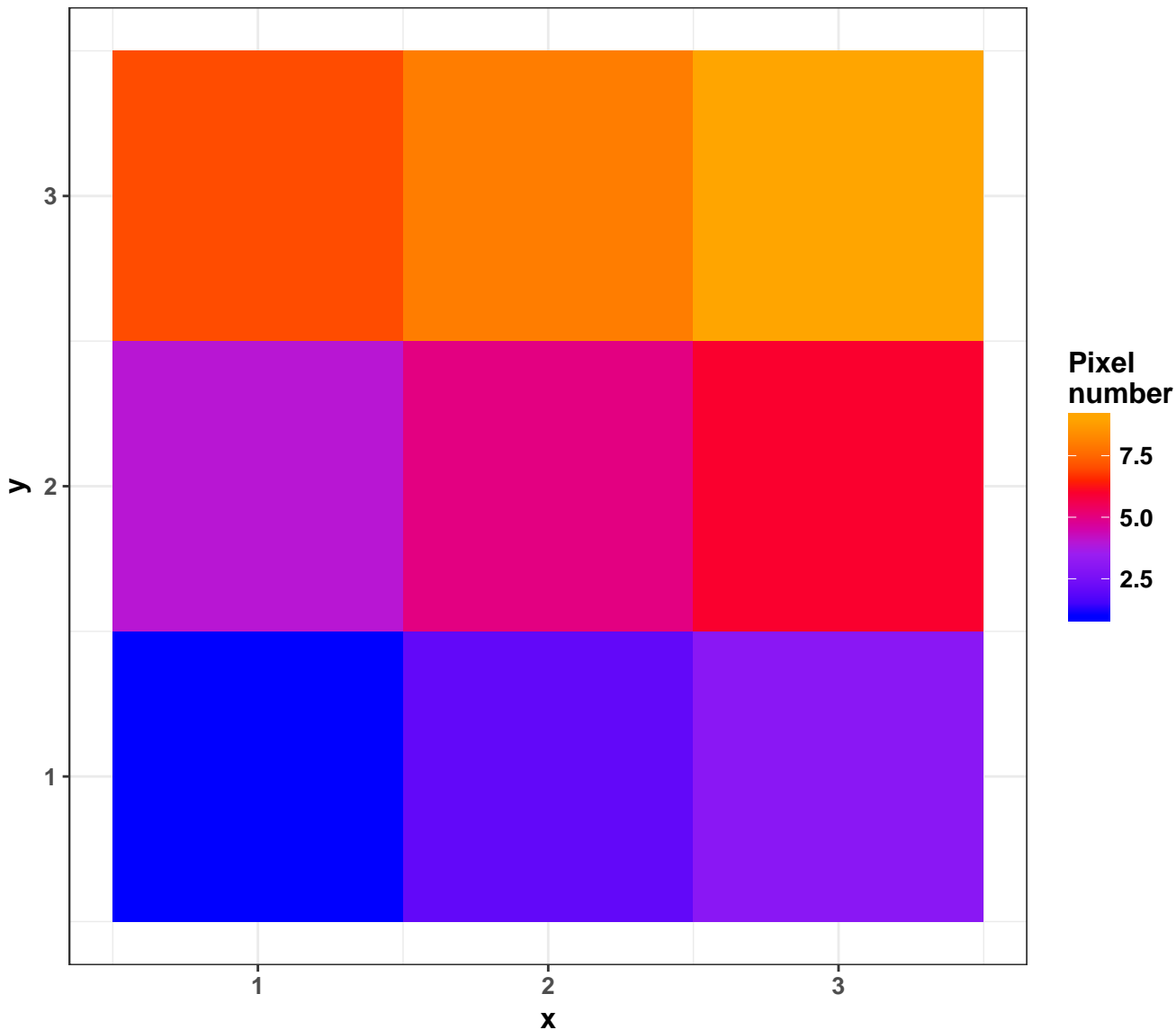


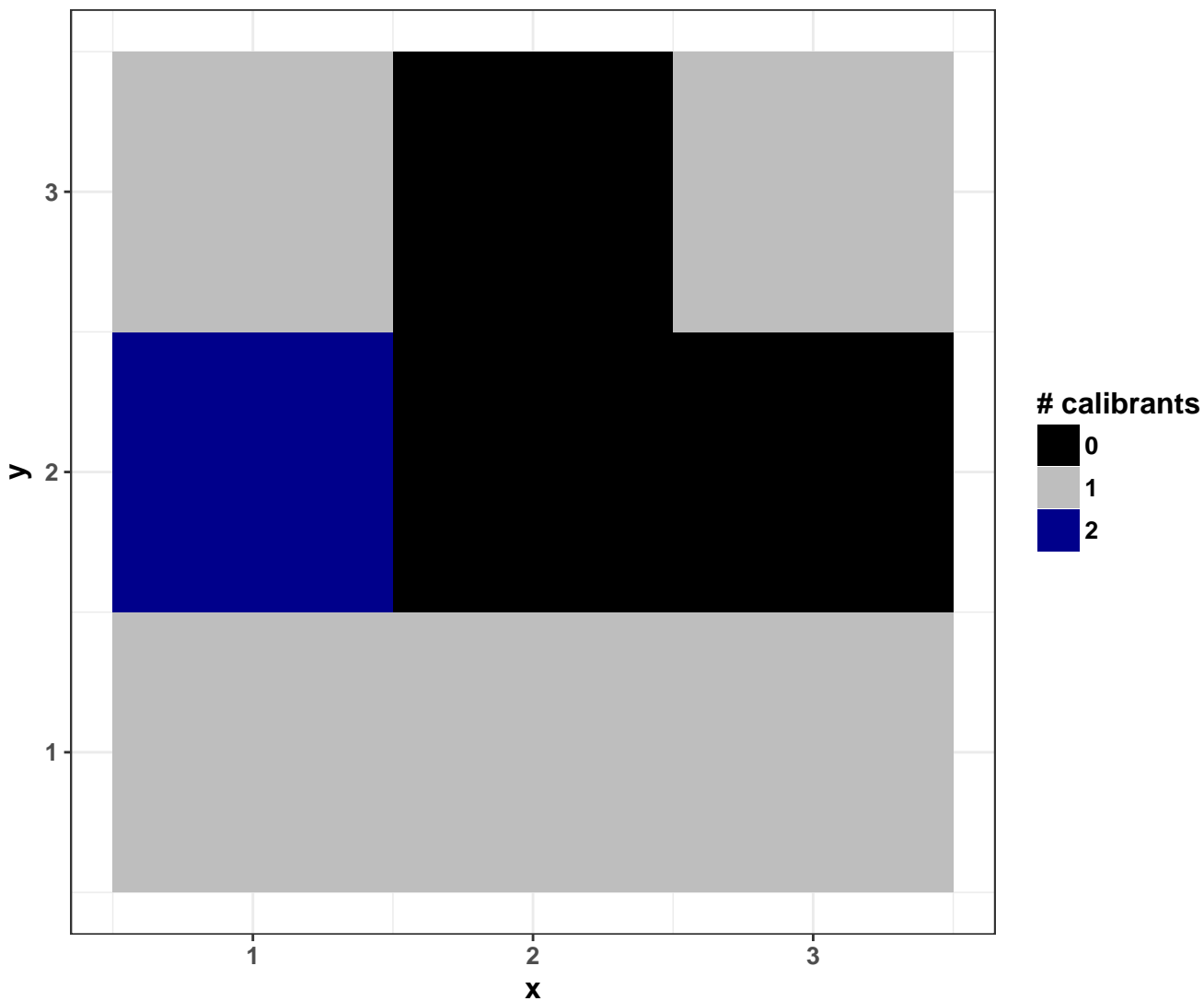
## Testfile\_imzml

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 $\pm$ sd	161.8 $\pm$ 43
Median # peaks per spectrum $\pm$ sd	1961 $\pm$ 260
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.txt	3 / 3

Pixel order

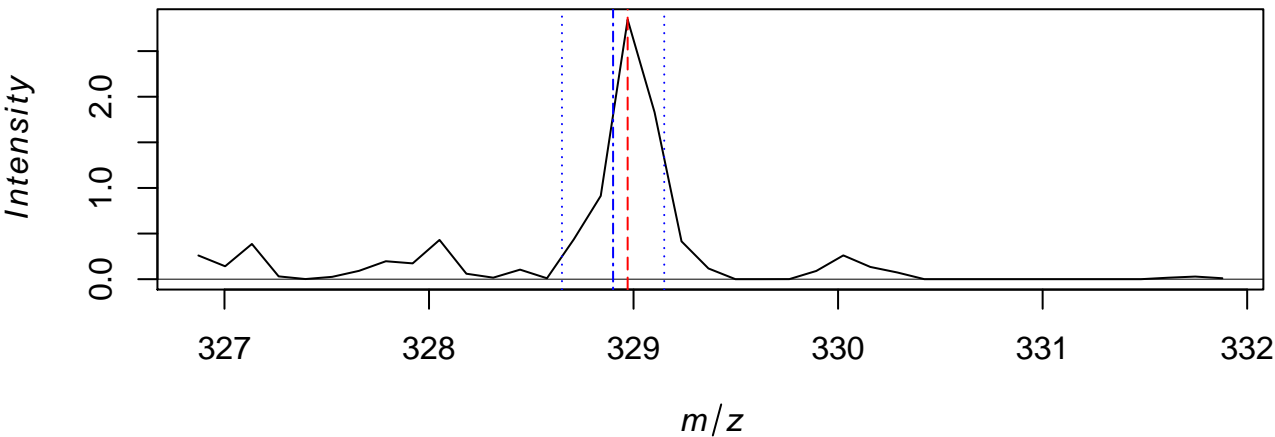


Number of calibrants per pixel ( $\pm 100$  ppm)

