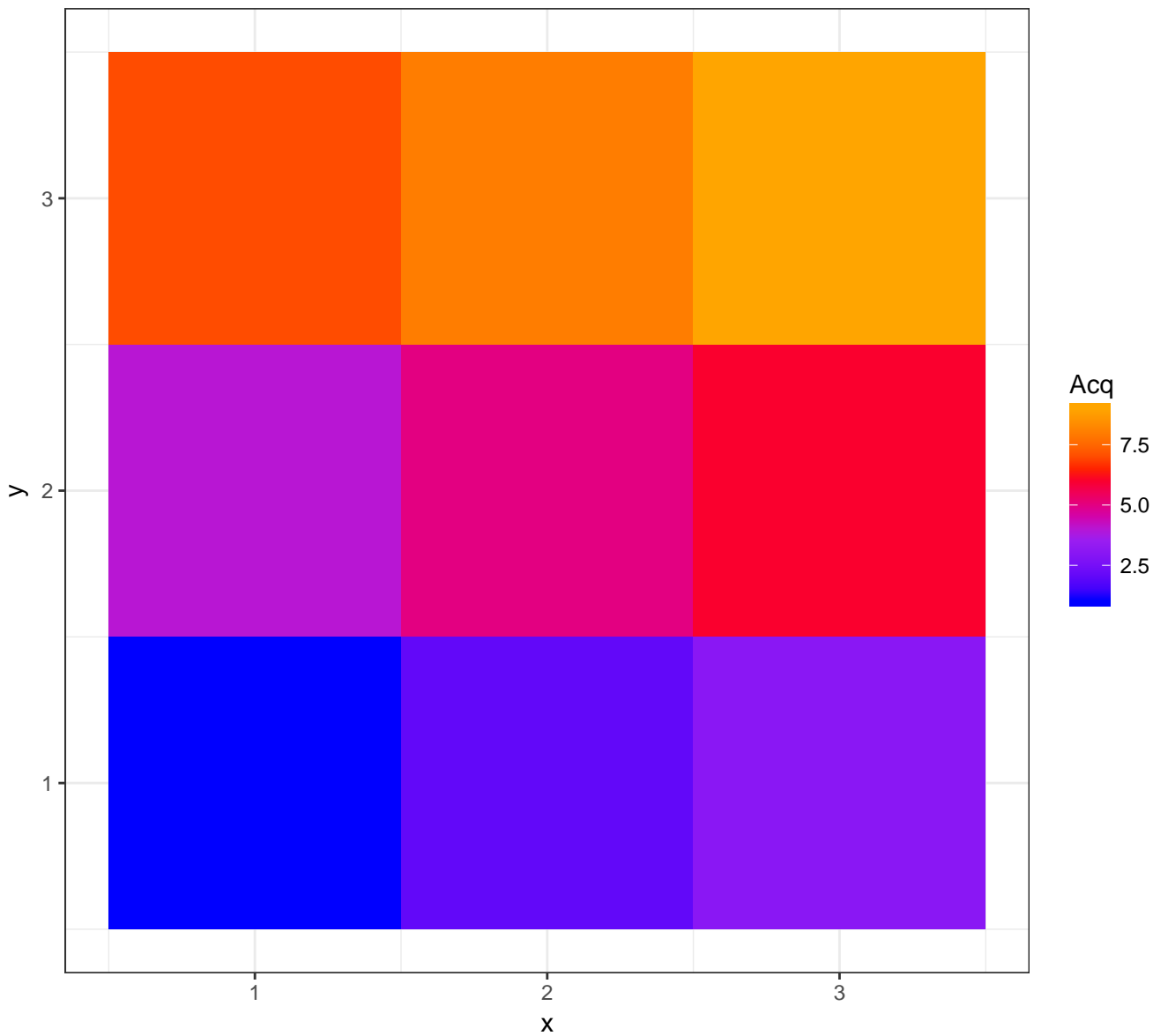


Quality control of MSI data

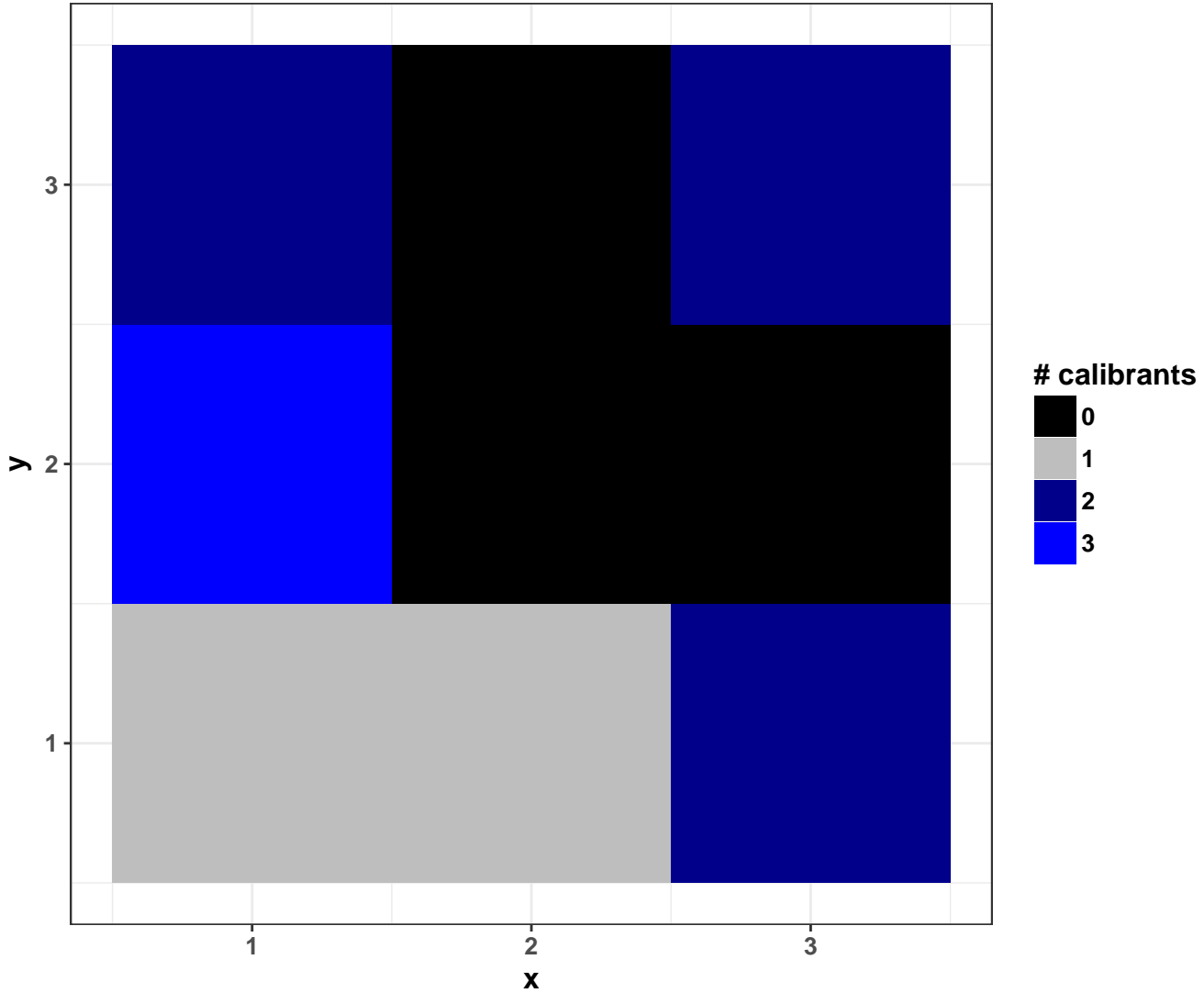
Filename: Testfile_rdata

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 input masses	6

