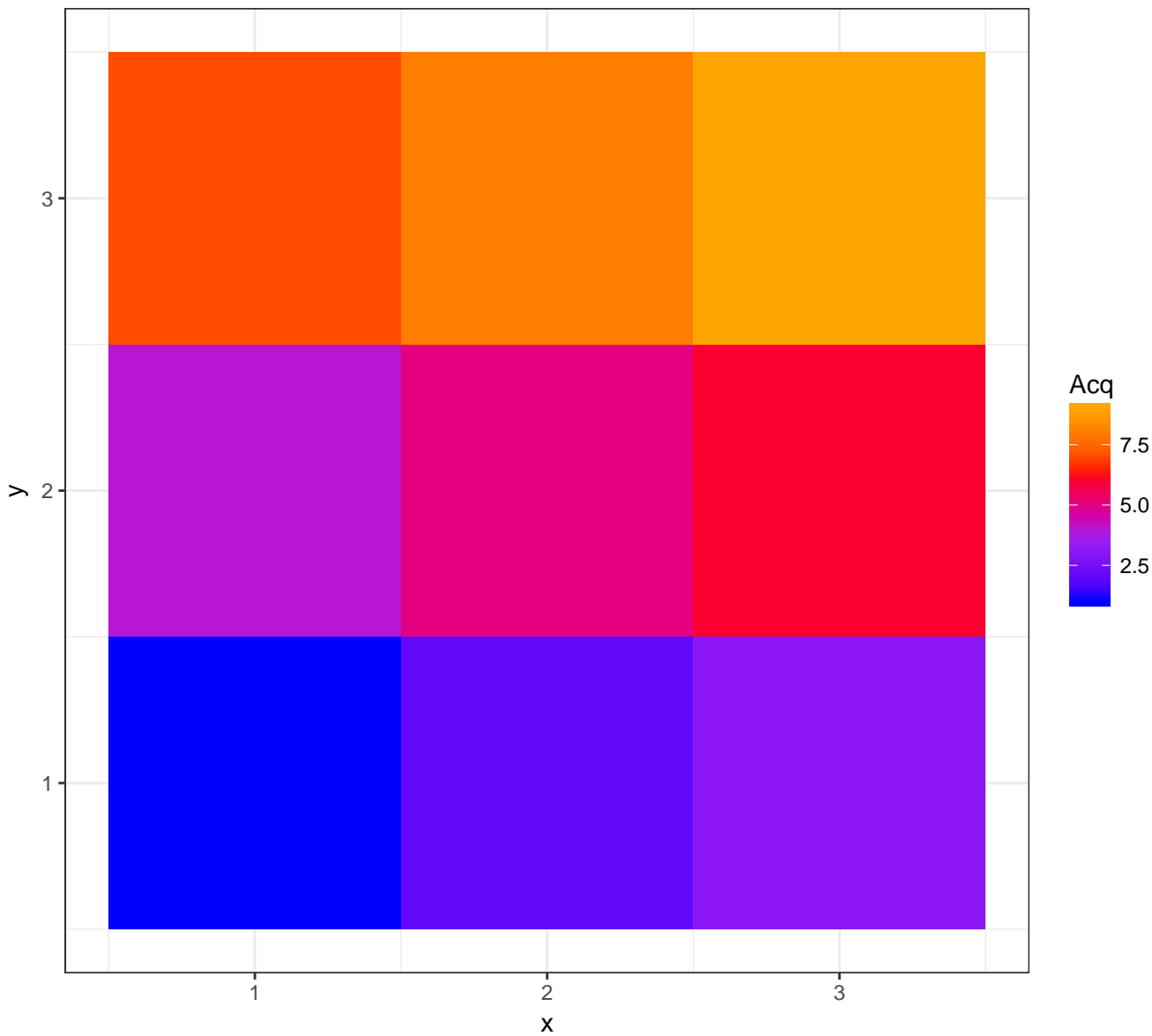


# Quality control of MSI data

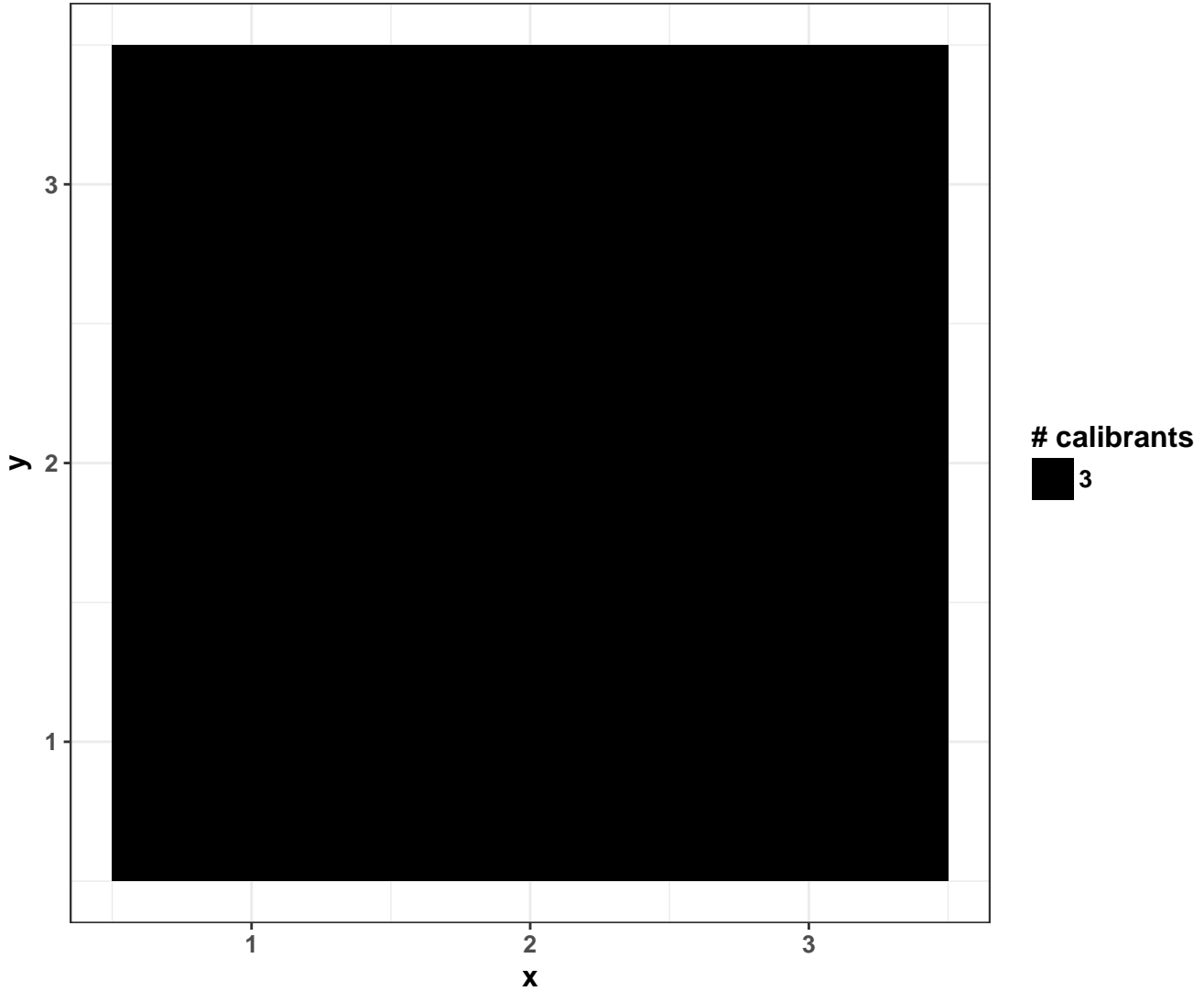
Filename: Testfile\_analyze75

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	2 / 3

