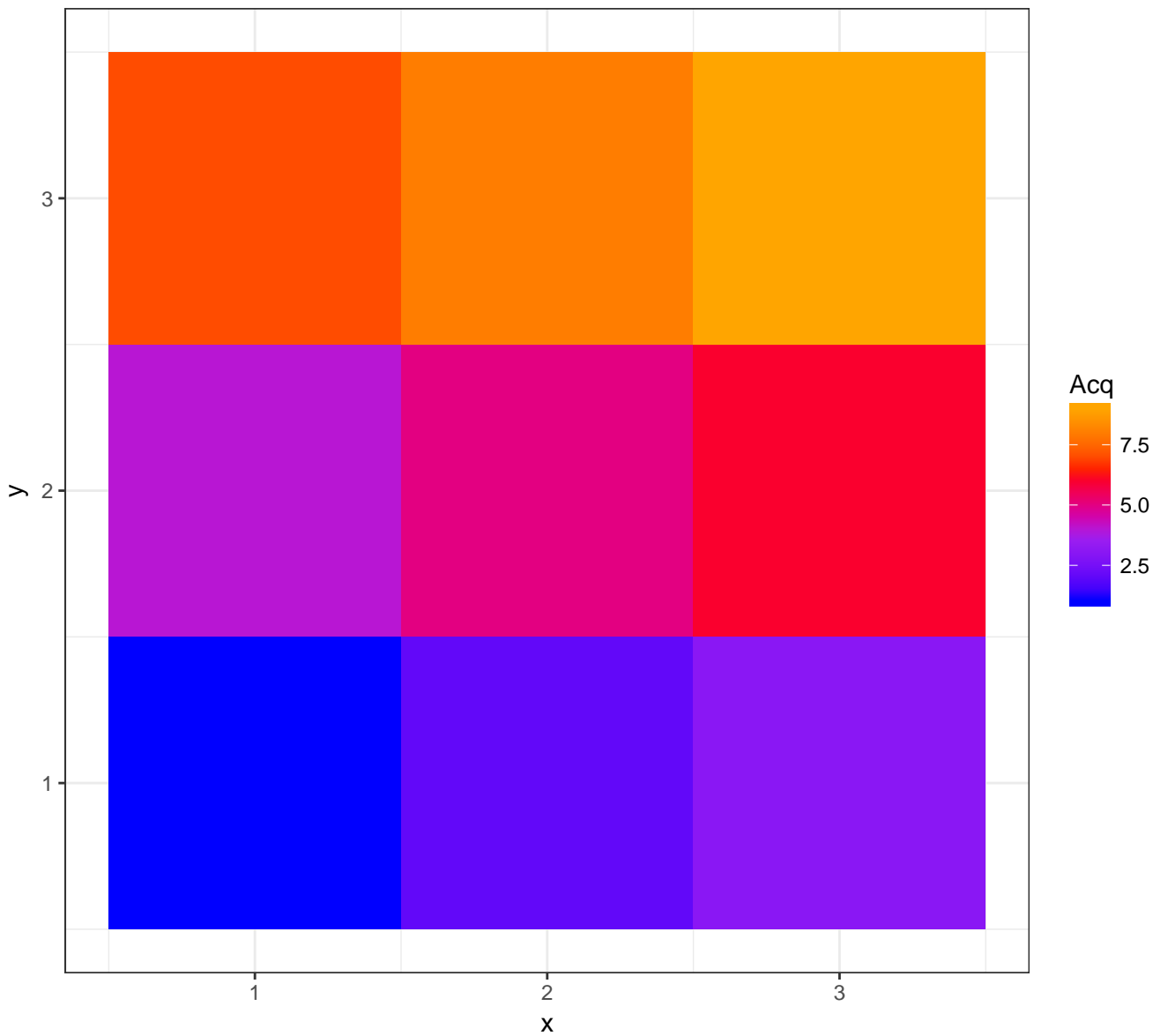


# Quality control of MSI data

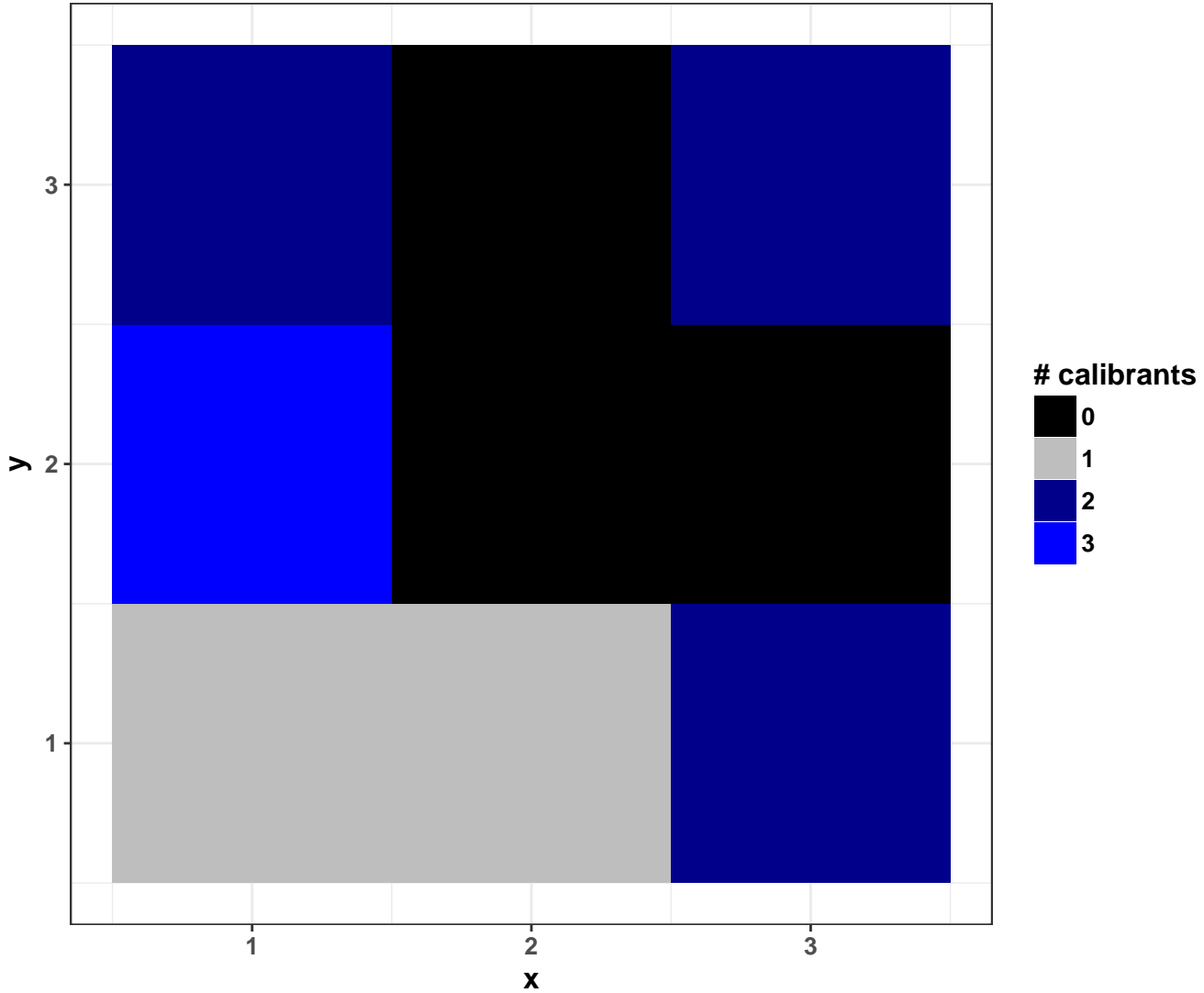
Filename: Testfile\_rdata

properties	values
Number of mz features	8399
Range of mz values [Da]	100.08 – 799.92
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	0 – 318.82
Median of intensities	0
Intensities > 0	30.92 %
Number of zero TICs	0
Preprocessing	
Normalization	tic
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# valid masses in Testfile_rdata	6/6

