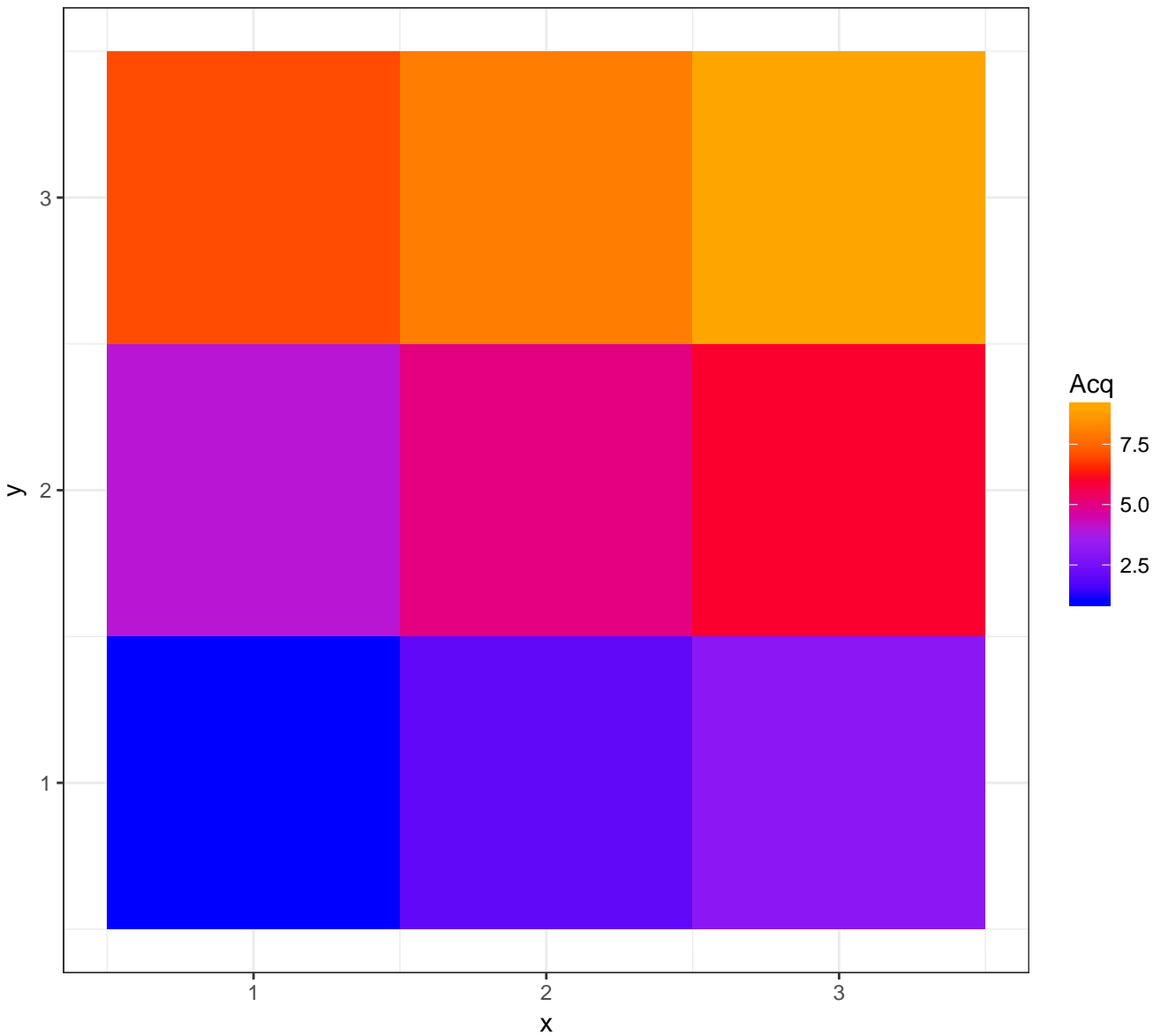


Quality control of MSI data

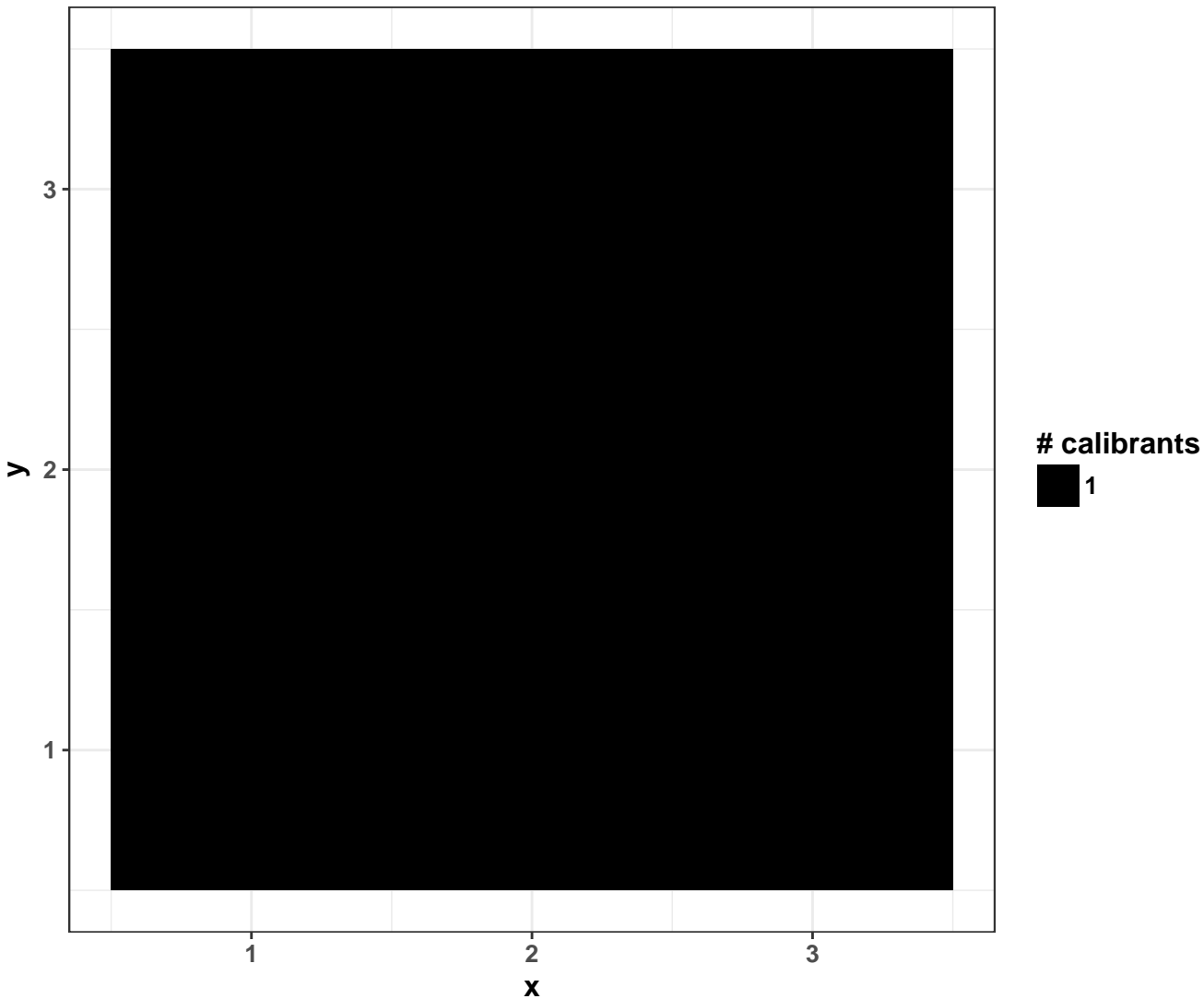
Filename: Testfile_analyze75

properties	values
Number of mz features	3672
Range of mz values [Da]	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 zero TICs	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in inputpeptides.txt	1 / 6
# calibrants in inputcalibrantfile2.txt	1 / 3