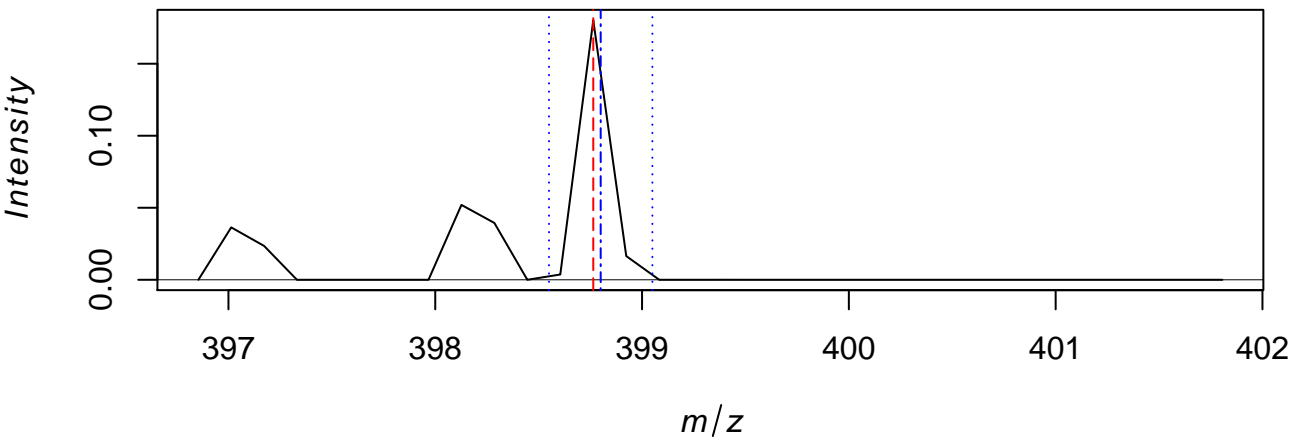


## Control of fold change plot

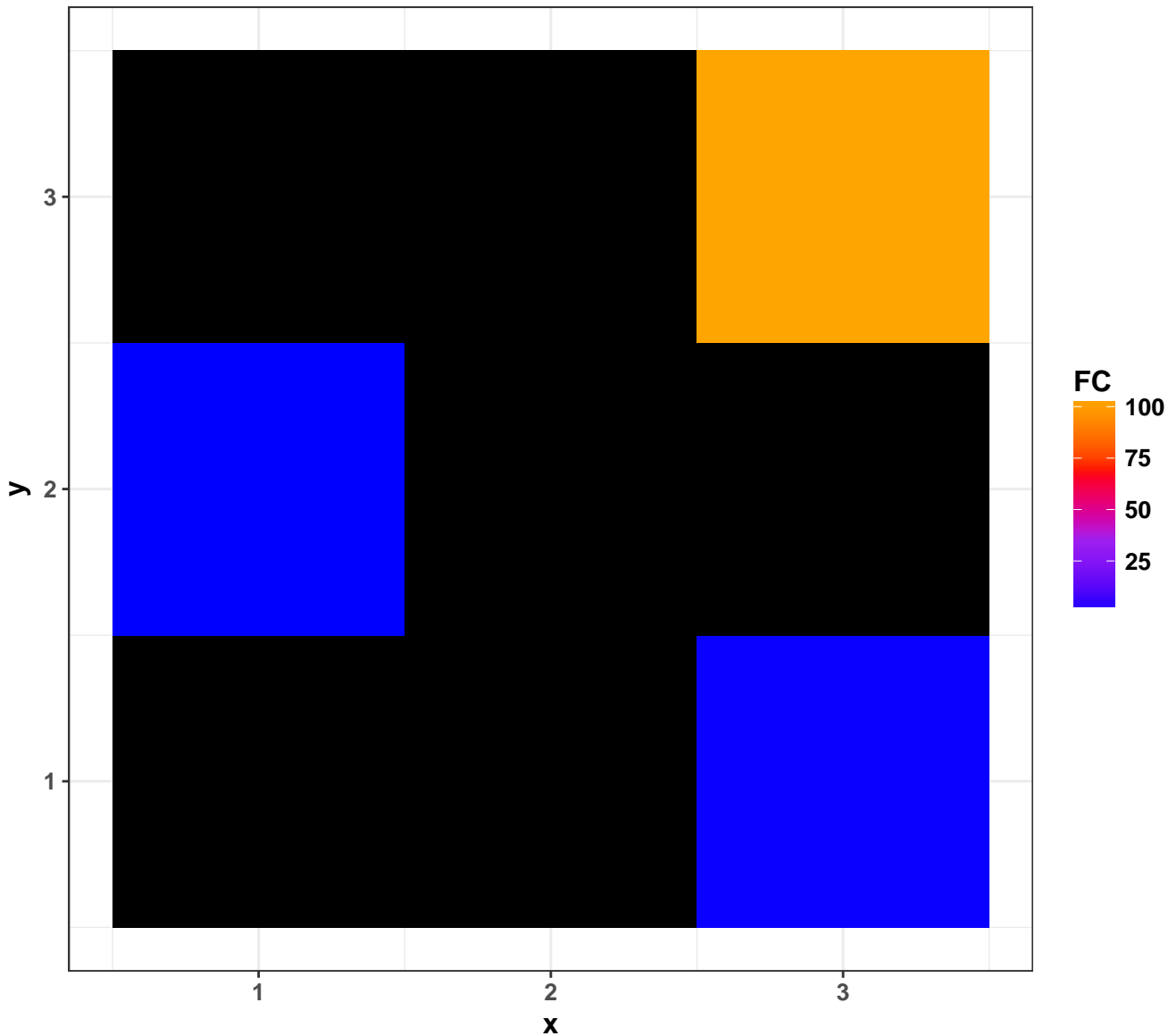
Average spectrum 328.9 Da



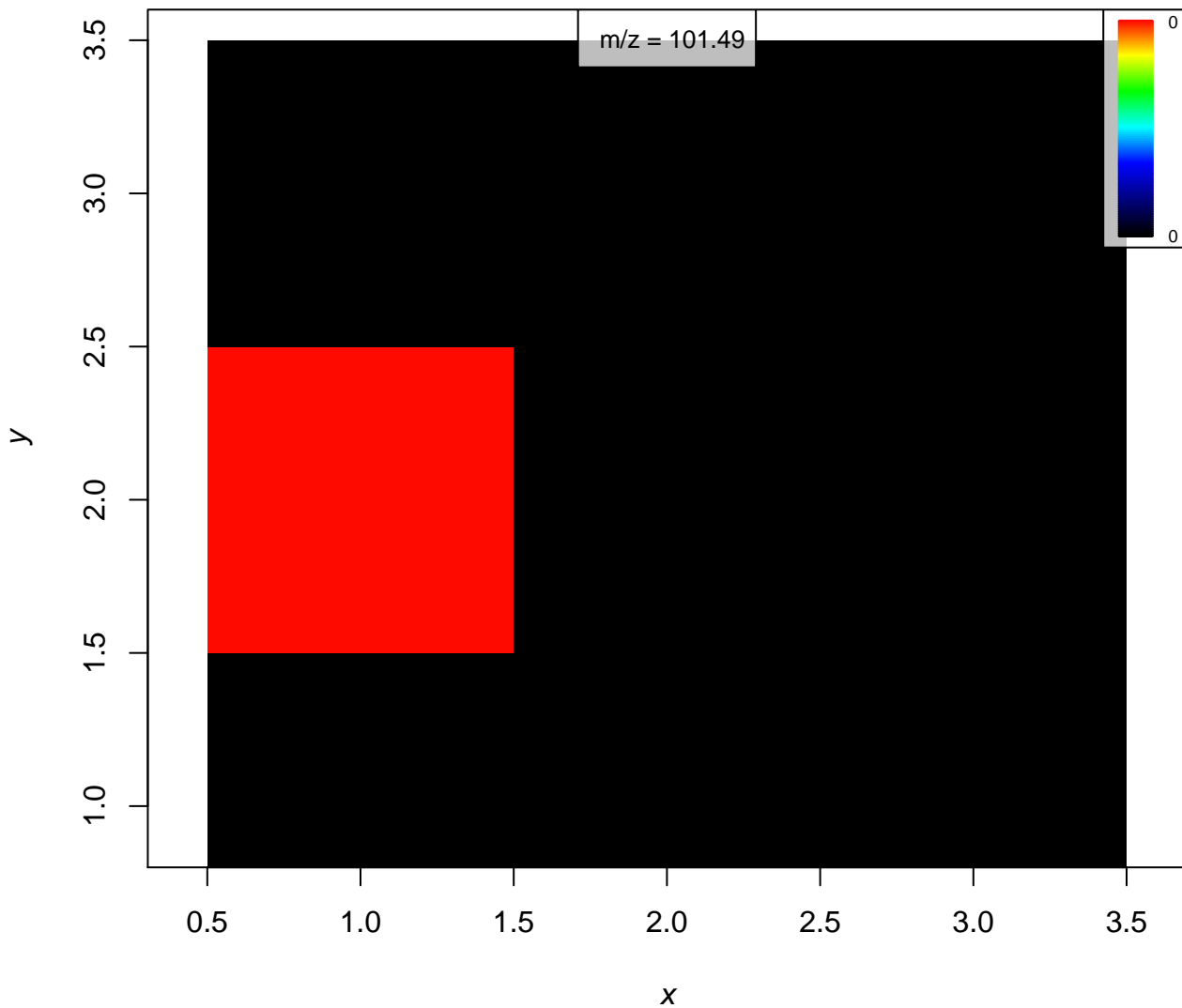
Average spectrum 398.8 Da



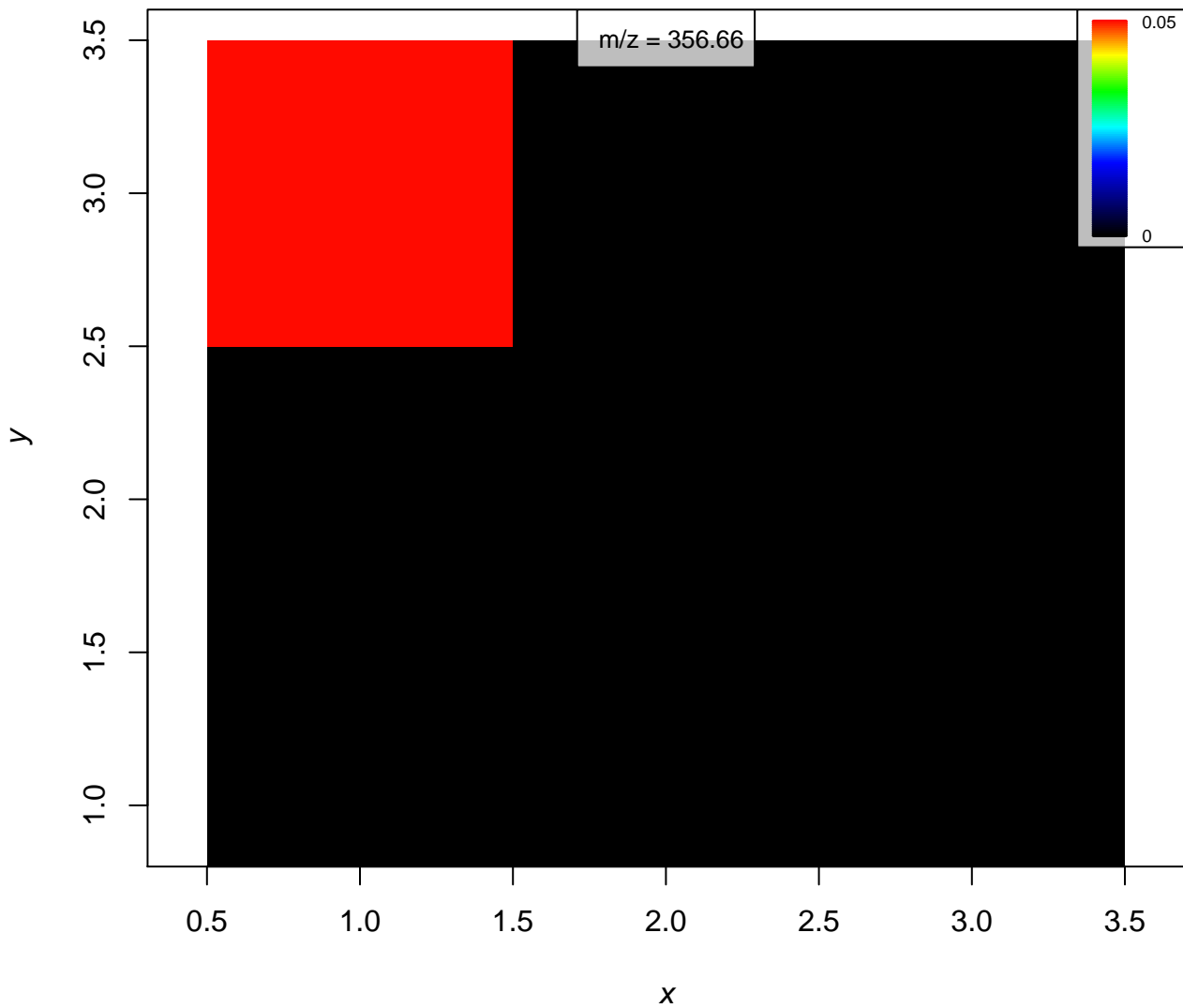
Ratio of mass1 (328.9) / mass2 (398.8)



