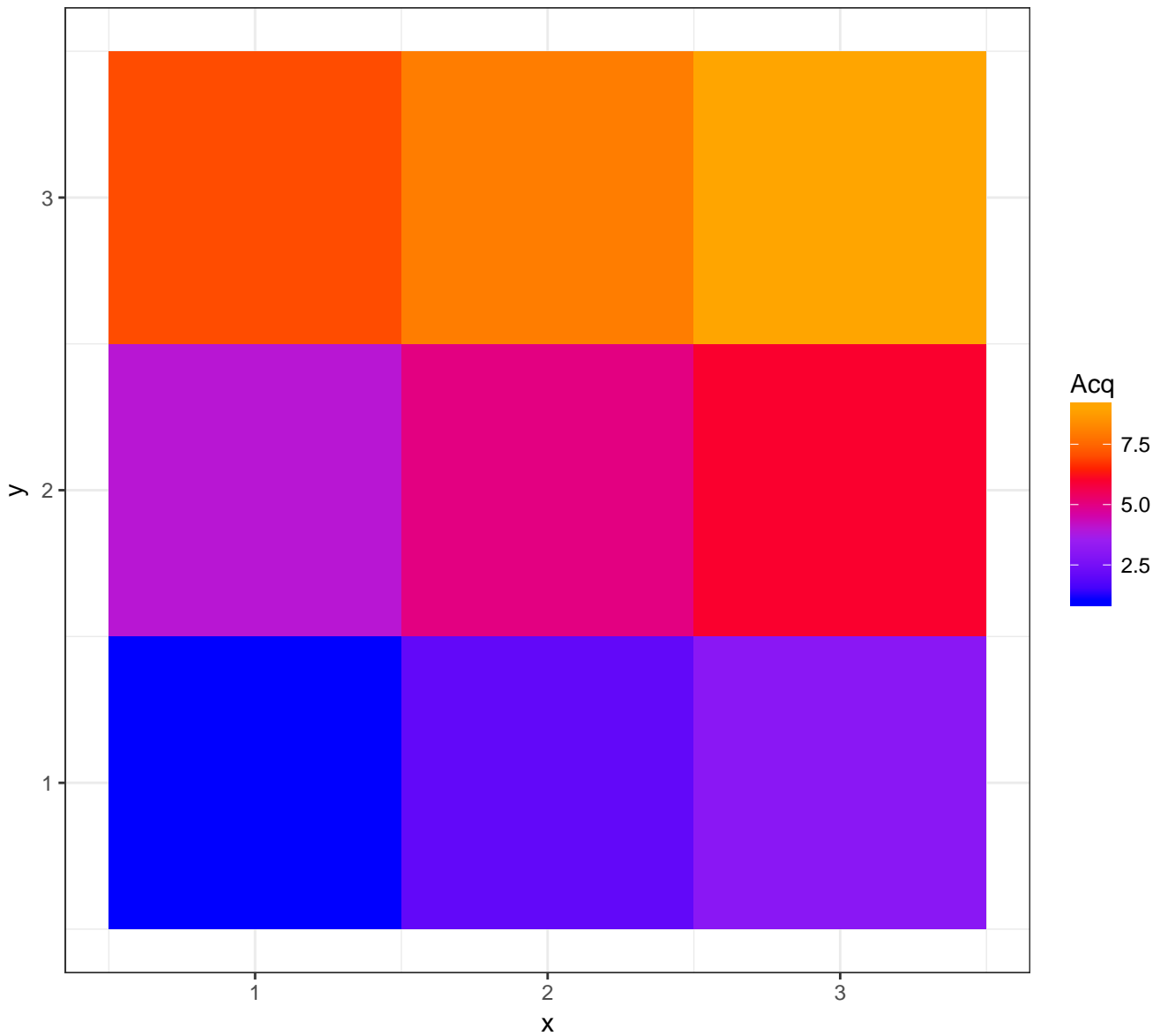


# Quality control of MSI data

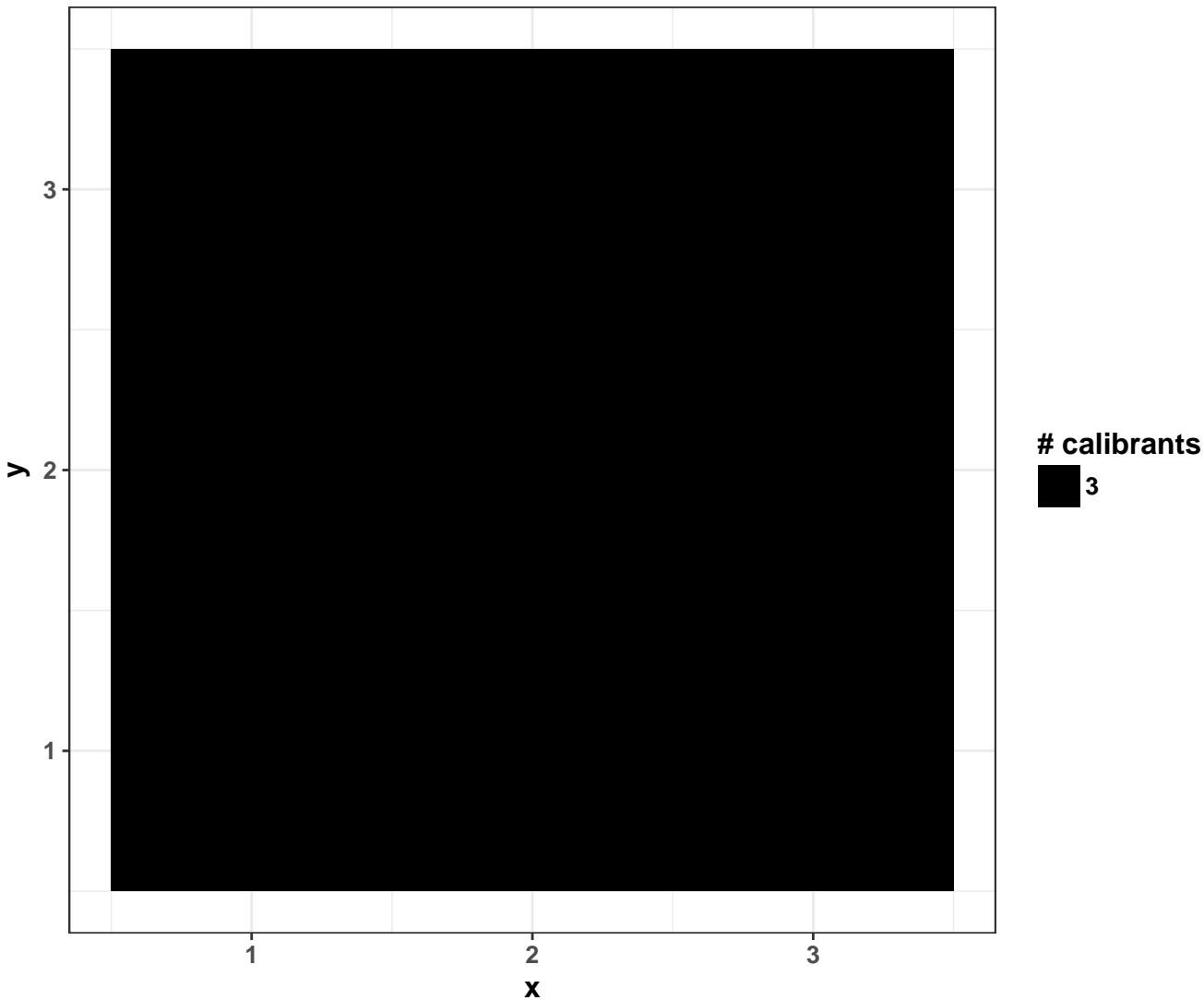
## Filename: Testfile\_analyze75

properties	values
Number of mz features	58031
Range of mz values [Da]	699.75 – 1916.29
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	0 – 146
Median of intensities	0
Intensities > 0	28.02 %
Number of zero TICs	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in inputpeptides.txt	2 / 3
# calibrants in inputcalibrantfile2.txt	3 / 3

