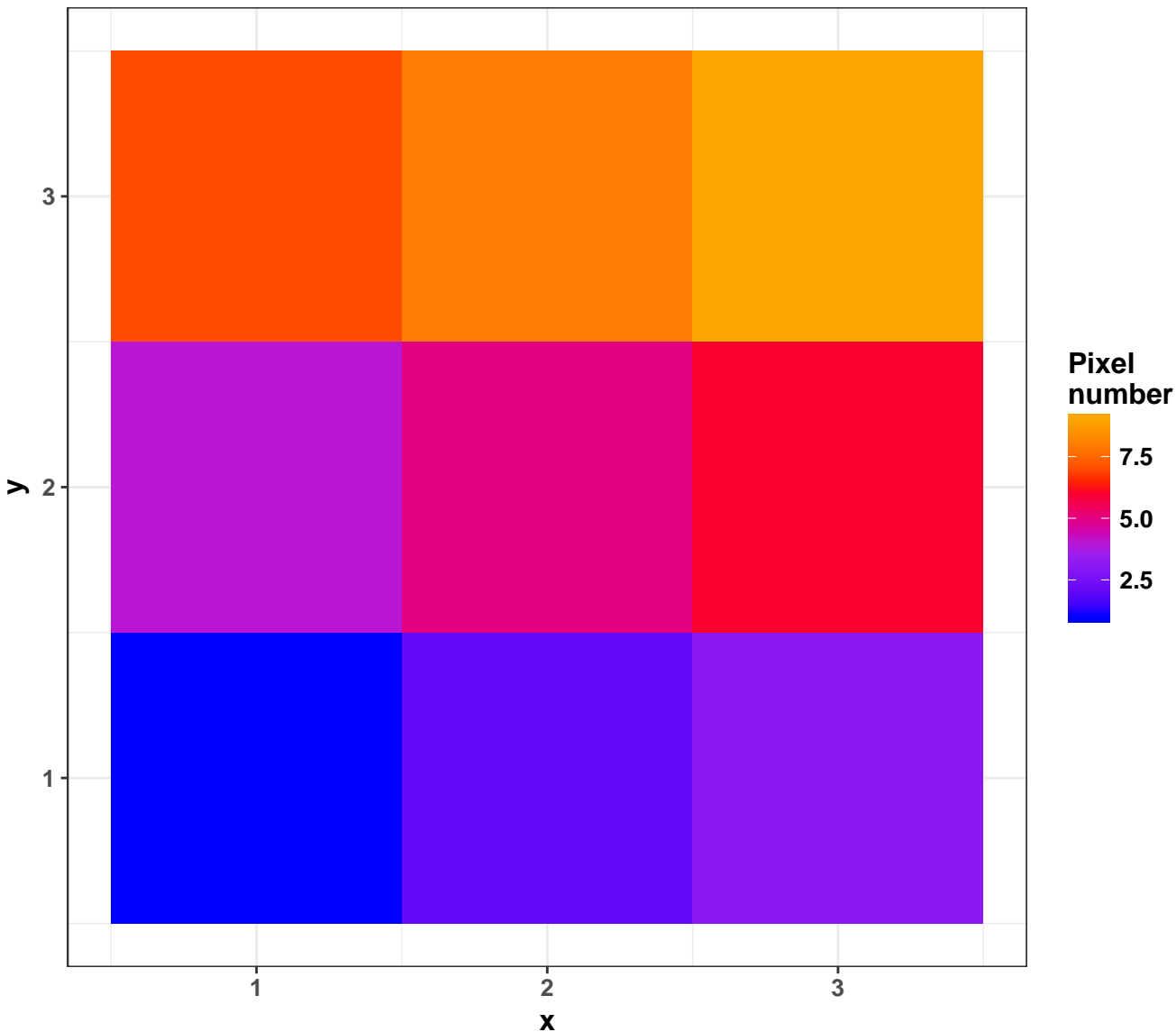


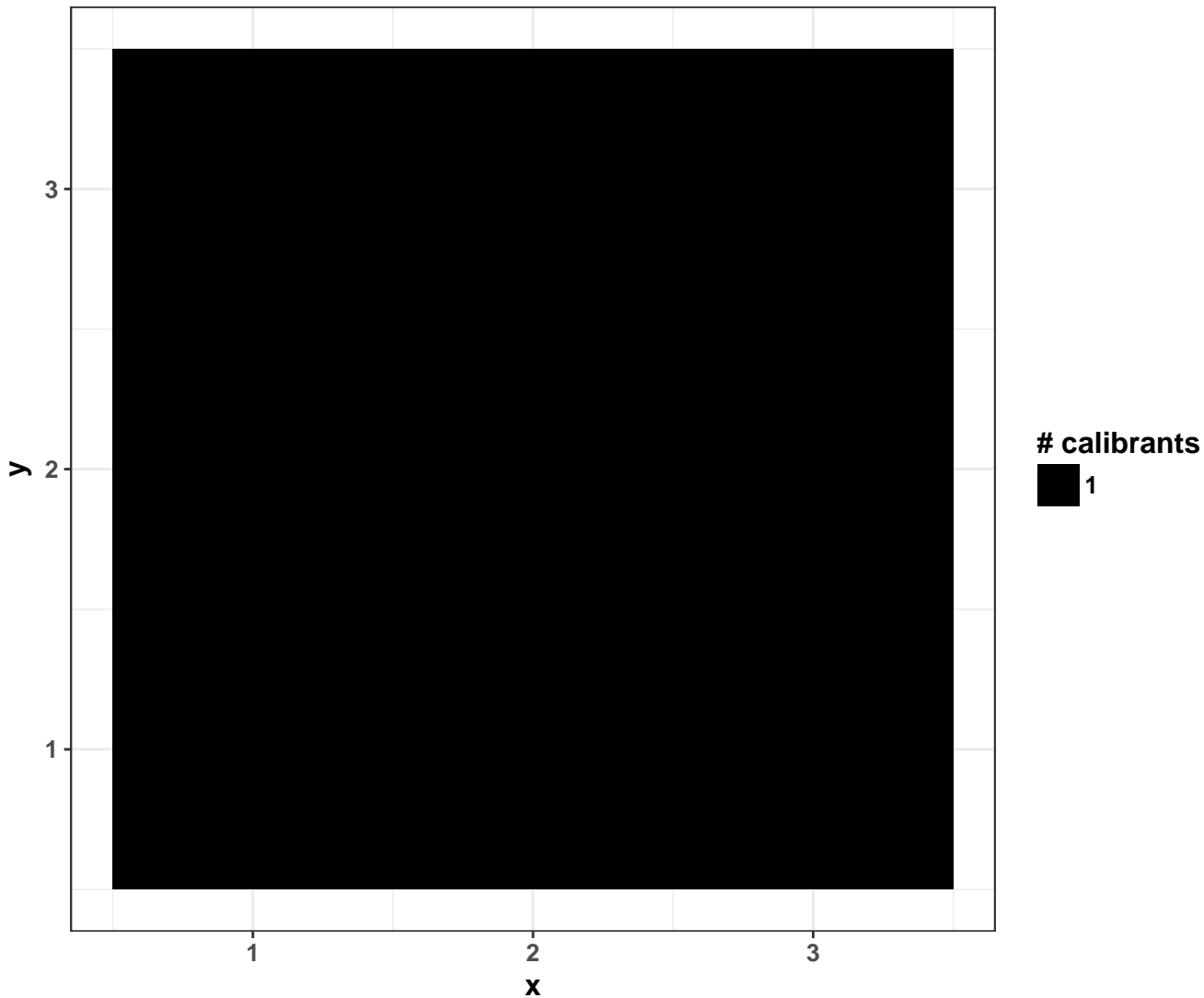
## Testfile\_analyze75

properties	values
Number of m/z features	3672
Range of m/z values	1199.47 – 1356.08
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	3 – 84
Median of intensities	9
Intensities > 0	100 %
Number of empty spectra	0
Median TIC	37005
Median # peaks per spectrum	3672
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile2.txt	1 / 3