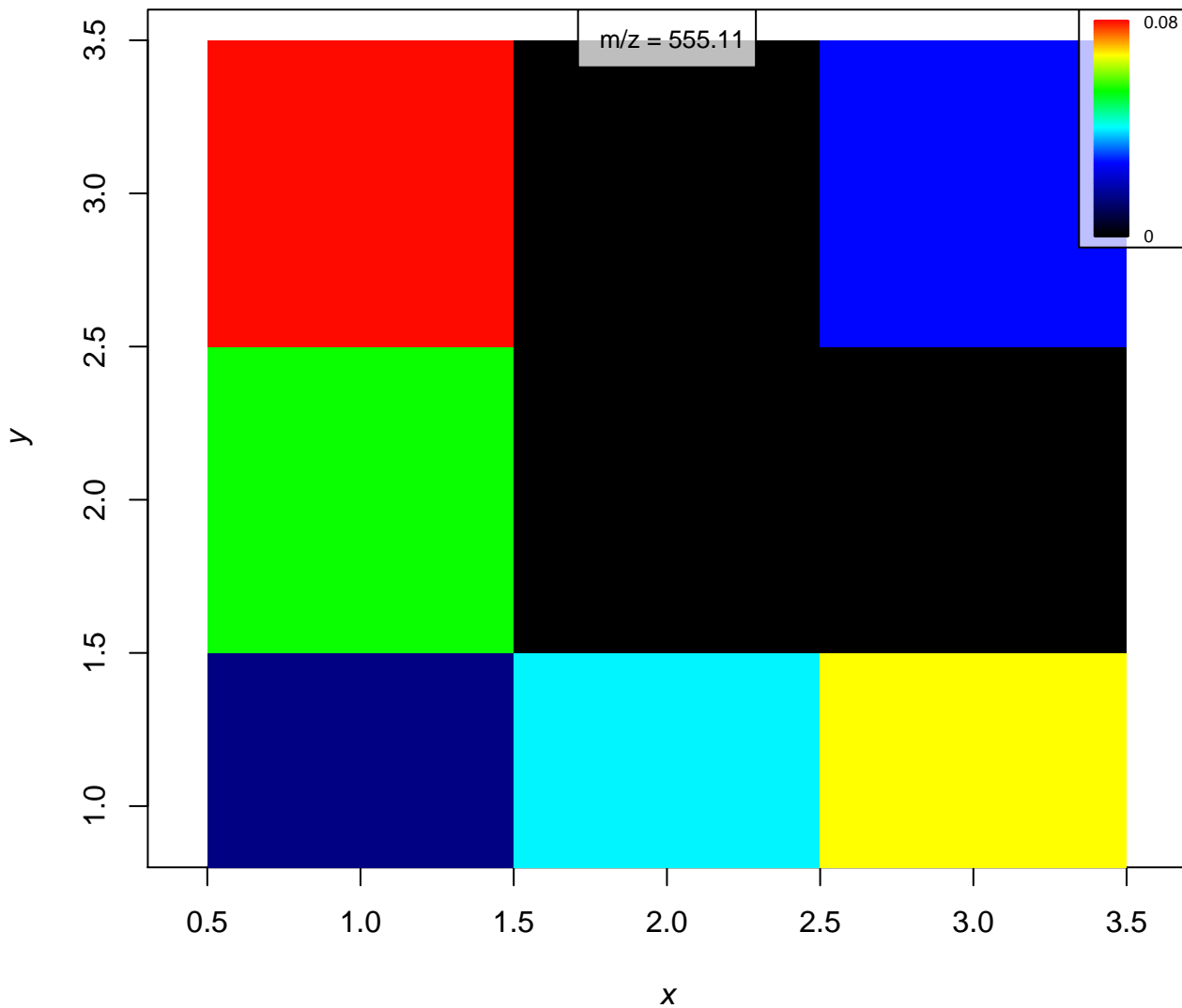
101.5: 101.5 ( $\pm 100$  ppm)



