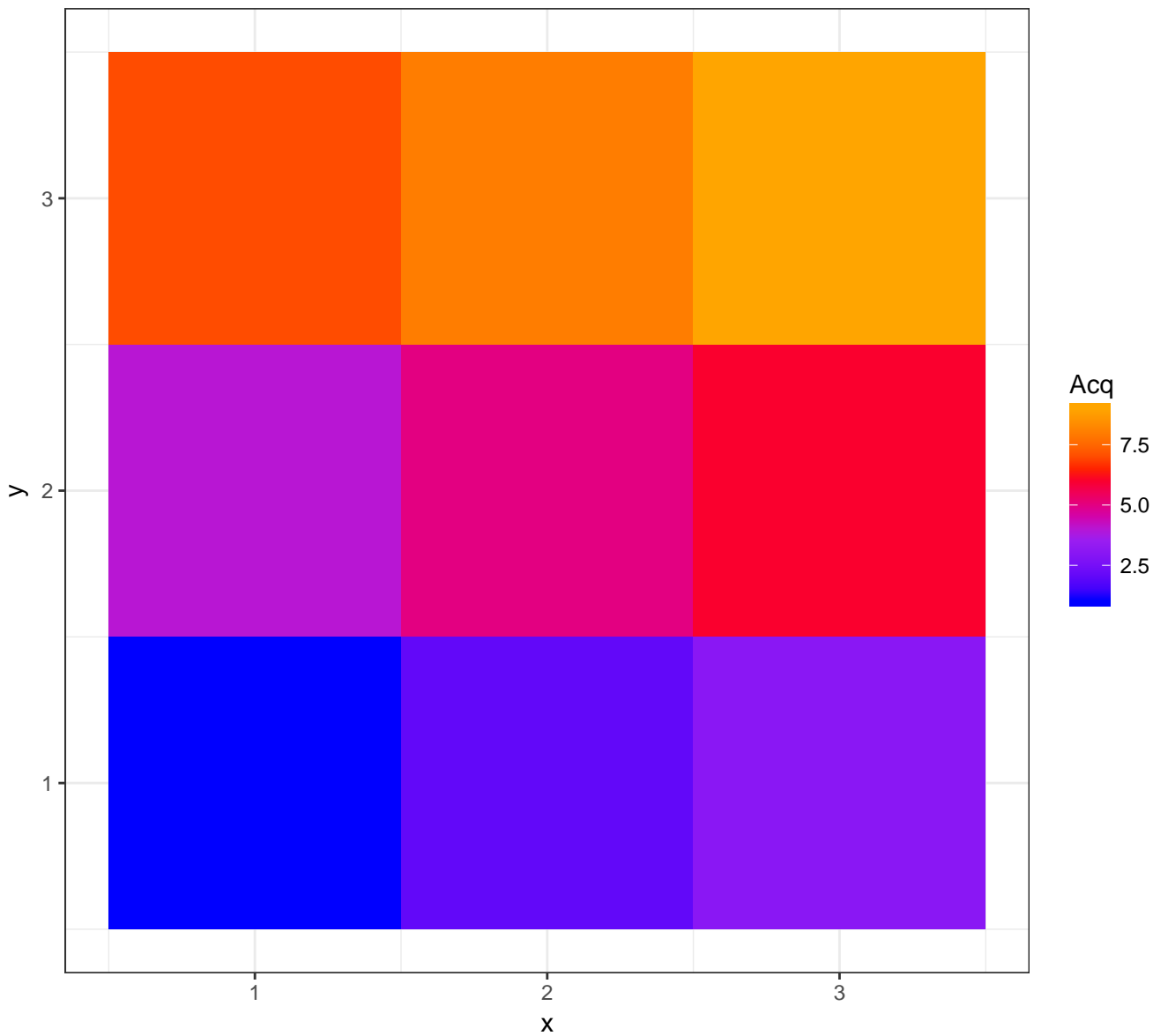


Quality control of MSI data

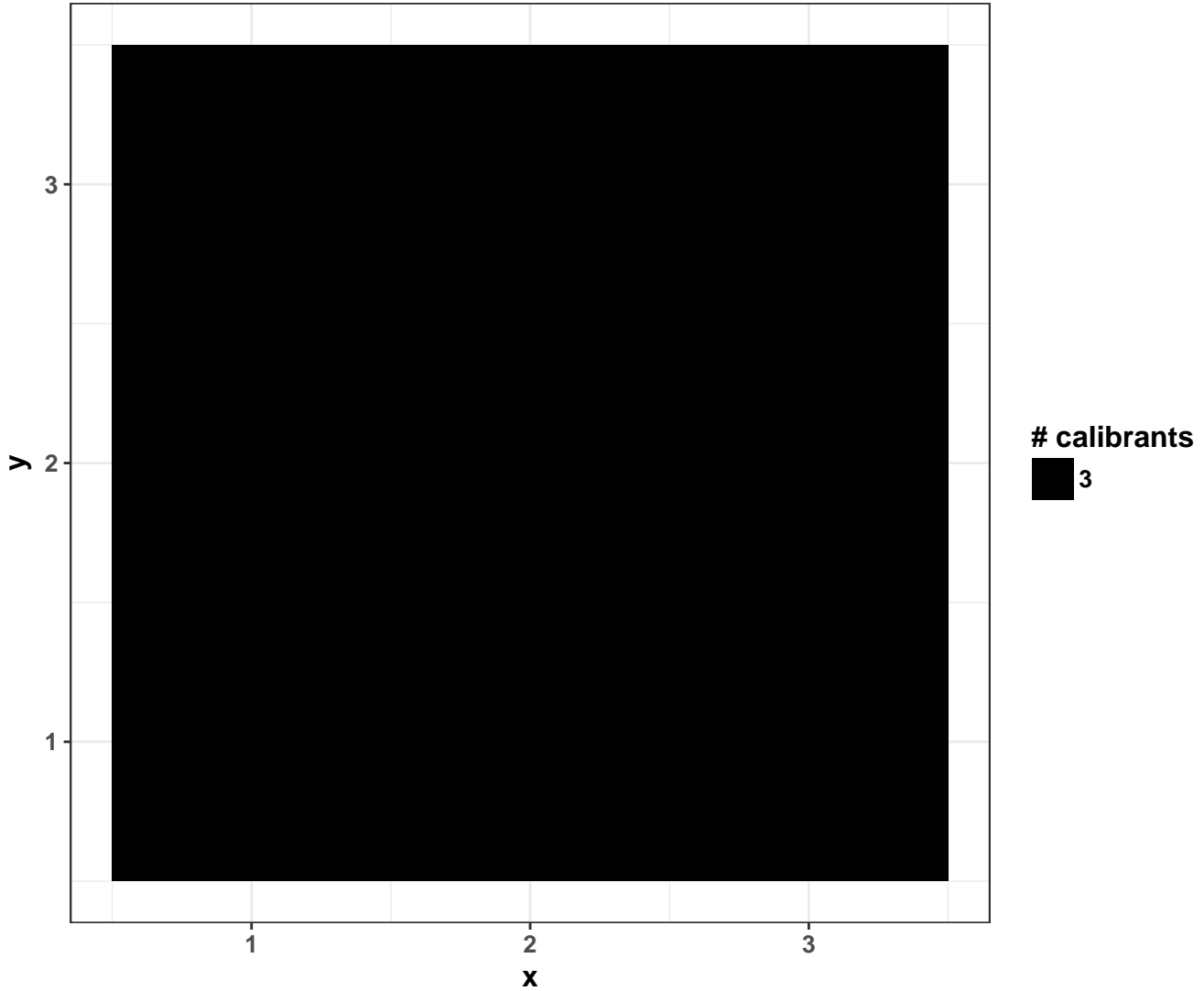
Filename: Testfile_analyze75

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