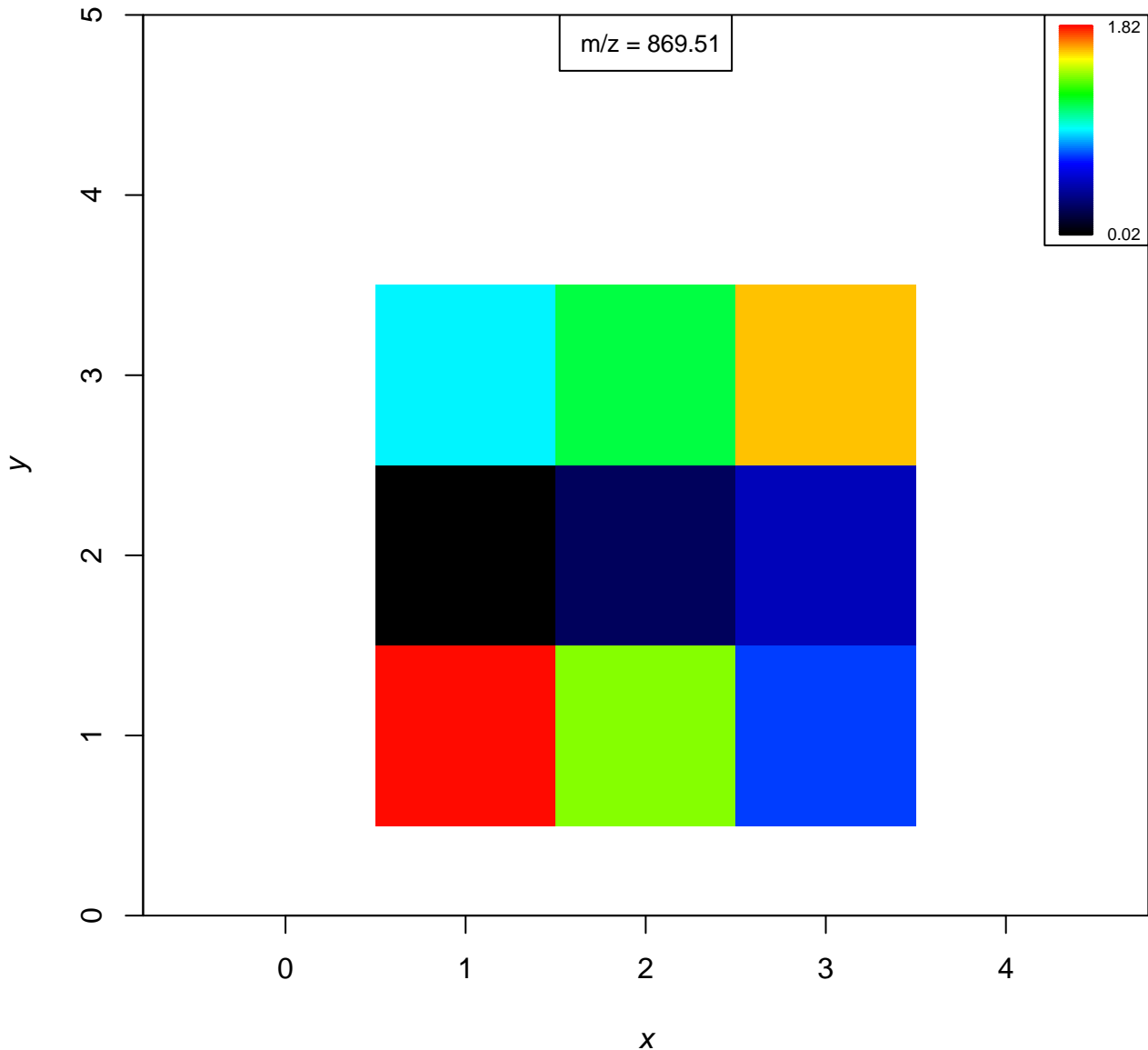
# 1) Order of Acquisition



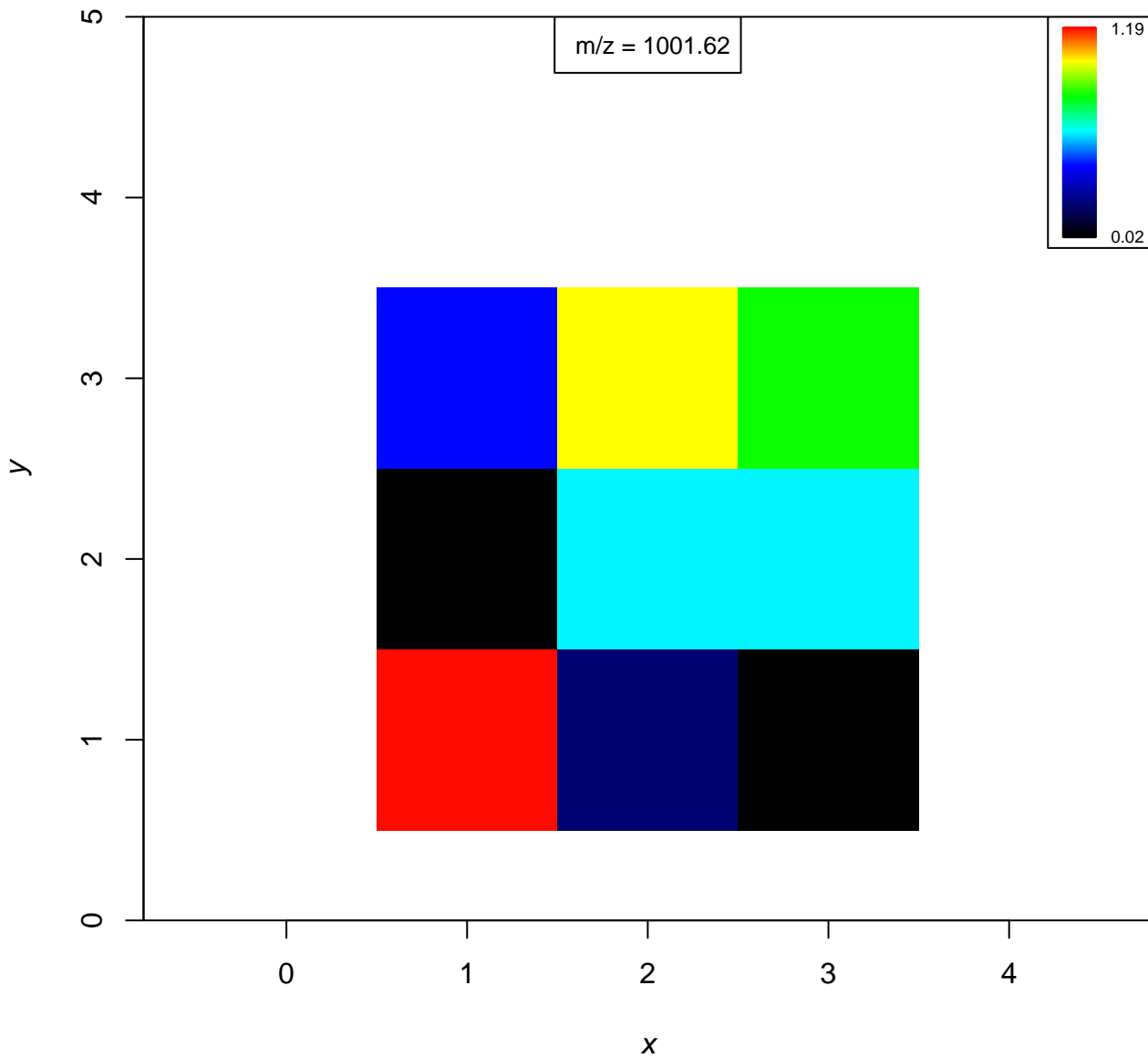
## 2) Number of calibrants per pixel



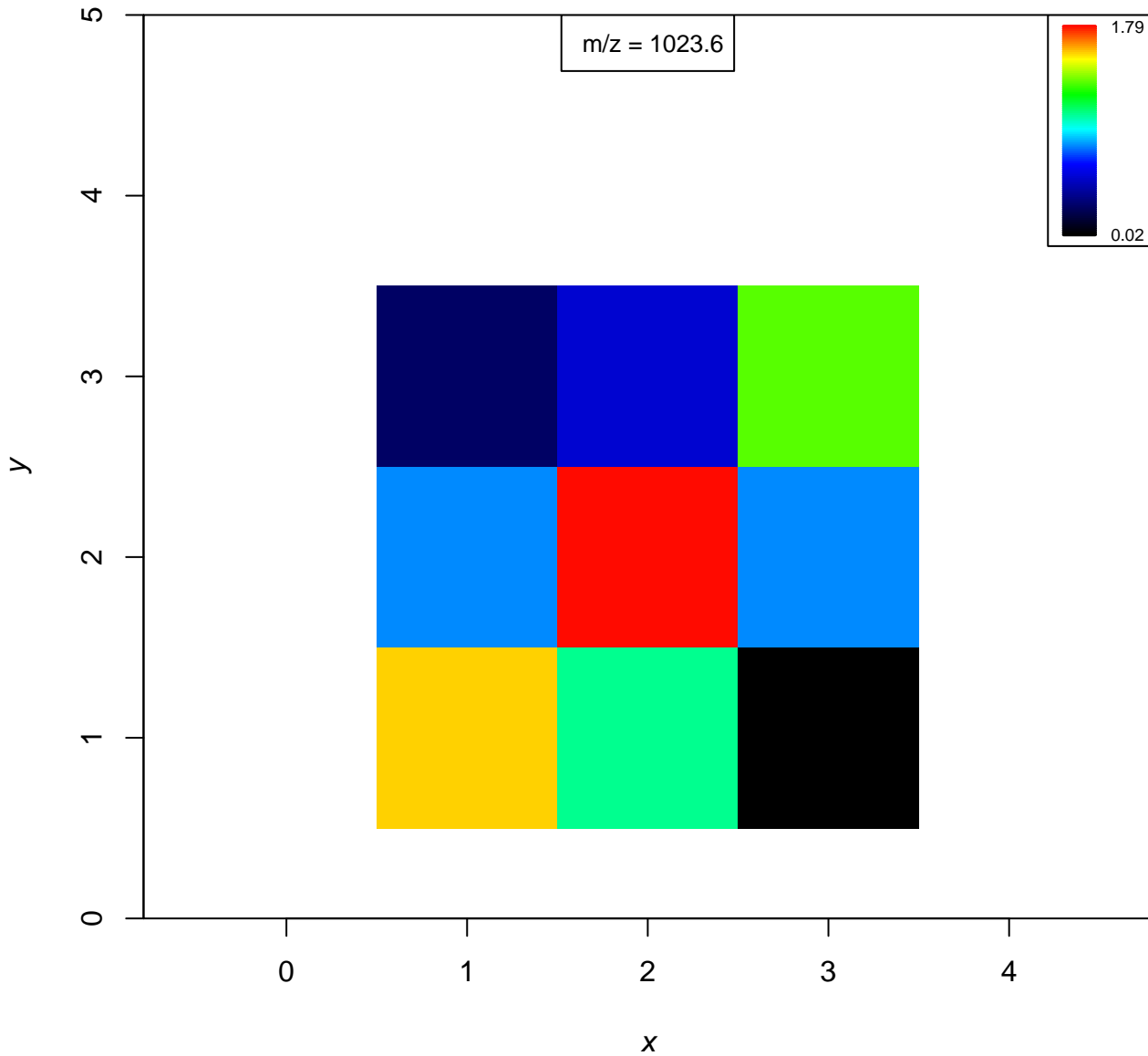
### 3A) mass1 (869.51 ± 0.5 Da)



