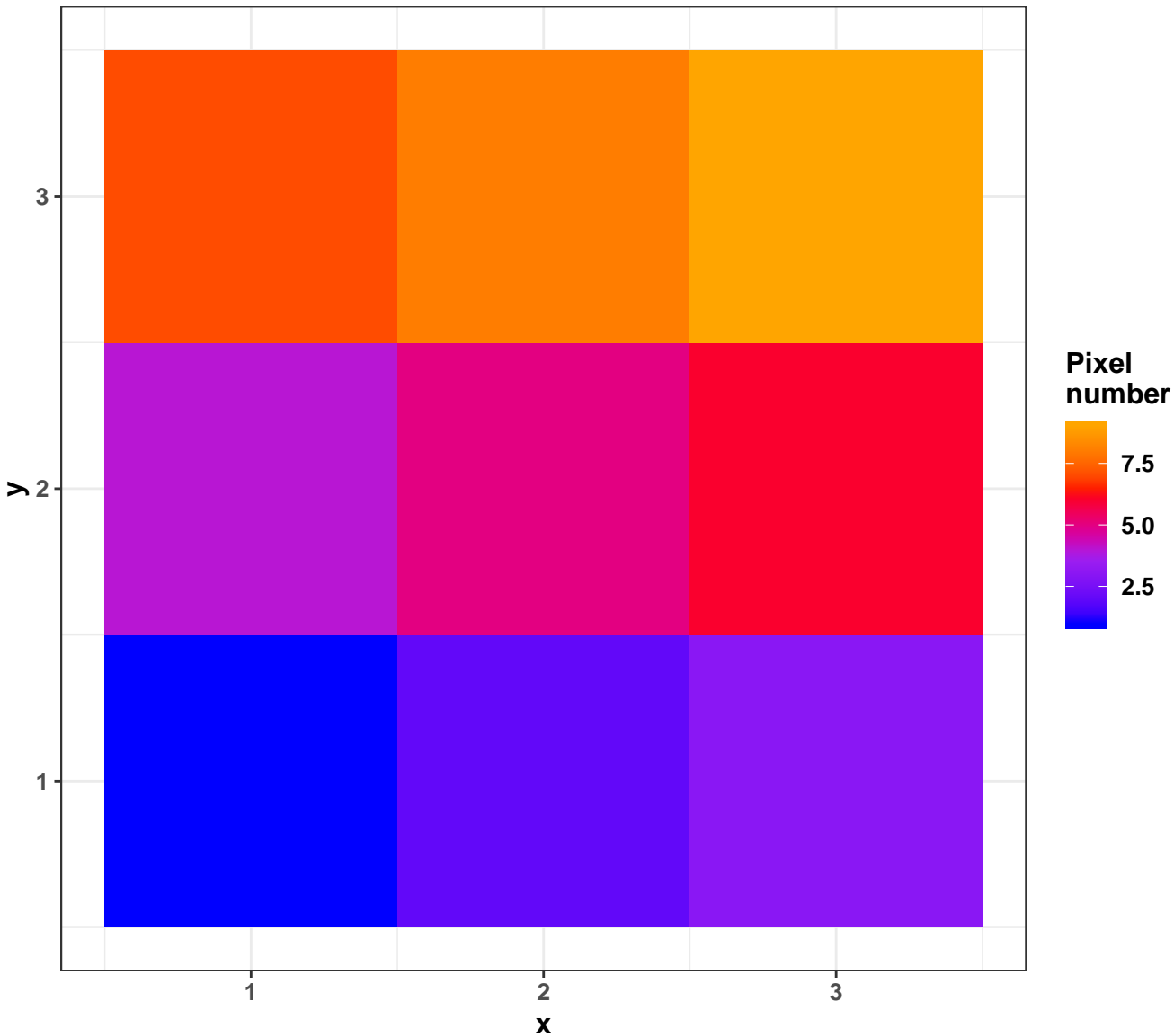


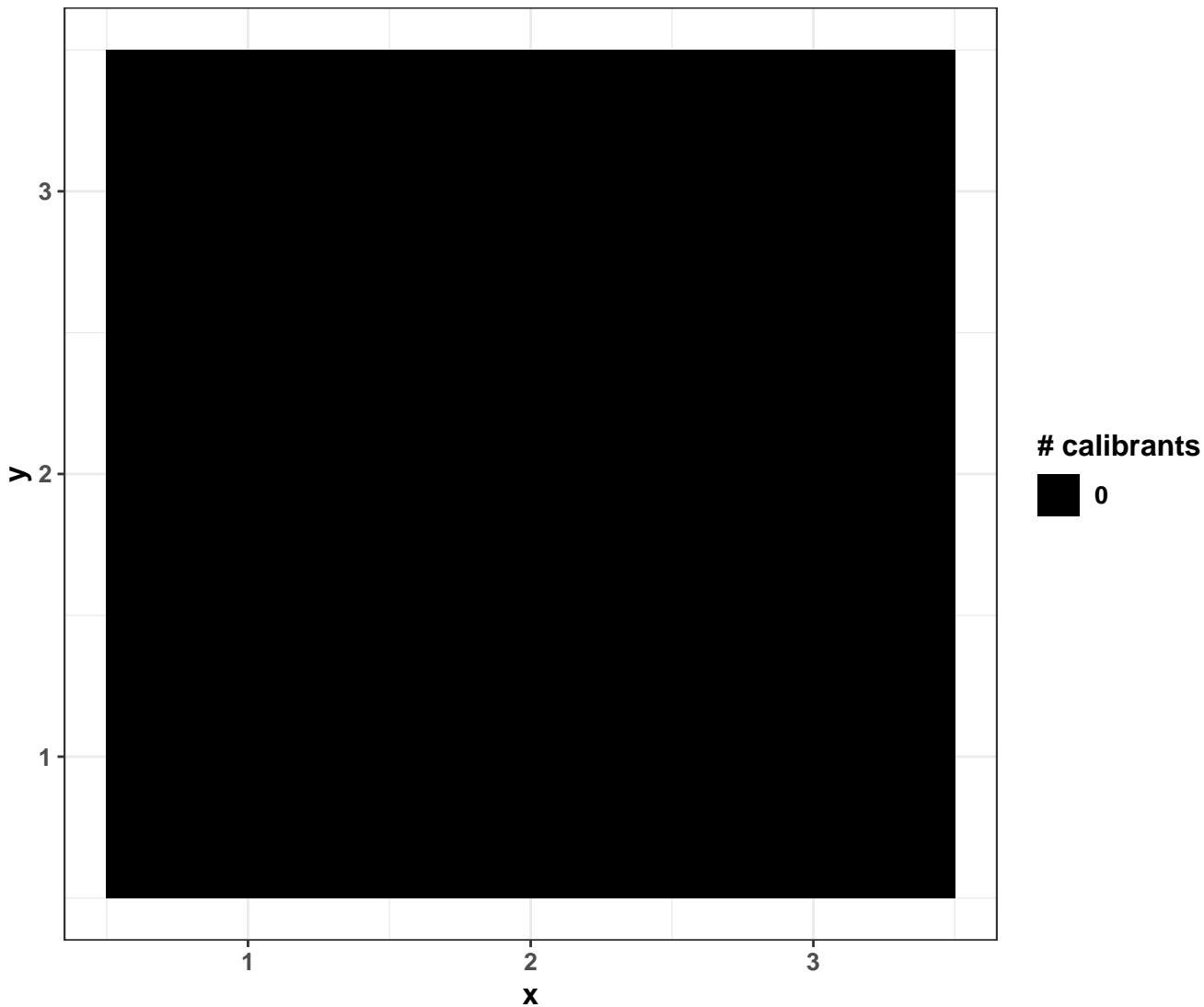
## Testfile\_imzml

properties	values
Number of m/z features	1199
Range of m/z values	300.08 – 399.92
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	0 – 2.59
Median of intensities	0
Intensities > 0	26.17 %
Number of empty spectra	0
Median TIC $\pm$ sd	24.4 $\pm$ 9
Median # peaks per spectrum $\pm$ sd	323 $\pm$ 65
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.tabular	1 / 3