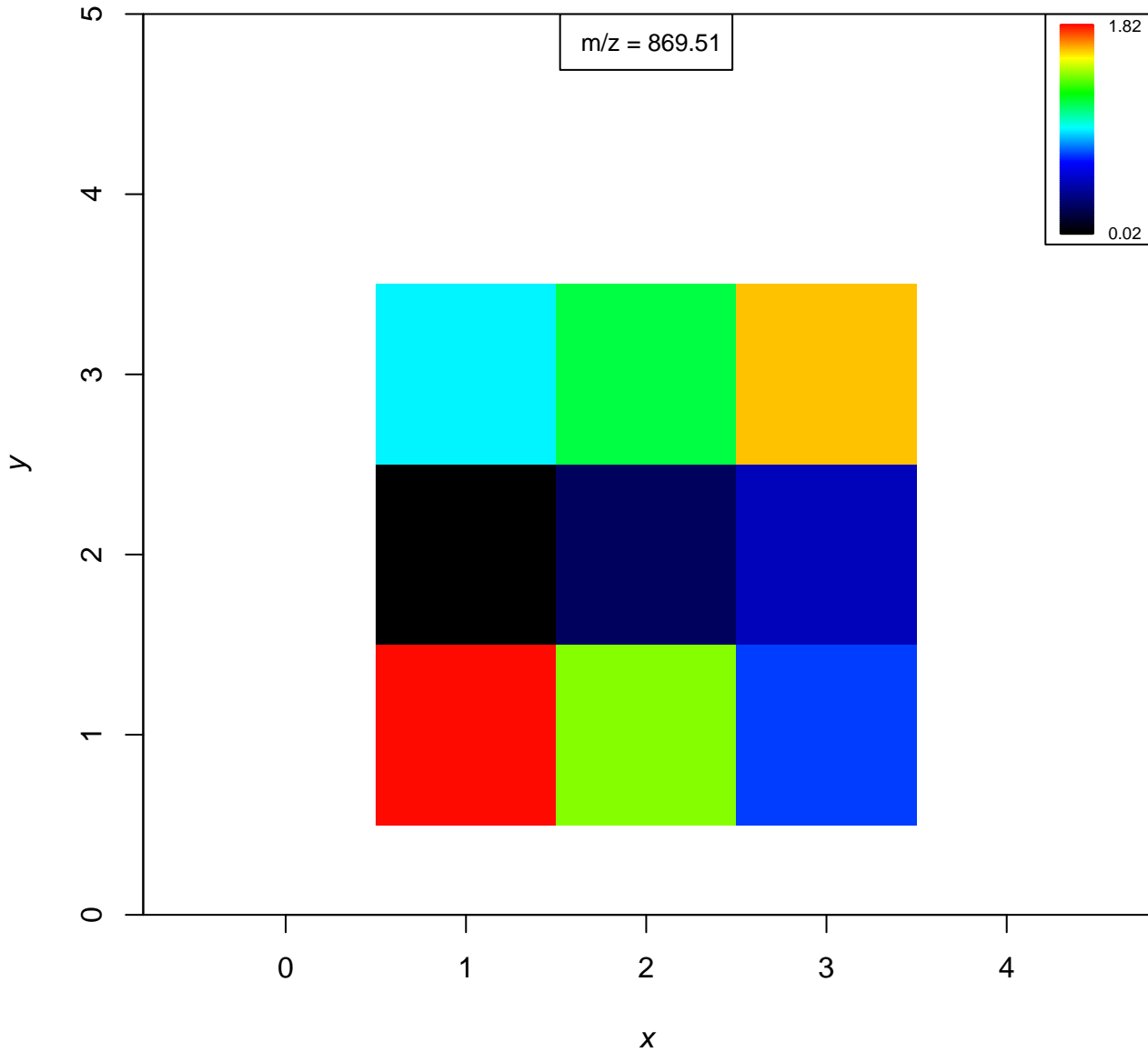
Order of Acquisition



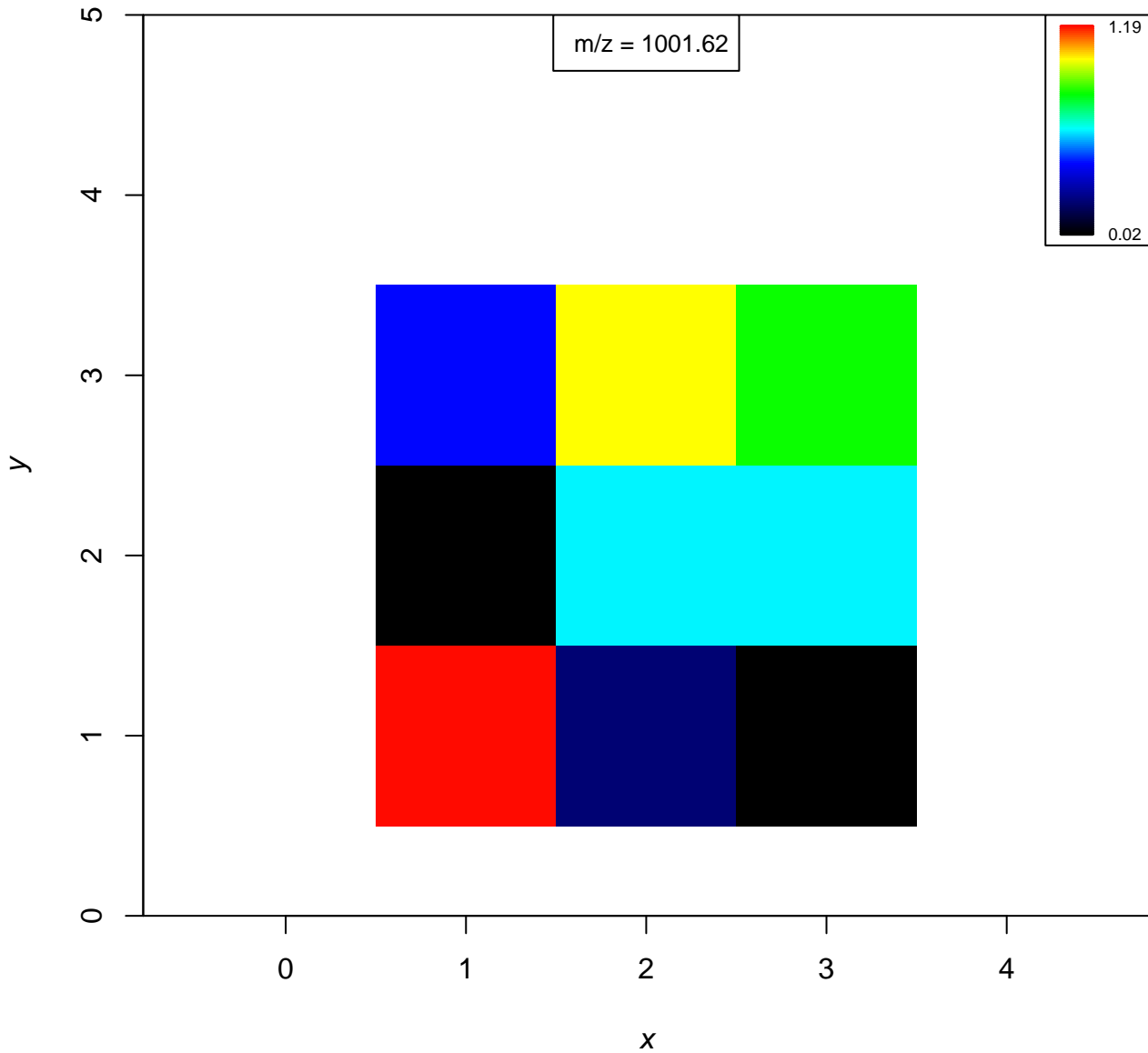
# Number of calibrants per pixel



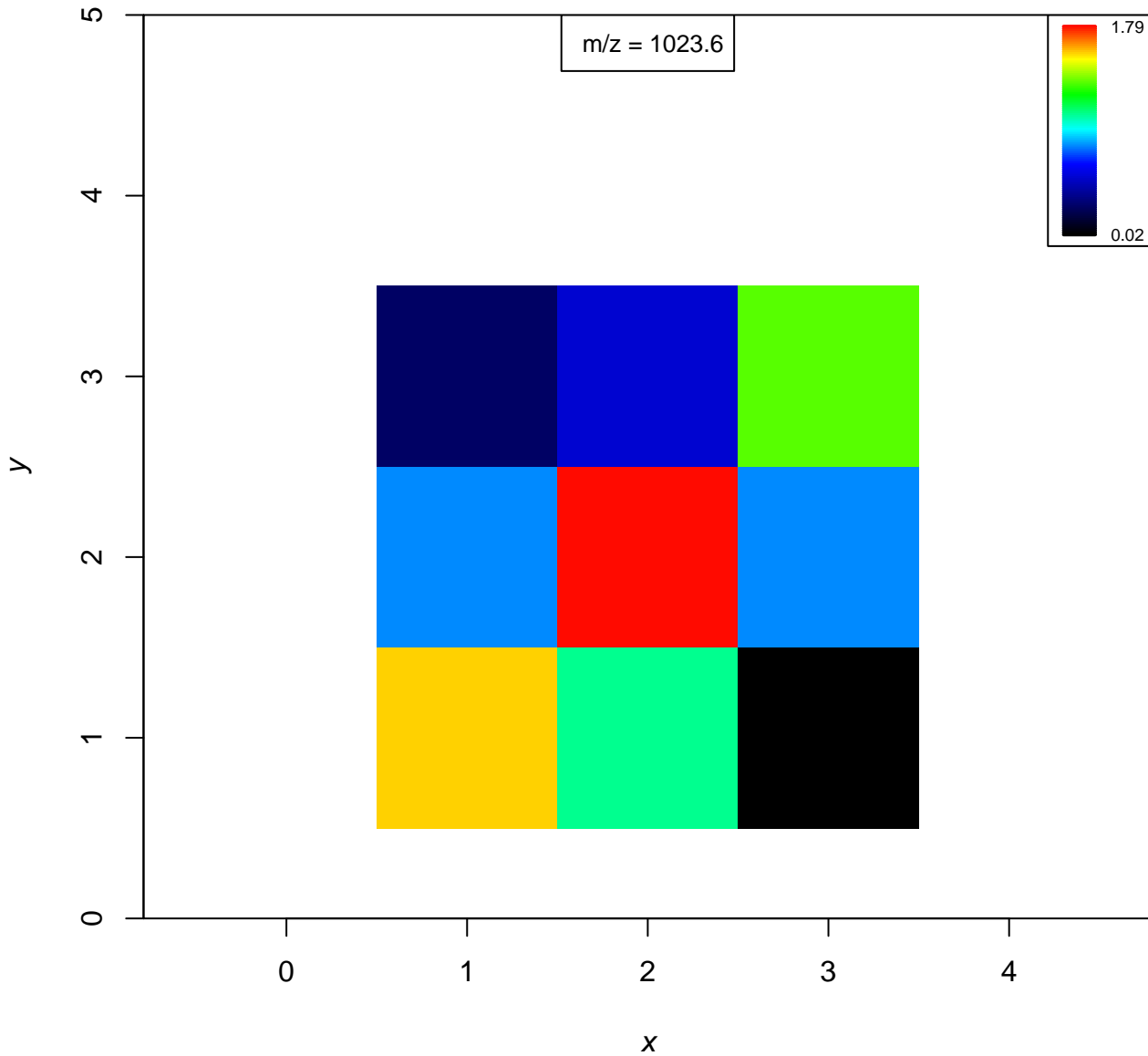
# mass1 (869.51 ± 0.5 Da)



