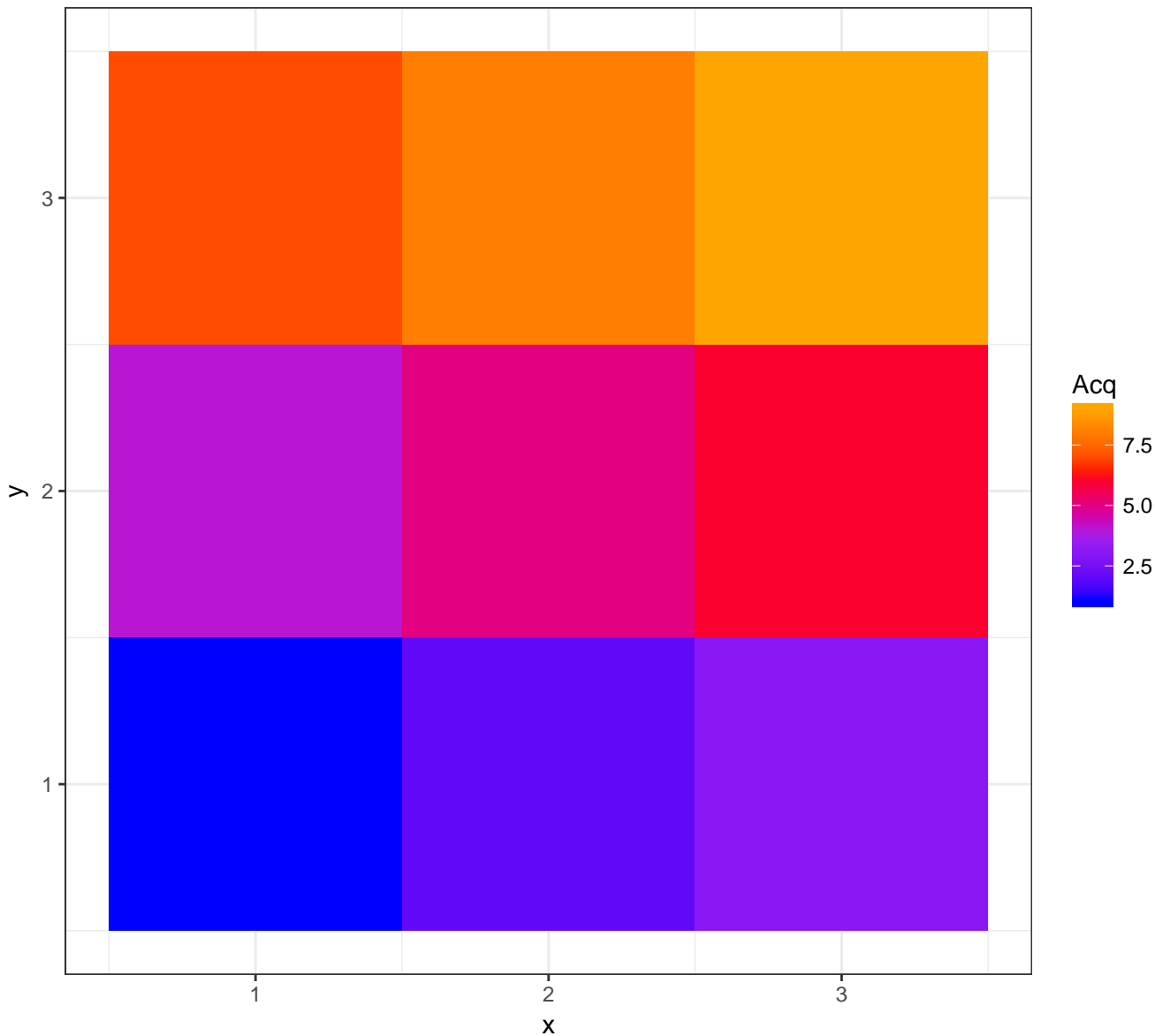


Quality control of MSI data

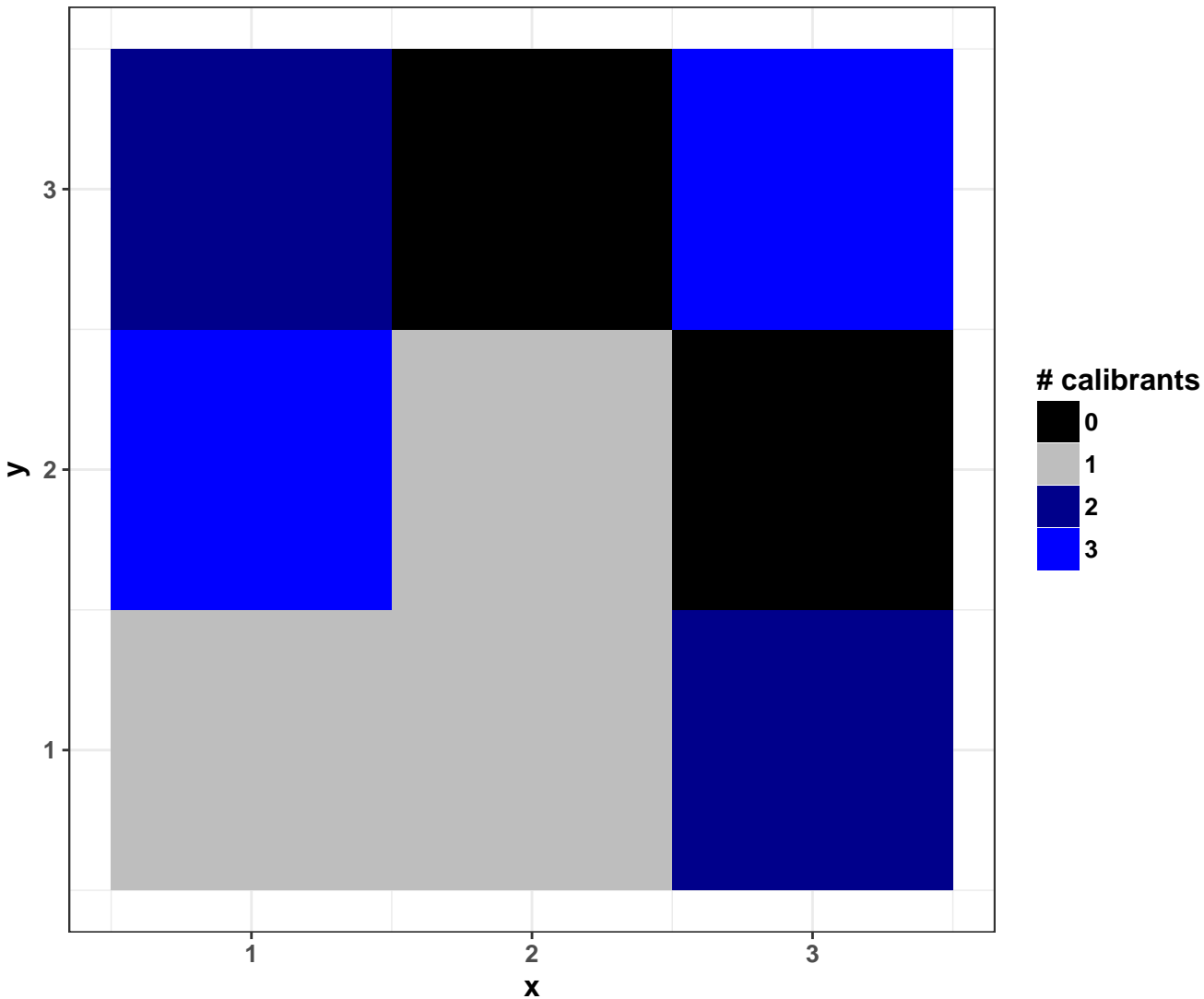
Filename: Testfile_imzml

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 – 9.24
Median of intensities	0
Intensities > 0	30.92 %
Number of zero TICs	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in inputpeptides.txt	3 / 6
# calibrants in inputcalibrantfile1.txt	3 / 3