# Pixel order

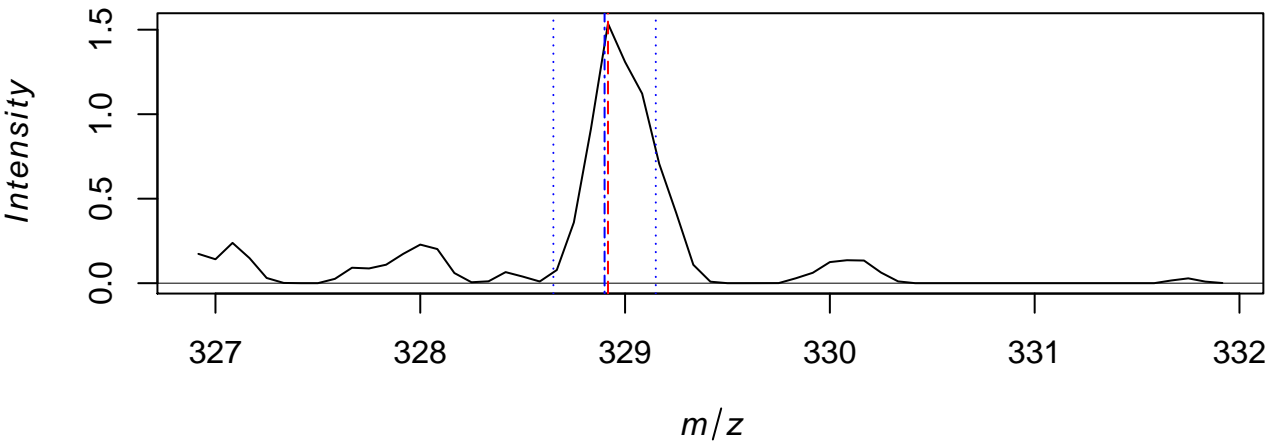


# Number of calibrants per pixel ( $\pm 100$ ppm)

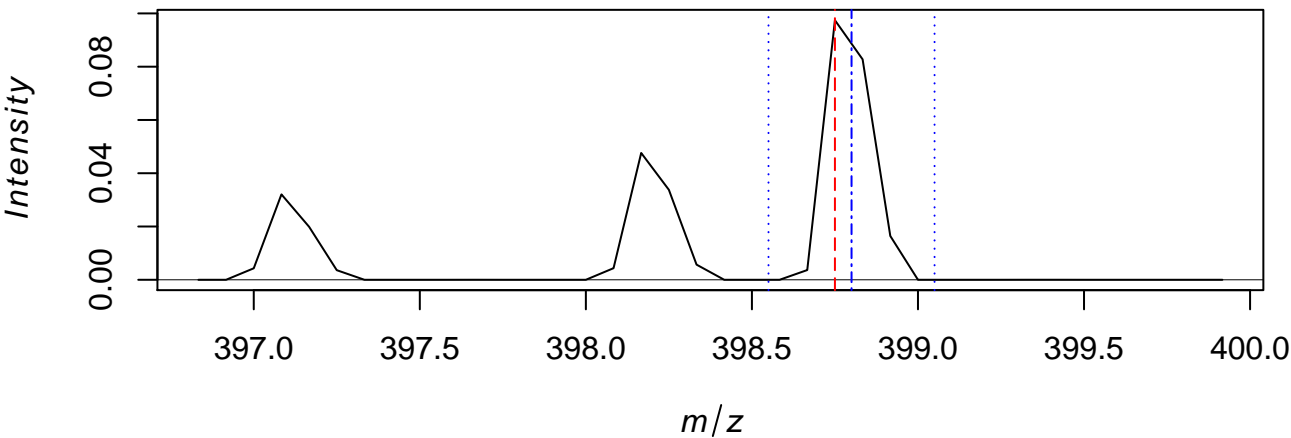


# Control of fold change plot

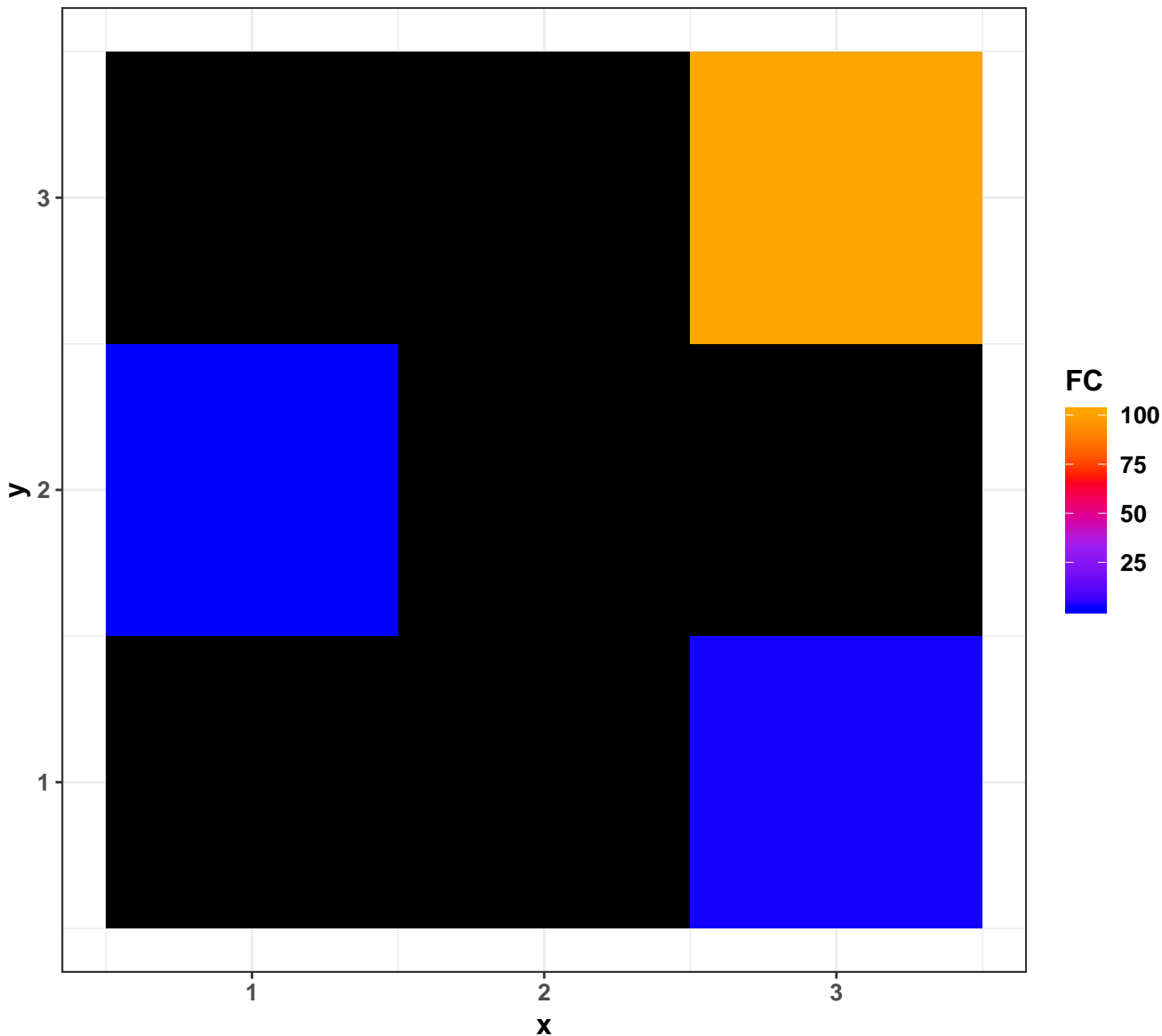