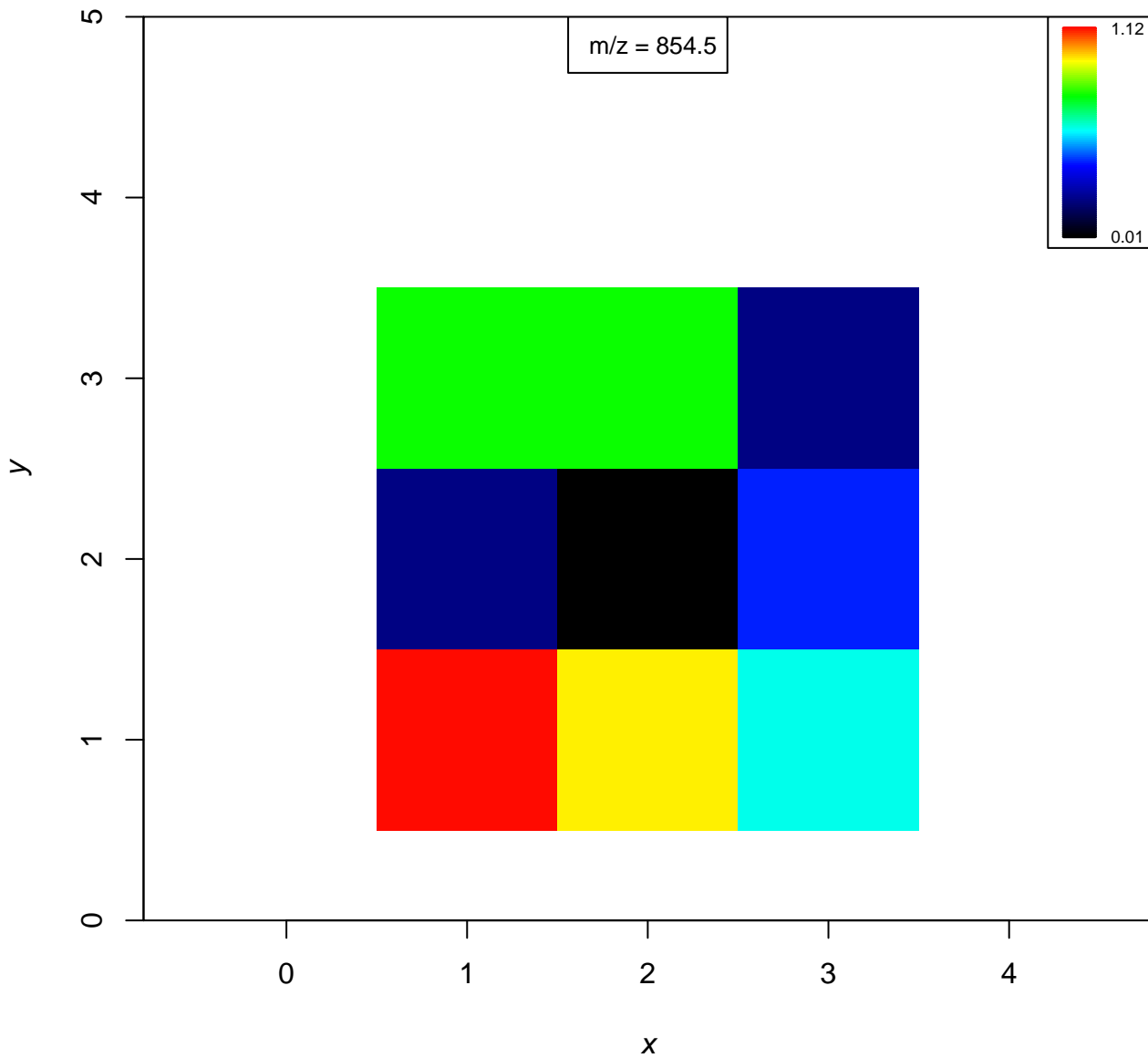
### 3B) mass2 (1001.62 ± 0.5 Da)



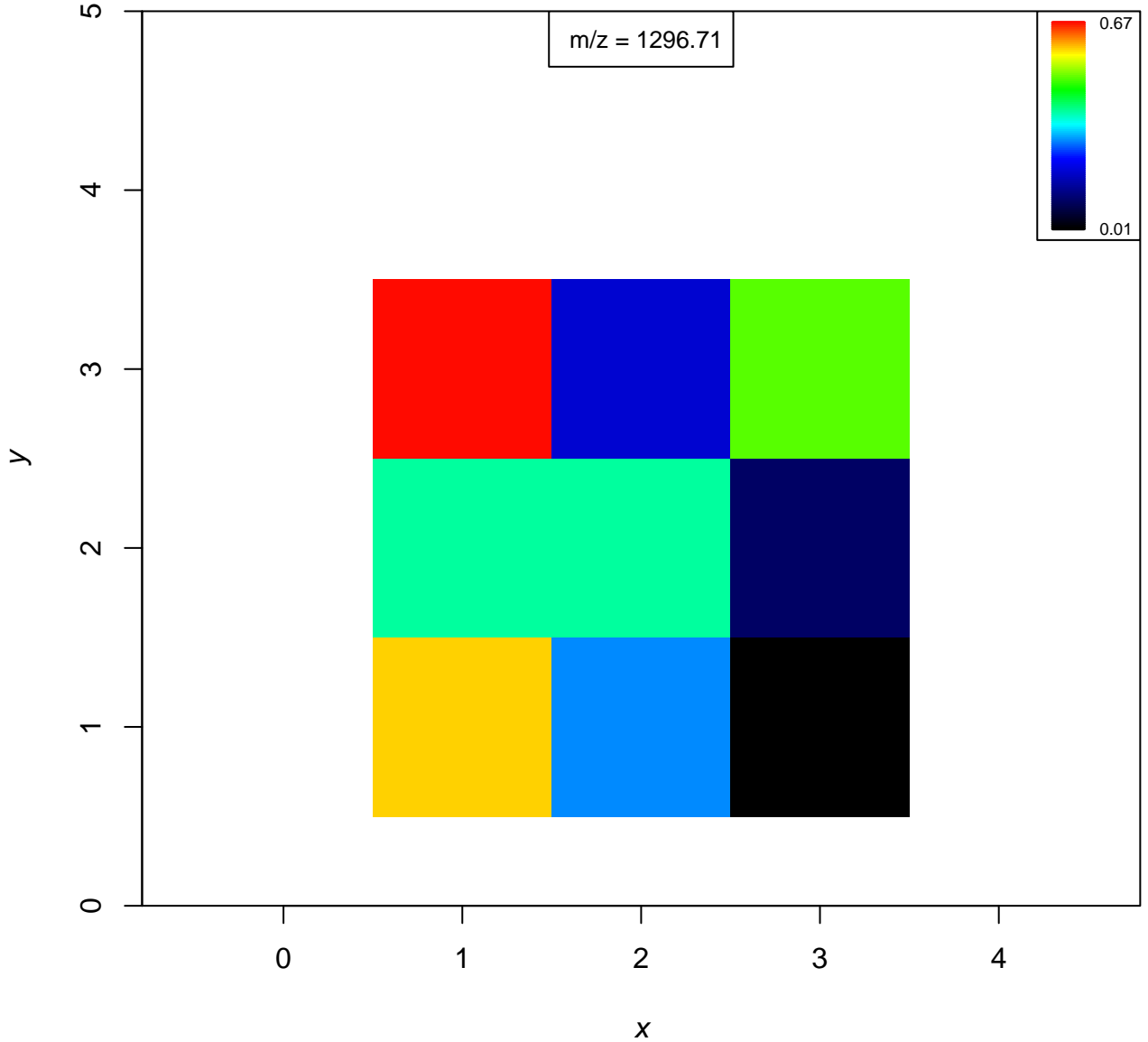
### 3C) mass3 (1023.6 ± 0.5 Da)