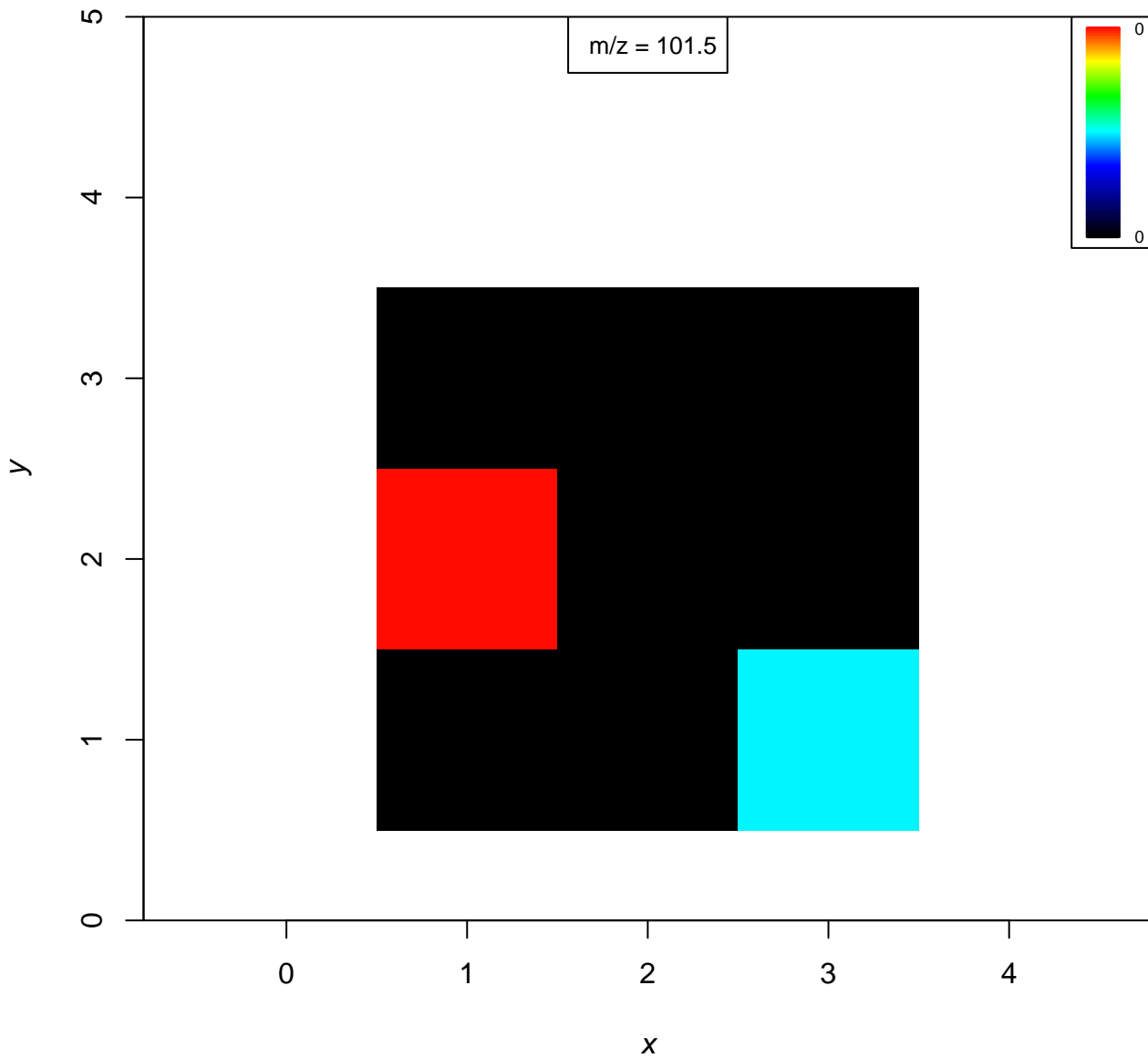
# 1) Order of Acquisition



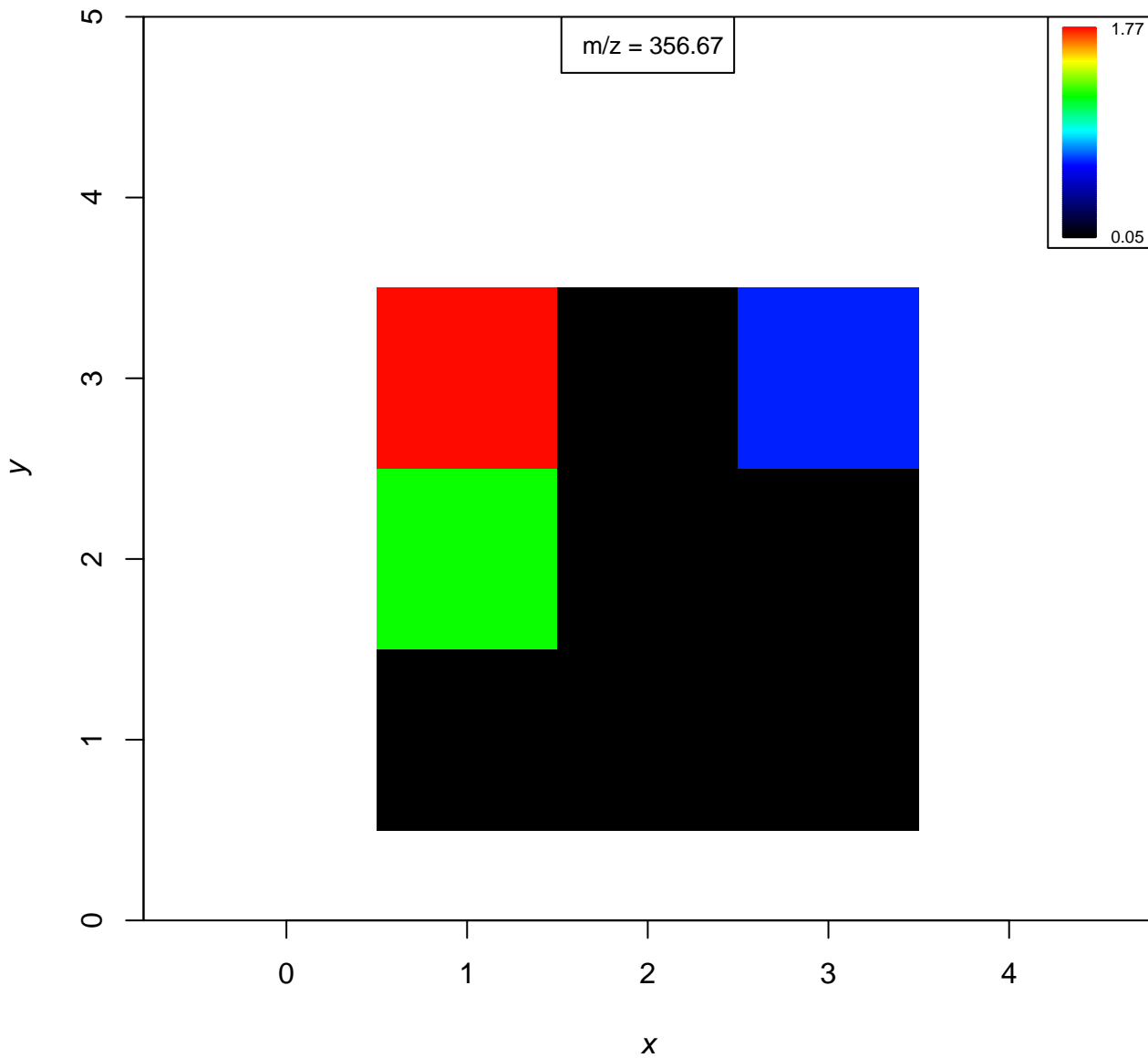
## 2) Number of calibrants per pixel



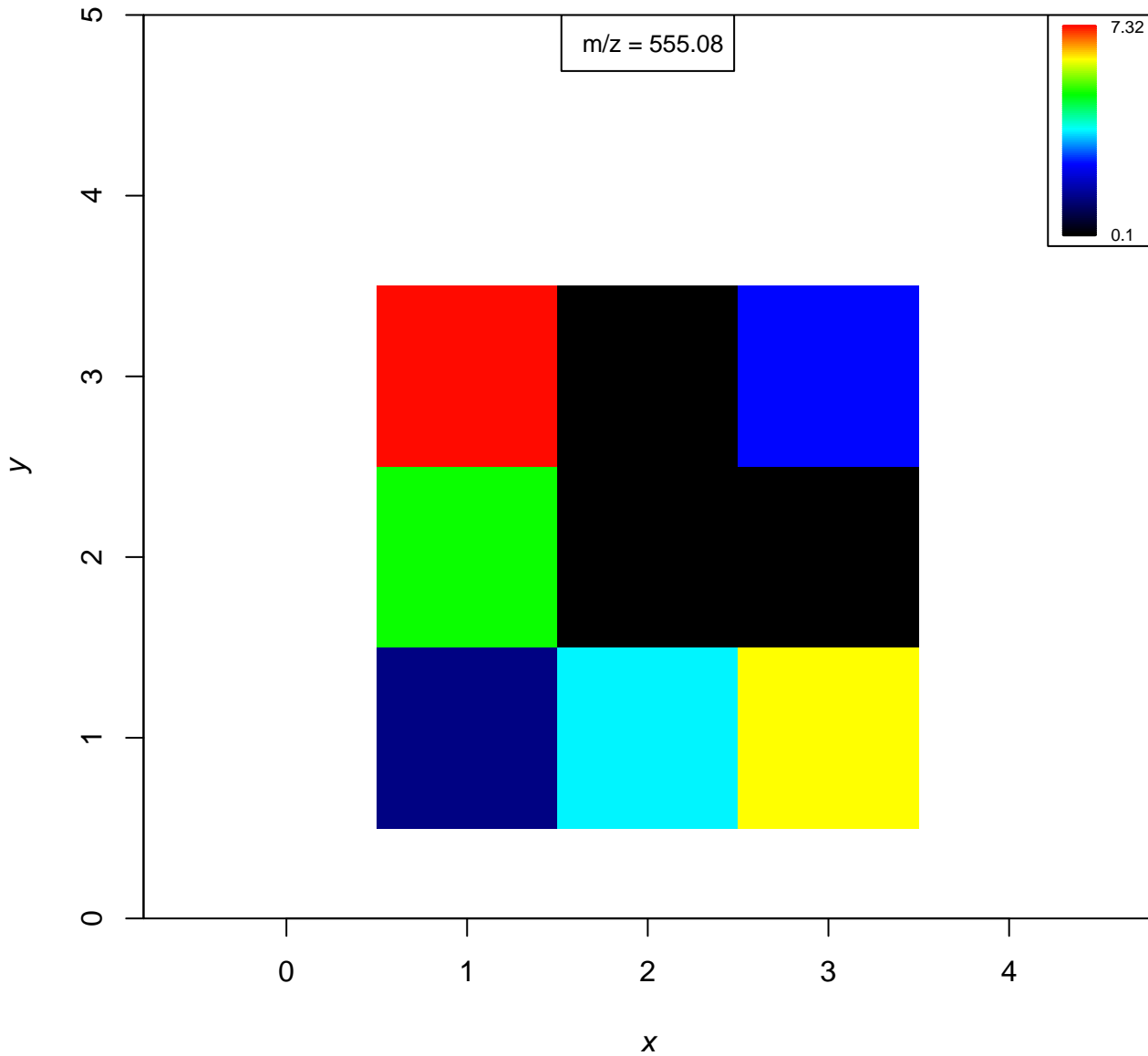
### 3A) 101.5 (101.5 ± 0.1 Da)