## Average spectrum 328.9 Da



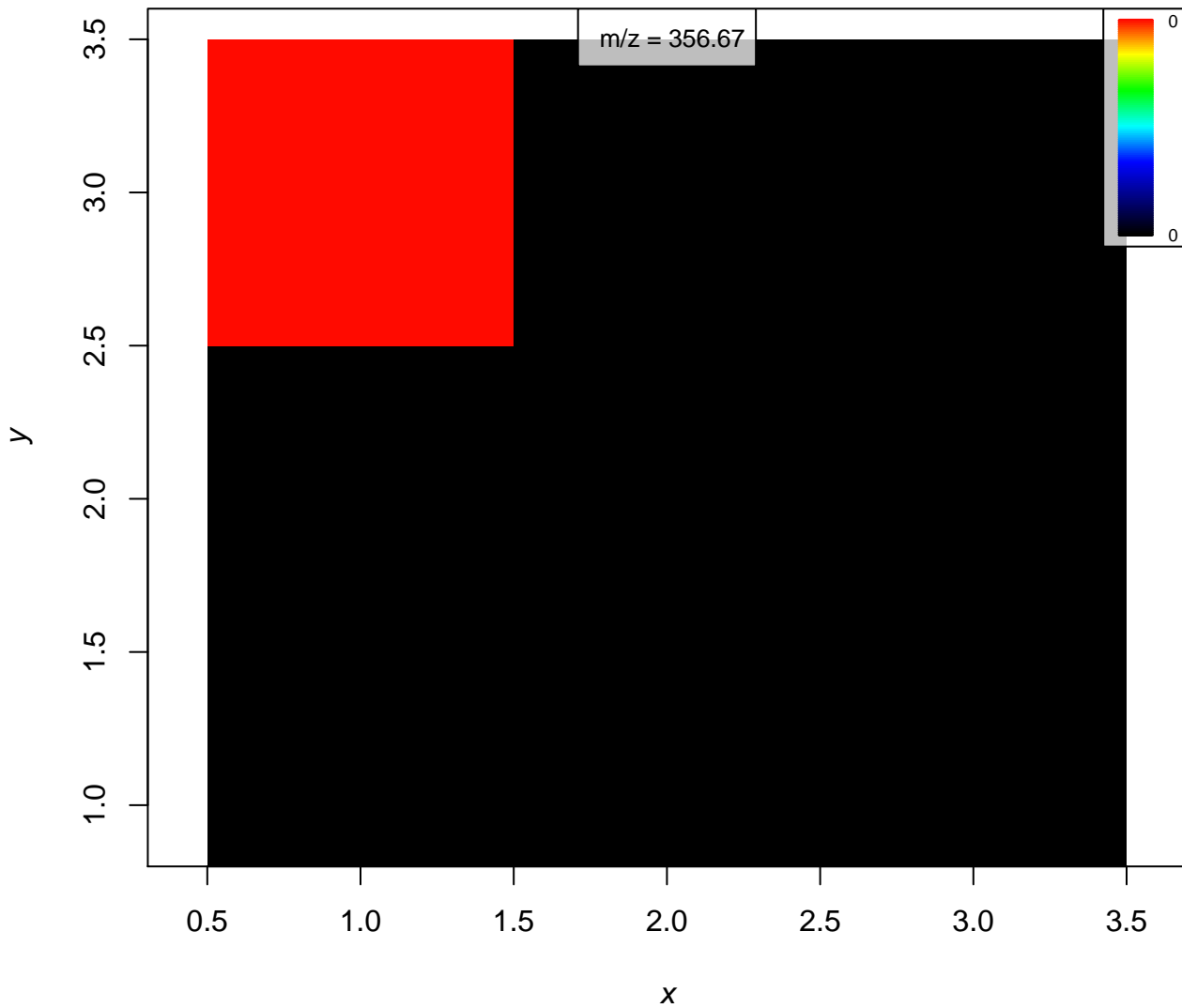
## Average spectrum 398.8 Da



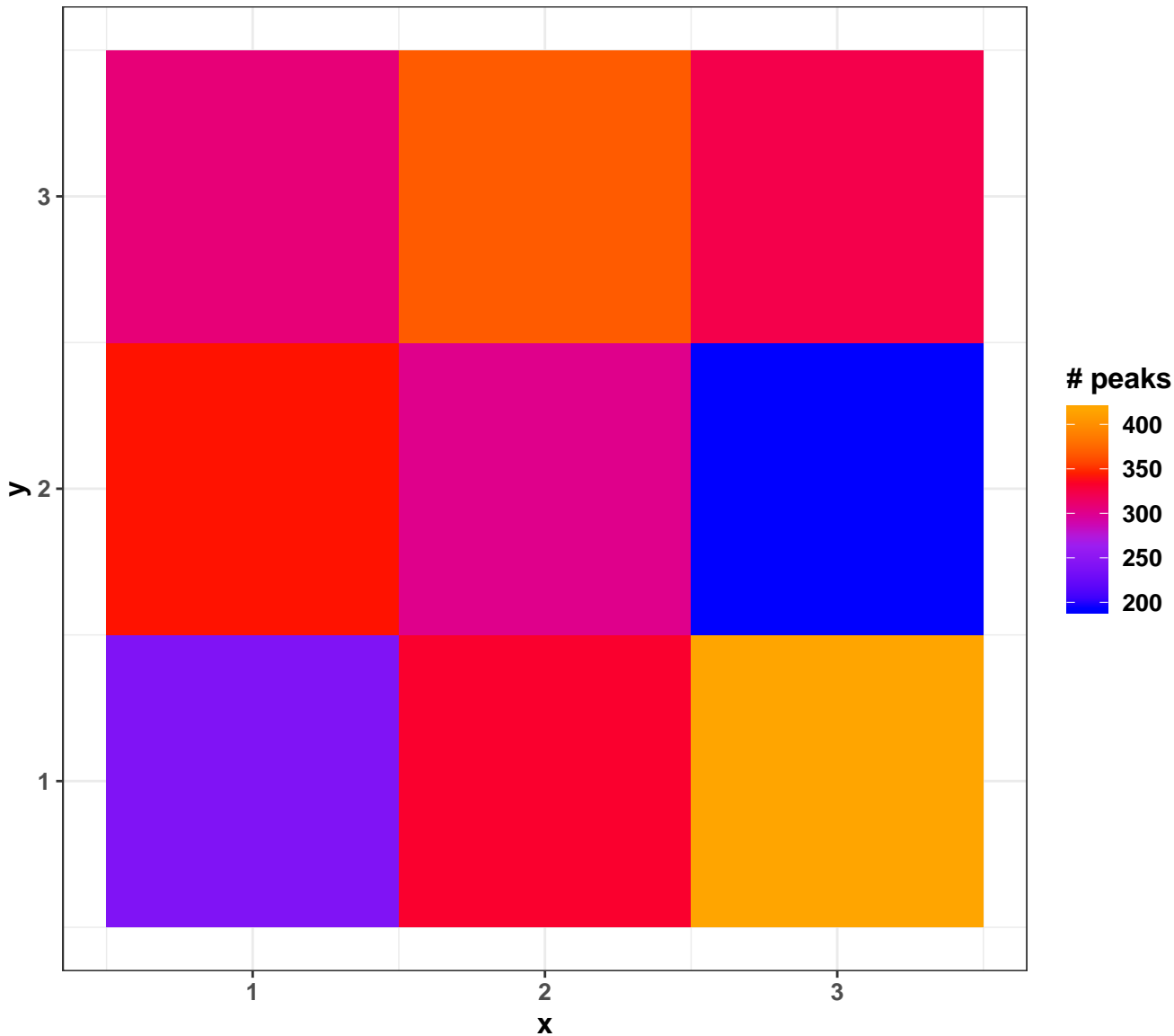
Ratioofmass13289mass23988



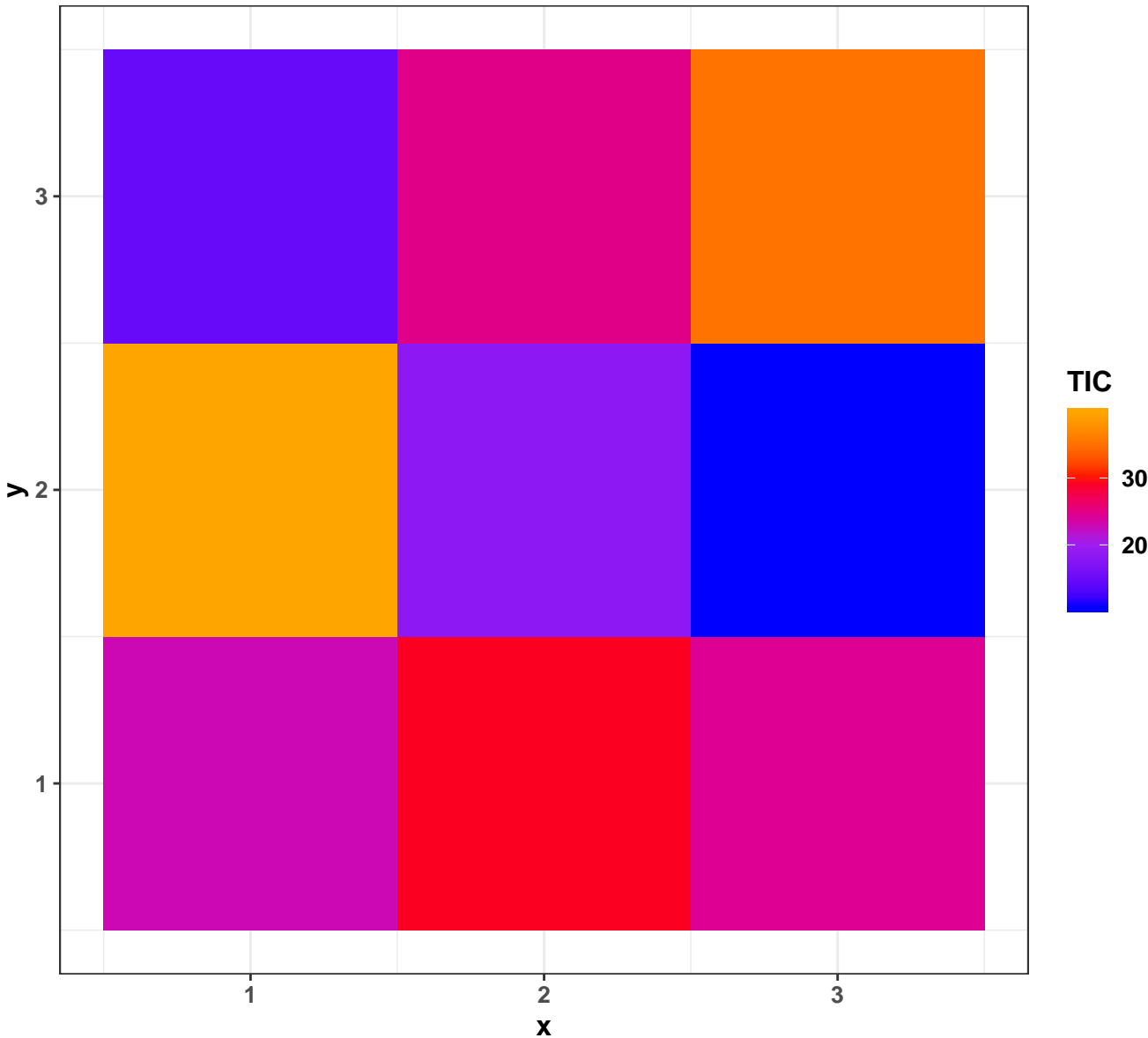
**356.7: 356.7 ( $\pm 100$  ppm)**



# Number