Order of Acquisition

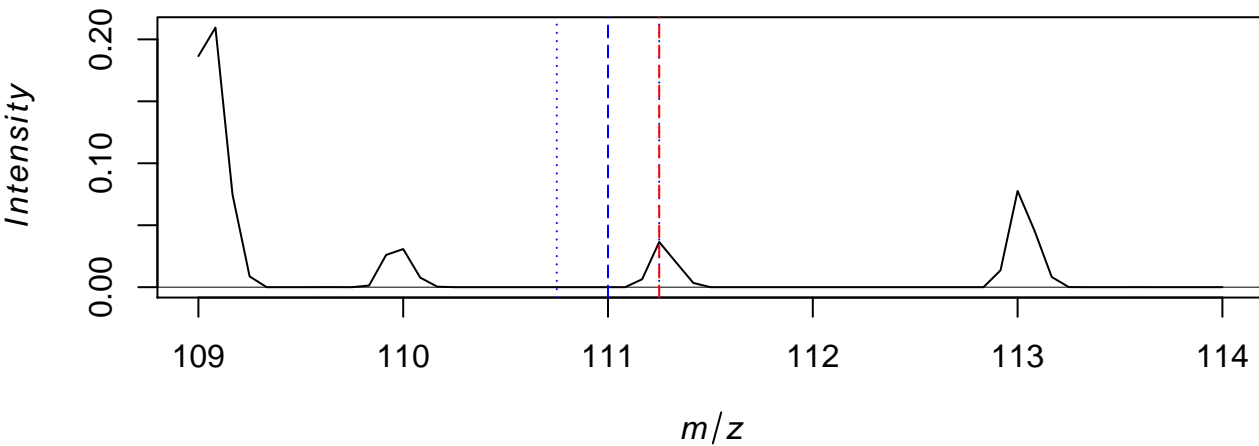


Number of calibrants per pixel

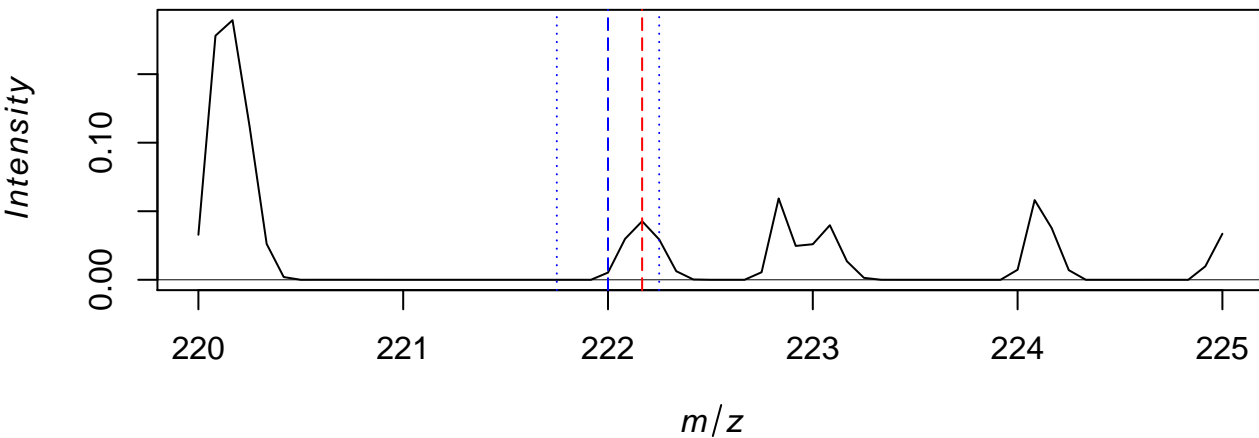


Control of fold change plot

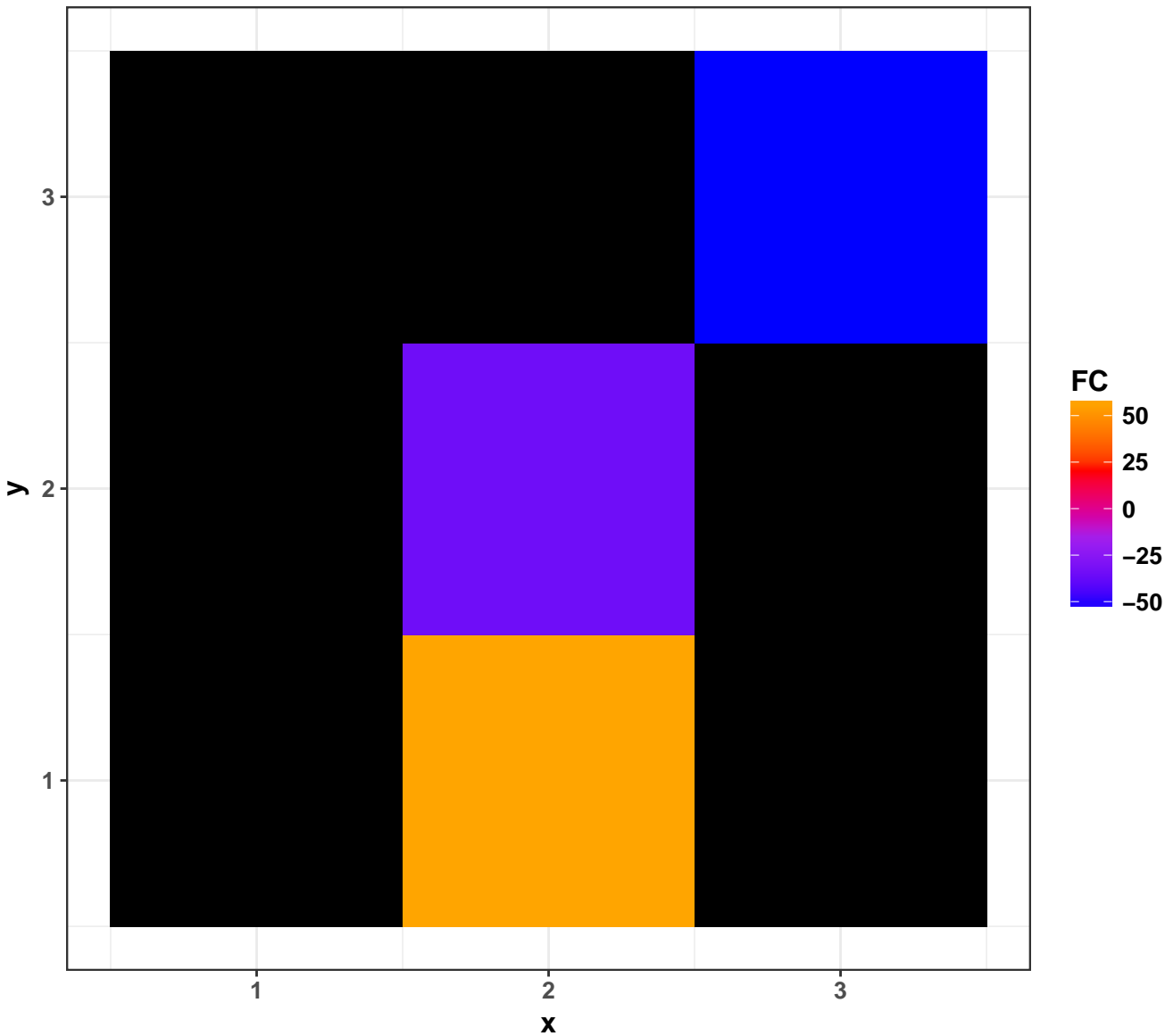
average spectrum 111 Da



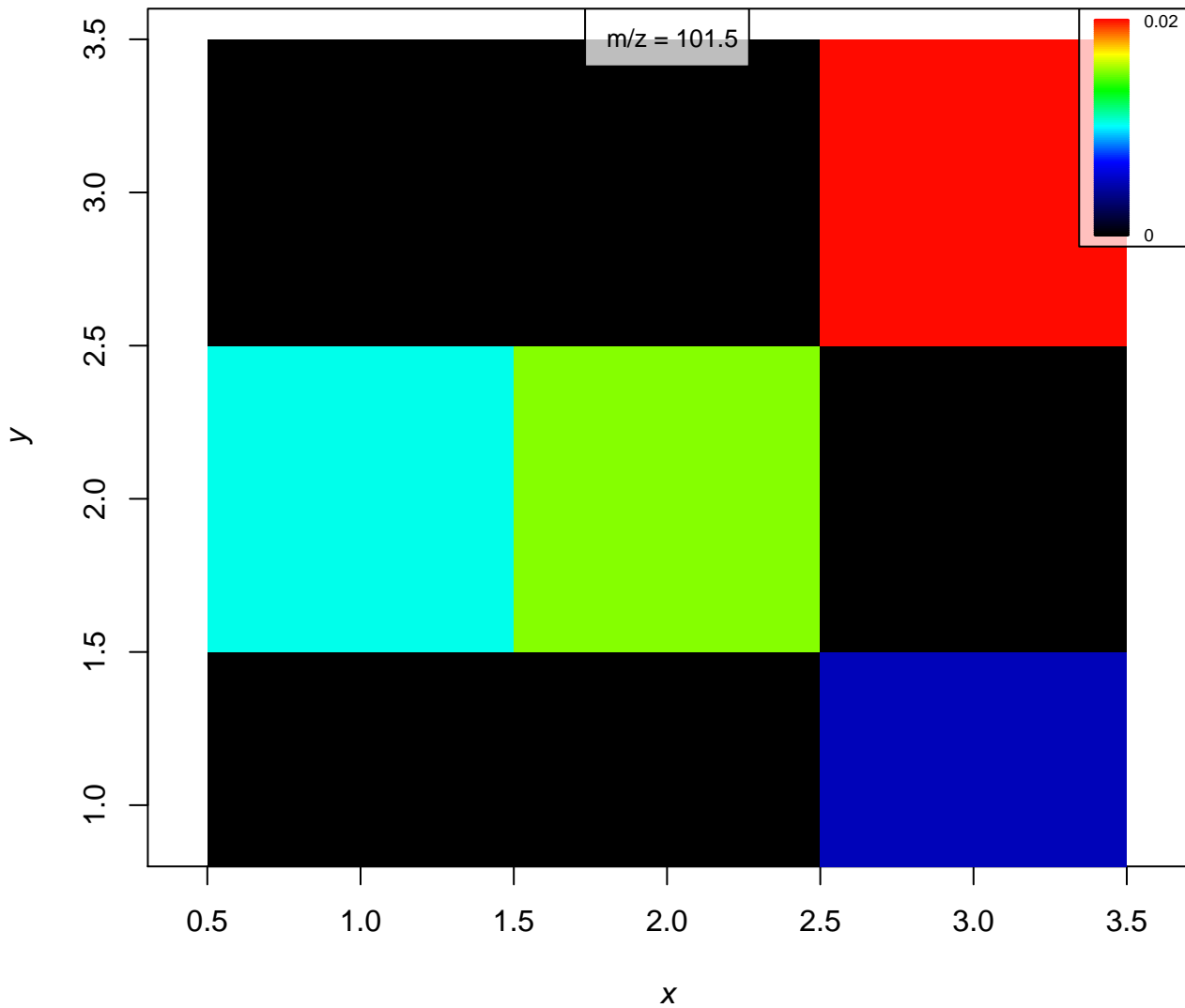
average spectrum 222 Da



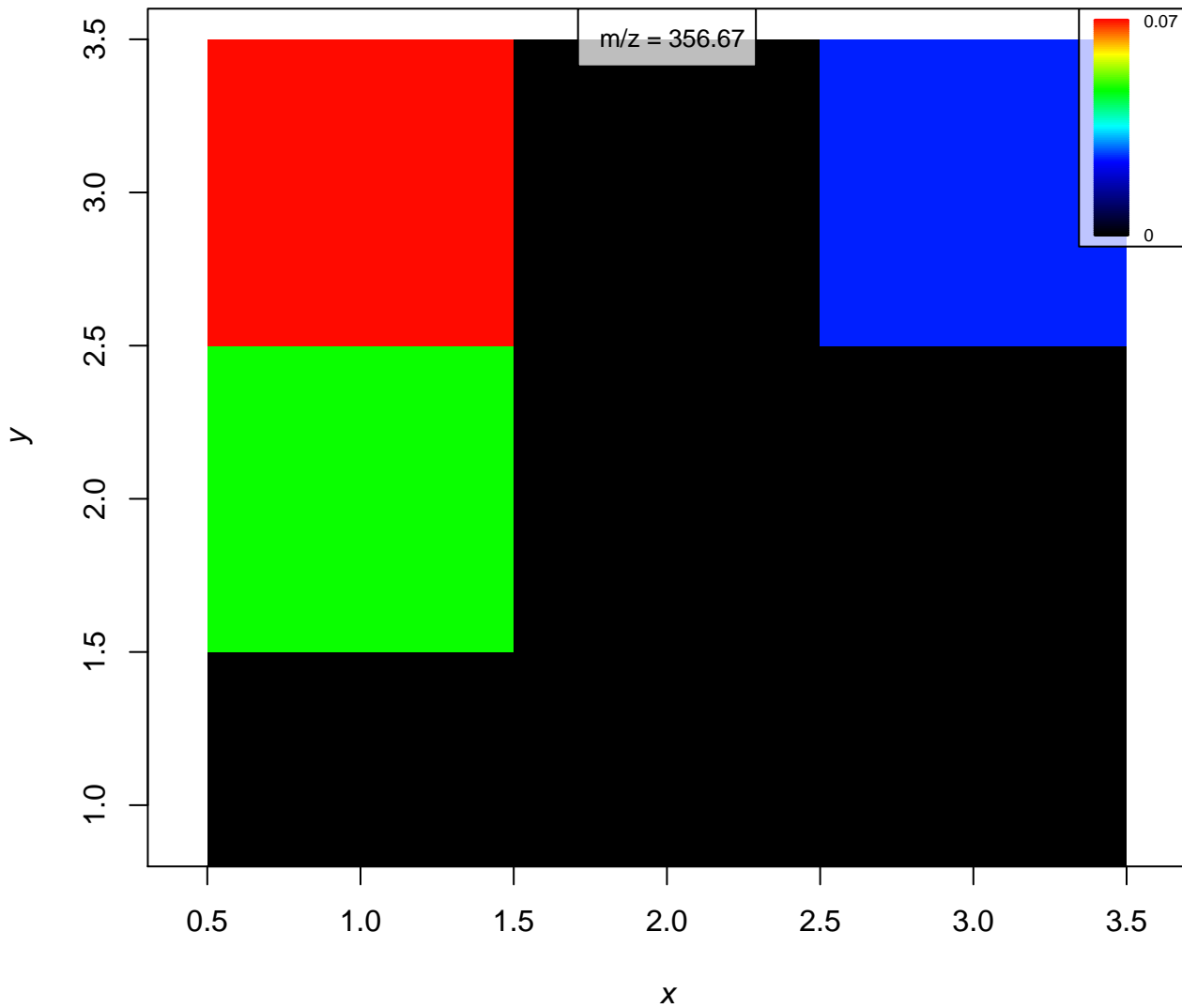
Ratio of mass1 (111) / mass2 (222)