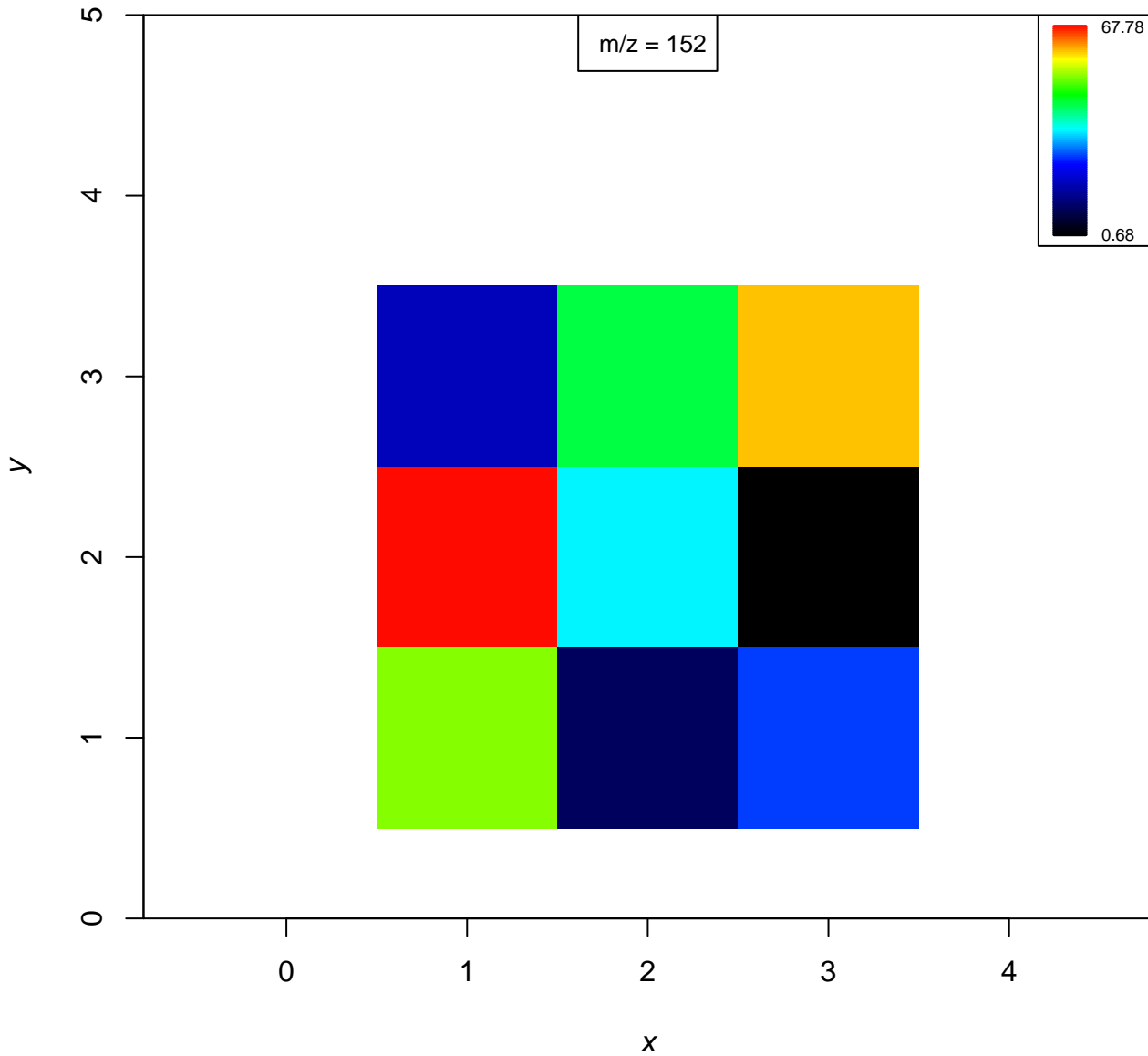
### 3B) 356.7 (356.7 ± 0.1 Da)



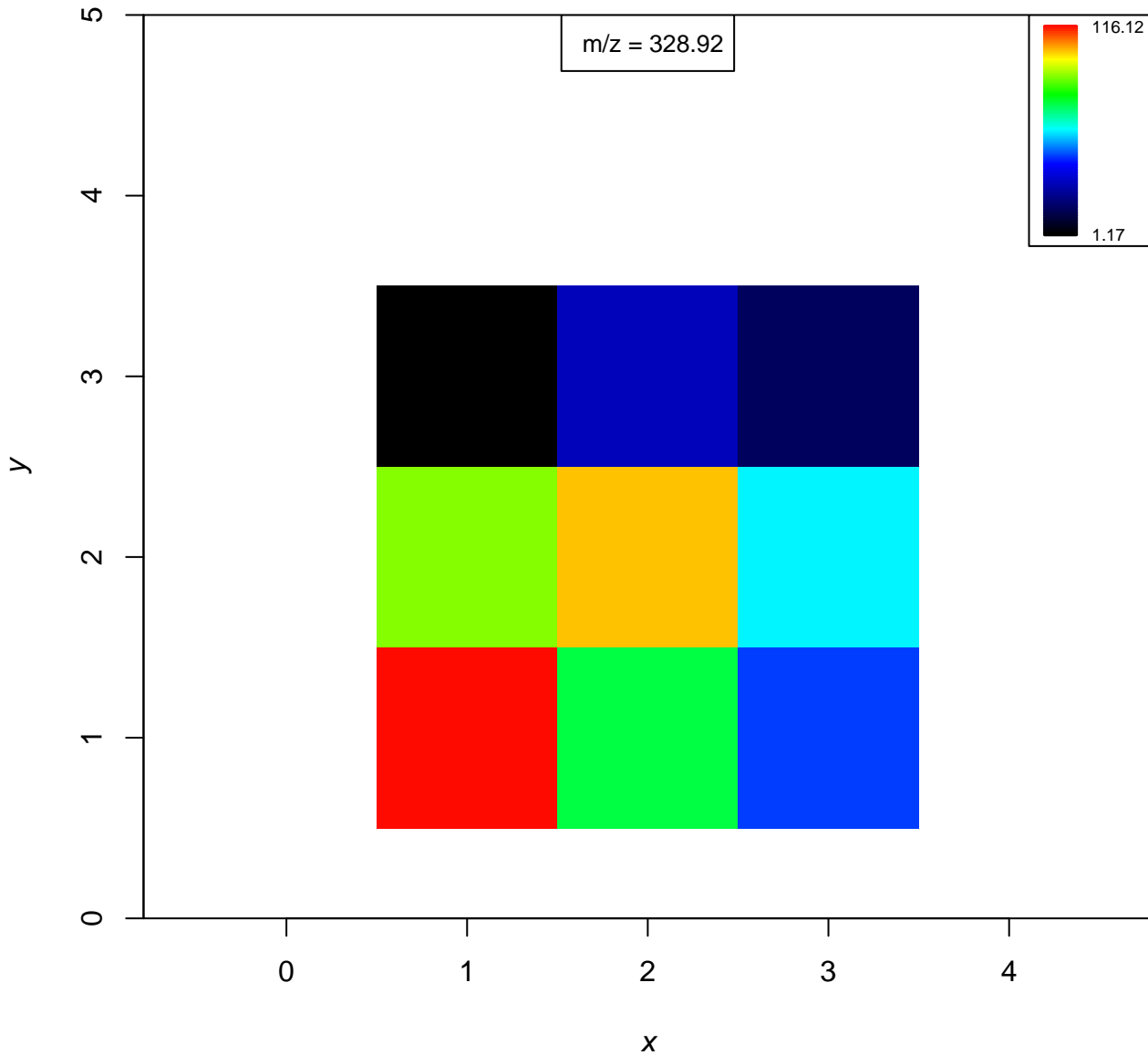
### 3C) 555.1 (555.1 ± 0.1 Da)