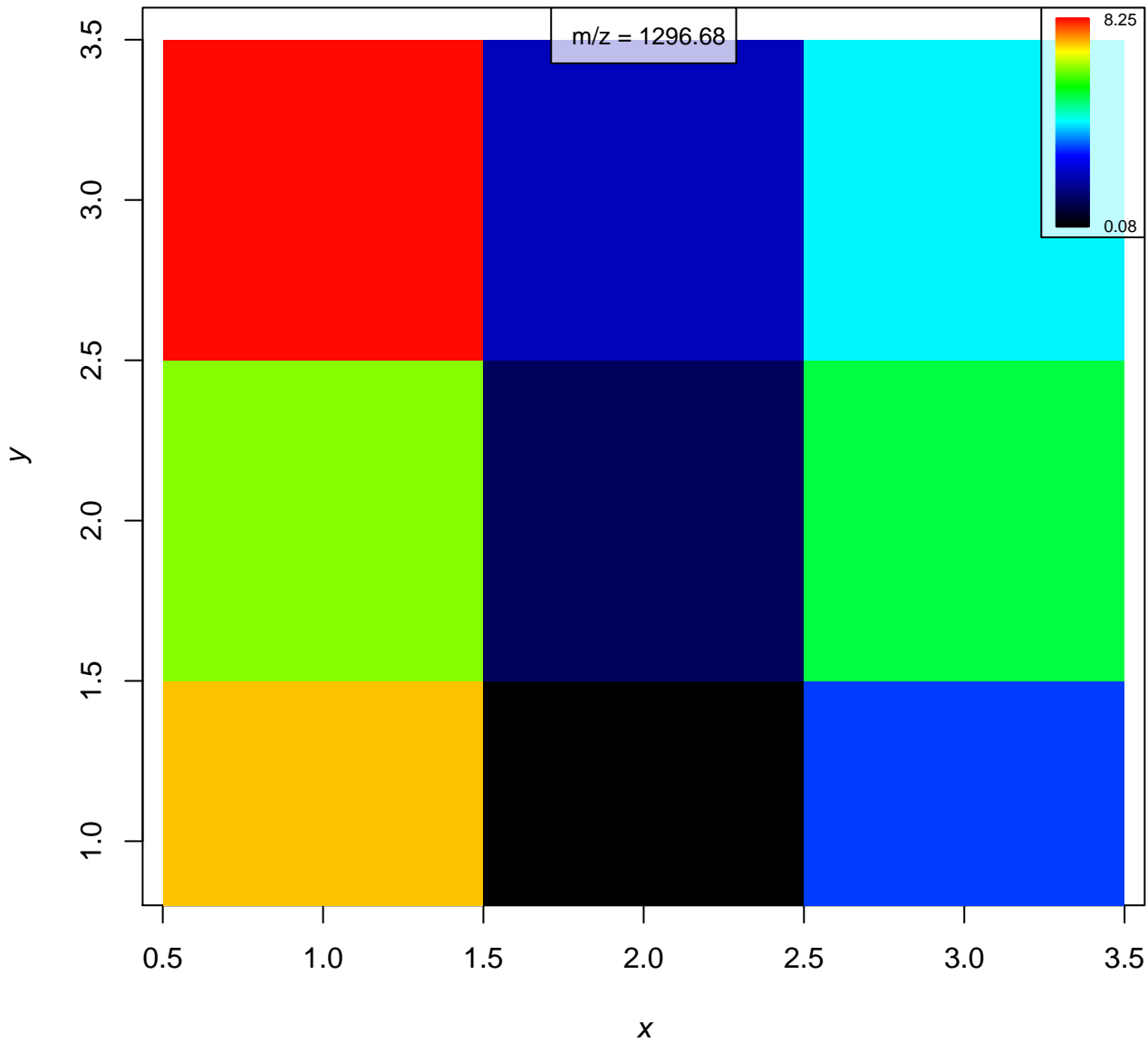
Order of Acquisition



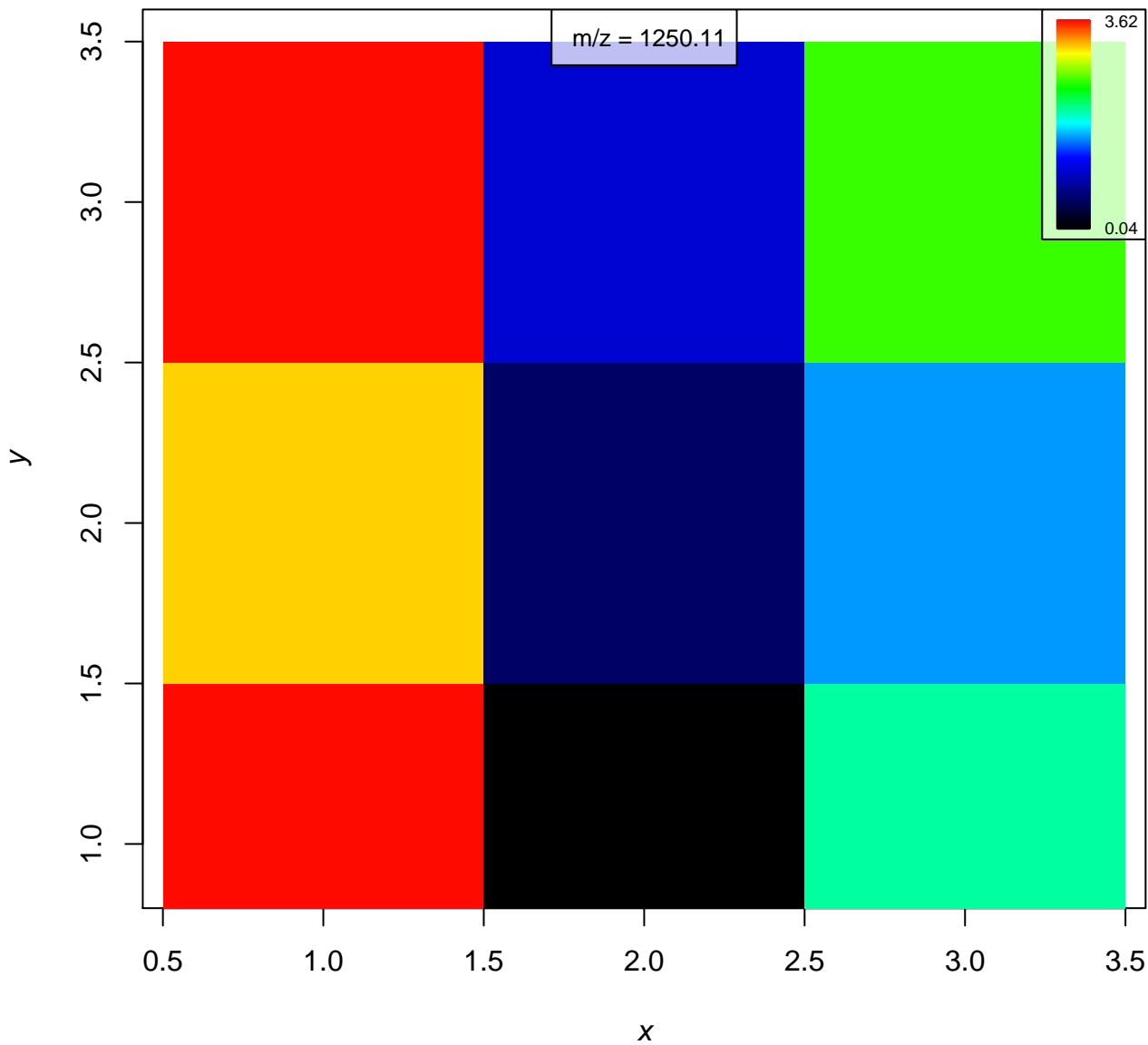
Number of calibrants per pixel