### 3D) 854.5 (854.5 ± 0.5 Da)

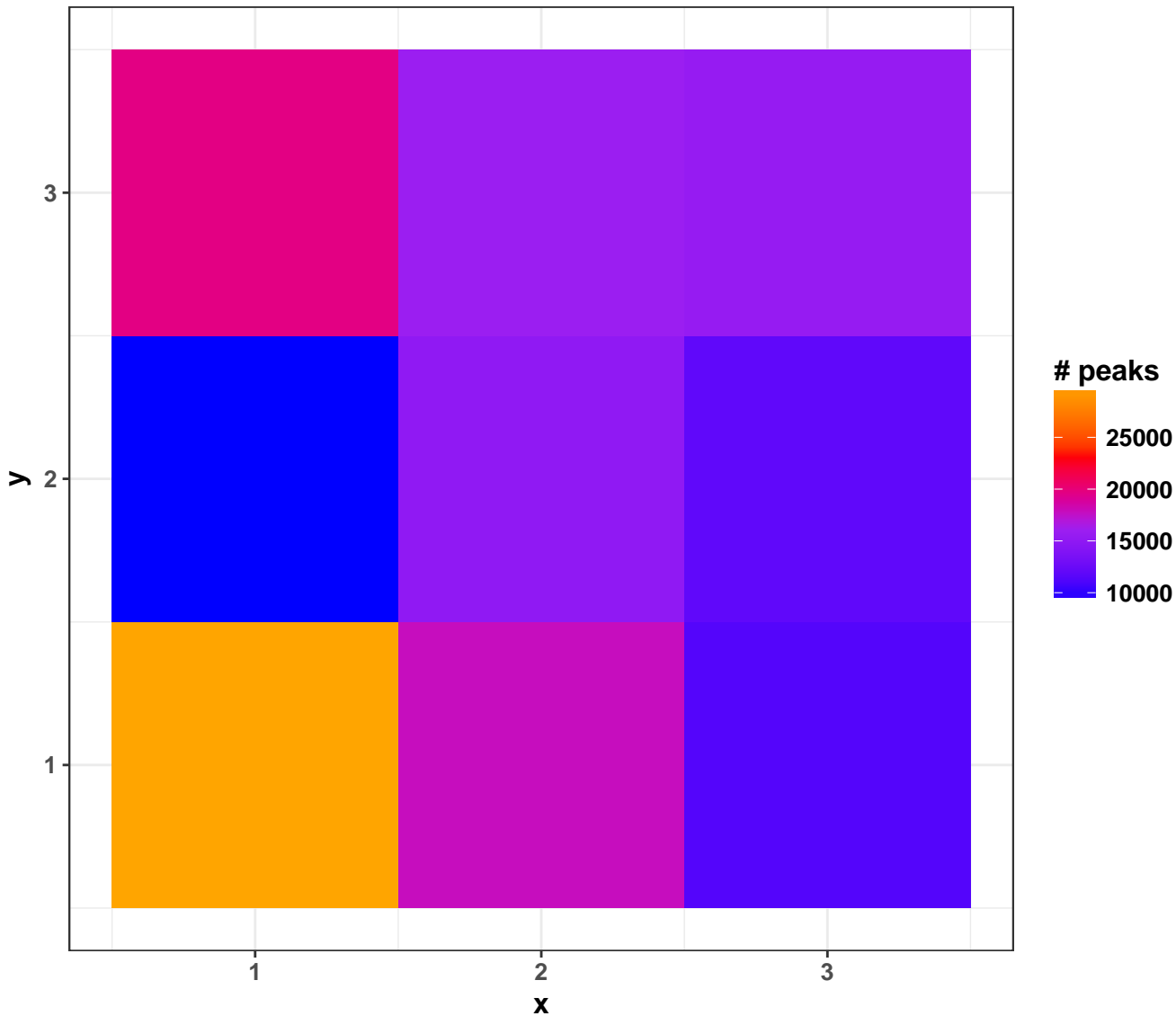


# 3E) 1296.7 (1296.7 ± 0.5 Da)

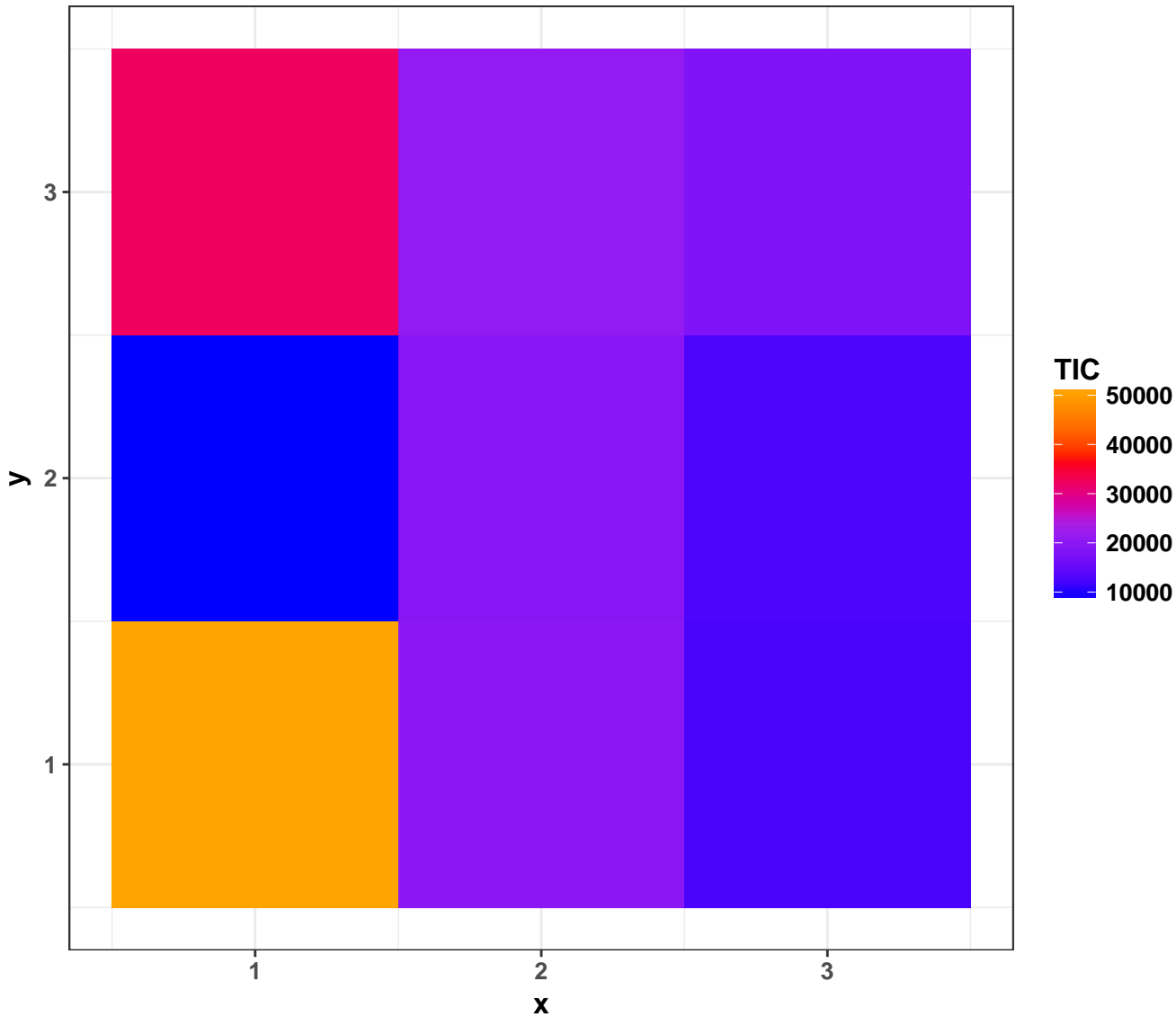




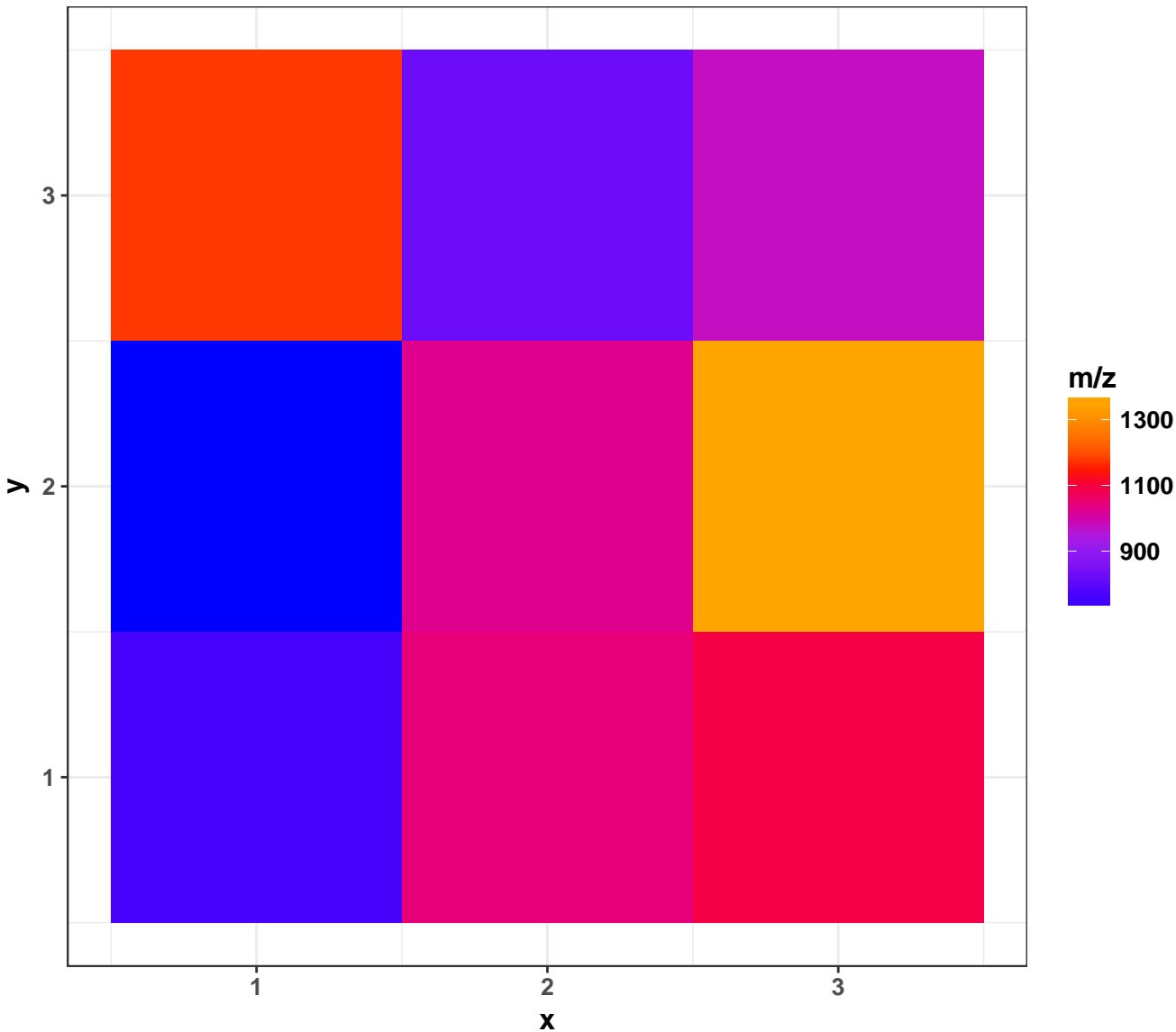
#### 4) Number of peaks per pixel



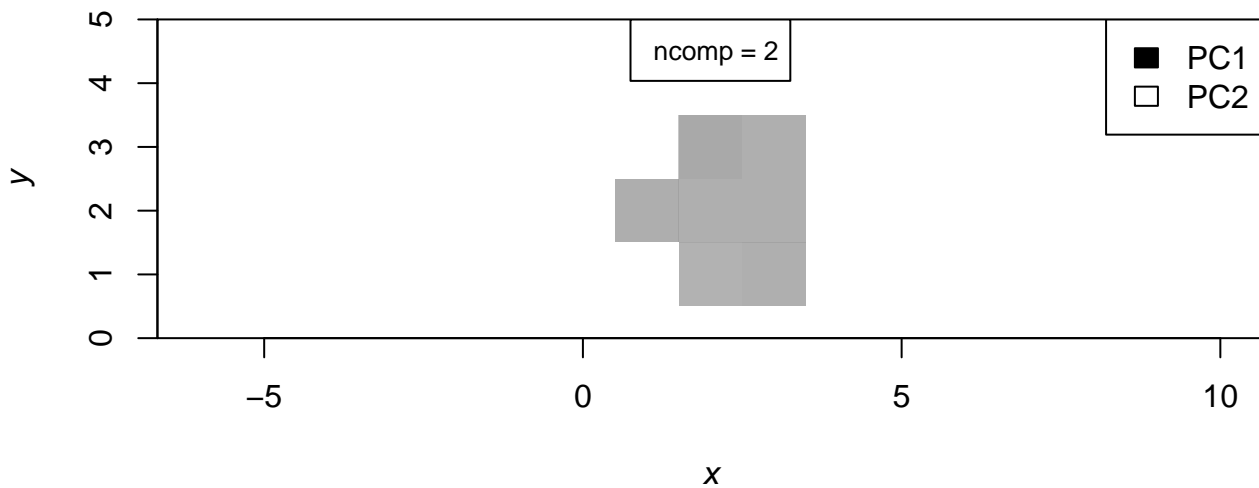
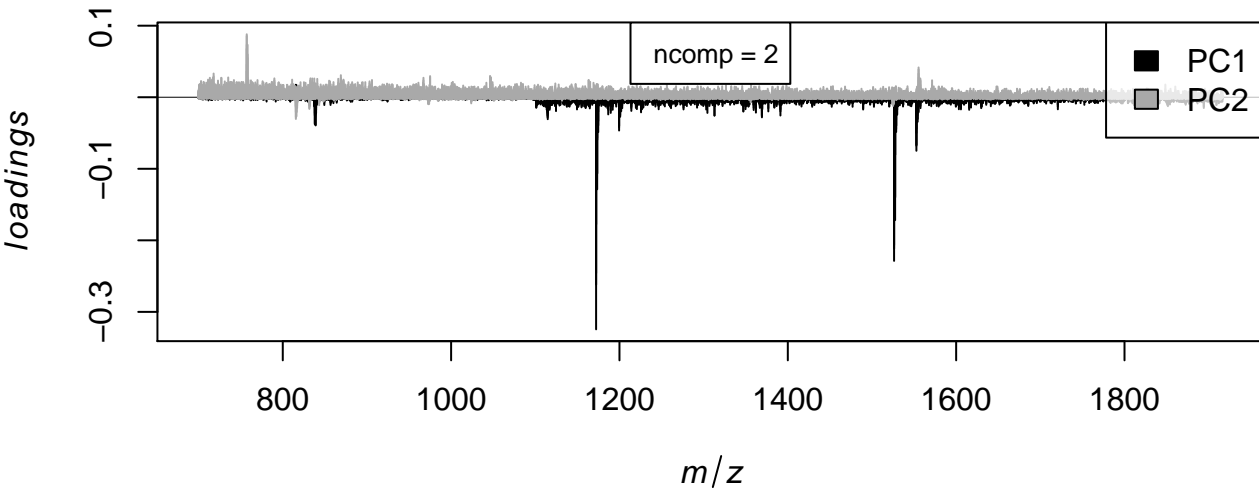
## 5) Total Ion Chromatogram