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

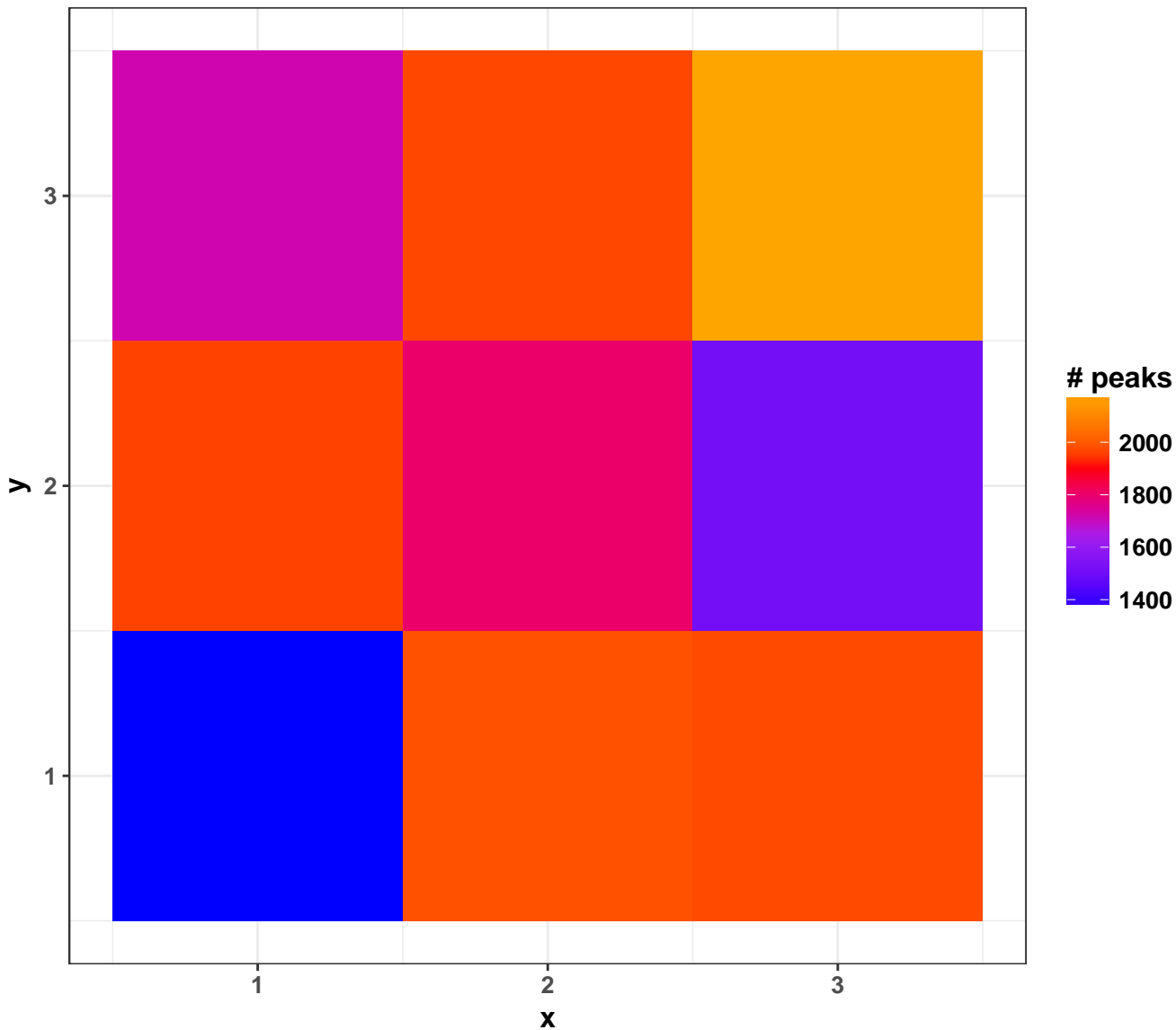


**555.1: 555.1 ( $\pm 100$  ppm)**

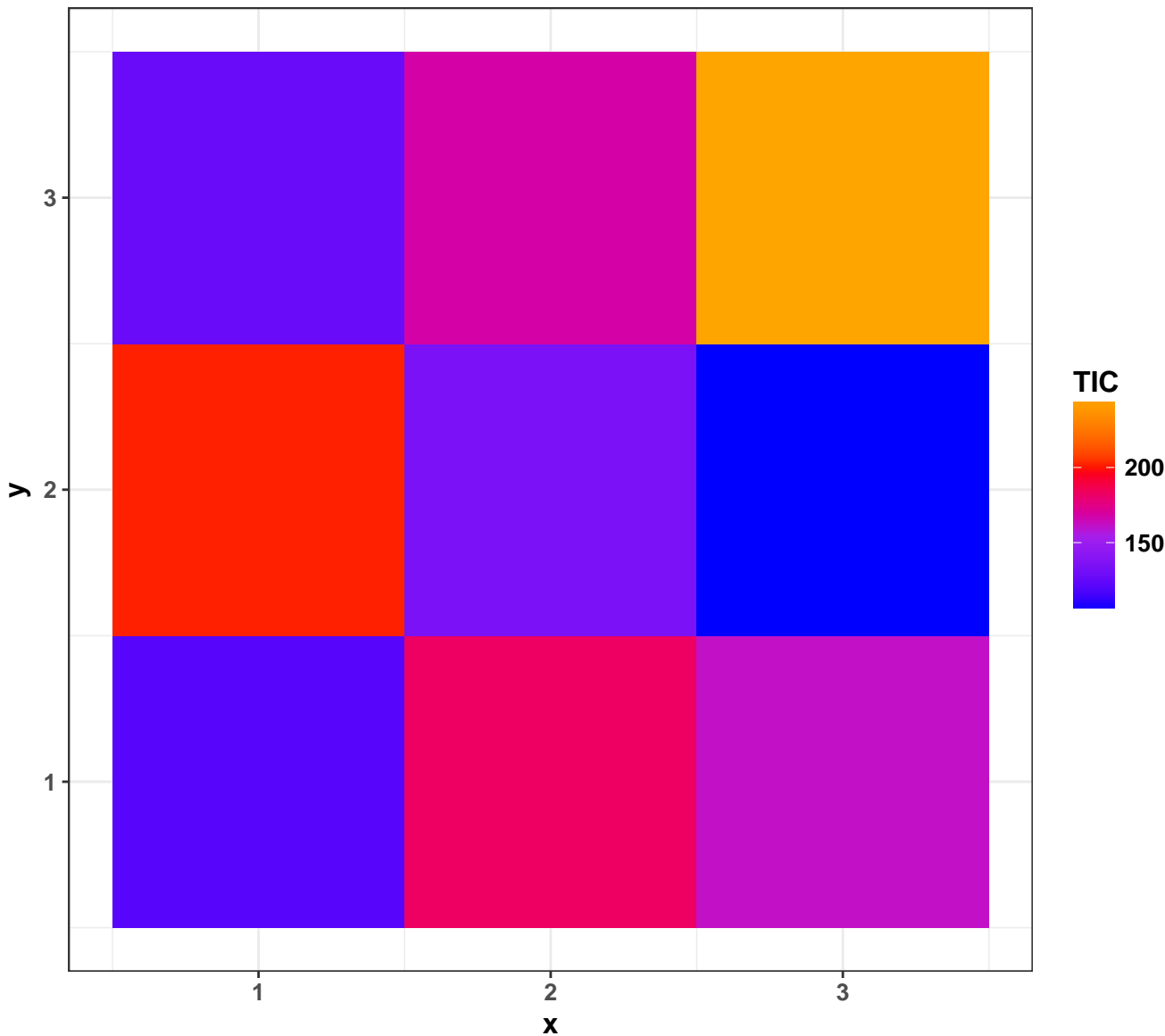




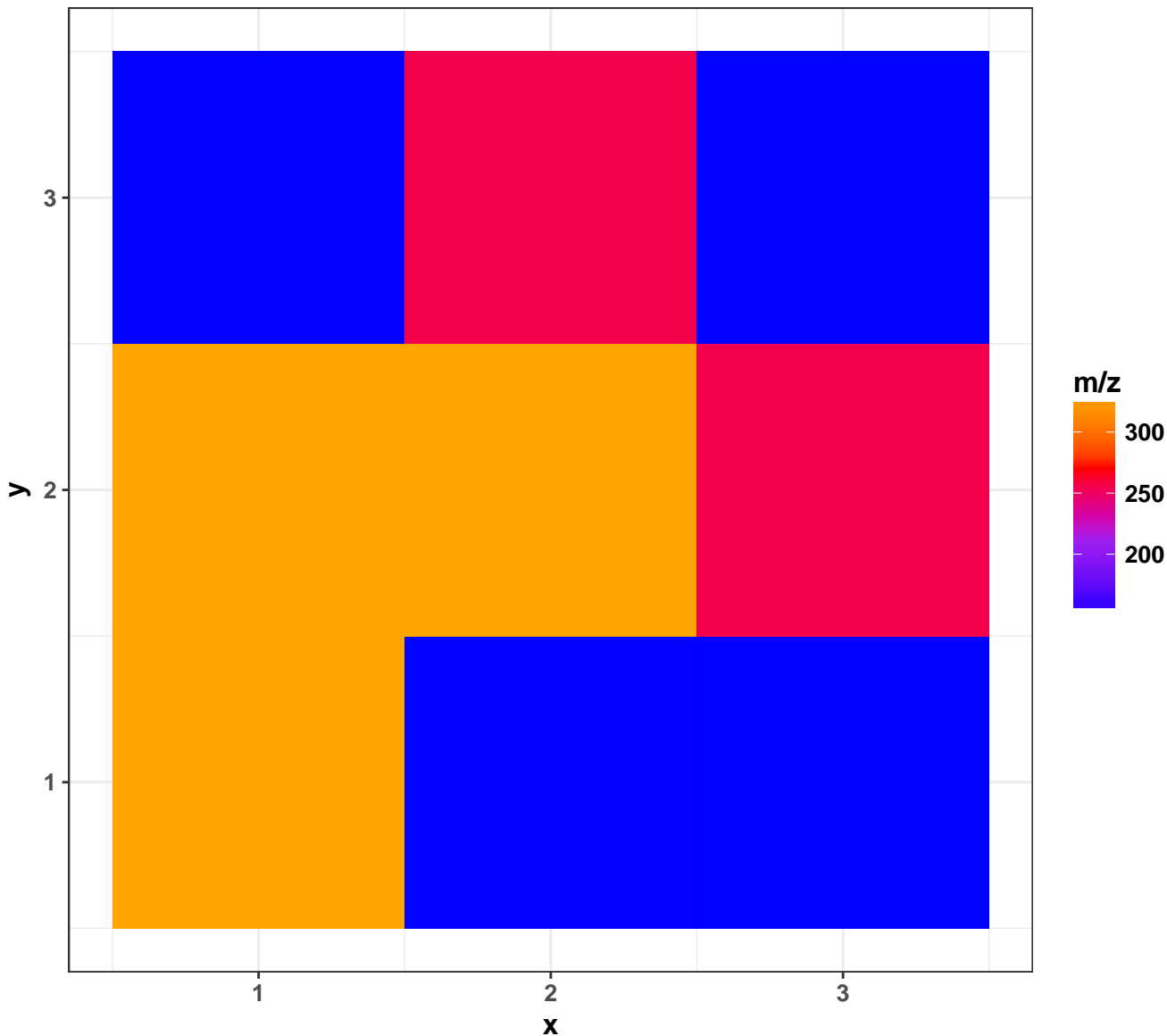
Number of peaks per spectrum



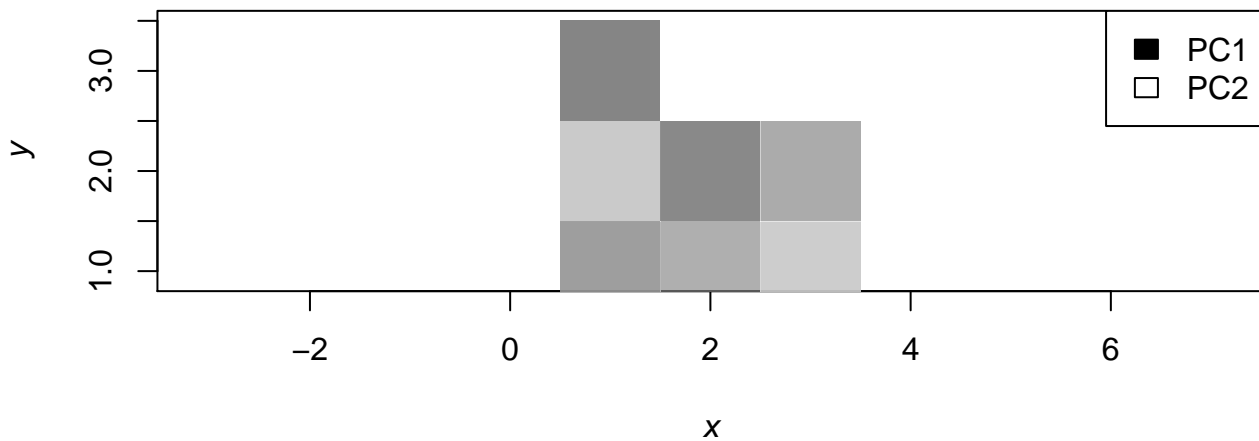
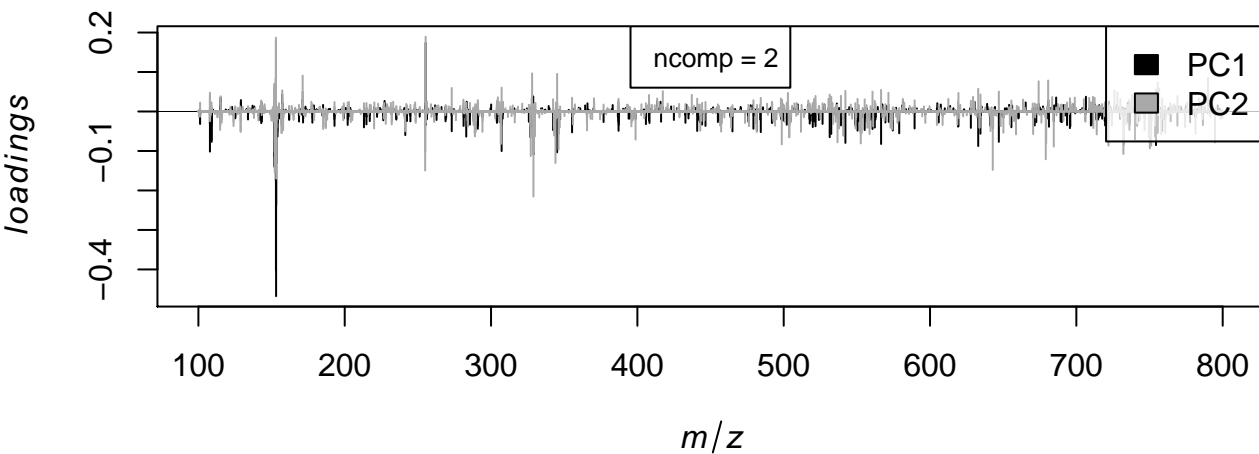
Total Ion Chromatogram