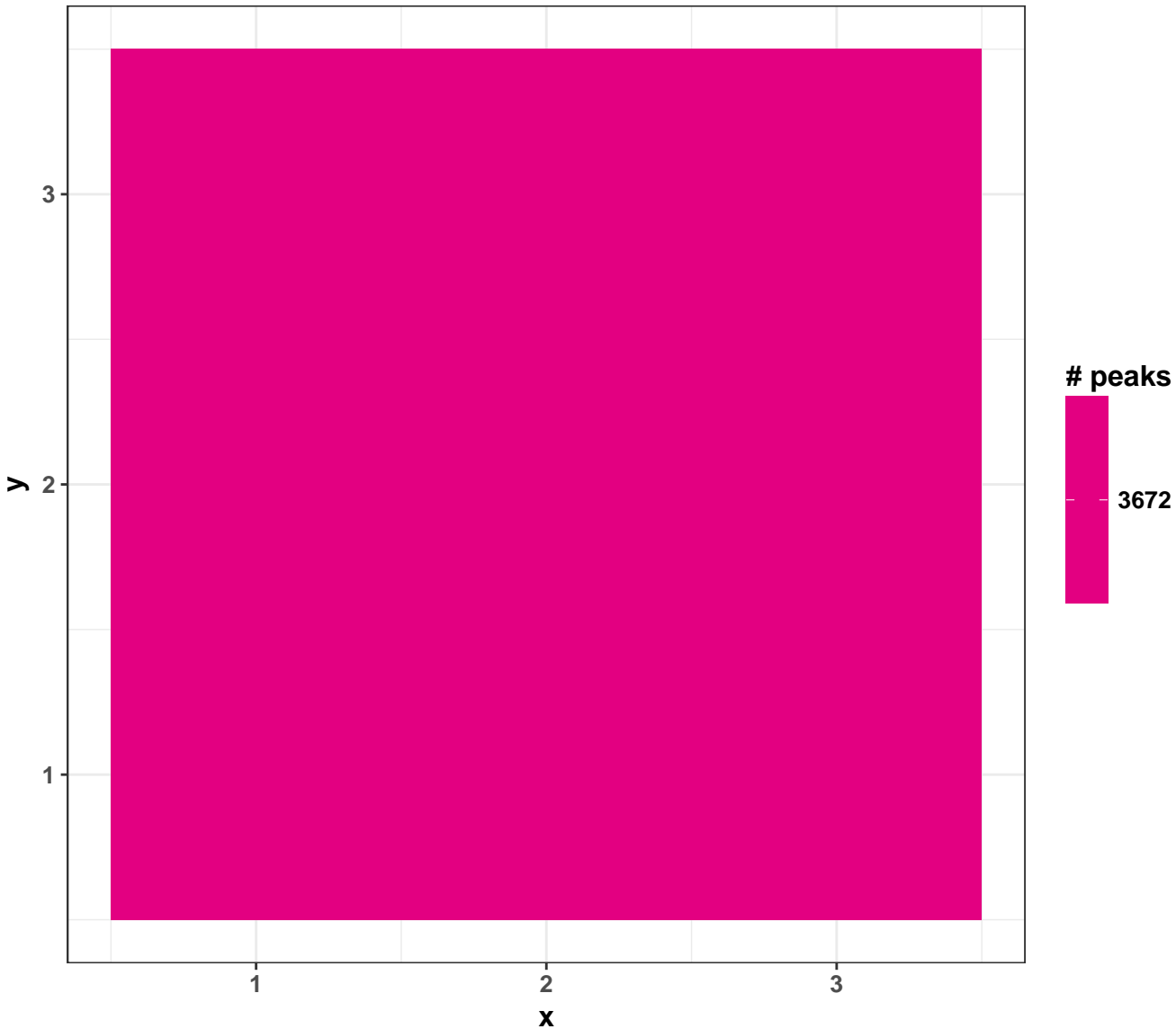
mass3 (1296.7 ± 0.5 Da)



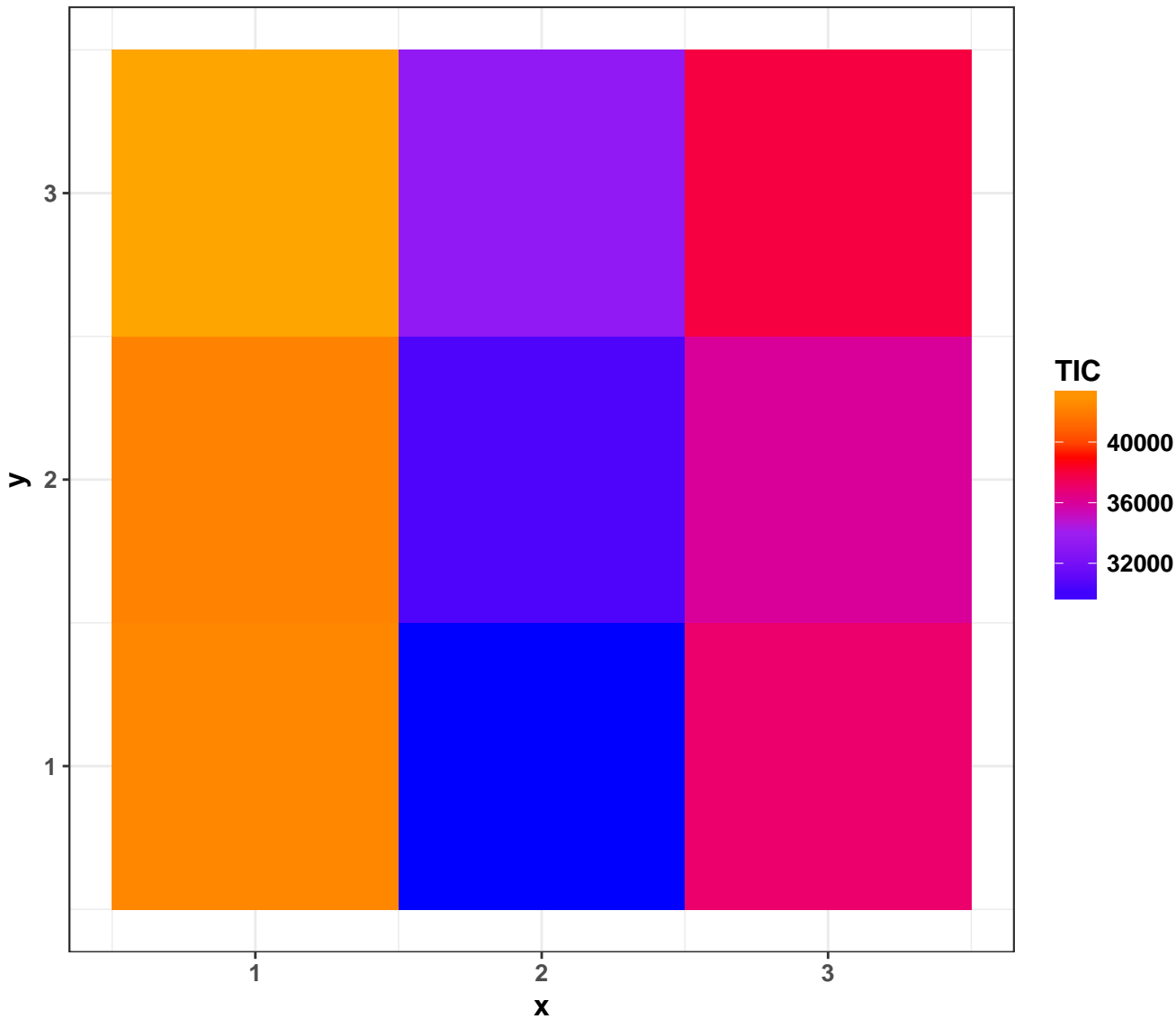
1250.1 (1250.1 ± 0.5 Da)