# 3D) mass1 ( $152 \pm 0.1$ Da)

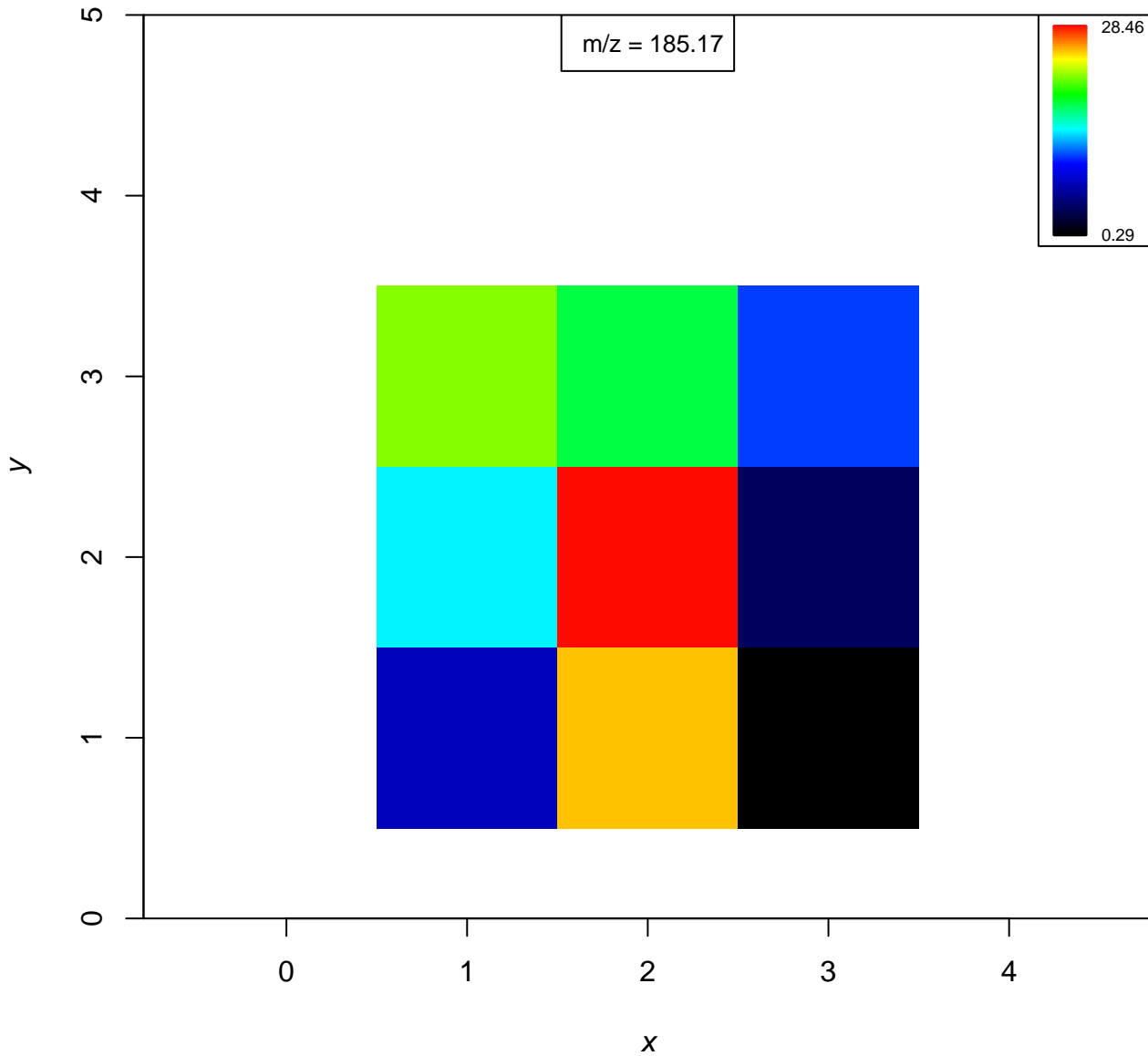


### 3E) mass2 (328.9 ± 0.1 Da)

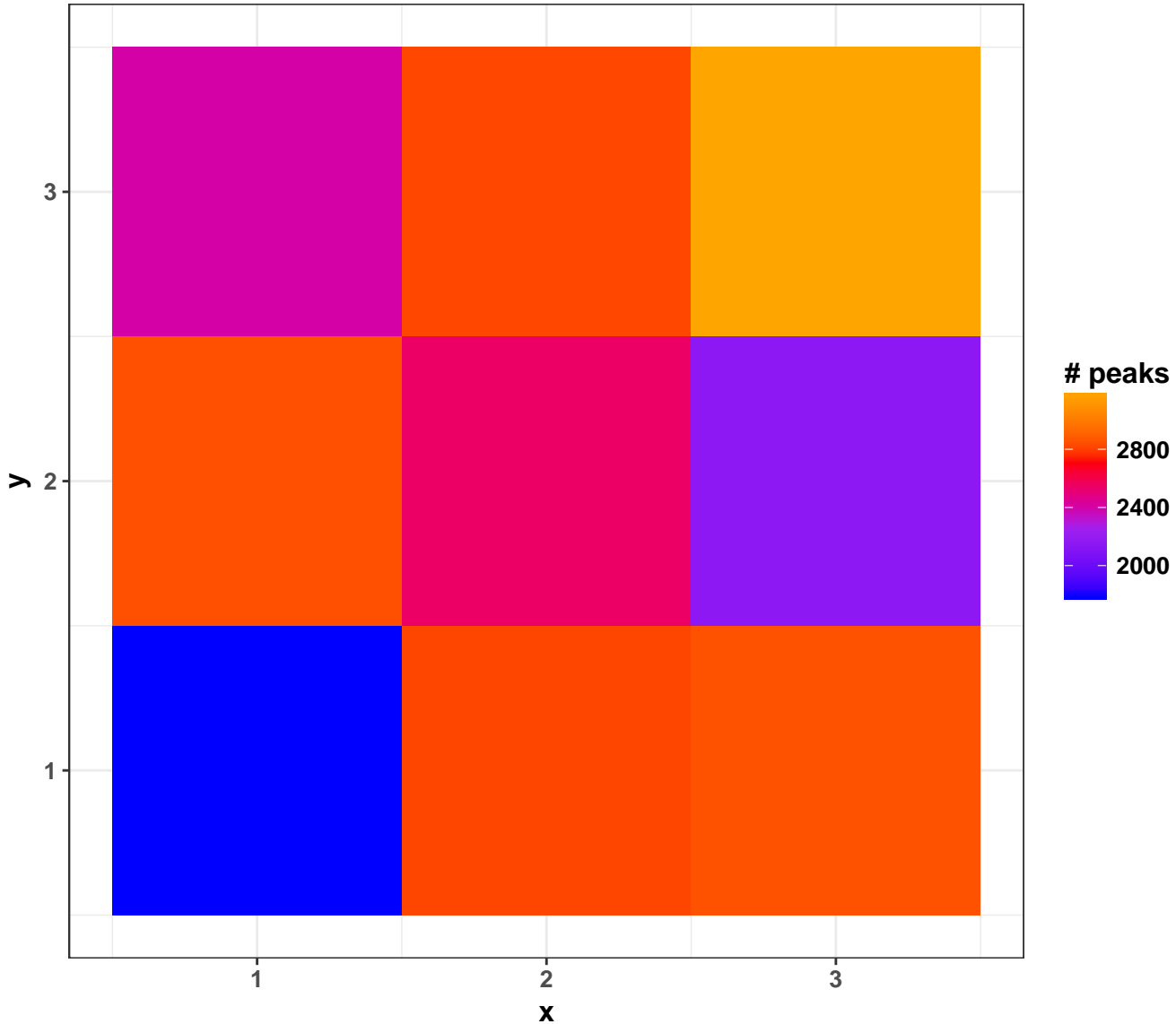




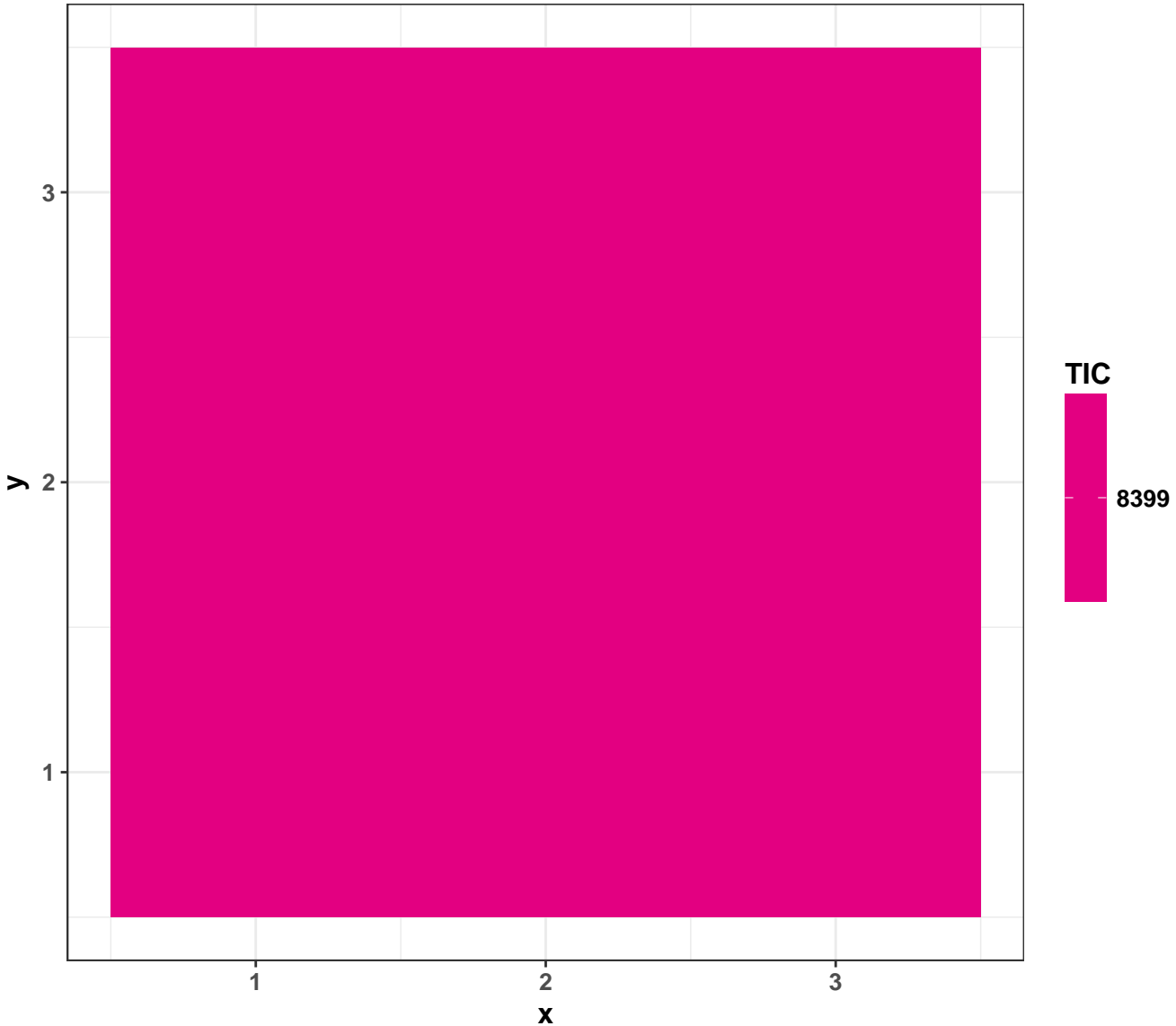
### 3F) mass3 (185.2 ± 0.1 Da)