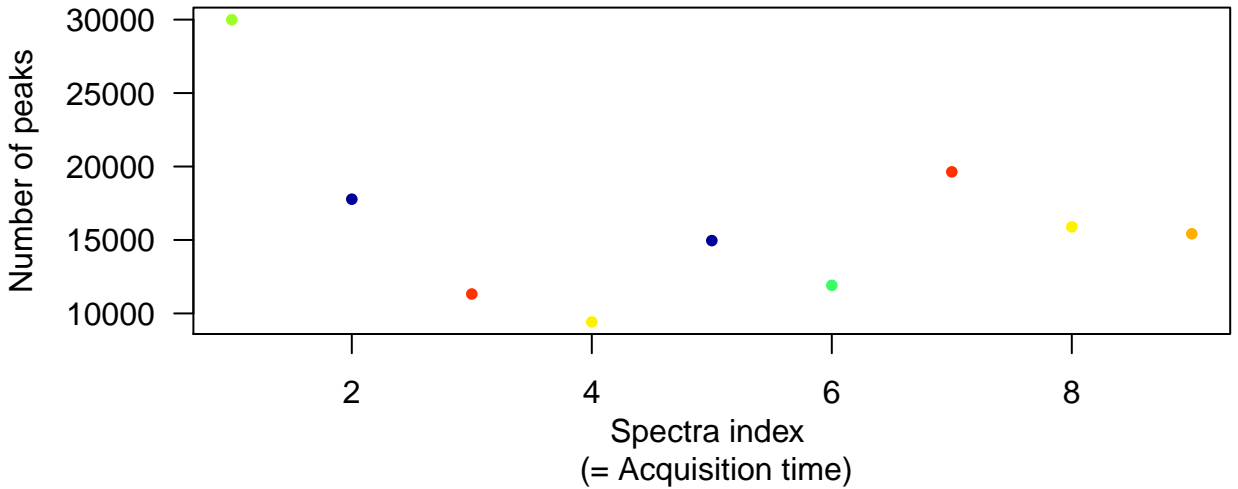
## 6) Most abundant m/z in each pixel



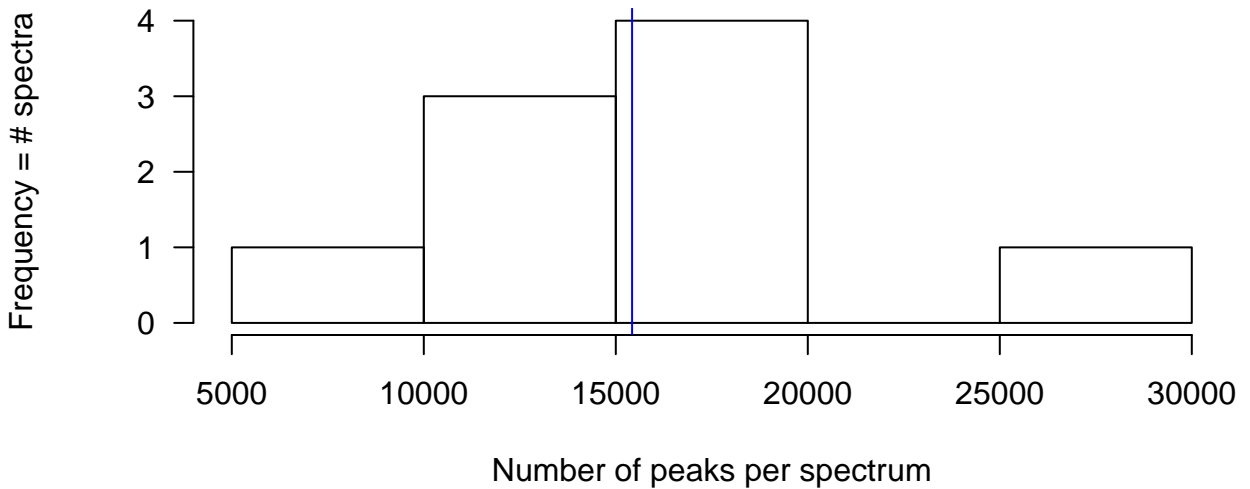
## 7) PCA for two components



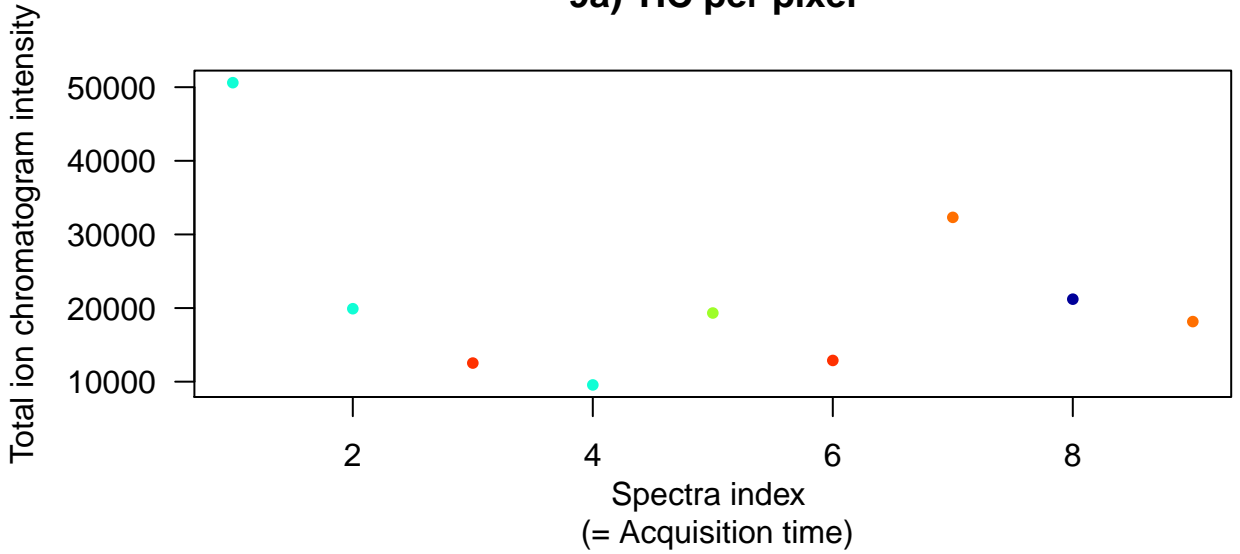
### 8a) Number of peaks per spectrum



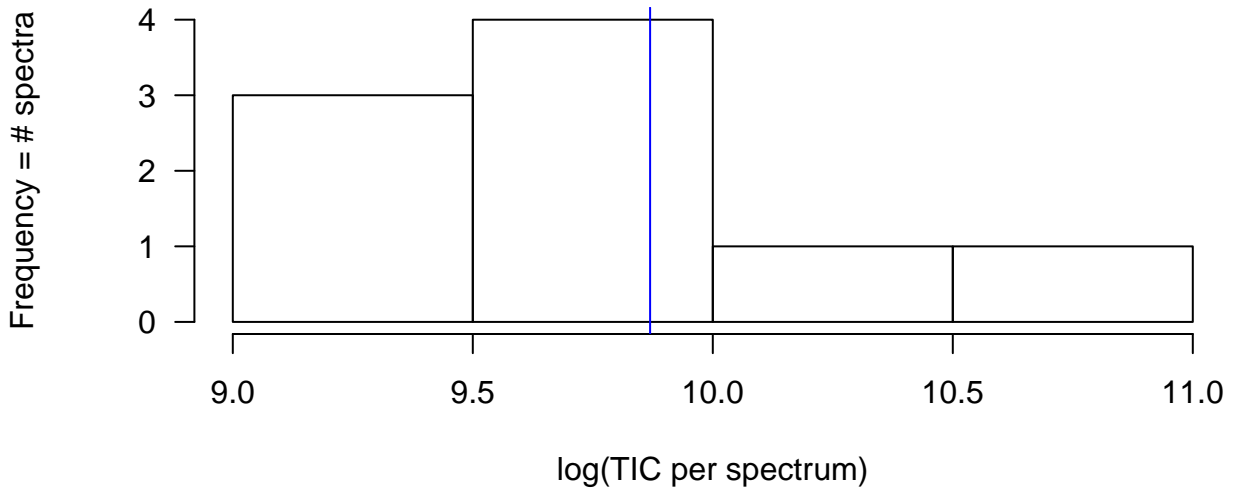
### 8b) Number of peaks per spectrum



### 9a) TIC per pixel

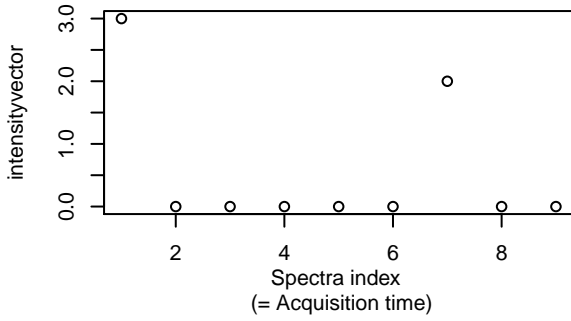


### 9b) TIC per spectrum

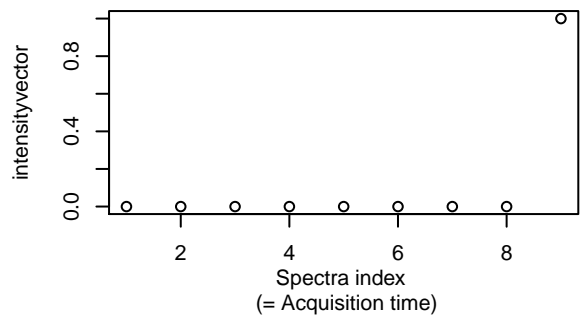