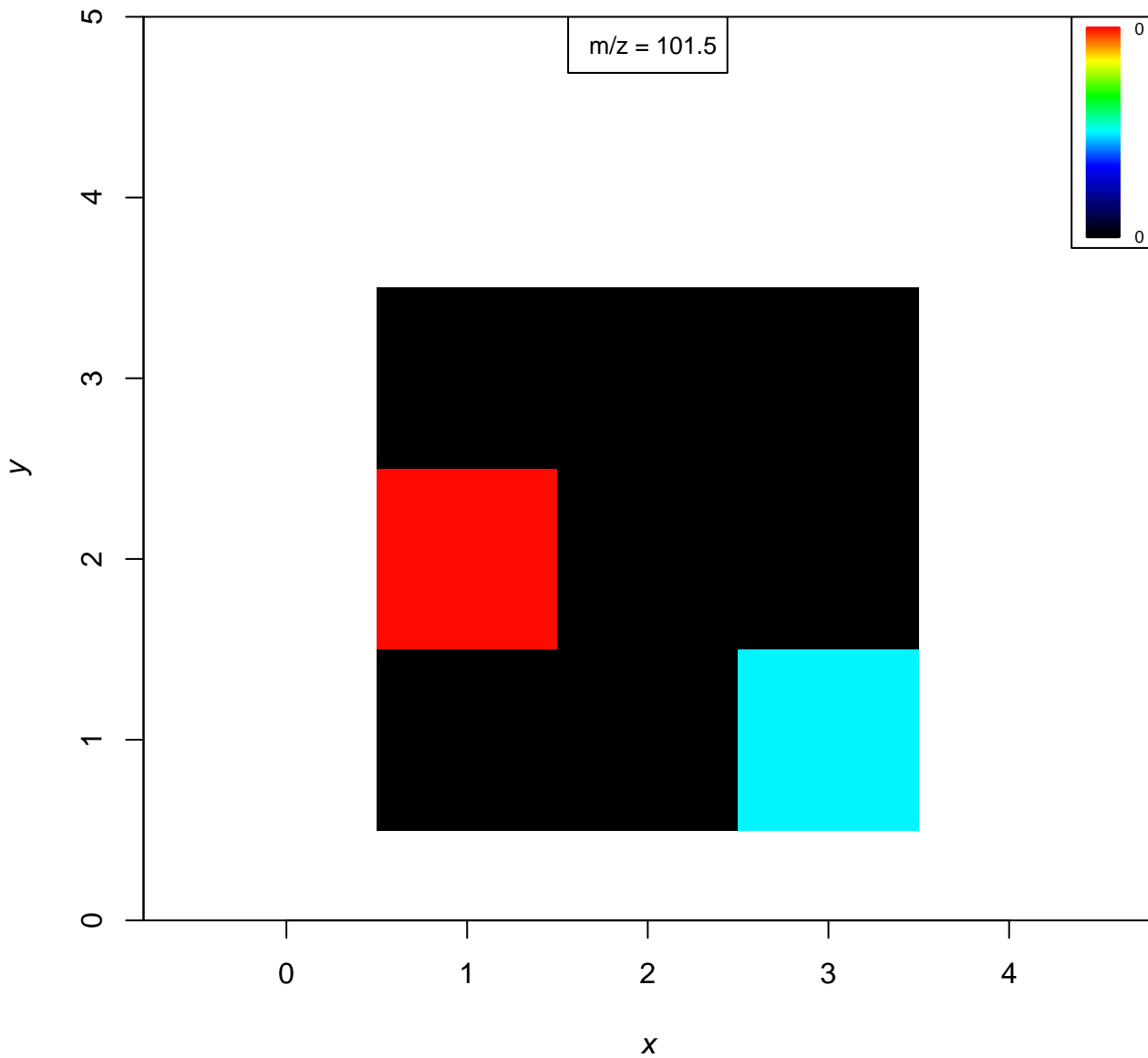
1) Order of Acquisition



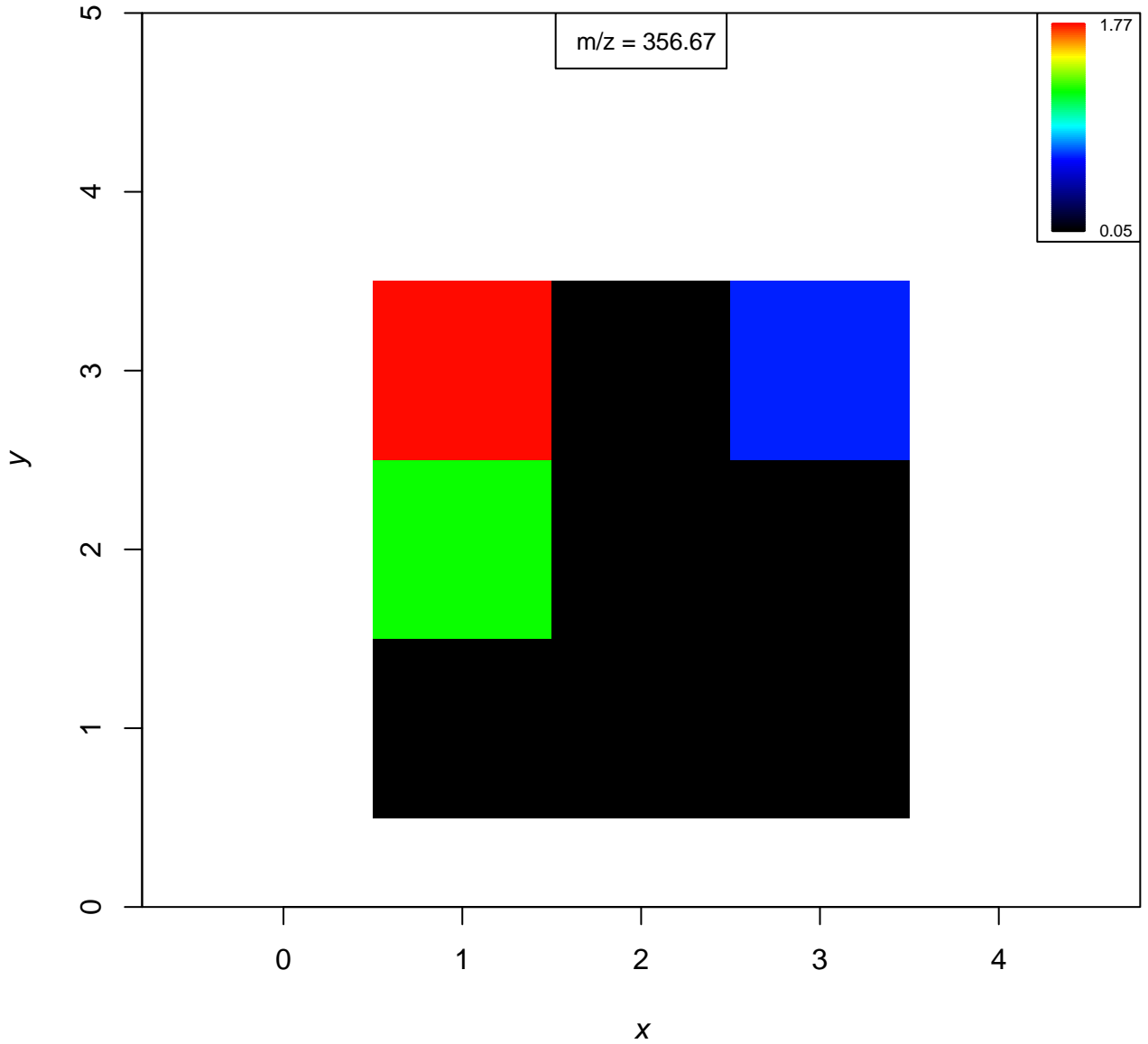
2) Number of calibrants per pixel



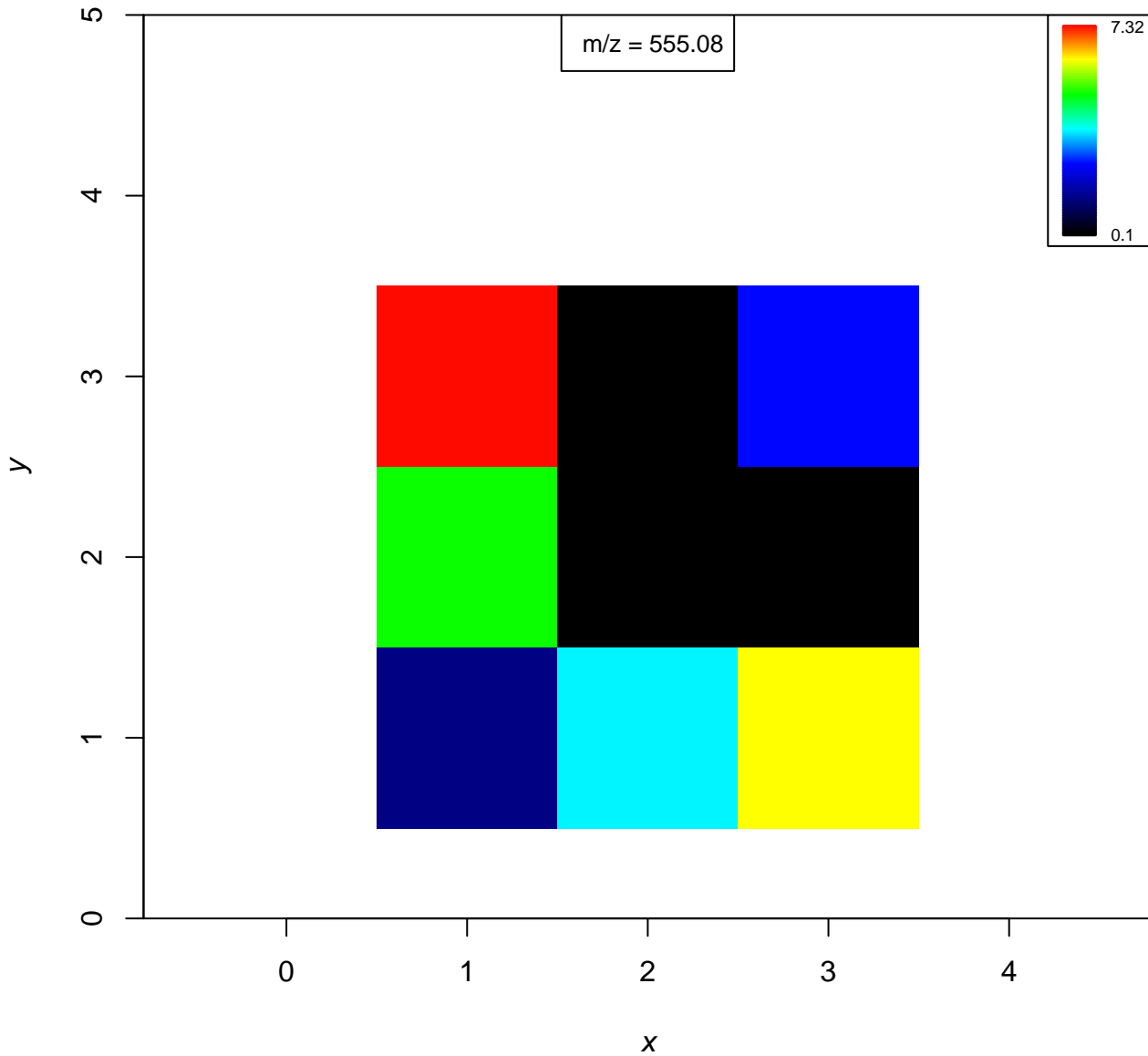
3A) 101.5 (101.5 Da)