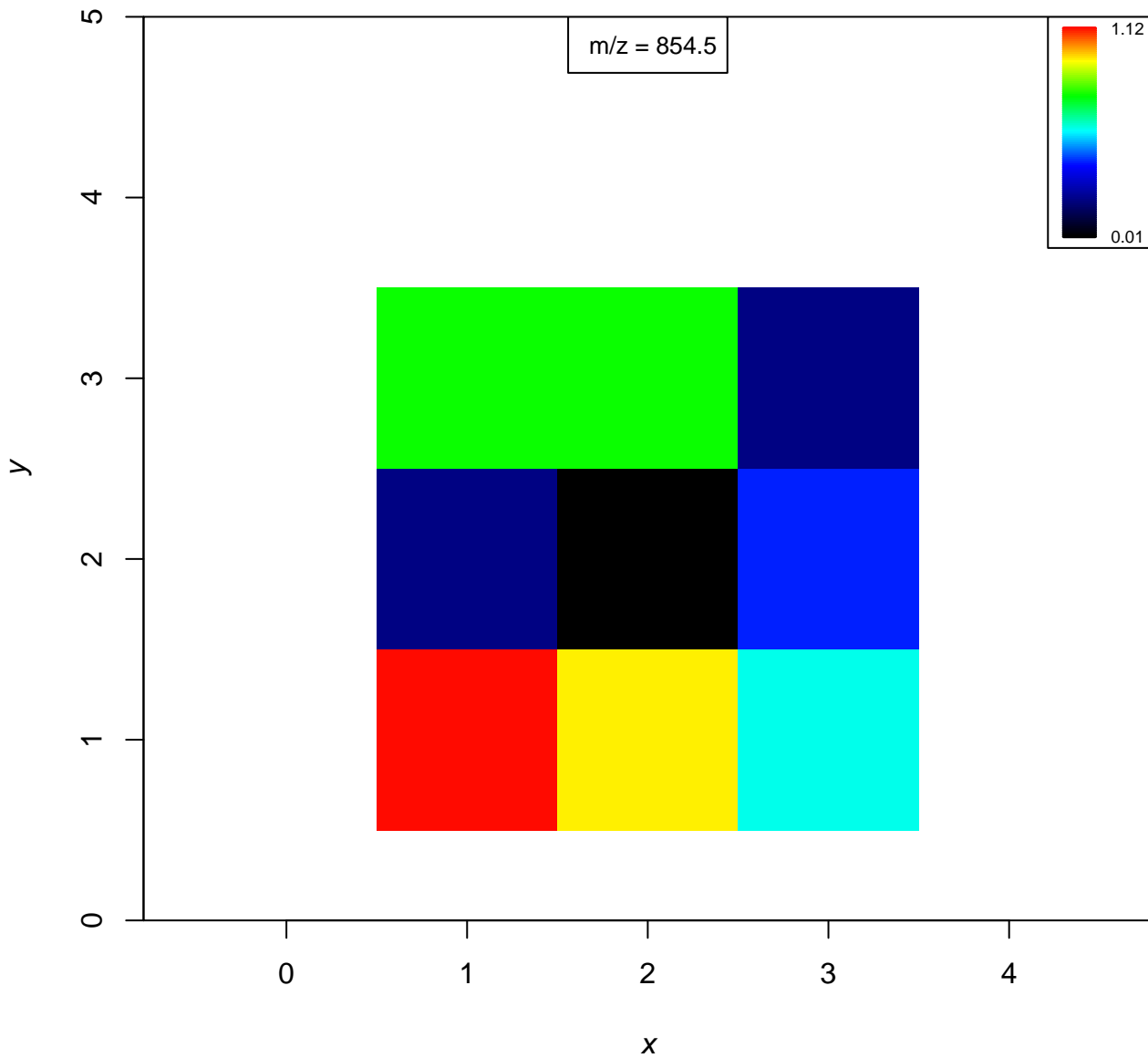
# mass2 (1001.62 ± 0.5 Da)



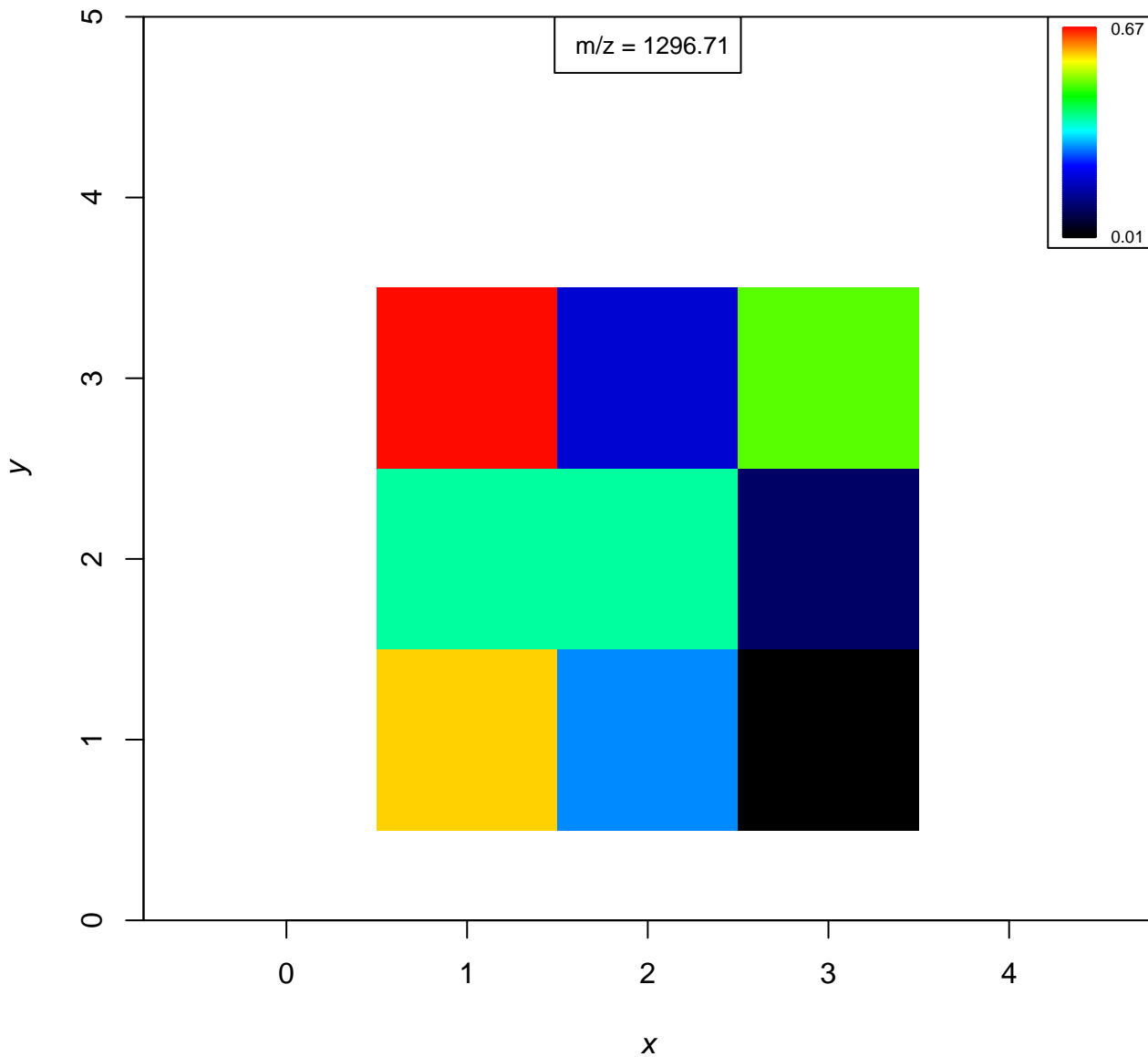
# mass3 (1023.6 ± 0.5 Da)



