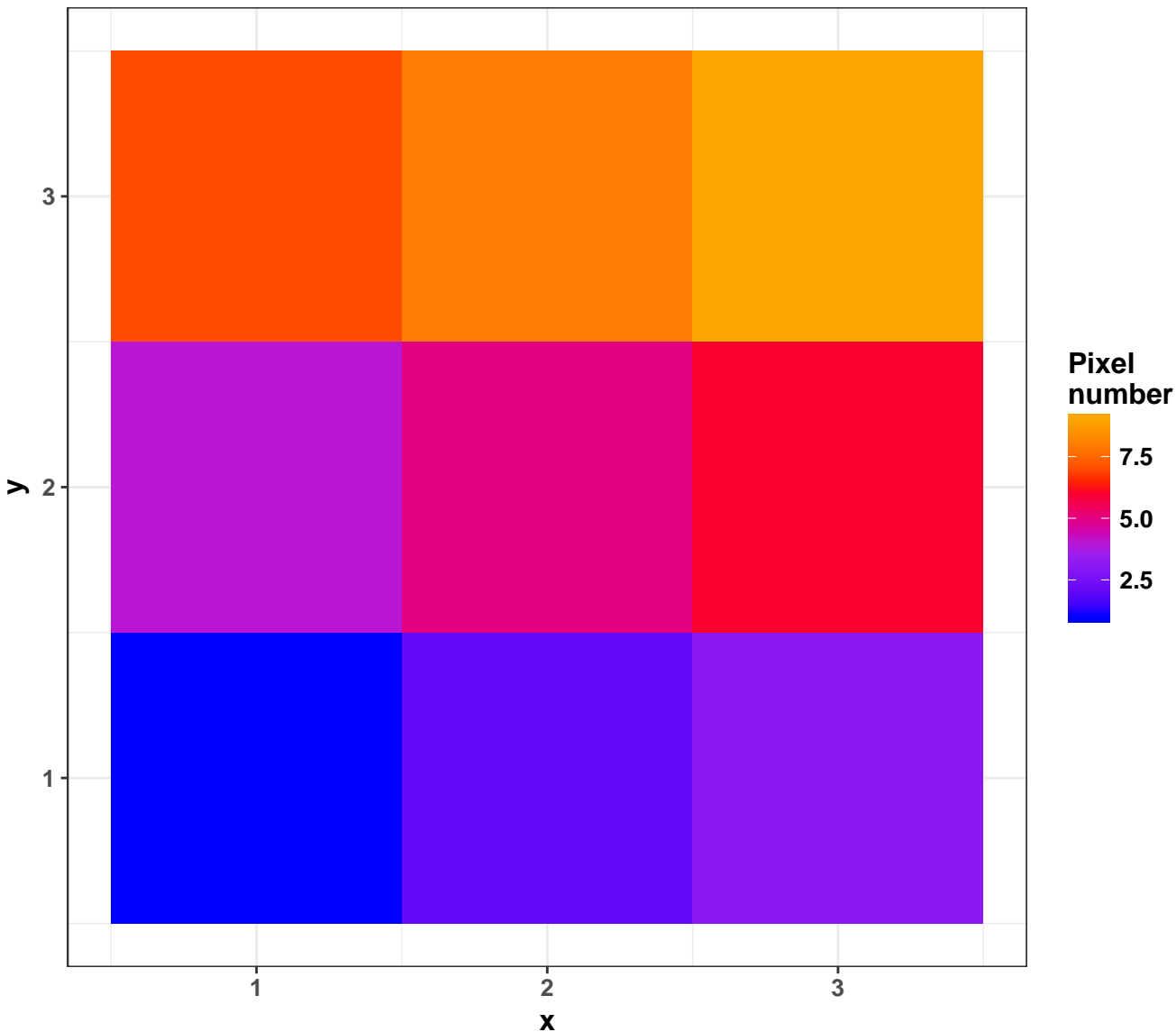


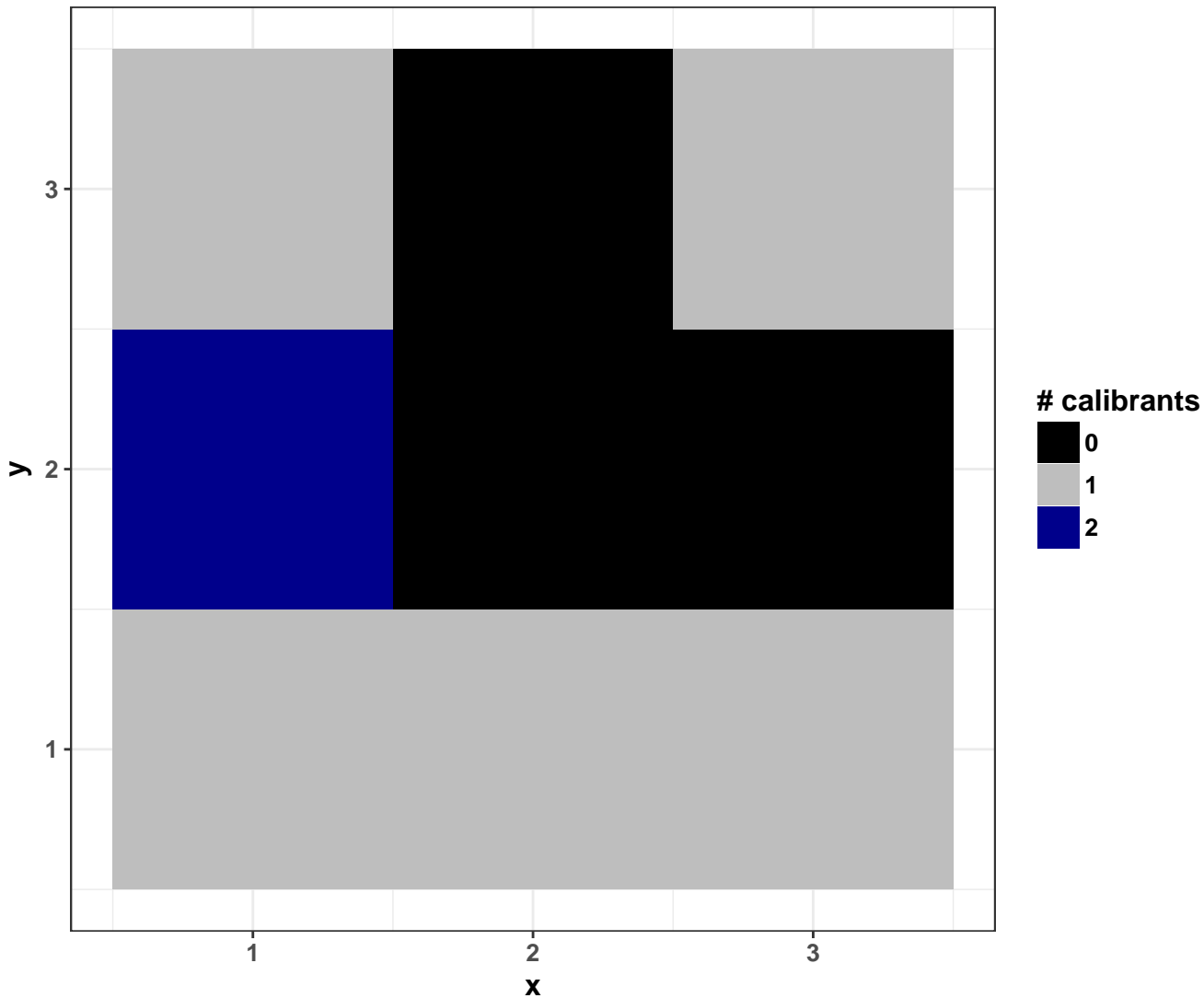
## Testfile\_imzml

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
Median of intensities	0
Intensities > 0	35.16 %
Number of empty spectra	0
Median TIC	161.81
Median # peaks per spectrum	1961
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.txt	3 / 3

# Pixel order

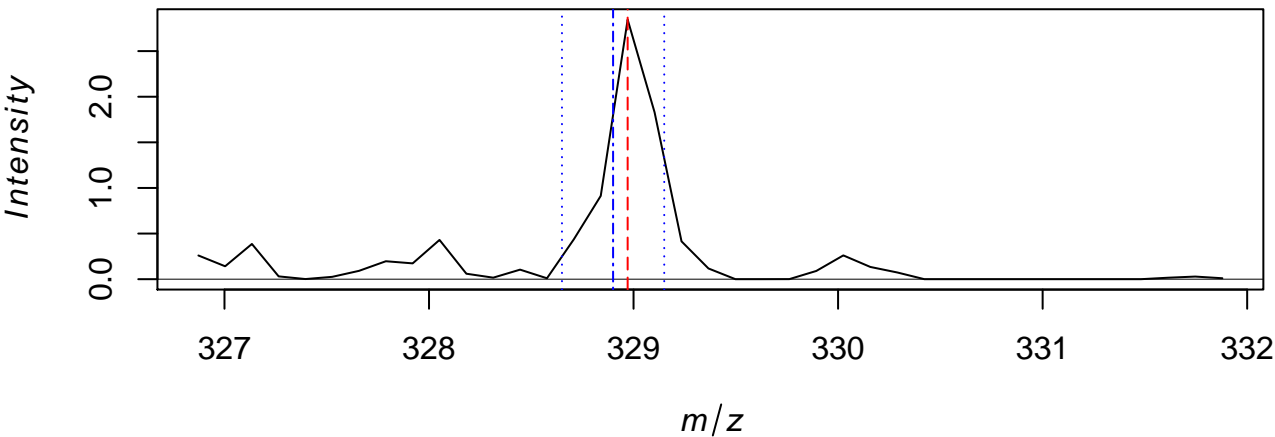


Number of calibrants per pixel ( $\pm 100$  ppm)