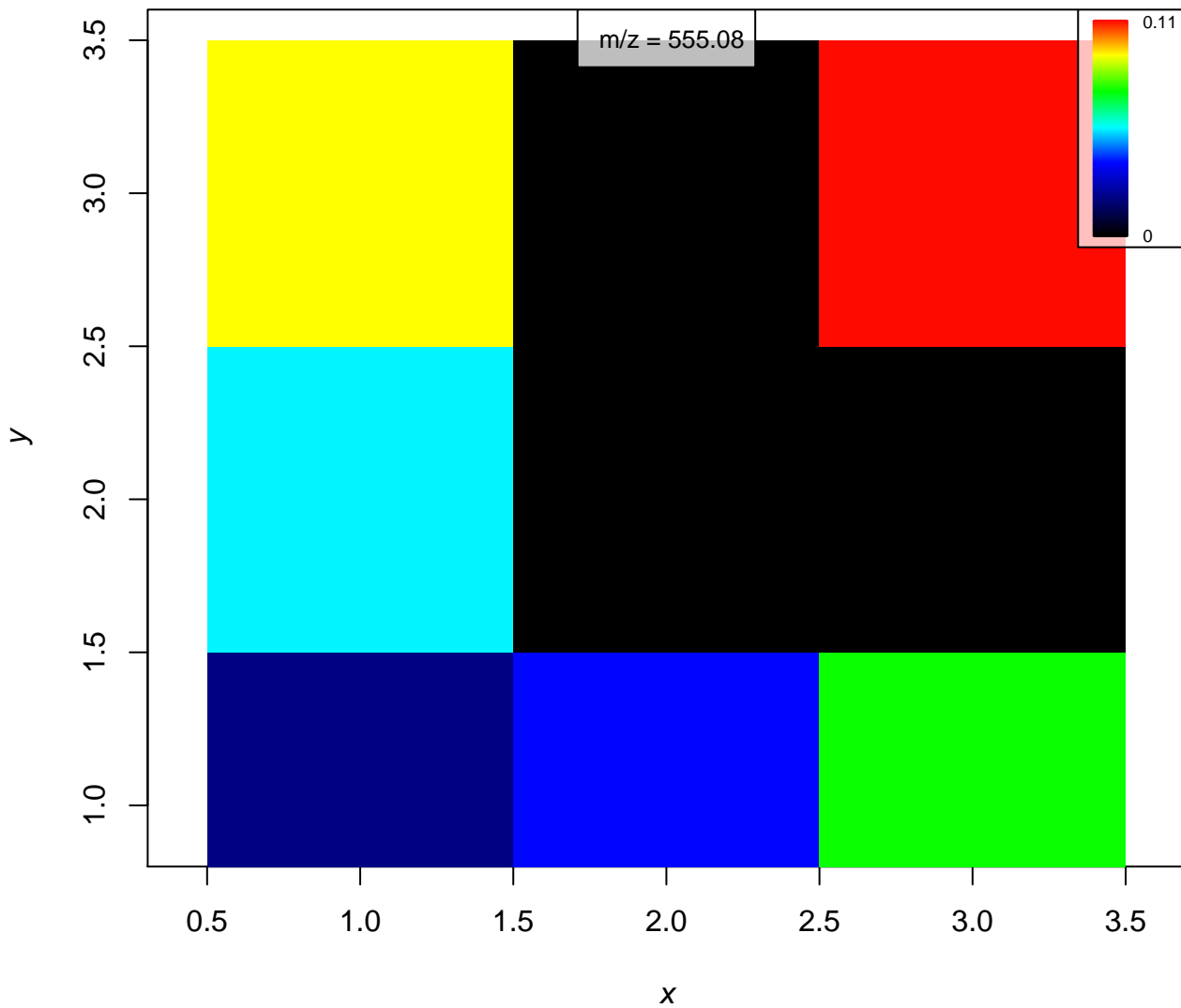
101.5 (101.5 ± 0.25 Da)



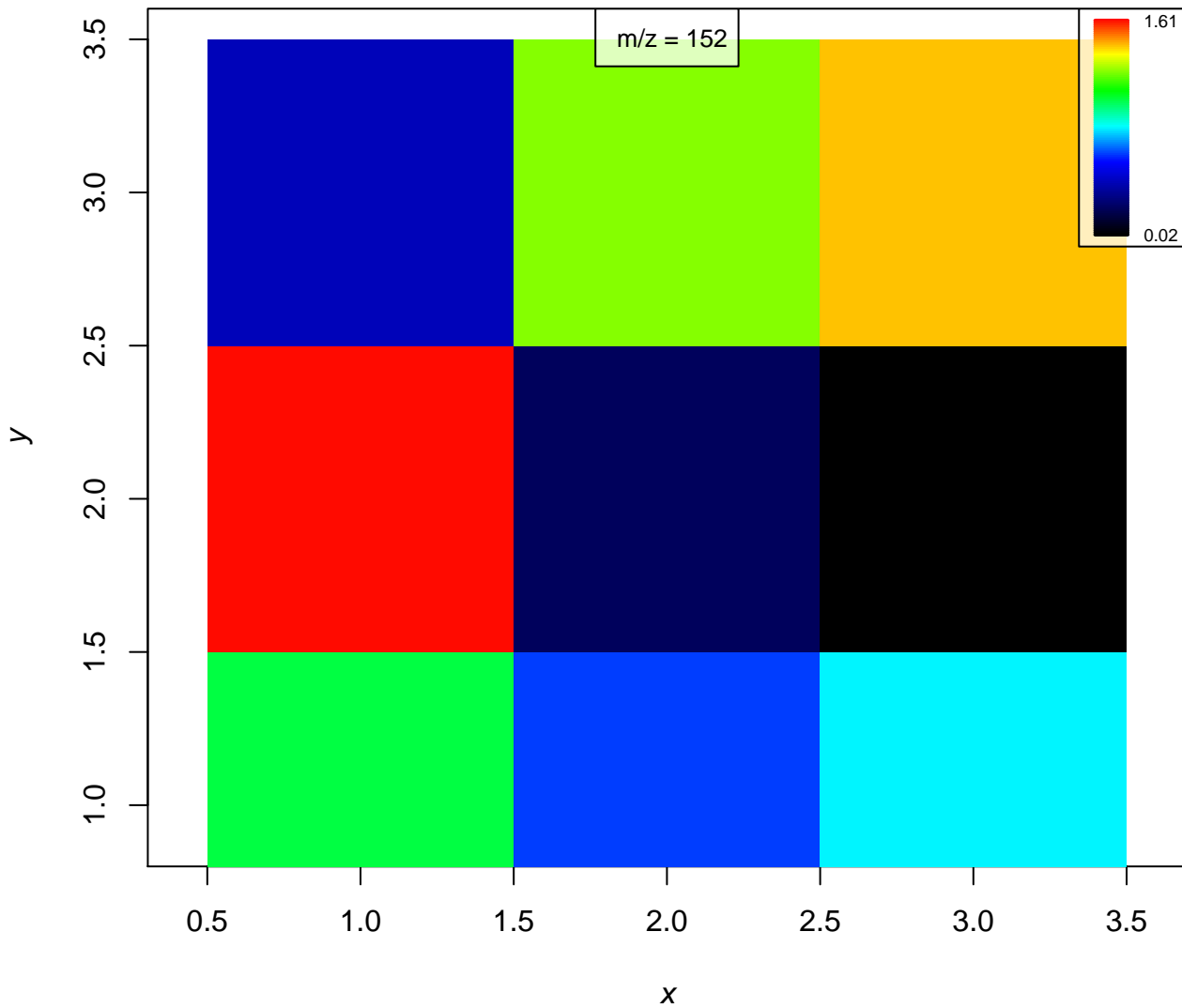
356.7 (356.7 ± 0.25 Da)



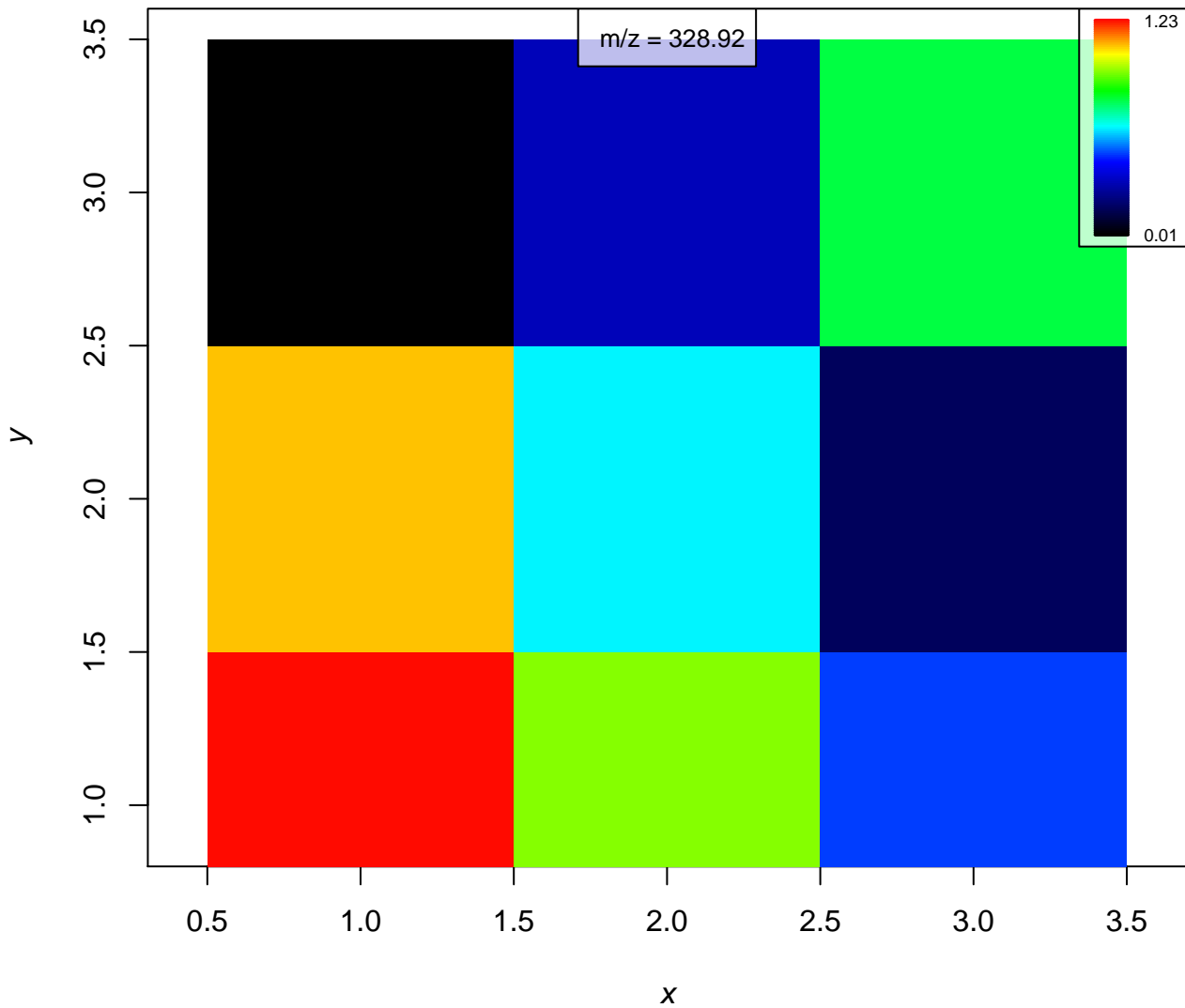
555.1 (555.1 \pm 0.25 Da)



