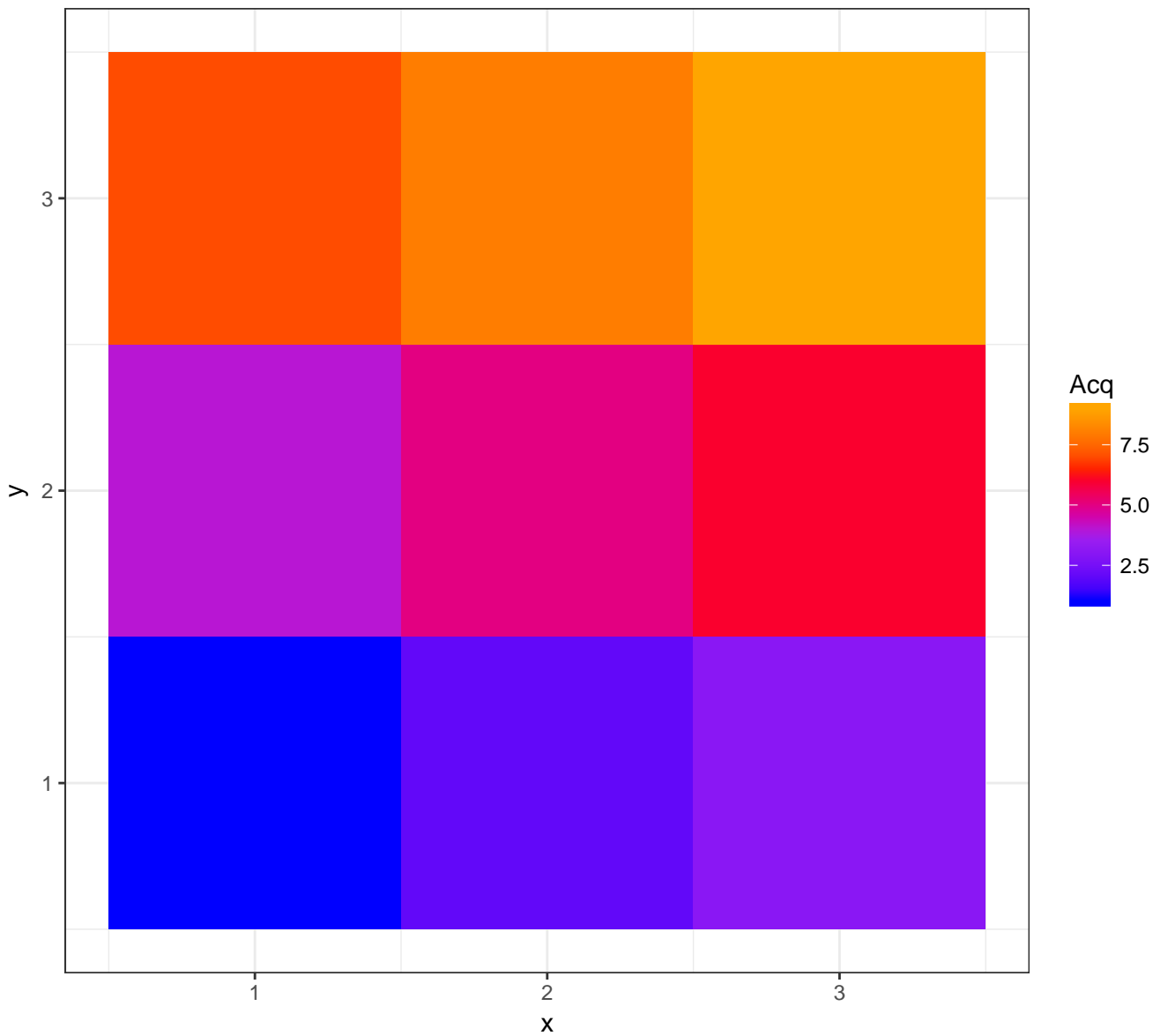


Quality control of MSI data

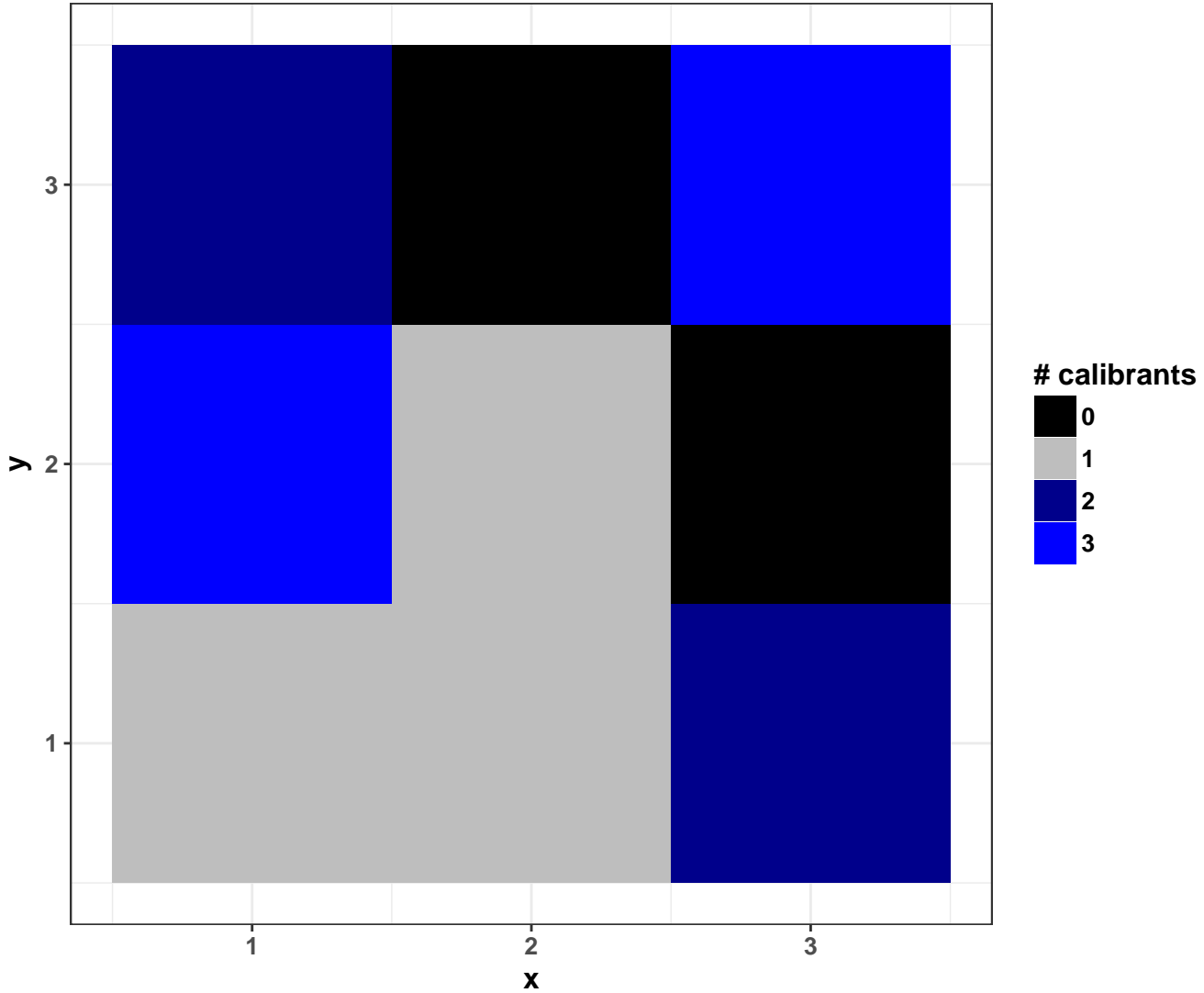
Filename: Testfile_imzml

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
# valid masses in Testfile_imzml	6/6