# 10) intensity of calibrants over acquisition

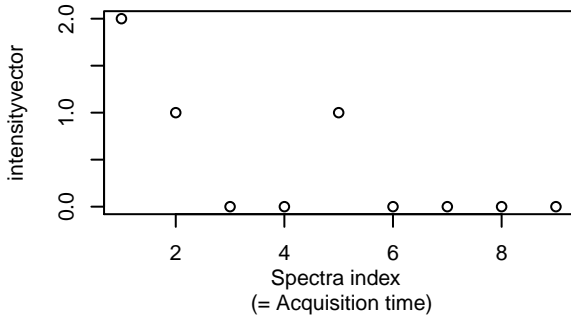
## mass1



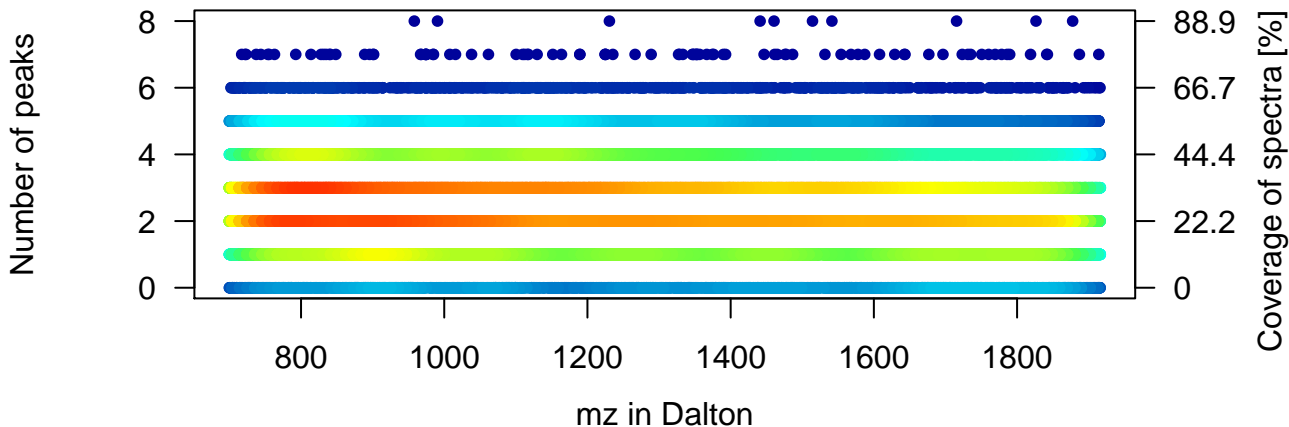
## mass2



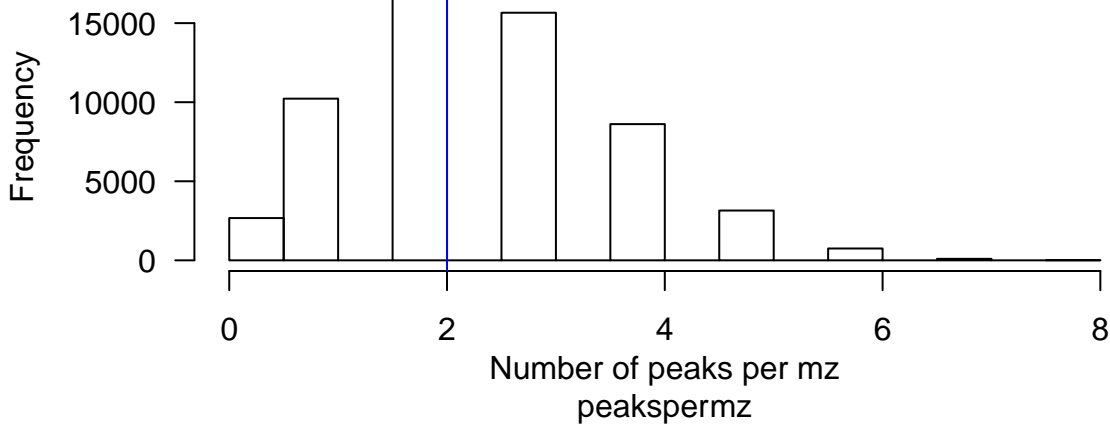
## mass3



### 11a) Number of peaks for each mz

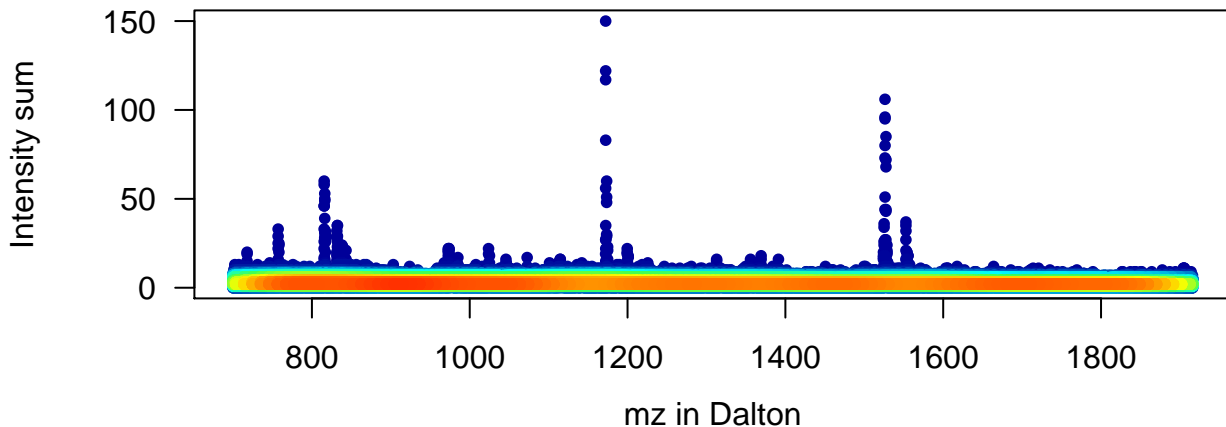


### 11b) Number of peaks per mz

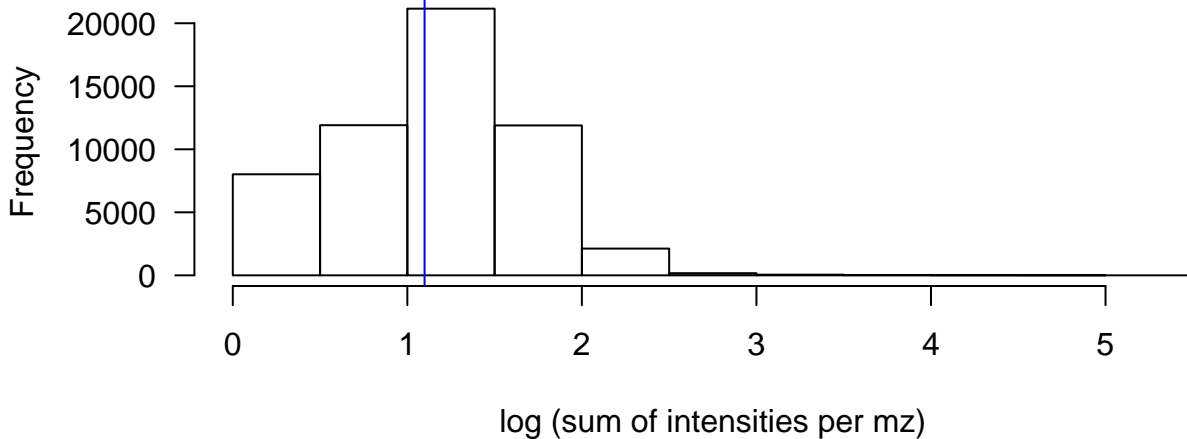




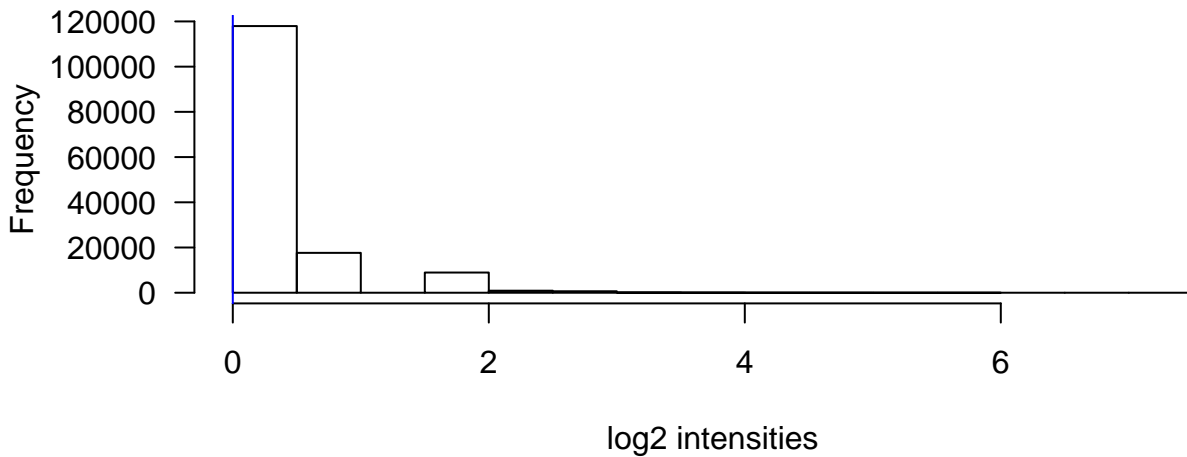
**12a) Sum of all peak intensities for each mz**