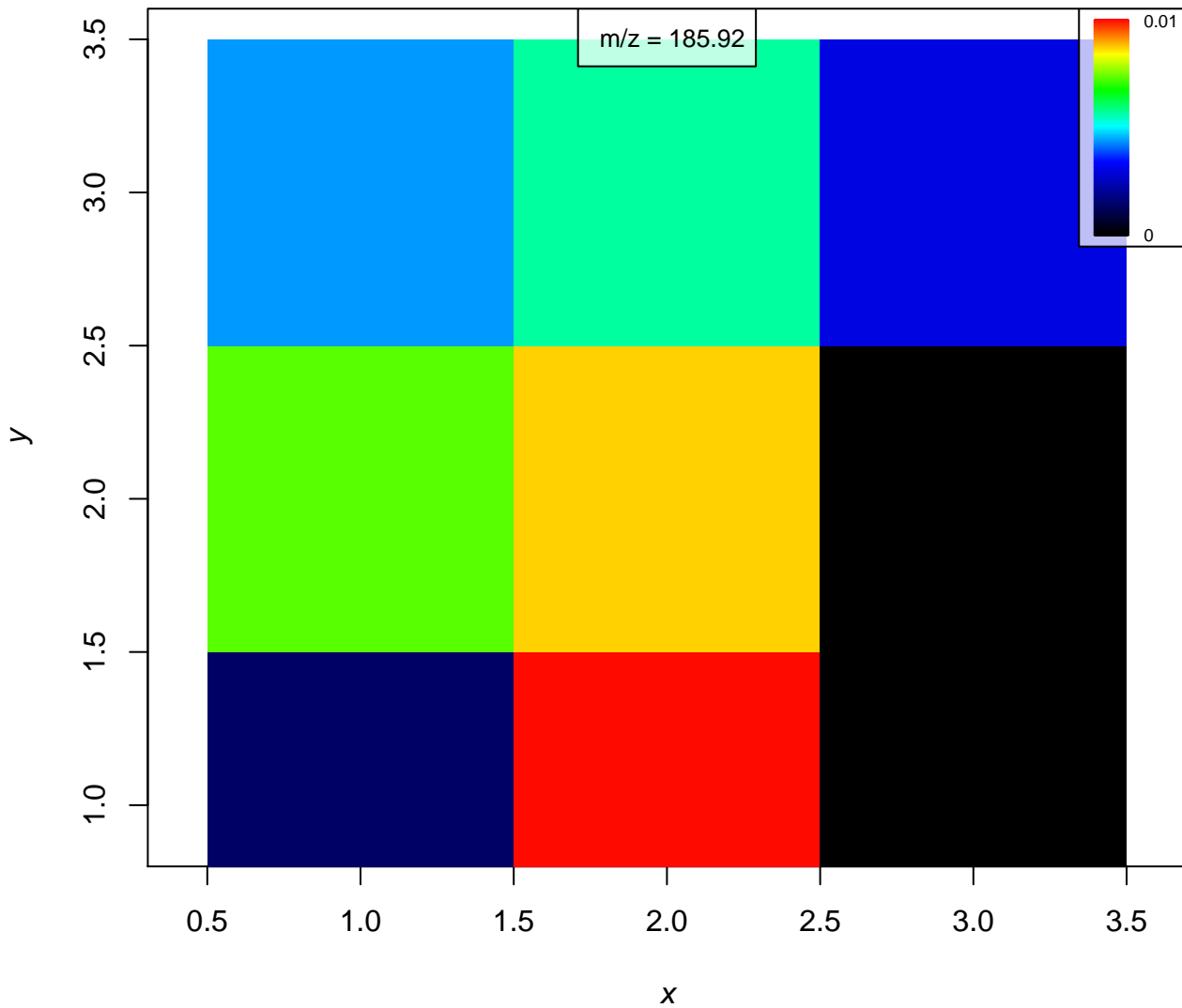
152 (152 ± 0.25 Da)



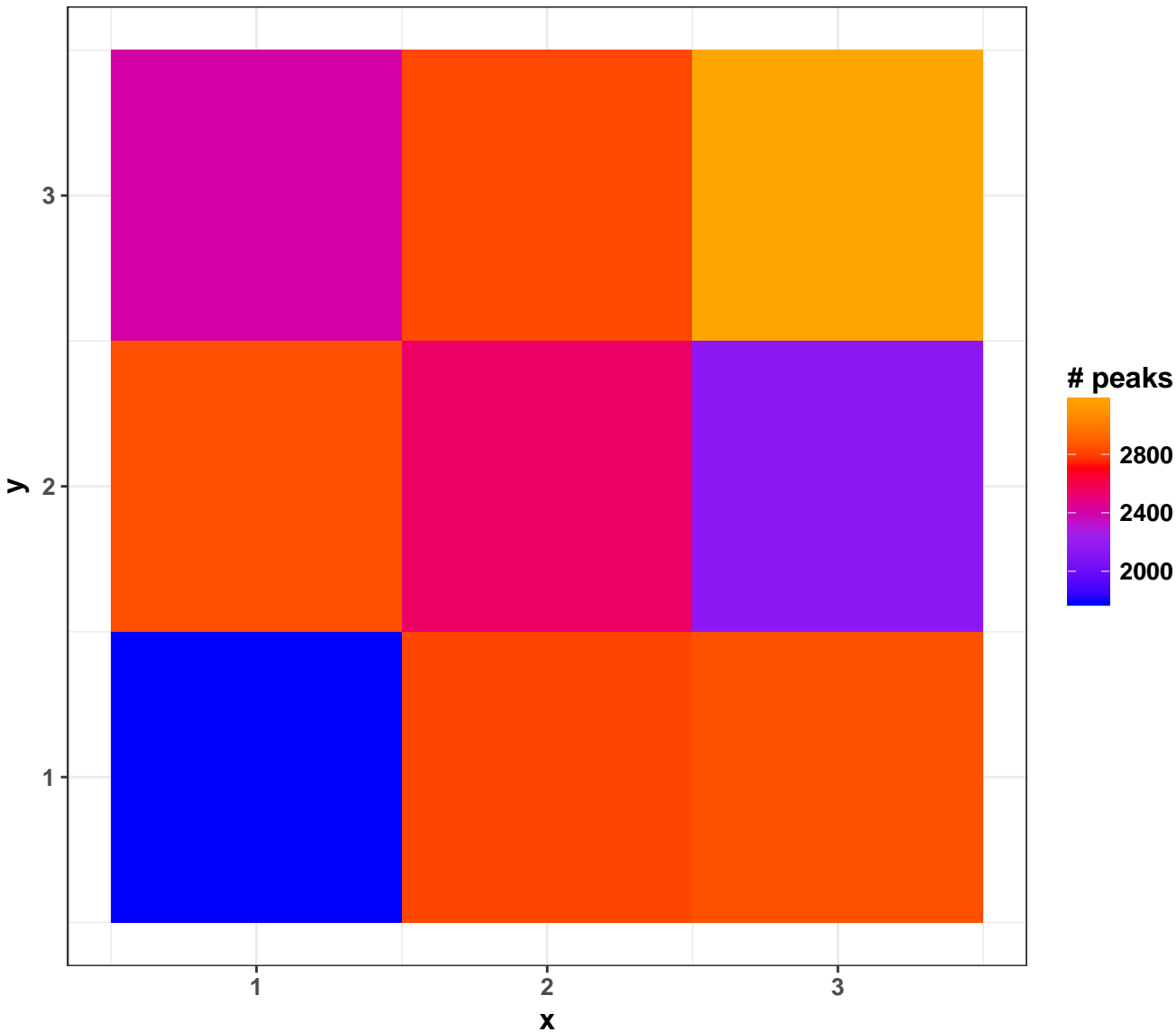
328.9 (328.9 ± 0.25 Da)



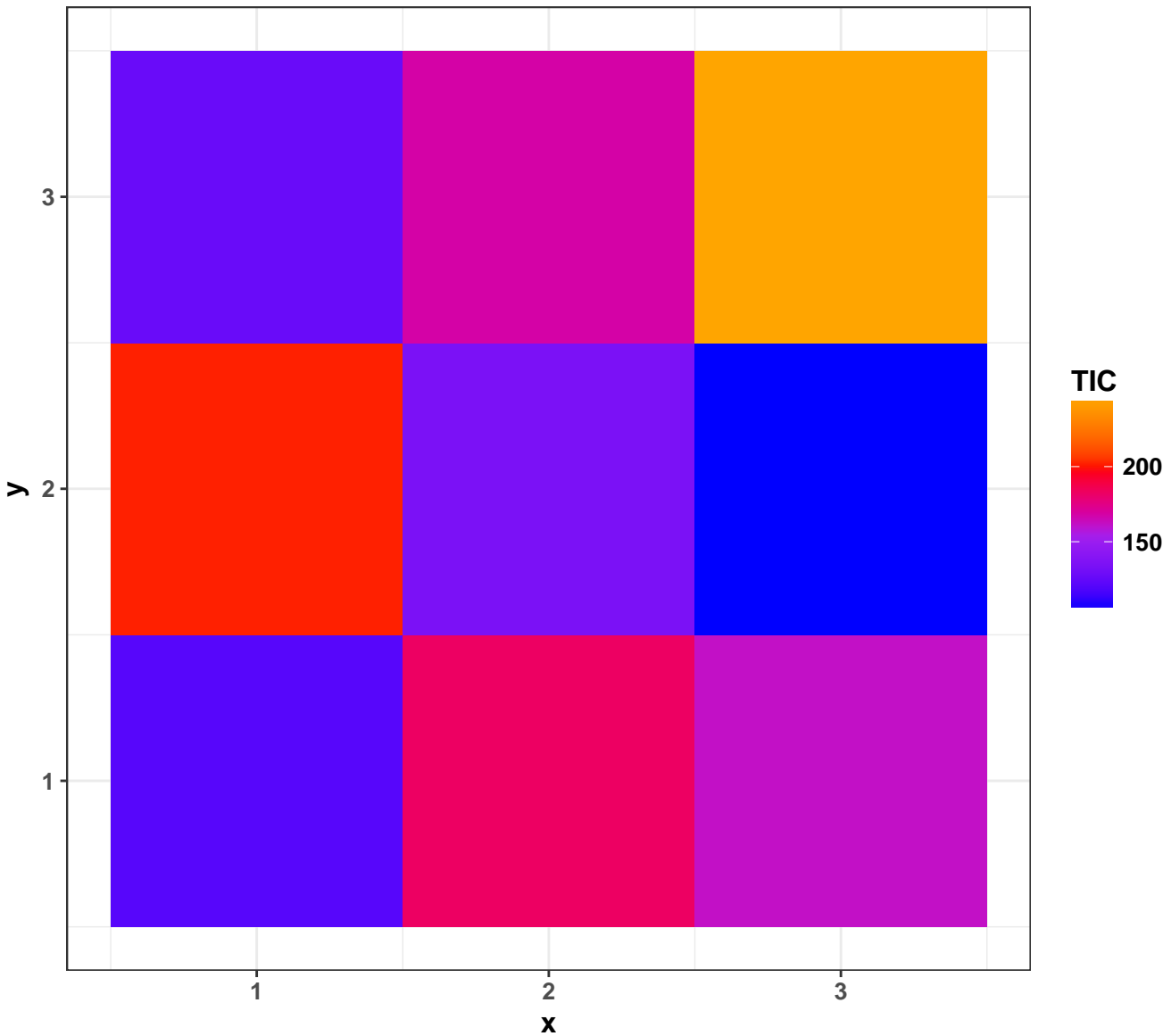
185.9 (185.9 ± 0.25 Da)