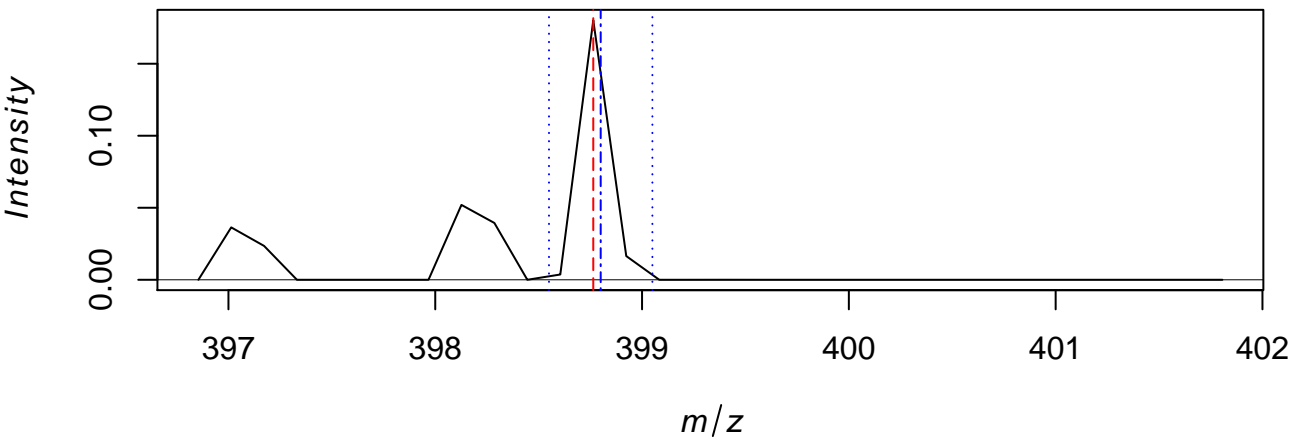


# Control of fold change plot

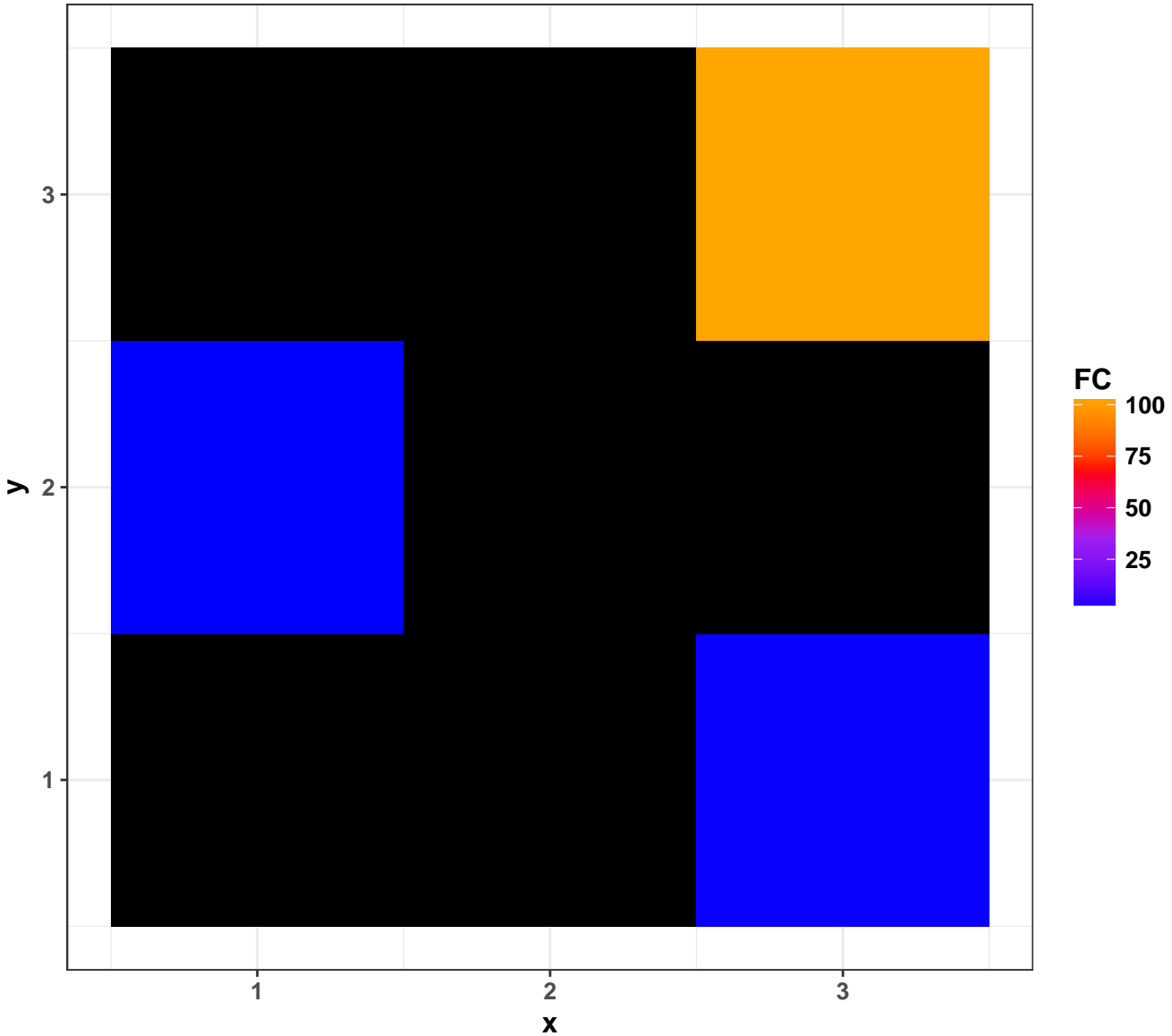
## average spectrum 328.9 Da



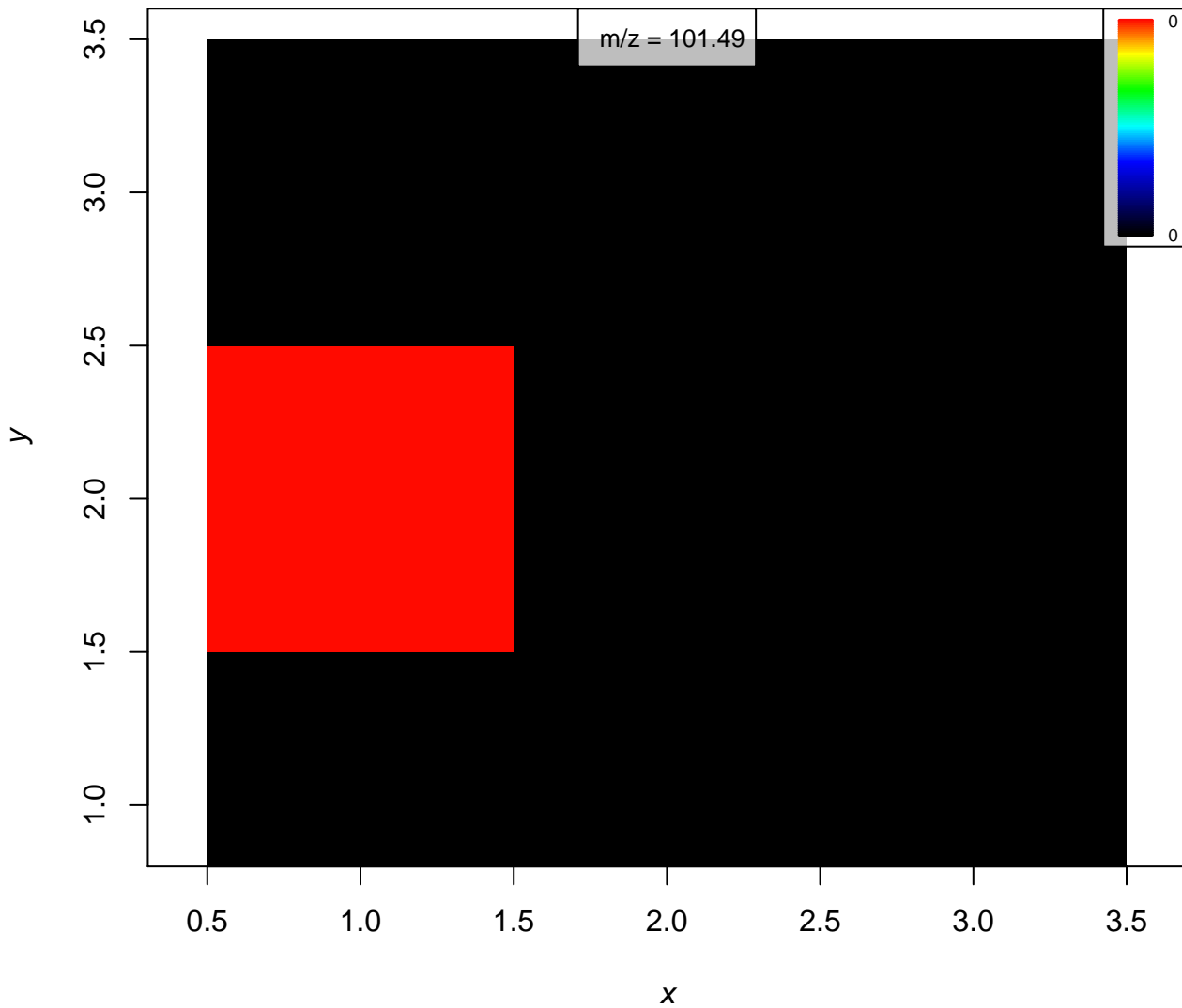
## average spectrum 398.8 Da



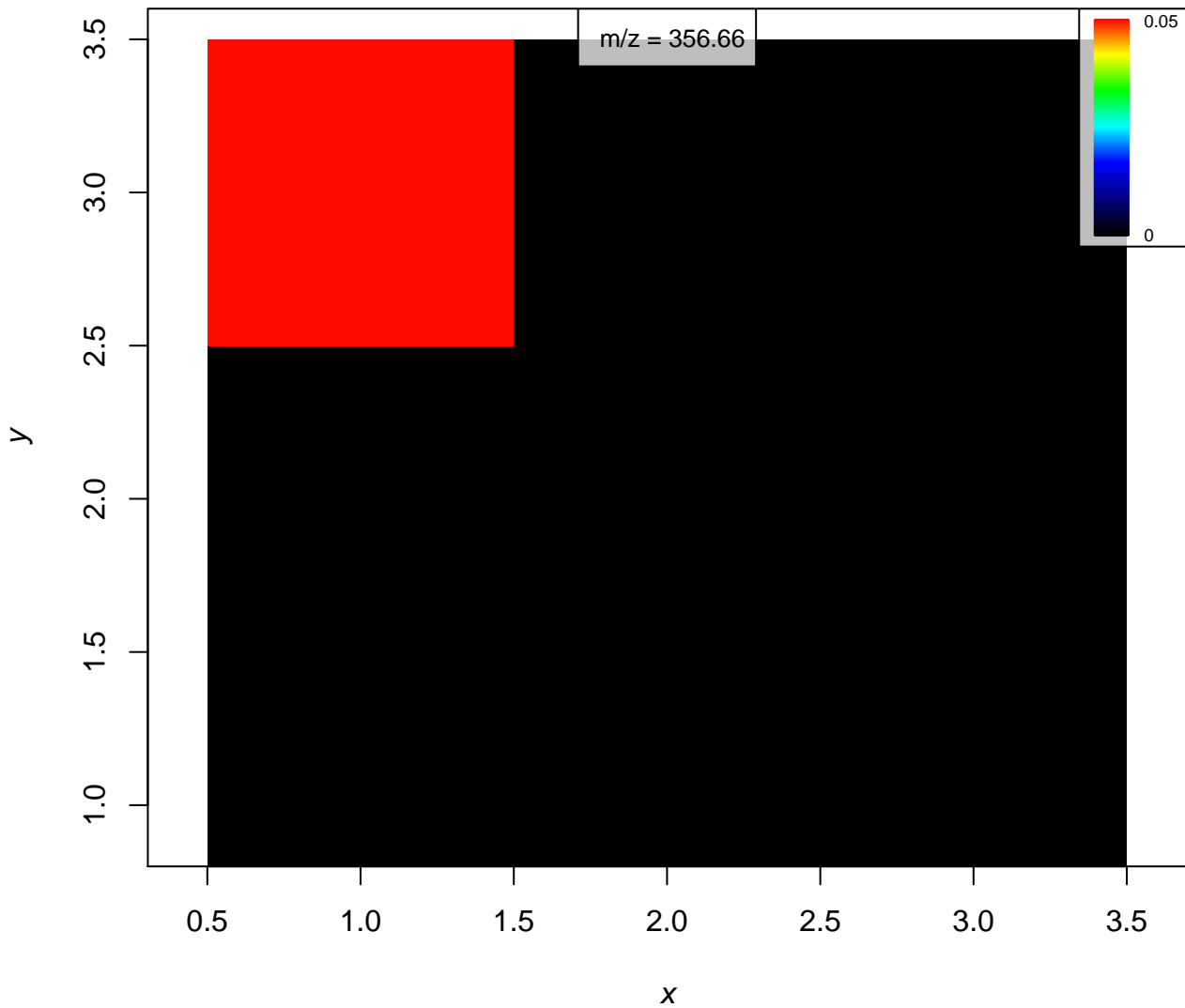
Ratio of mass1 (328.9) / mass2 (398.8)