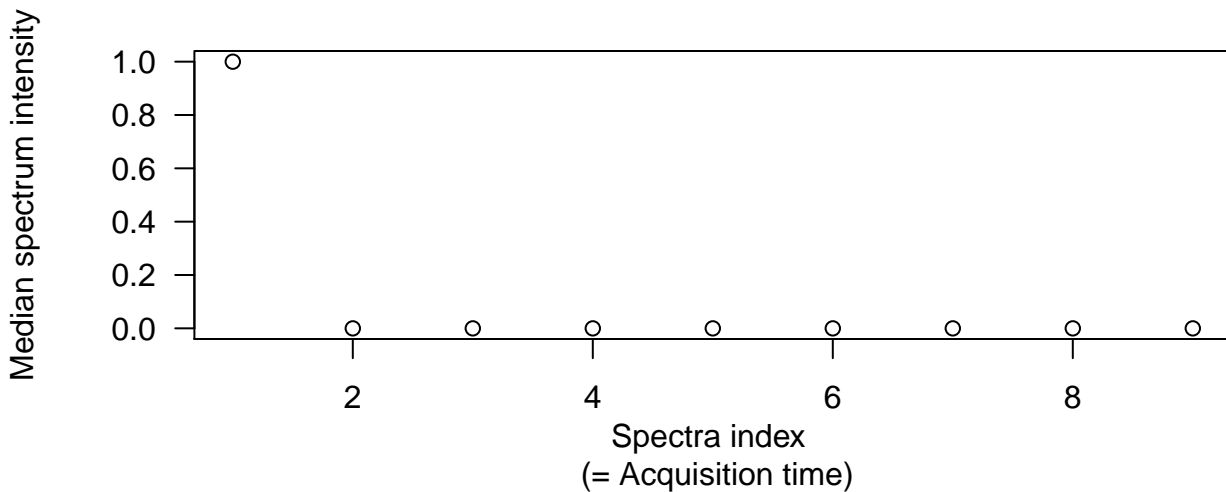
**12b) Sum of intensities per mz**



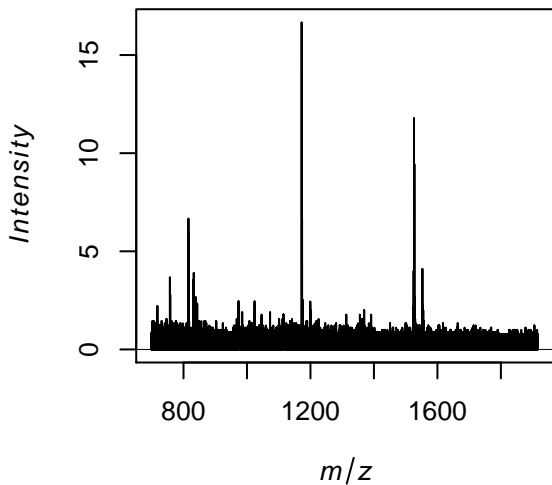
### 13a) Log2-transformed intensities



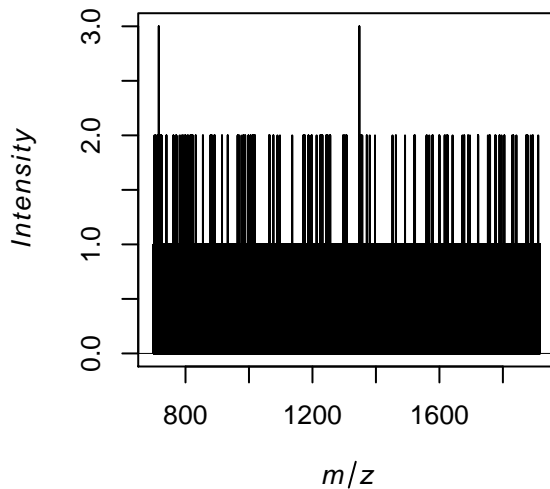
### 13b) Median intensity per spectrum



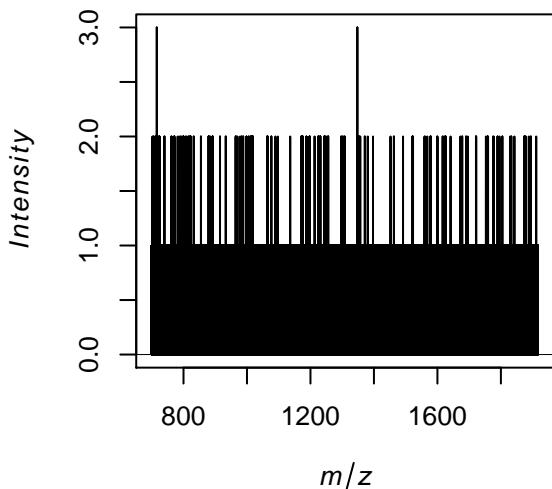
**Average spectrum**



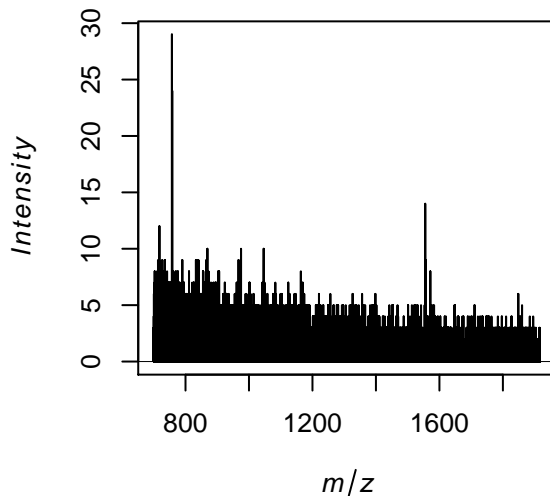
**Spectrum in middle of acquisition**



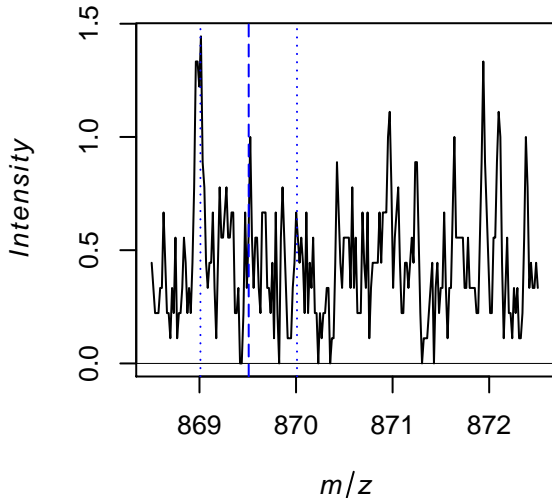
**Spectrum at x = 1, y = 2**



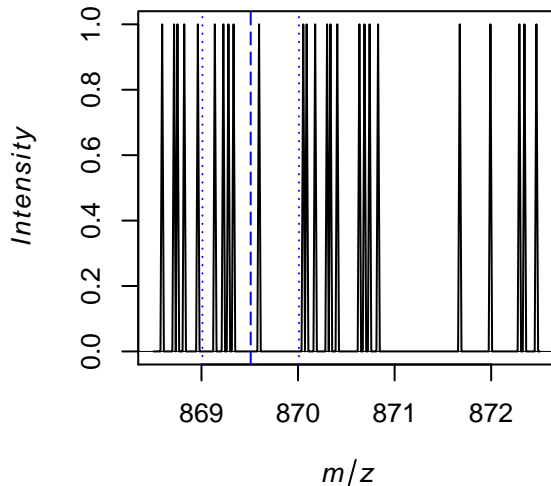
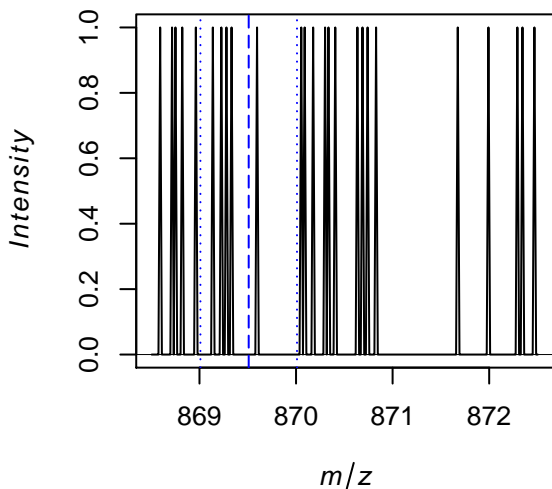
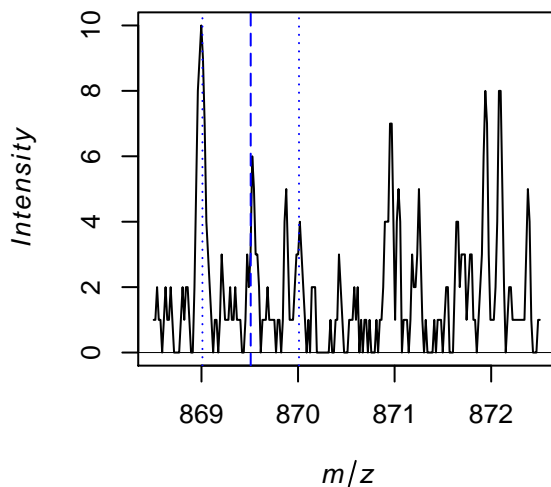