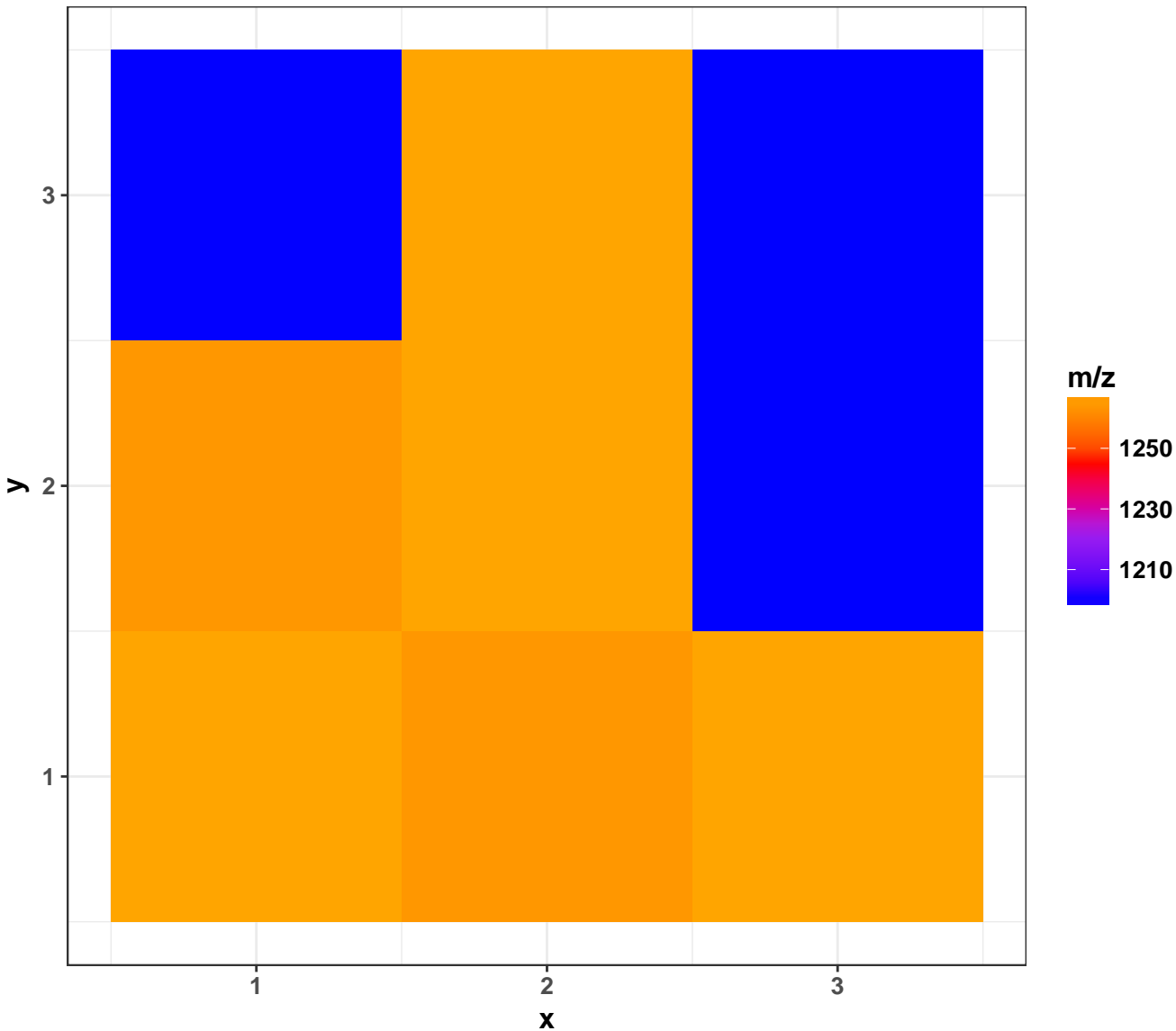
Number of peaks per pixel



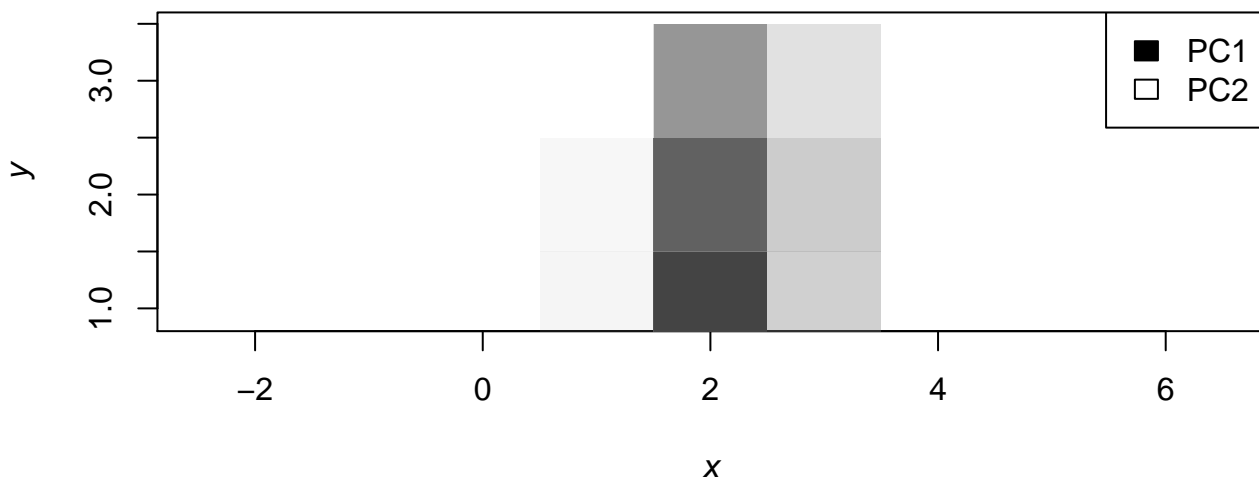
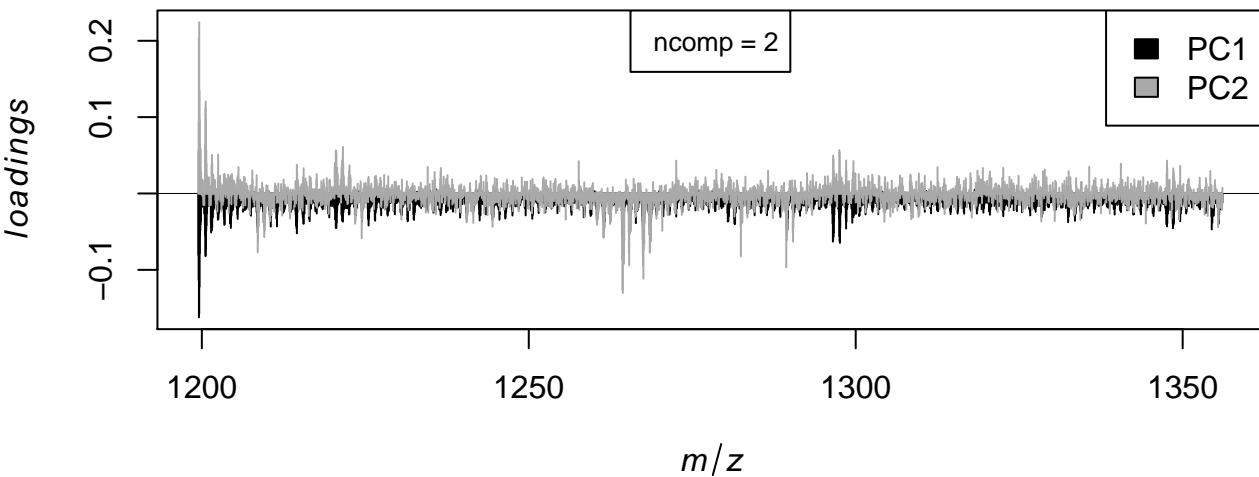
Total Ion Chromatogram