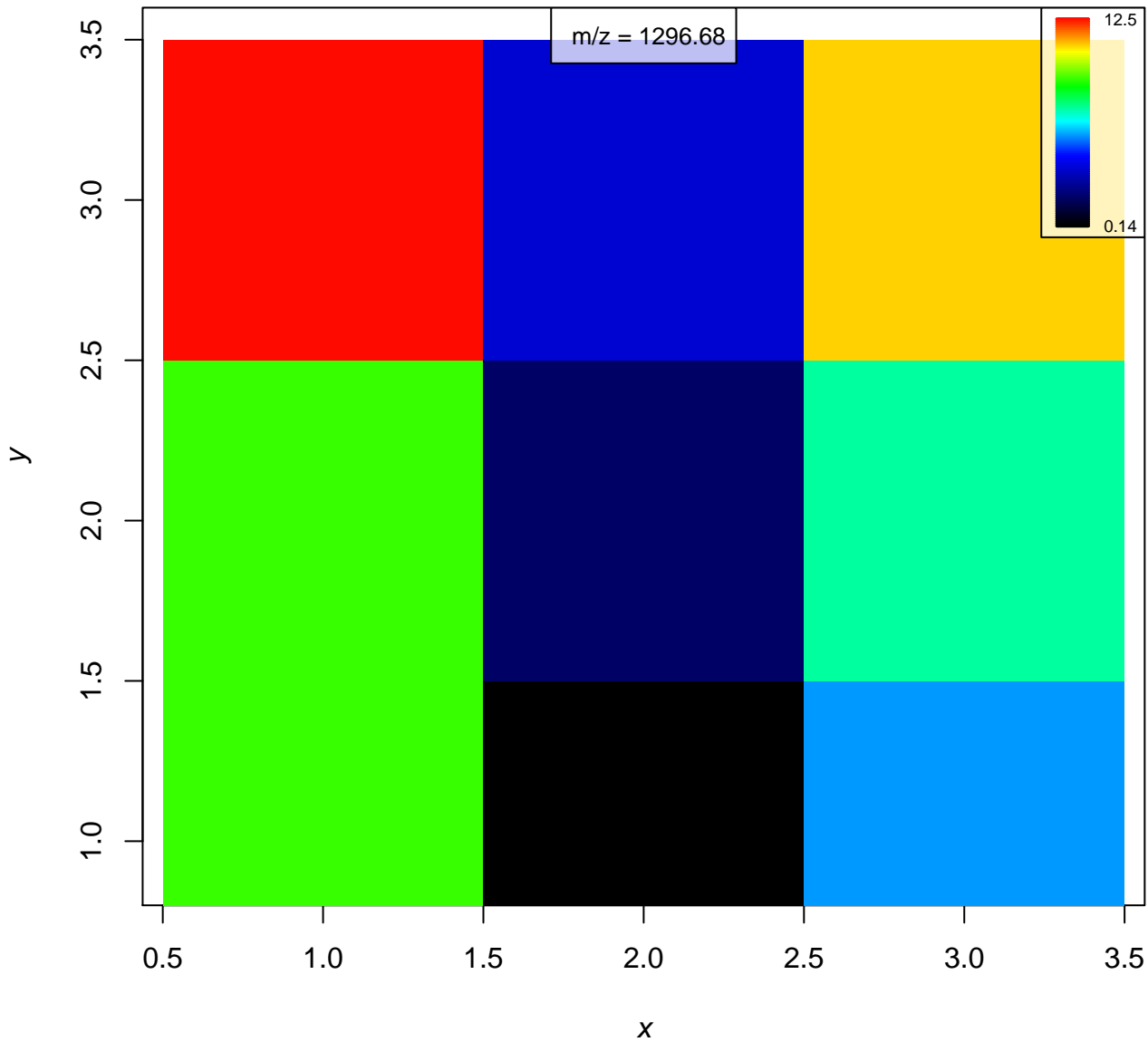
# Pixel order



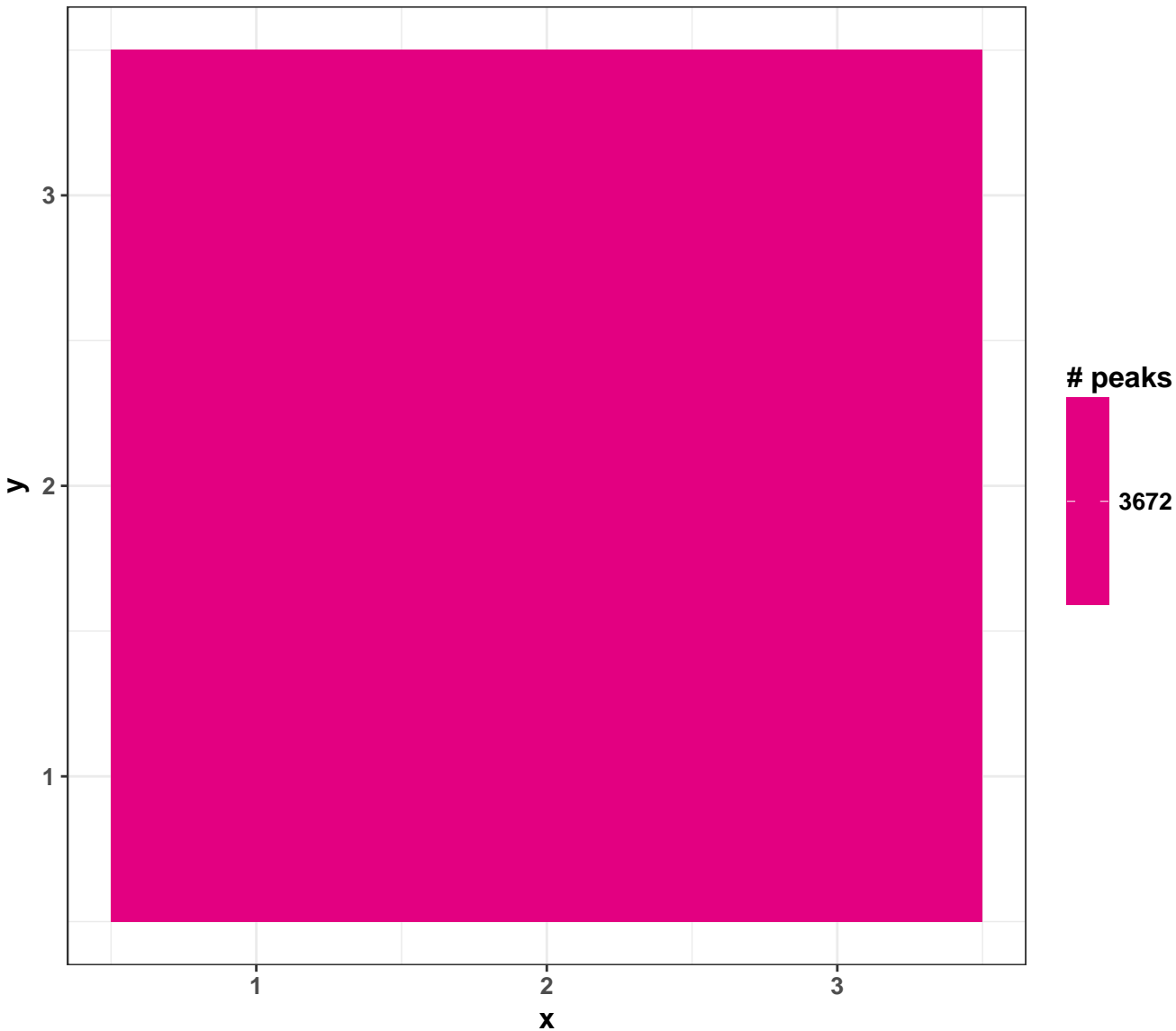
# Number of calibrants per pixel ( $\pm 50$ ppm)