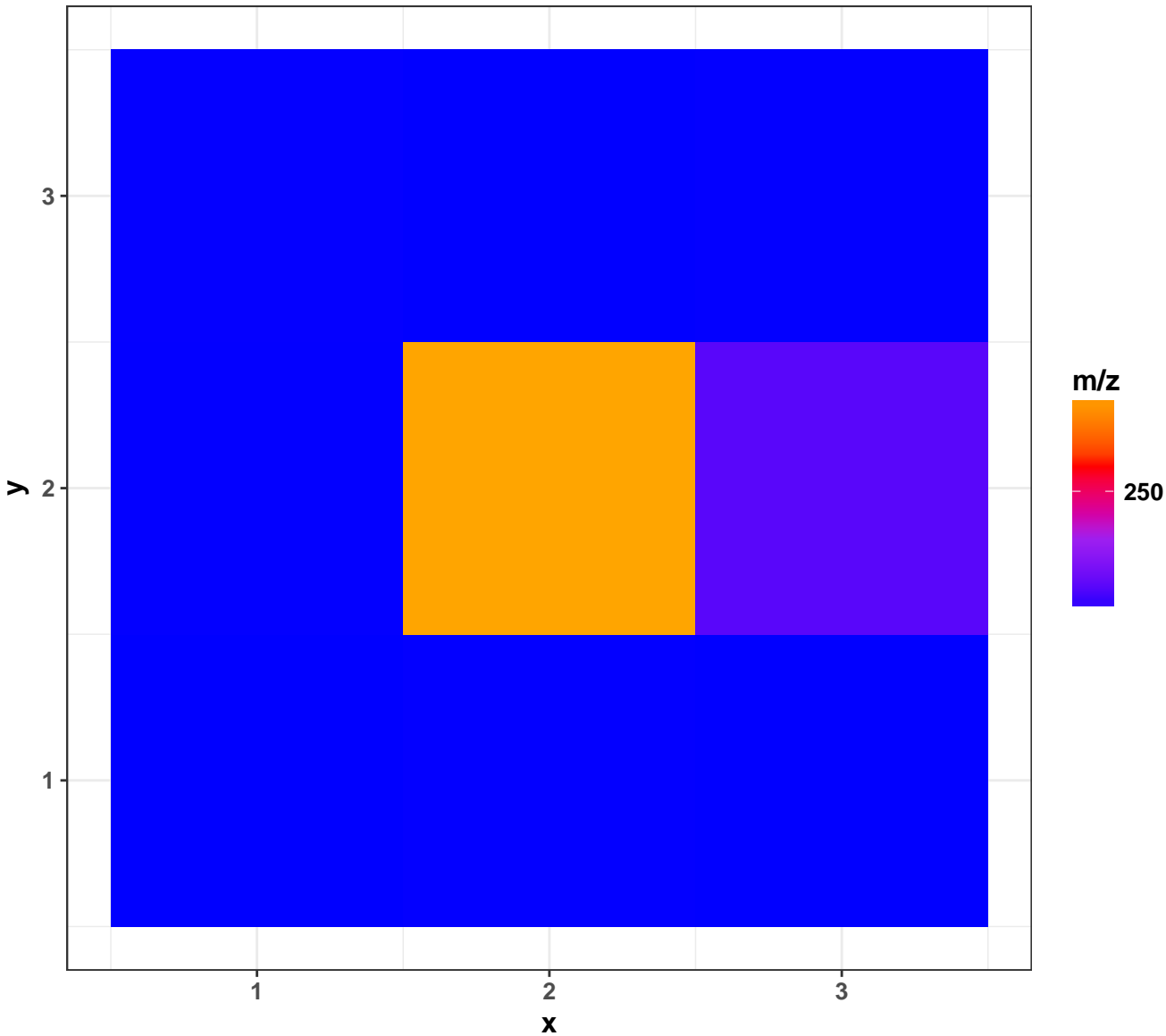
#### 4) Number of peaks per pixel



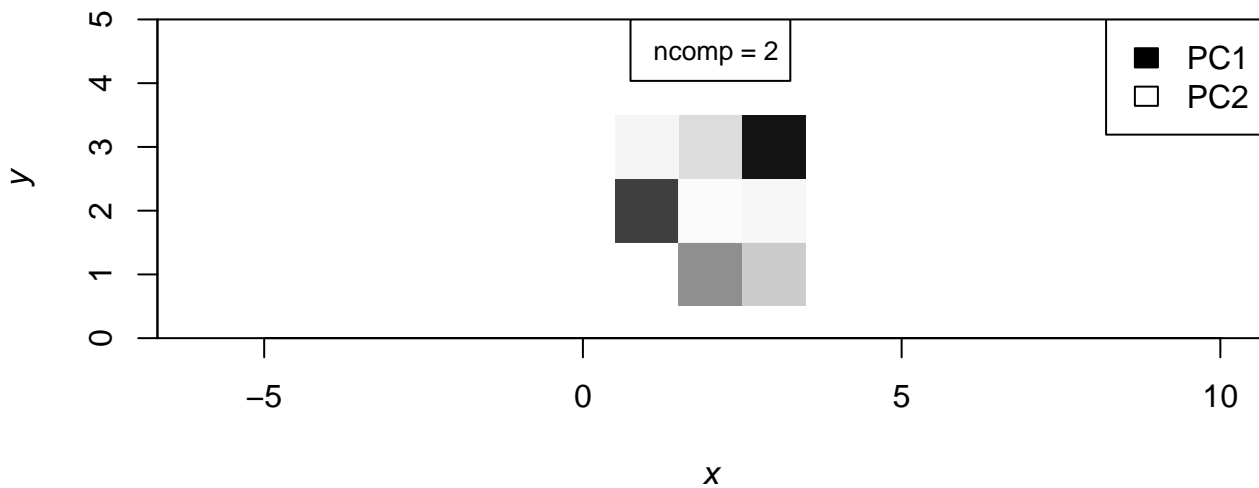
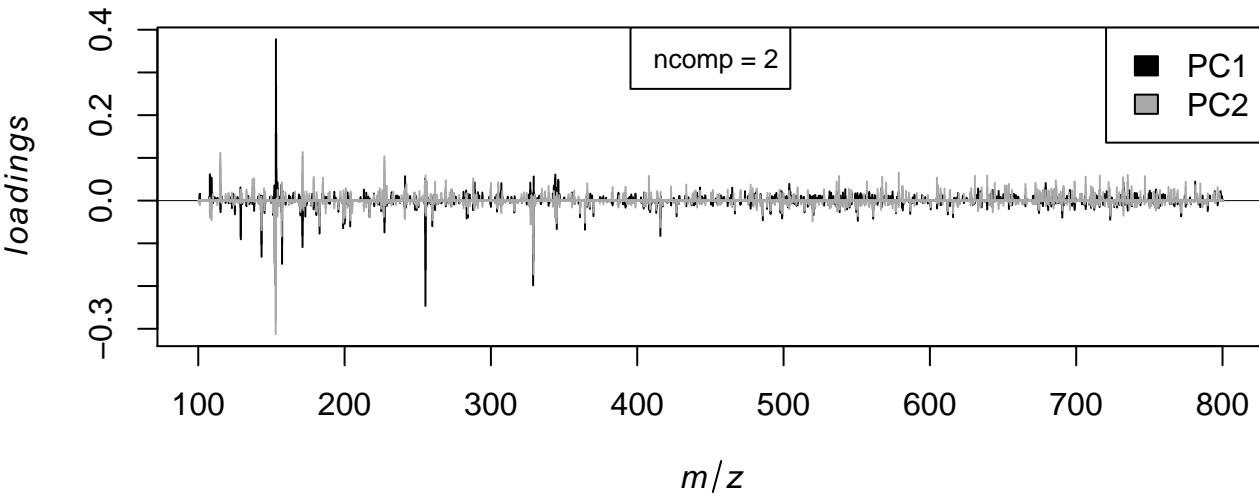
## 5) Total Ion Chromatogram