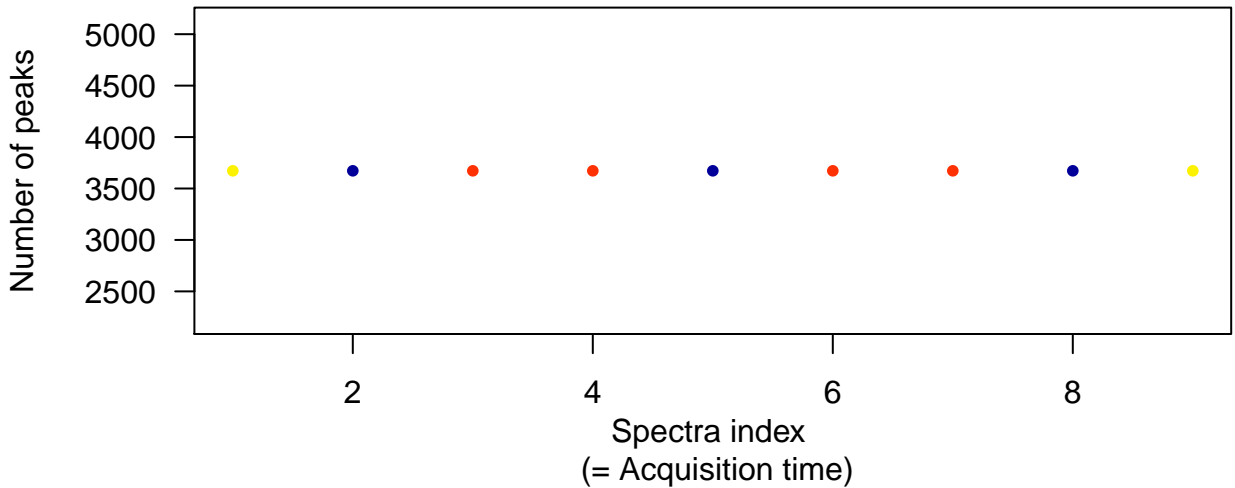
Most abundant m/z in each pixel



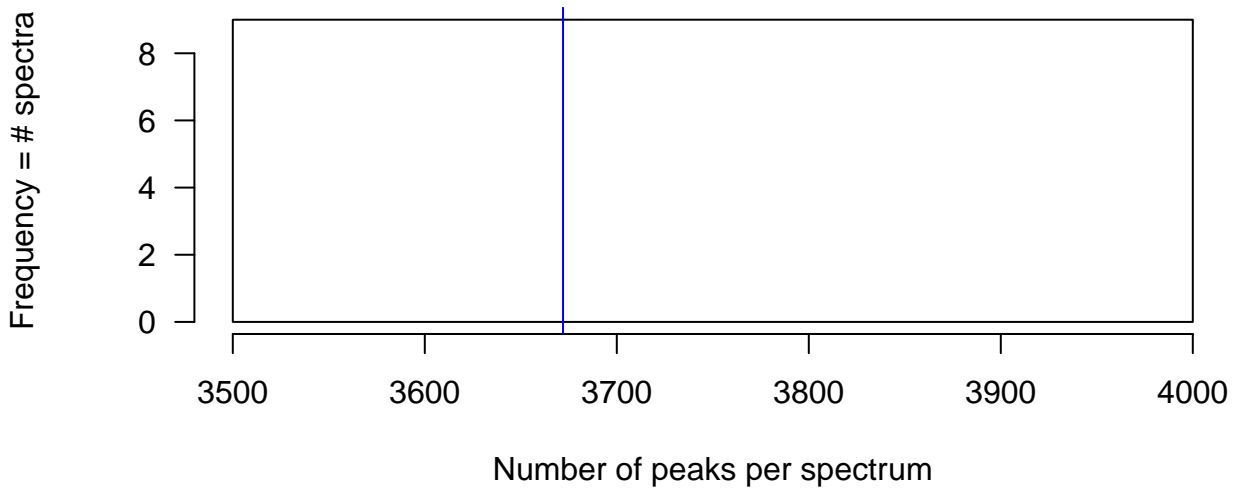
PCA for two components



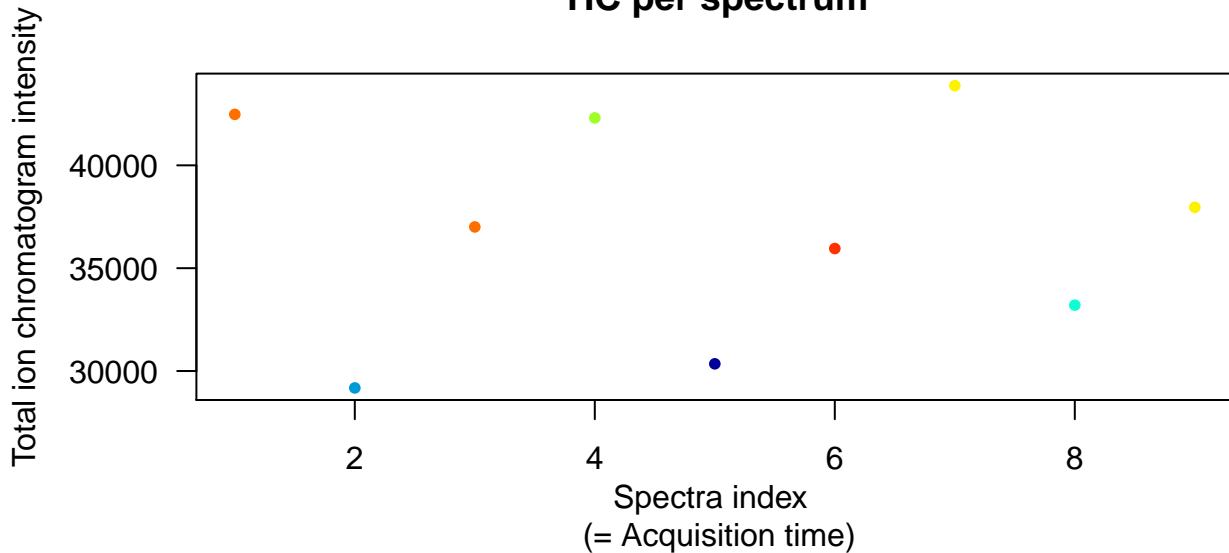
Number of peaks per spectrum



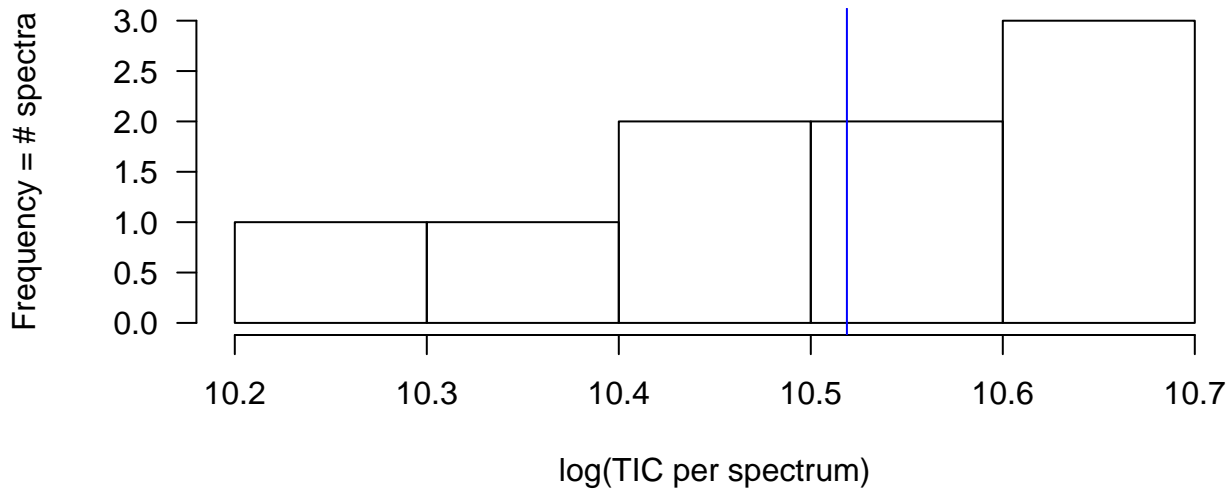
Number of peaks per spectrum



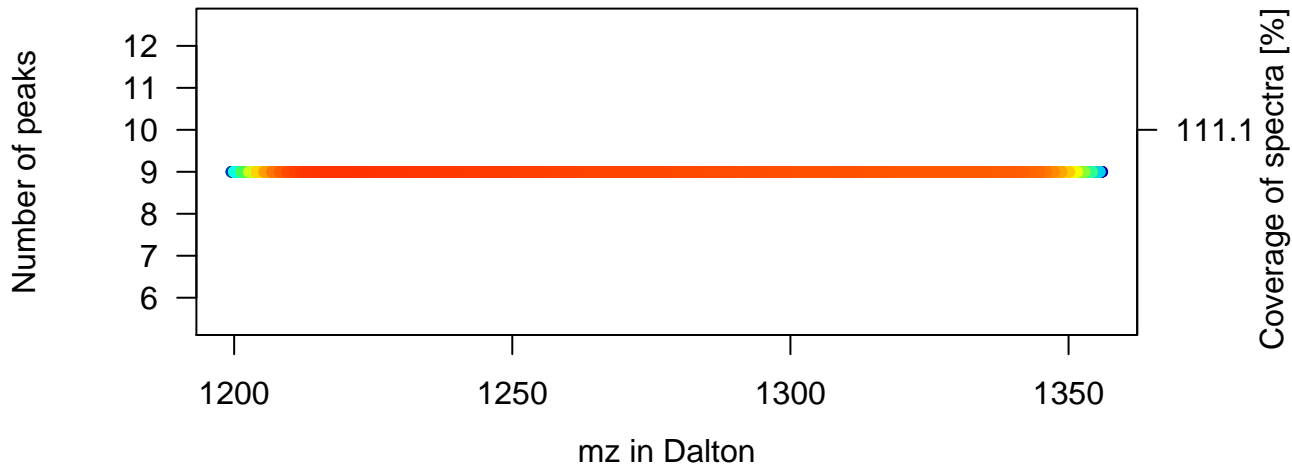
TIC per spectrum