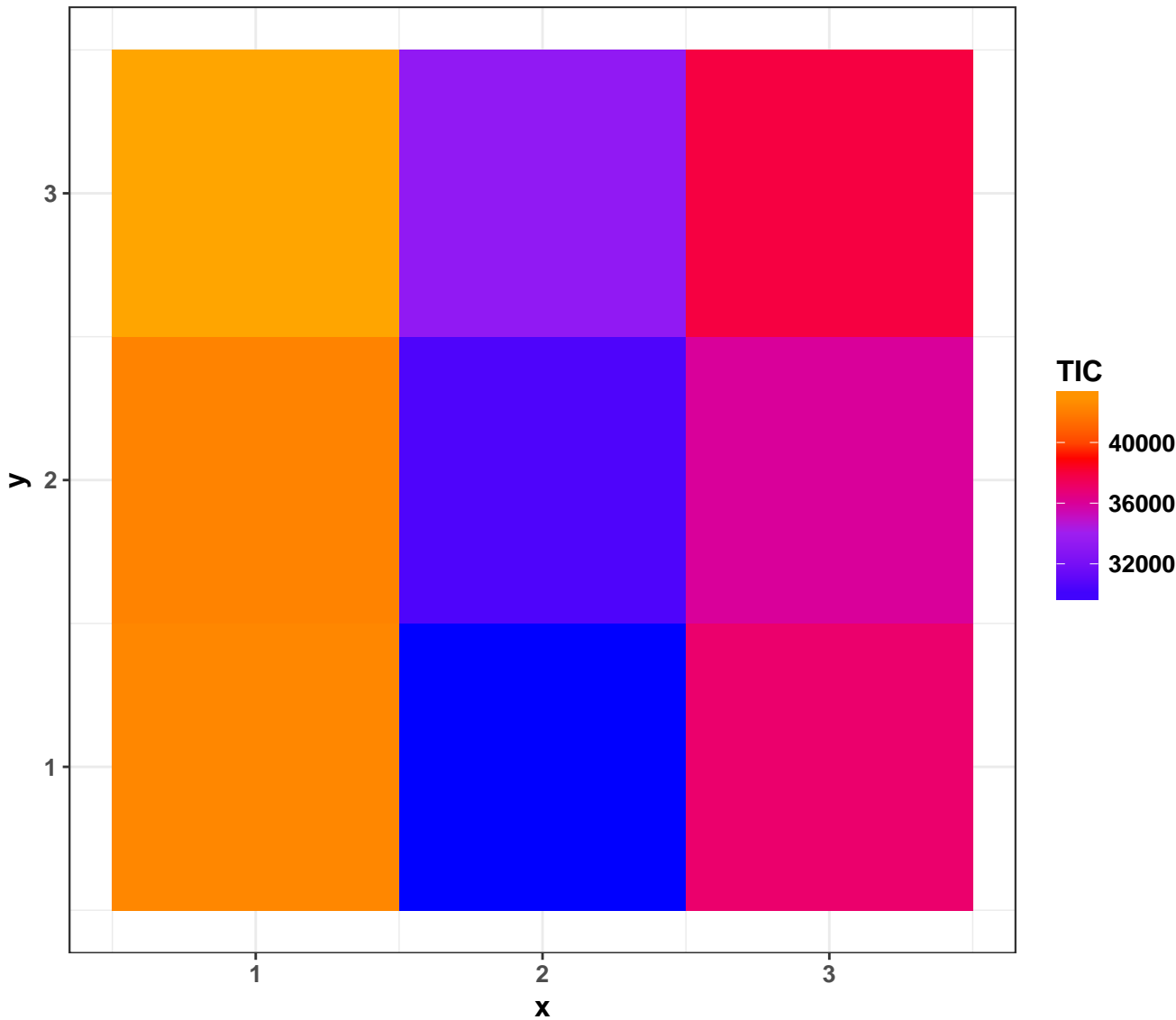
mass3: 1296.7 ( $\pm 50$  ppm)