1) Order of Acquisition

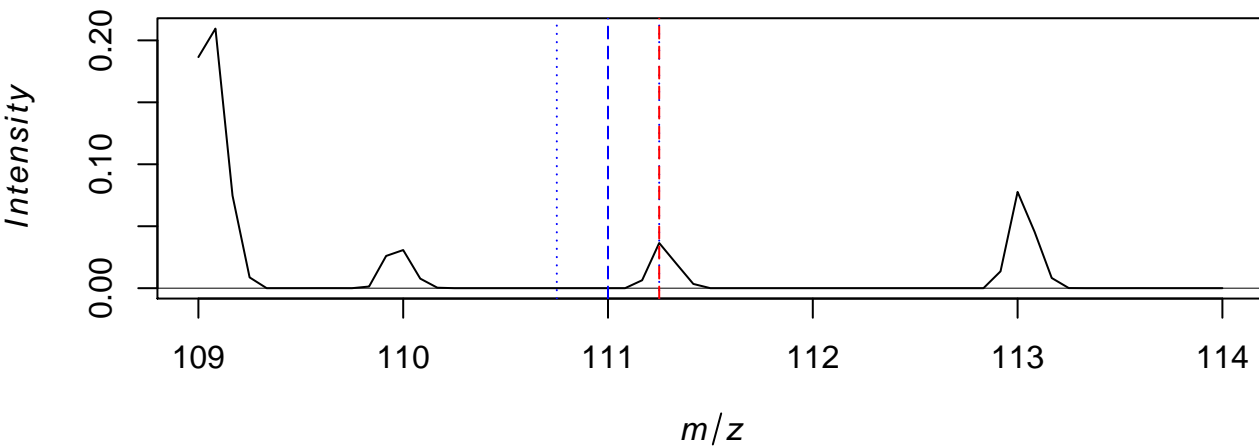


2) Number of calibrants per pixel

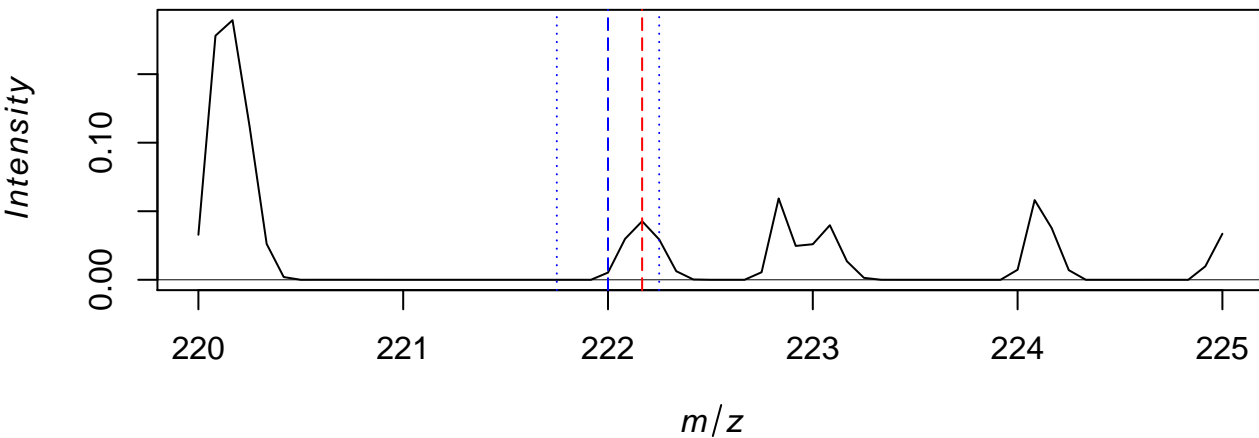