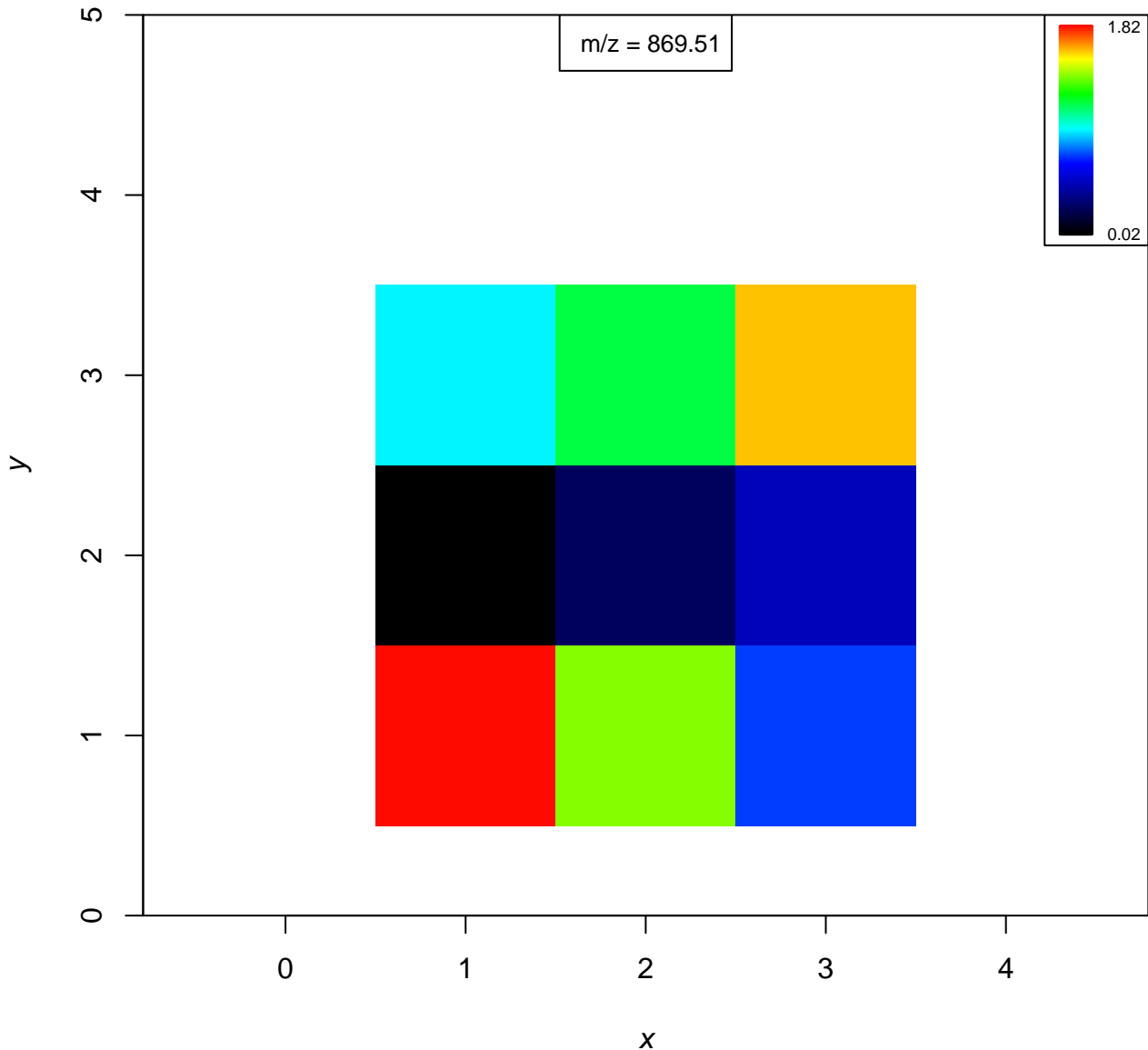
1) Order of Acquisition



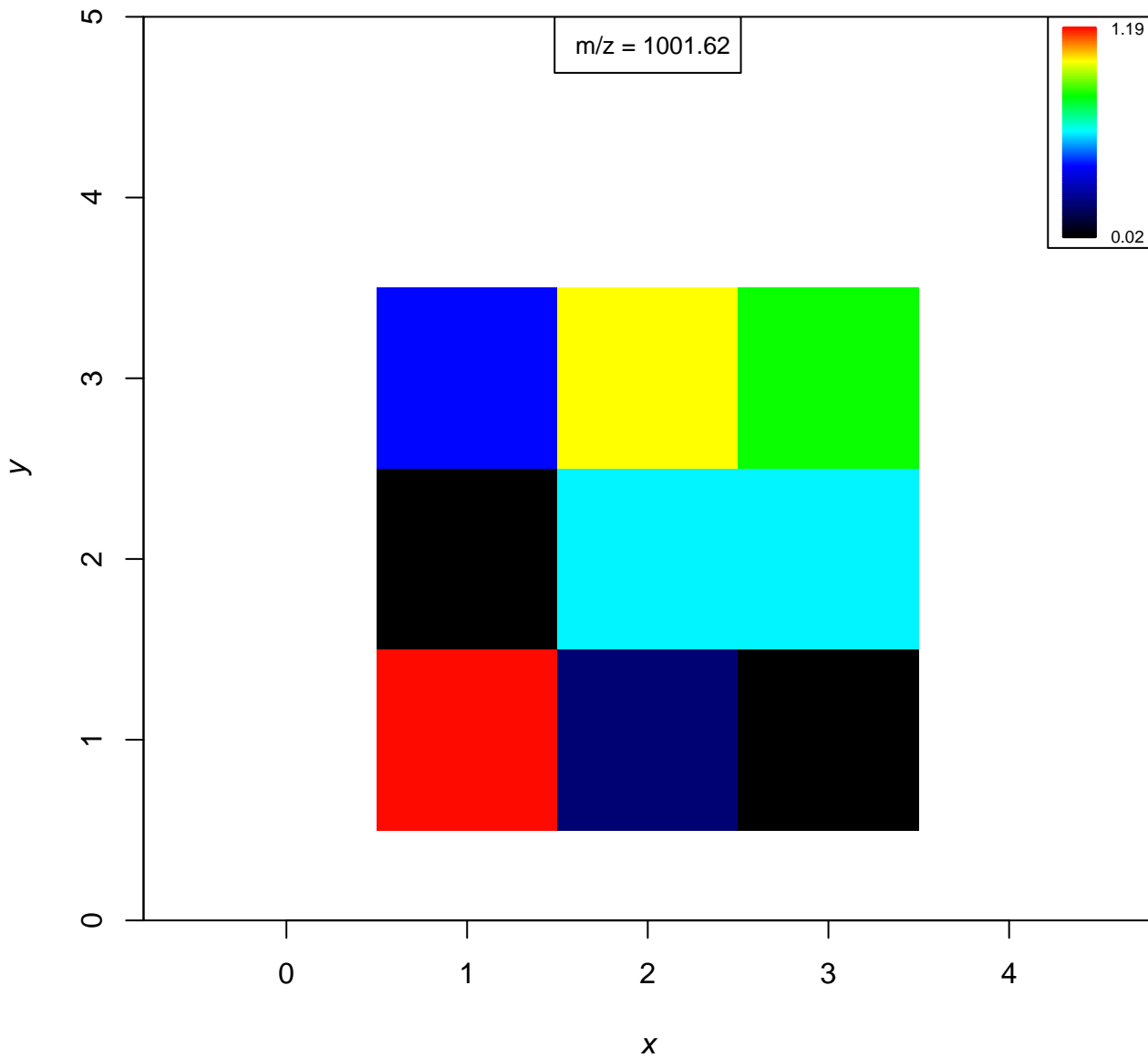
2) Number of calibrants per pixel



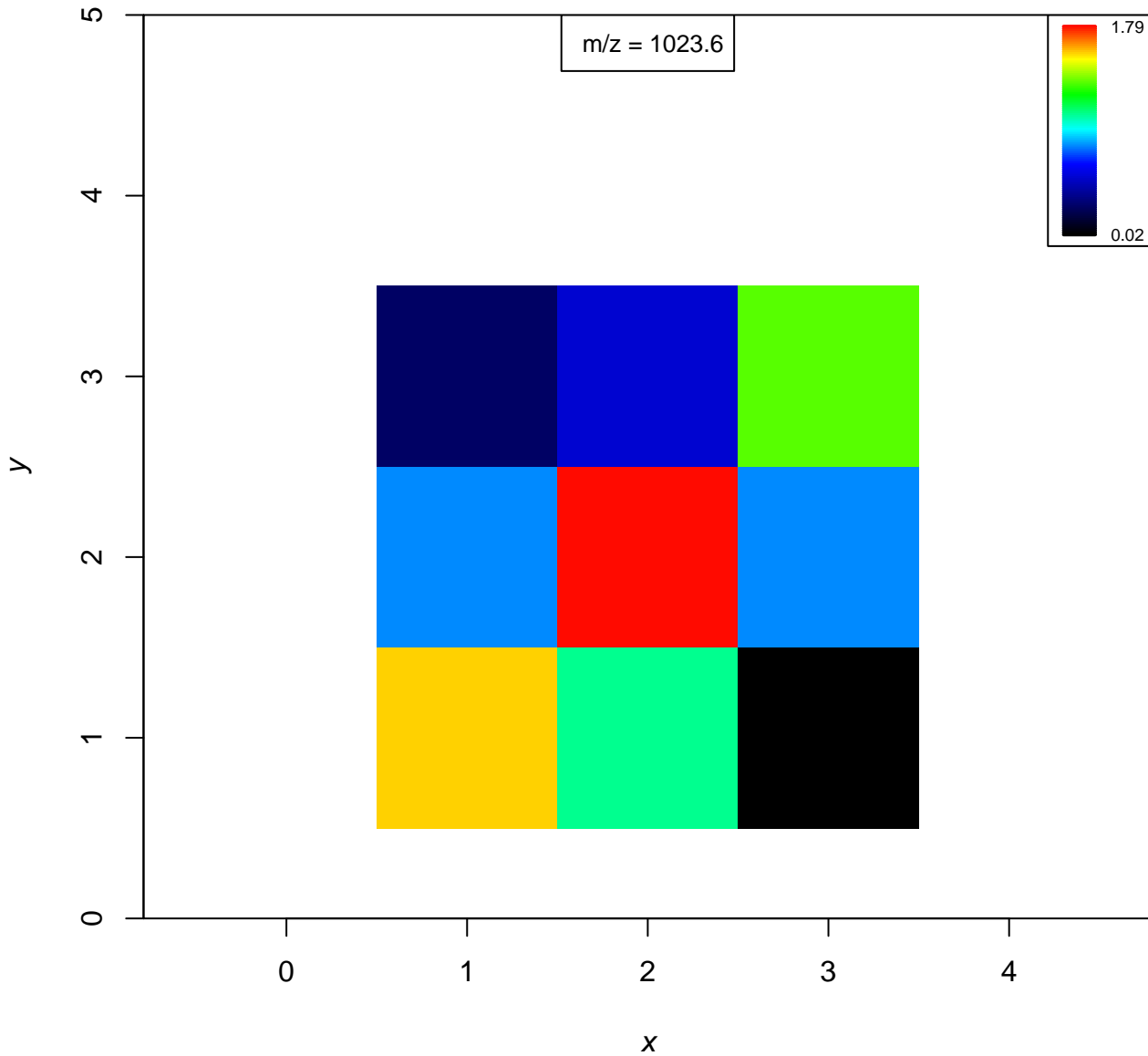
3A) mass1 (869.51 ± 0.5 Da)