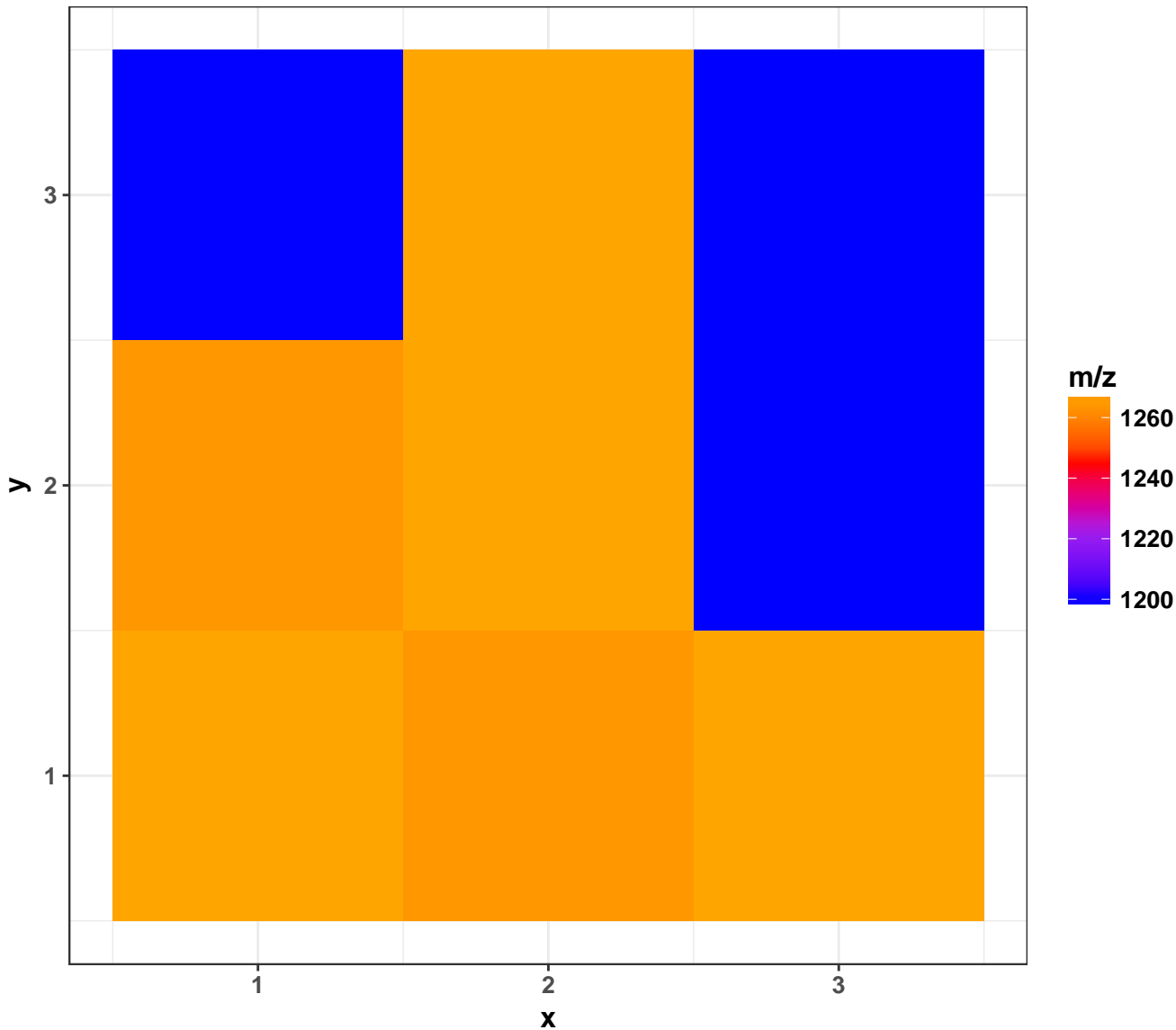
# Number of peaks per spectrum



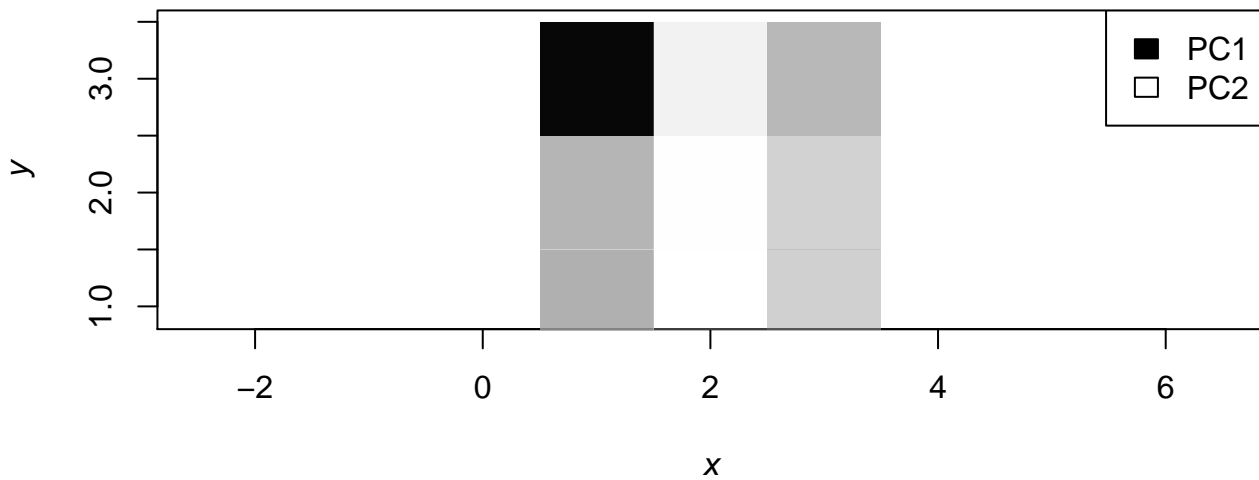
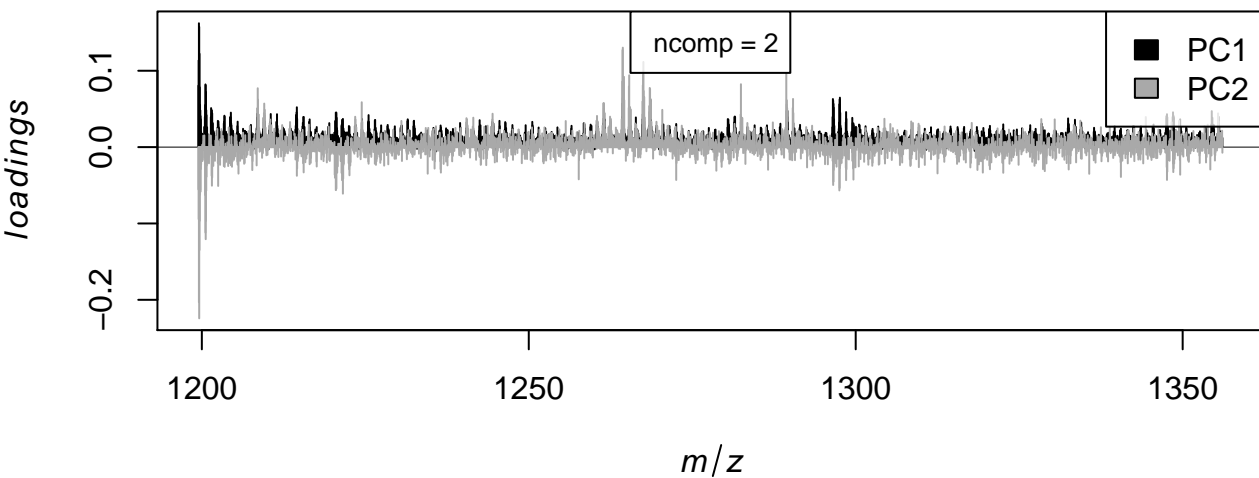
# Total Ion Chromatogram