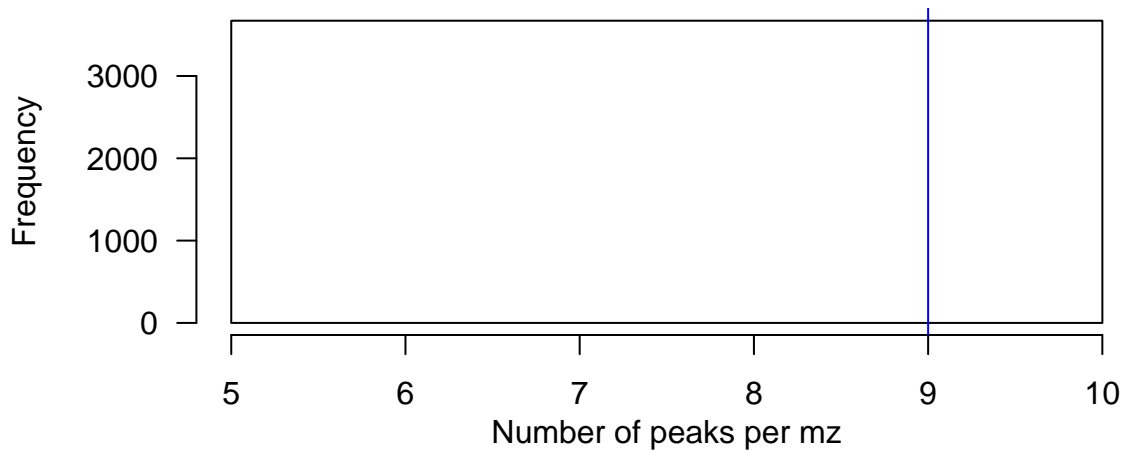
TIC per spectrum



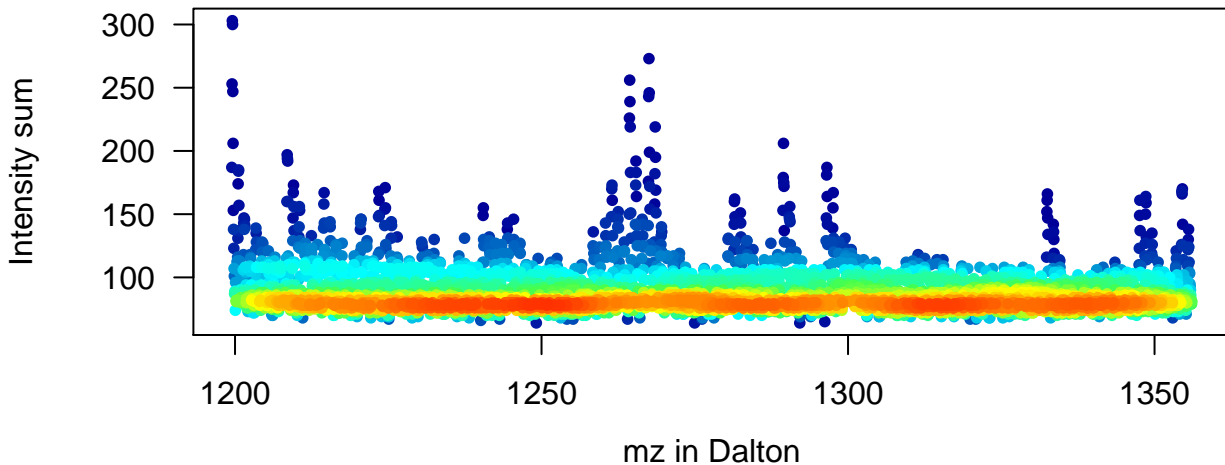
Number of peaks per mz



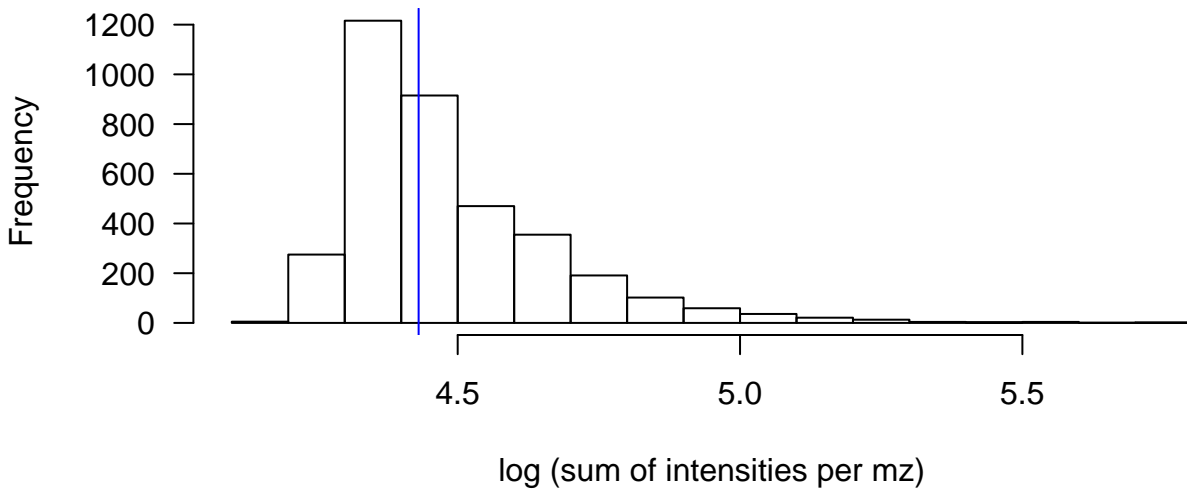
Number of peaks per mz



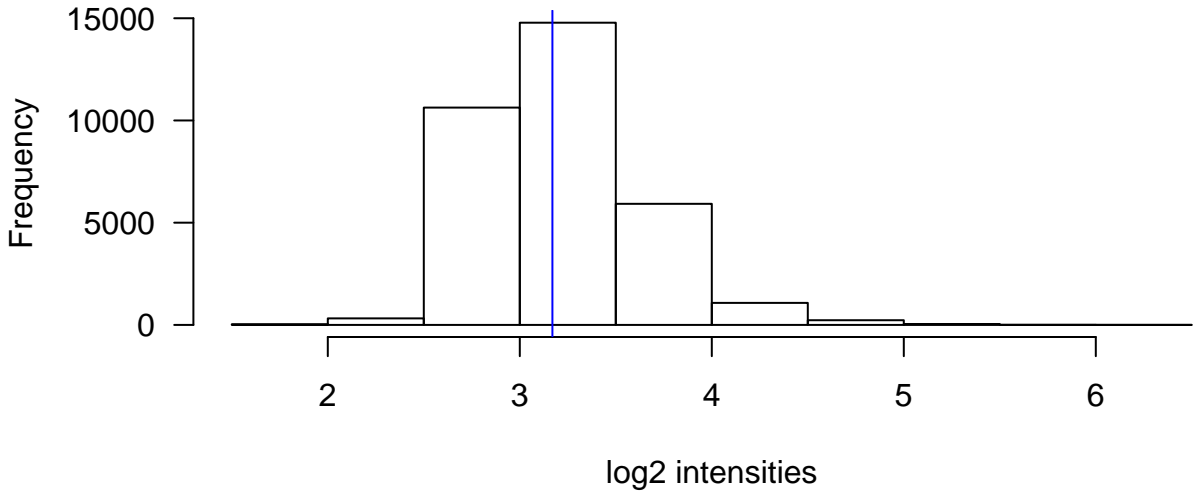
Sum of intensities per mz



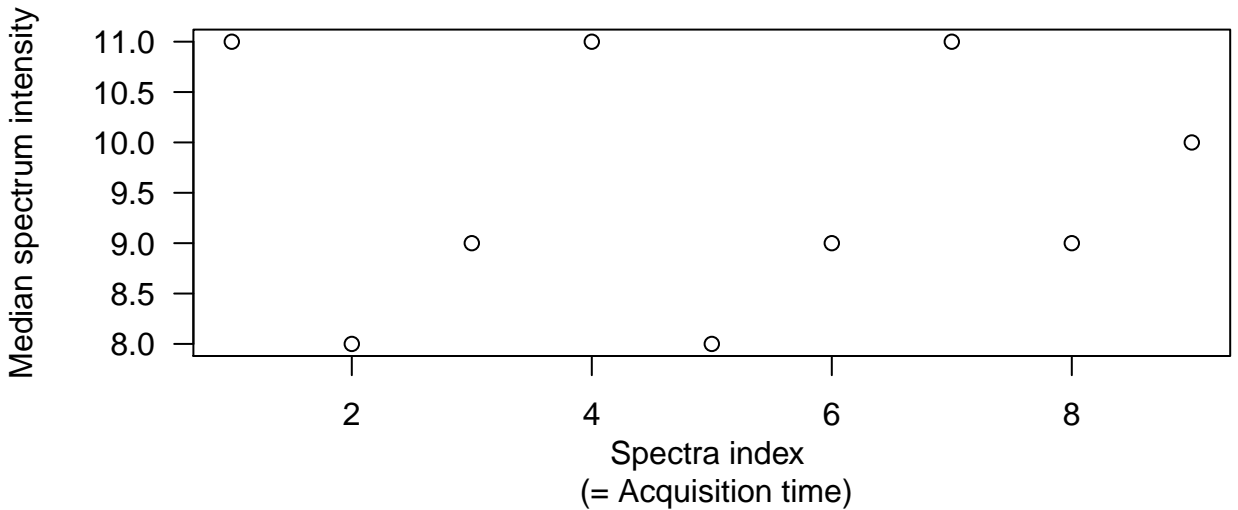
Sum of intensities per mz



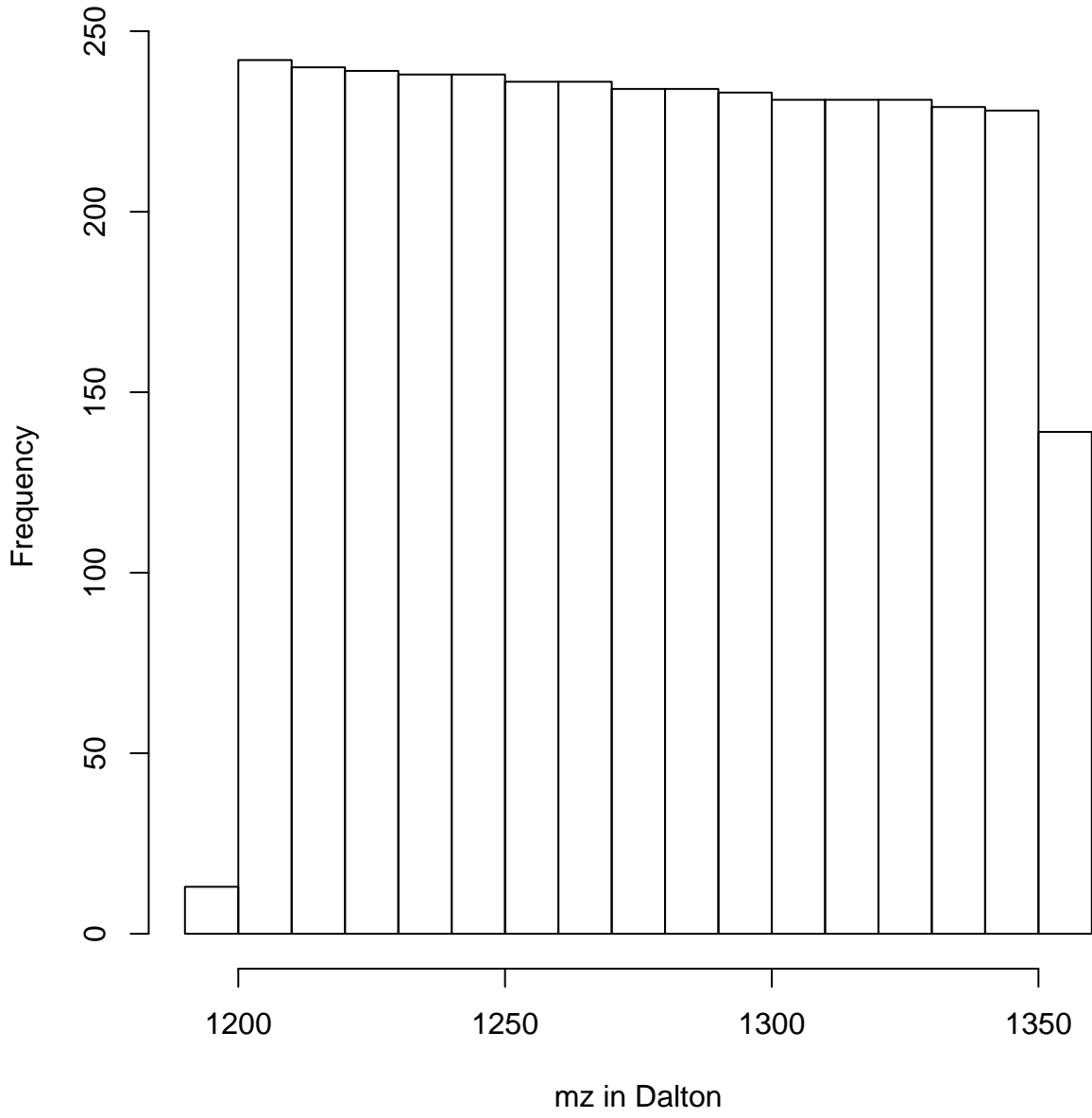