Control of fold change plot

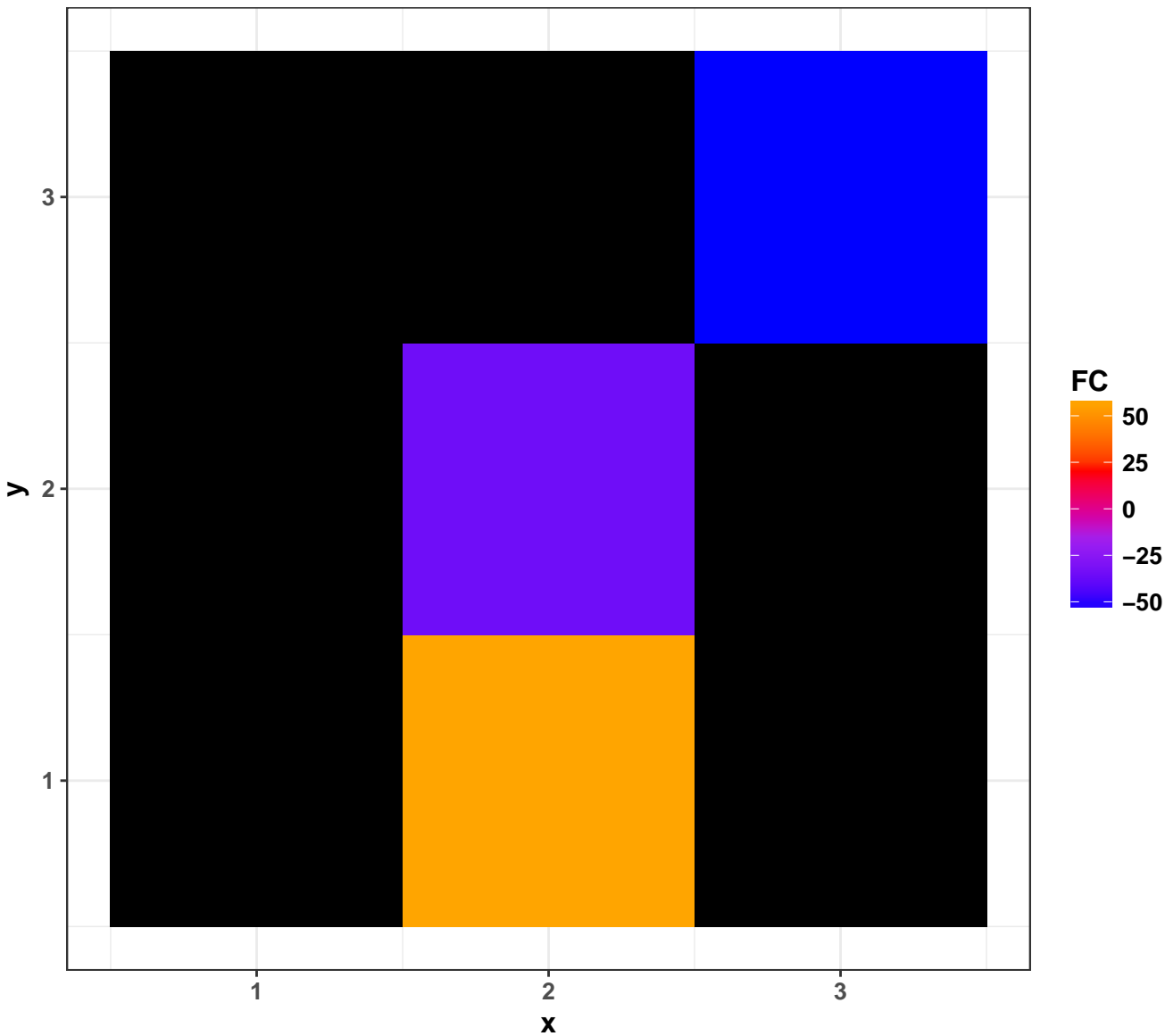
average spectrum 111 Da



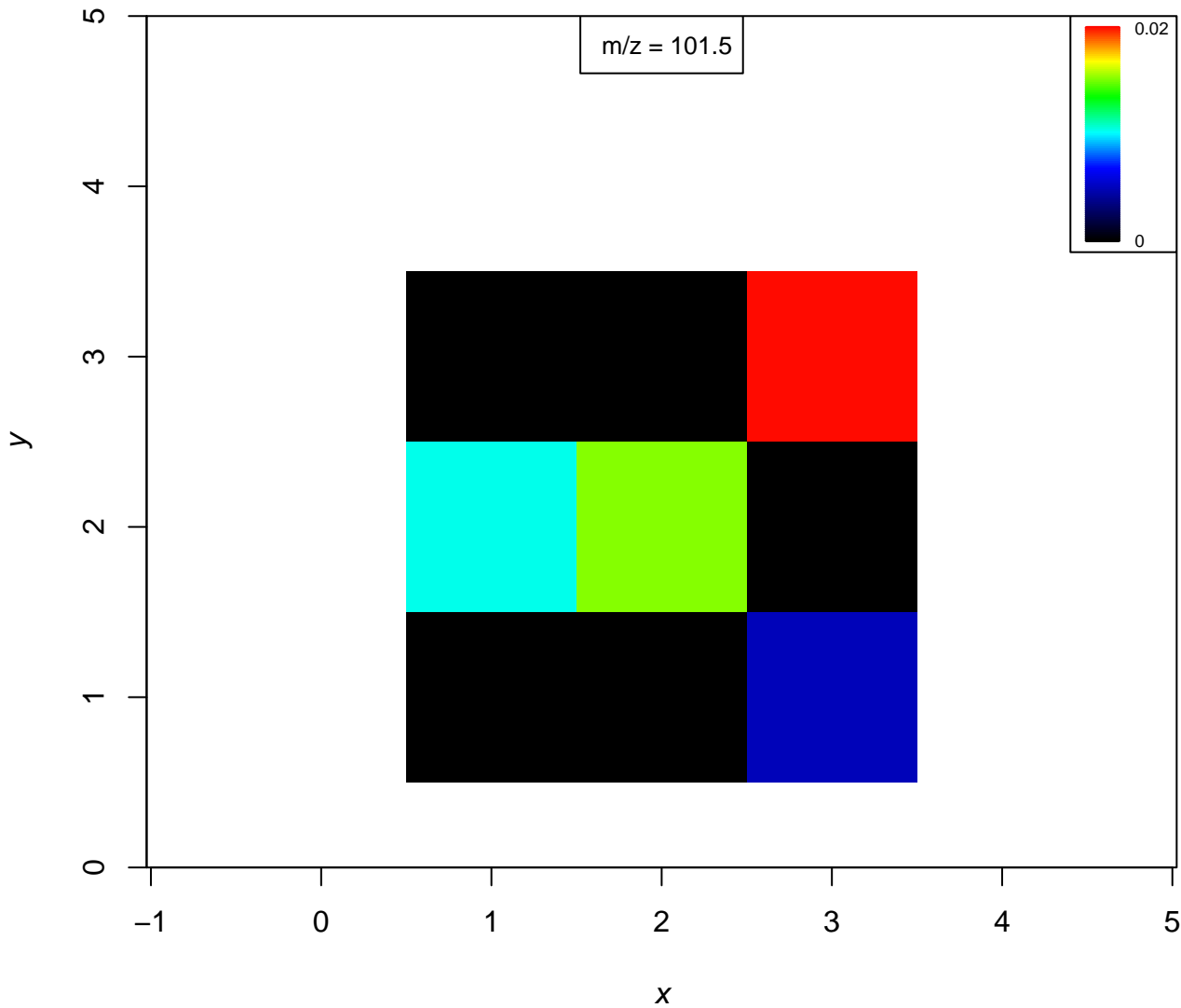
average spectrum 222 Da