# 854.5 (854.5 ± 0.5 Da)

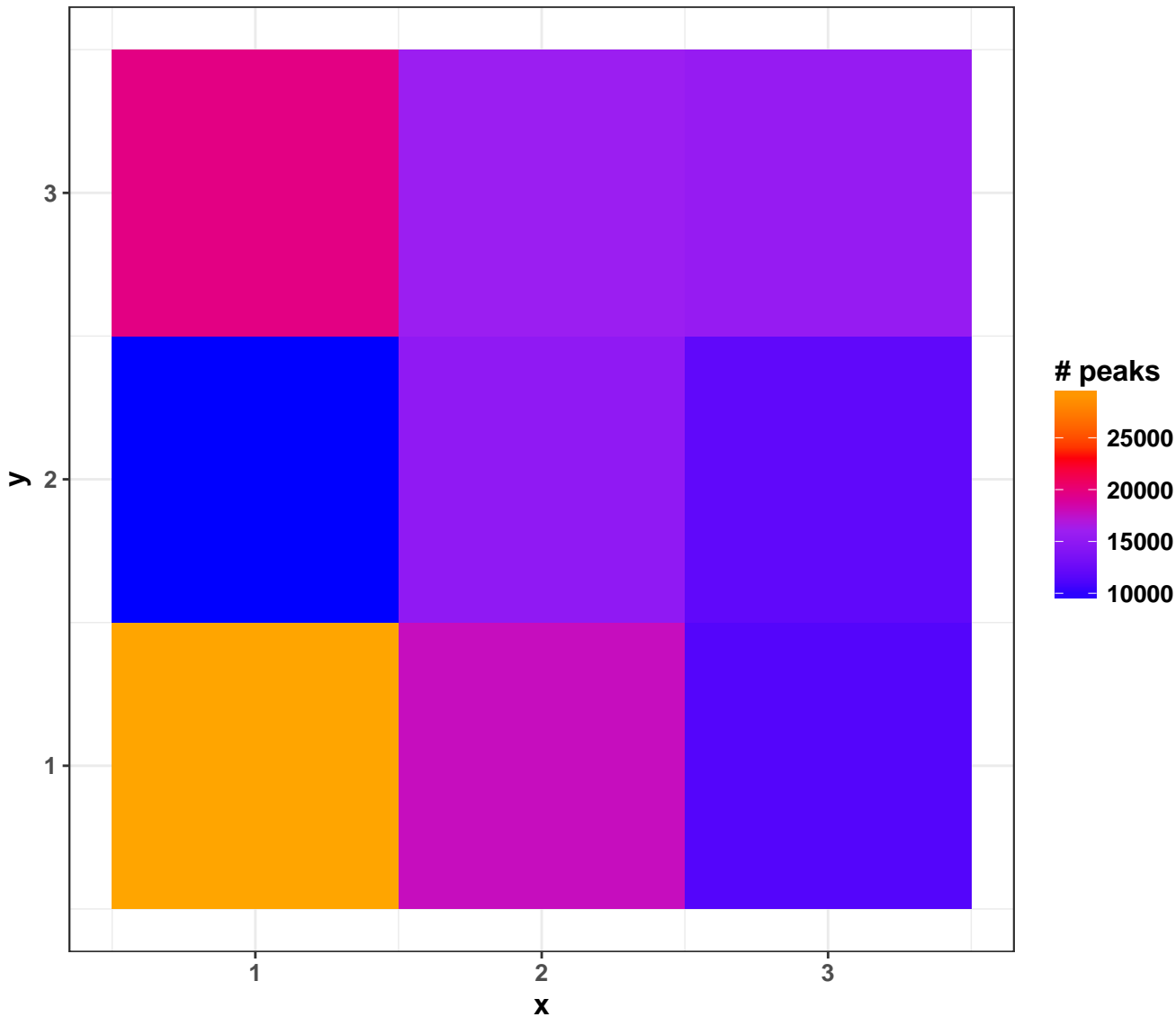


# 1296.7 (1296.7 ± 0.5 Da)

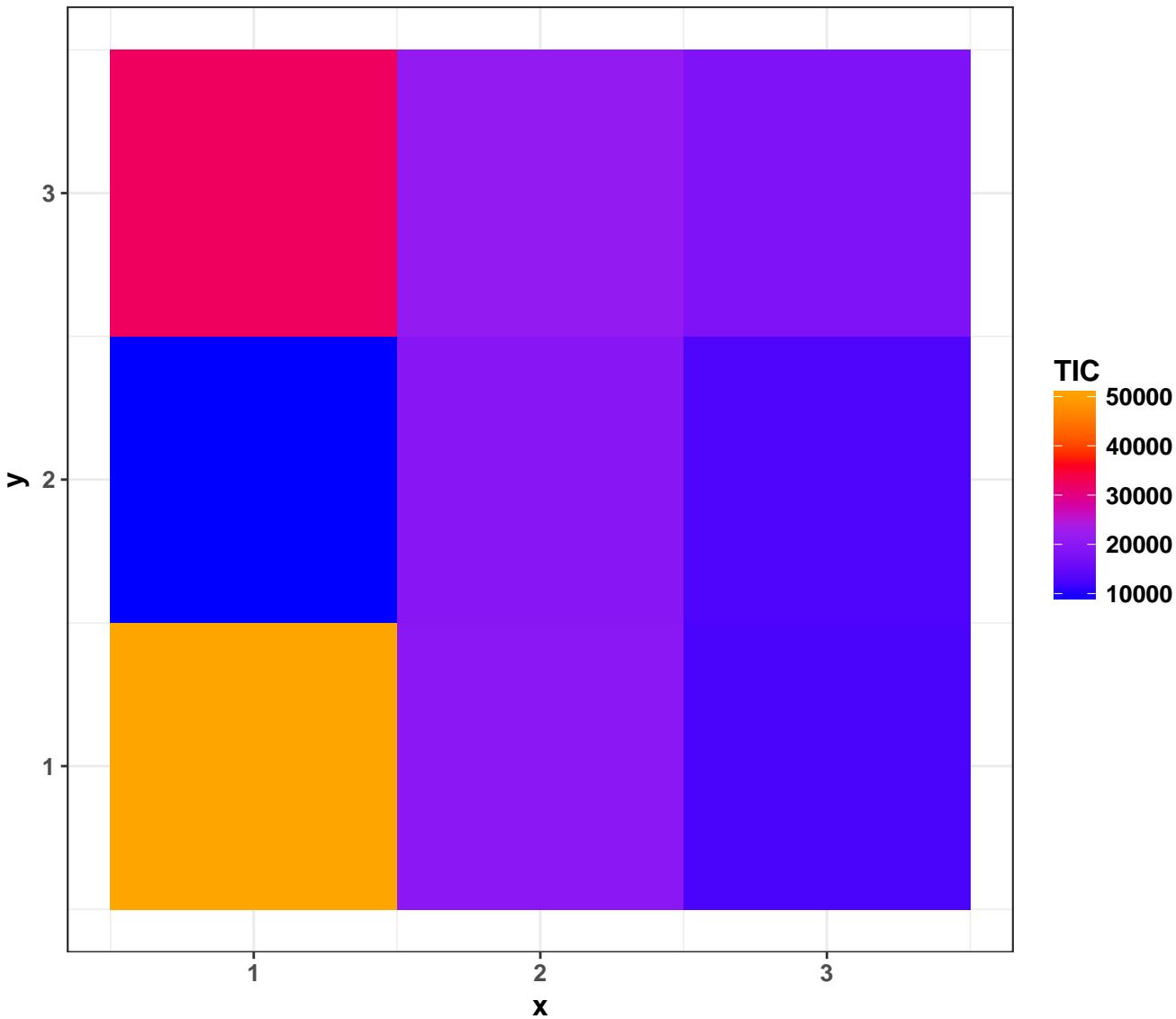




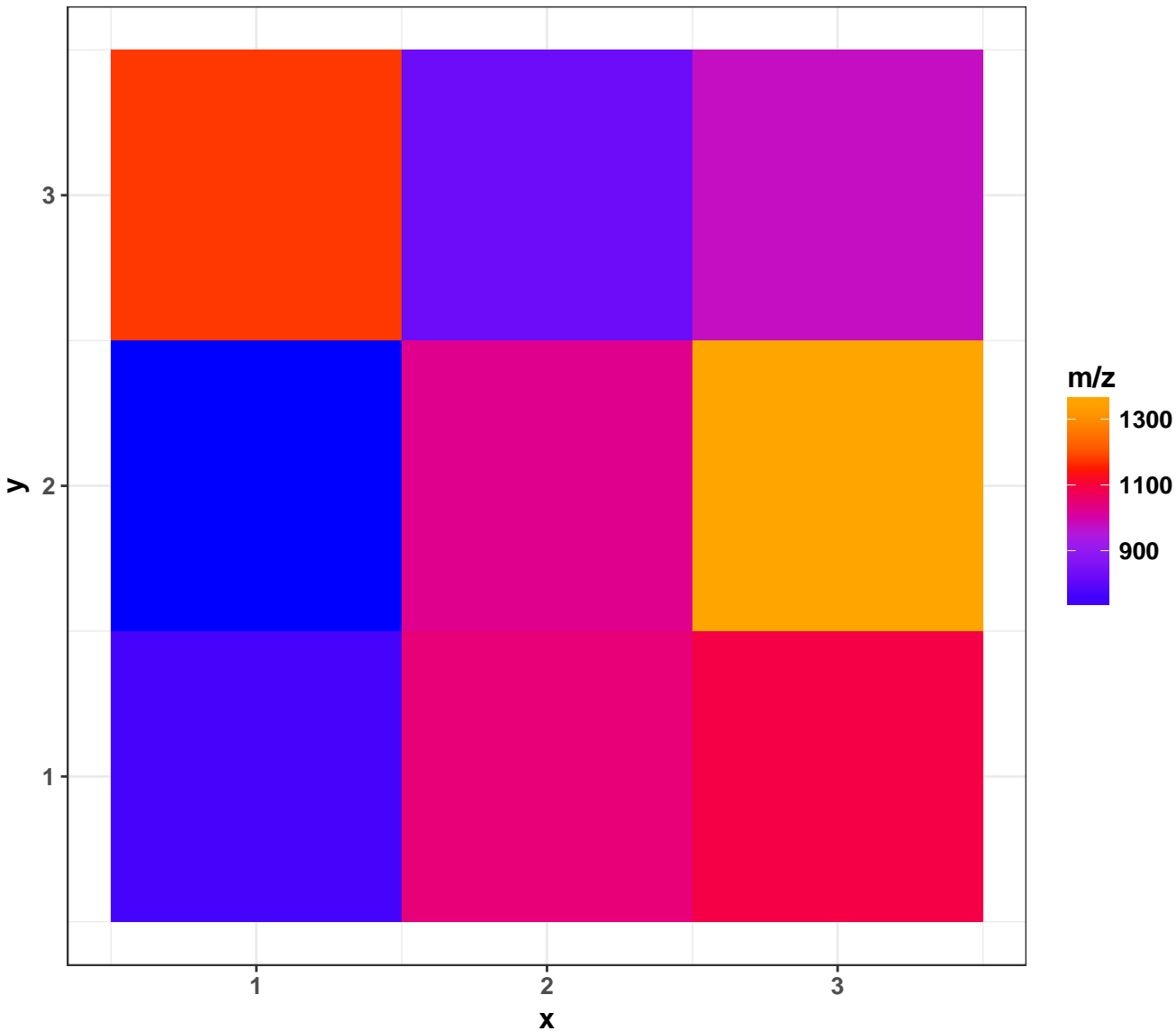
# Number of peaks per pixel



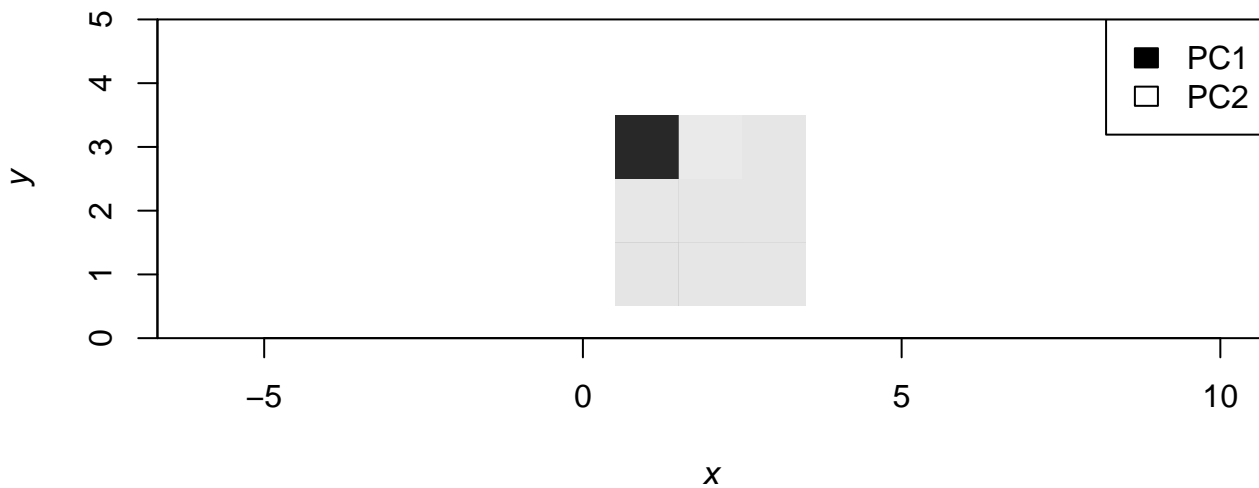
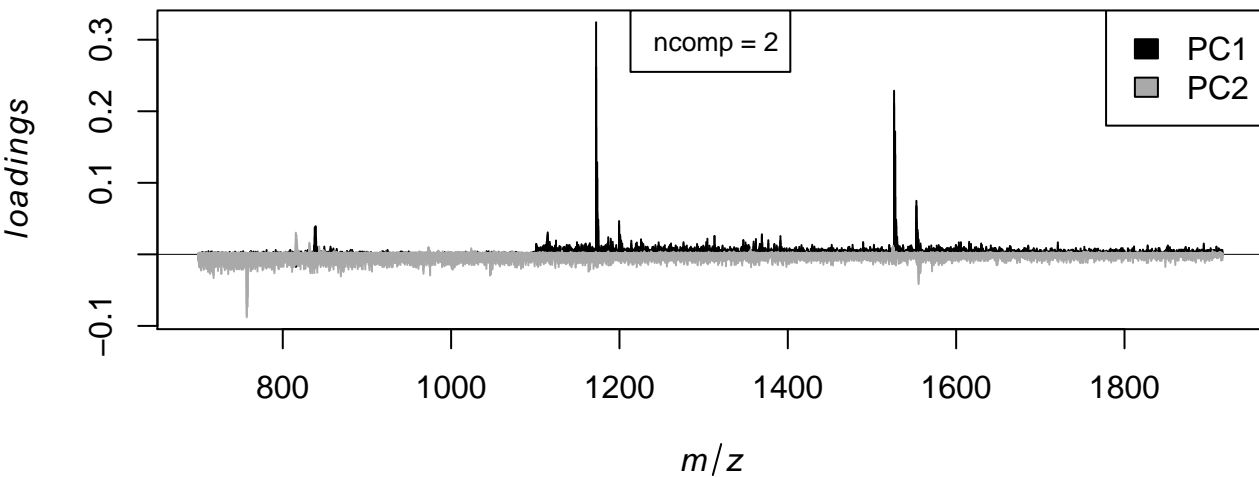
# Total Ion Chromatogram