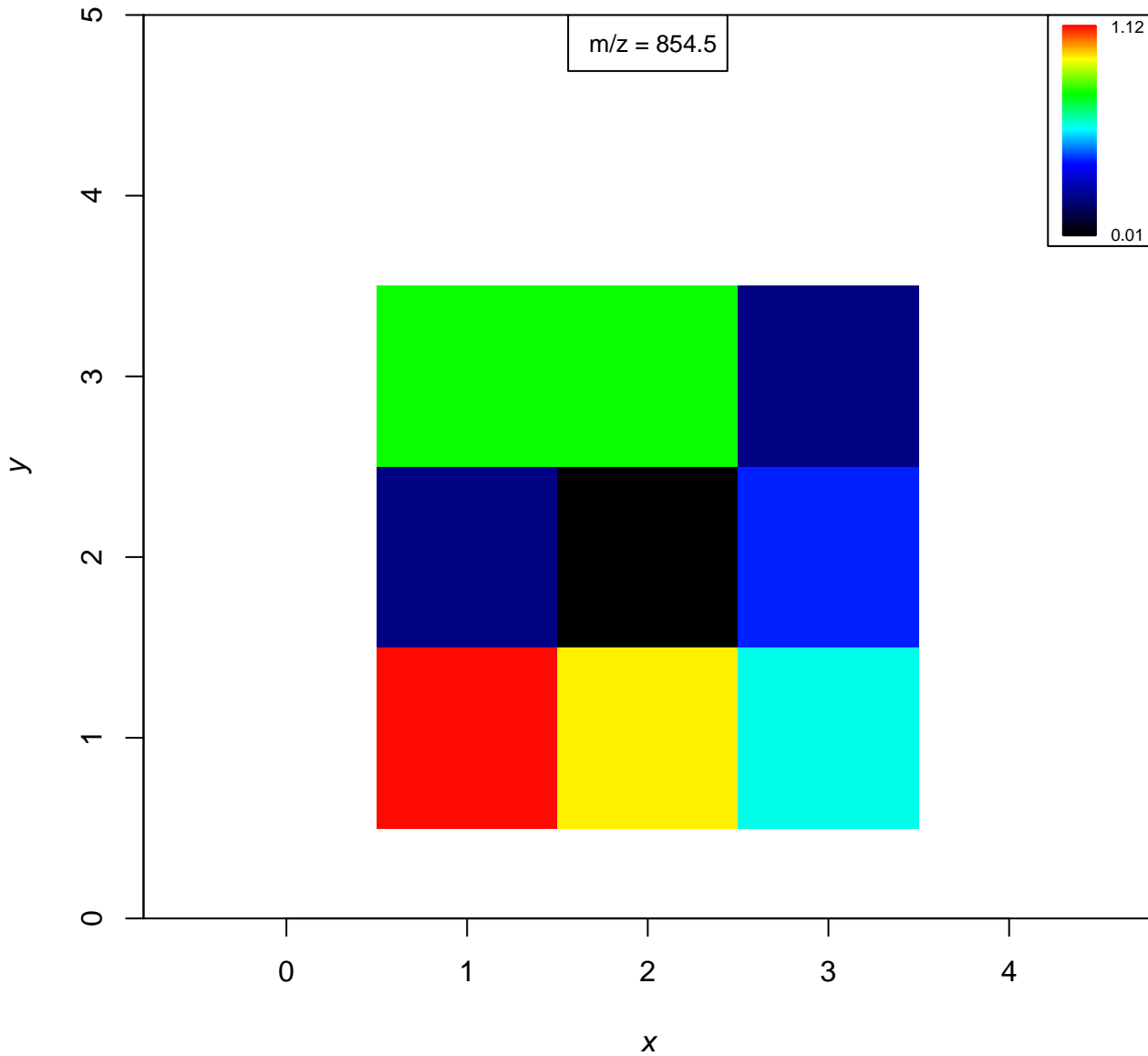
3B) mass2 (1001.62 ± 0.5 Da)



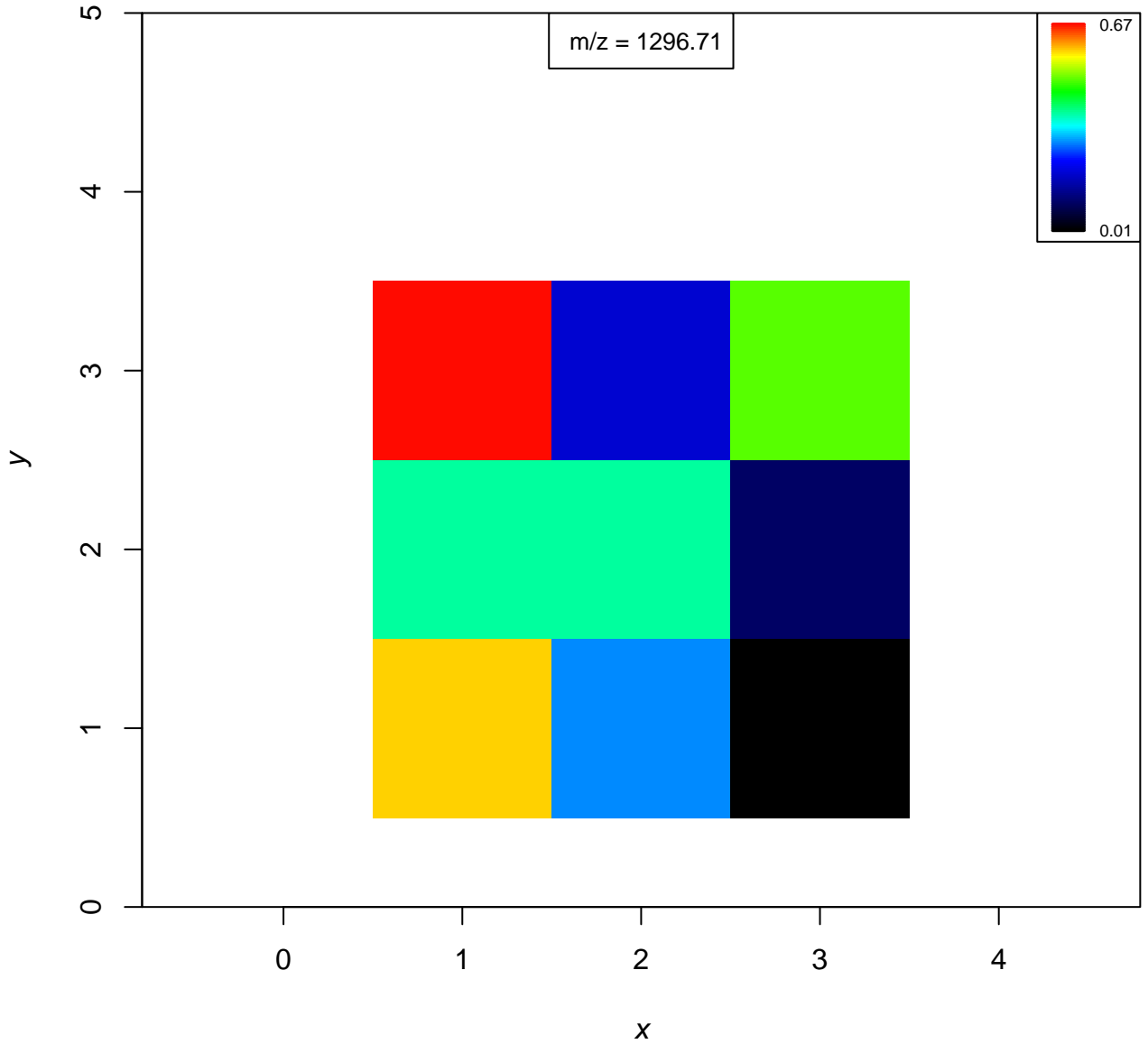
3C) mass3 (1023.6 ± 0.5 Da)



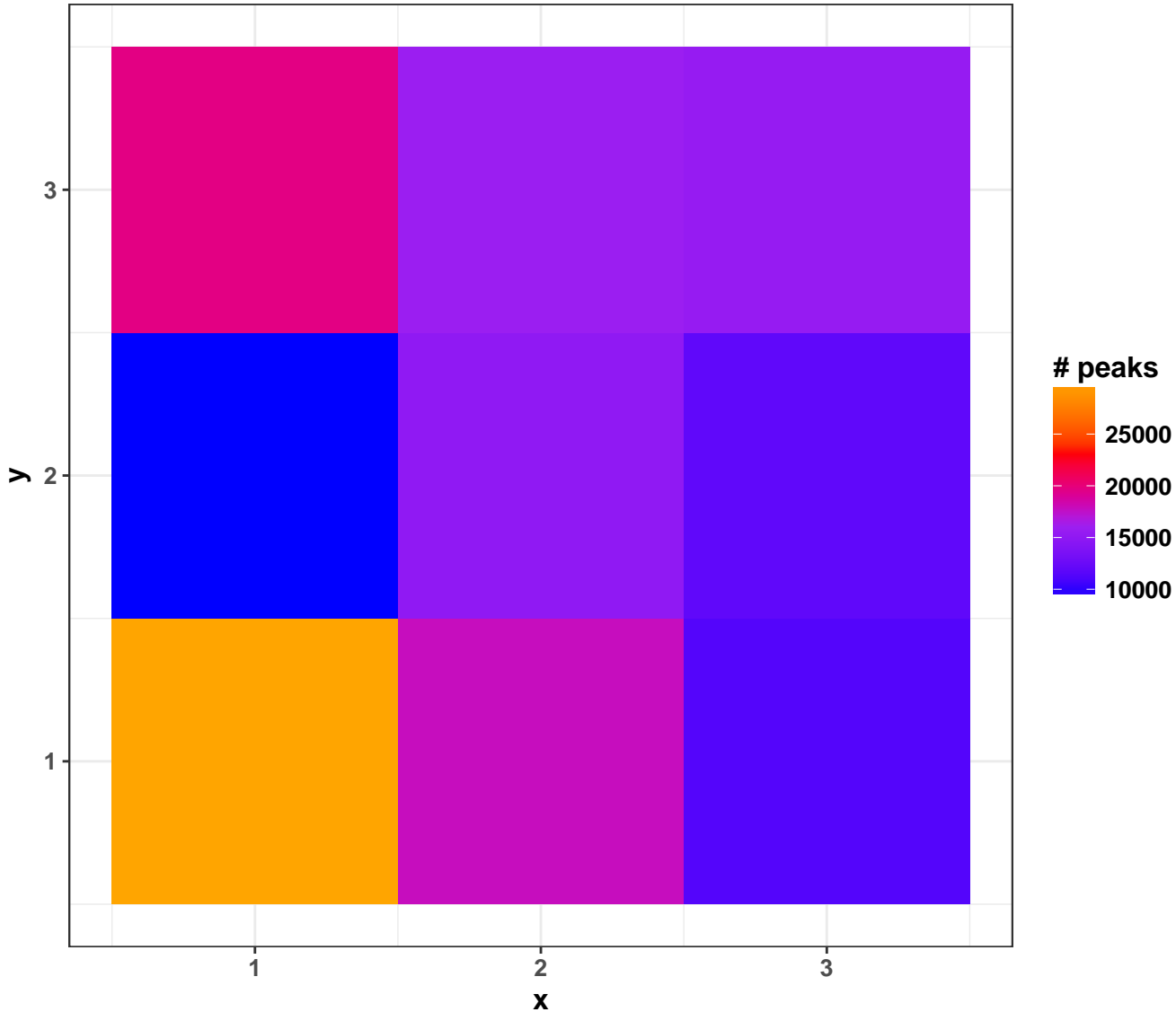
3D) 854.5 (854.5 \pm 0.5 Da)