# Most abundant m/z in each spectrum

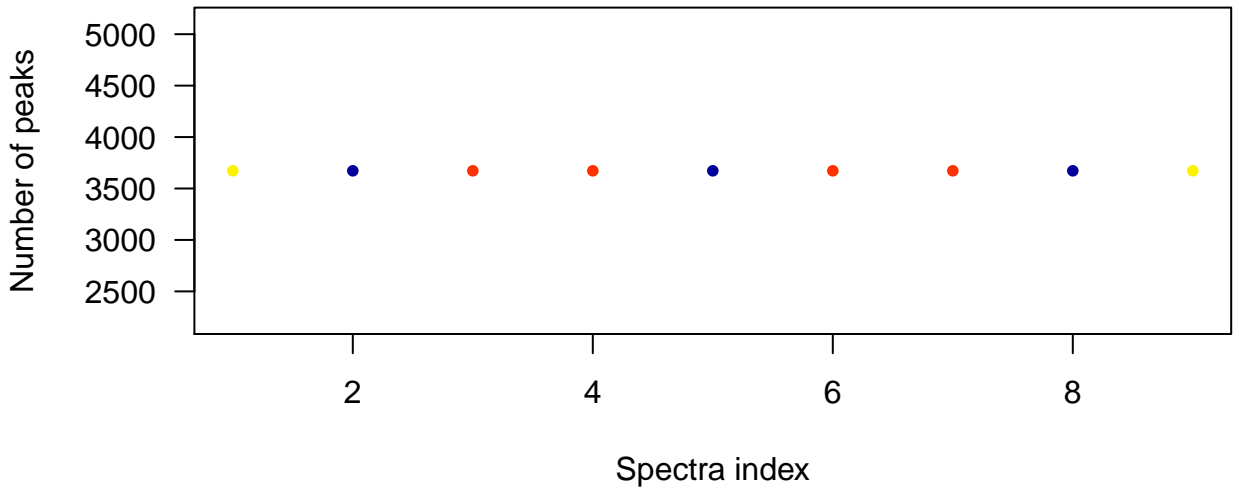


# PCA for two components

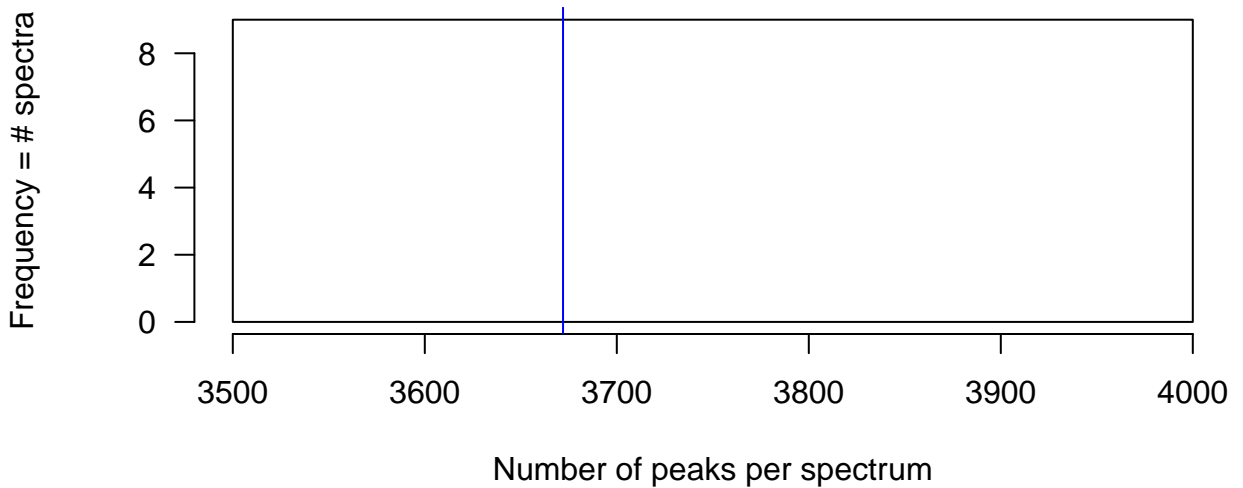




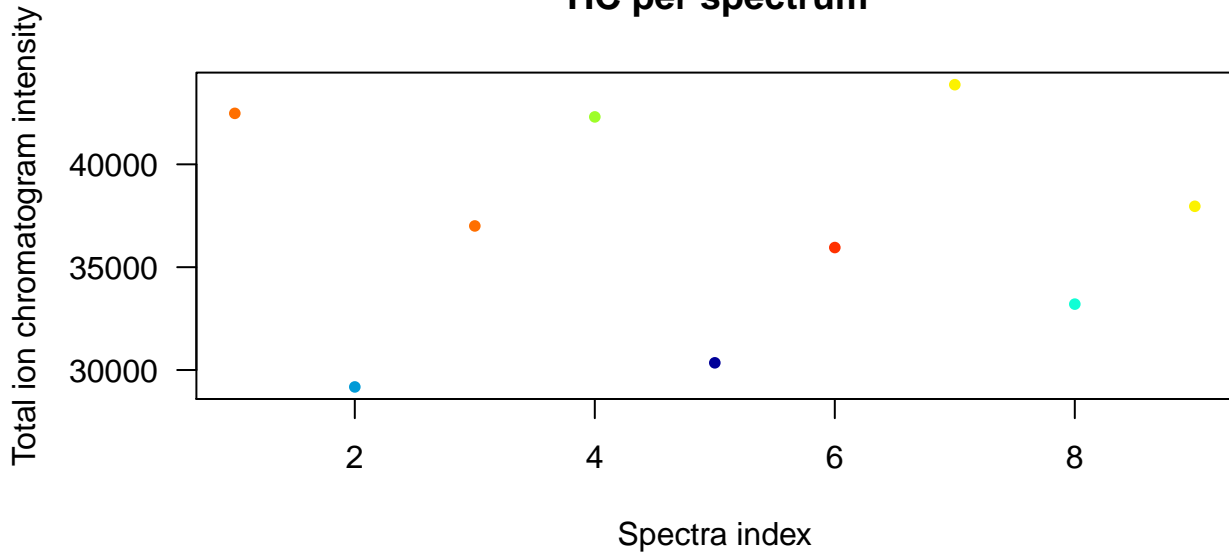
### Number of peaks per spectrum



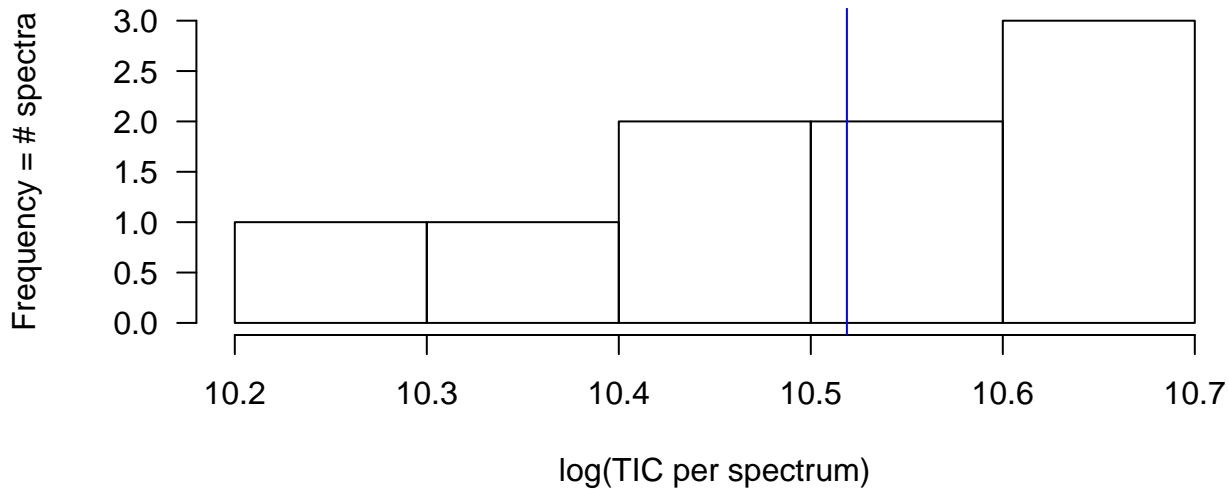
### Number of peaks per spectrum



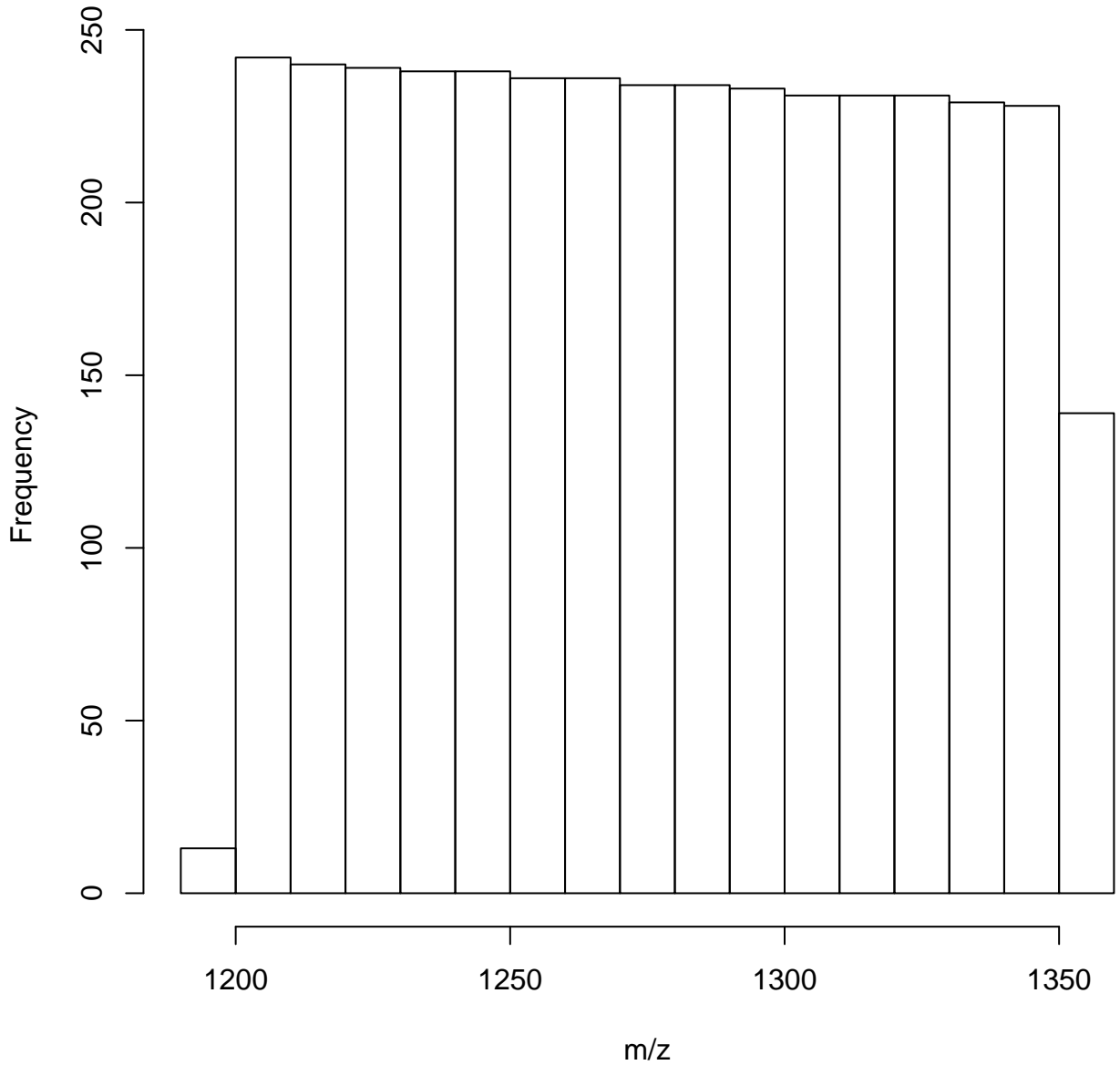
### TIC per spectrum



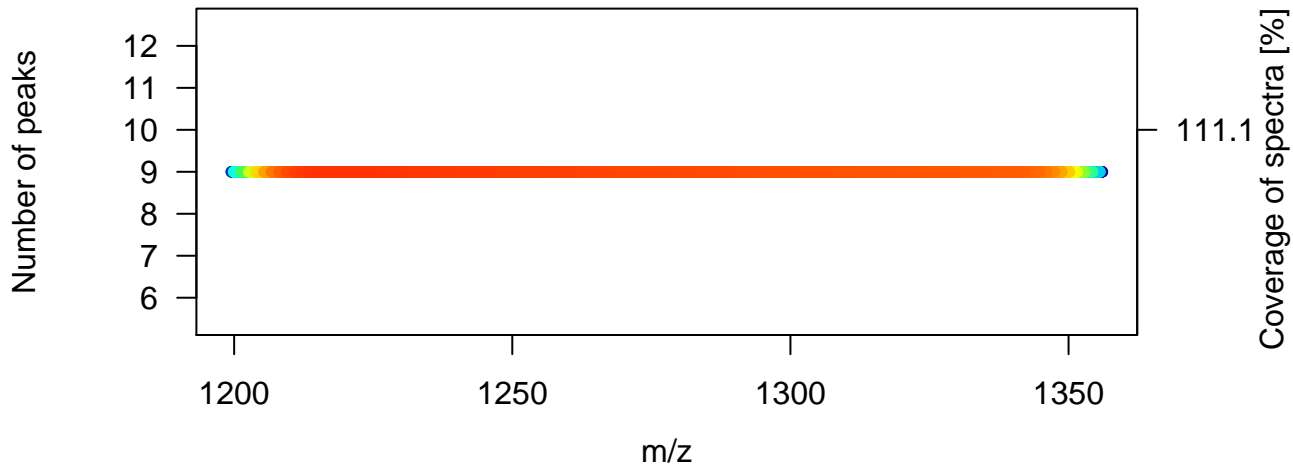