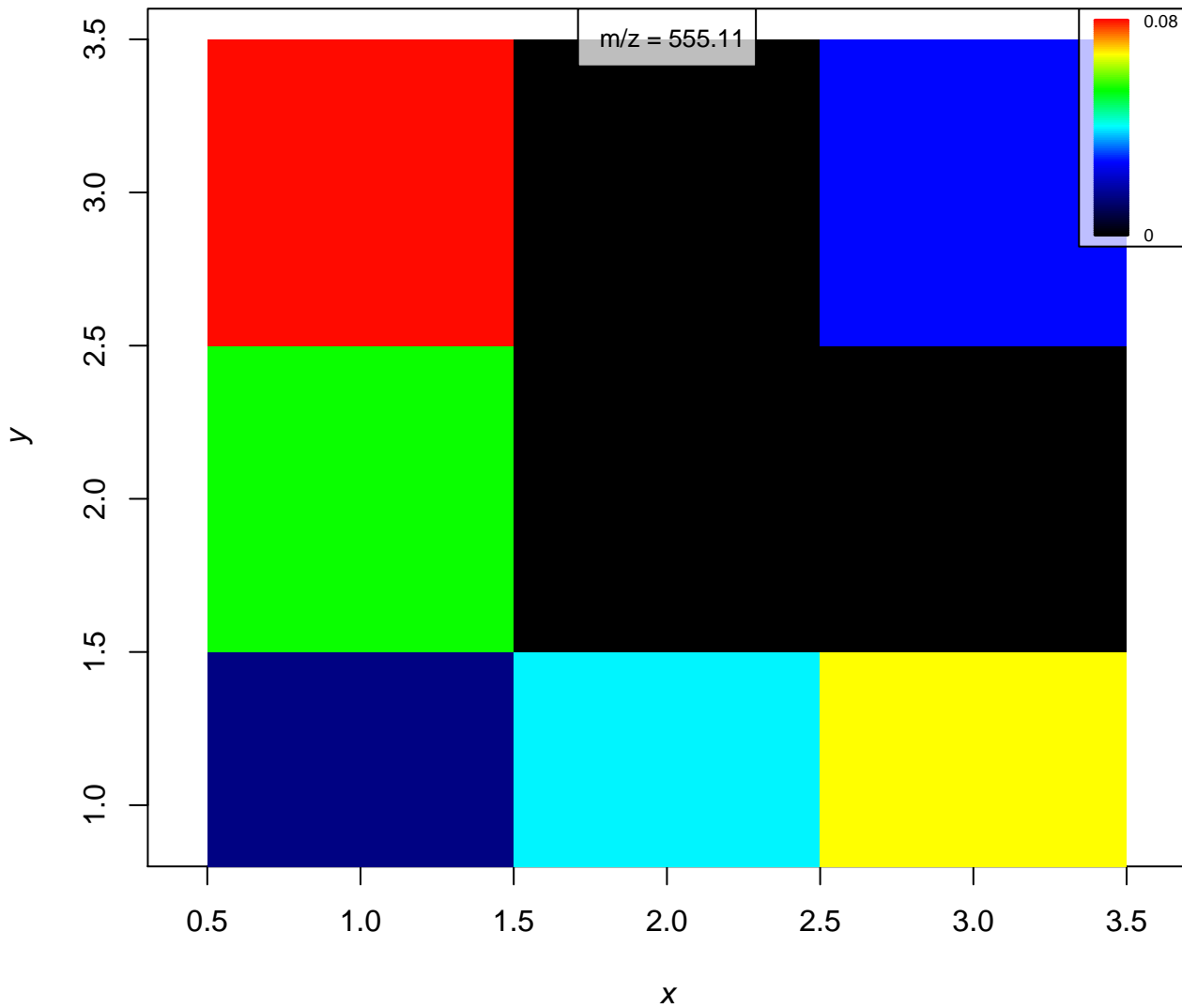
# 101.5: 101.5 ( $\pm 100$ ppm)



356.7: 356.7 ( $\pm 100$  ppm)

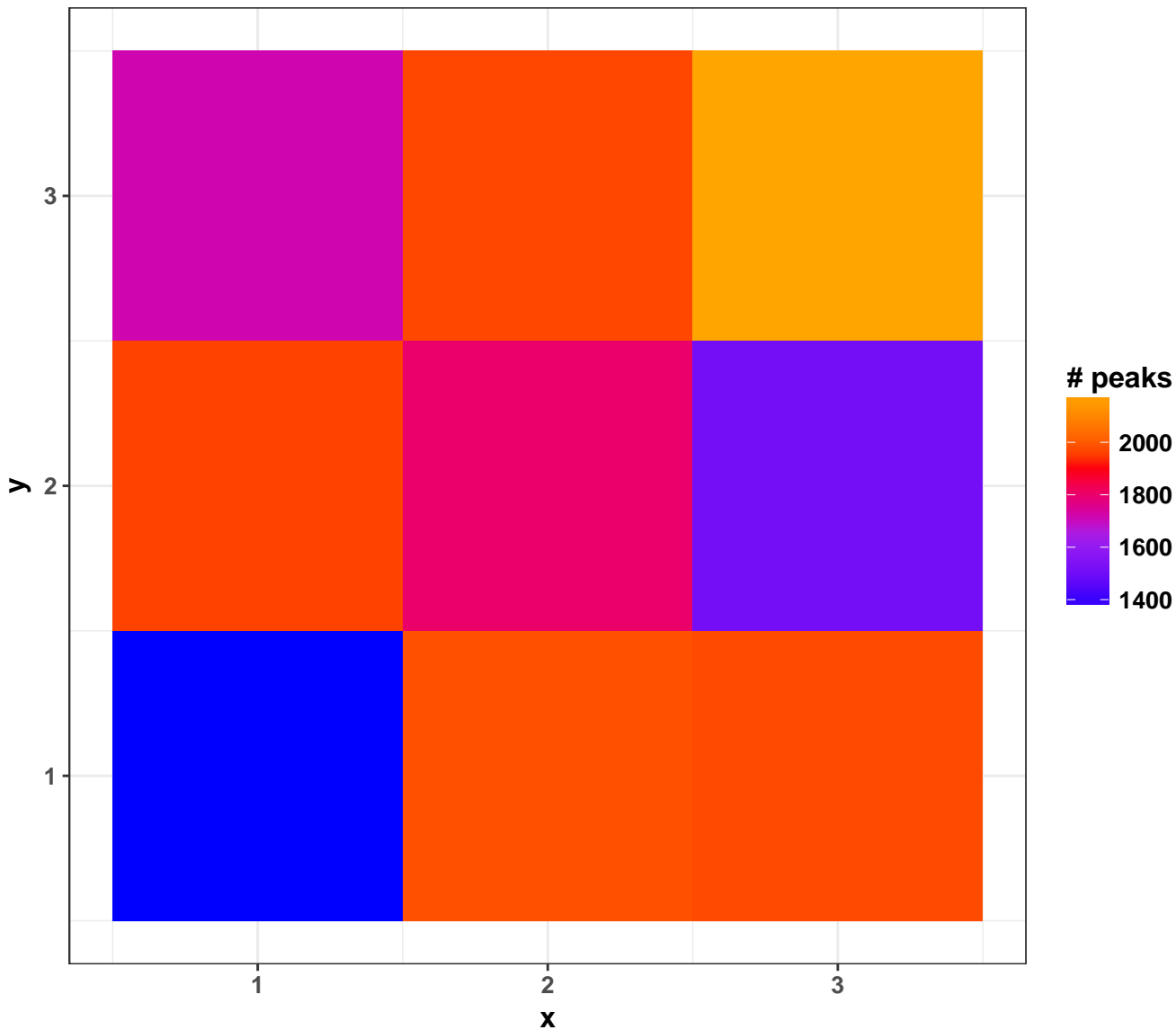


555.1: 555.1 ( $\pm 100$  ppm)