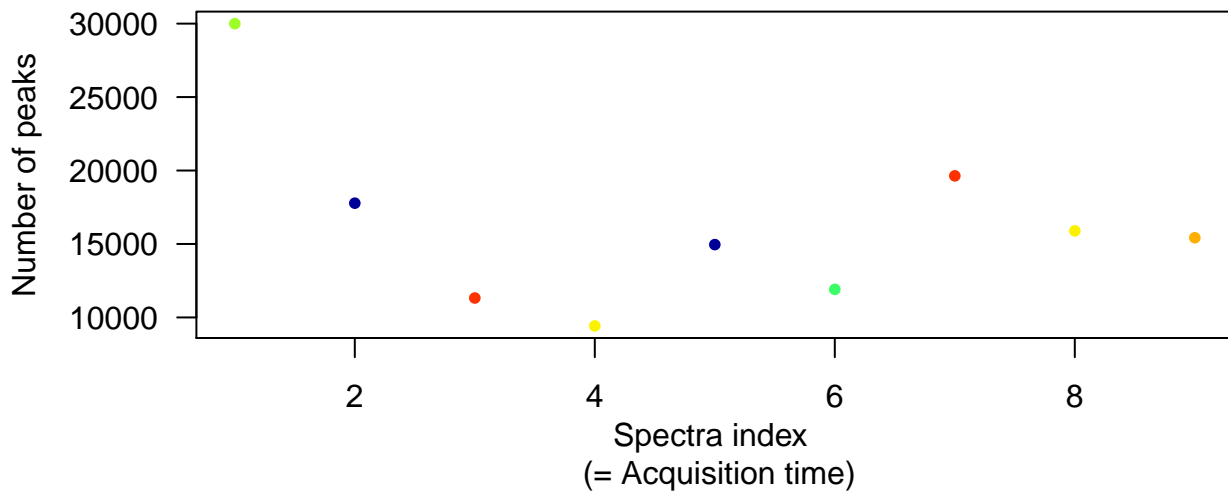
# Most abundant m/z in each pixel



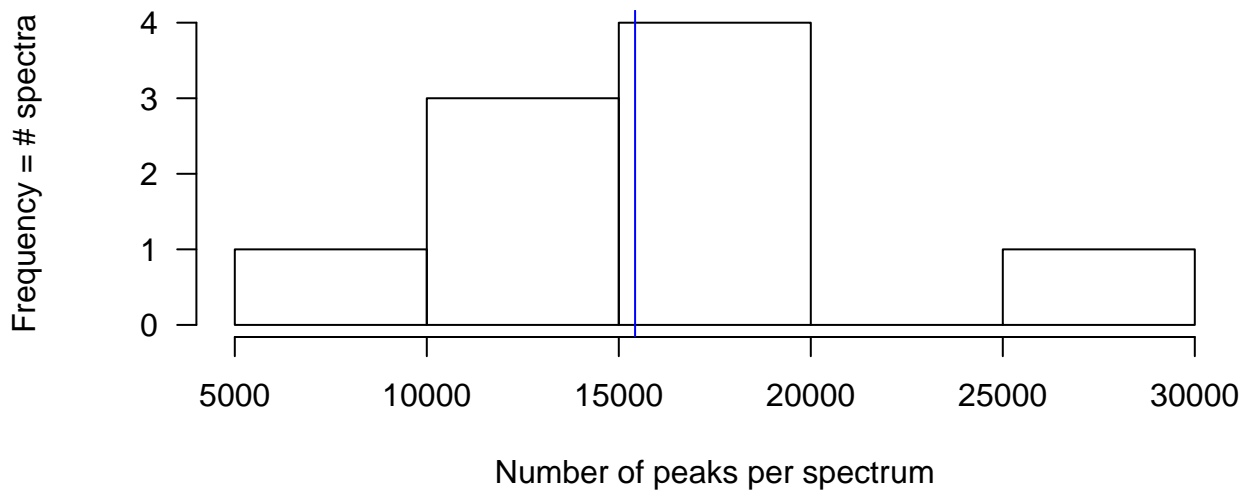
# PCA for two components



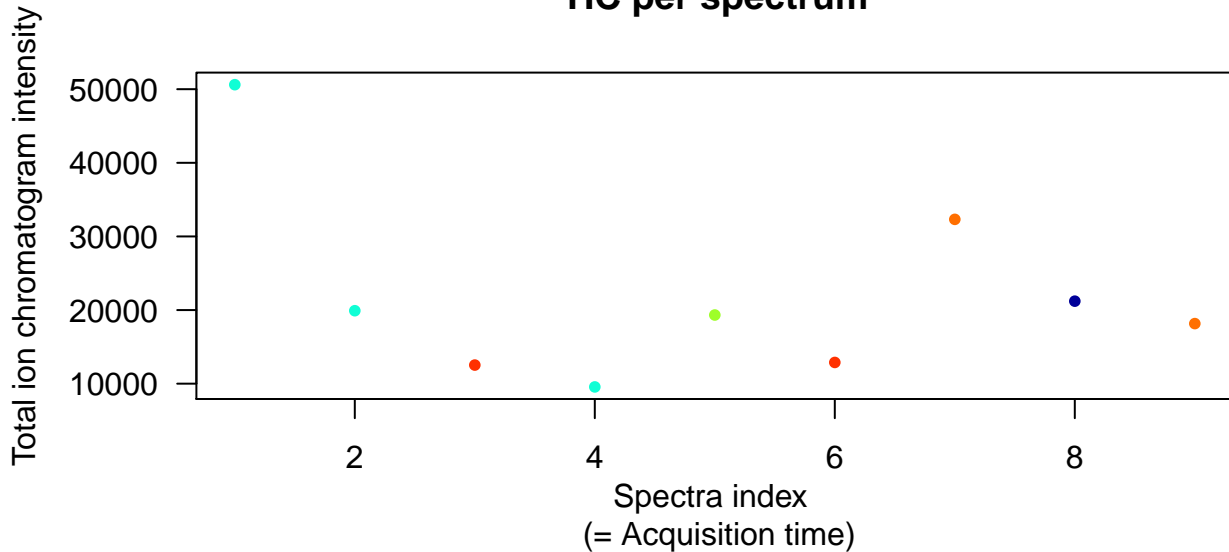
### Number of peaks per spectrum



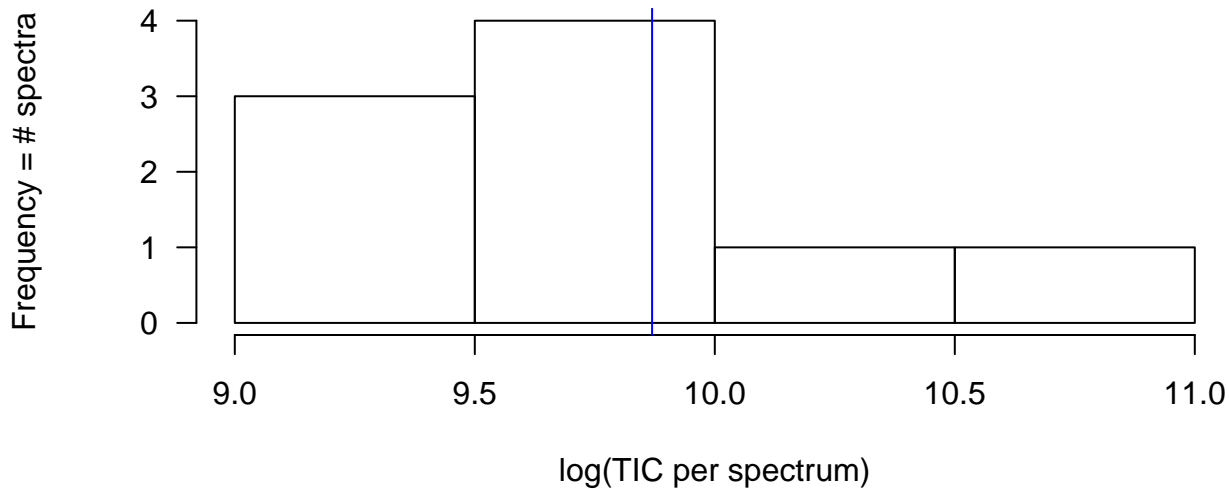
### Number of peaks per spectrum



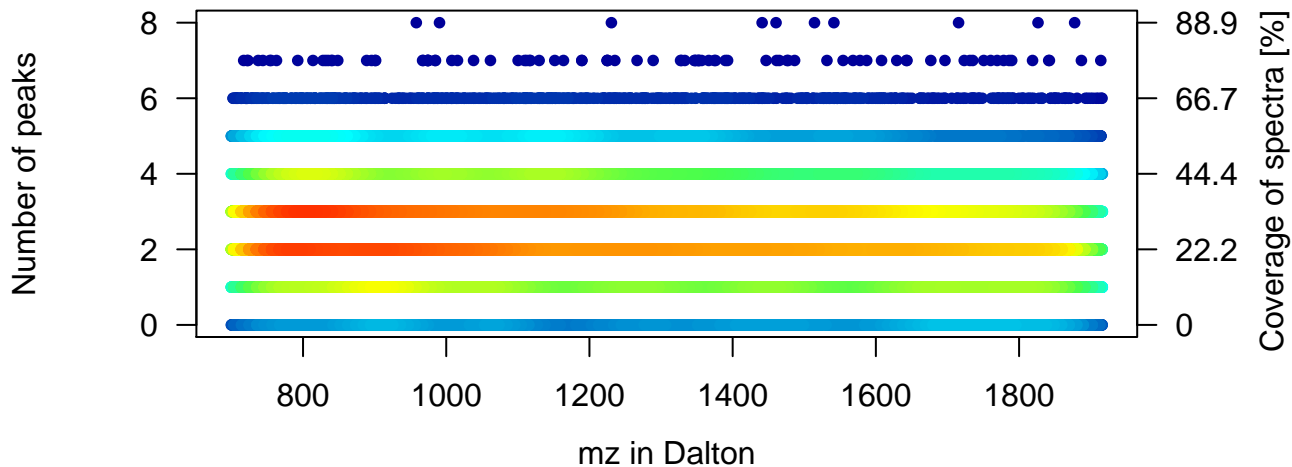
### TIC per spectrum



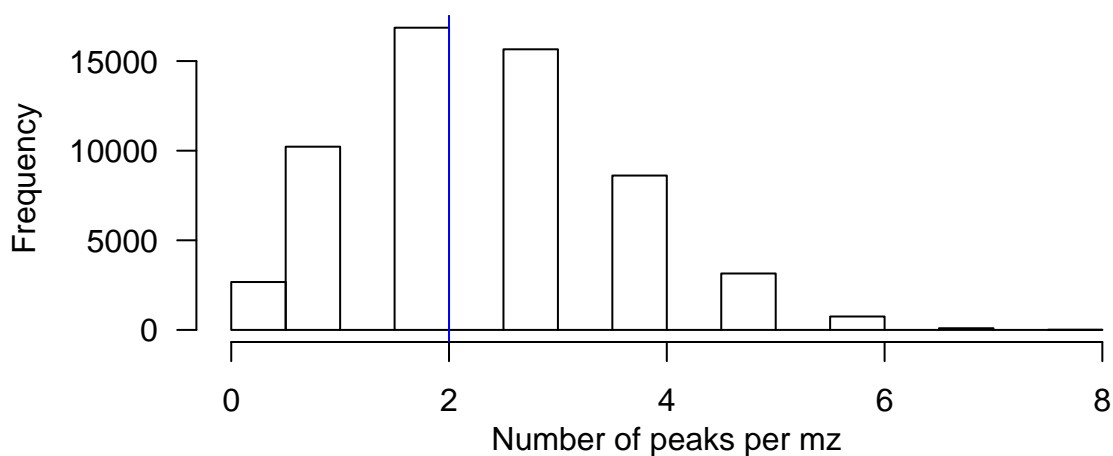
### TIC per spectrum



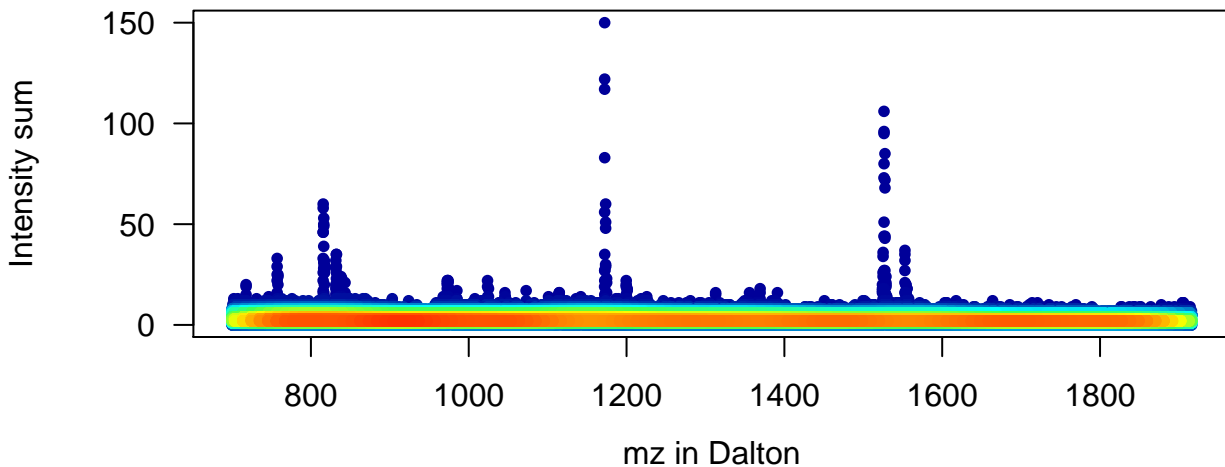
### Number of peaks per mz



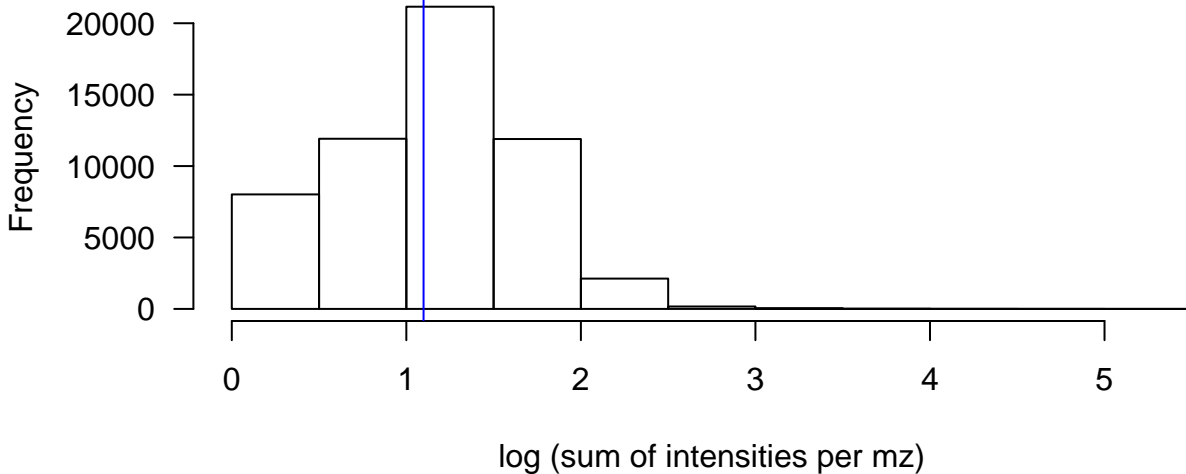