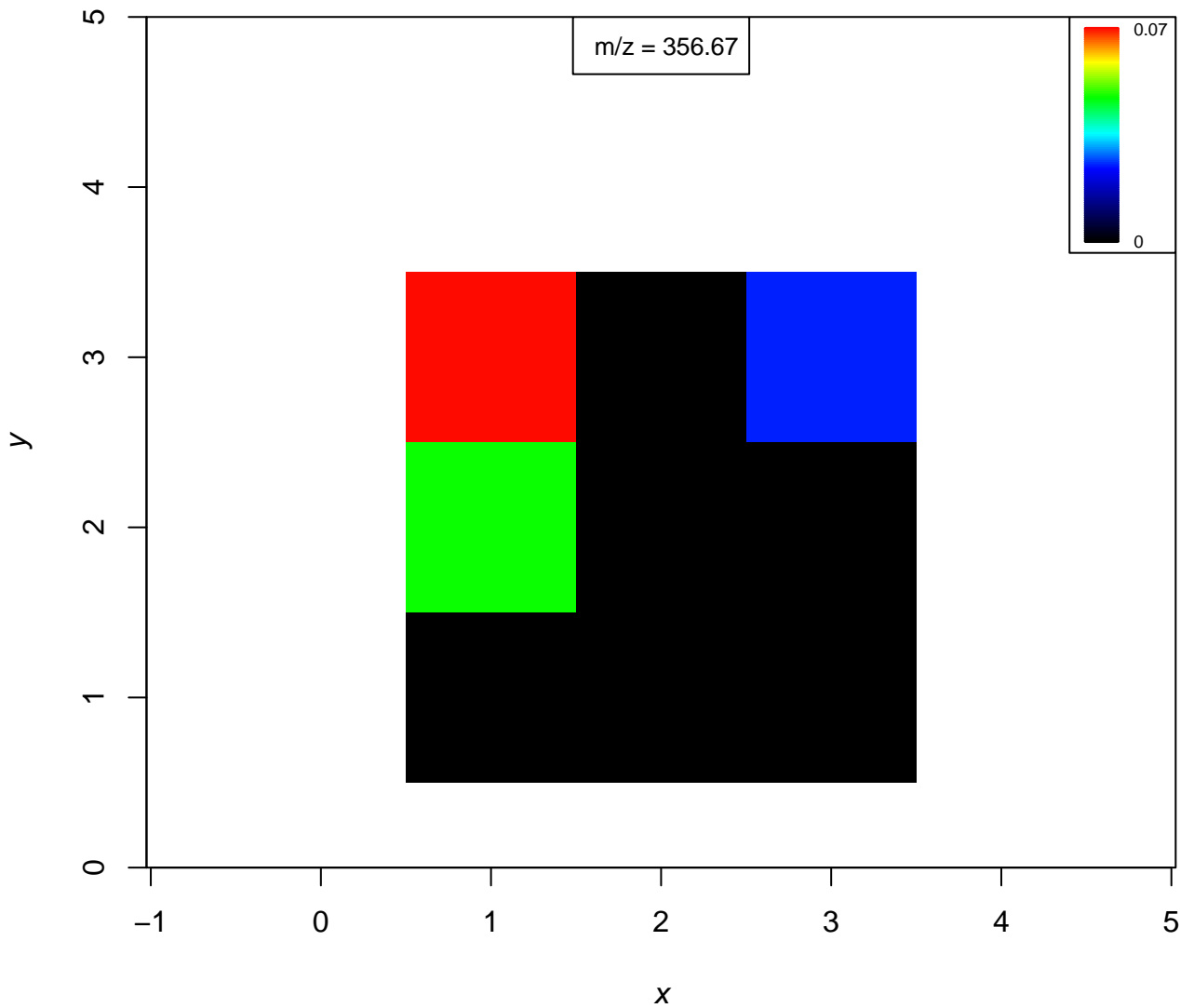
Fold change 111.0 Da / 222.0 Da



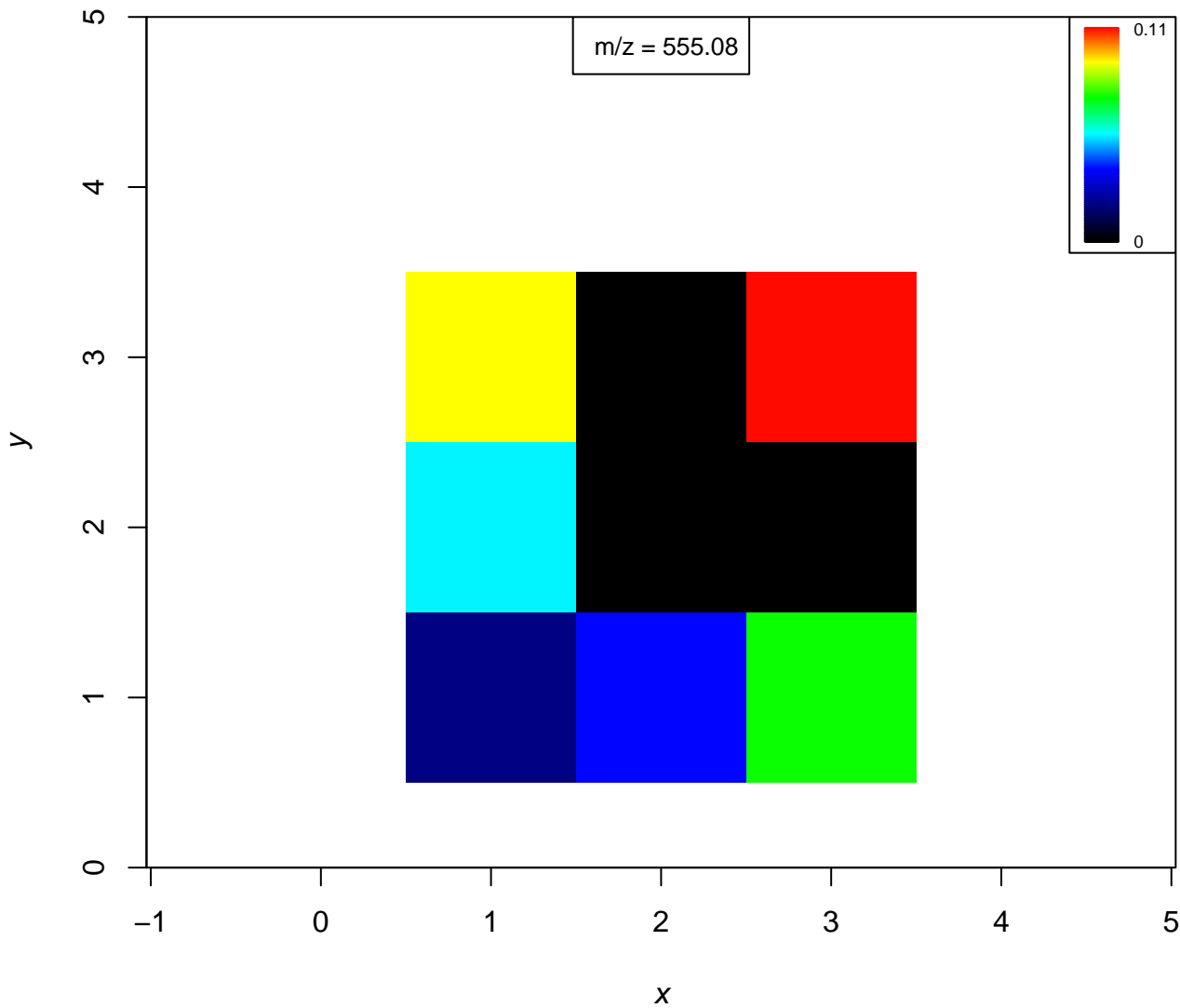
3A) 101.5 (101.5 ± 0.25 Da)