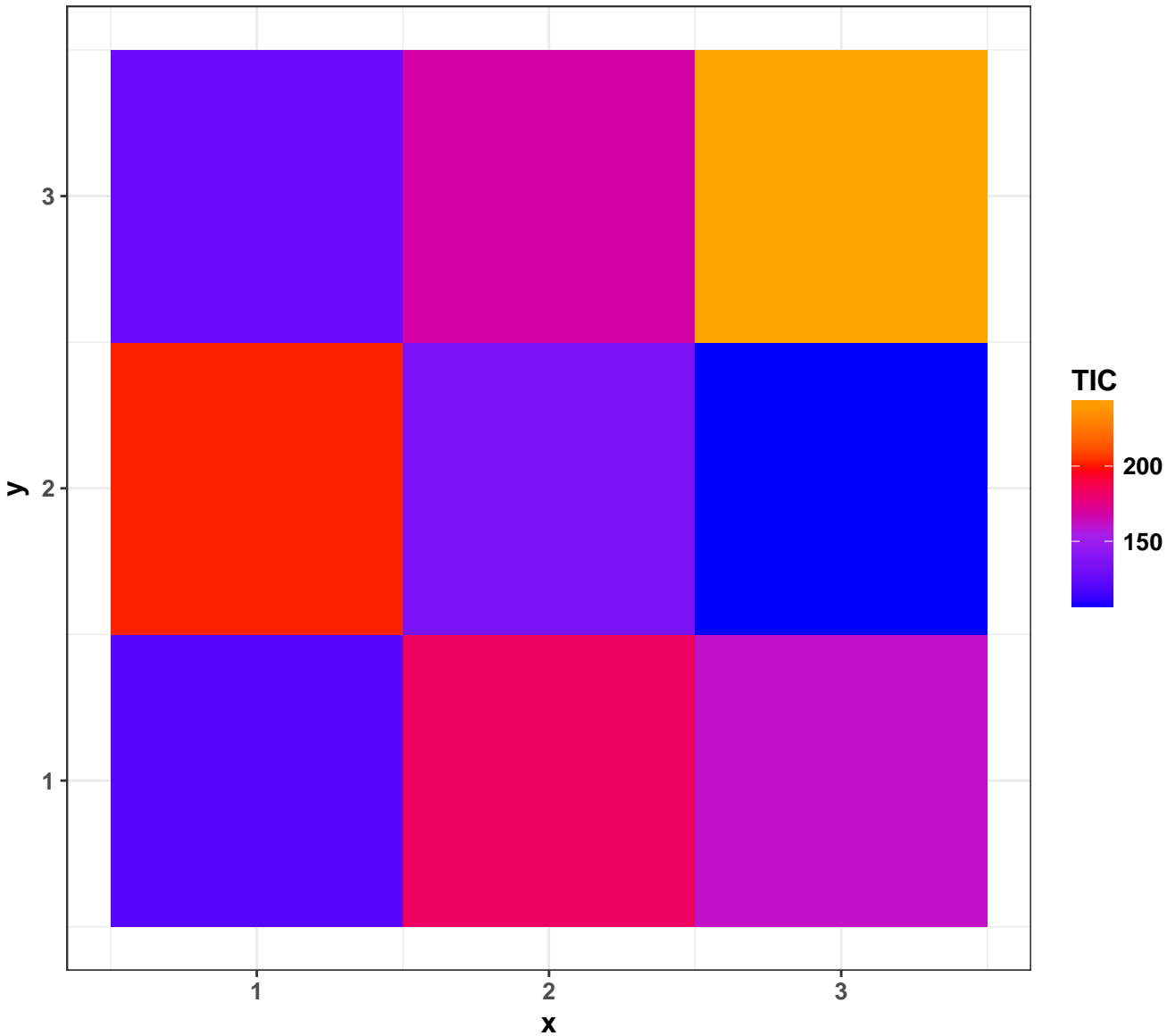




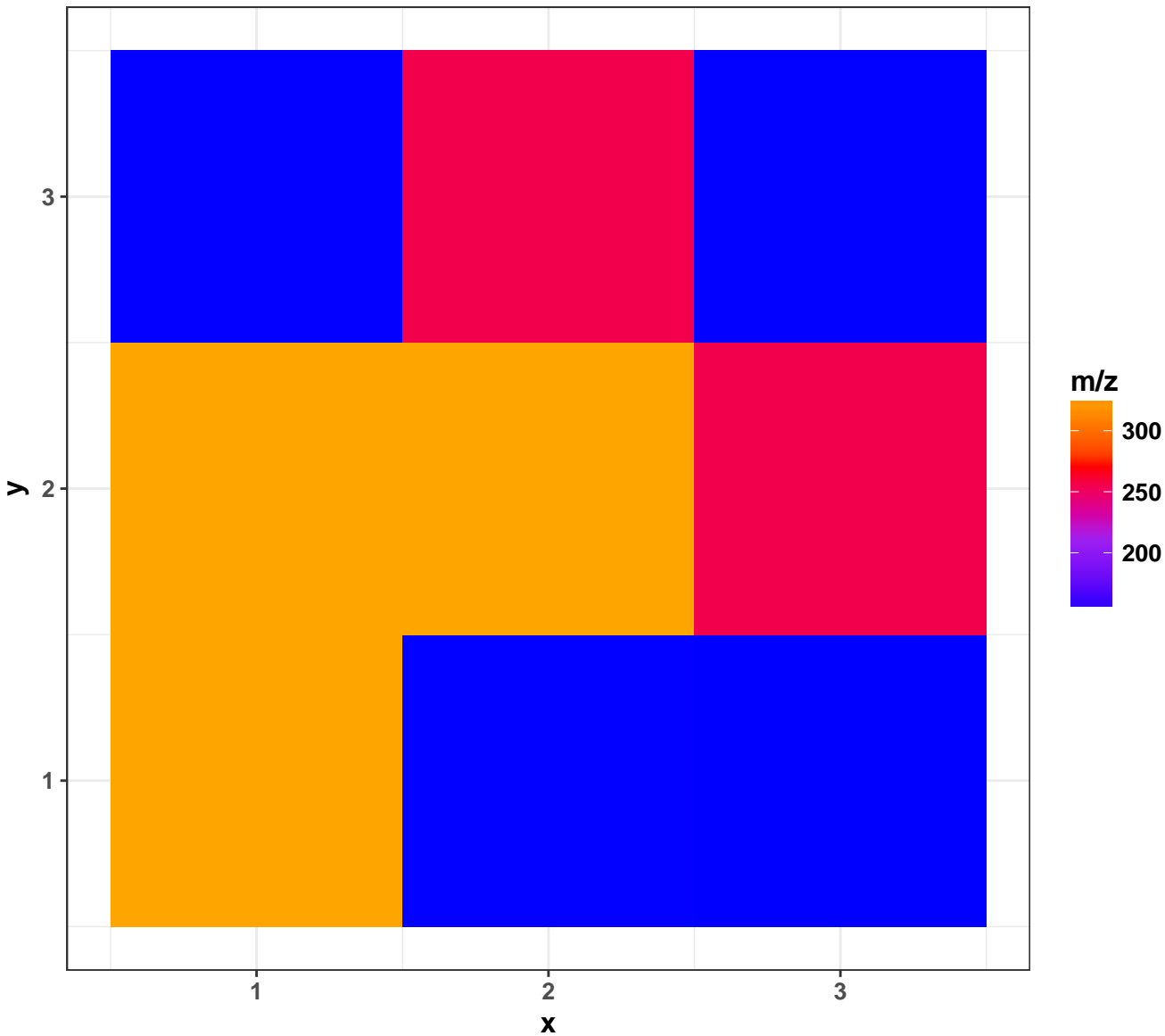
# Number of peaks per spectrum



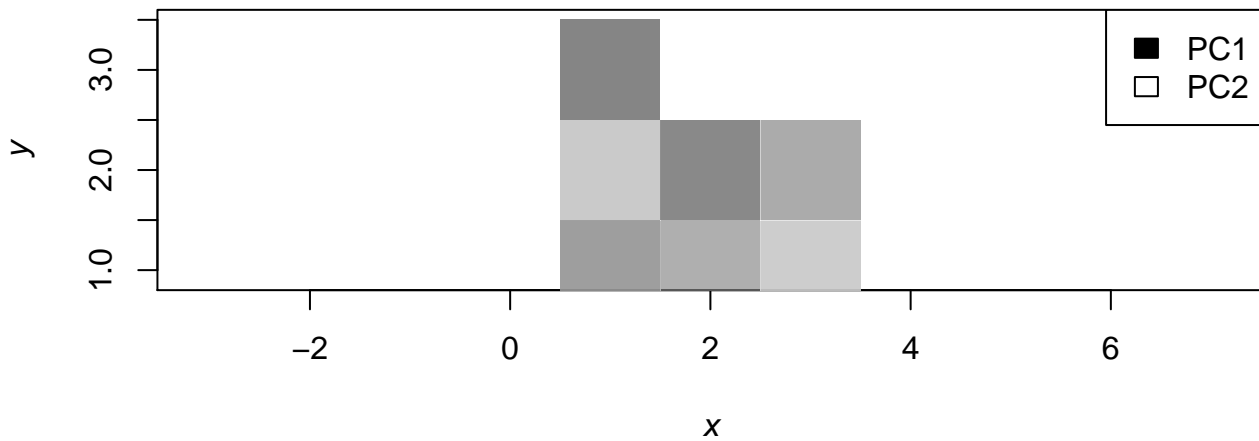
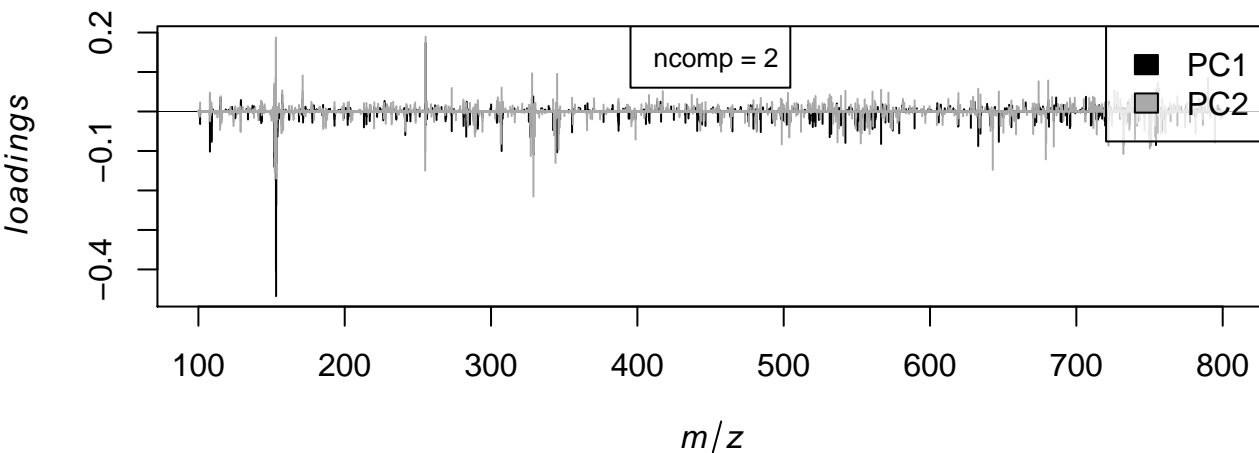
# Total Ion Chromatogram