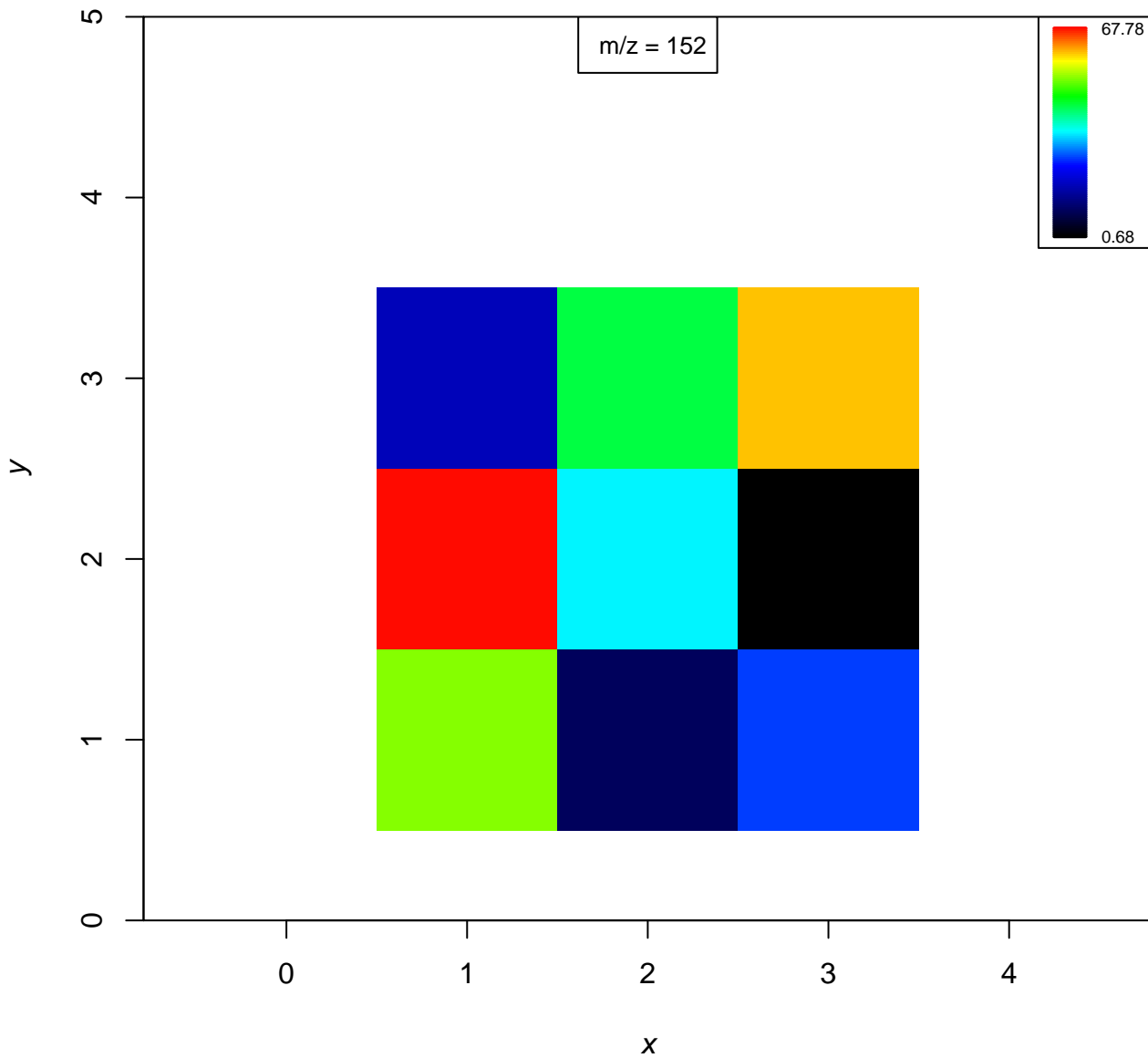
3B) 356.7 (356.7 Da)



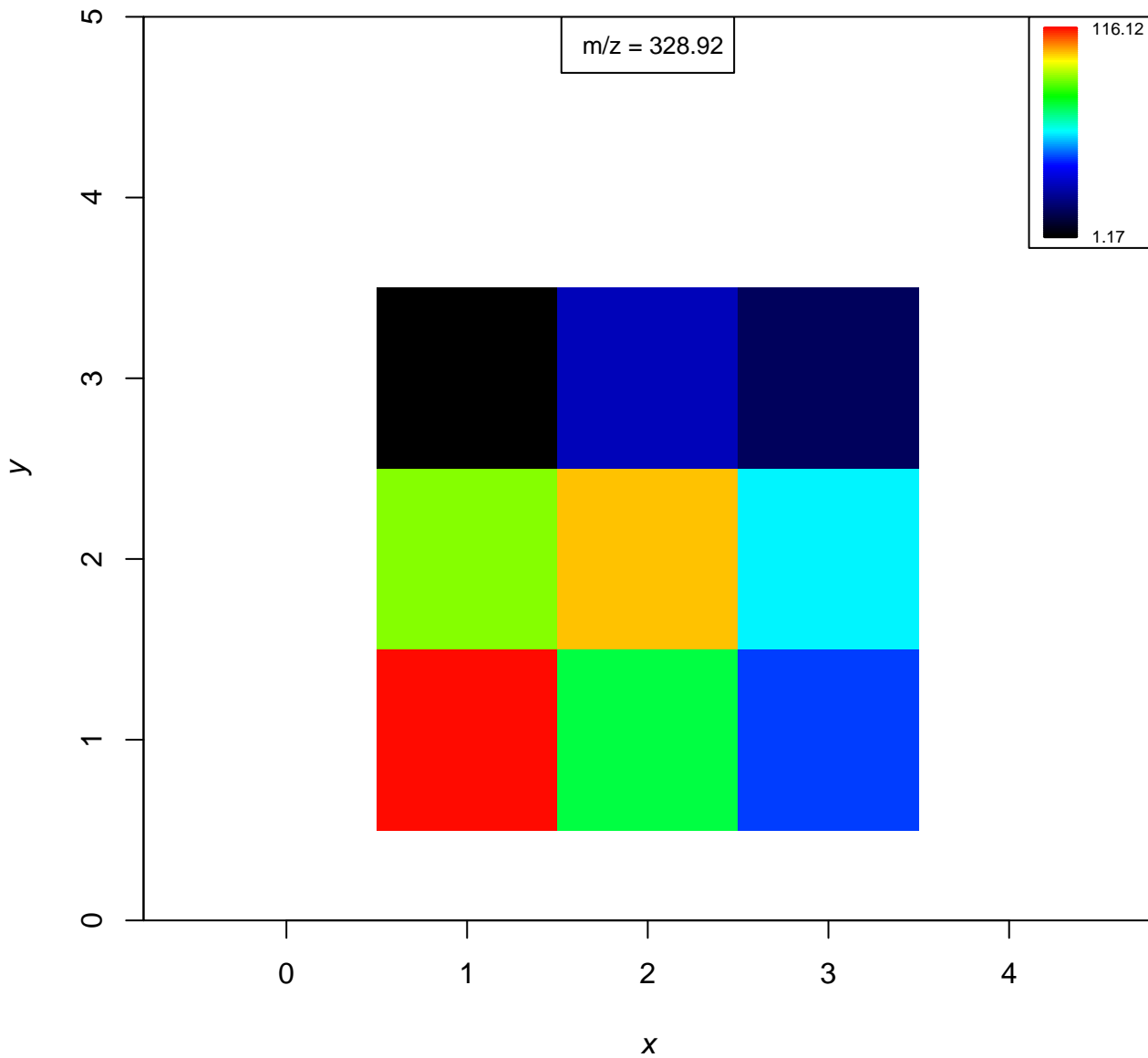
3C) 555.1 (555.1 Da)



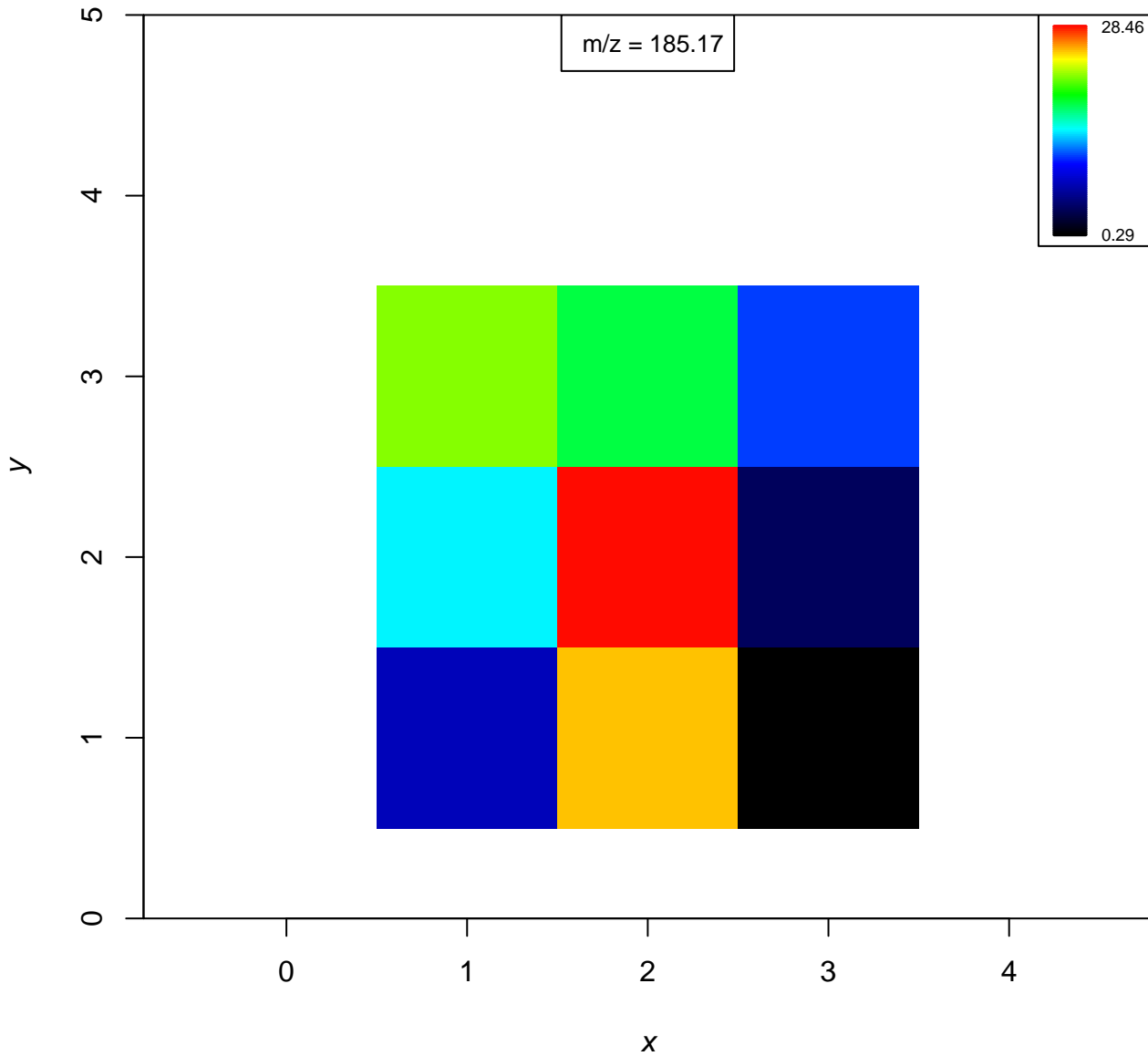
3D) mass1 (152 Da)