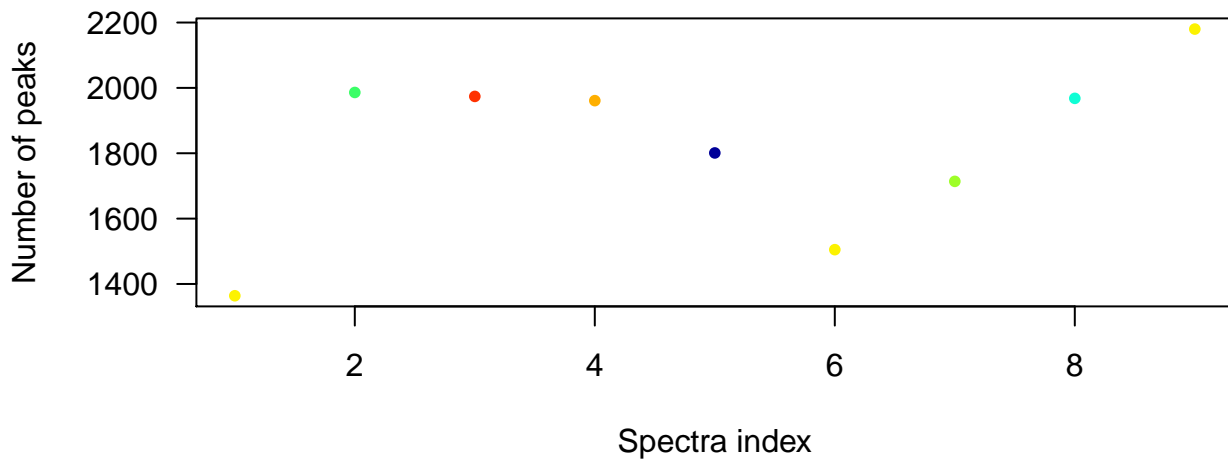
Most abundant m/z in each spectrum



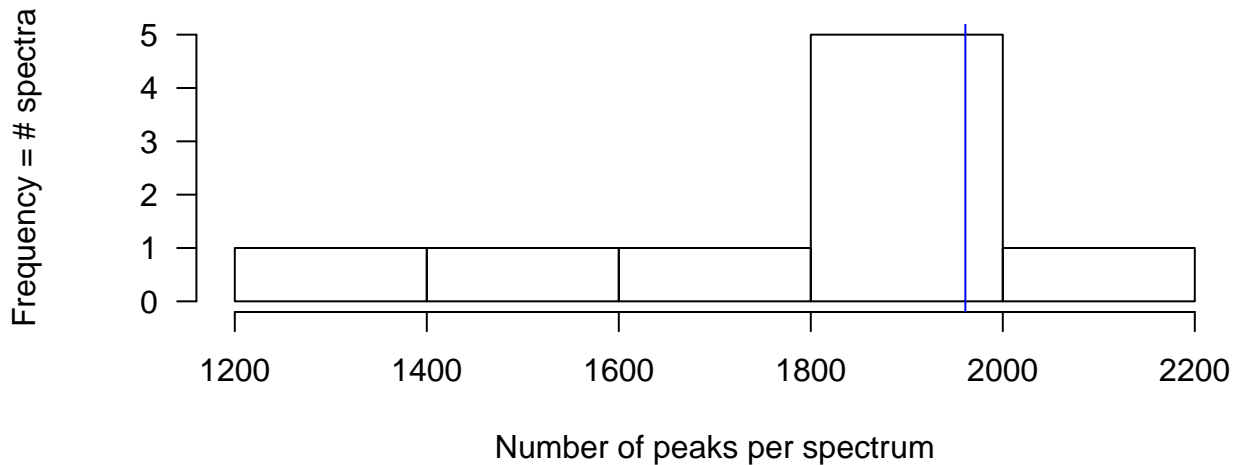
## PCA for two components

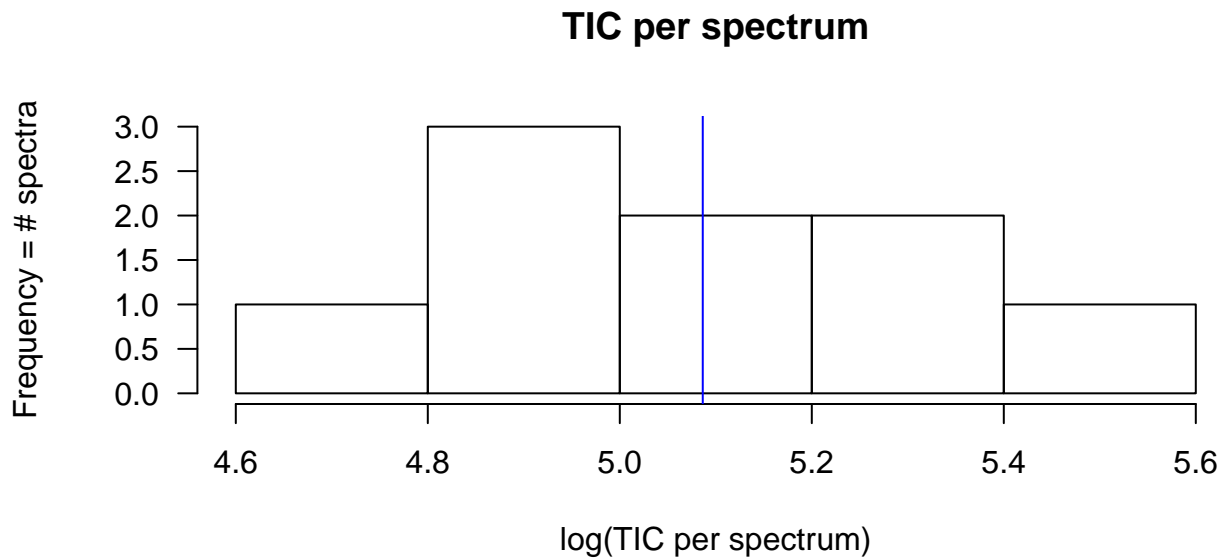
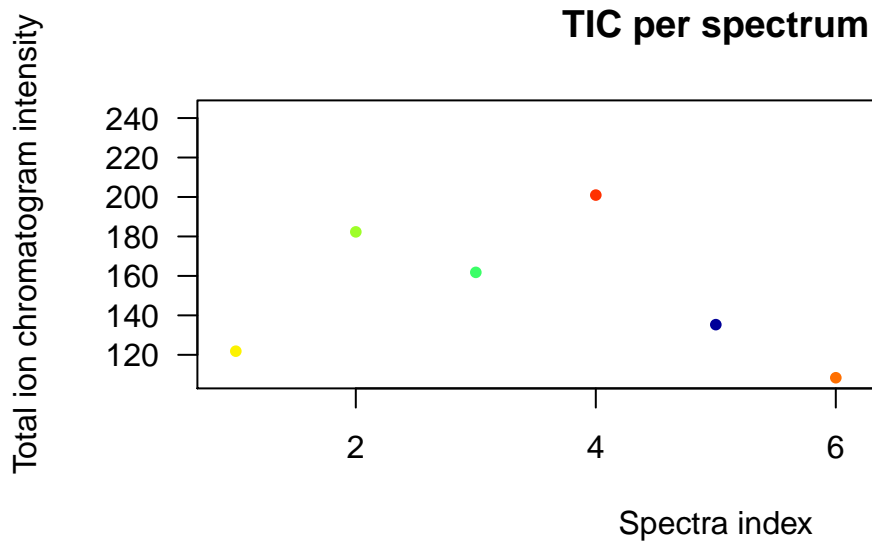