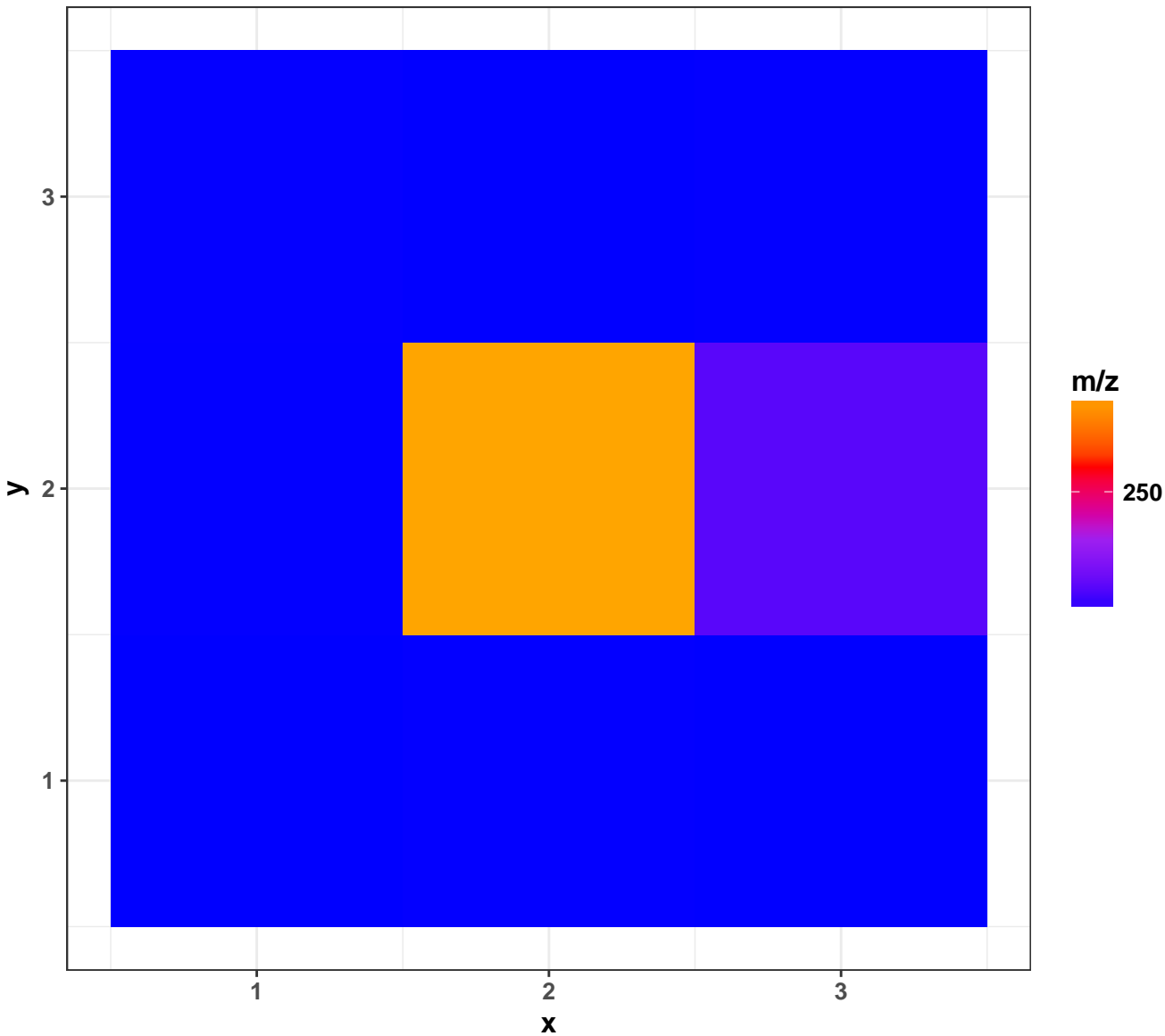
Number of peaks per pixel



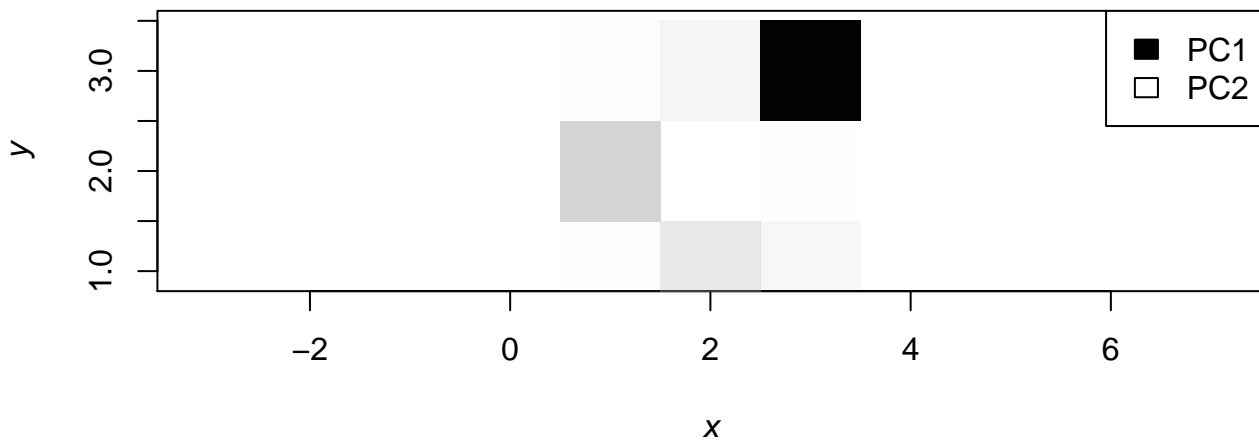
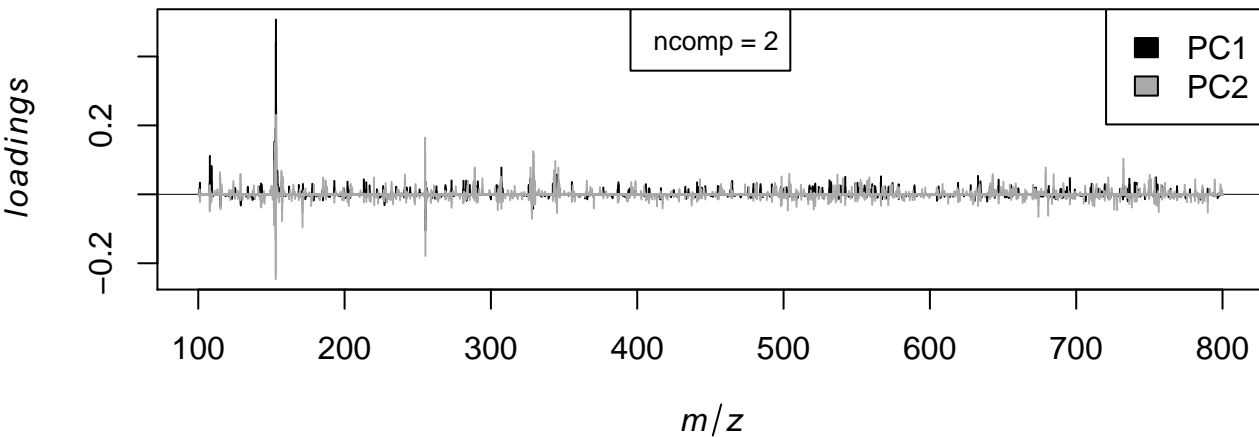
Total Ion Chromatogram