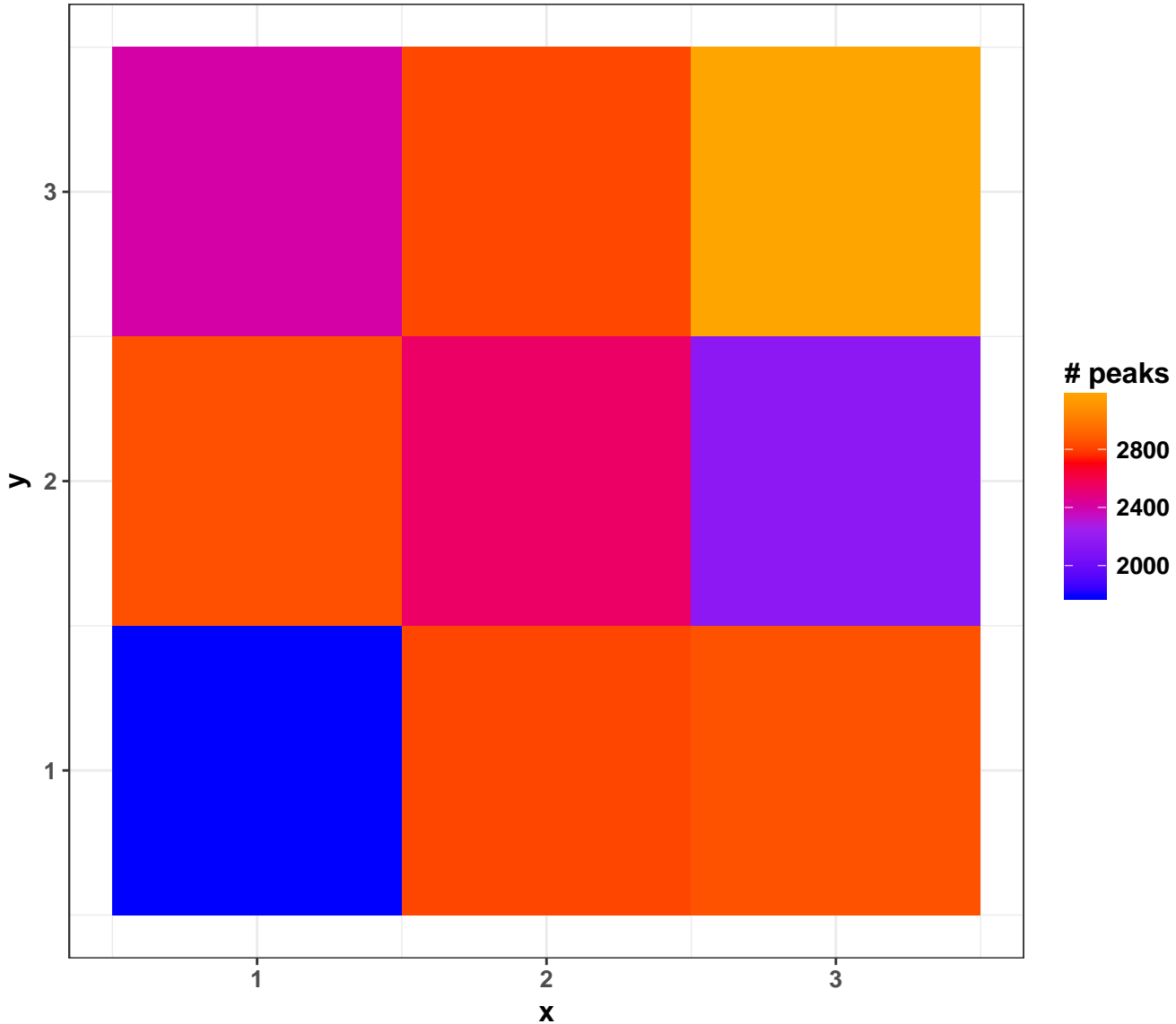
3E) mass2 (328.9 Da)



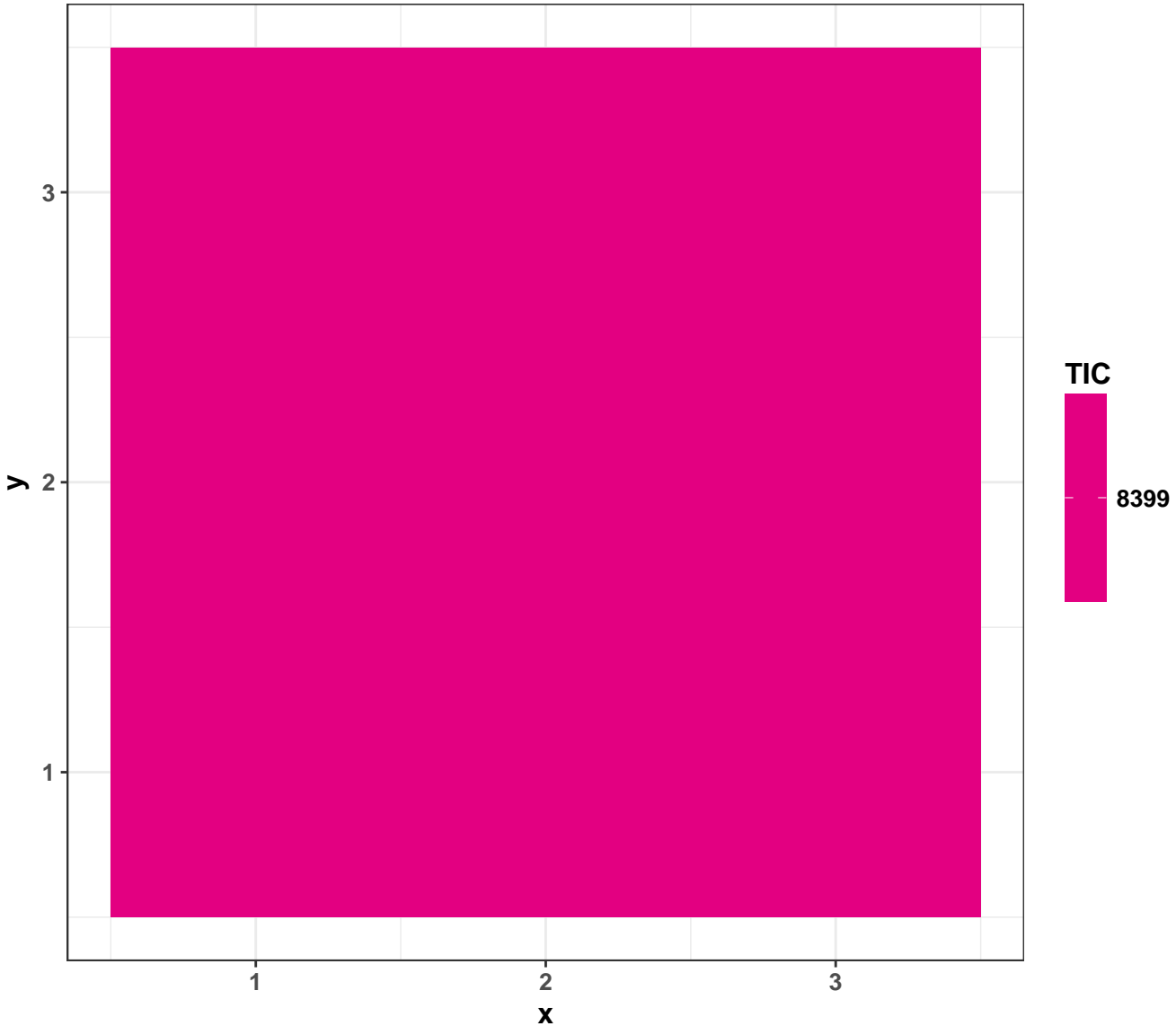
3F) mass3 (185.2 Da)