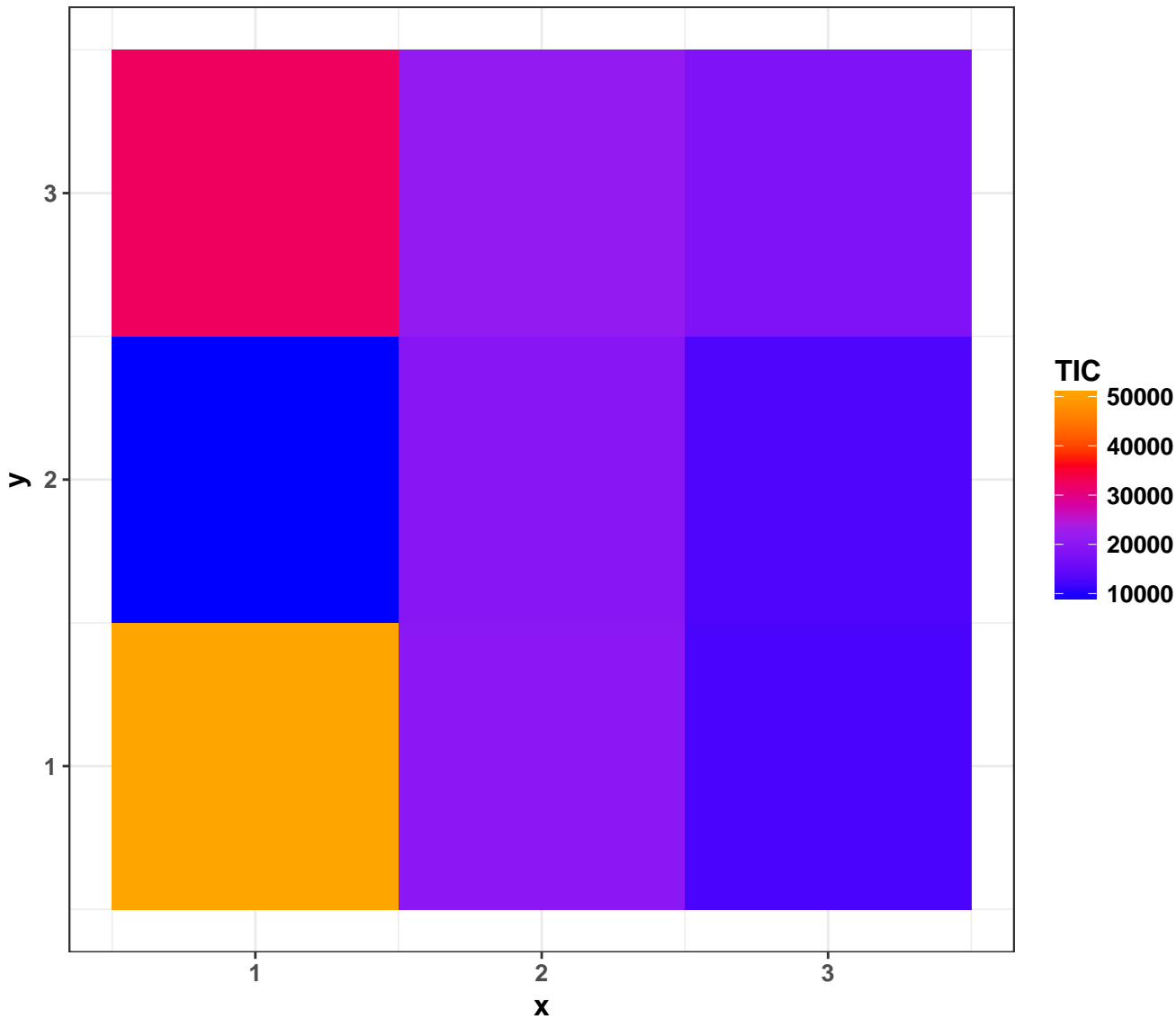
3E) 1296.7 (1296.7 ± 0.5 Da)