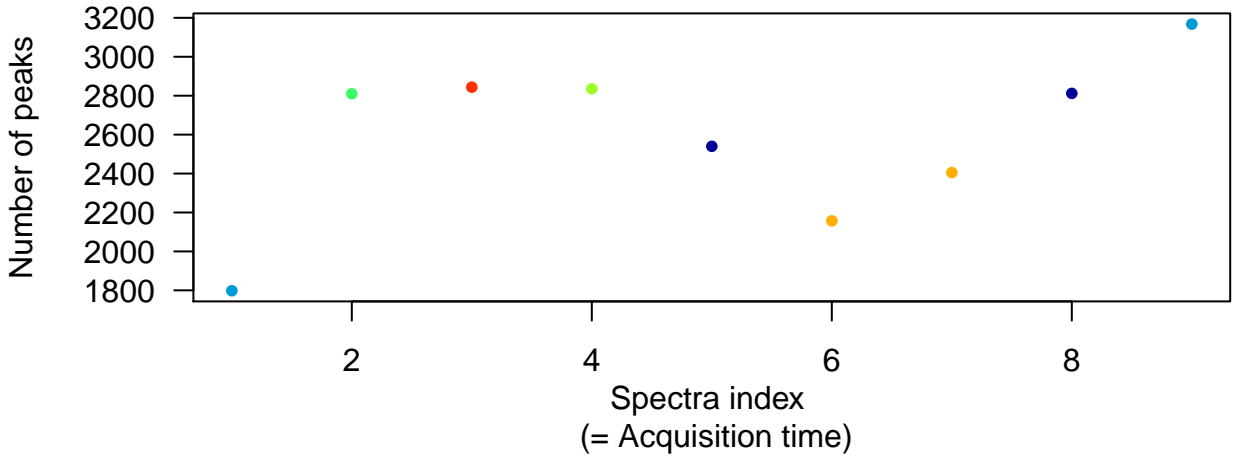
Most abundant m/z in each pixel



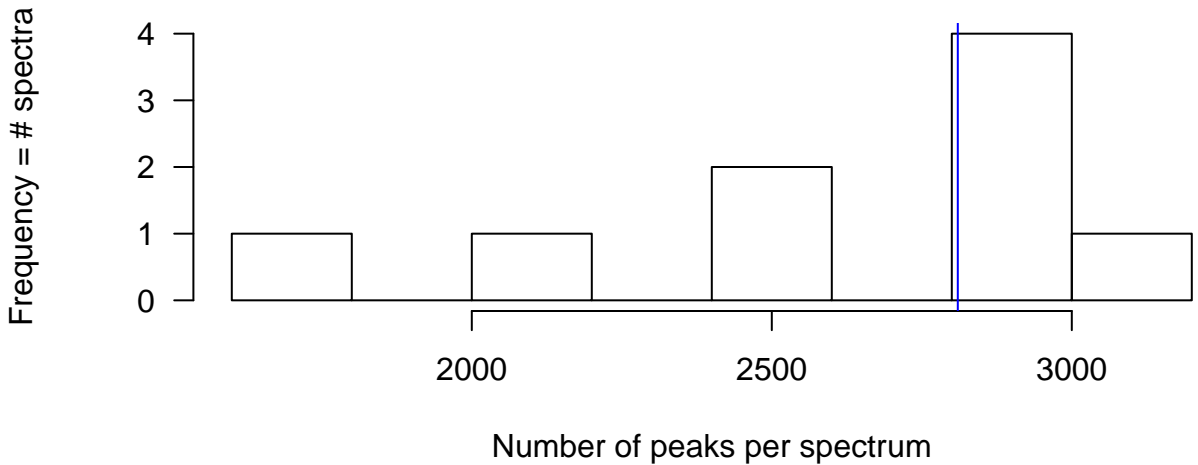
PCA for two components



Number of peaks per spectrum

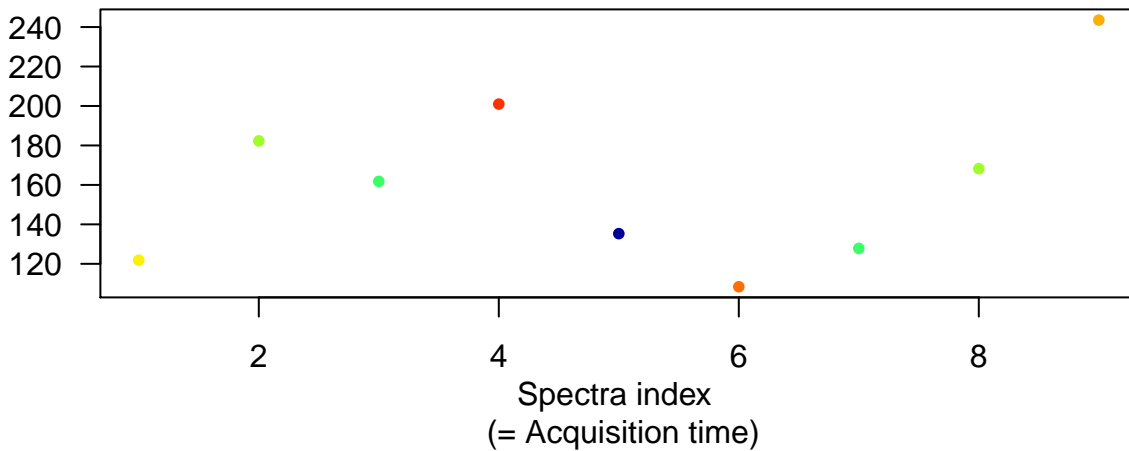


Number of peaks per spectrum



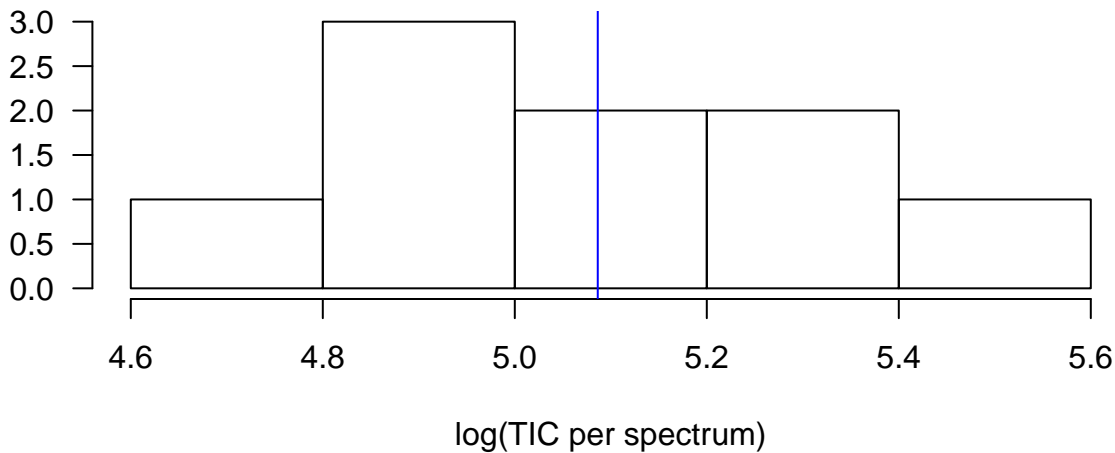
Total ion chromatogram intensity

TIC per spectrum

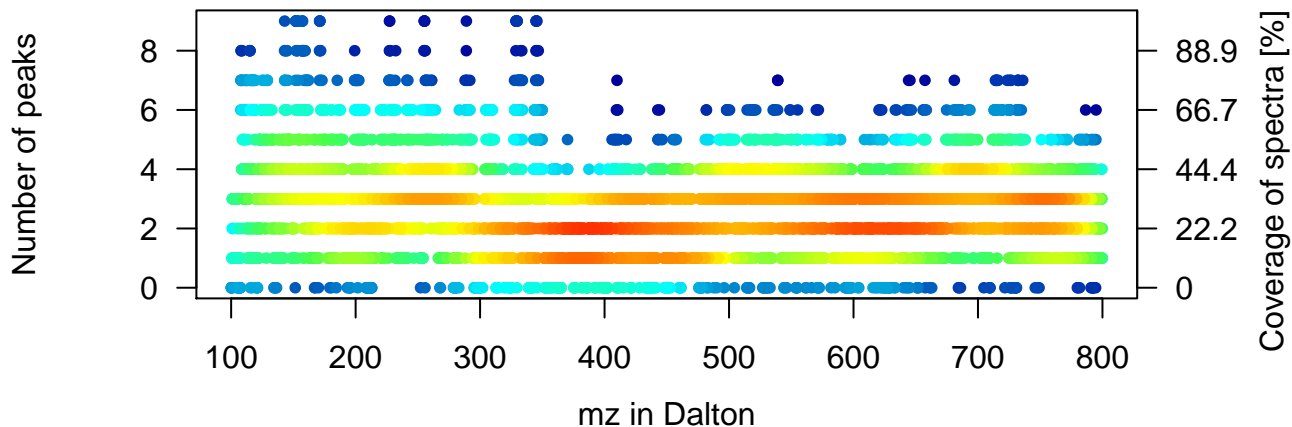


Frequency = # spectra

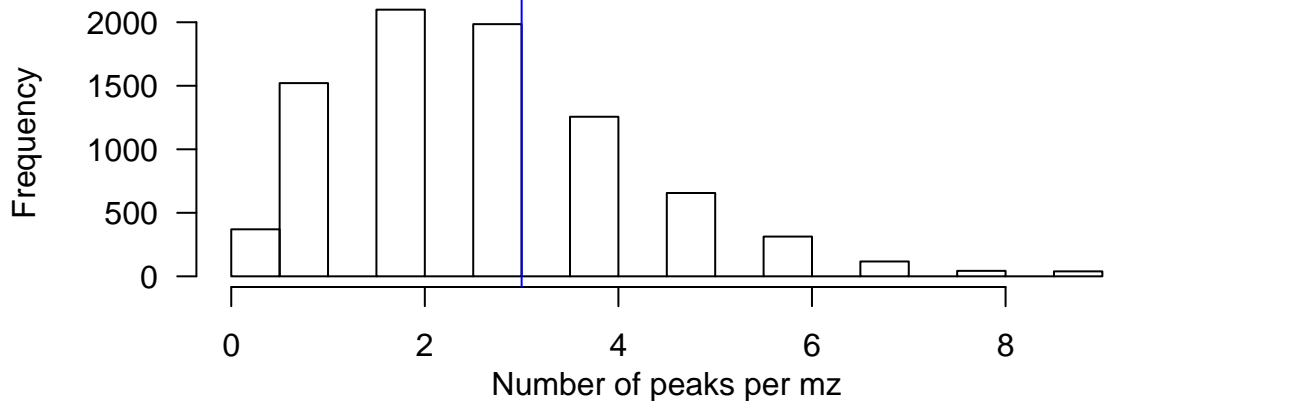
TIC per spectrum



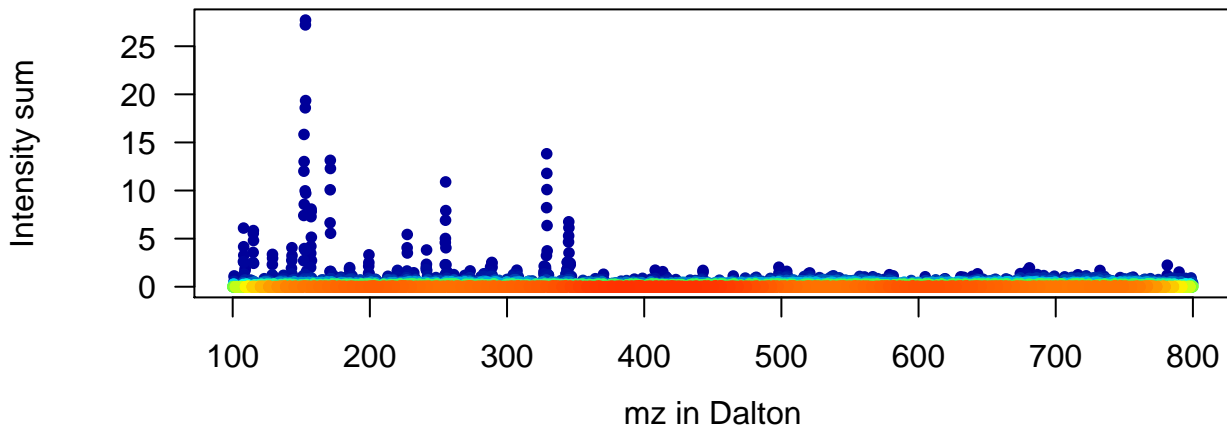
Number of peaks per mz



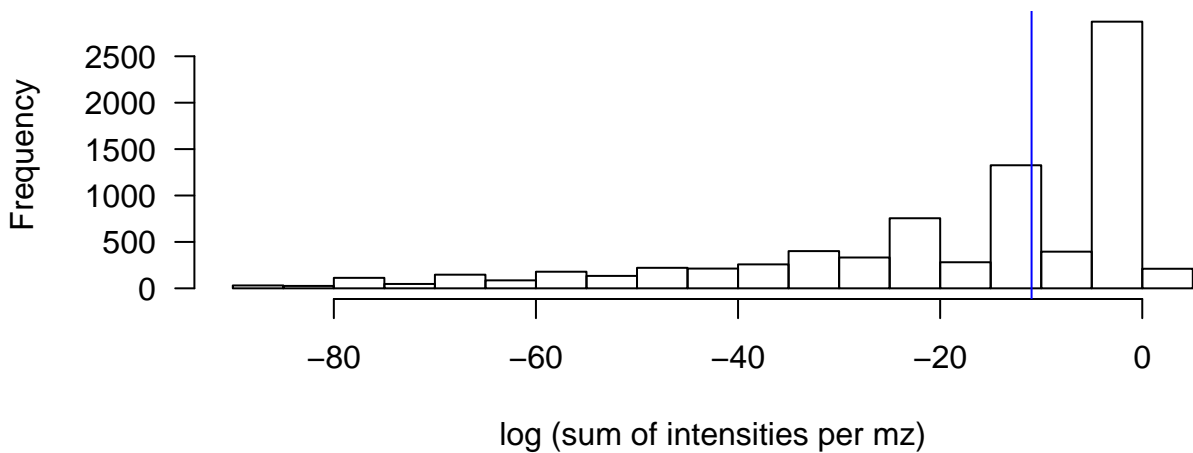
Number of peaks per mz



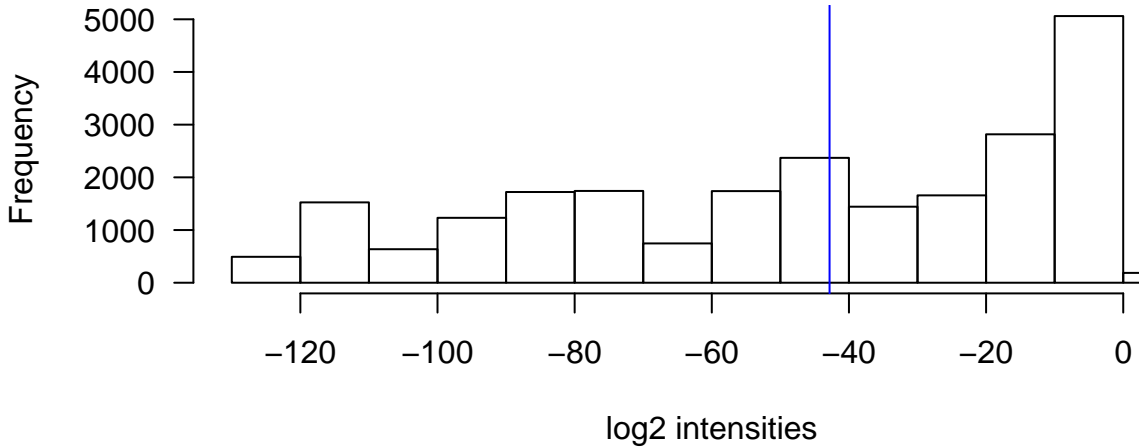
Sum of intensities per mz