of peaks per spectrum

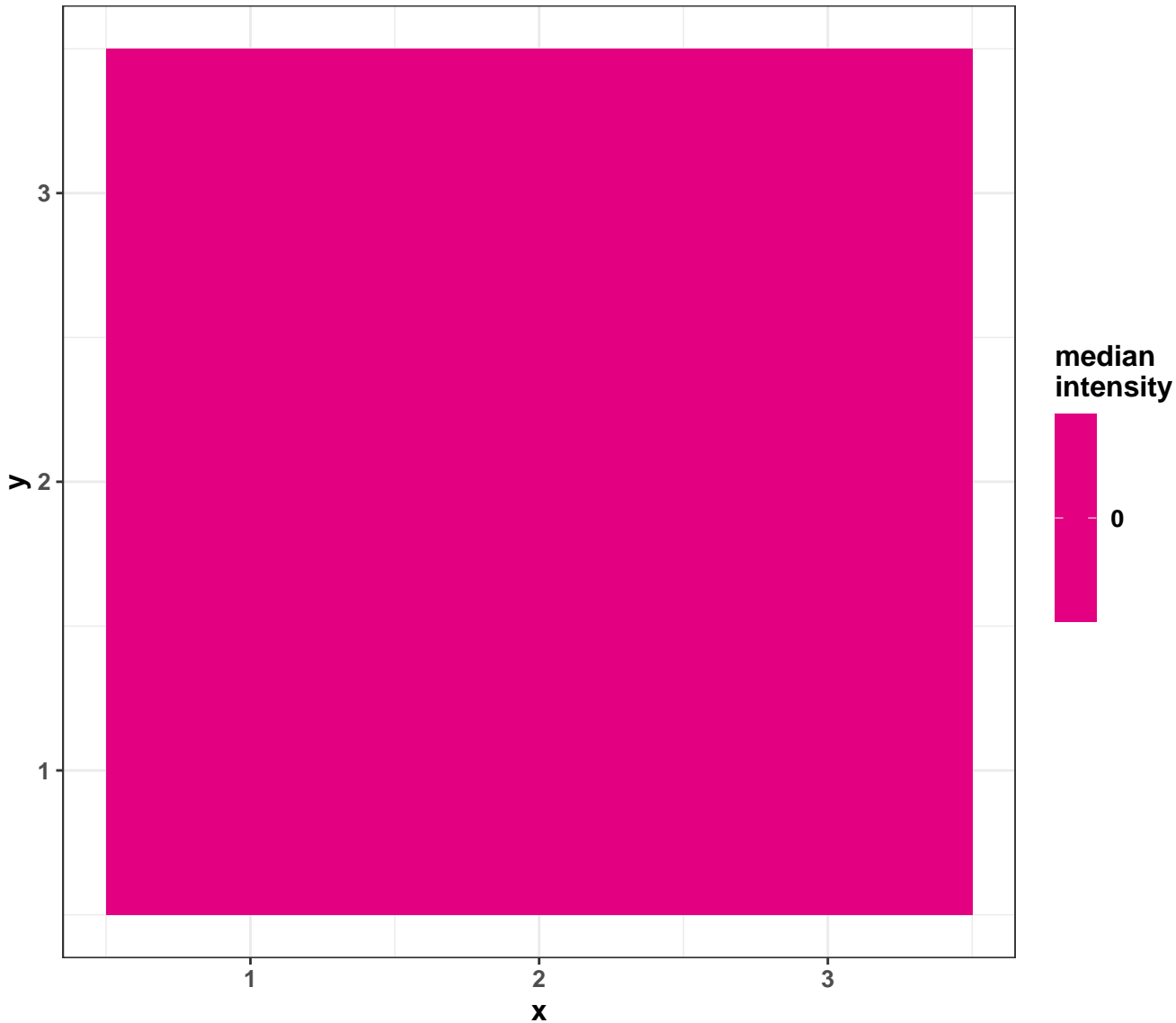


# Total Ion Chromatogram

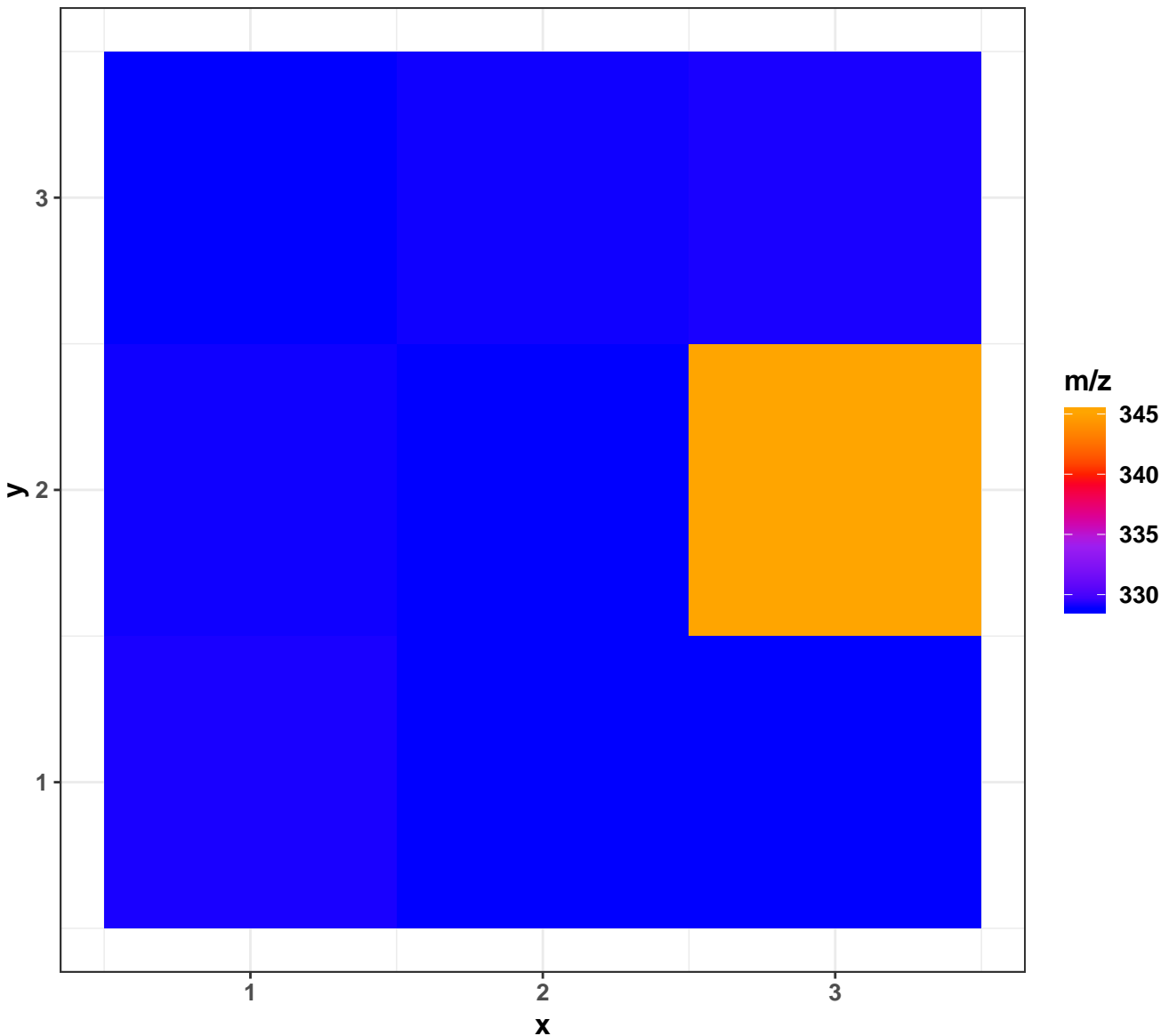




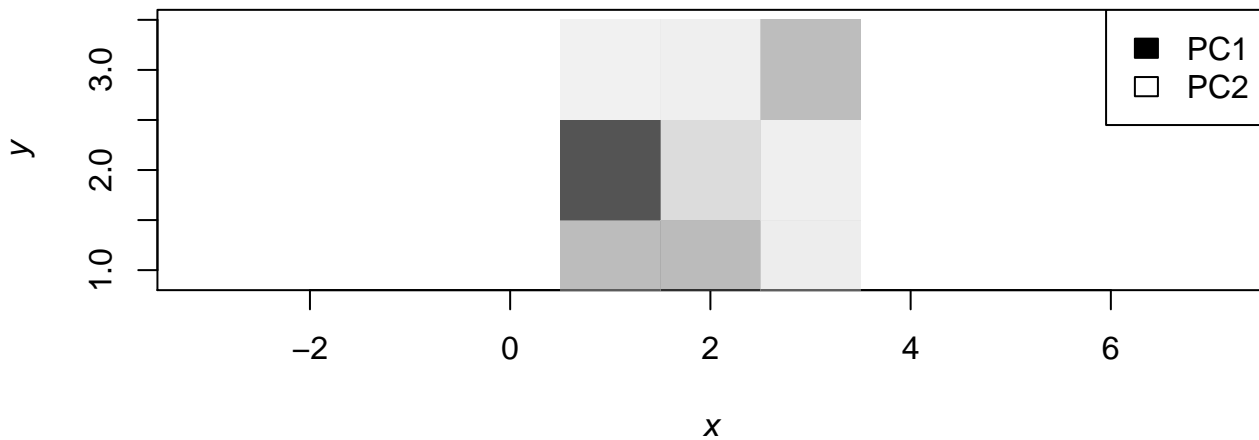
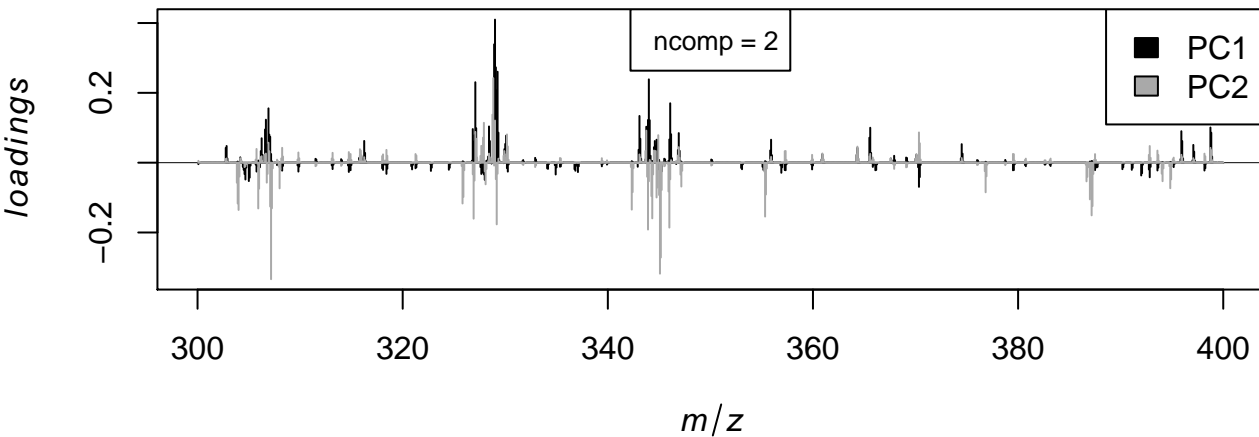