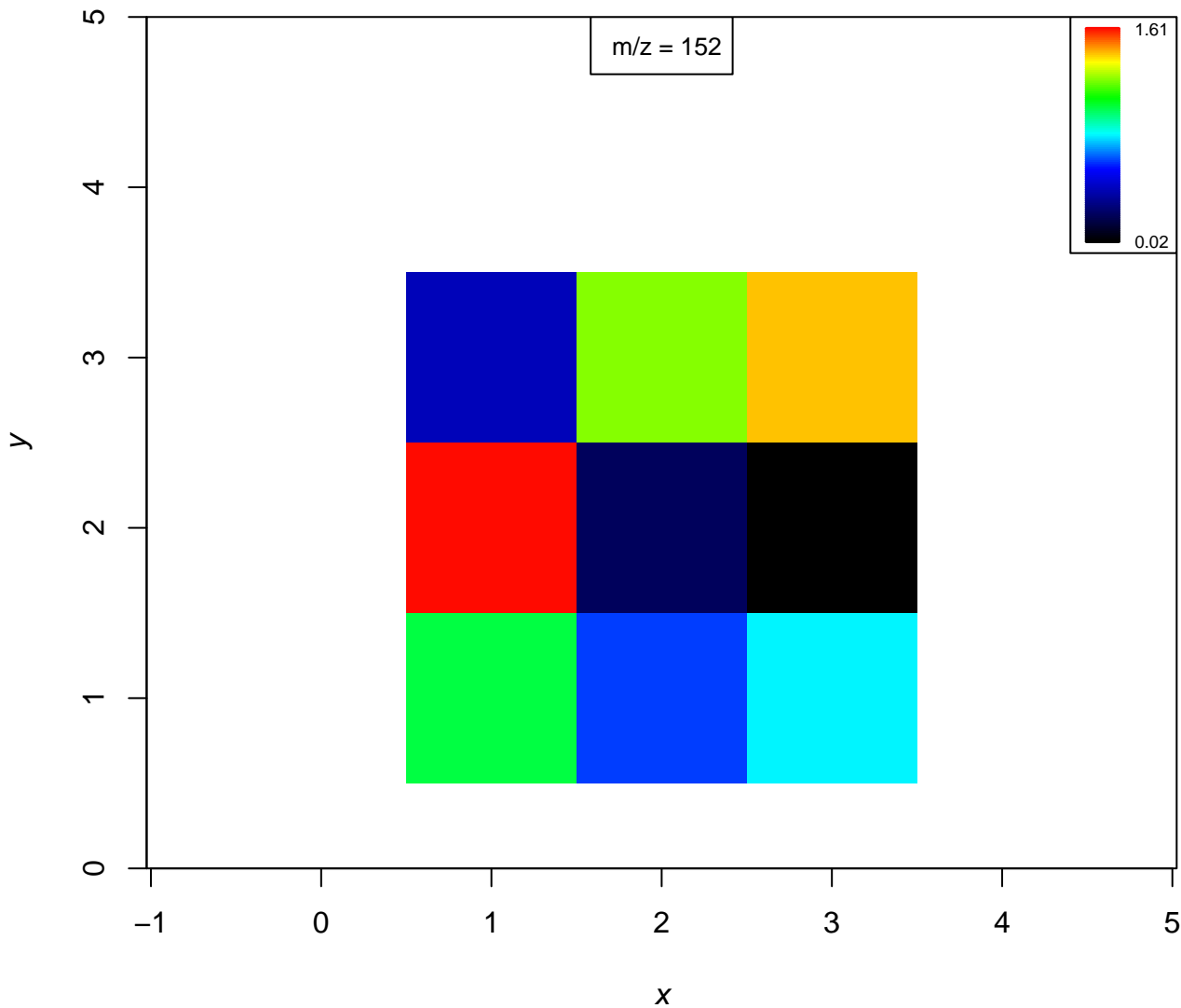
3B) 356.7 (356.7 ± 0.25 Da)



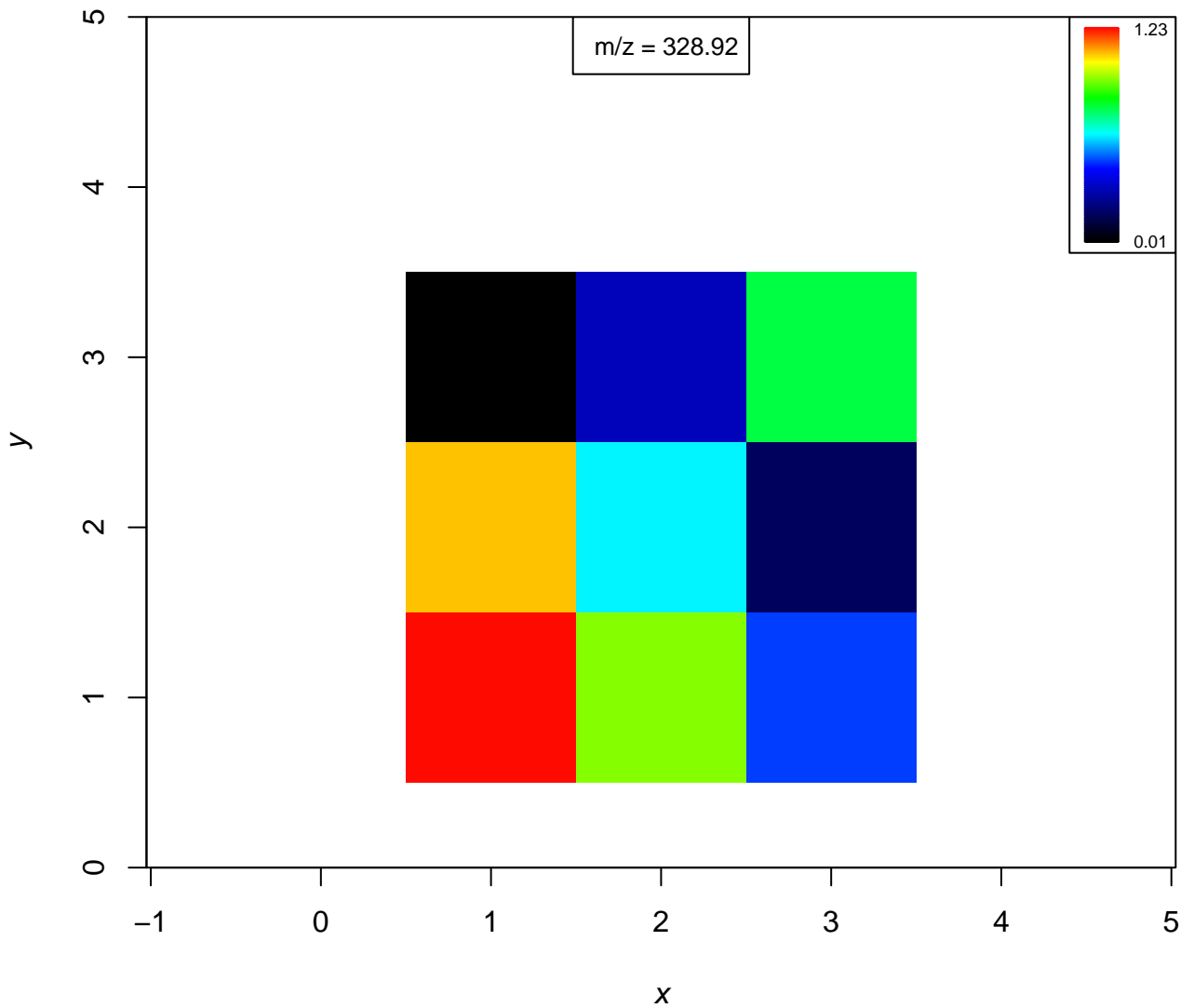
3C) 555.1 (555.1 ± 0.25 Da)