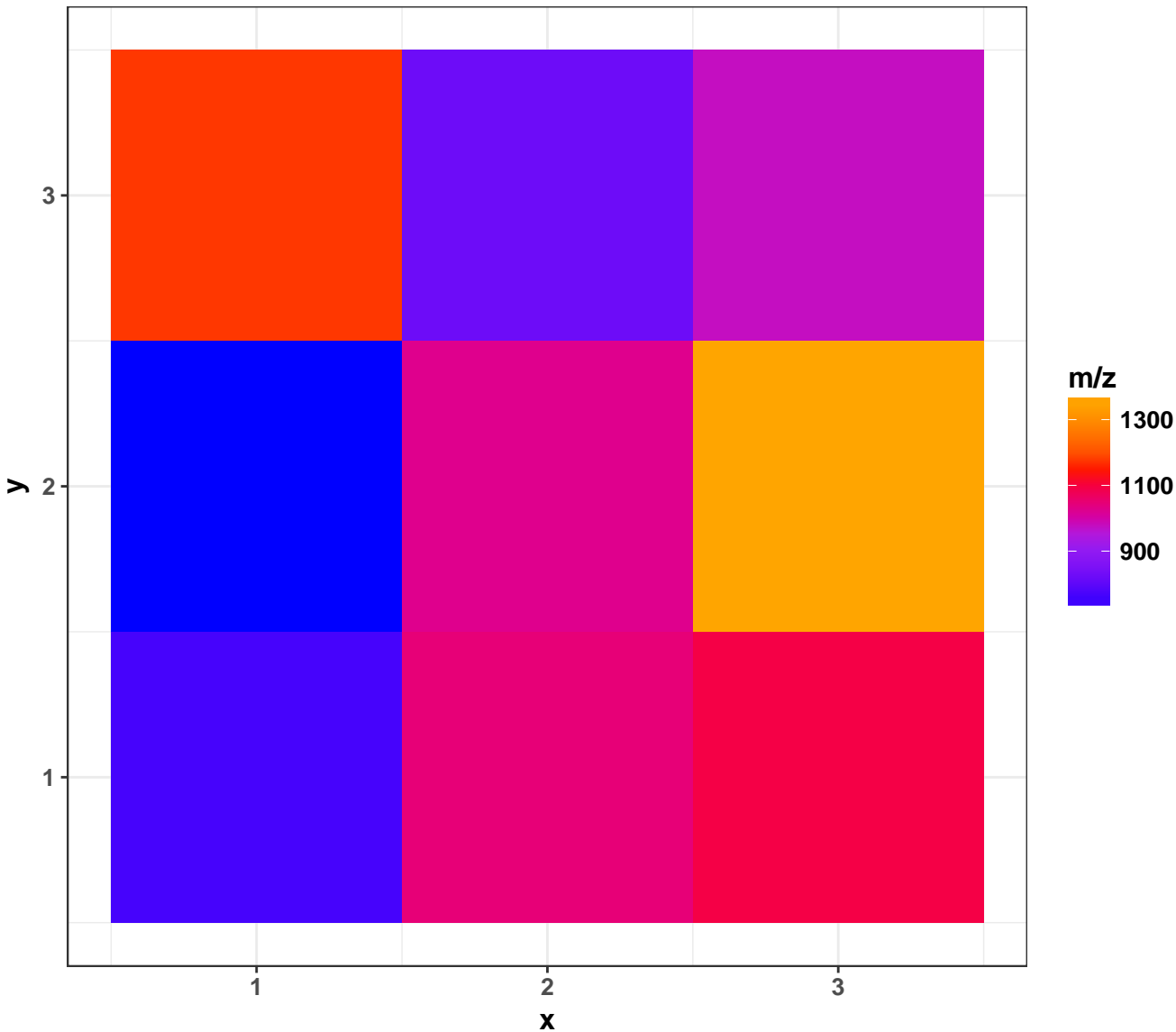
4) Number of peaks per pixel



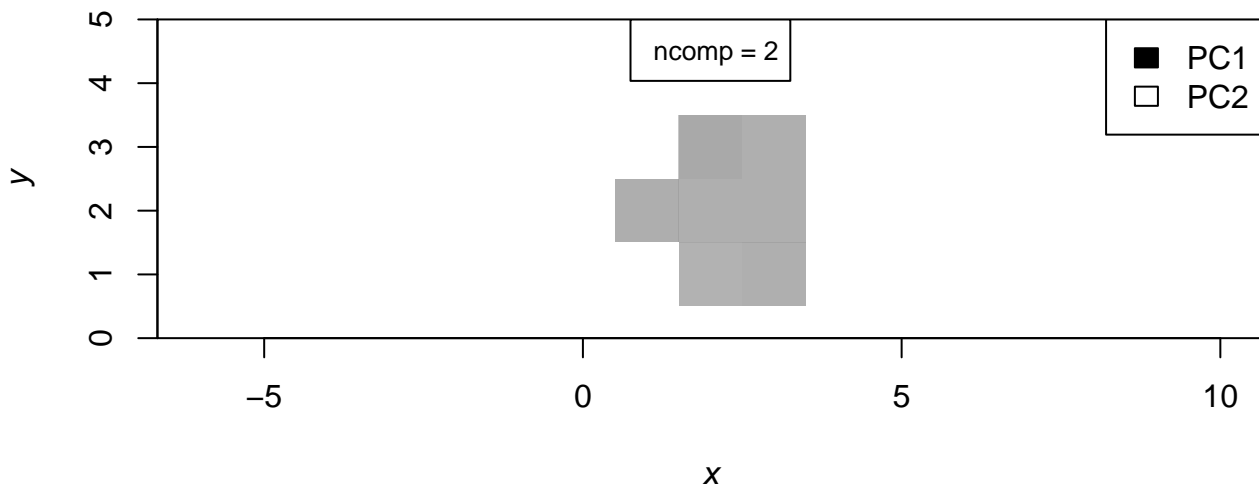
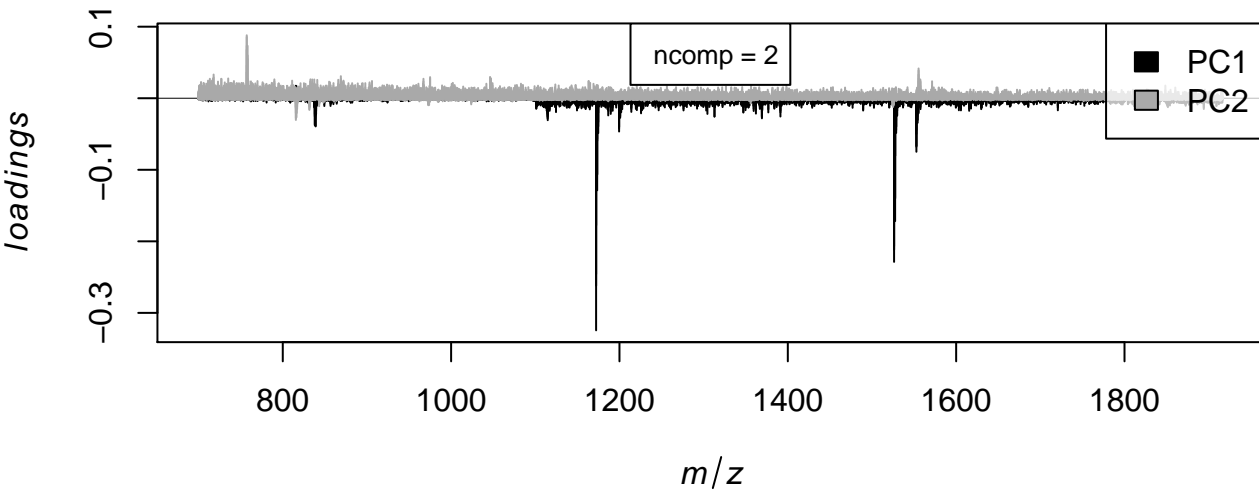
5) Total Ion Chromatogram