Log2-transformed intensities



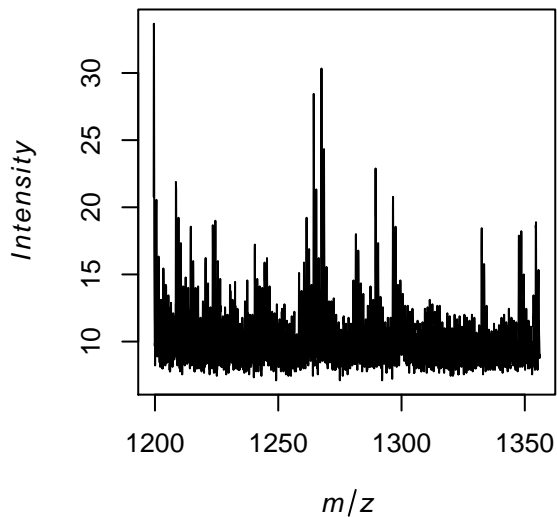
Median intensity per spectrum



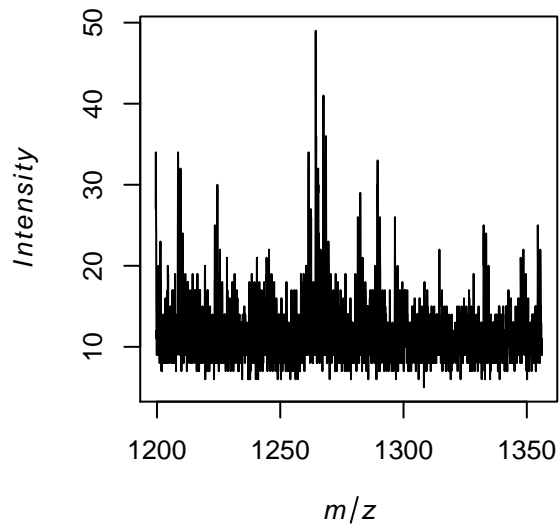
Histogram of mz values



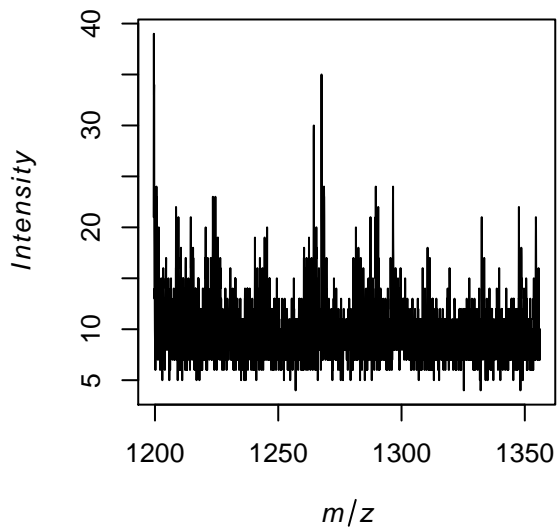
Average spectrum



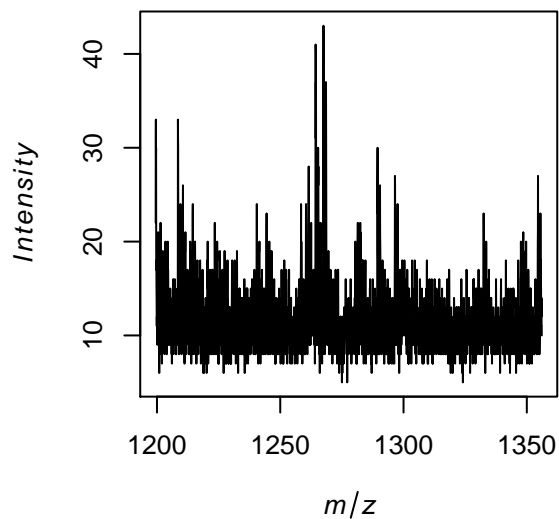
Spectrum in middle of acquisition



Spectrum at x = 3, y = 2