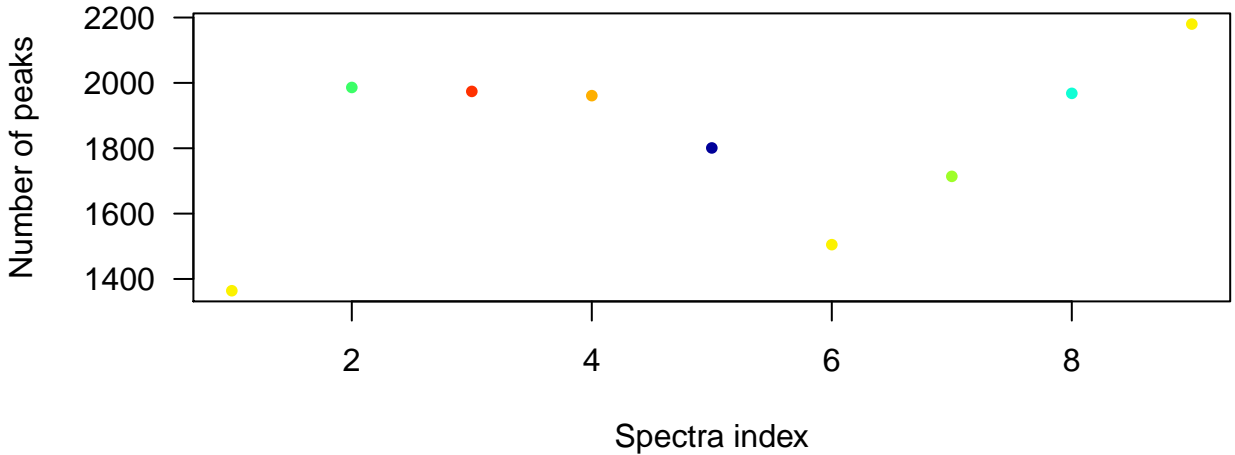
# Most abundant m/z in each spectrum



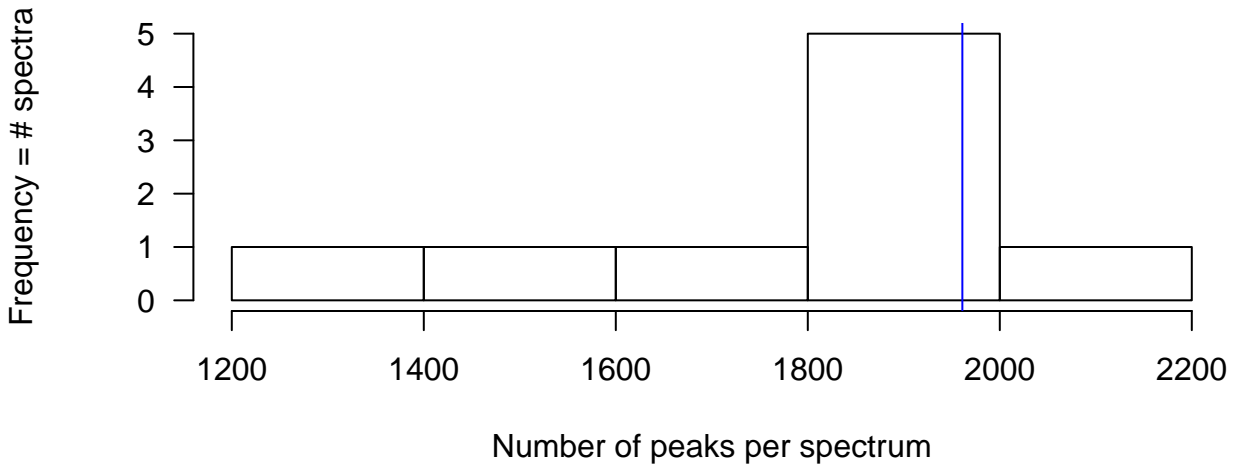
# PCA for two components



### Number of peaks per spectrum

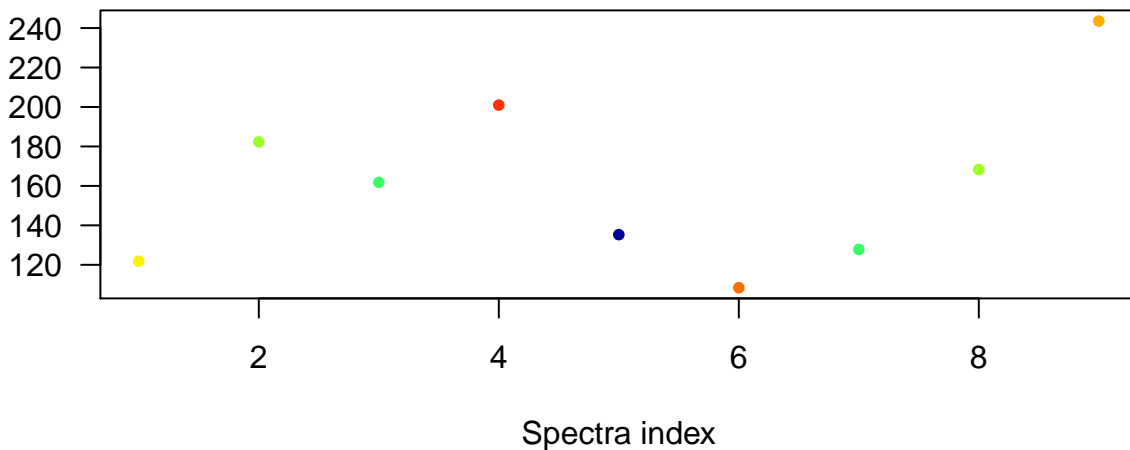


### Number of peaks per spectrum



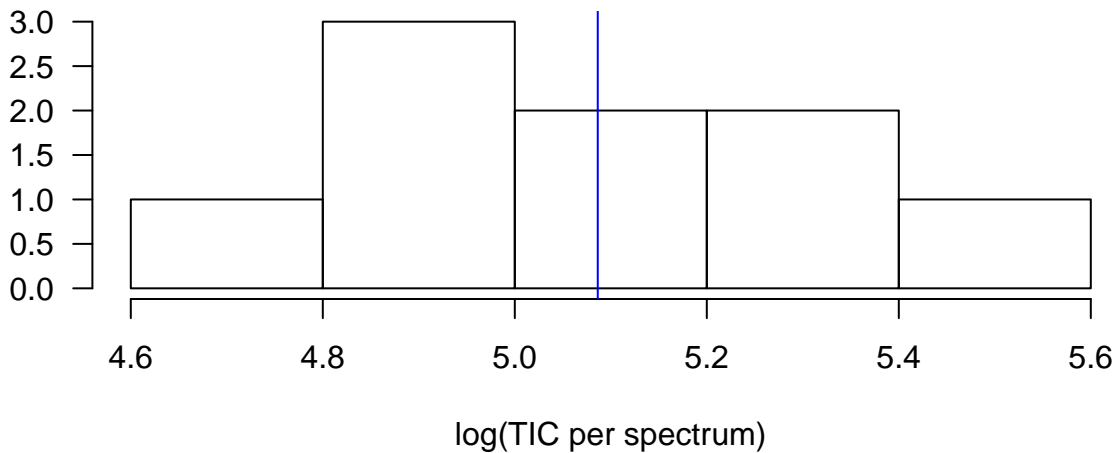
Total ion chromatogram intensity

TIC per spectrum

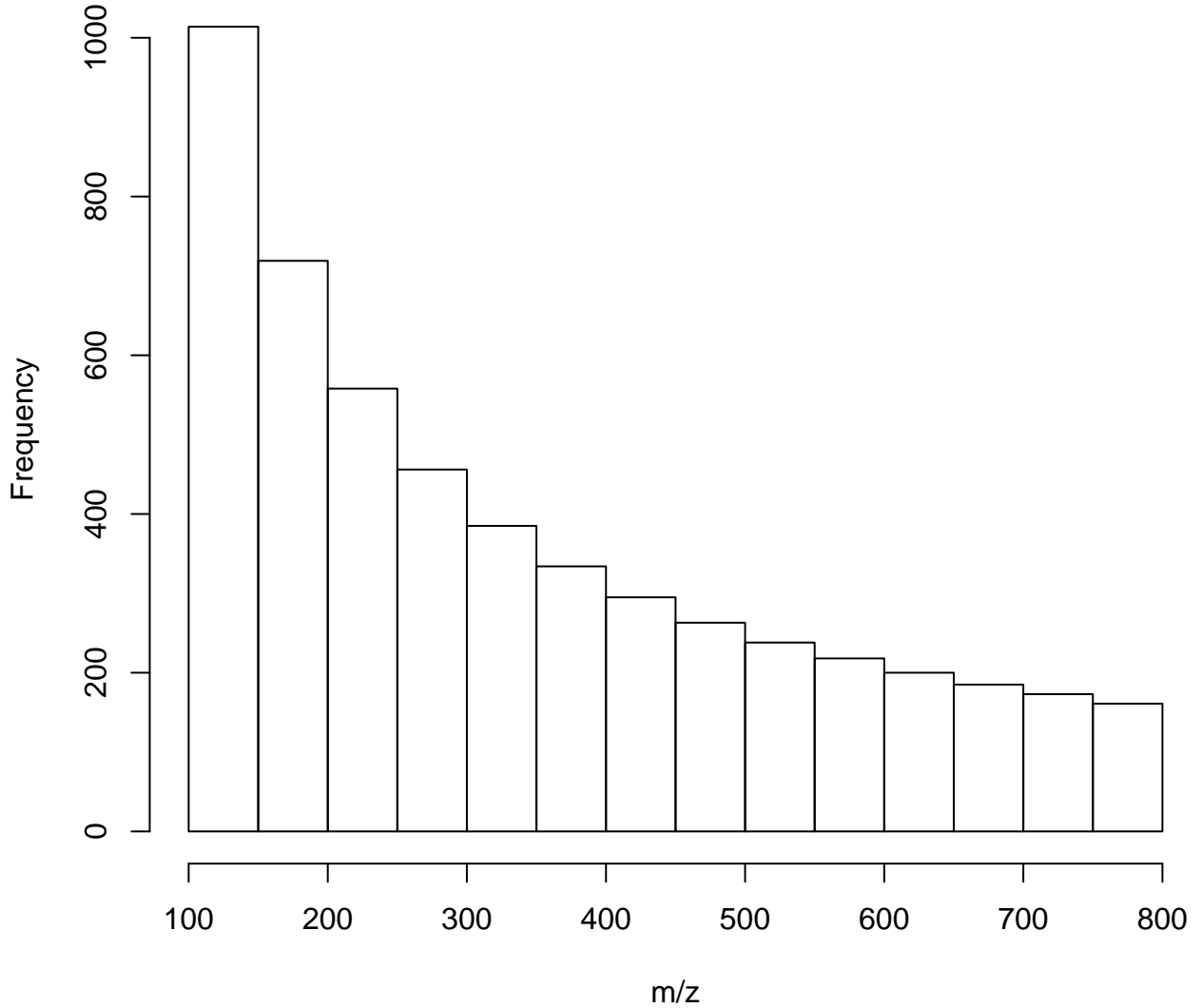


Frequency = # spectra

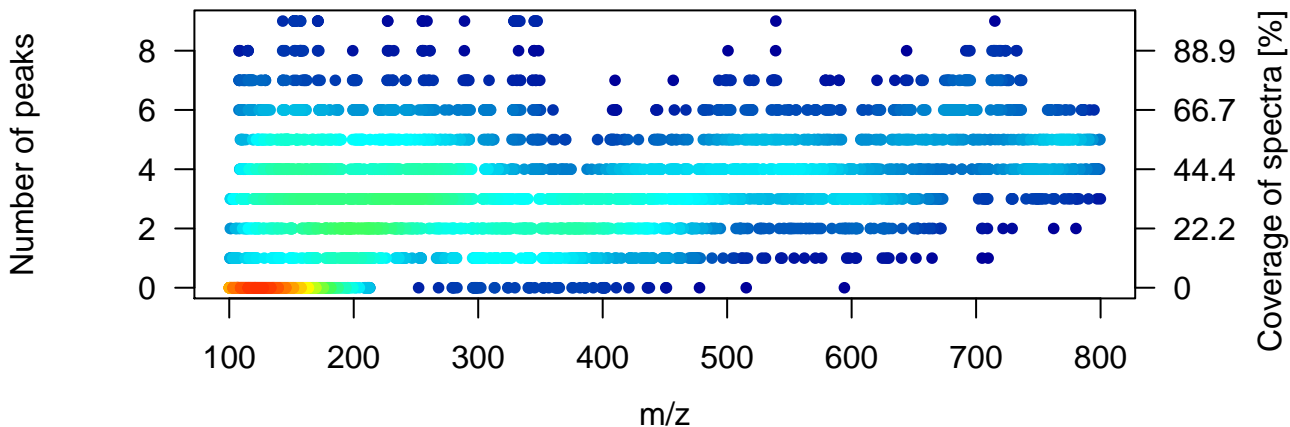
TIC per spectrum



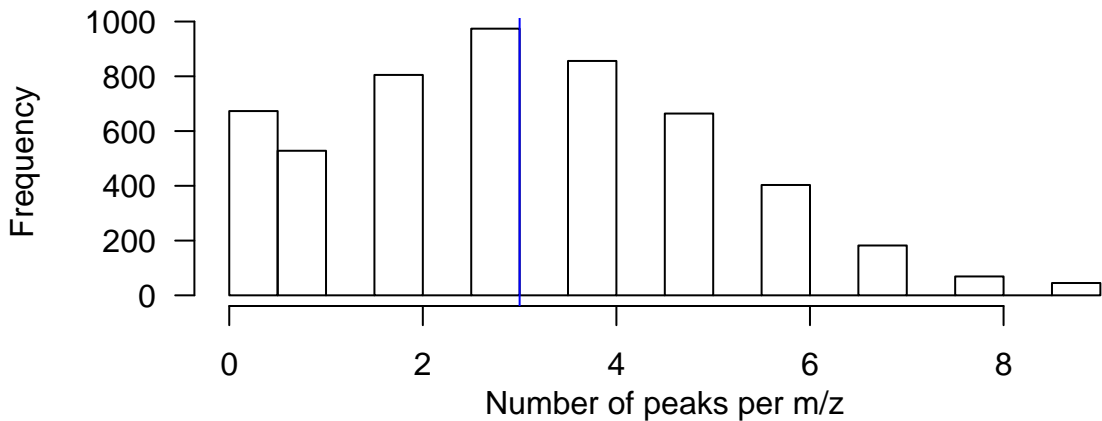
Histogram of m/z values



### Number of peaks per m/z

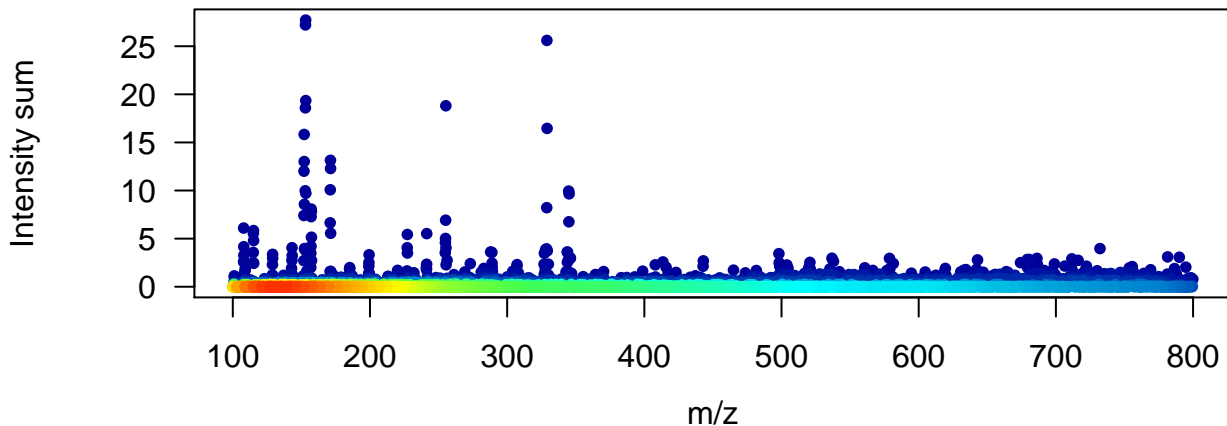