### TIC per spectrum



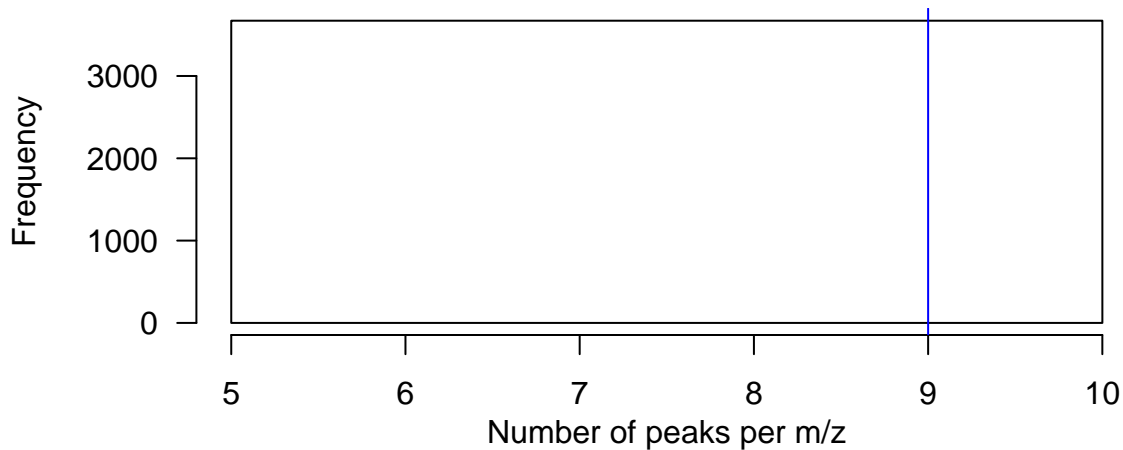
# Histogram of m/z values



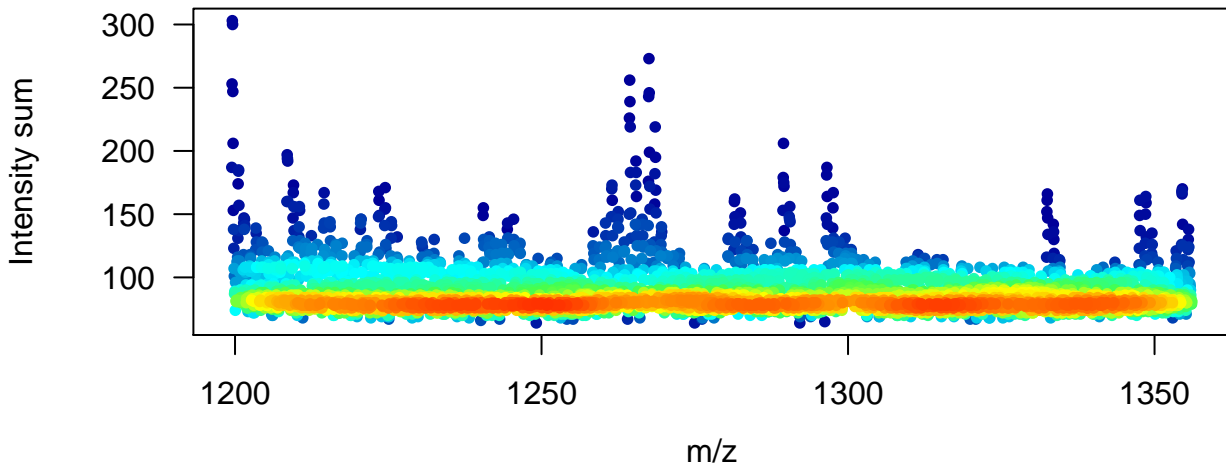
### Number of peaks per m/z



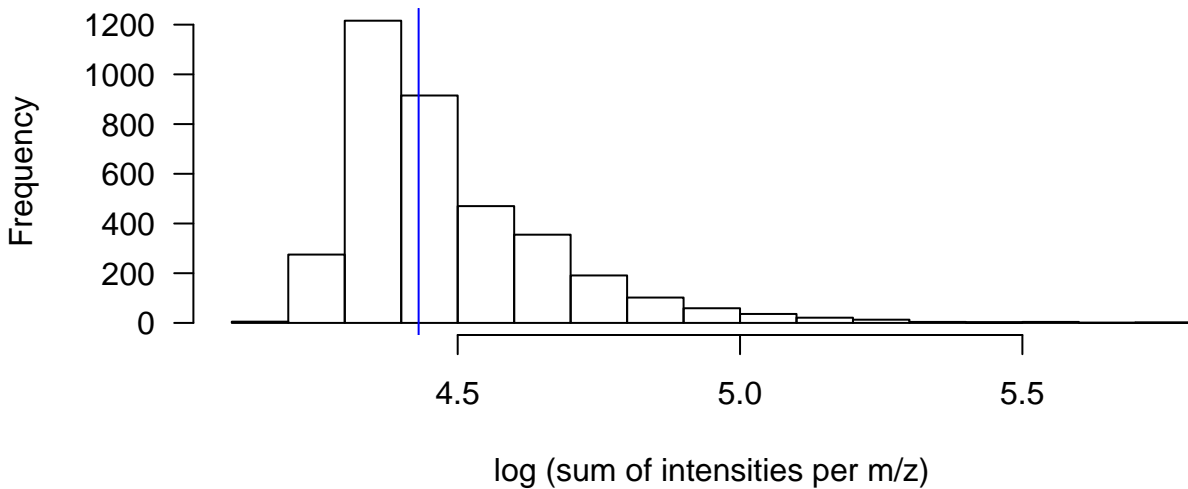
### Number of peaks per m/z



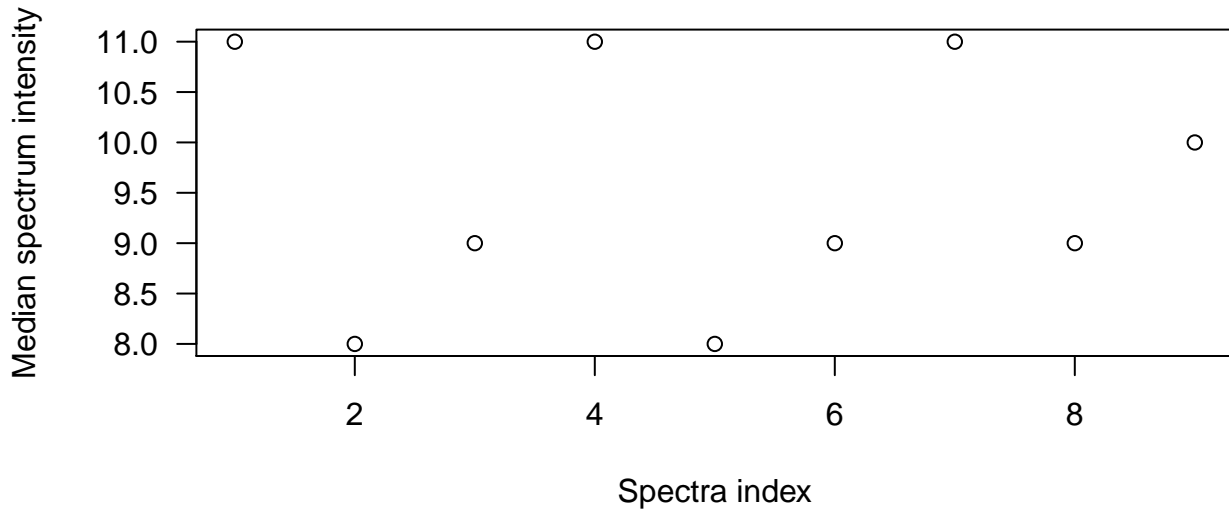
Sum of intensities per m/z



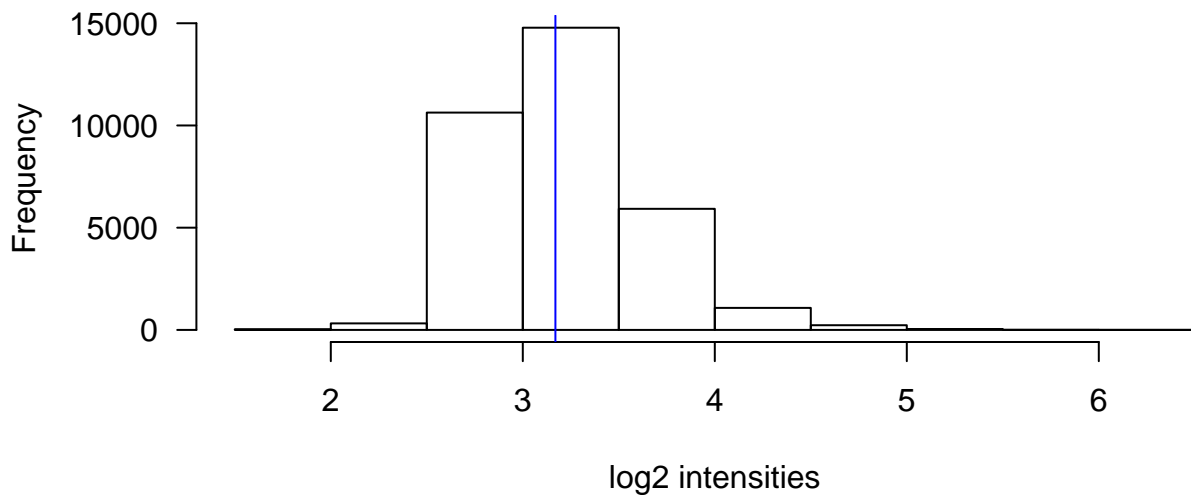
Sum of intensities per m/z



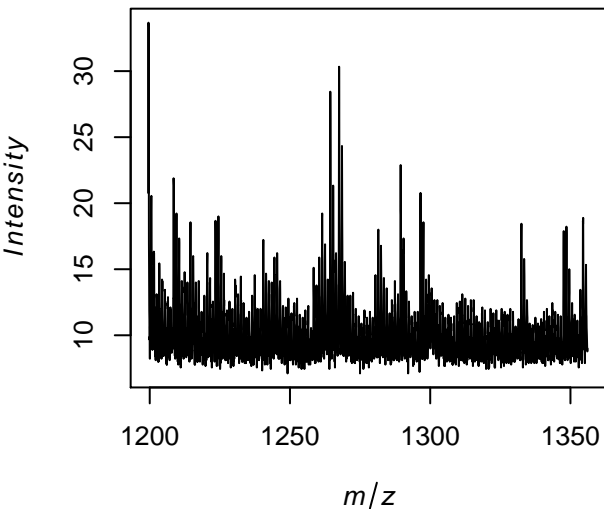
## Median intensity per spectrum



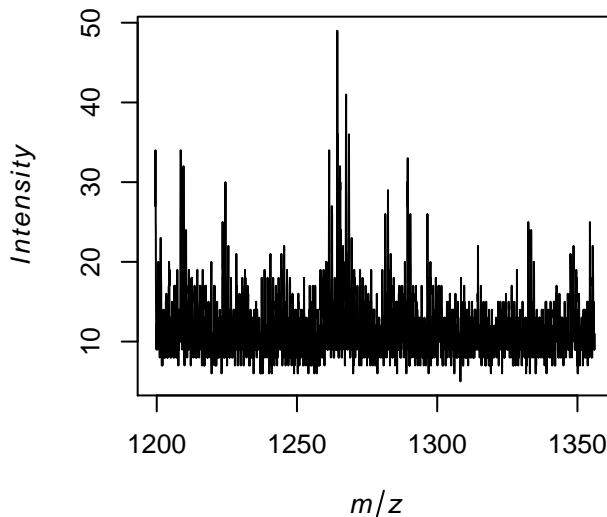