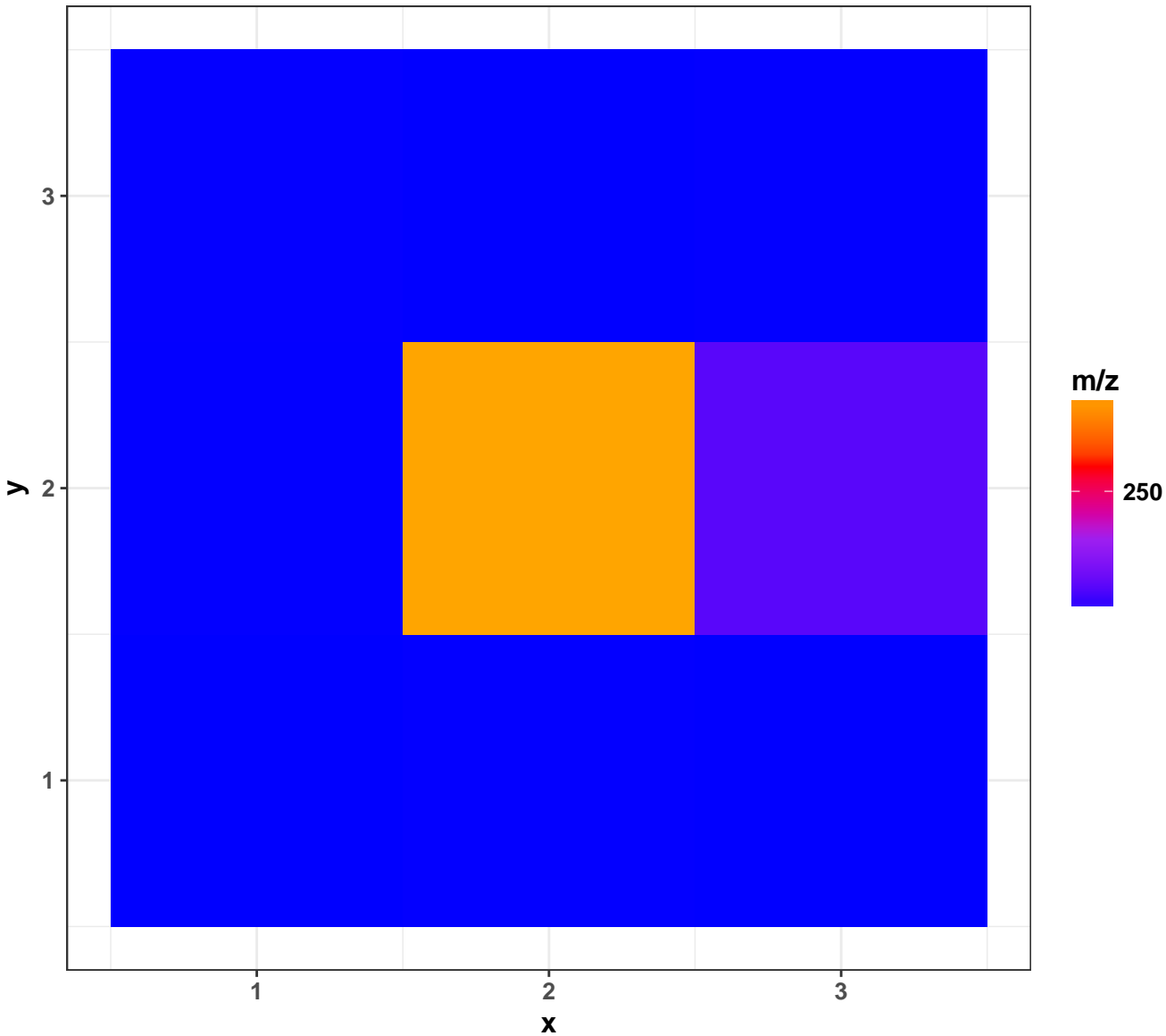
4) Number of peaks per pixel



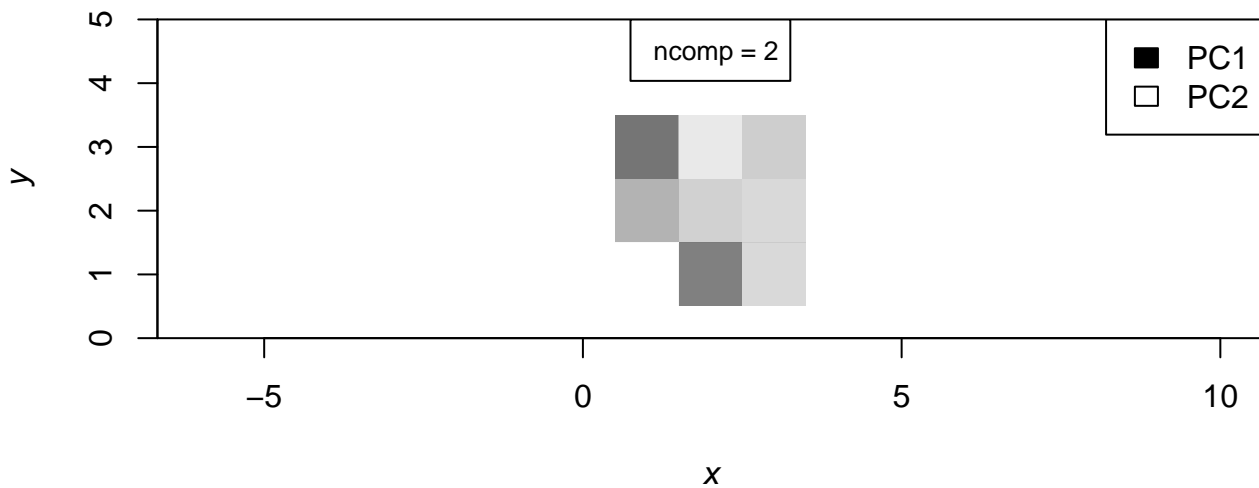
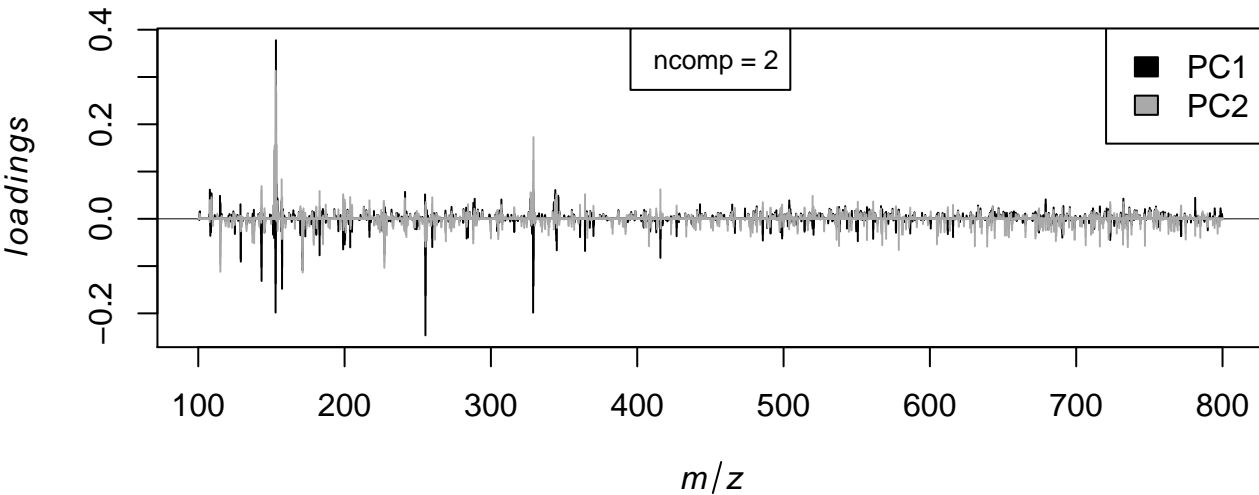
5) Total Ion Chromatogram