# Median intensity per pixel



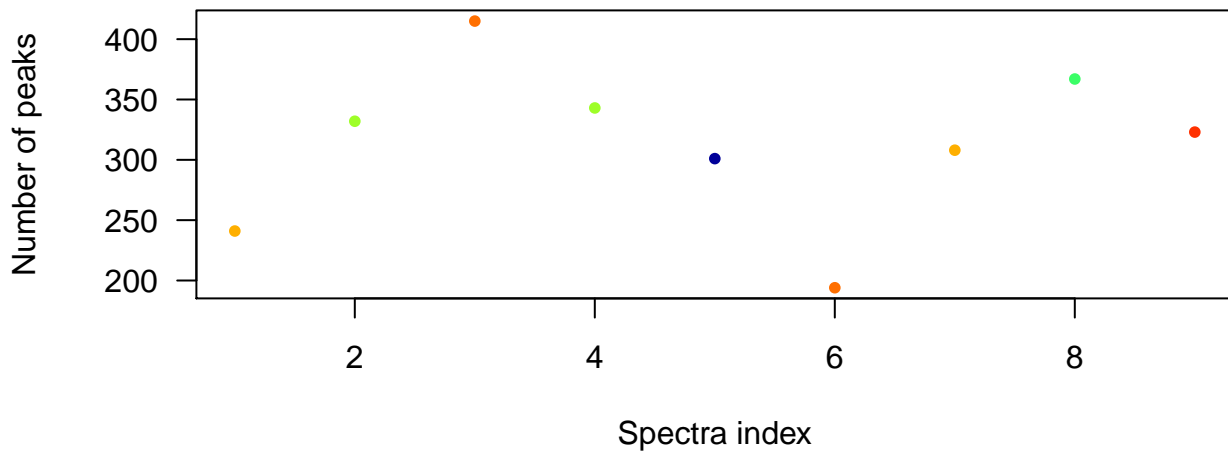
# Most abundant m/z in each spectrum



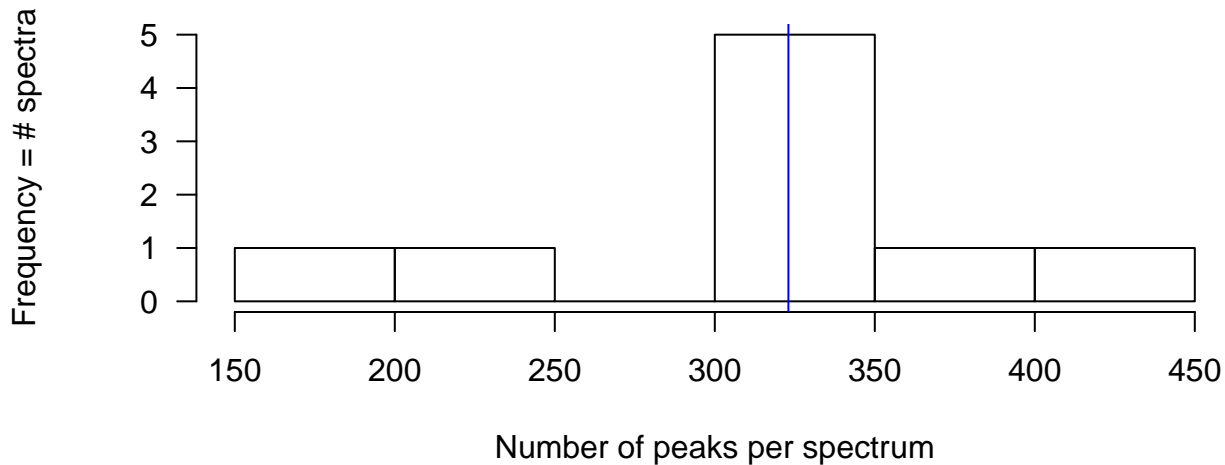
# PCA for two components

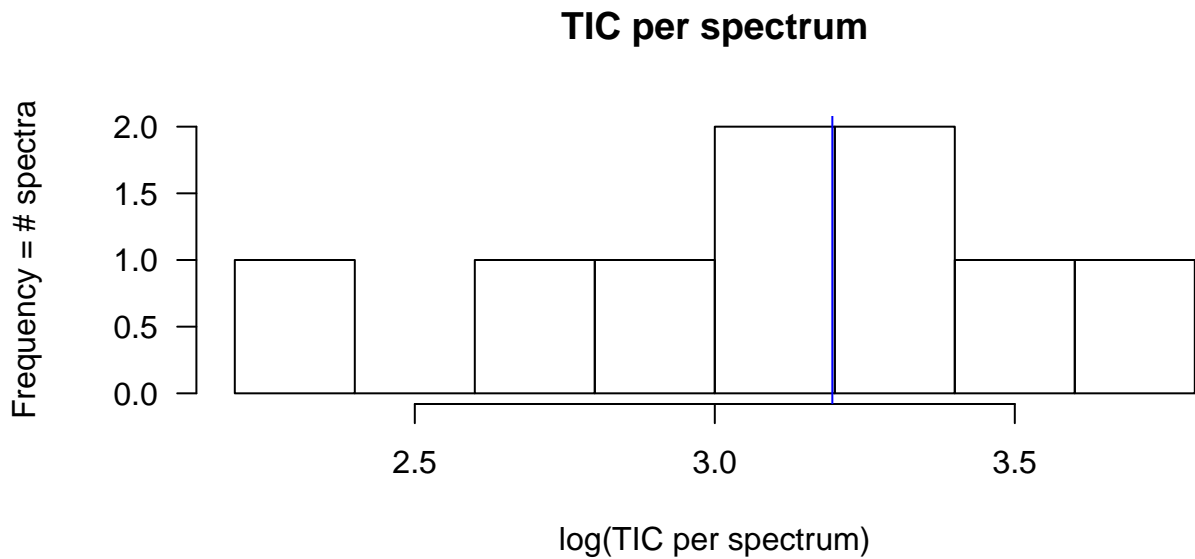
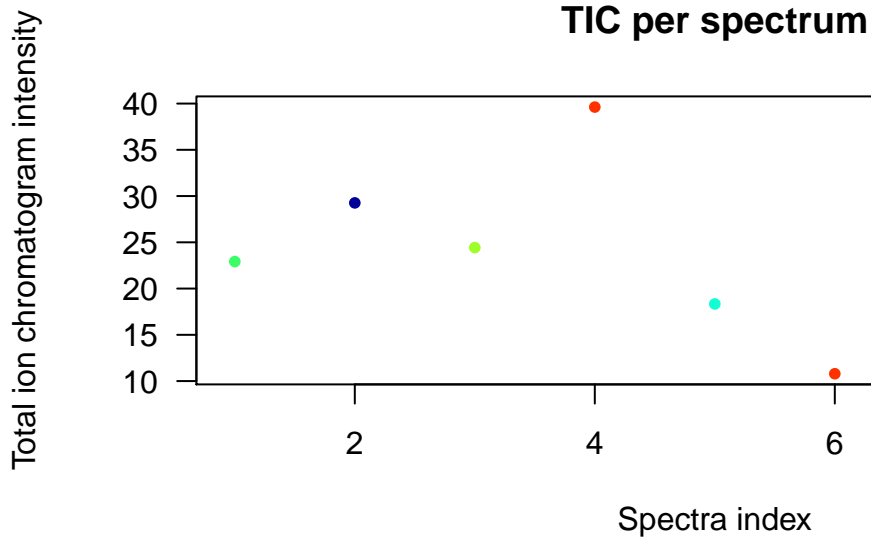