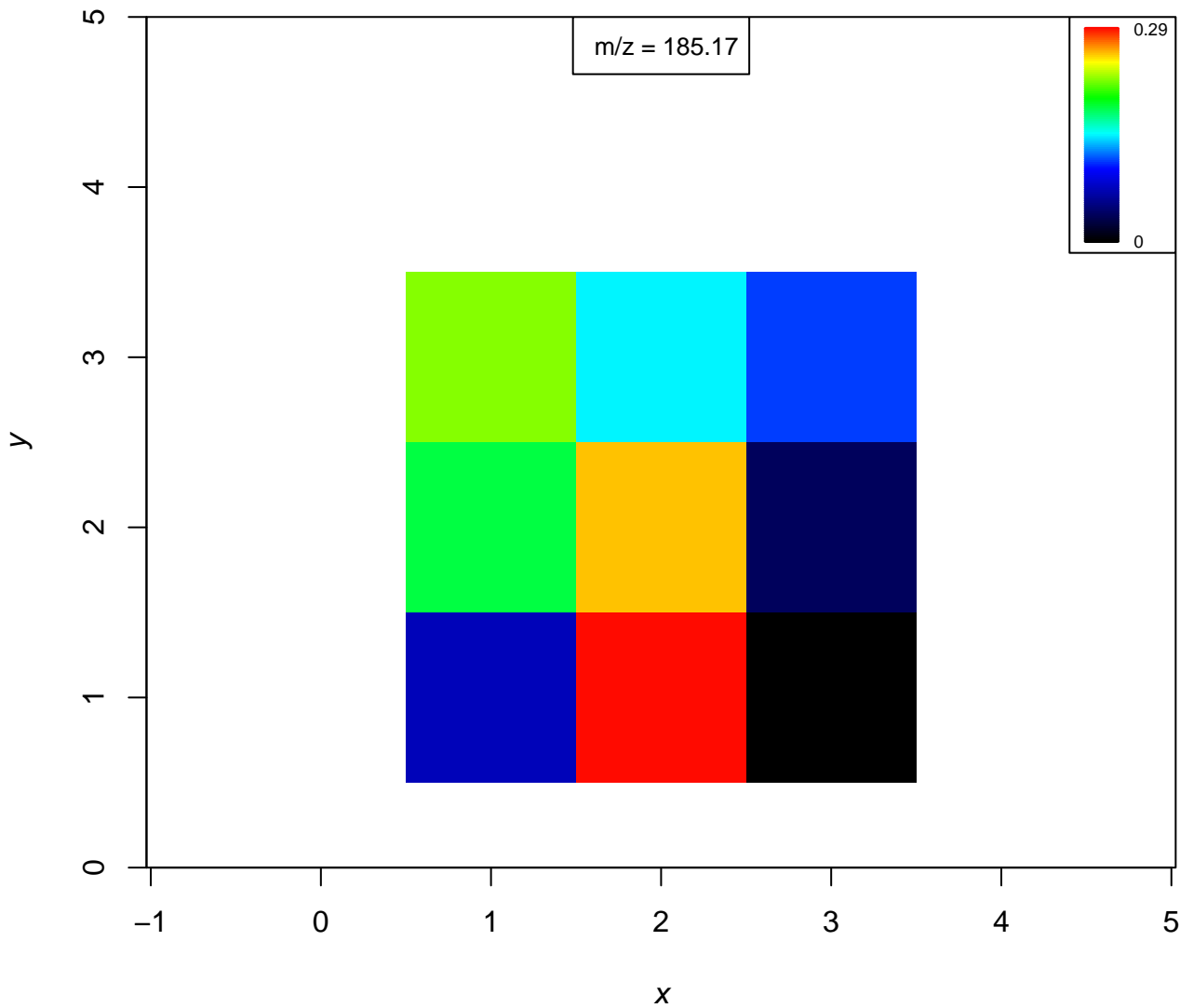
3D) mass1 (152 ± 0.25 Da)