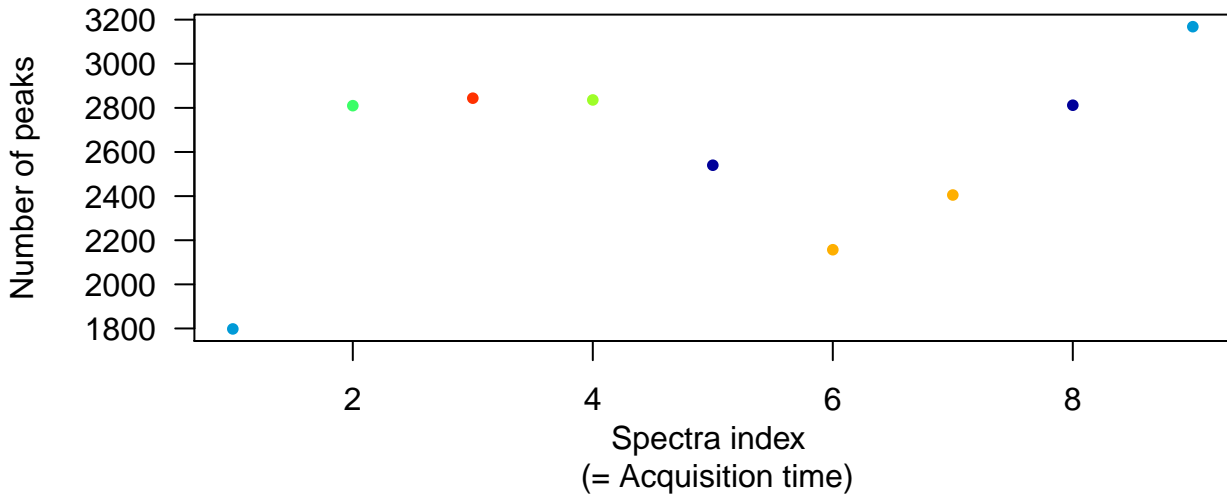
6) Most abundant m/z in each pixel



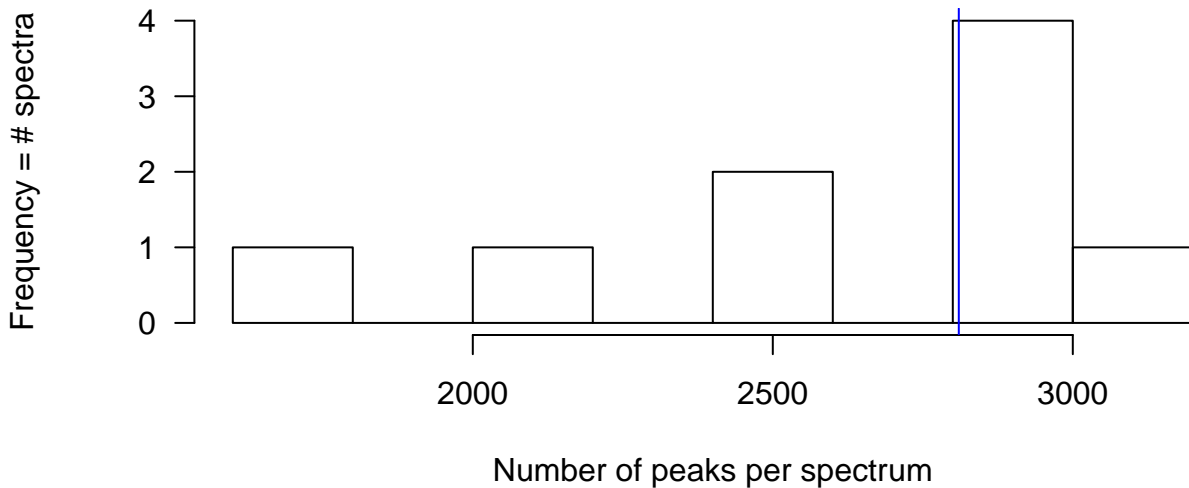
7) PCA for two components



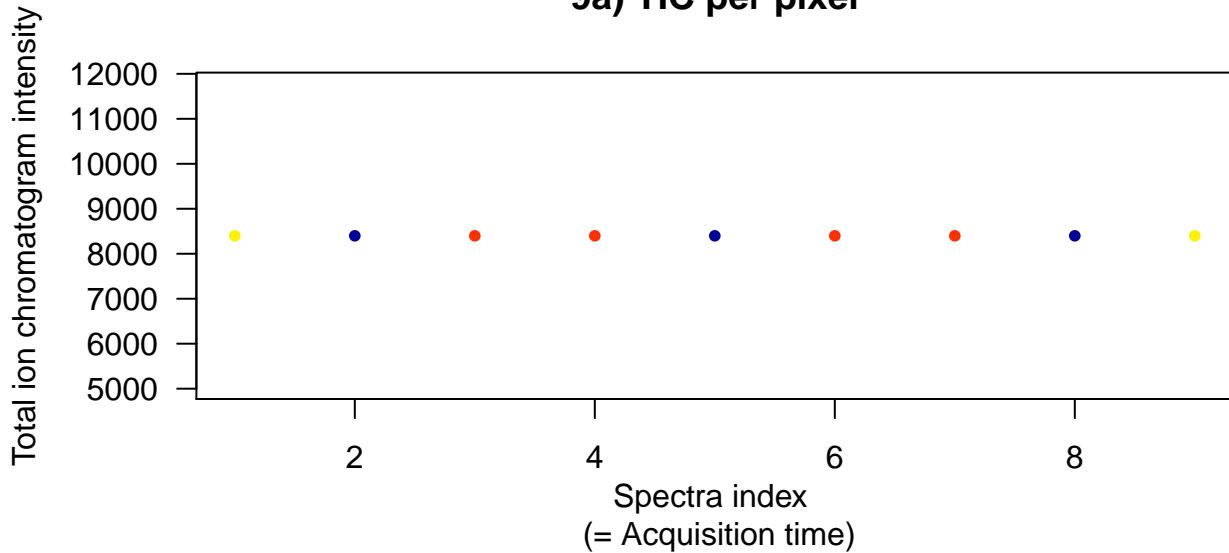
8a) Number of peaks per spectrum



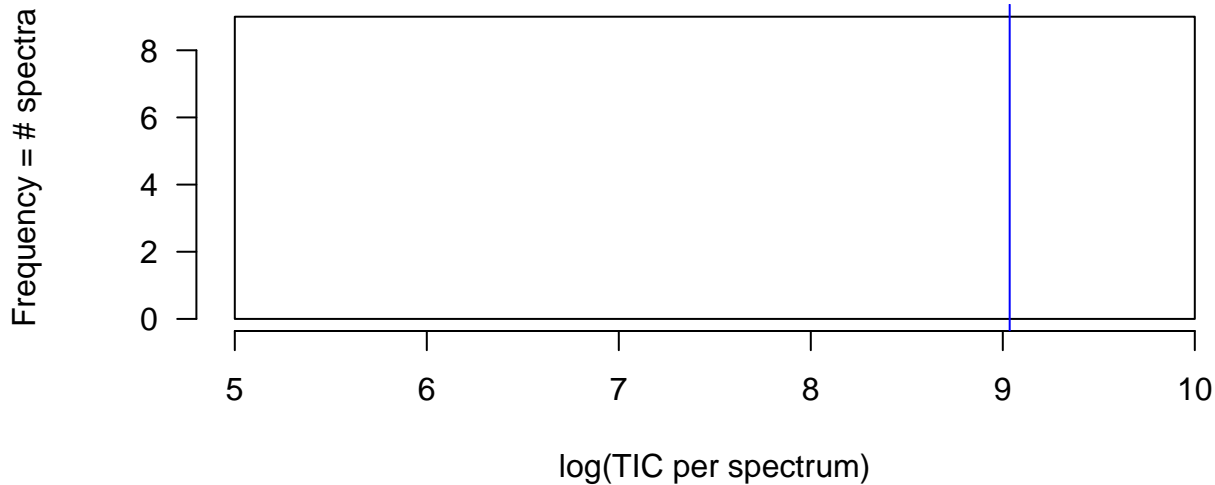
8b) Number of peaks per spectrum



9a) TIC per pixel

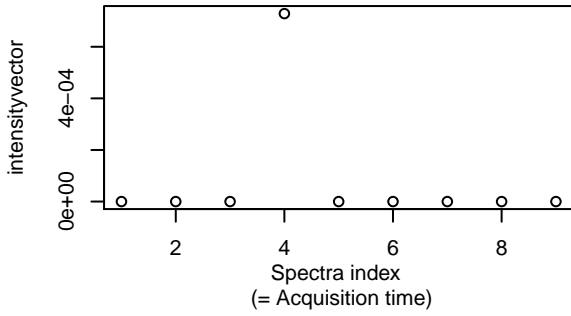


9b) TIC per spectrum

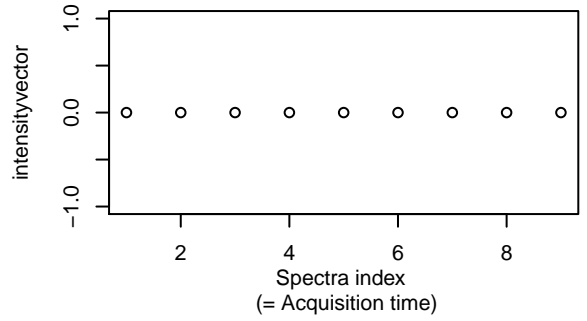