### Number of peaks per spectrum

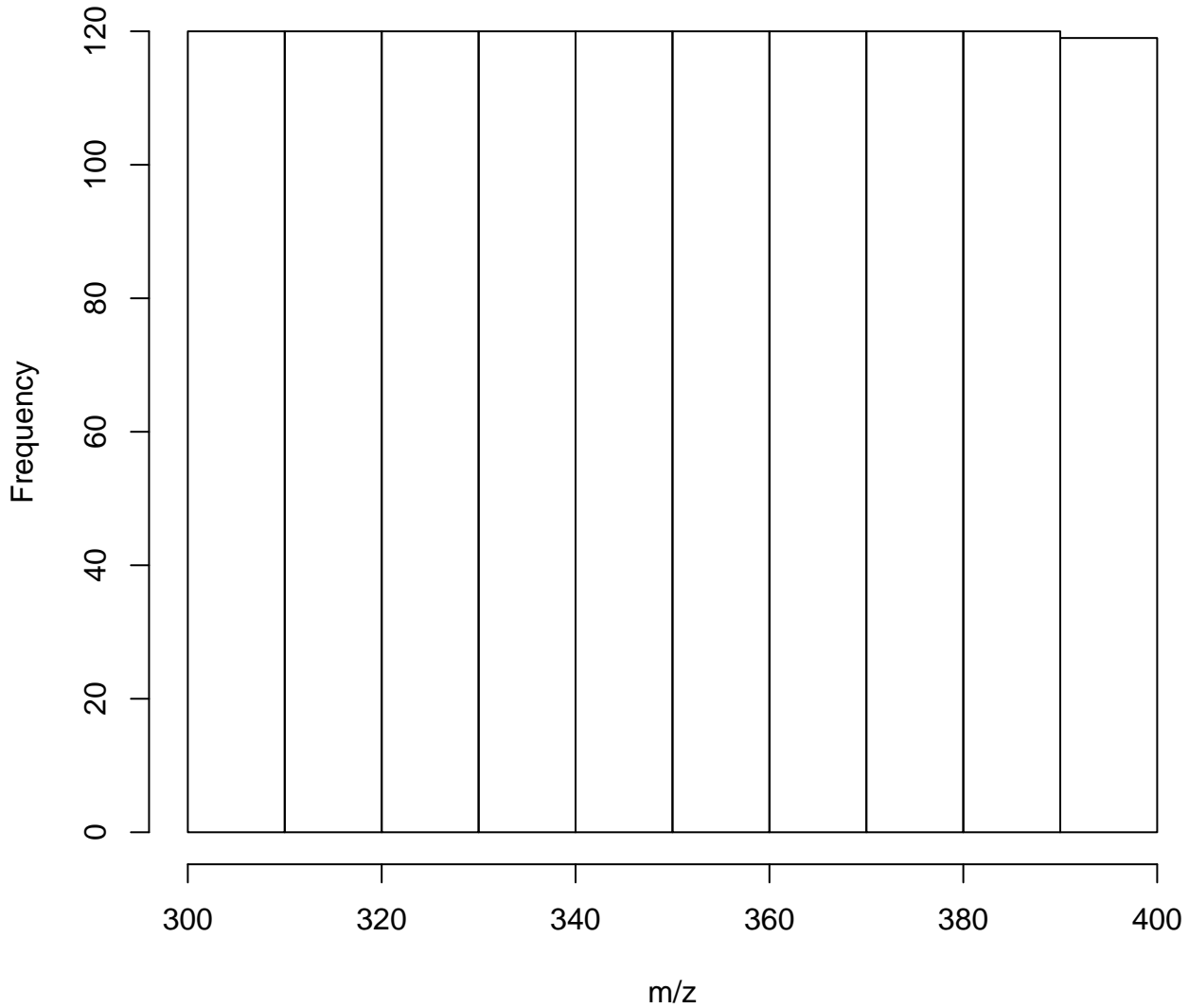


### Number of peaks per spectrum

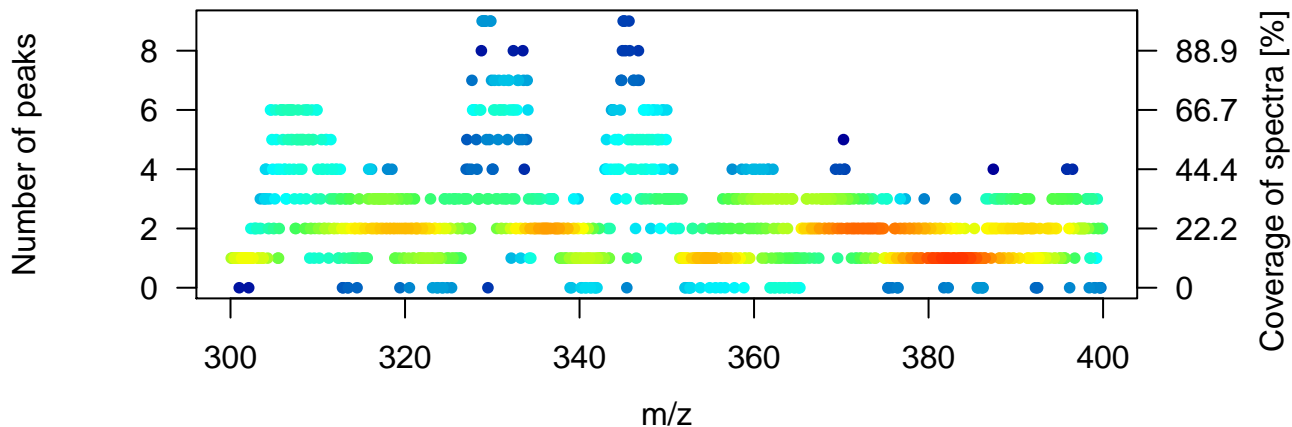




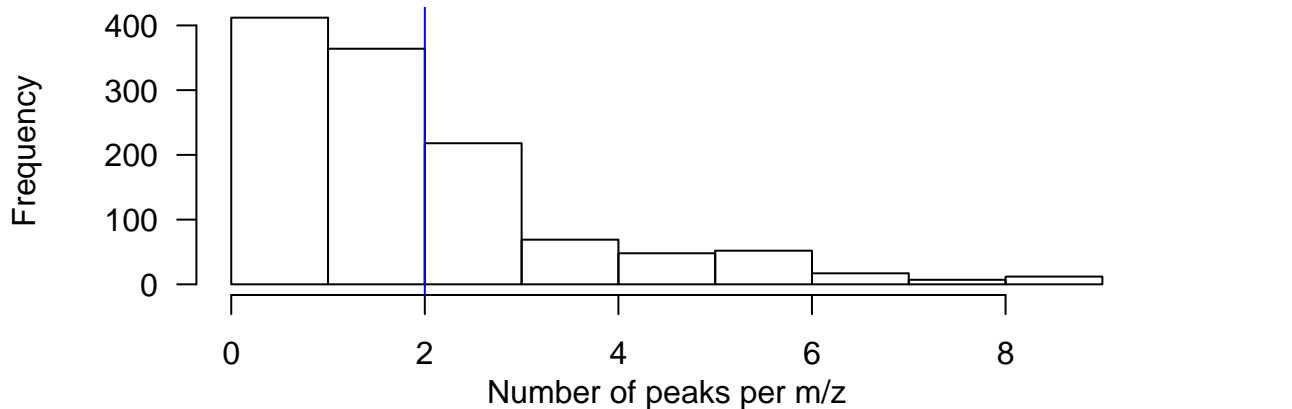
# Histogram of m/z values



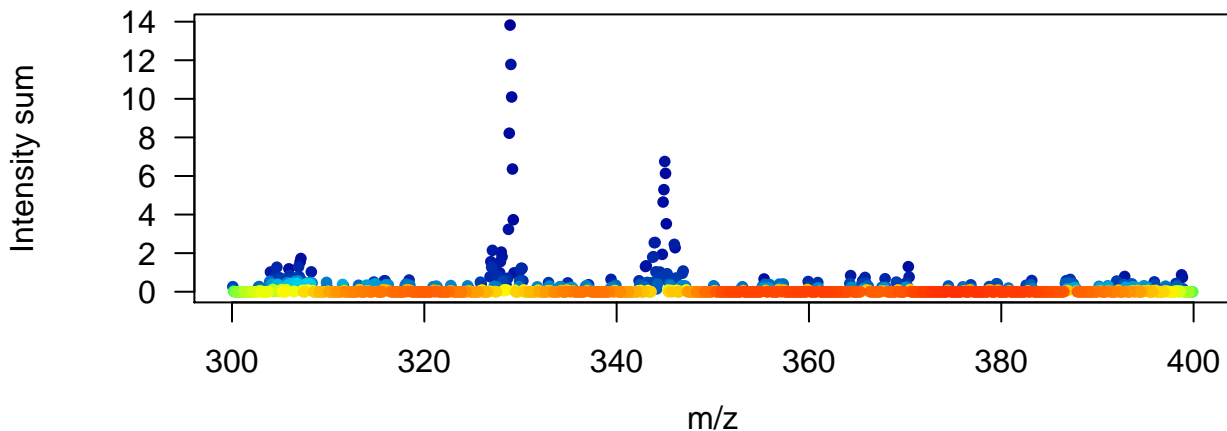
### Number of peaks per m/z



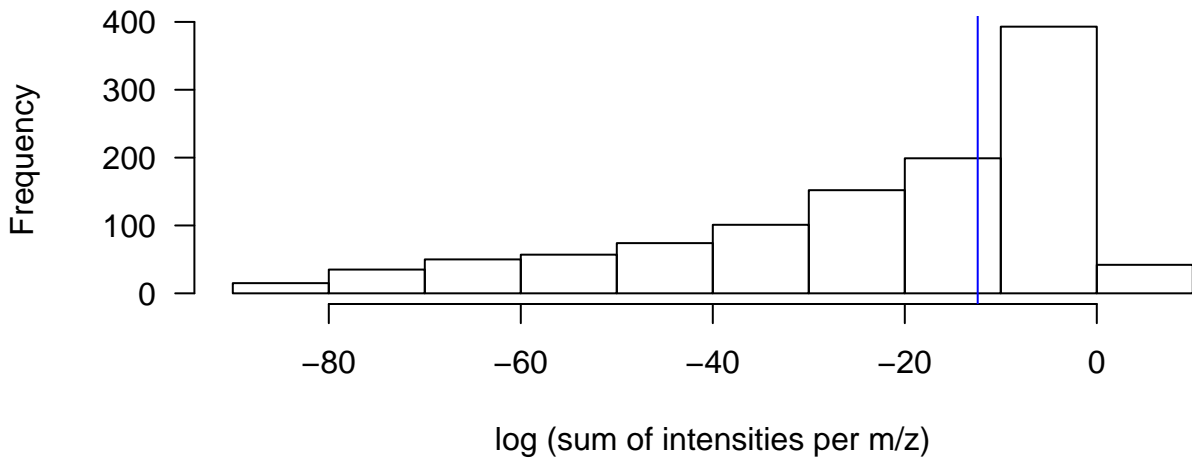
### Number of peaks per m/z



### Sum of intensities per m/z

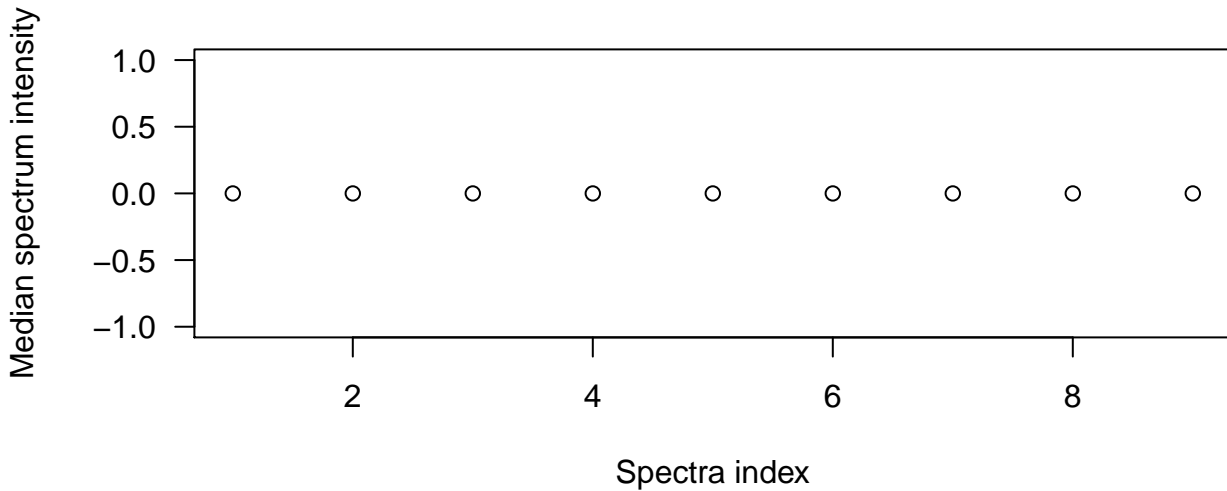


### Sum of intensities per m/z

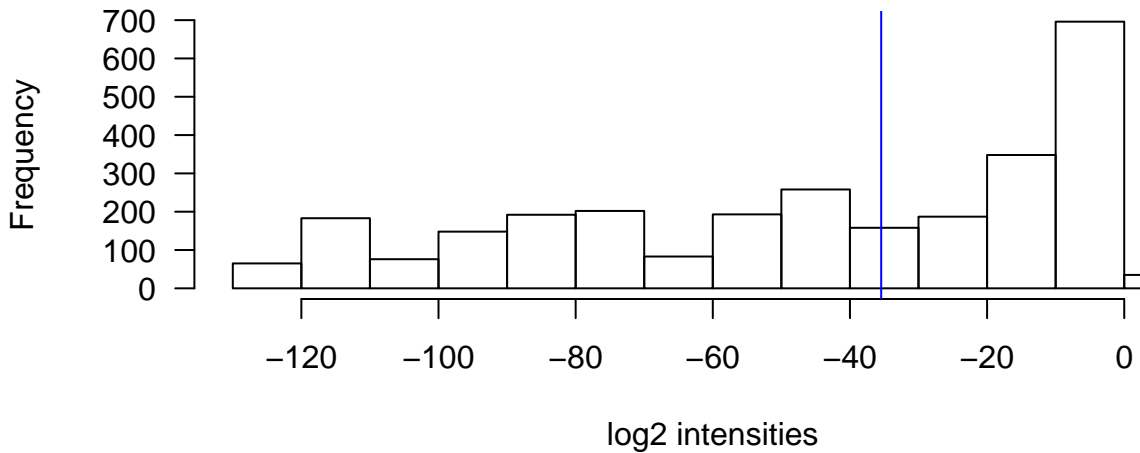