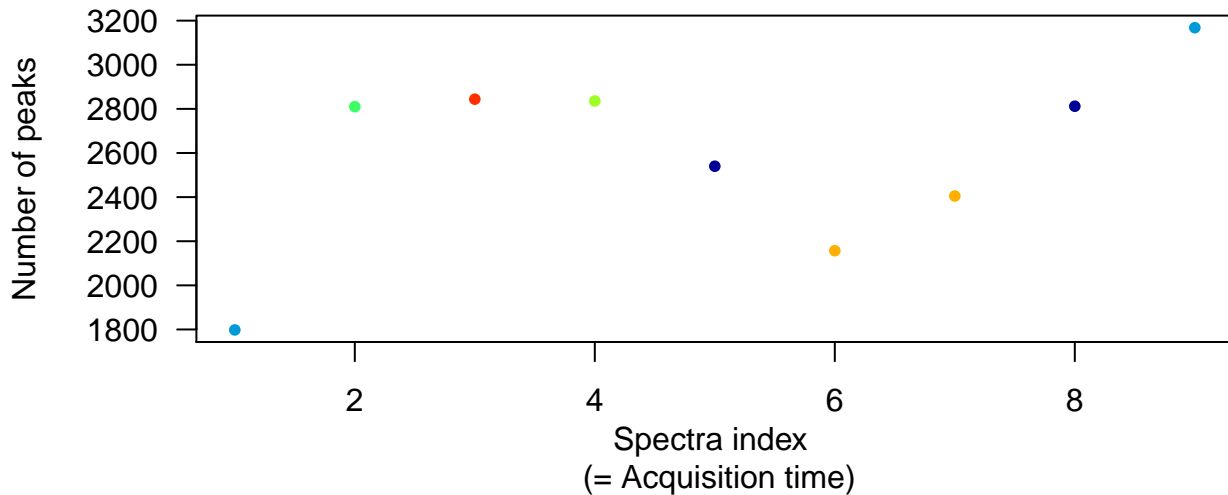
## 6) Most abundant m/z in each pixel



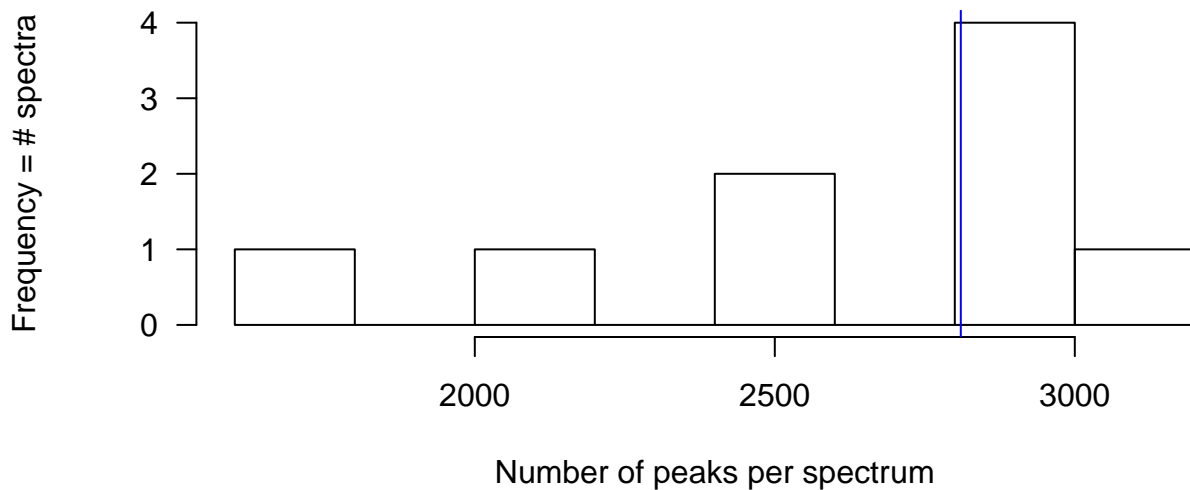
## 7) PCA for two components



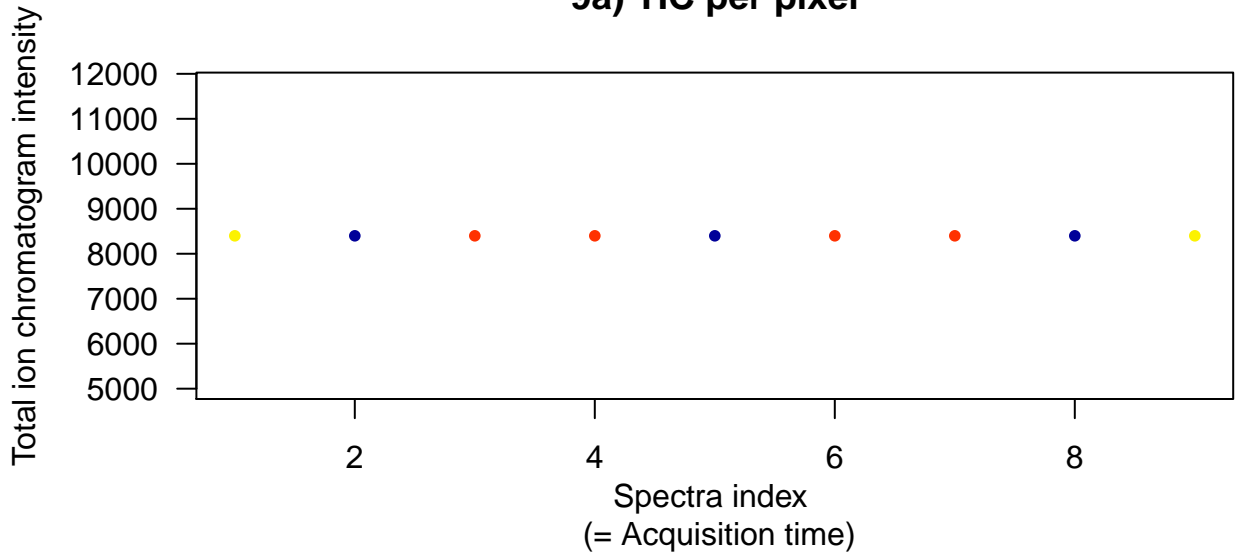
### 8a) Number of peaks per spectrum



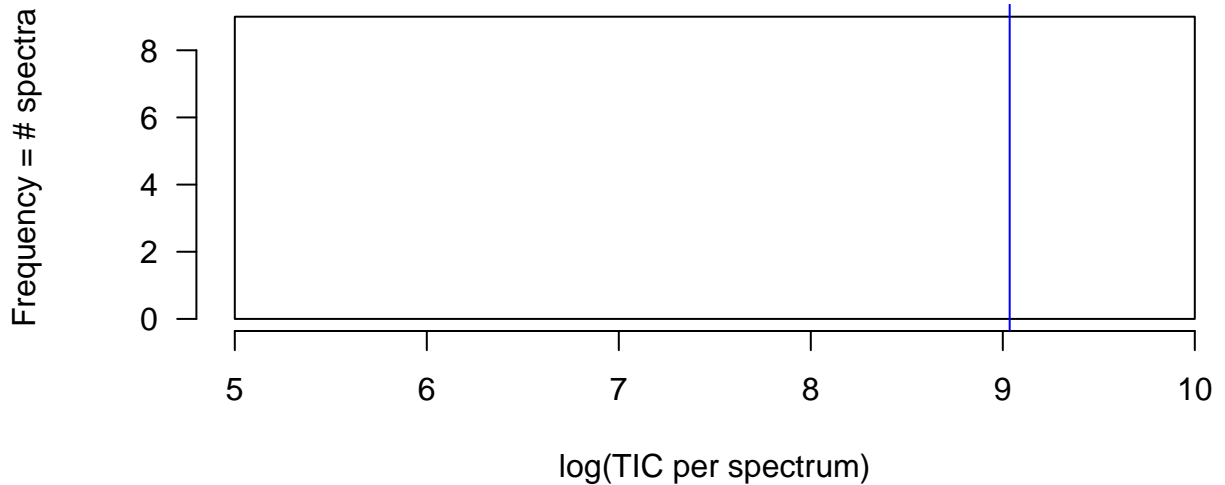
### 8b) Number of peaks per spectrum



### 9a) TIC per pixel

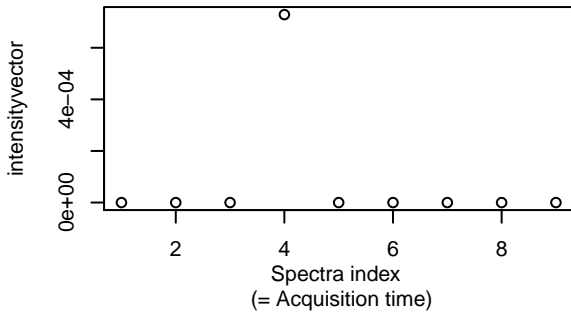


### 9b) TIC per spectrum

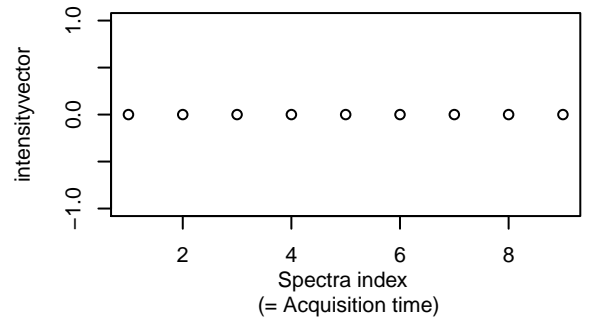