10) intensity of calibrants over acquisition

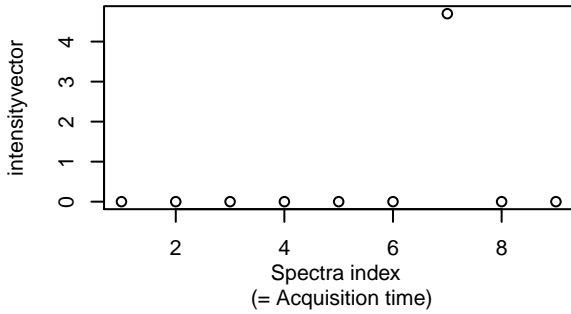
101.5



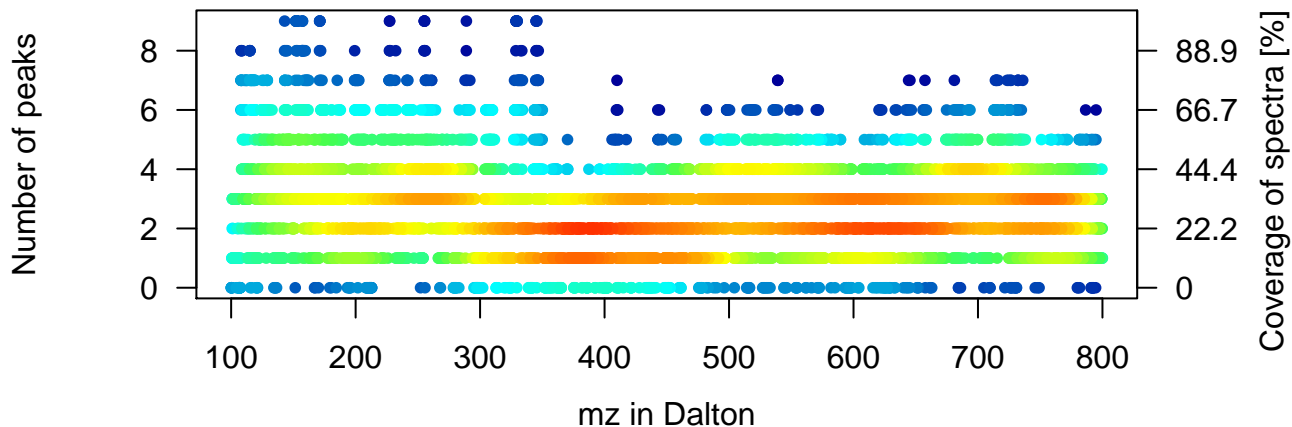
356.7



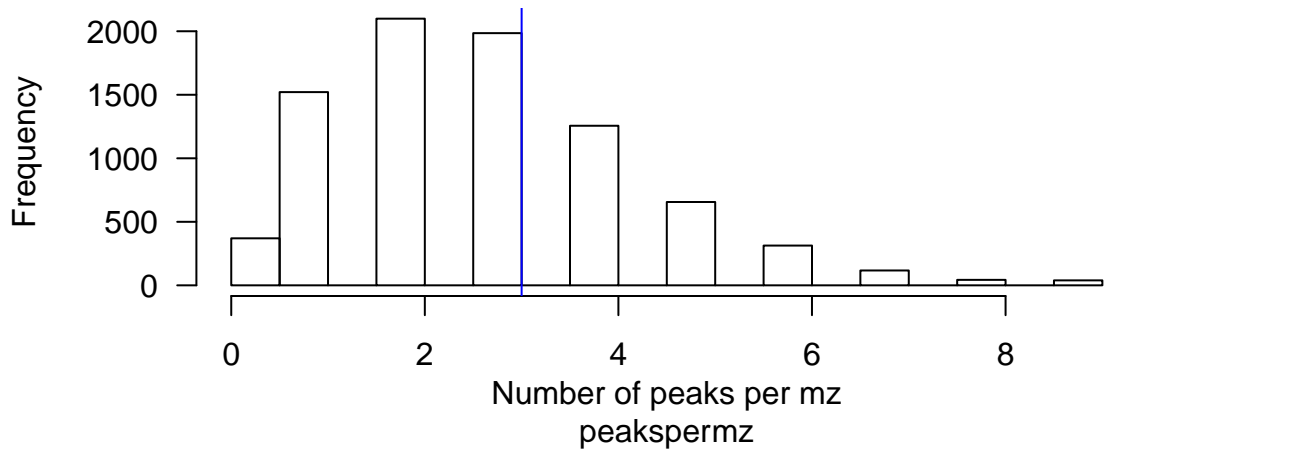
555.1



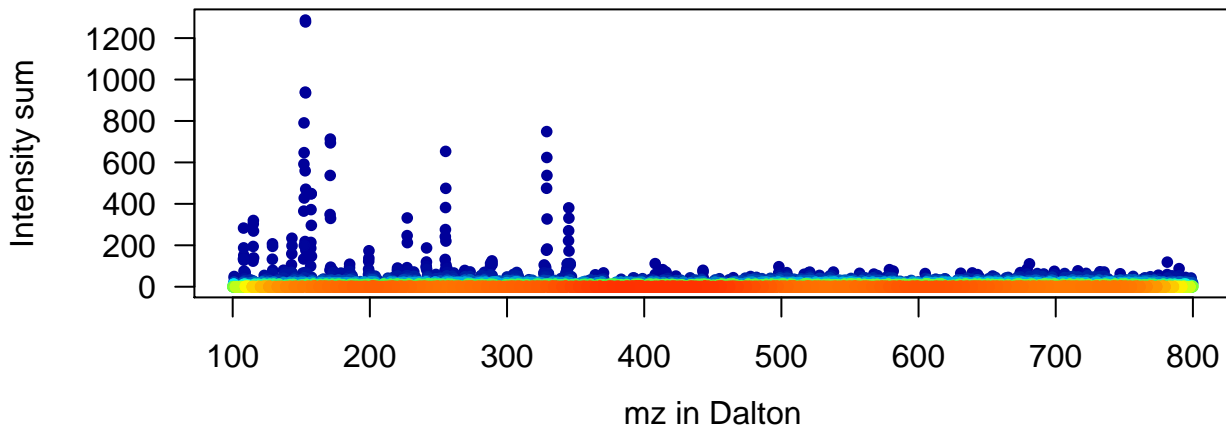
11a) Number of peaks for each mz



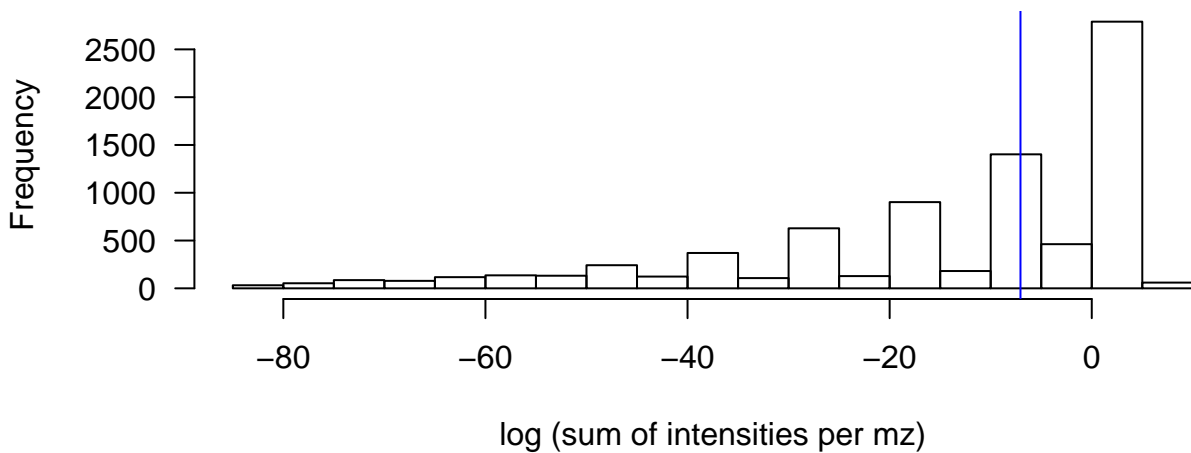
11b) Number of peaks per mz



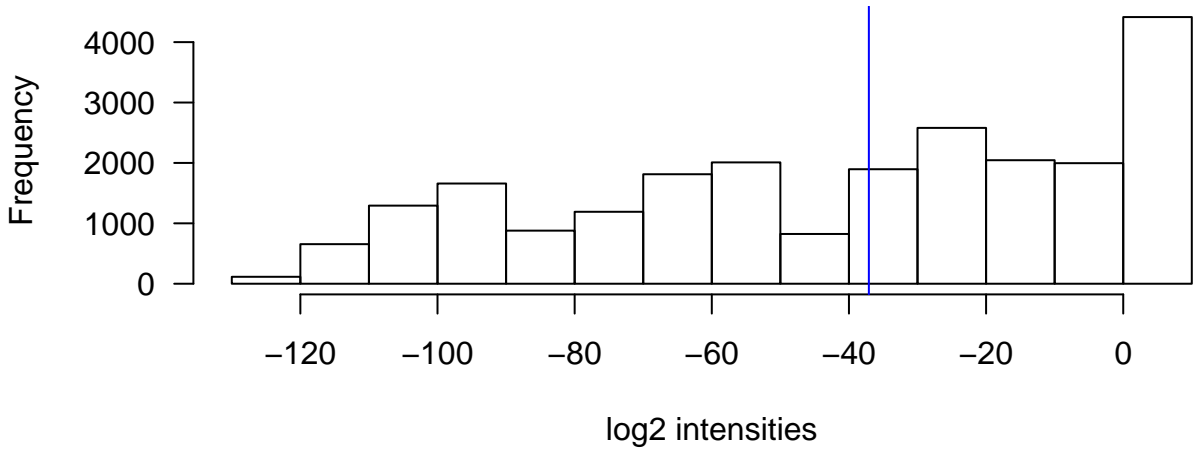
12a) Sum of all peak intensities for each mz