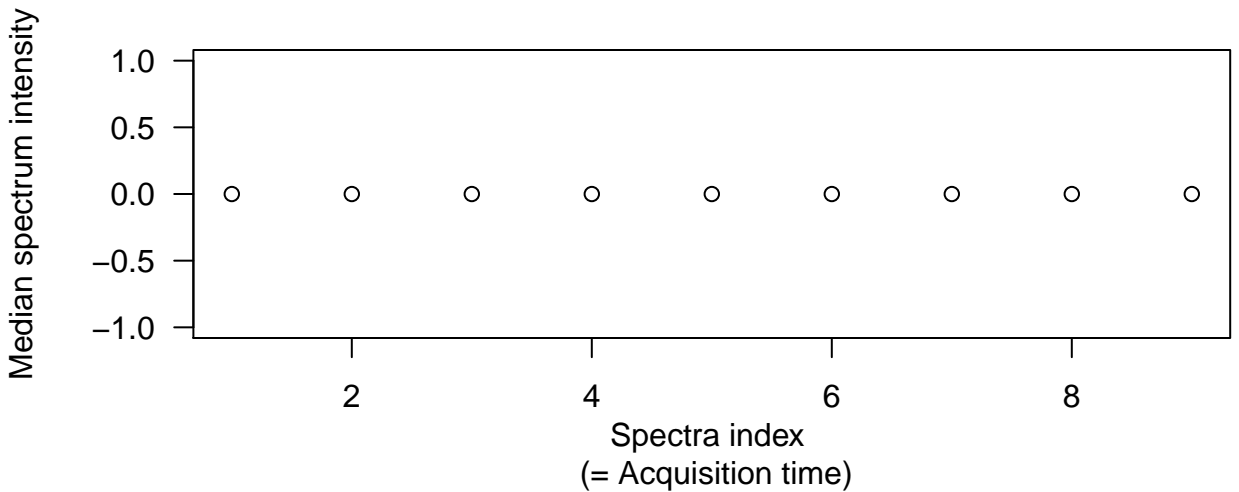
Sum of intensities per mz



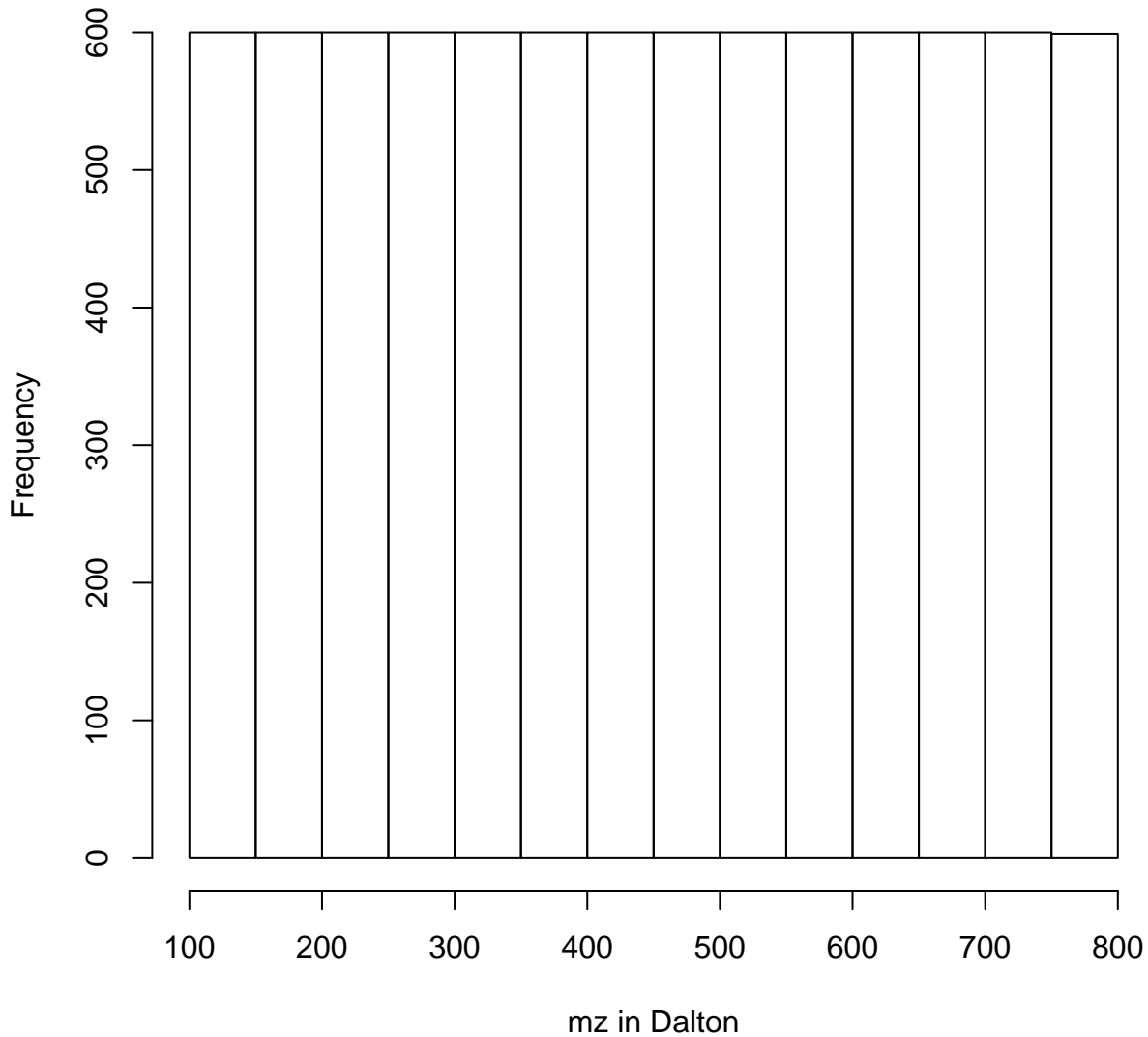
Log2-transformed intensities



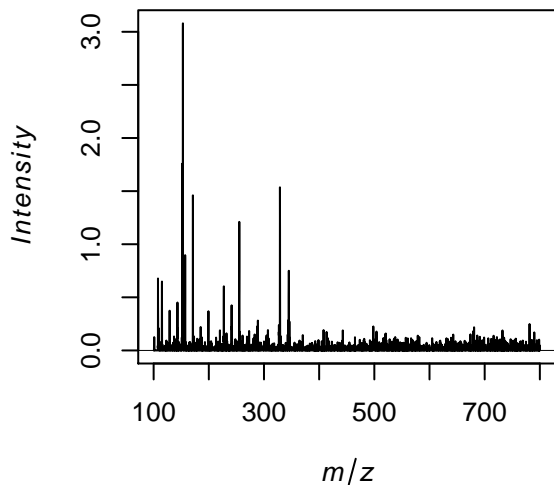
Median intensity per spectrum



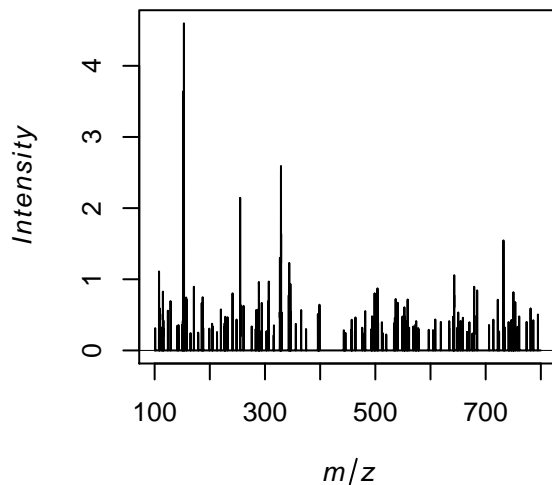
Histogram of mz values



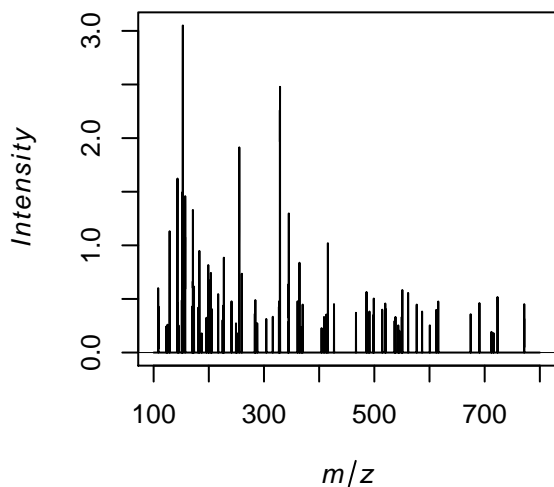
Average spectrum



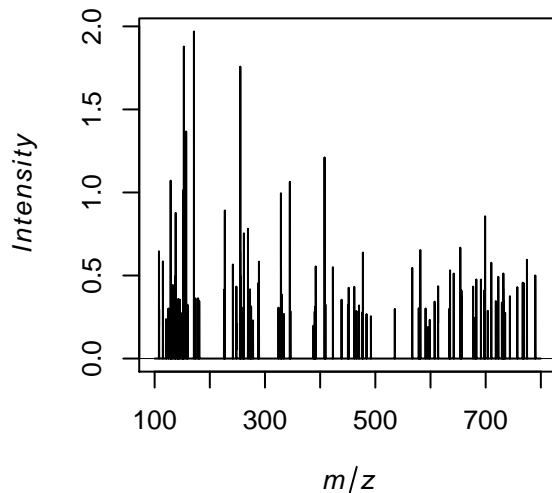
Spectrum in middle of acquisition



Spectrum at x = 1, y = 1

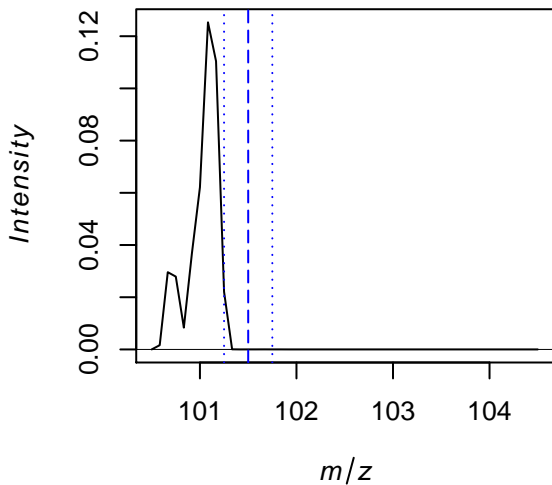


Spectrum at x = 3, y = 2

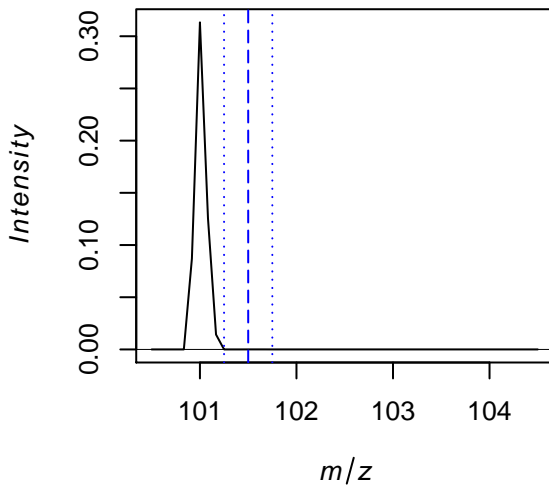


101.5

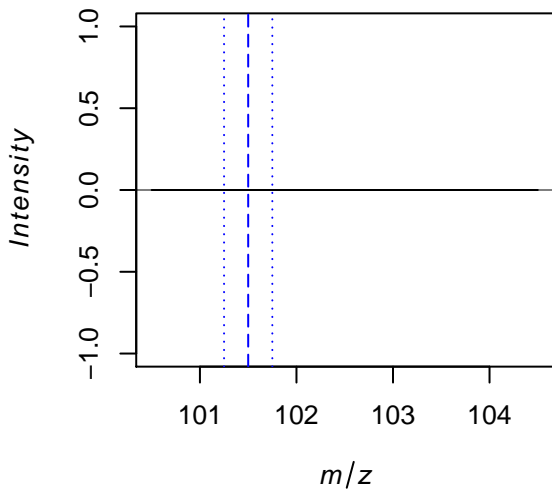
average spectrum



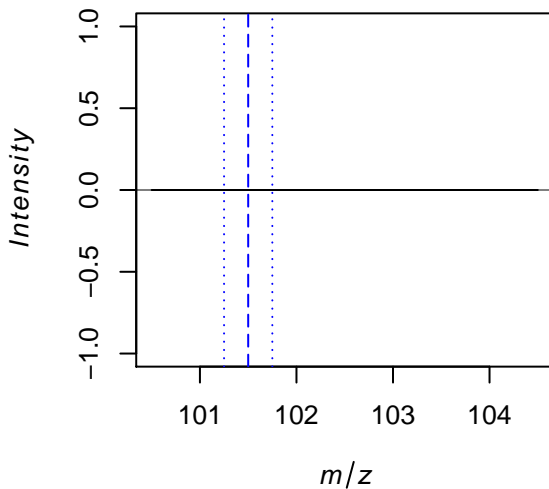
pixel in middle of acquisition