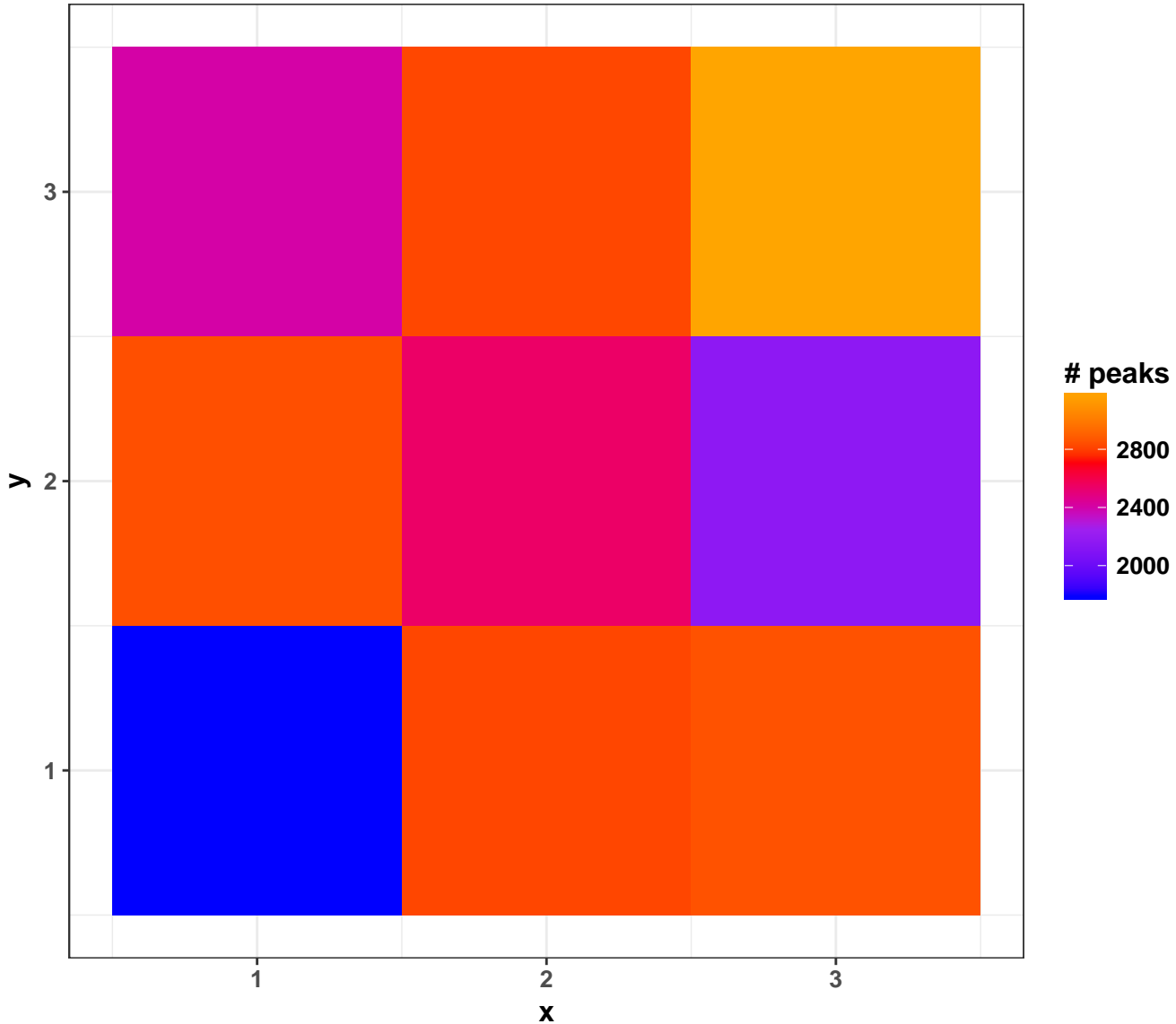
3E) mass2 (328.9 ± 0.25 Da)



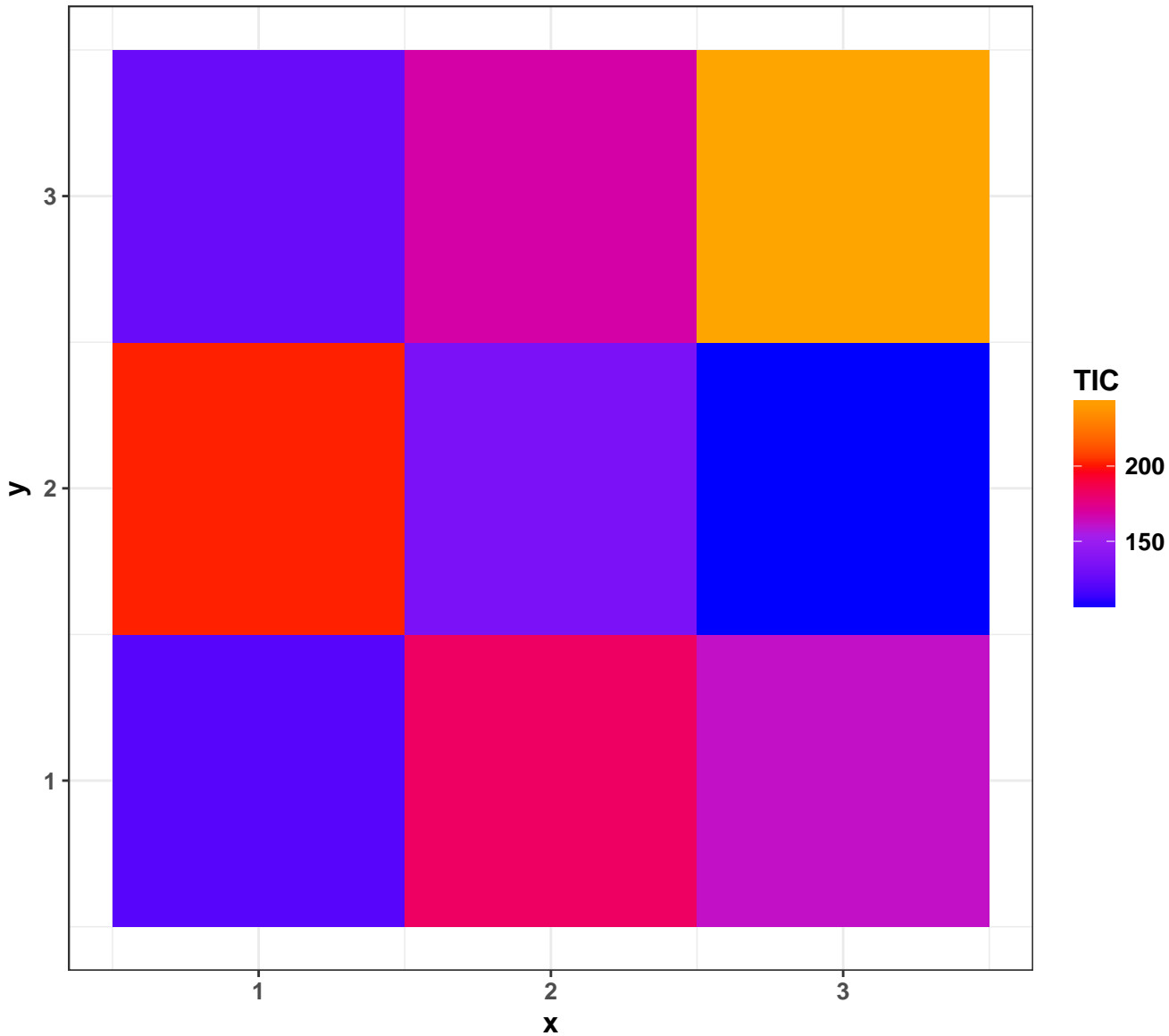
3F) mass3 (185.2 ± 0.25 Da)