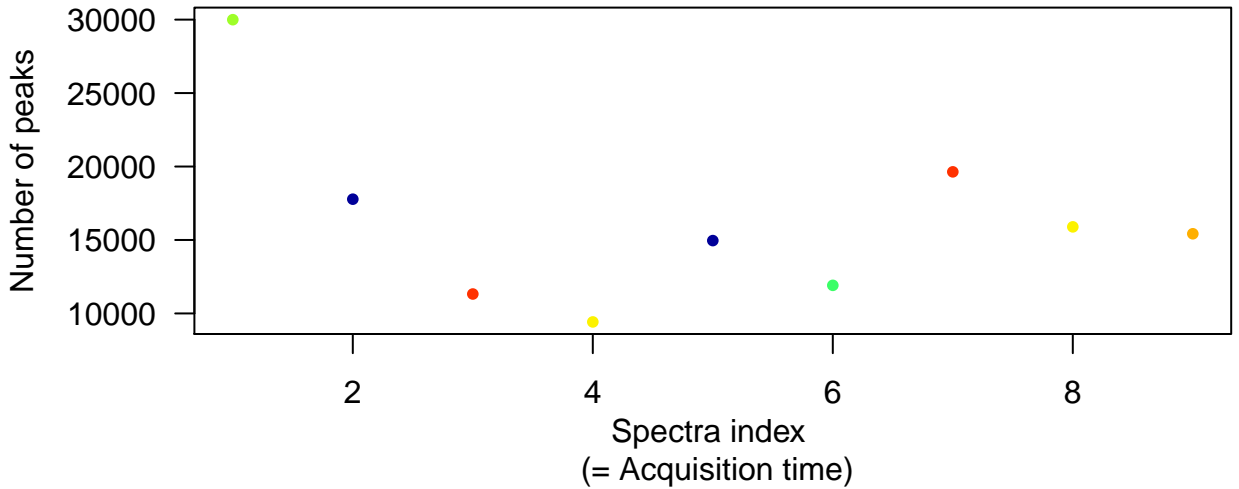
6) Most abundant m/z in each pixel



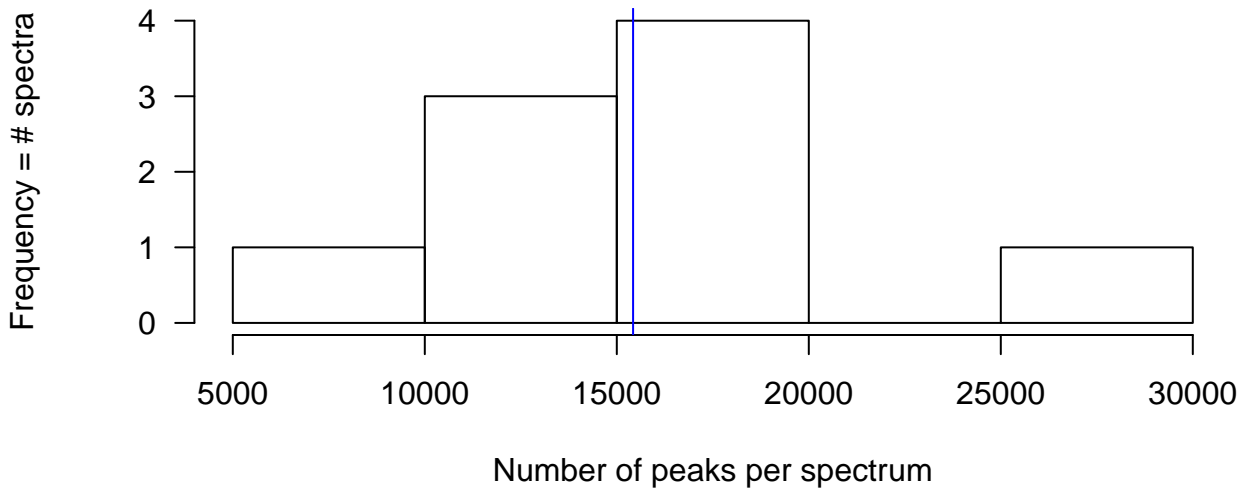
7) PCA for two components



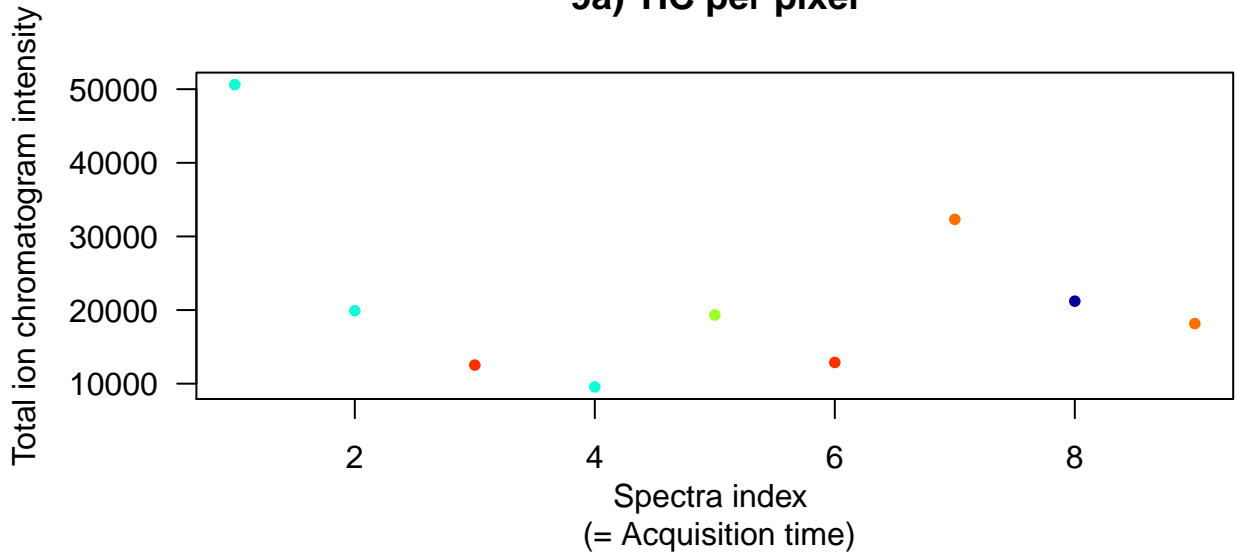
8a) Number of peaks per spectrum



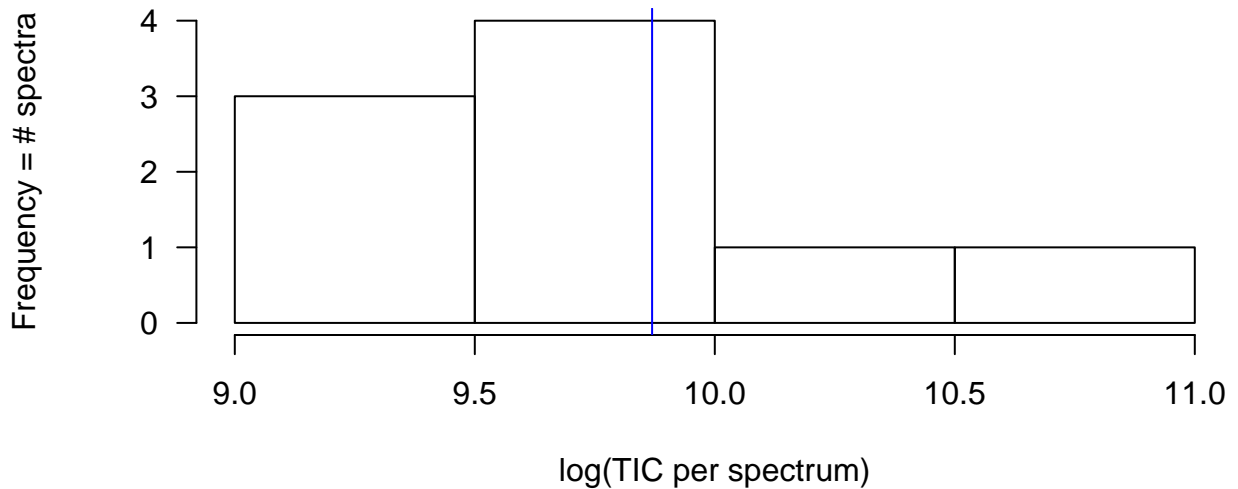
8b) Number of peaks per spectrum



9a) TIC per pixel

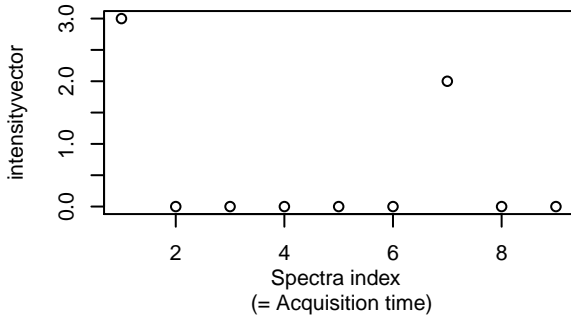


9b) TIC per spectrum

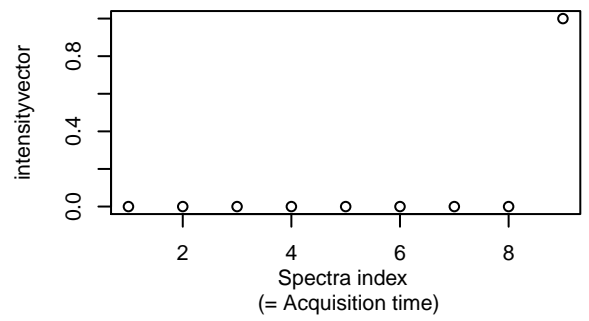