**Spectrum at x = 1, y = 1**



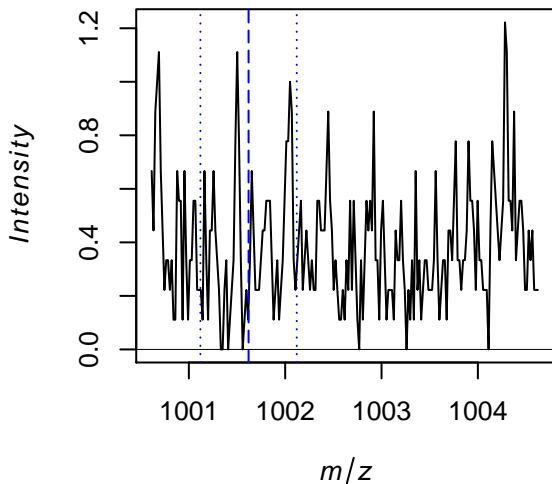
average spectrum



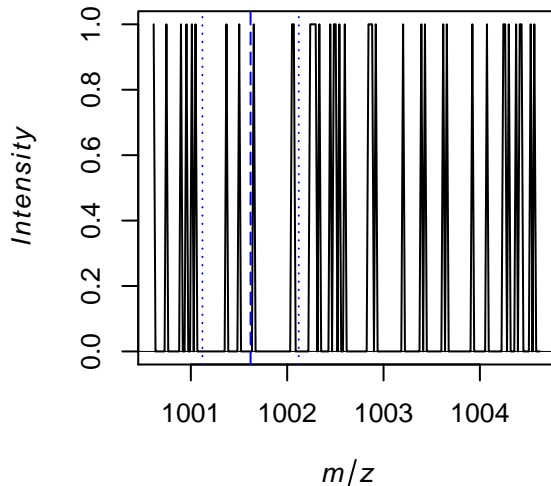
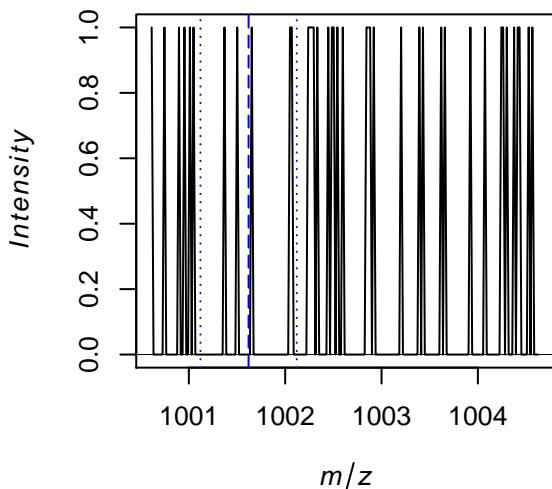
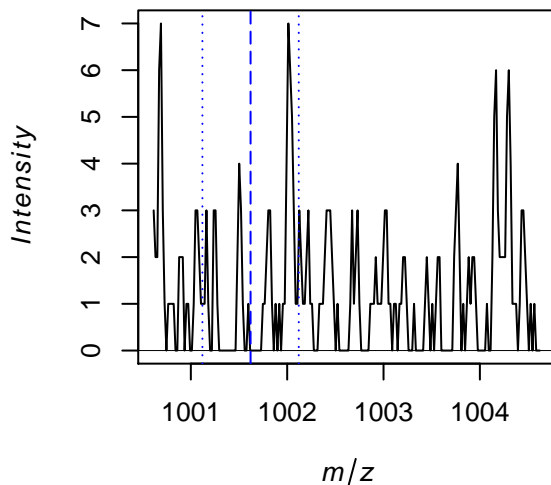
pixel in middle of acquisition

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

average spectrum

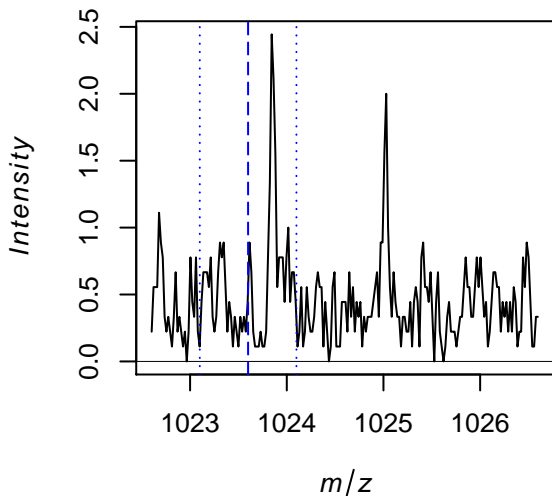


pixel in middle of acquisition

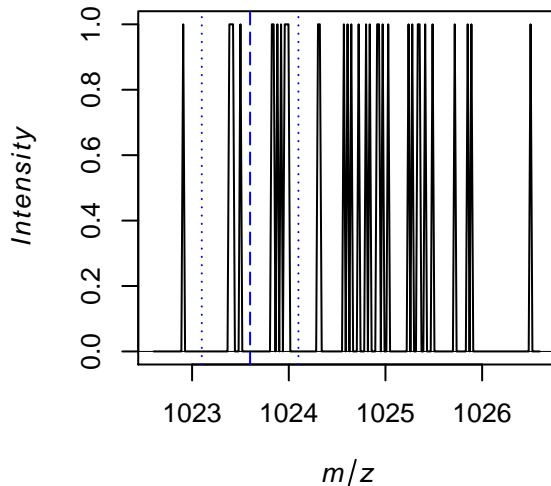
Spectrum at  $x = 1, y = 2$ Spectrum at  $x = 1, y = 1$ 

1023.6

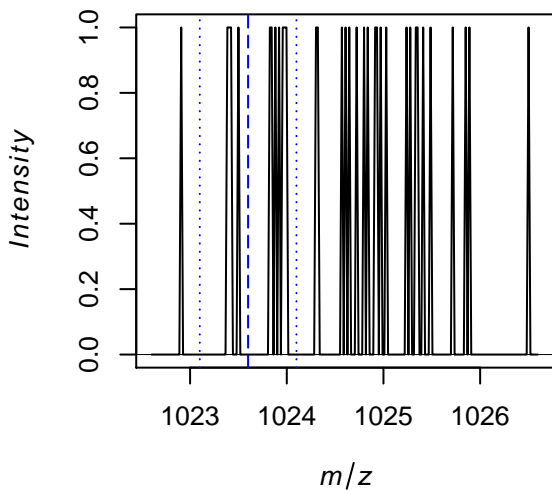
average spectrum



pixel in middle of acquisition



Spectrum at  $x = 1, y = 2$



Spectrum at  $x = 1, y = 1$