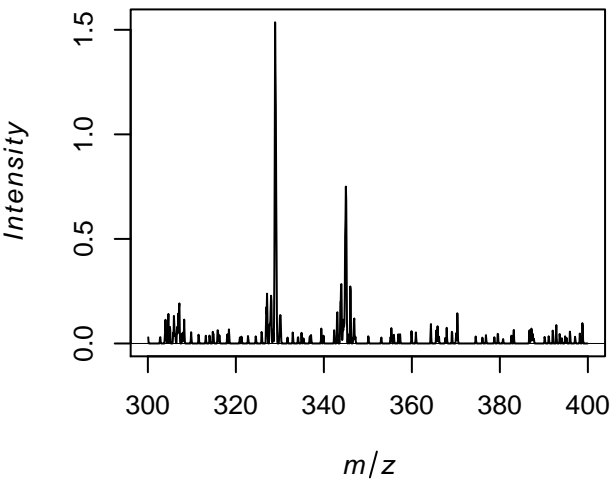
### Median intensity per spectrum



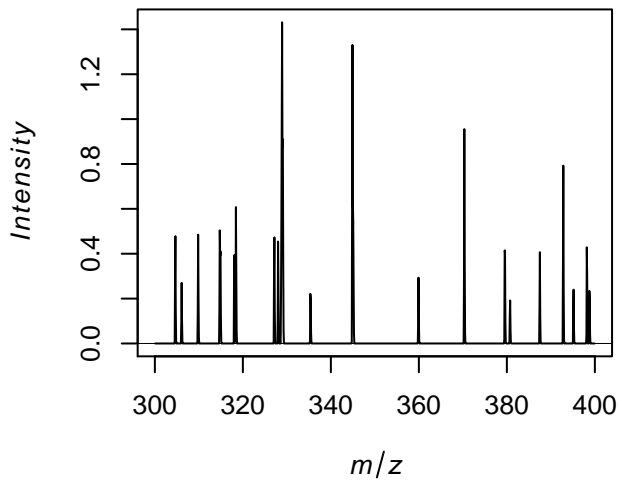
### Log2-transformed intensities



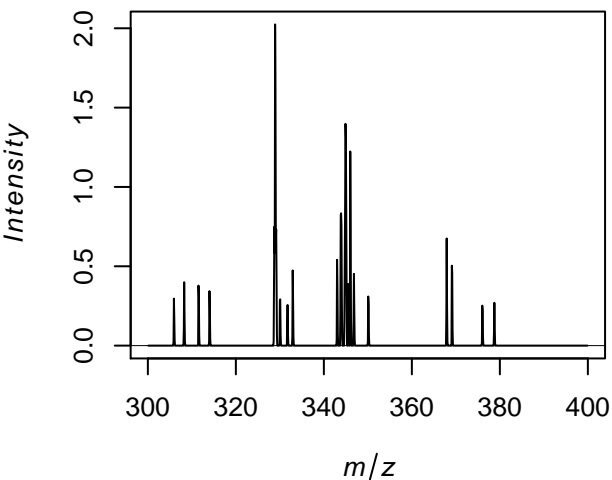
**Average spectrum**



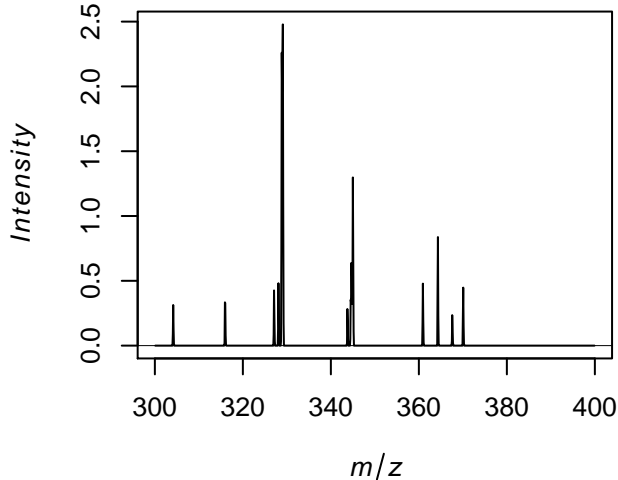
**Spectrum at x = 3, y = 1**



**Spectrum at x = 2, y = 1**



**Spectrum at x = 1, y = 1**

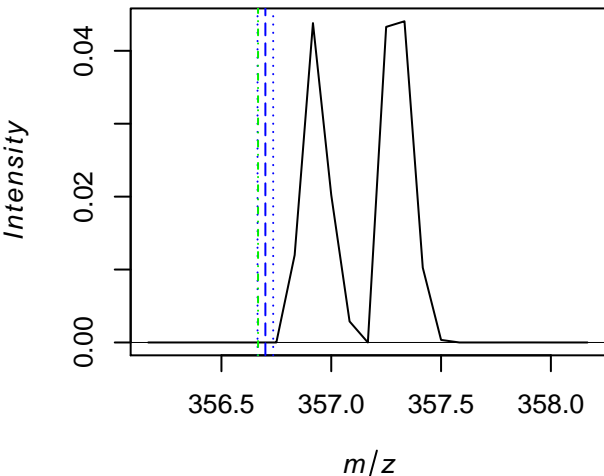


theor. m/z: 356.7

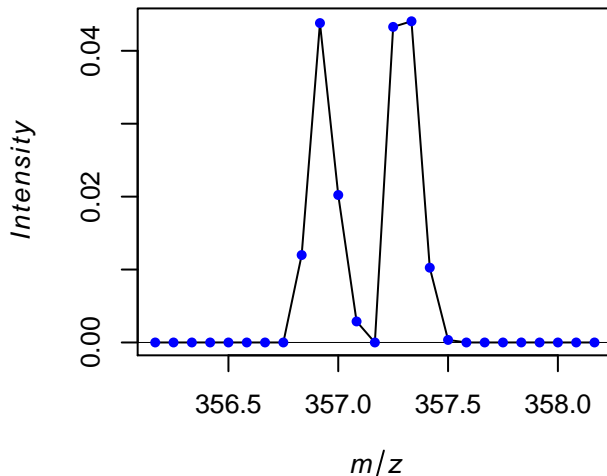