10) intensity of calibrants over acquisition

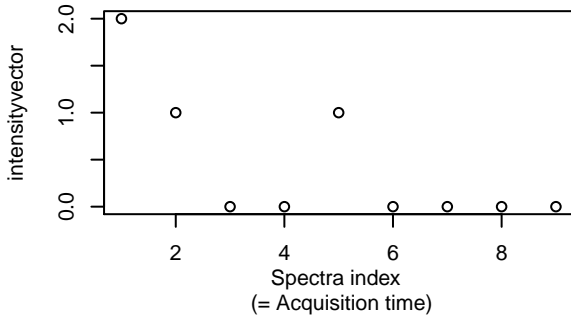
mass1



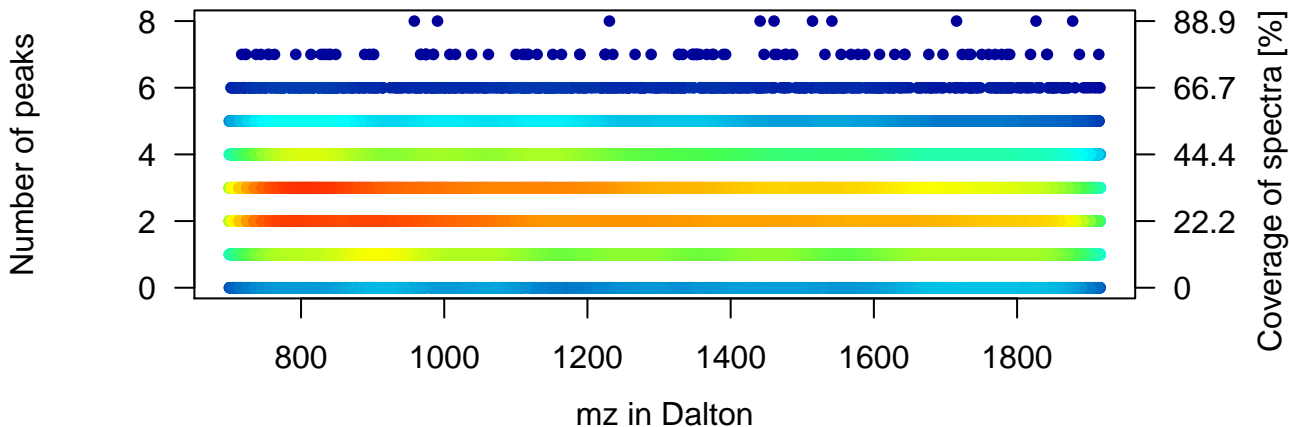
mass2



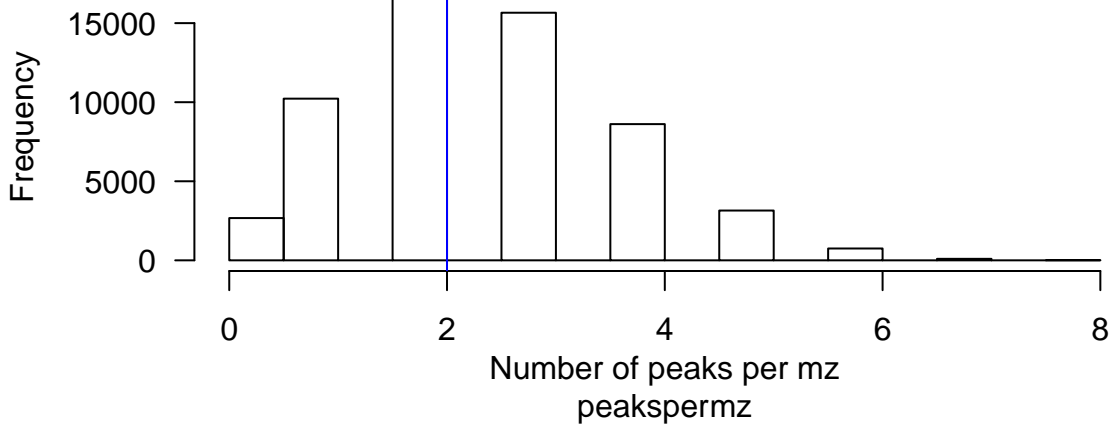
mass3



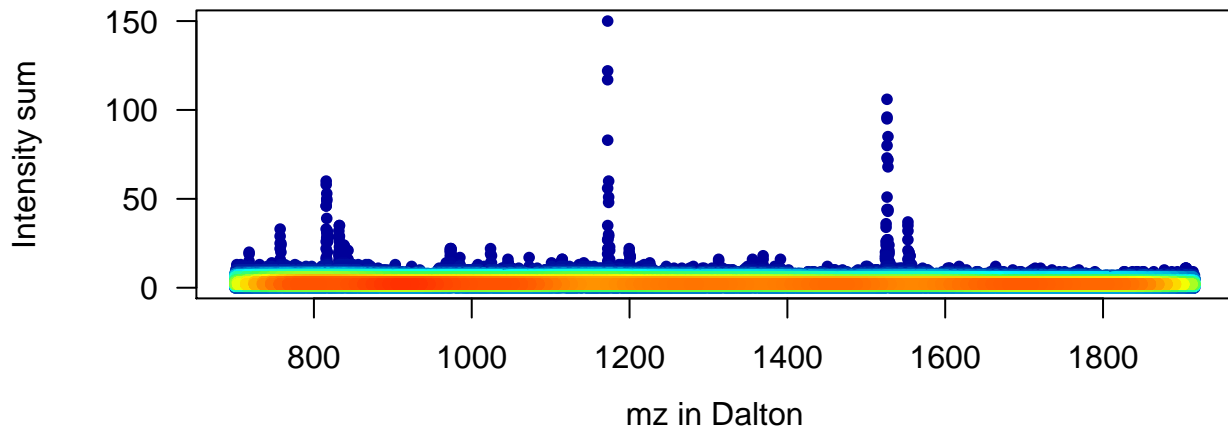
11a) Number of peaks for each mz



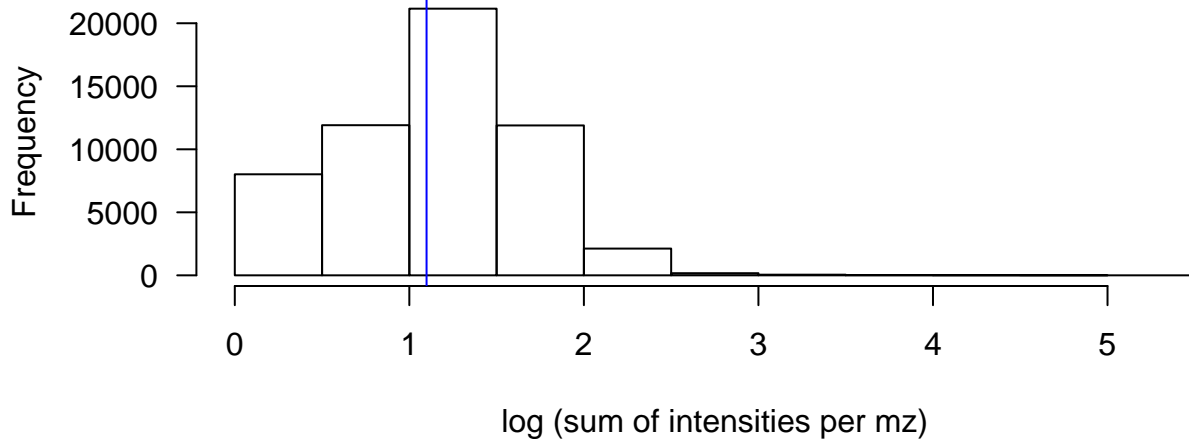
11b) Number of peaks per mz



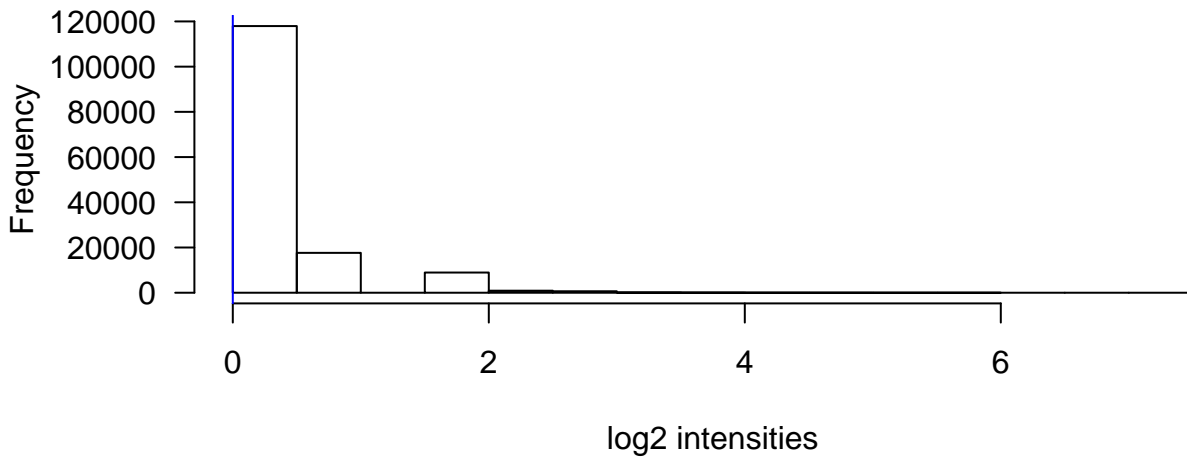
12a) Sum of all peak intensities for each mz