**Number of peaks per spectrum**

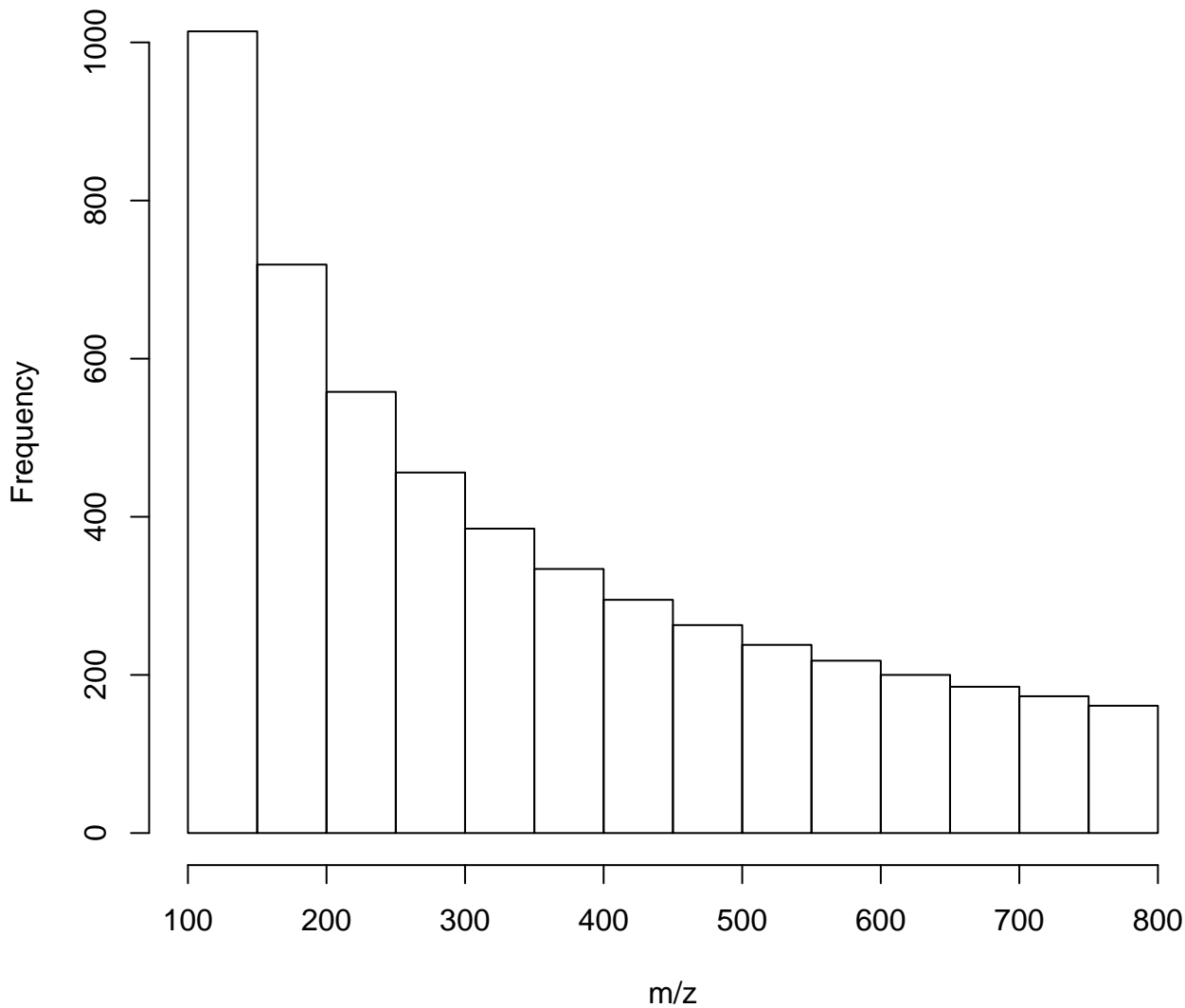


**Number of peaks per spectrum**

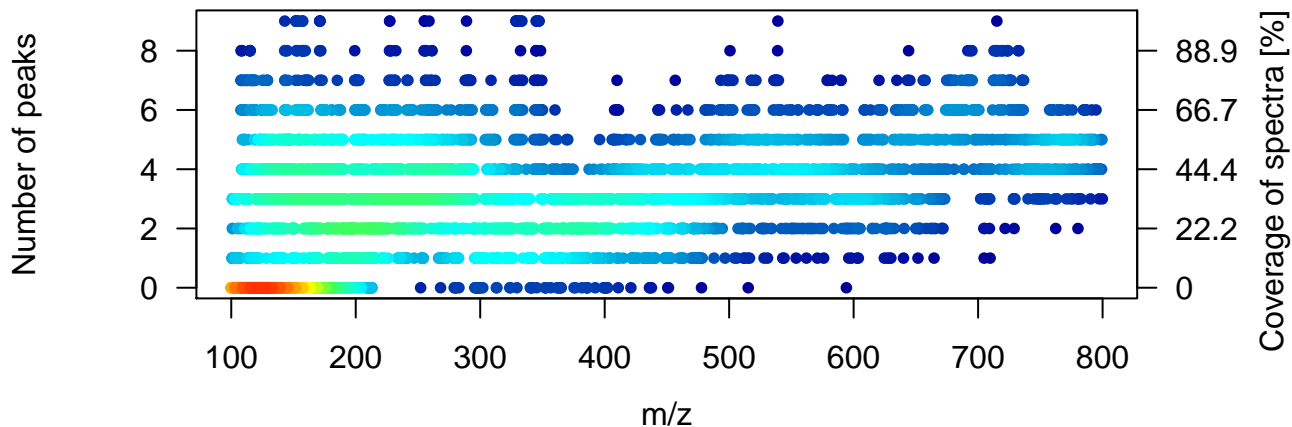




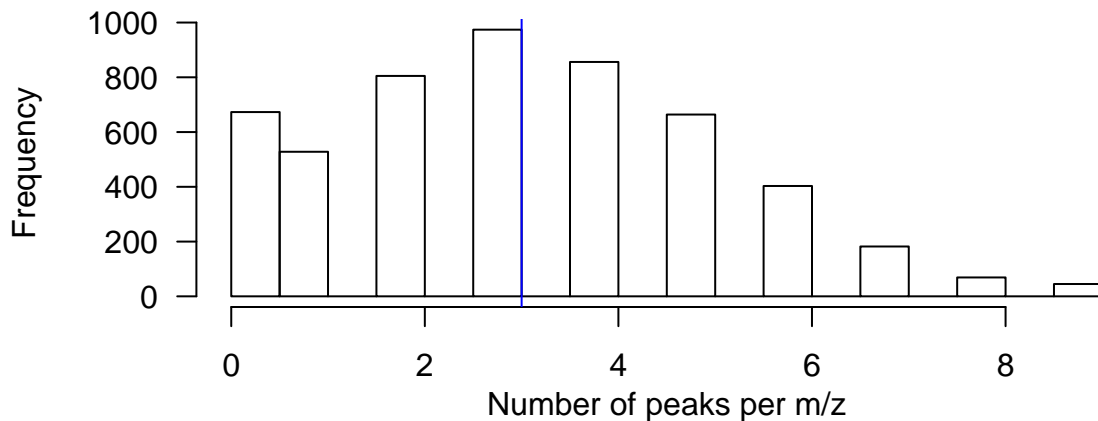
**Histogram of m/z values**



Number of peaks per m/z

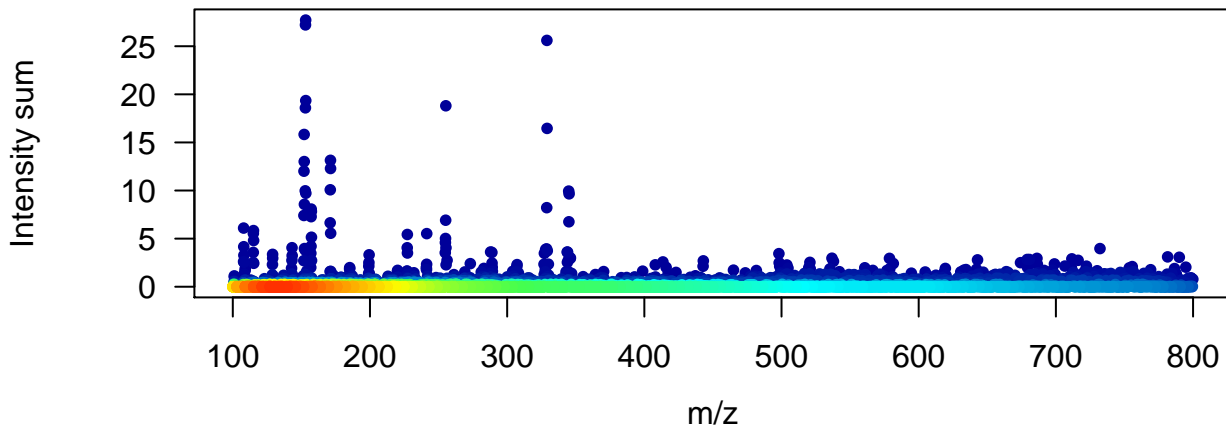


Number of peaks per m/z

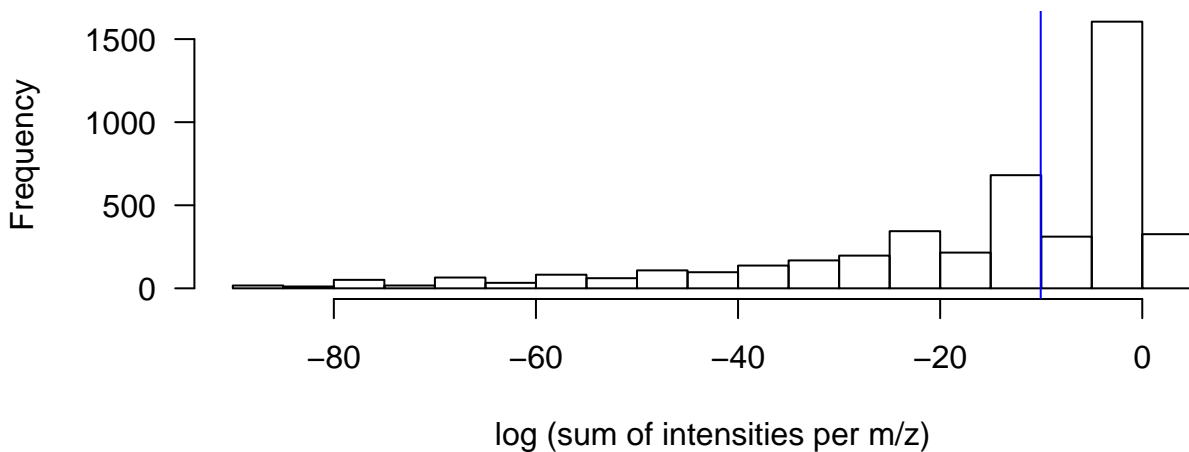




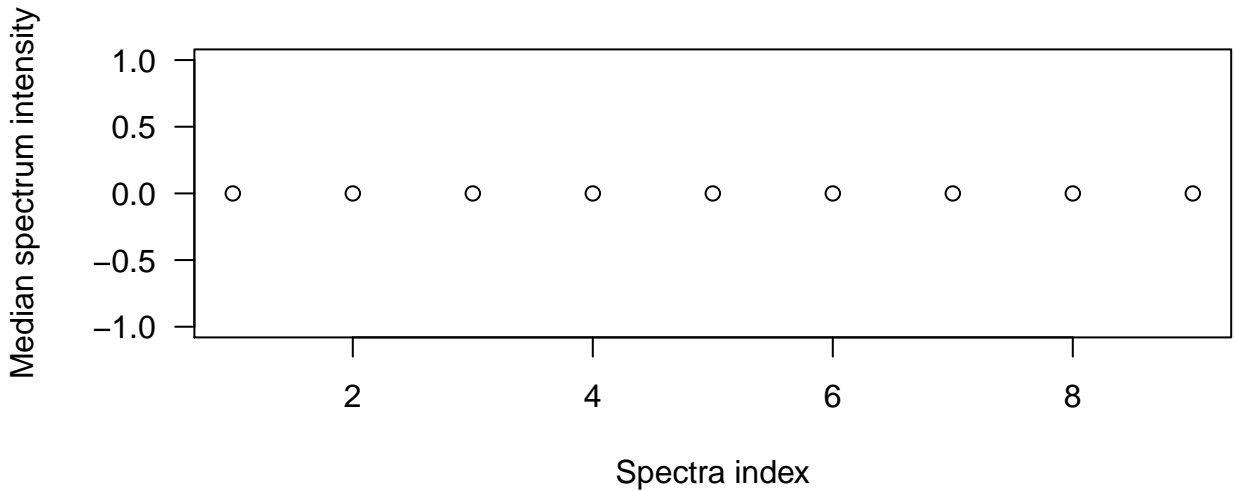
**Sum of intensities per m/z**



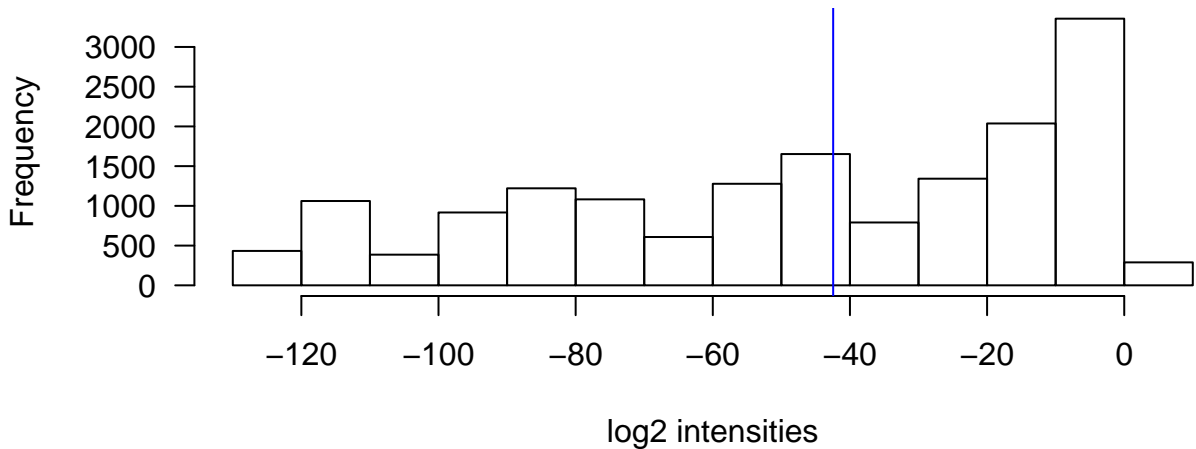
**Sum of intensities per m/z**



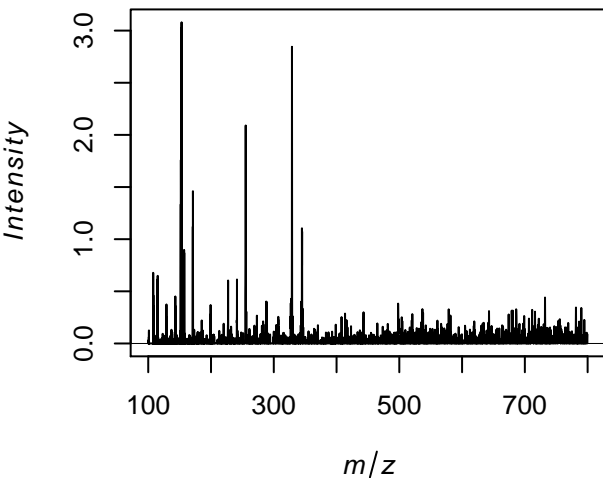
### Median intensity per spectrum



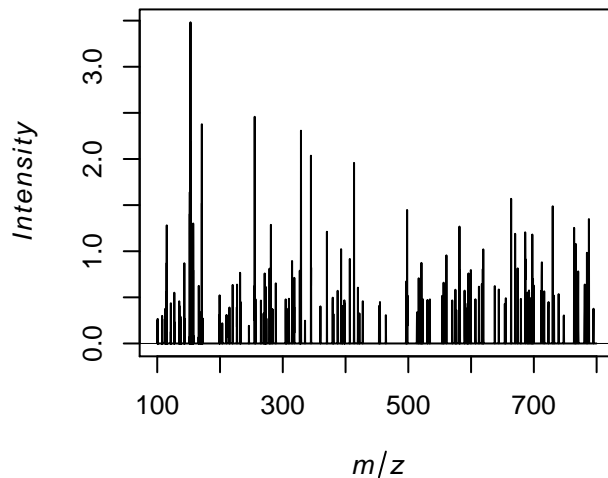
### Log2-transformed intensities



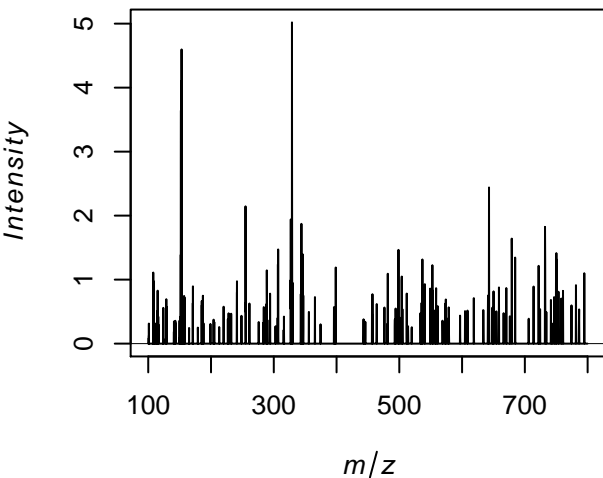