Spectrum at $x = 1, y = 1$

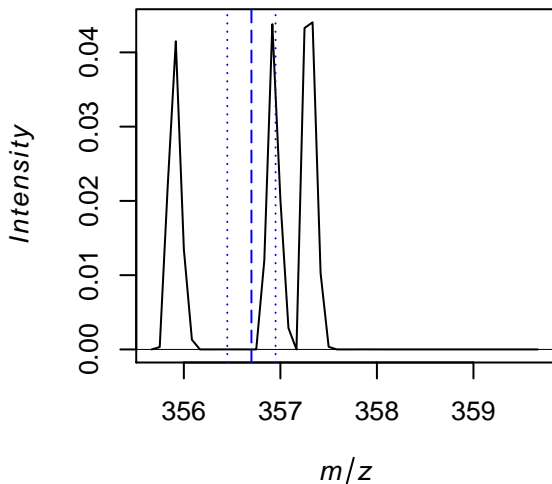


Spectrum at $x = 3, y = 2$

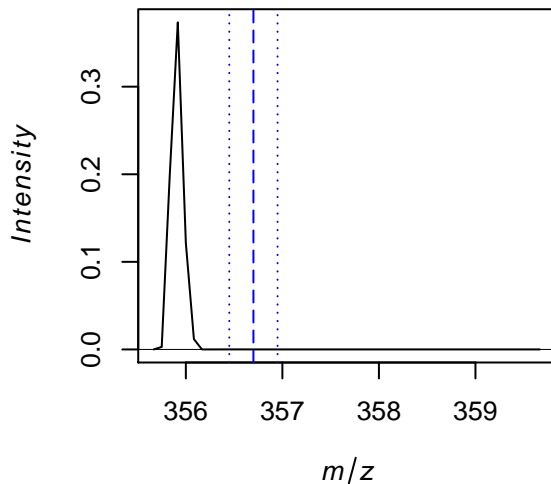


356.7

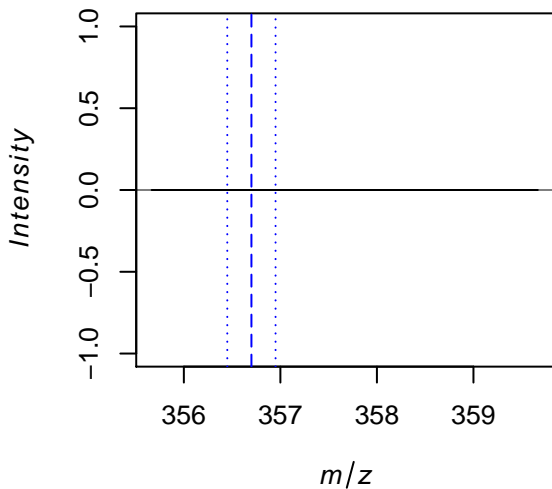
average spectrum



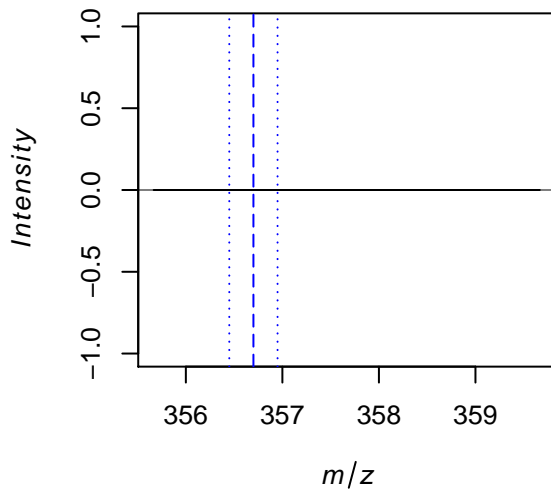
pixel in middle of acquisition



Spectrum at $x = 1, y = 1$

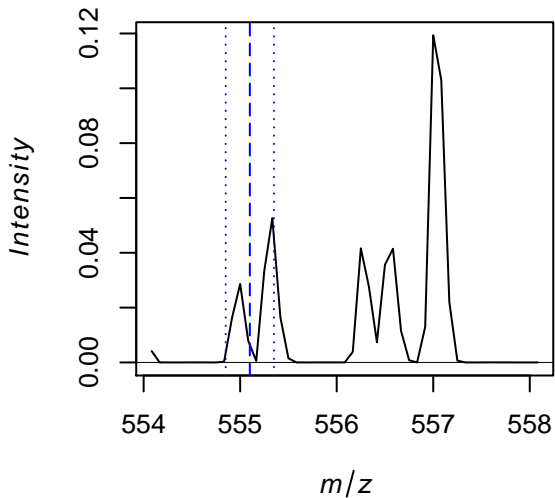


Spectrum at $x = 3, y = 2$

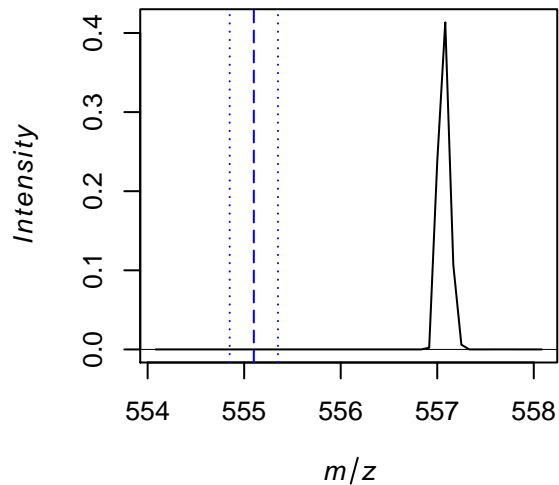


555.1

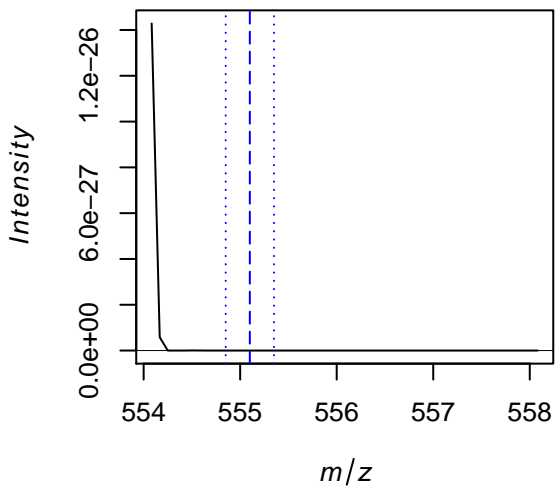
average spectrum



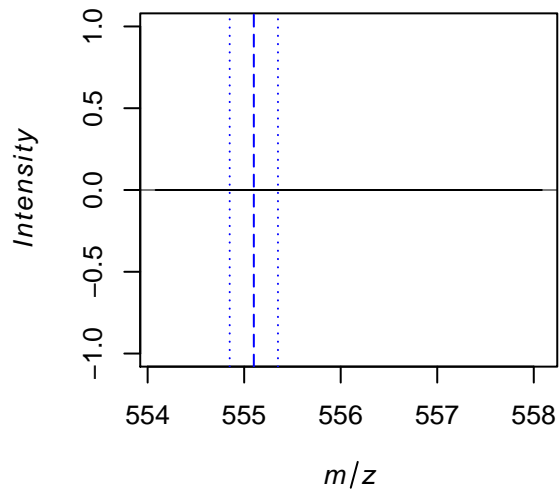
pixel in middle of acquisition



Spectrum at x = 1, y = 1



Spectrum at x = 3, y = 2



Theoretical calibrant mz vs. closest measured mz