### Number of peaks per mz



Sum of intensities per mz

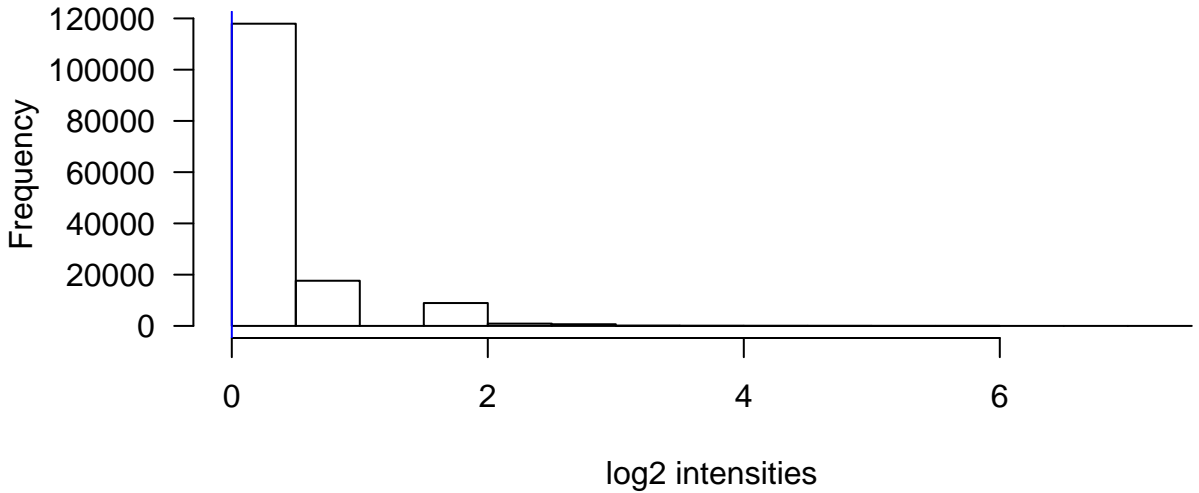


Sum of intensities per mz

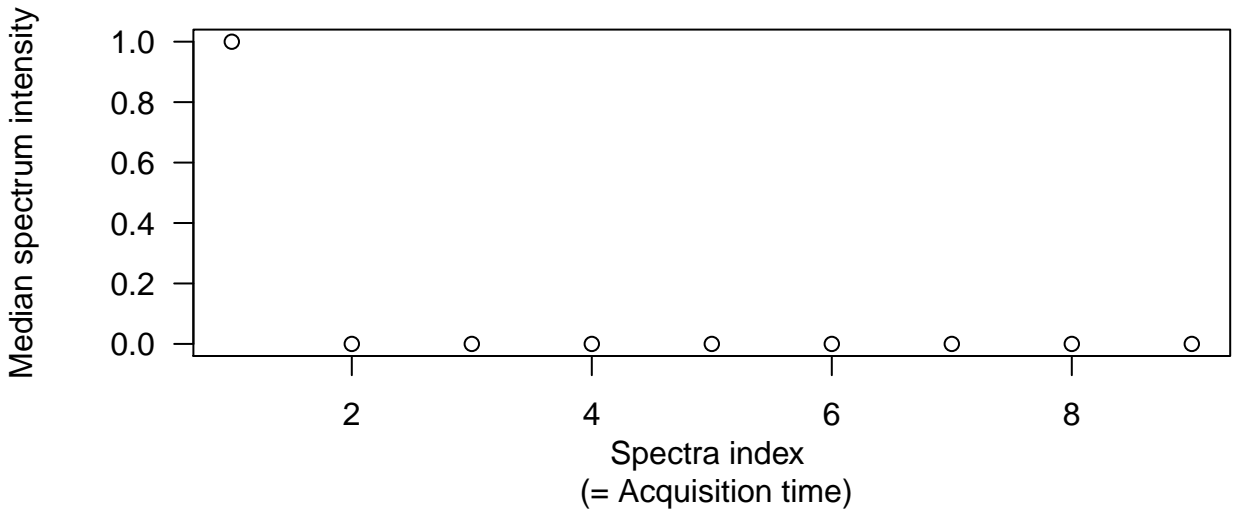




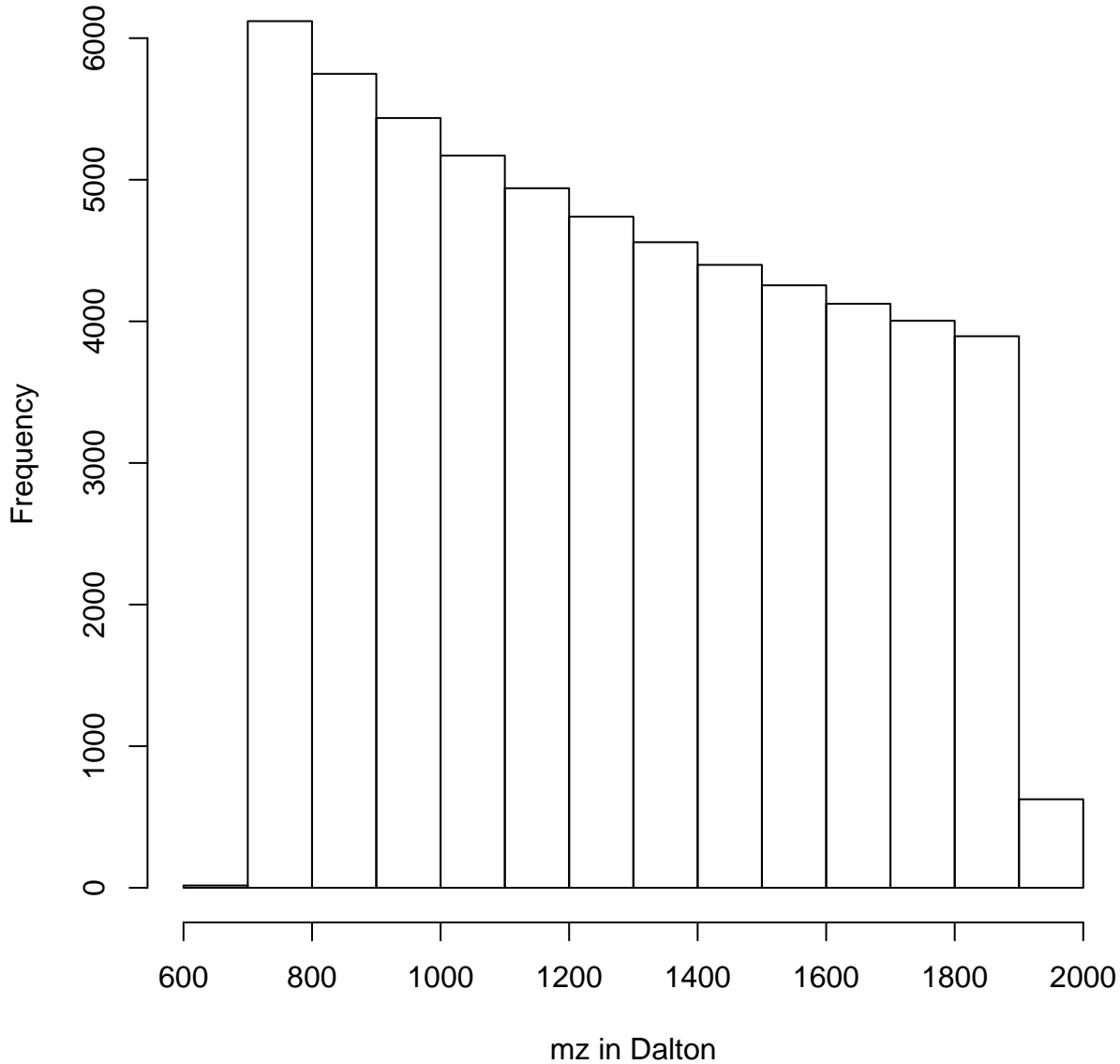
## Log2-transformed intensities



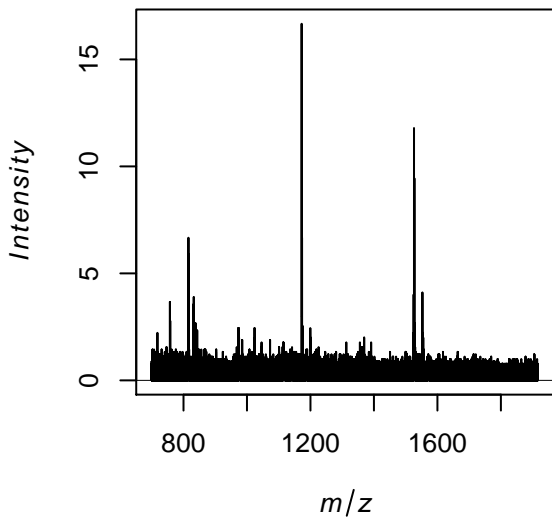
## Median intensity per spectrum



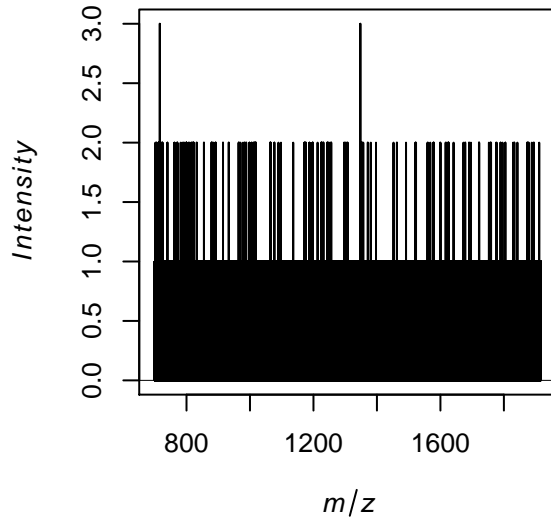
# Histogram of mz values



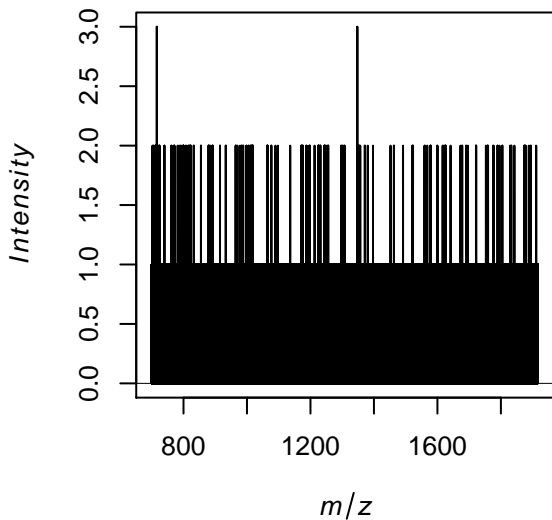
**Average spectrum**



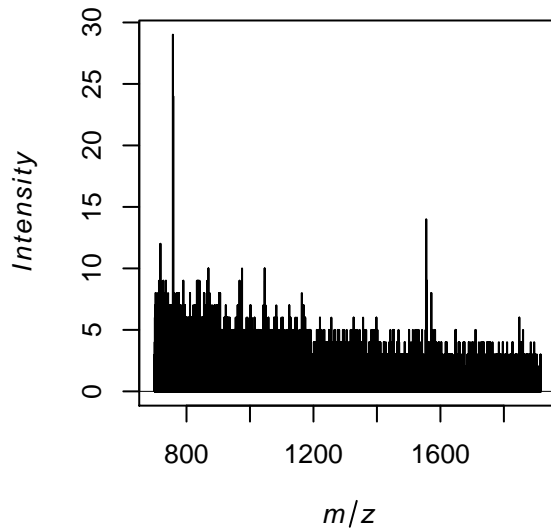