most abundant m/z: NA

closest m/z: 356.667

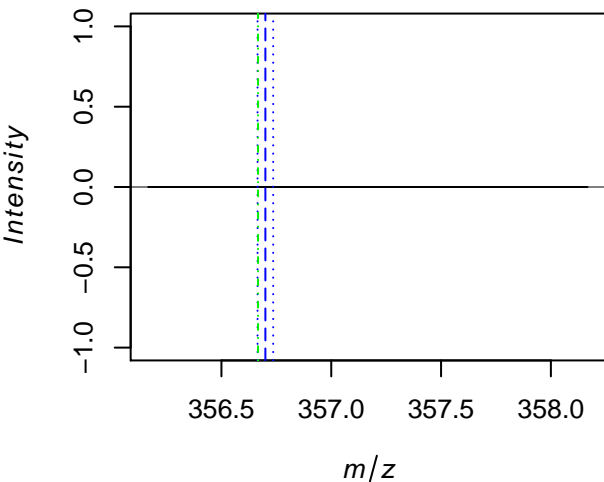
Average spectrum



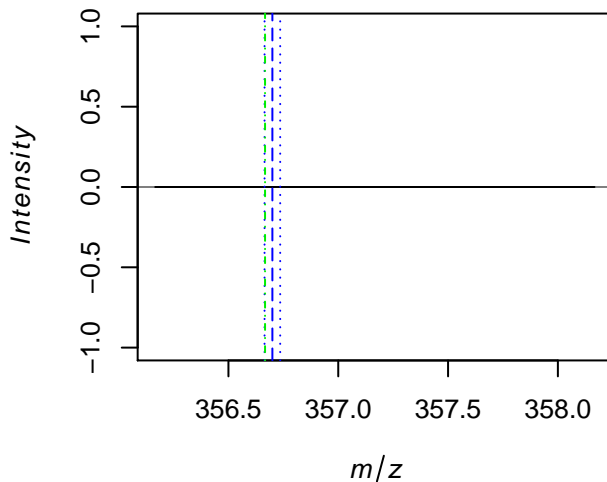
Average spectrum with data points



Spectrum at x = 2, y = 1

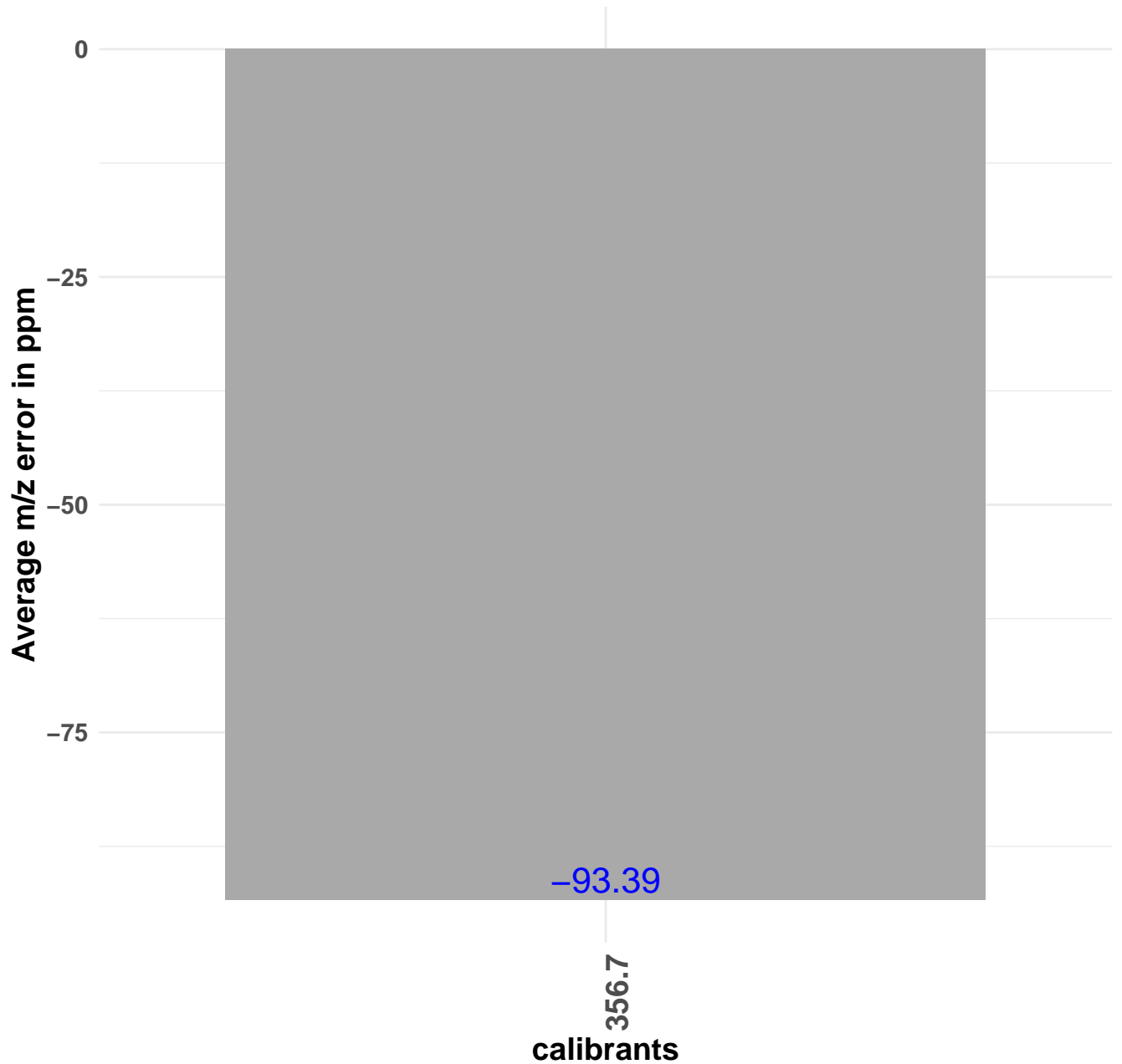


Spectrum at x = 1, y = 1



**plot 17: no peaks in the chosen region, repeat with higher ppm range**

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



**plot 19: no peaks in the chosen region, repeat with higher ppm range**