### Number of peaks per m/z

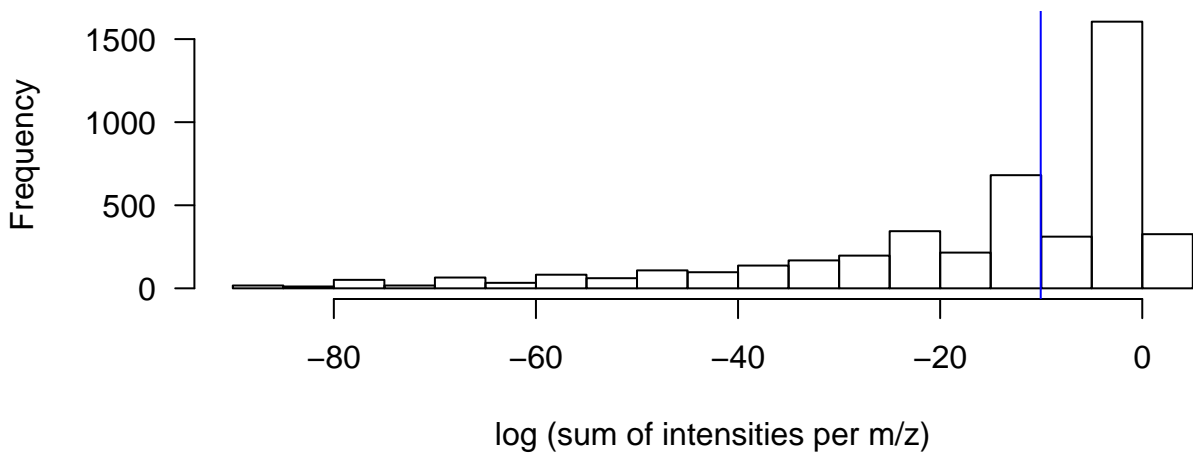




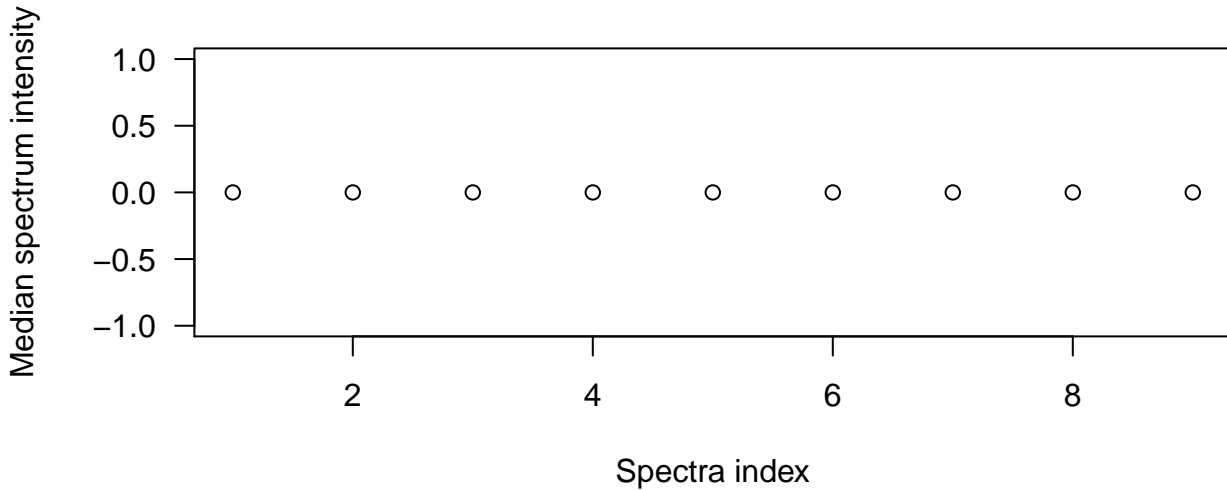
### Sum of intensities per m/z



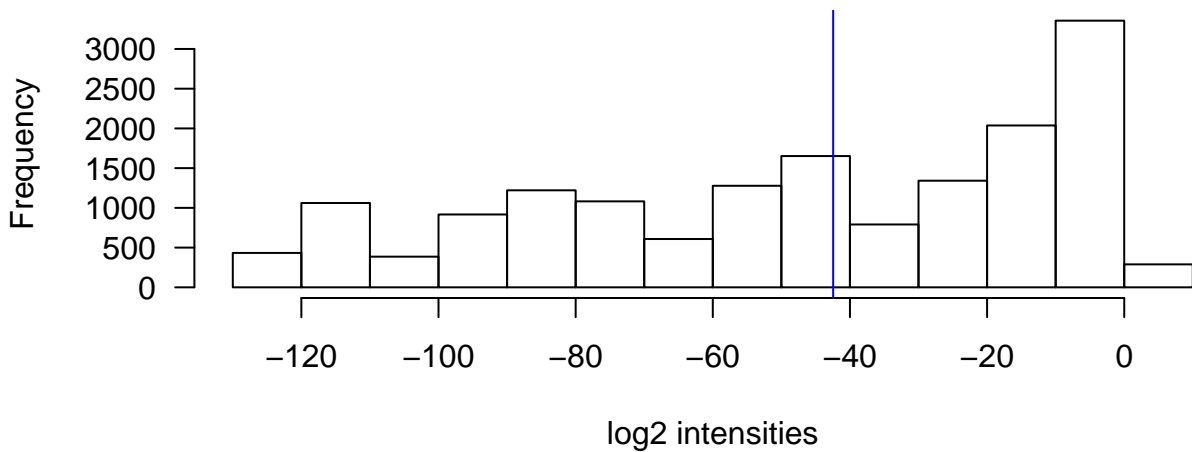
### Sum of intensities per m/z



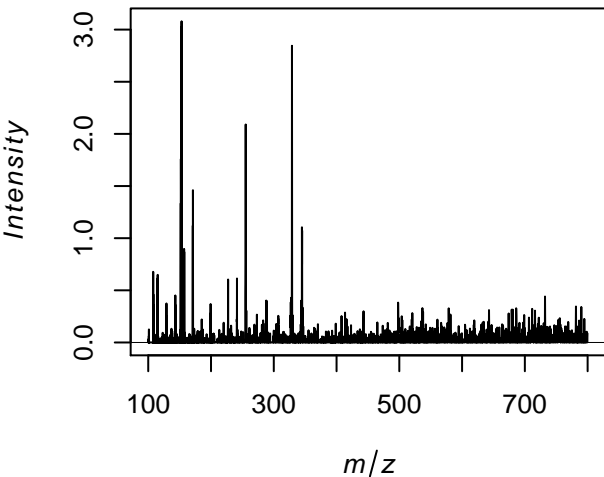
### Median intensity per spectrum



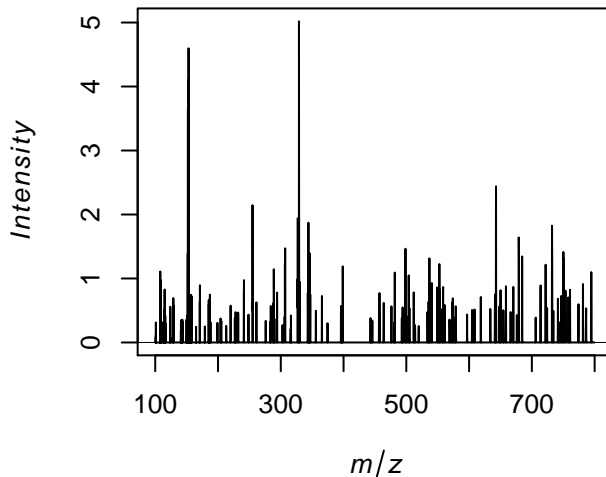
### Log2-transformed intensities



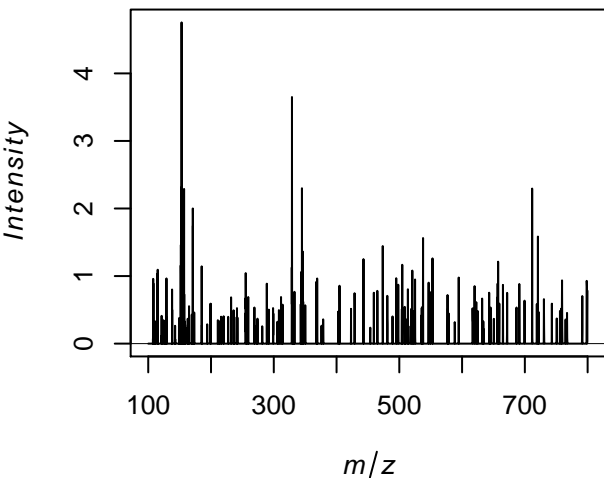
**Average spectrum**



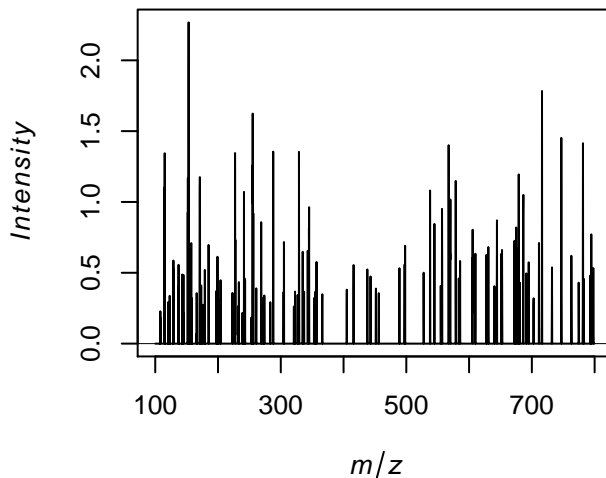
**Spectrum at x = 1, y = 2**



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



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