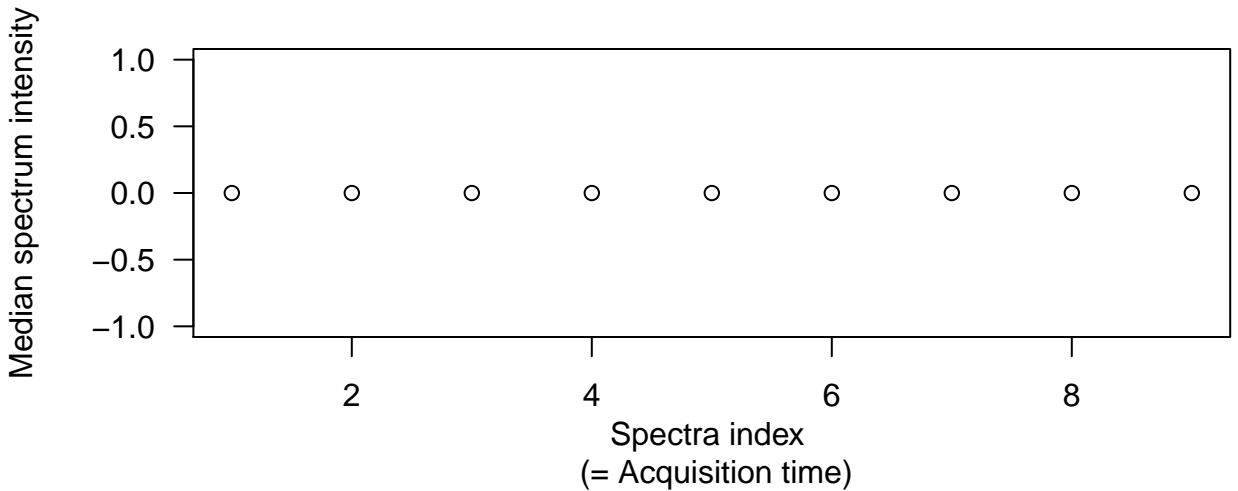
12b) Sum of intensities per mz



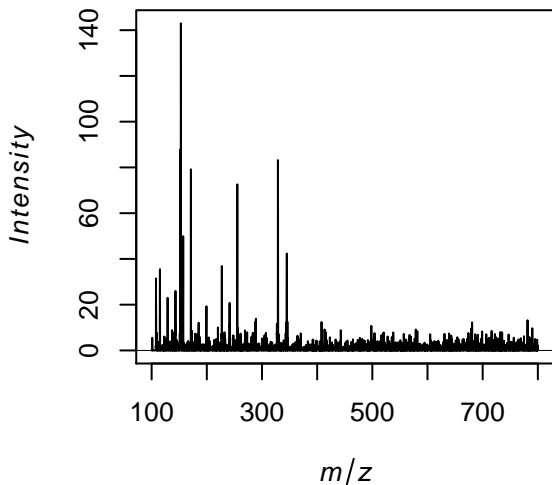
13a) Log2-transformed intensities



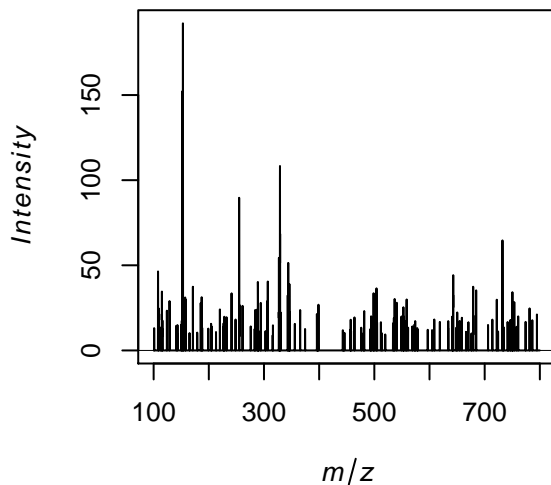
13b) Median intensity per spectrum



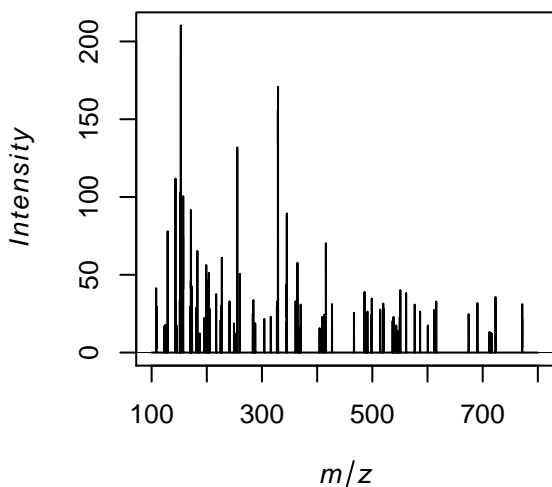
Average spectrum



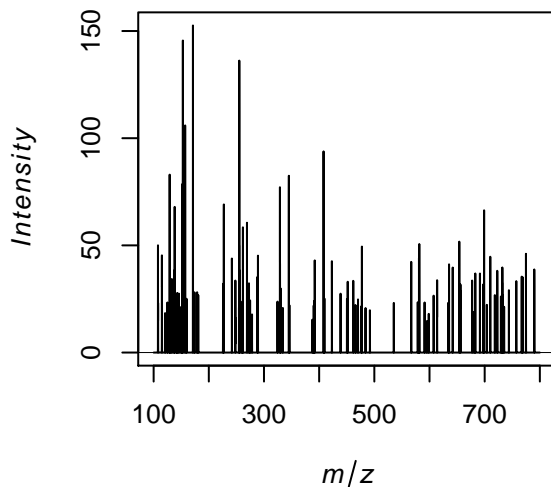
Spectrum in middle of acquisition



Spectrum at $x = 1, y = 1$

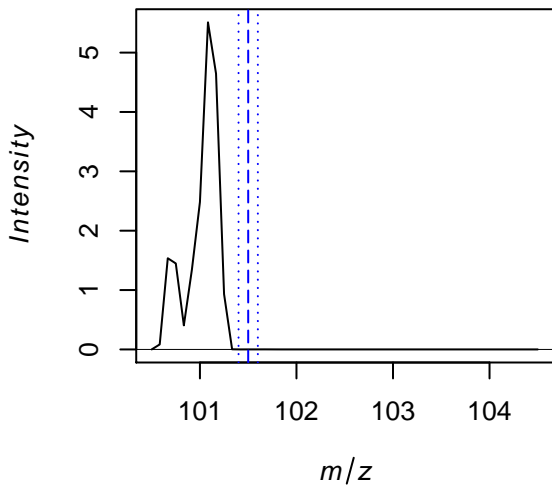


Spectrum at $x = 3, y = 2$

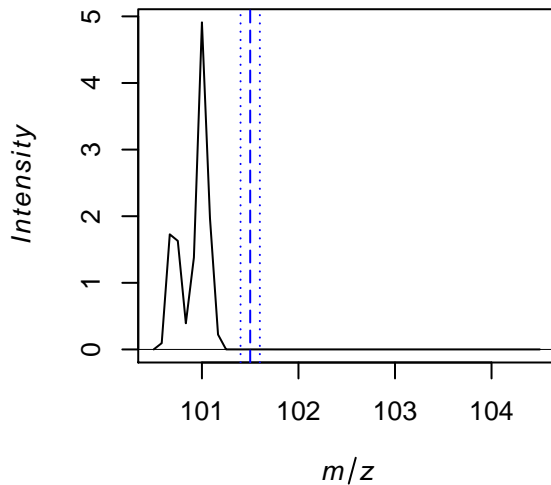


101.5

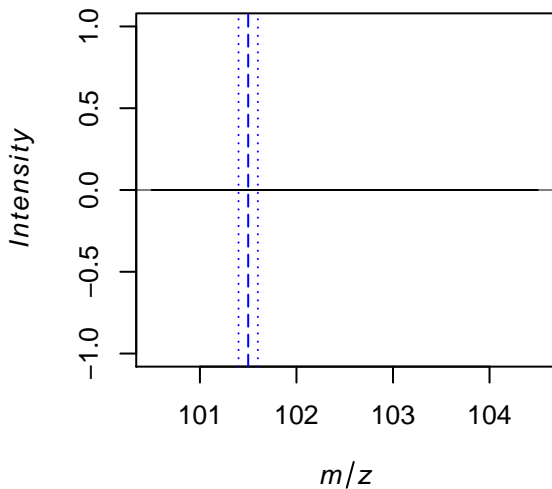
average spectrum



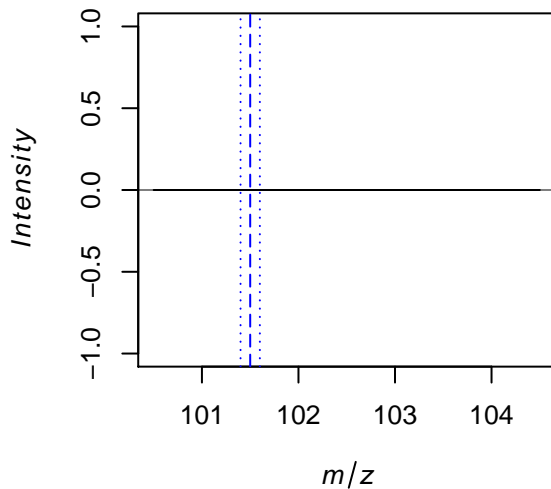
pixel in middle of acquisition



Spectrum at $x = 1, y = 1$

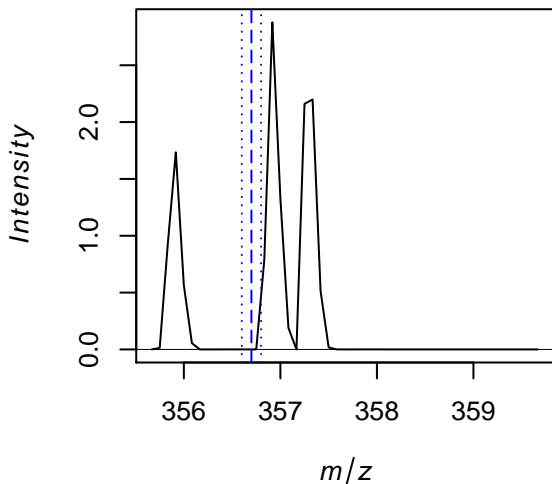


Spectrum at $x = 3, y = 2$

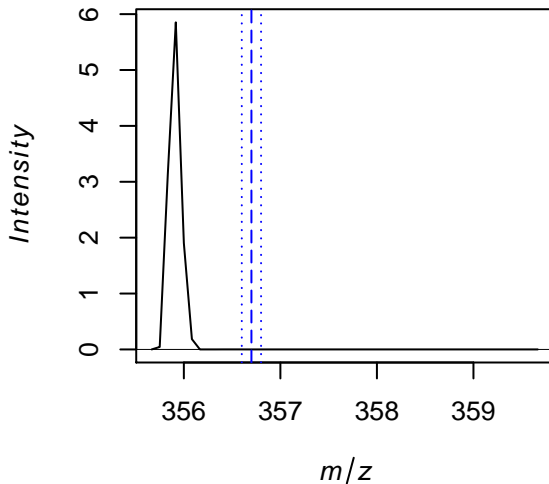


356.7

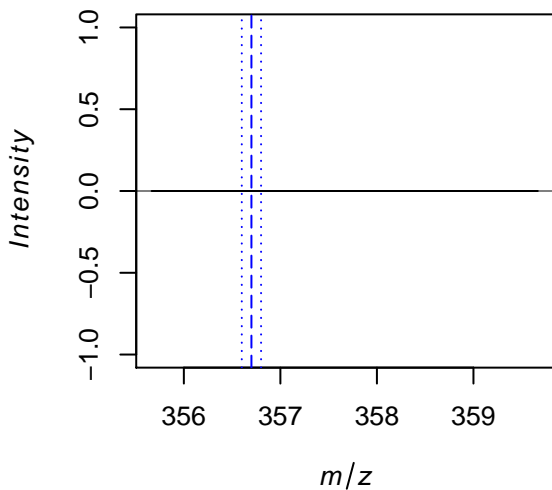
average spectrum



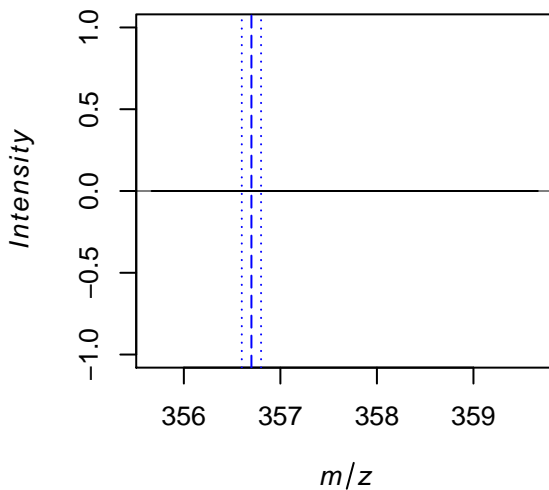
pixel in middle of acquisition



Spectrum at $x = 1, y = 1$

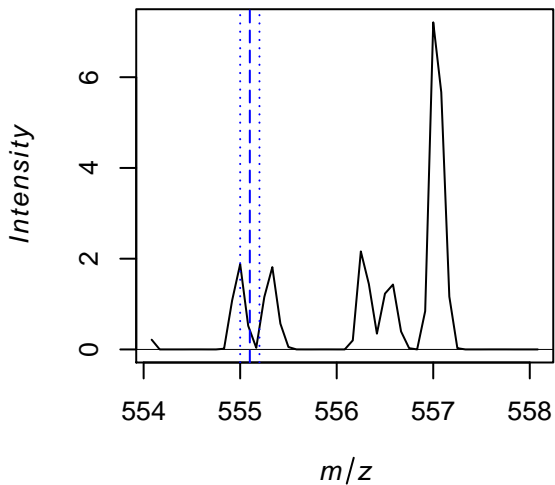


Spectrum at $x = 3, y = 2$

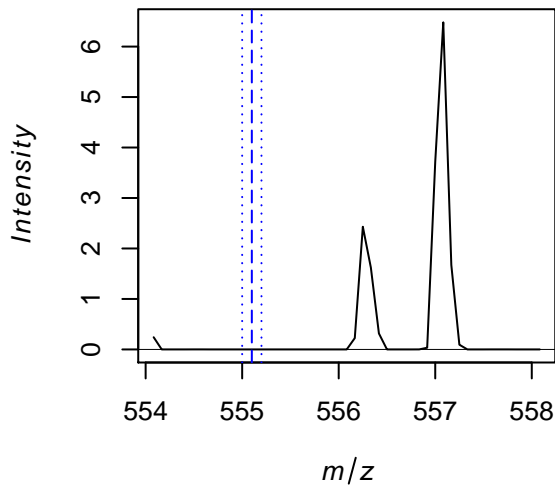


555.1

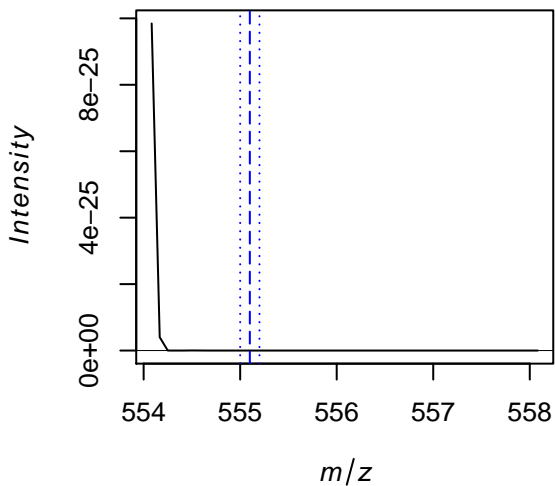
average spectrum



pixel in middle of acquisition



Spectrum at x = 1, y = 1



Spectrum at x = 3, y = 2