# 10) intensity of calibrants over acquisition

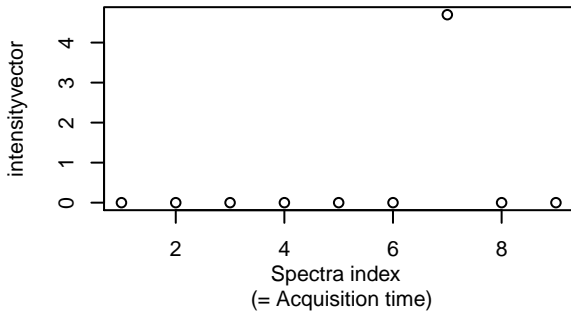
## 101.5



## 356.7

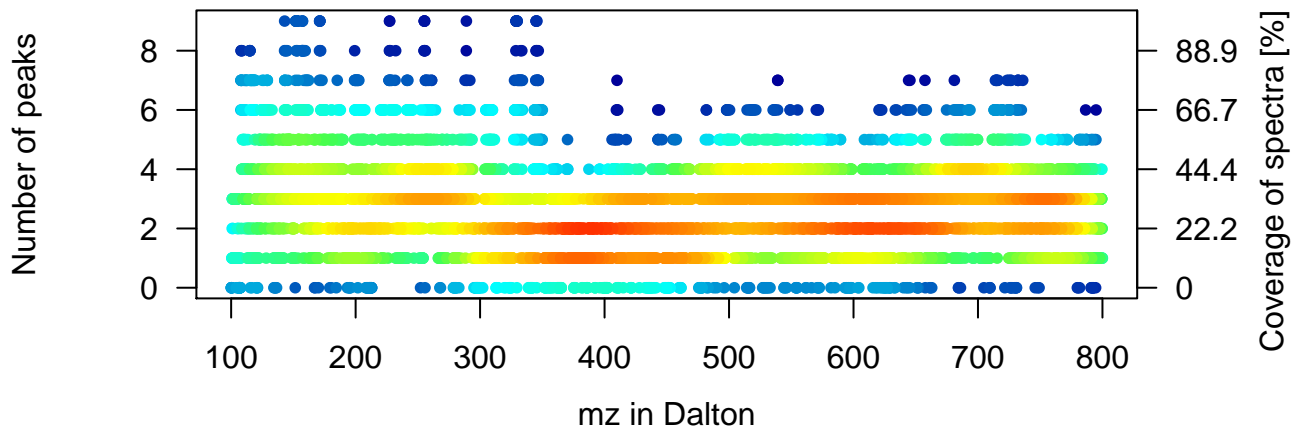


## 555.1

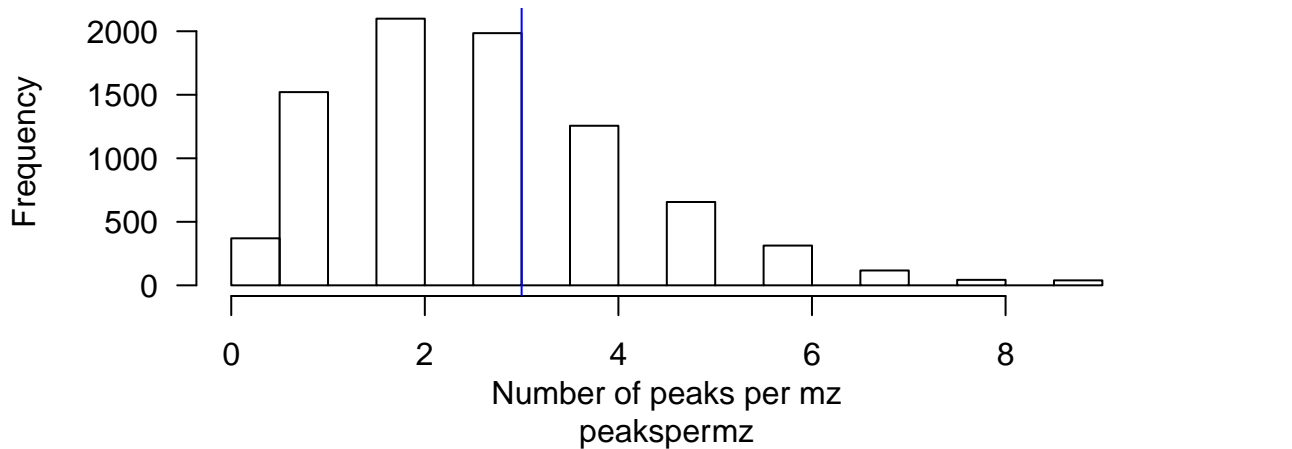




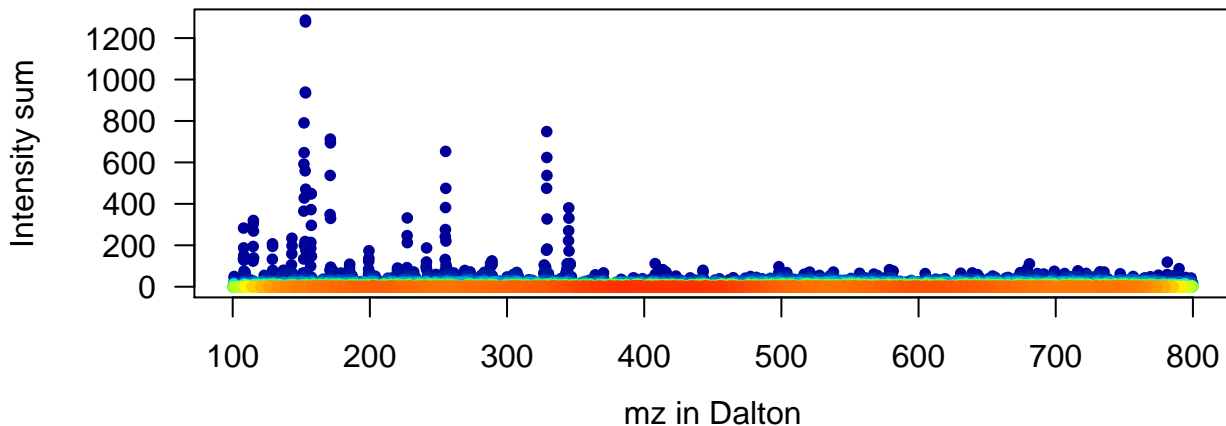
### 11a) Number of peaks for each mz



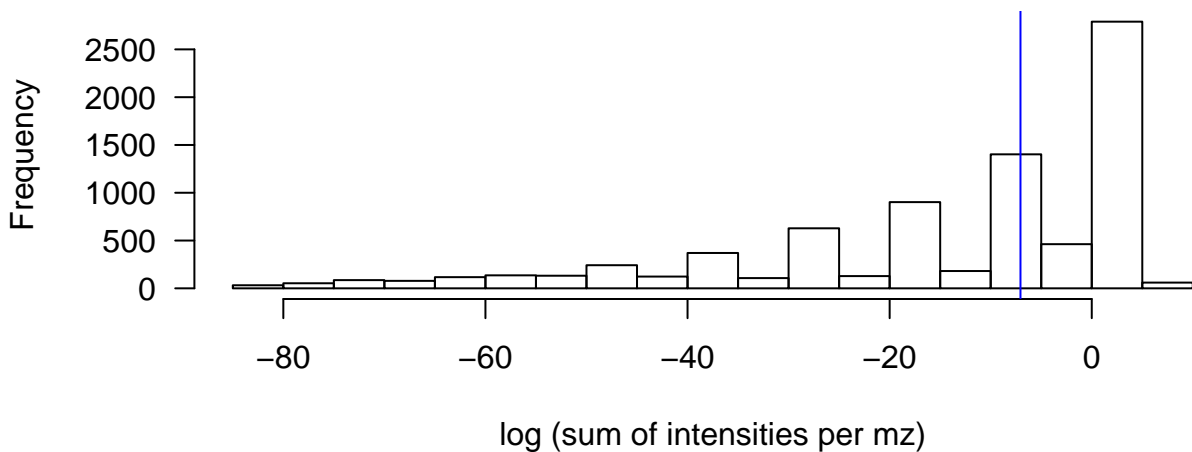
### 11b) Number of peaks per mz



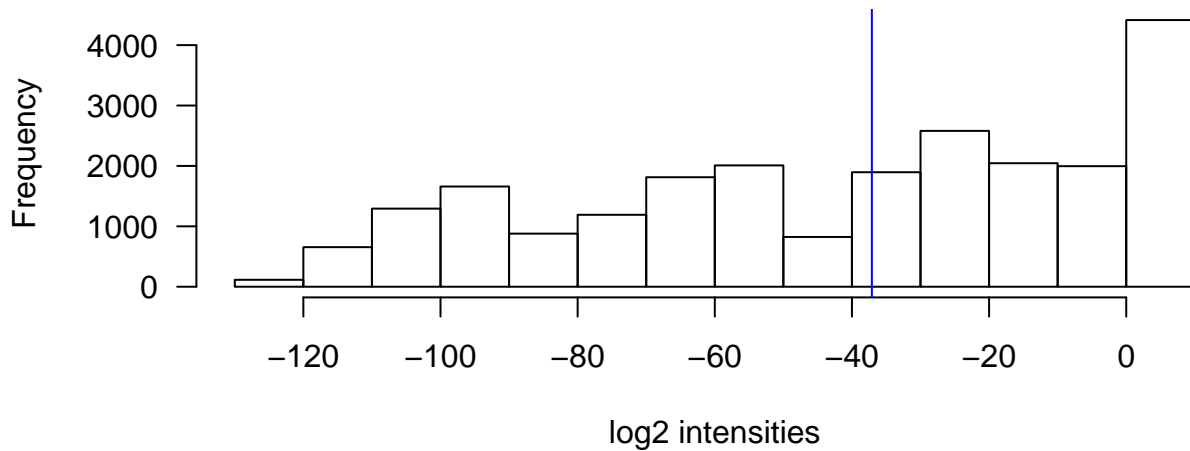
### 12a) Sum of all peak intensities for each mz