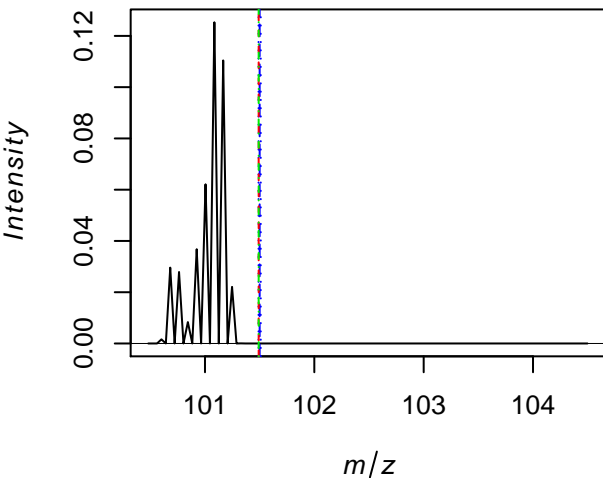


theor. m/z: 101.5

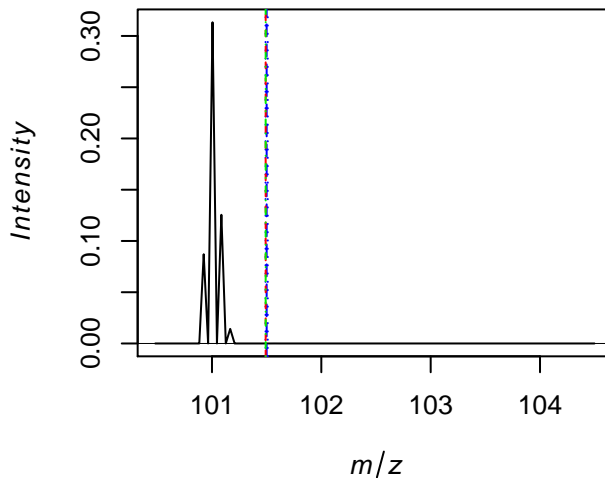
most abundant m/z: 101.491

closest m/z: 101.491

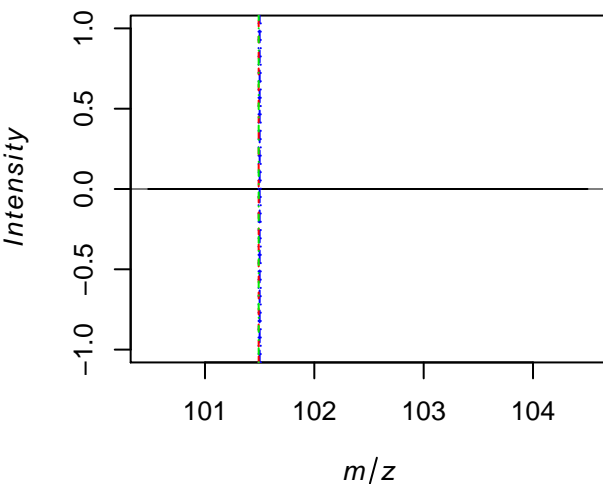
average spectrum



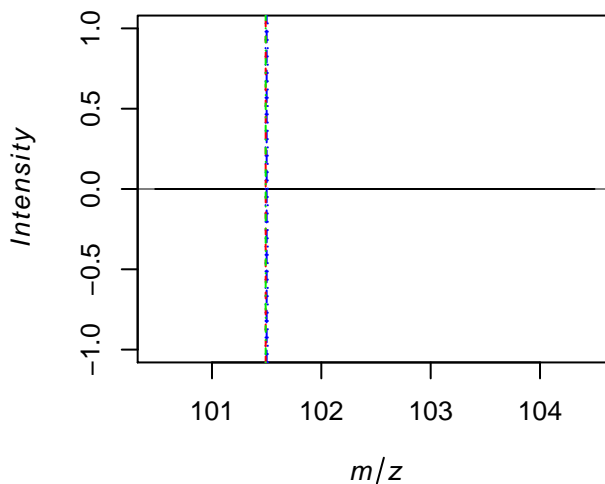
Spectrum at  $x = 1, y = 2$



Spectrum at  $x = 2, y = 1$



Spectrum at  $x = 1, y = 3$

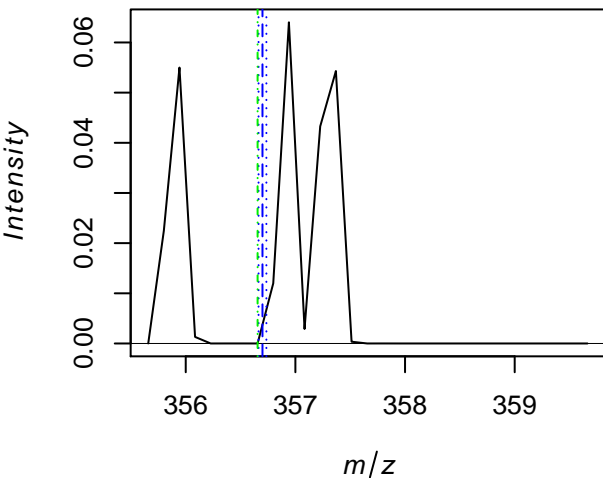


theor. m/z: 356.7

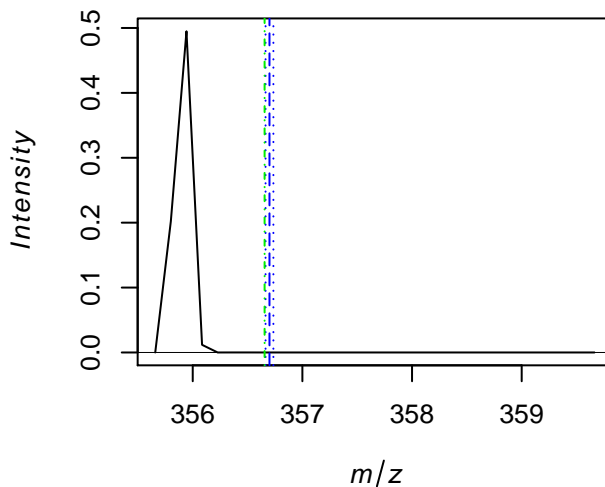
most abundant m/z: NA

closest m/z: 356.6555

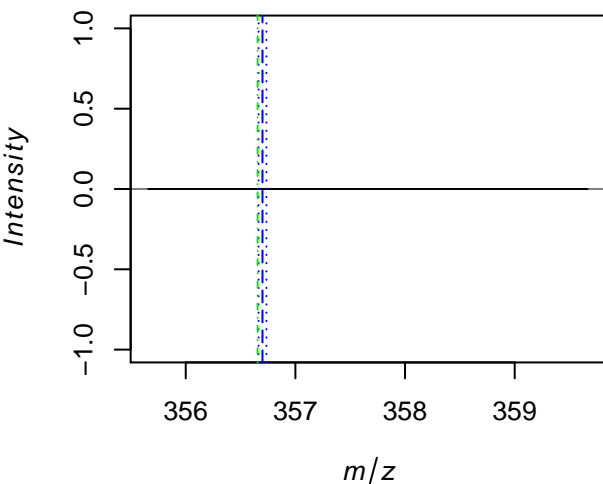
average spectrum



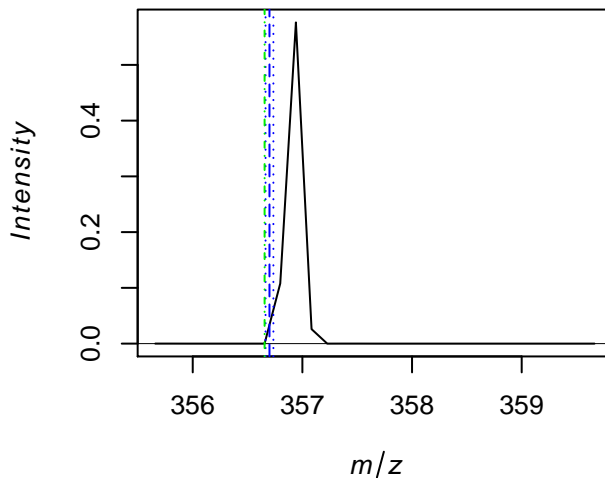