**Spectrum in middle of acquisition**



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

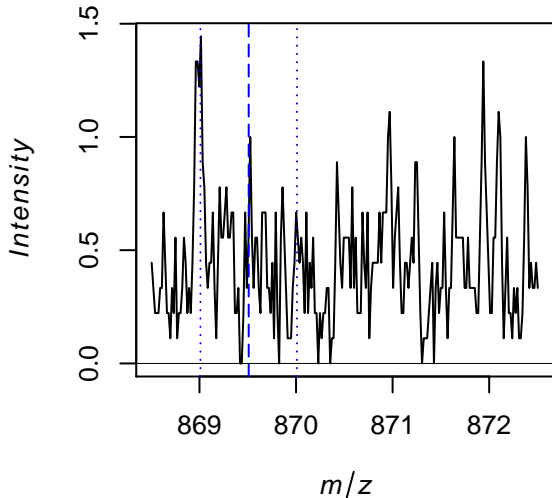


**Spectrum at x = 1, y = 1**

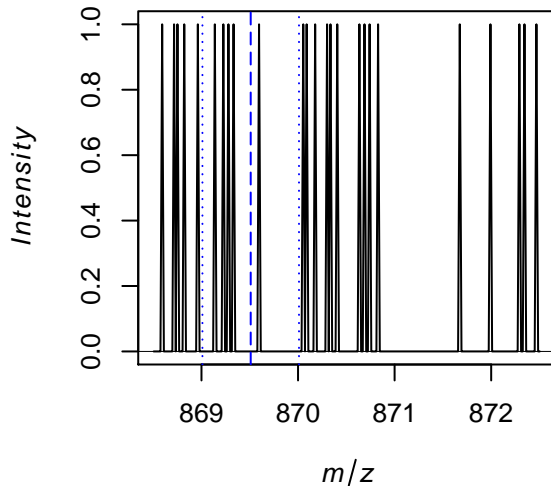


869.51

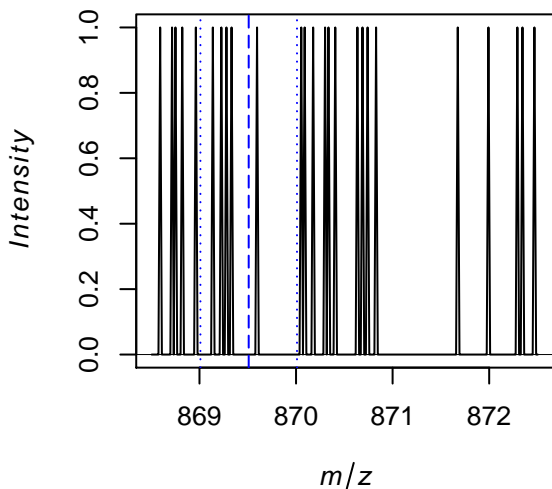
average spectrum



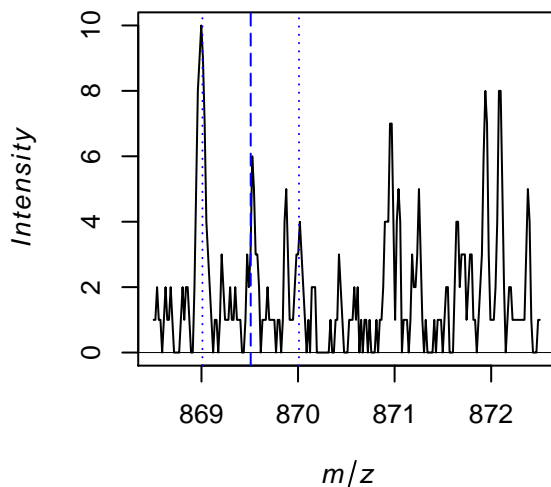
pixel in middle of acquisition



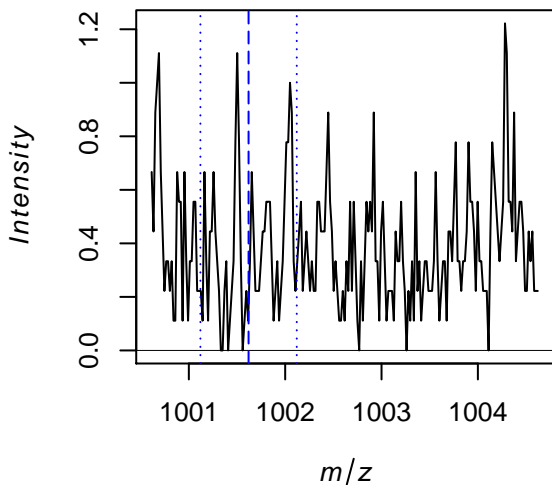
Spectrum at  $x = 1, y = 2$



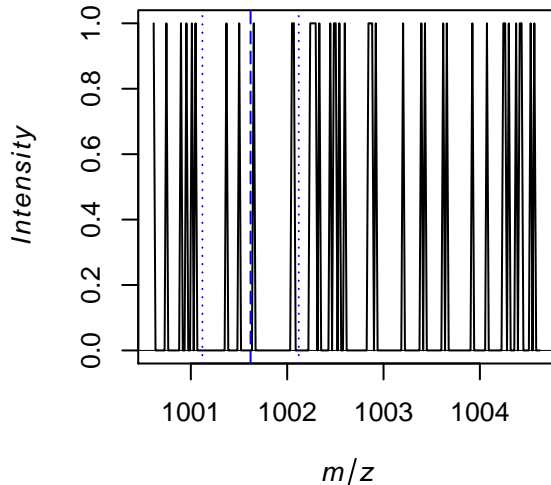
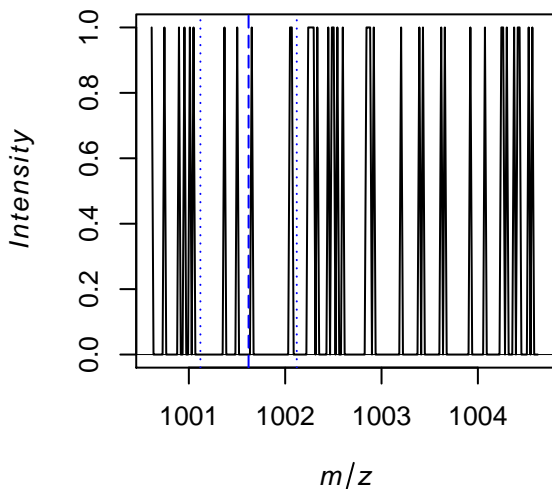