## Log2-transformed intensities



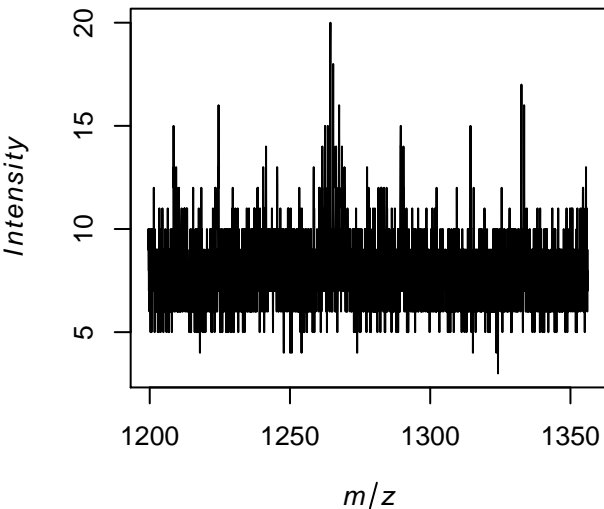
**Average spectrum**



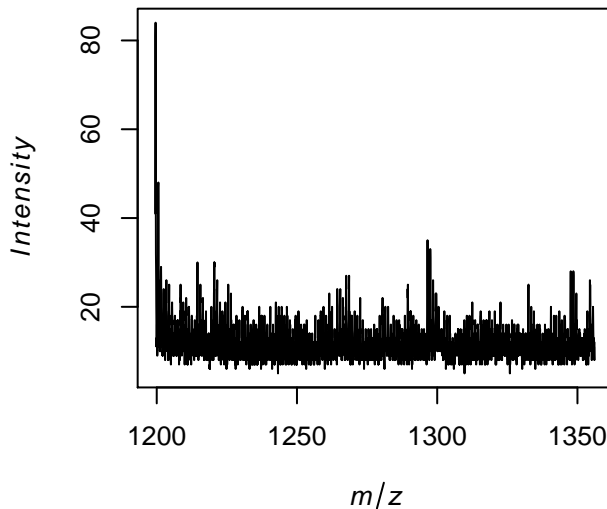
**Spectrum at  $x = 1, y = 2$**



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



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

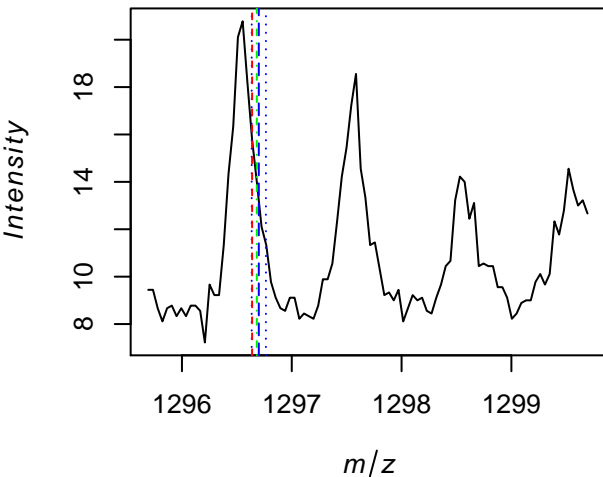


theor. m/z: 1296.7

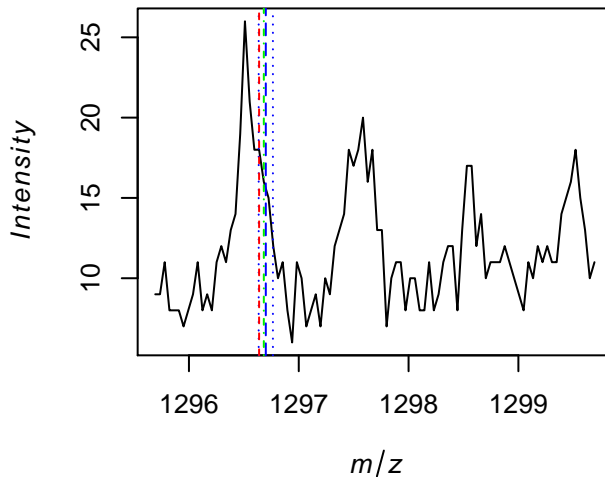