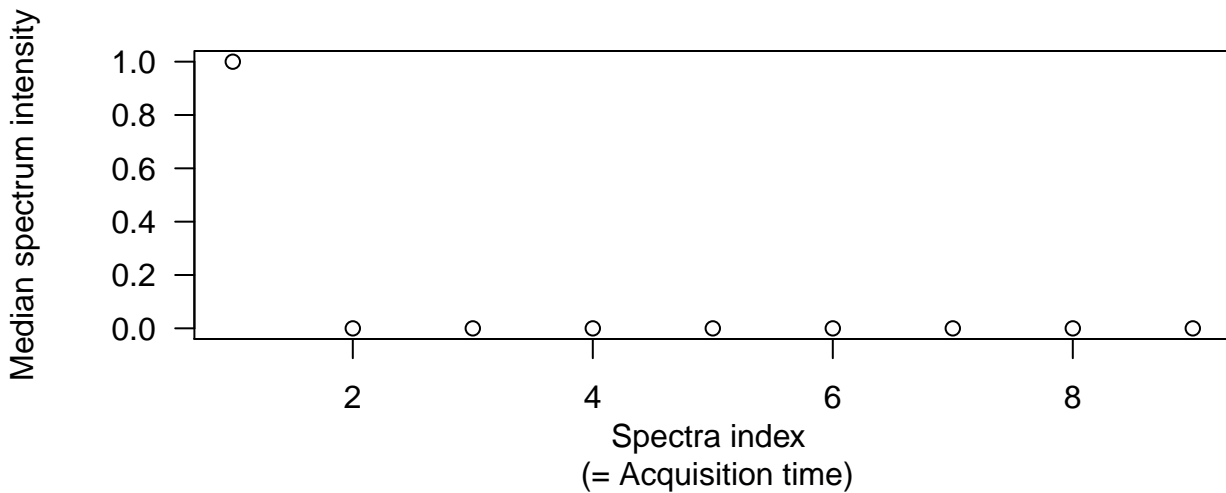
12b) Sum of intensities per mz



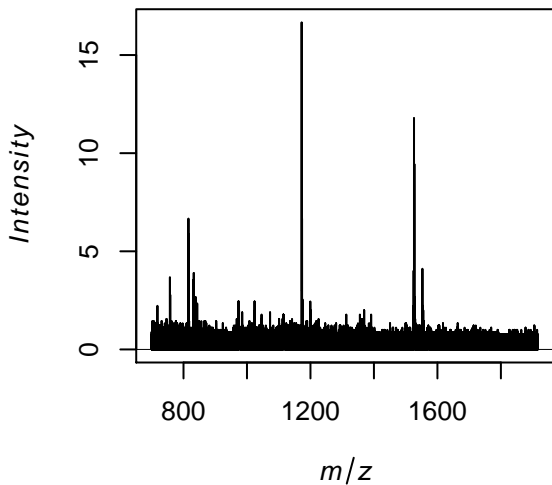
13a) Log2-transformed intensities



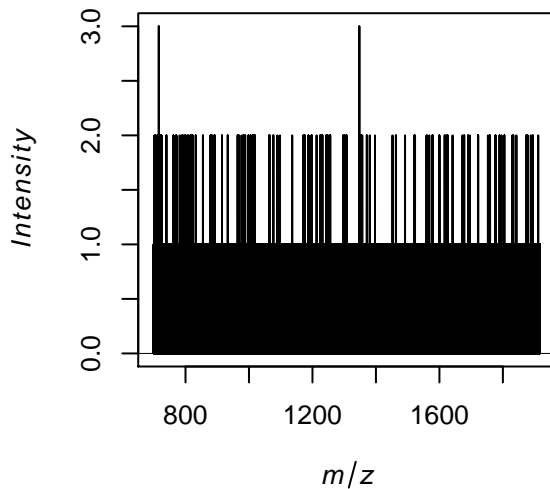
13b) Median intensity per spectrum



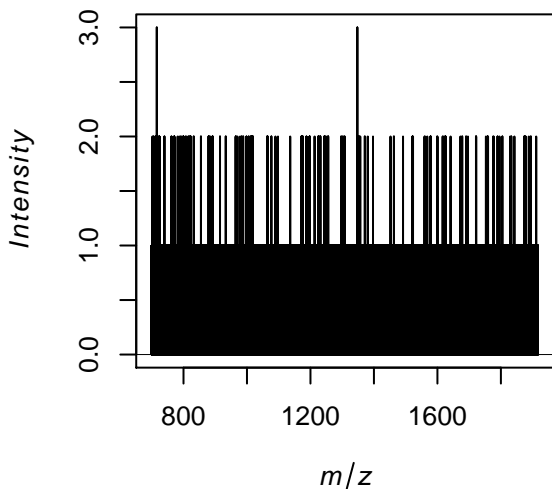
Average spectrum



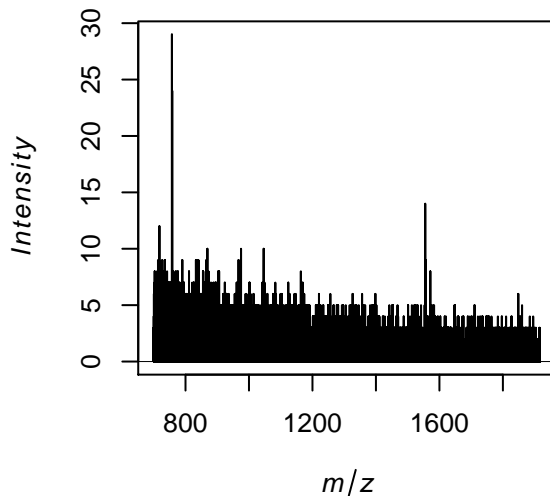
Spectrum in middle of acquisition



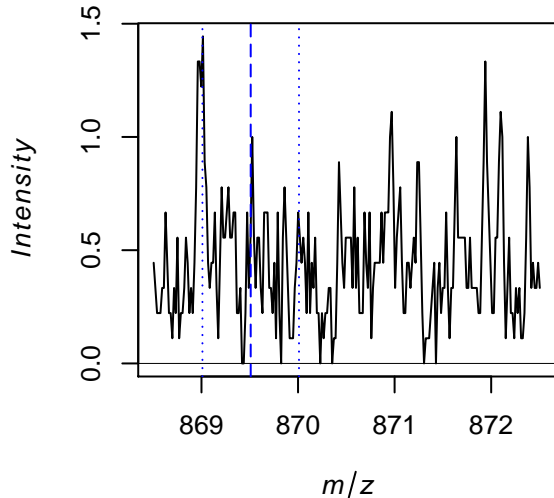
Spectrum at $x = 1, y = 2$



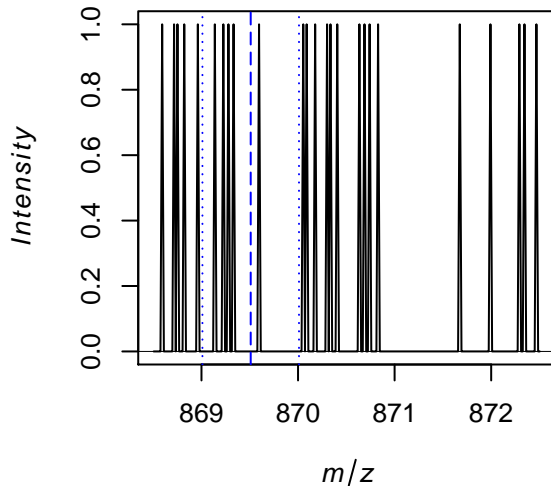
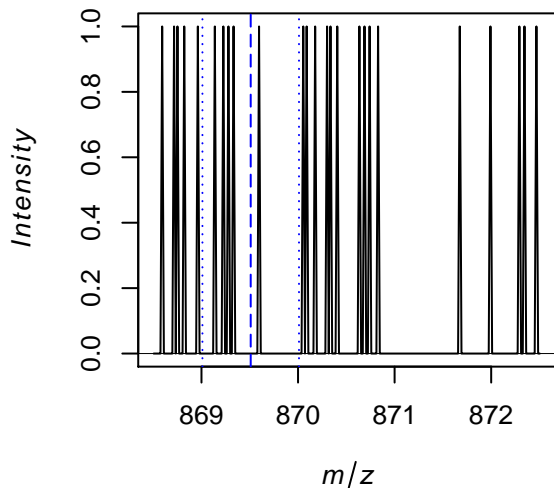
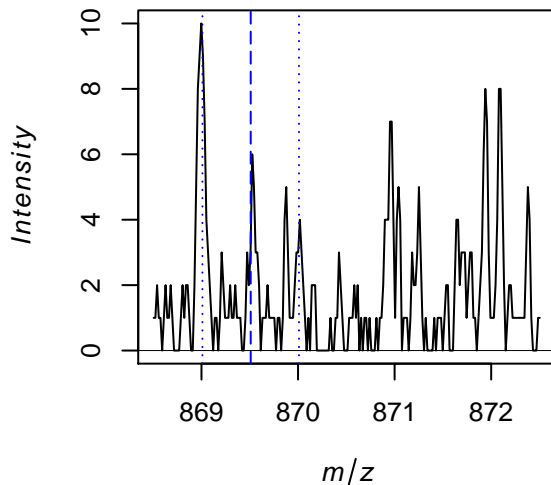
Spectrum at $x = 1, y = 1$



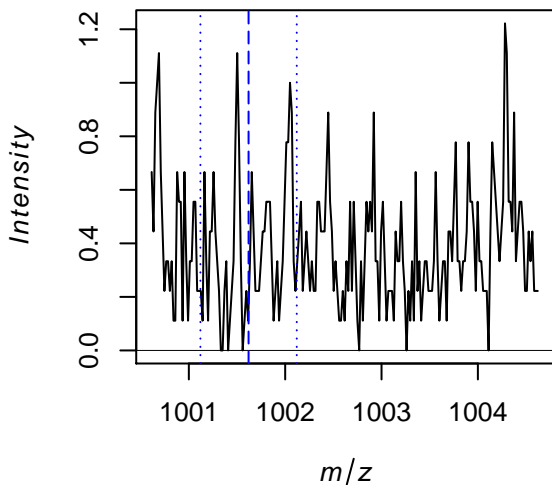
average spectrum



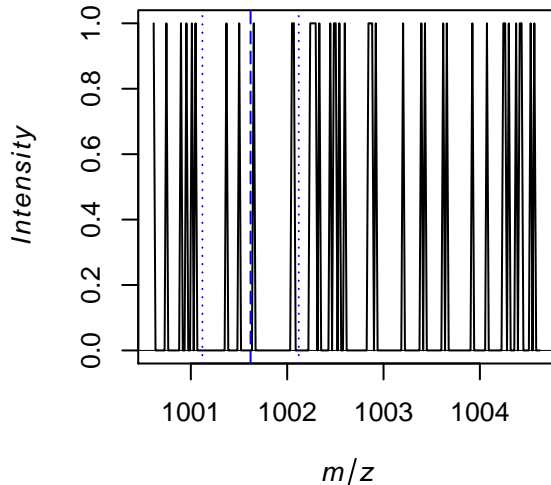
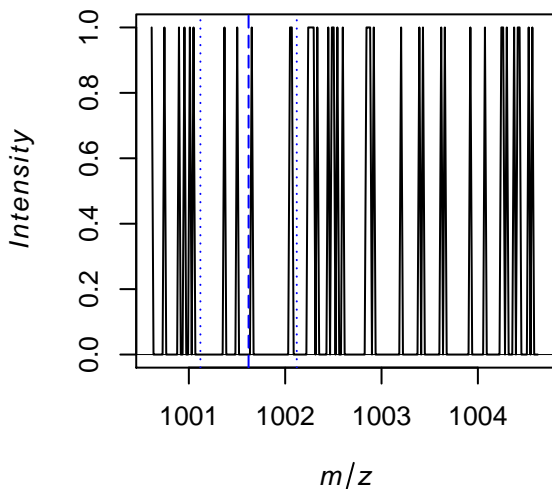
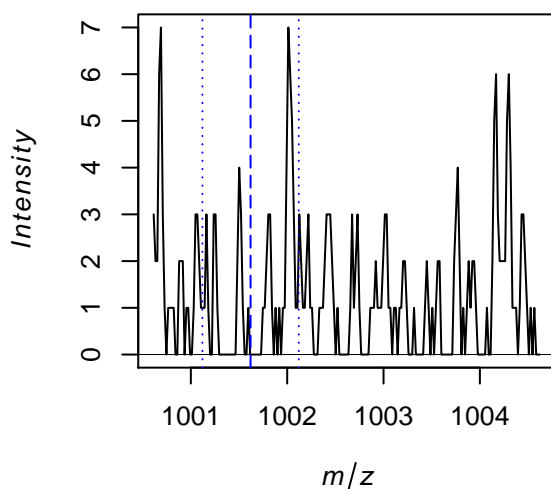
pixel in middle of acquisition

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

average spectrum

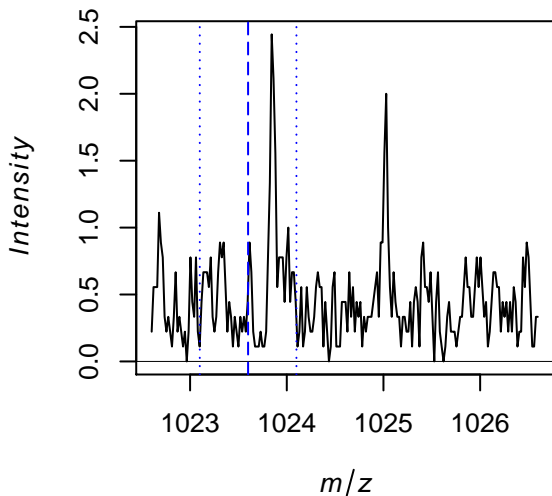


pixel in middle of acquisition

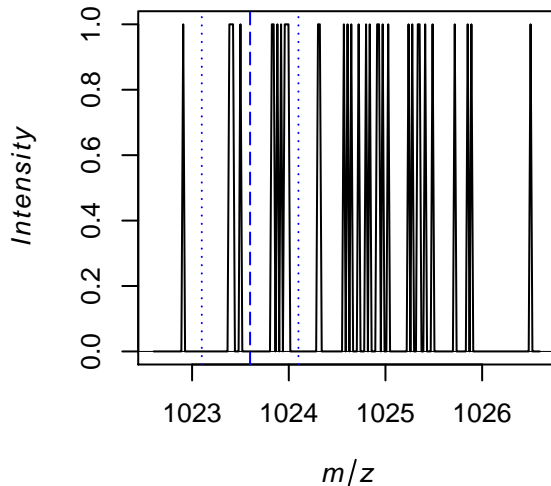
Spectrum at $x = 1, y = 2$ Spectrum at $x = 1, y = 1$ 

1023.6

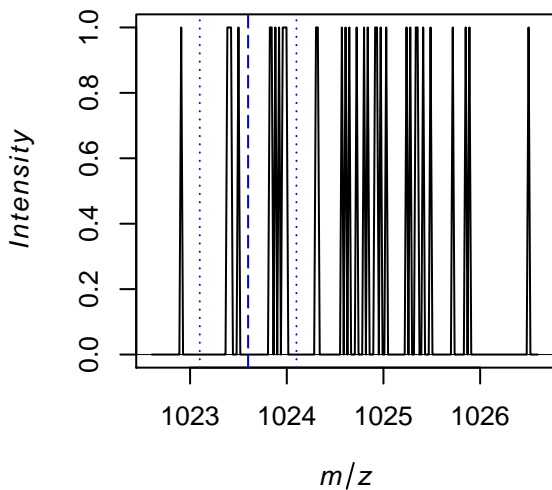
average spectrum



pixel in middle of acquisition



Spectrum at $x = 1, y = 2$



Spectrum at $x = 1, y = 1$