Spectrum at x = 1, y = 2



Spectrum at x = 2, y = 1



Spectrum at x = 1, y = 3

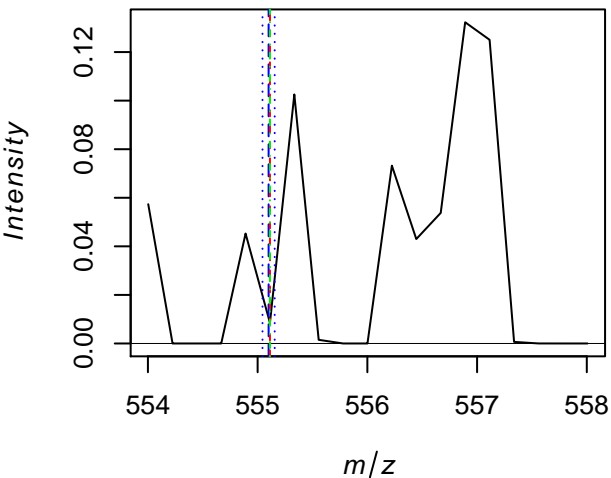


theor. m/z: 555.1

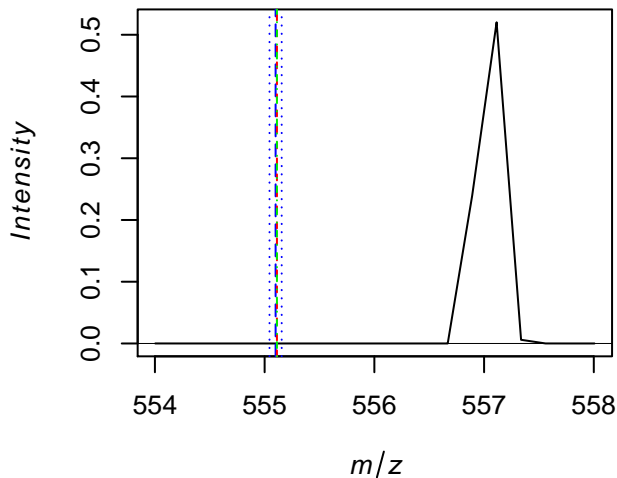
most abundant m/z: 555.122

closest m/z: 555.122

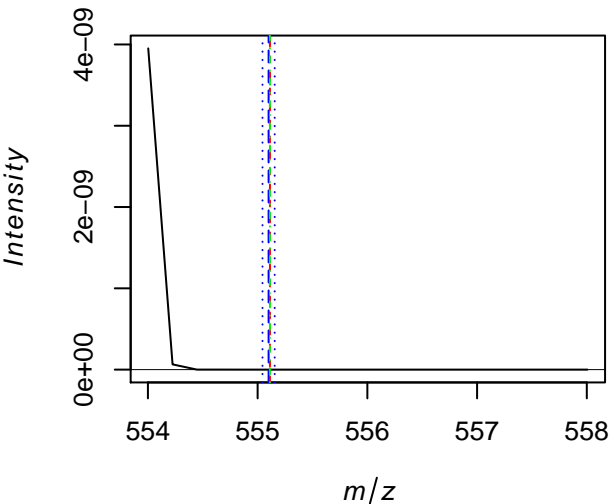
average spectrum



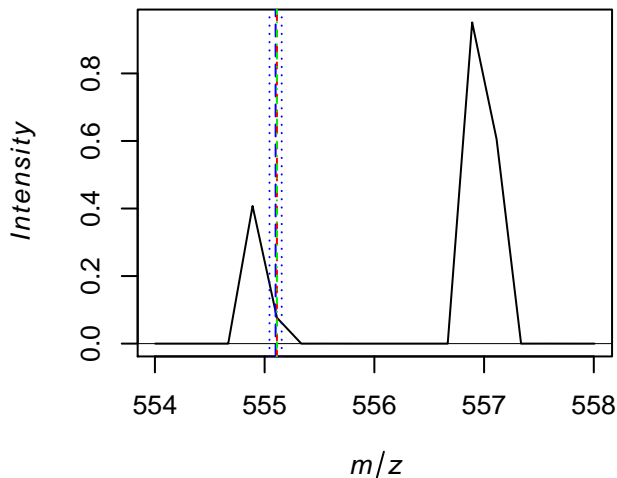
Spectrum at x = 1, y = 2



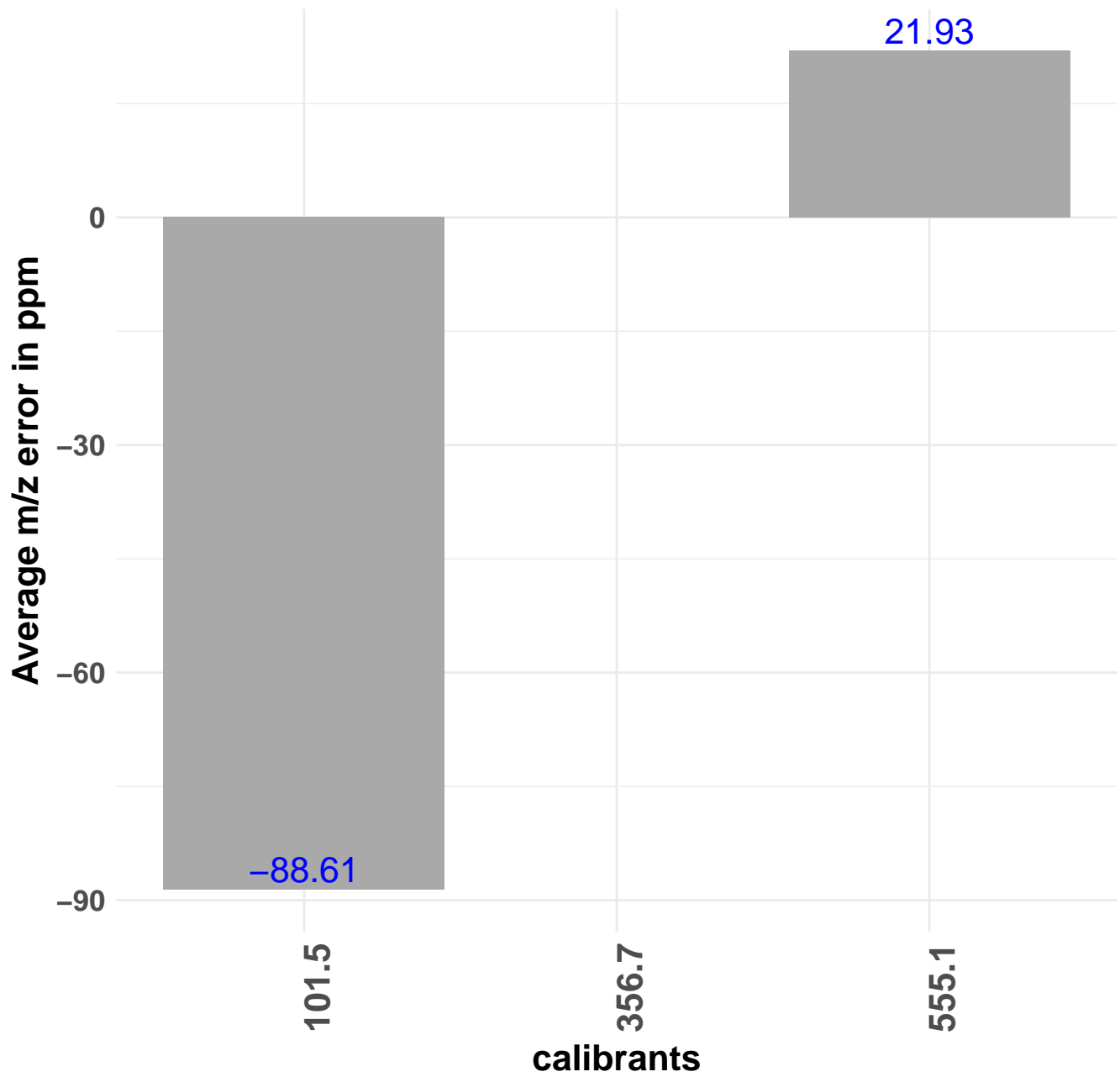
Spectrum at x = 2, y = 1



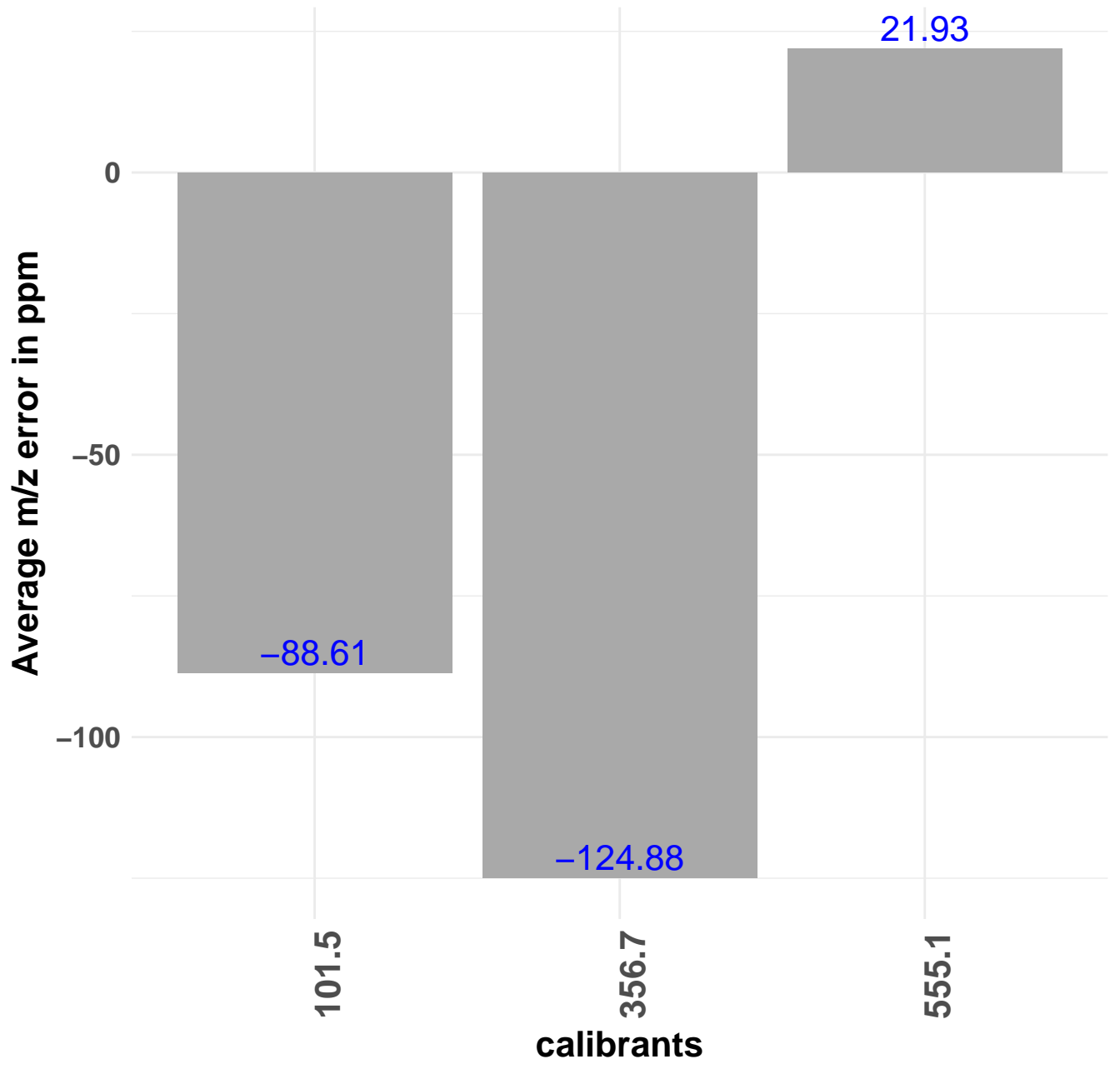
Spectrum at x = 1, y = 3



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)





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