**Average spectrum**



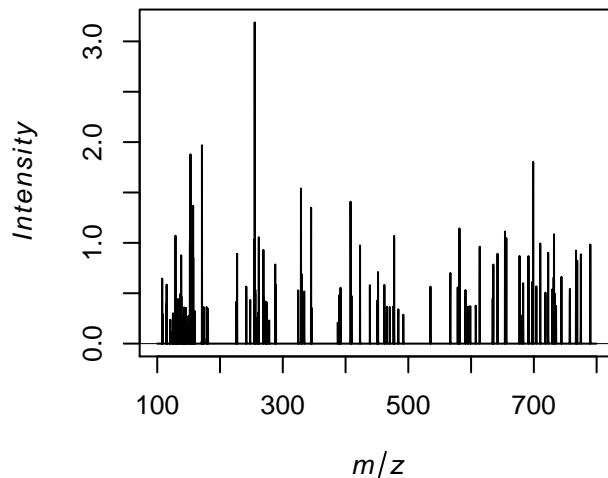
**Spectrum at x = 3, y = 1**



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



**Spectrum at x = 3, y = 2**

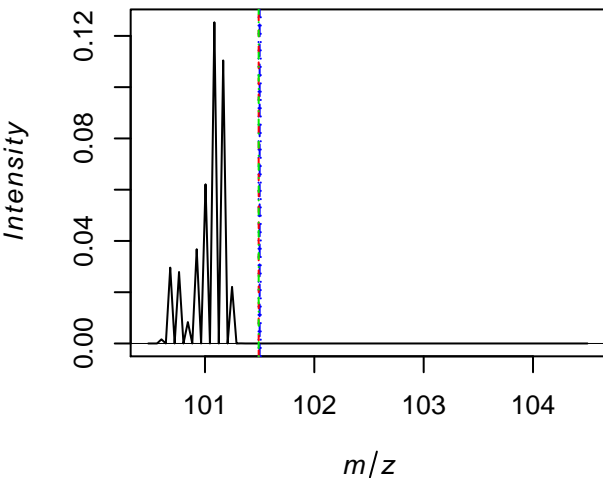


theor. m/z: 101.5

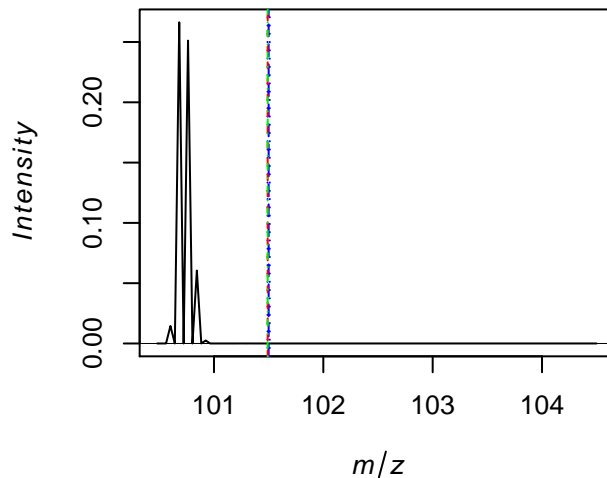
most abundant m/z: 101.491

closest m/z: 101.491

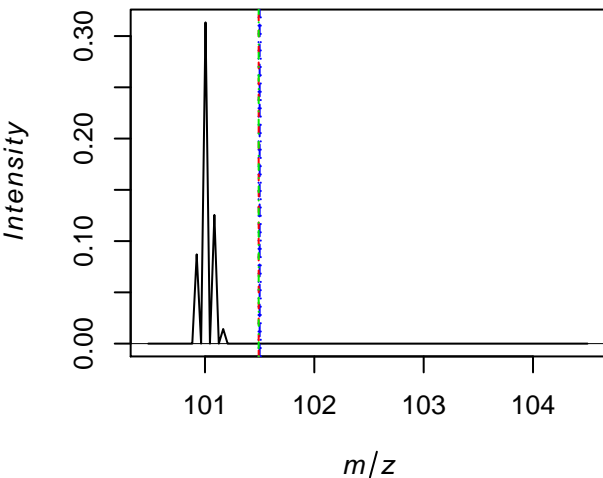
Average spectrum



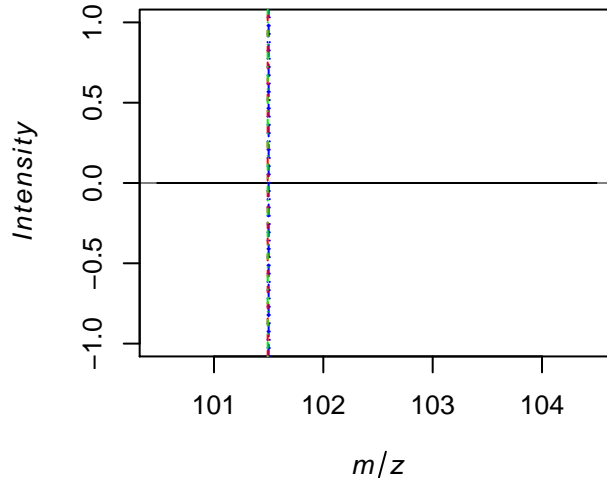
Spectrum at x = 3, y = 1



Spectrum at x = 1, y = 2



Spectrum at x = 3, y = 2

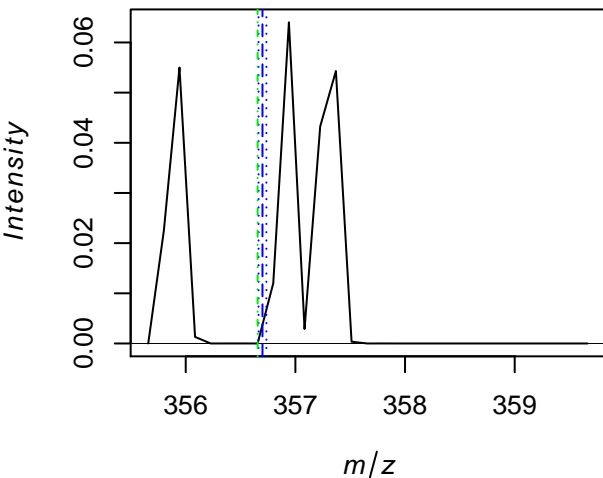


theor. m/z: 356.7

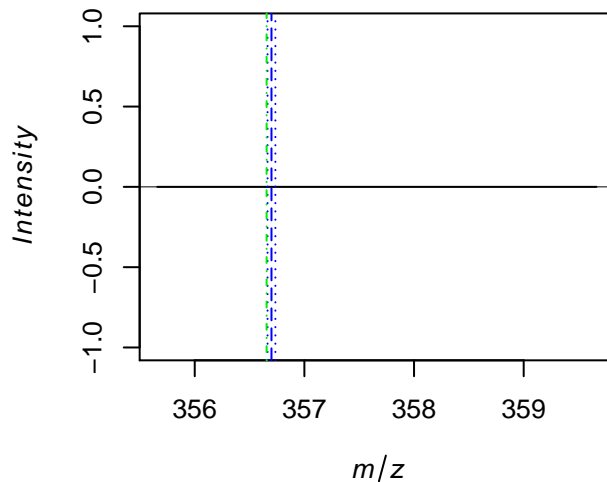
most abundant m/z: NA

closest m/z: 356.6555

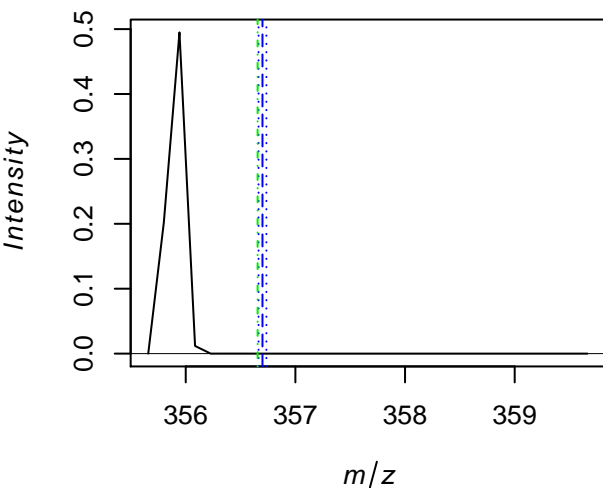