most abundant m/z: 1296.6389

closest m/z: 1296.6819

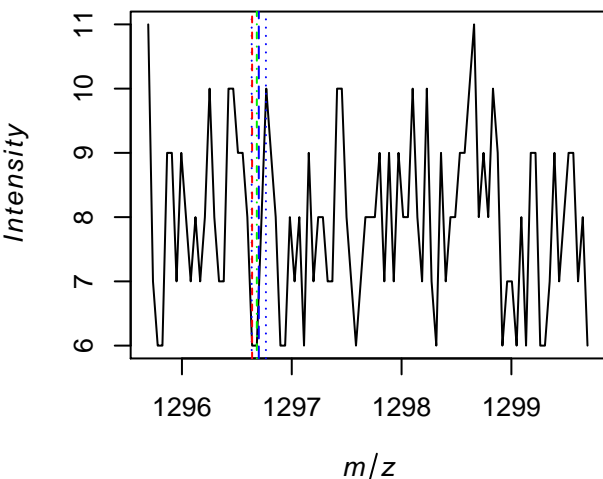
average spectrum



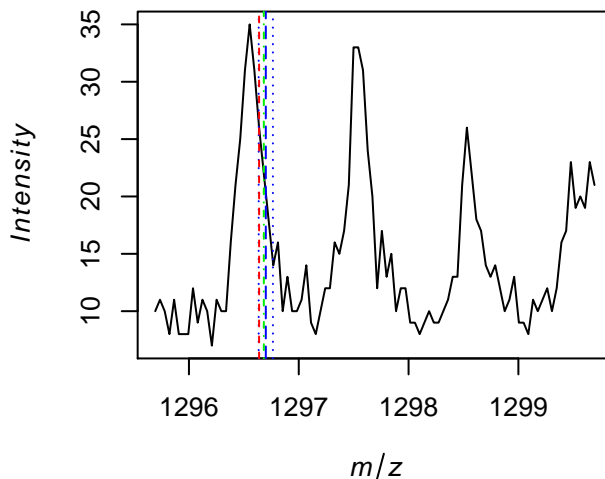
Spectrum at x = 1, y = 2



Spectrum at x = 2, y = 1

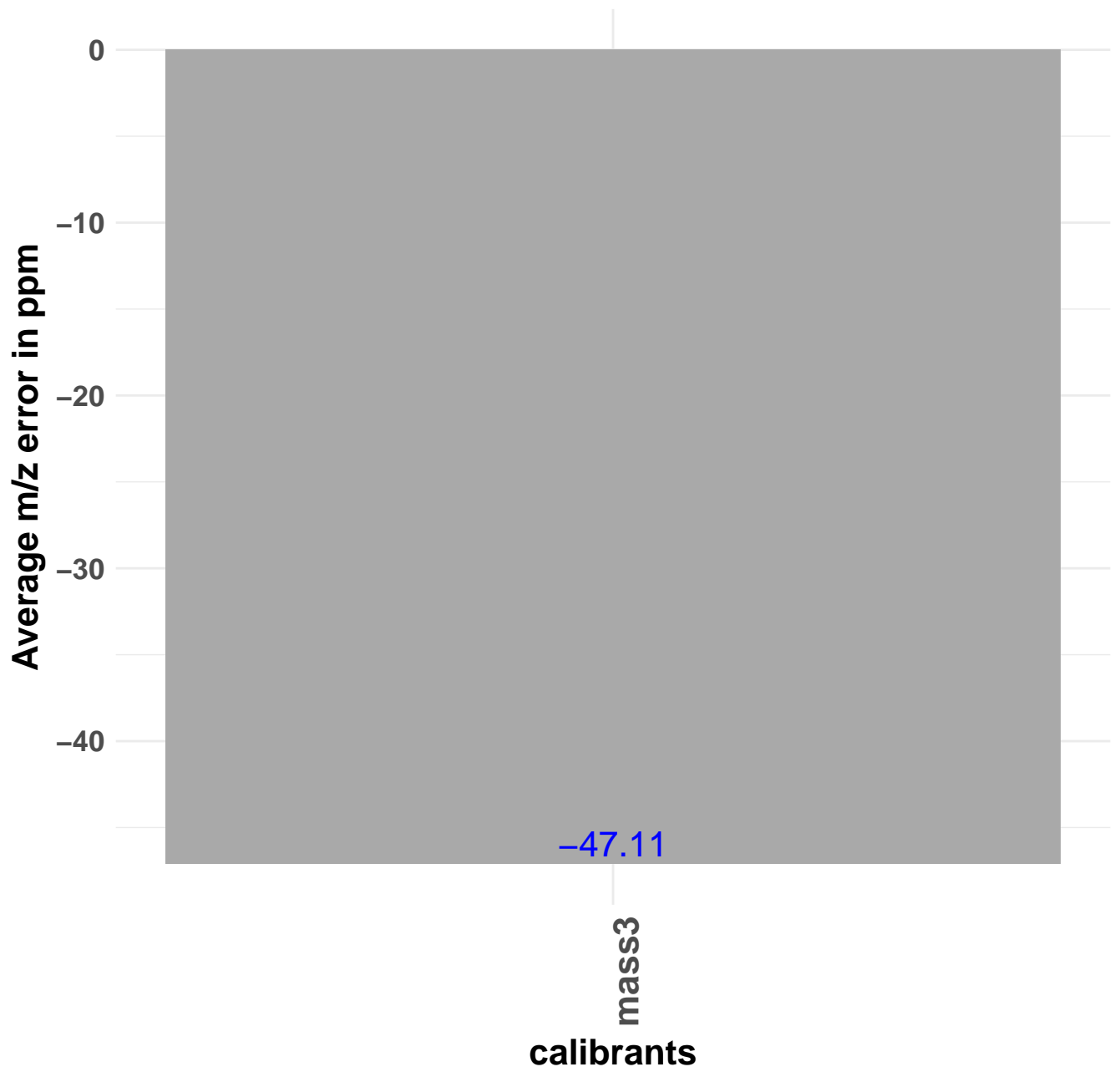


Spectrum at x = 1, y = 3

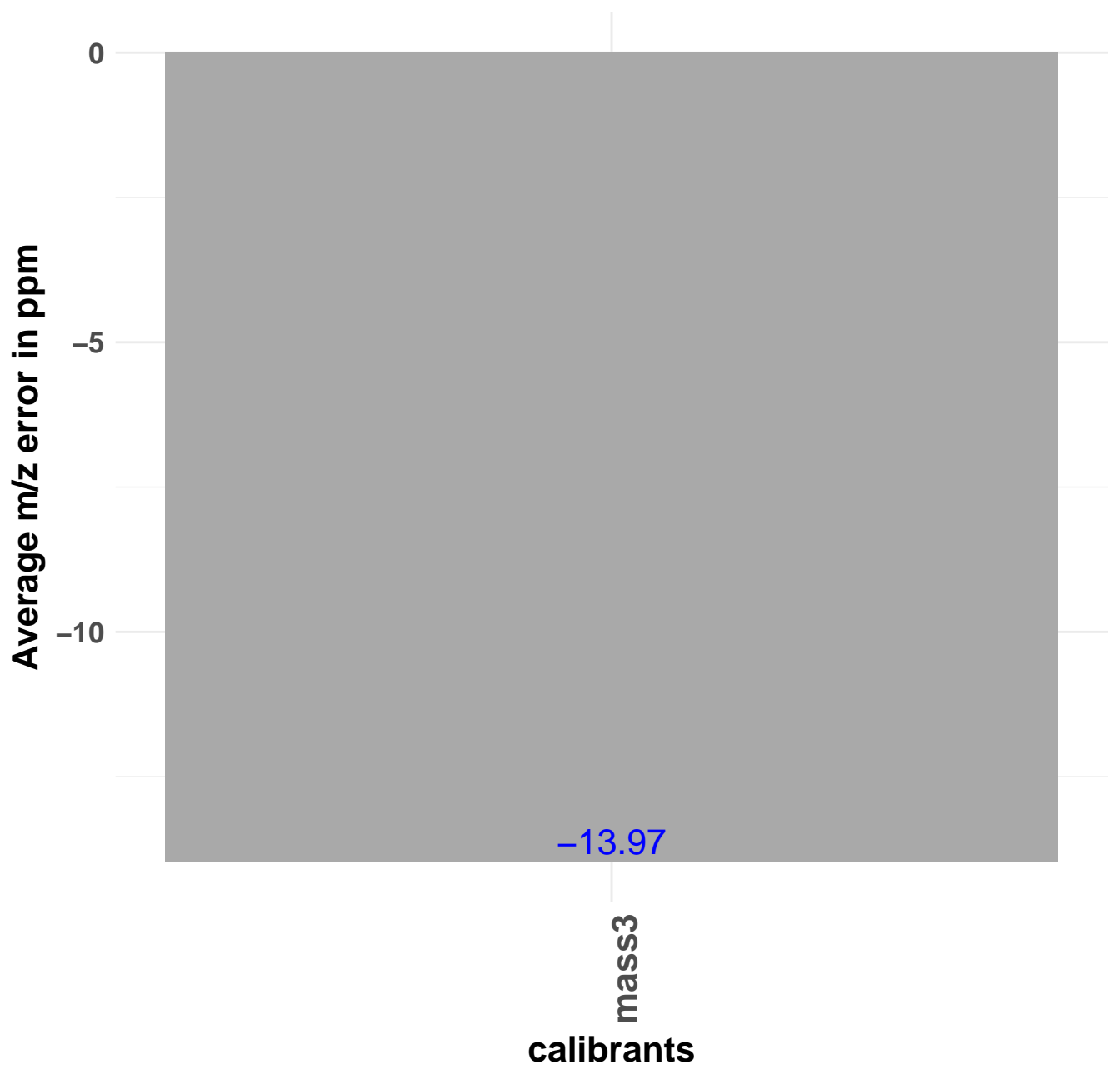




# Average m/z error (max. average intensity vs. theor. calibrant m/z)



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)