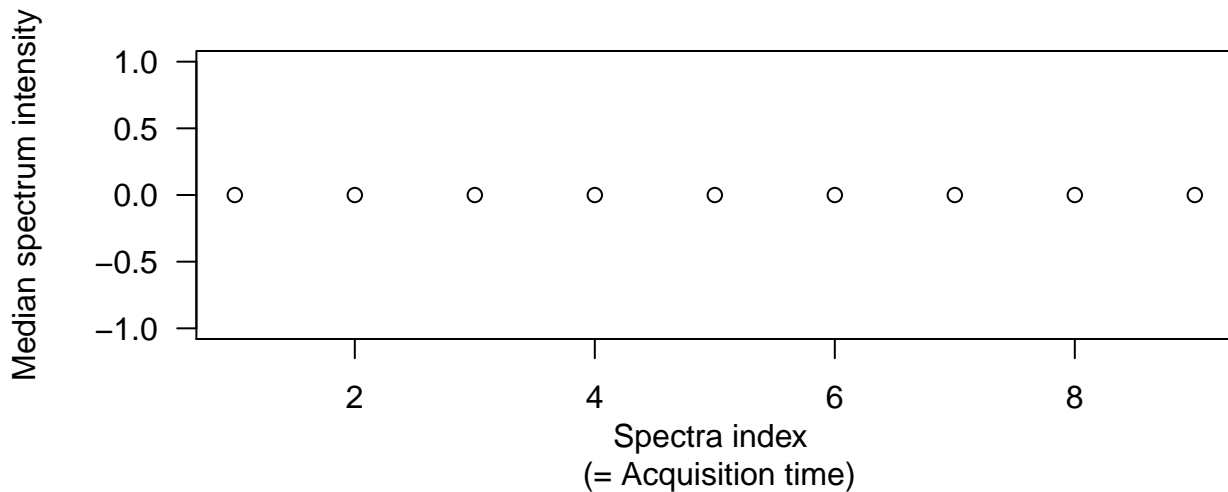
### 12b) Sum of intensities per mz



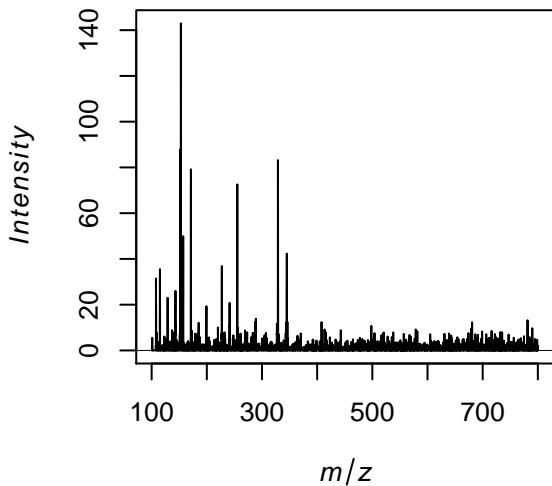
### 13a) Log2-transformed intensities



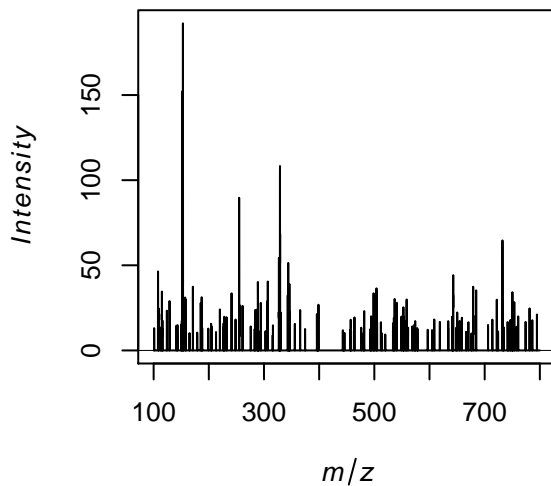
### 13b) Median intensity per spectrum



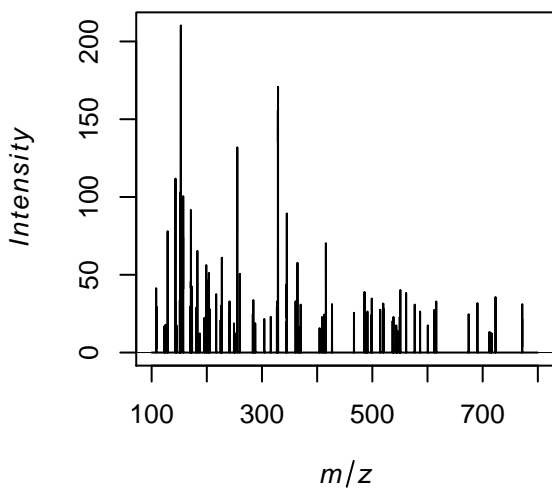
**Average spectrum**



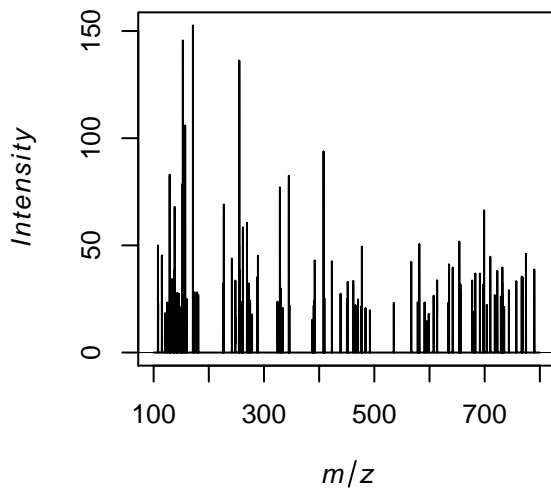
**Spectrum in middle of acquisition**



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

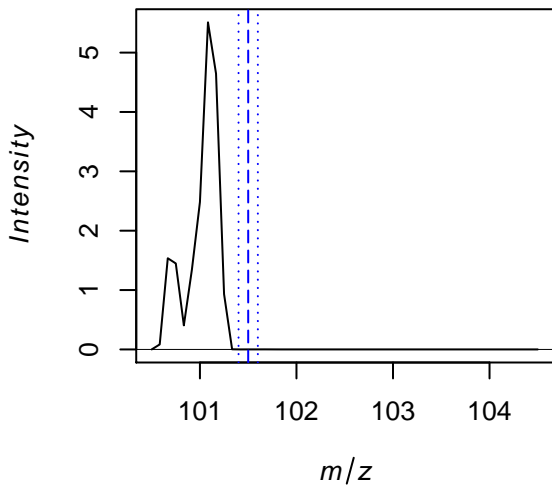


**Spectrum at  $x = 3, y = 2$**

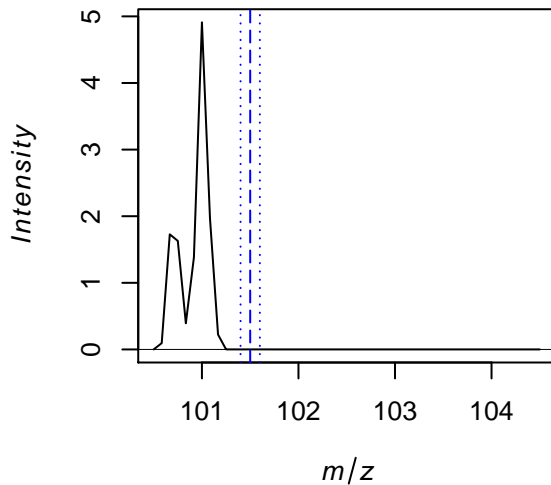


101.5

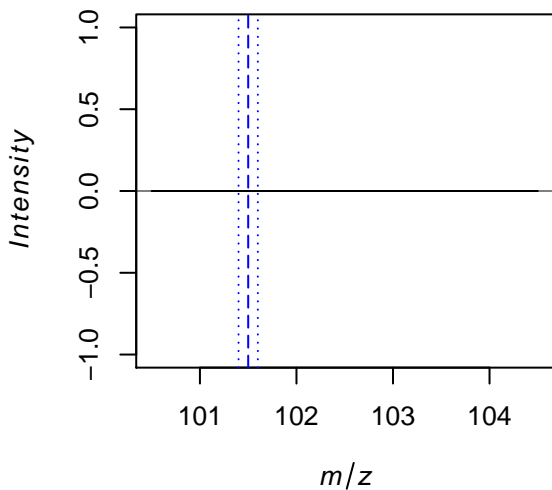
average spectrum



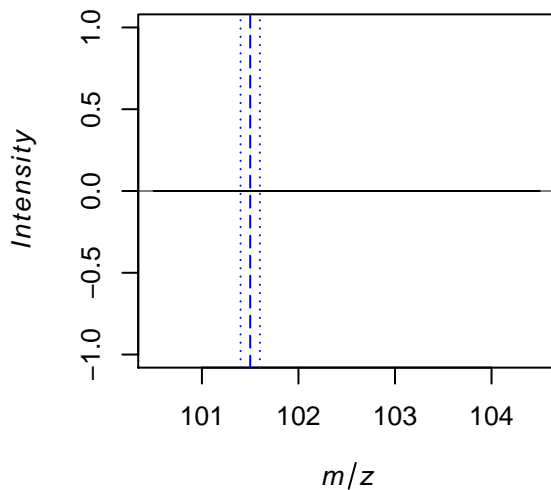
pixel in middle of acquisition



Spectrum at  $x = 1, y = 1$

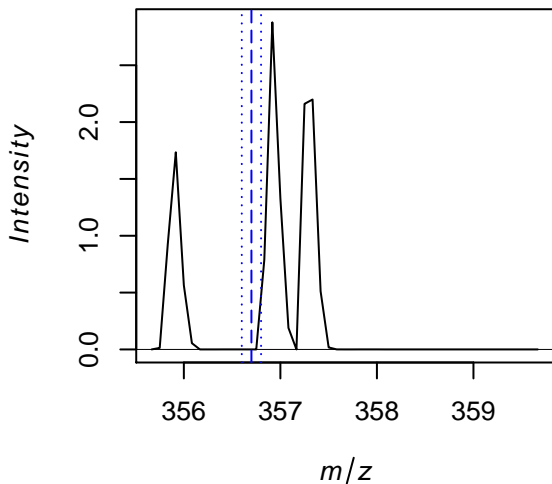


Spectrum at  $x = 3, y = 2$

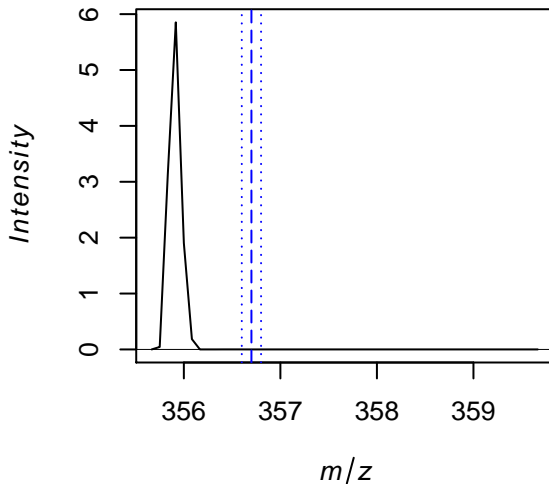


356.7

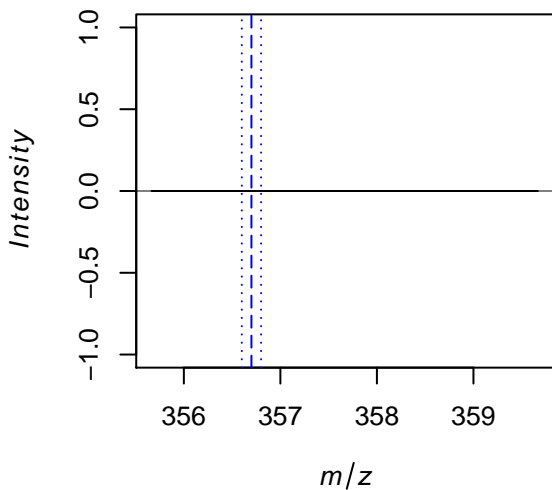
average spectrum



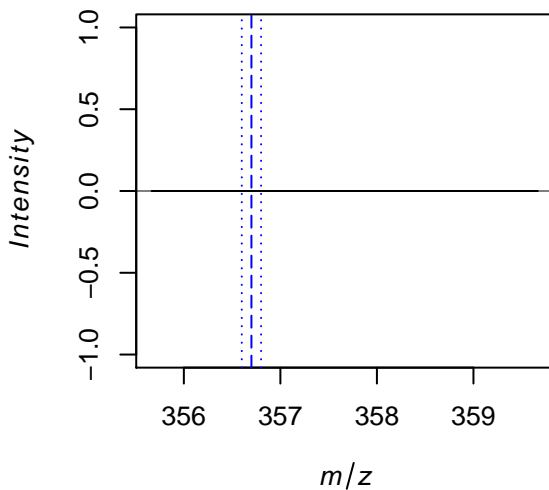
pixel in middle of acquisition



Spectrum at  $x = 1, y = 1$

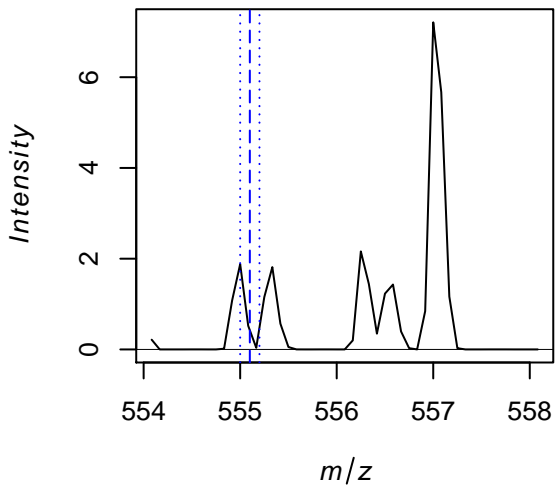


Spectrum at  $x = 3, y = 2$

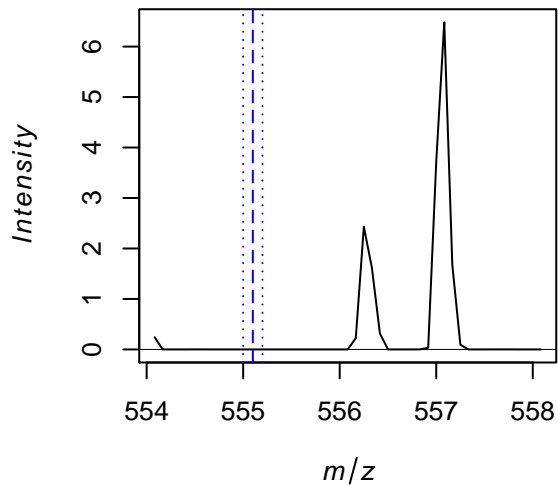


555.1

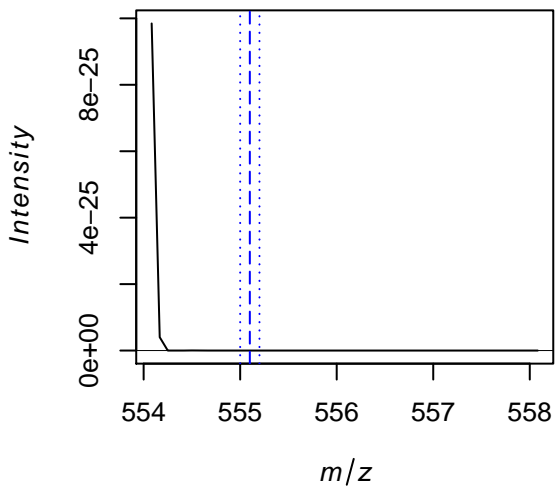
average spectrum



pixel in middle of acquisition



Spectrum at x = 1, y = 1



Spectrum at x = 3, y = 2