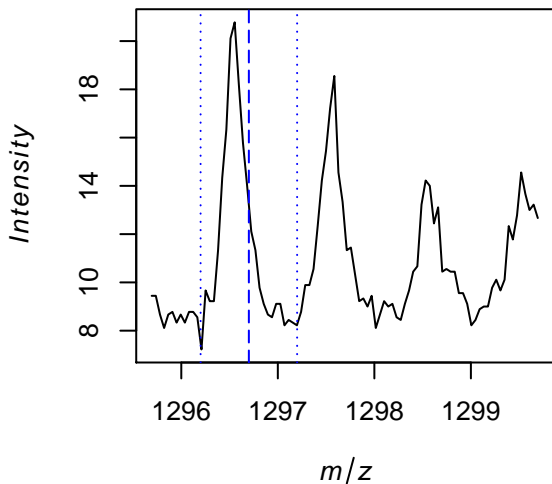


Spectrum at x = 1, y = 1

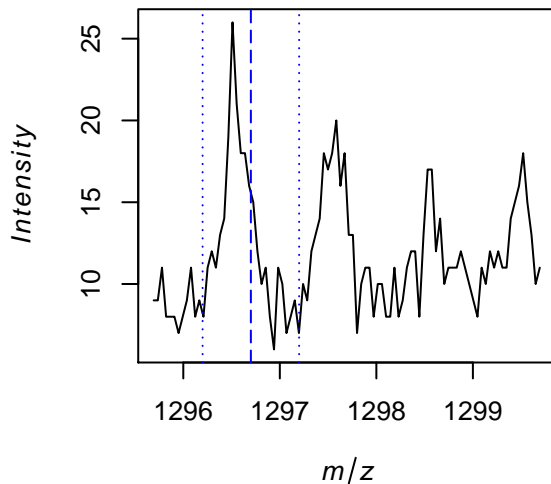


1296.7

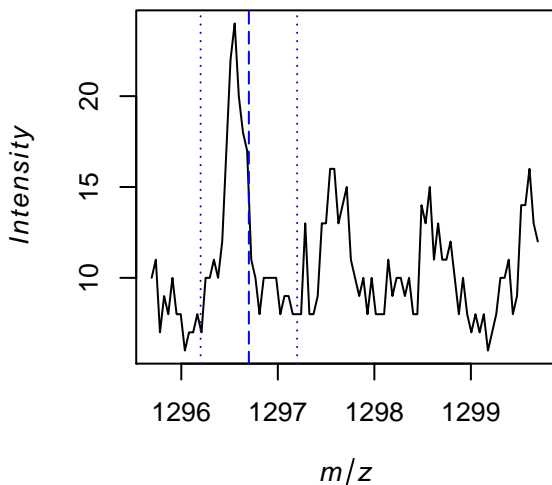
average spectrum



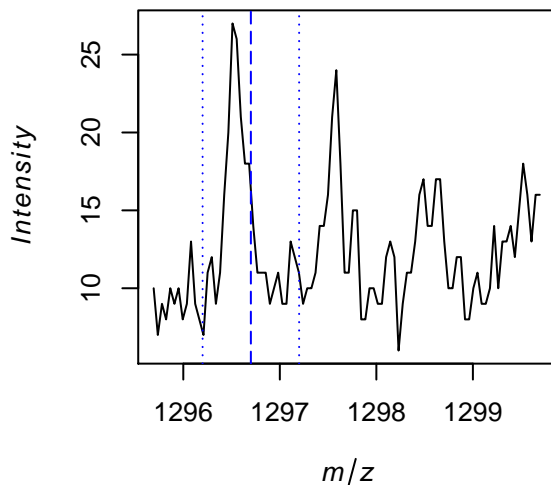
pixel in middle of acquisition



Spectrum at $x = 3, y = 2$



Spectrum at $x = 1, y = 1$



Theoretical calibrant mz vs. closest measured mz