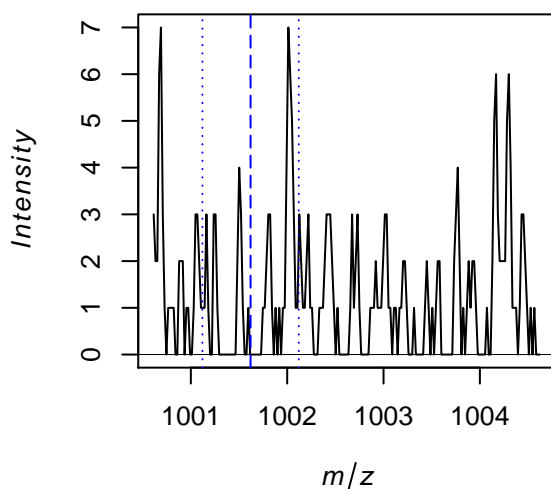
Spectrum at  $x = 1, y = 1$



average spectrum

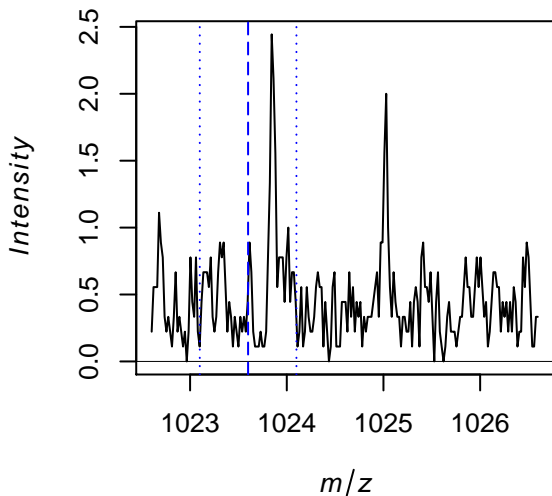


pixel in middle of acquisition

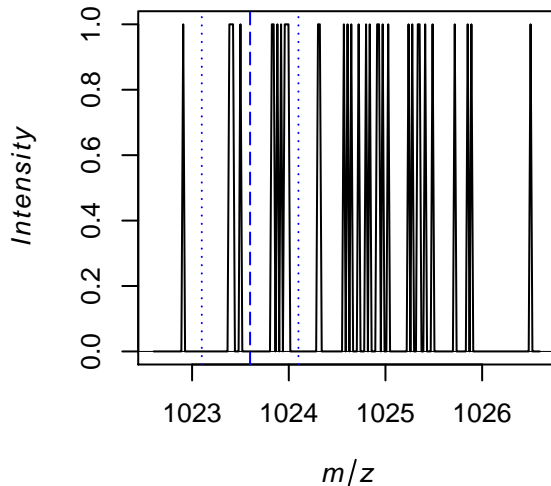
Spectrum at  $x = 1, y = 2$ Spectrum at  $x = 1, y = 1$ 

1023.6

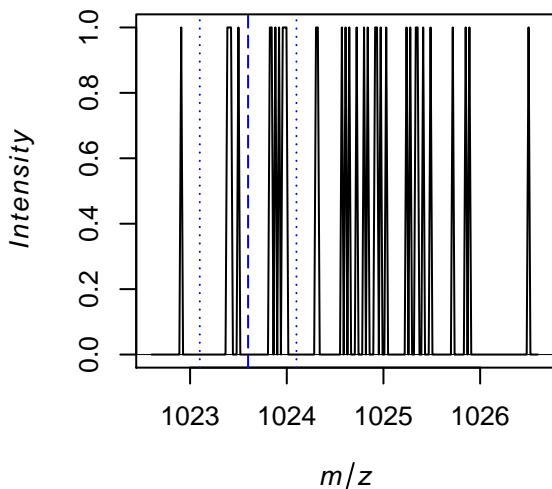
average spectrum



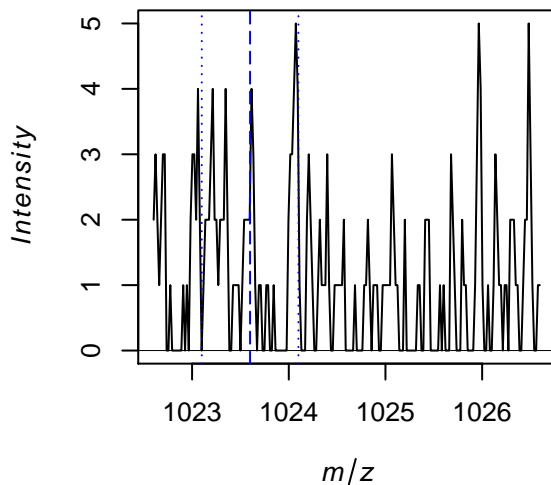
pixel in middle of acquisition



Spectrum at  $x = 1, y = 2$



Spectrum at  $x = 1, y = 1$



Theoretical calibrant mz vs. closest measured mz