Average spectrum



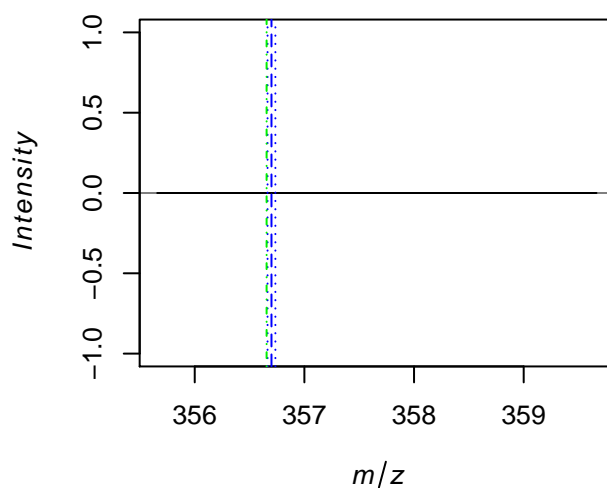
Spectrum at x = 3, y = 1



Spectrum at x = 1, y = 2



Spectrum at x = 3, y = 2

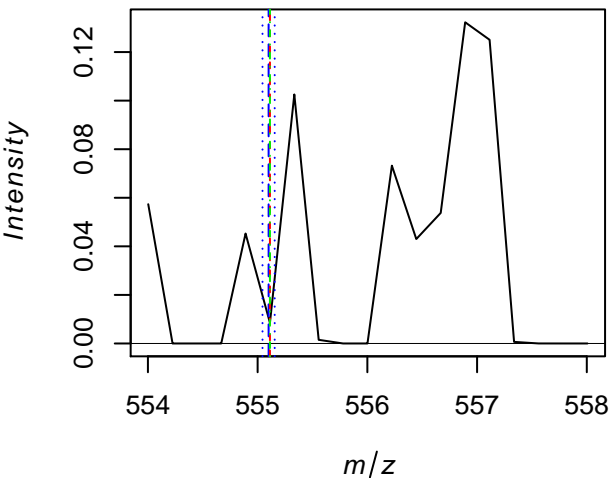


theor. m/z: 555.1

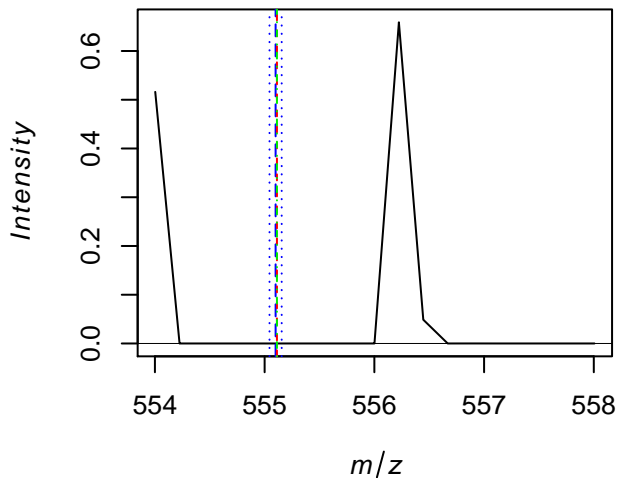
most abundant m/z: 555.1122

closest m/z: 555.1122

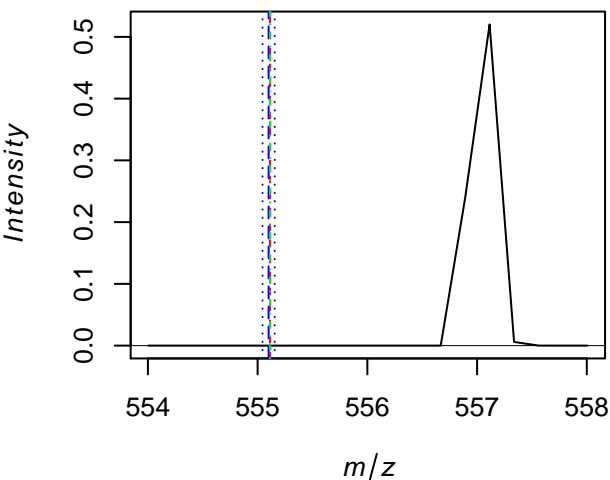
Average spectrum



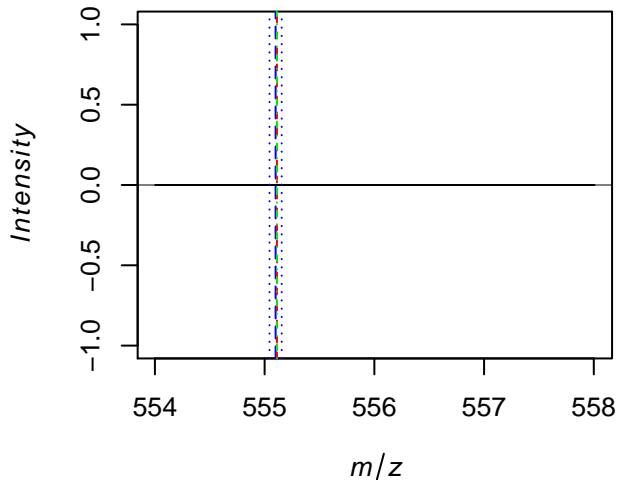
Spectrum at x = 3, y = 1



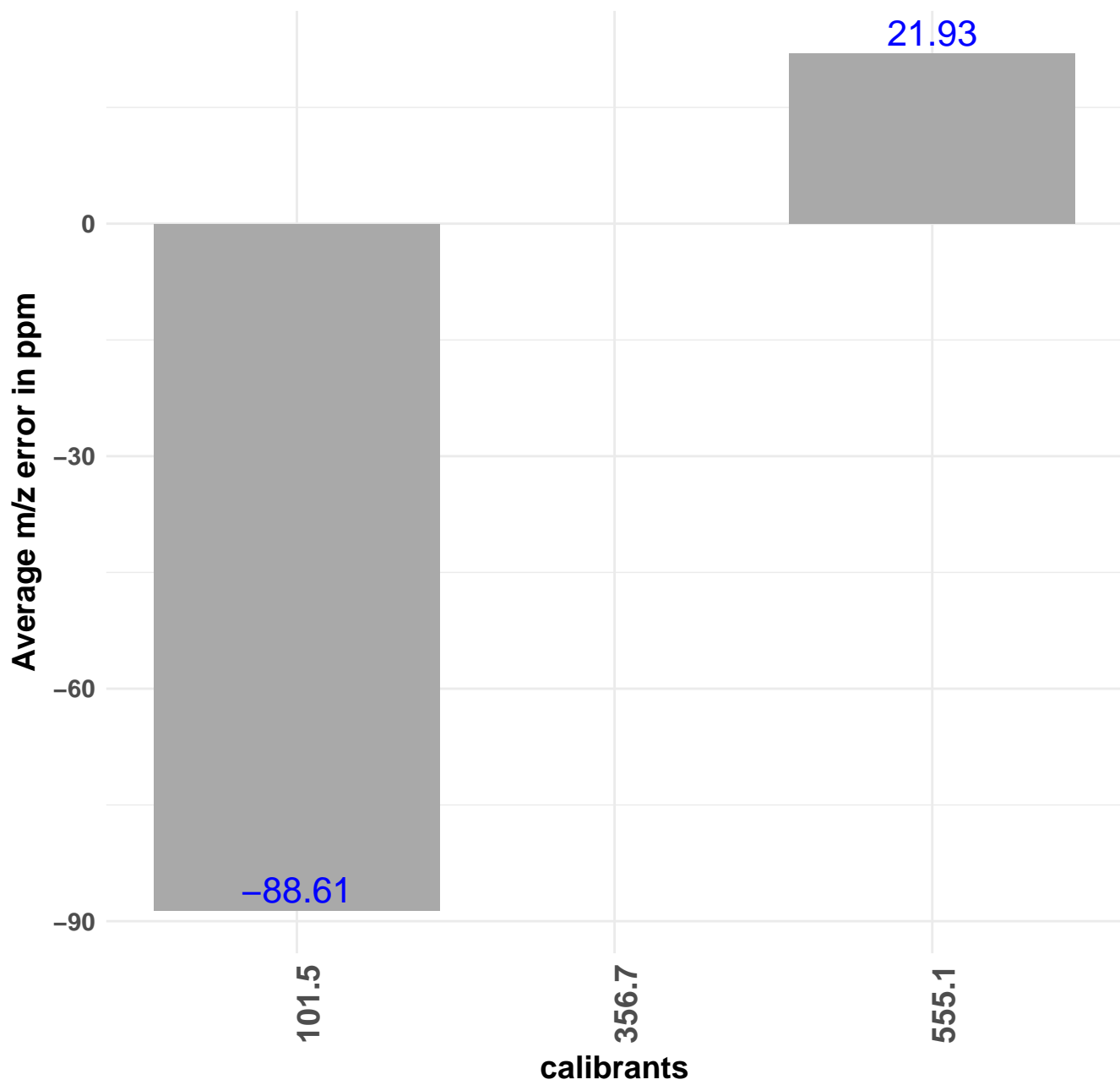
Spectrum at x = 1, y = 2



Spectrum at x = 3, y = 2

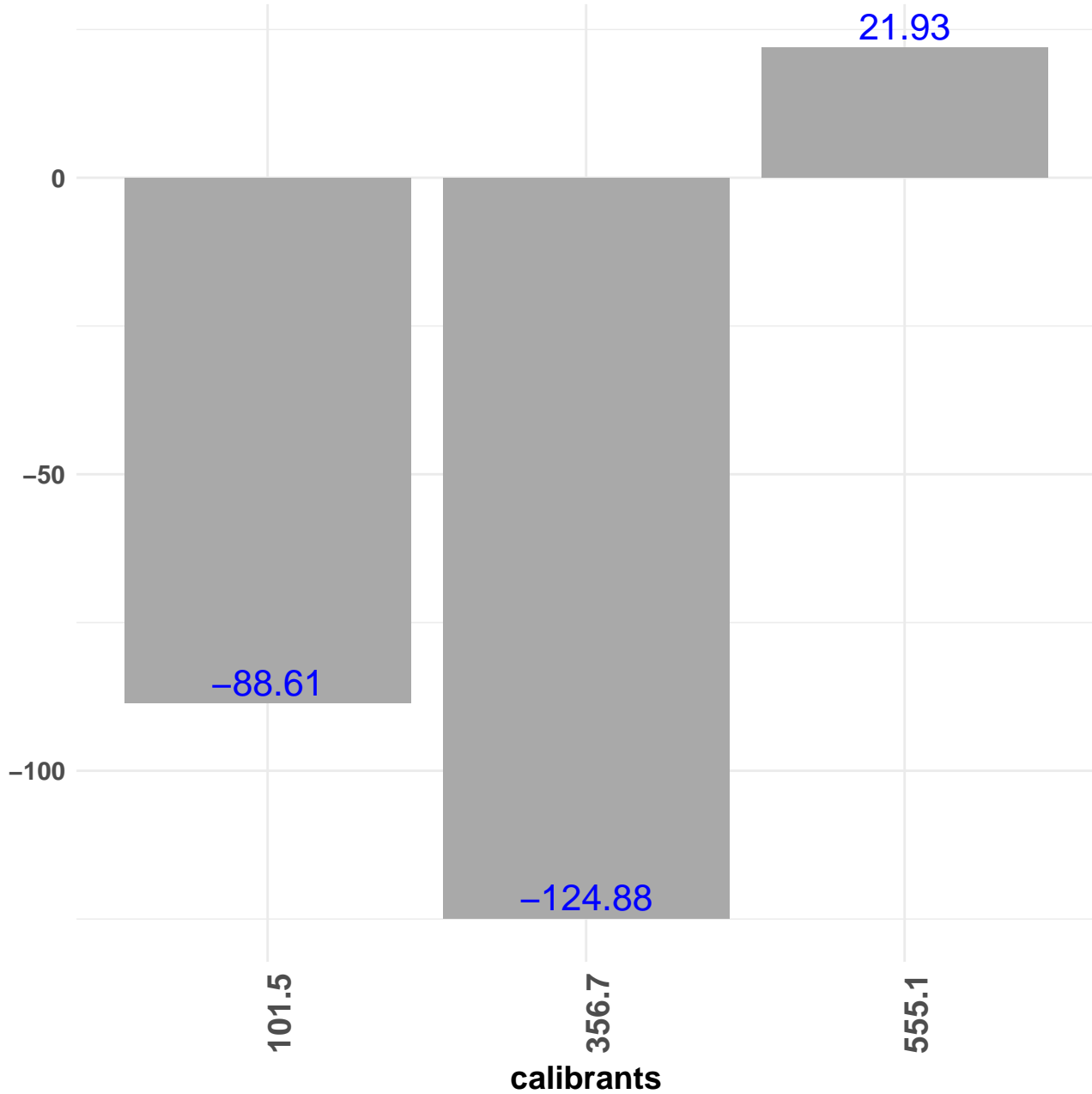


Average m/z error (max. average intensity vs. theor. calibrant m/z)



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)