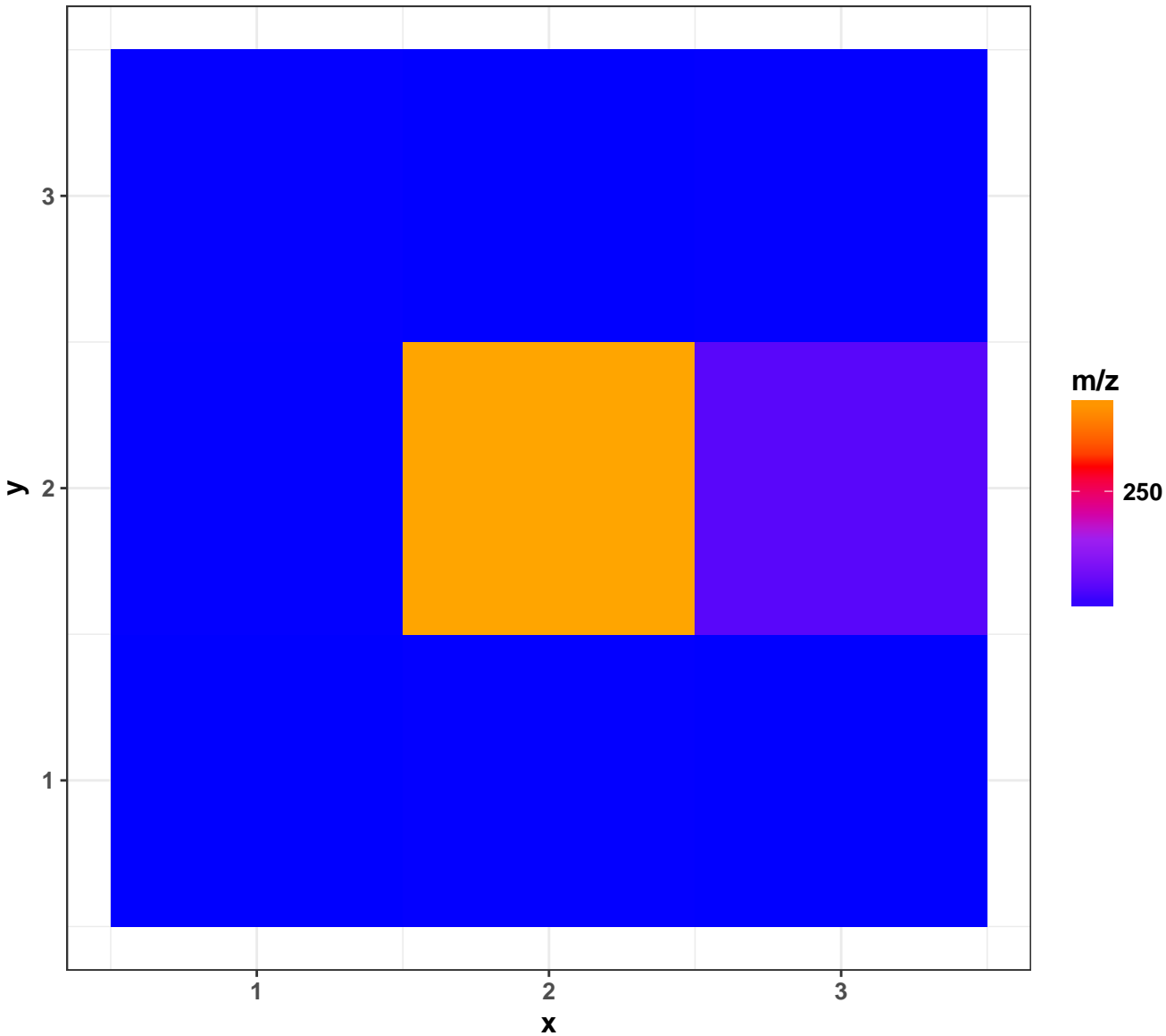
4) Number of peaks per pixel



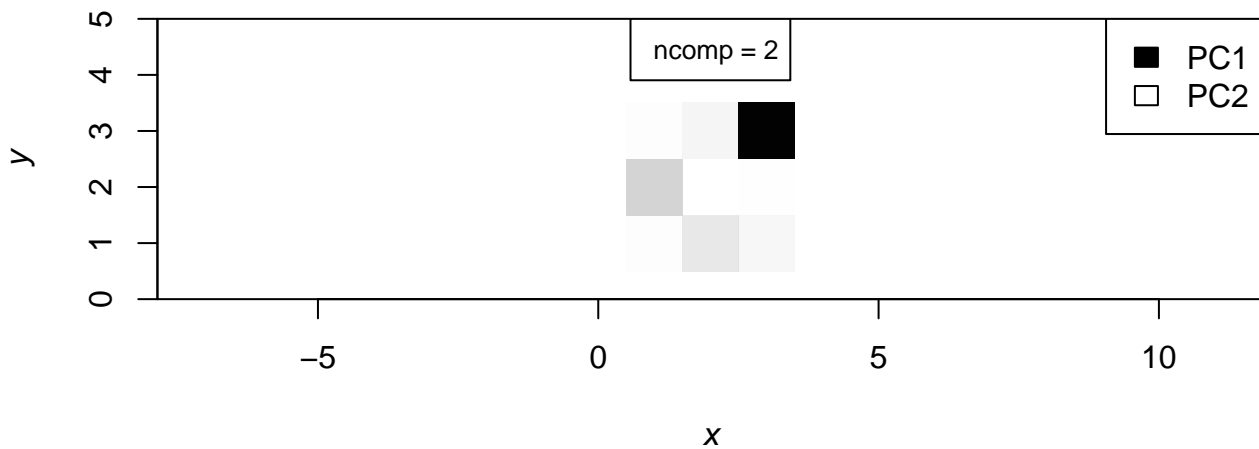
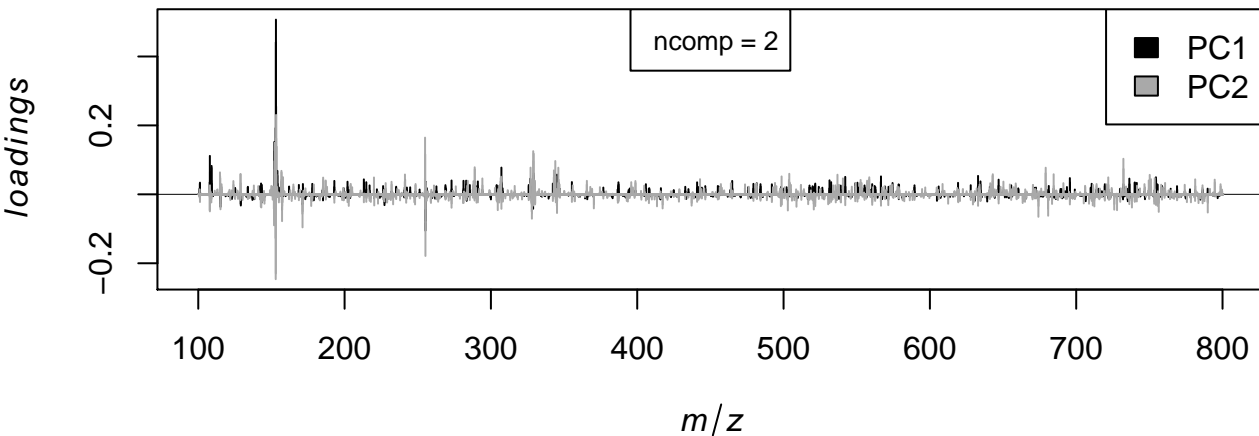
5) Total Ion Chromatogram



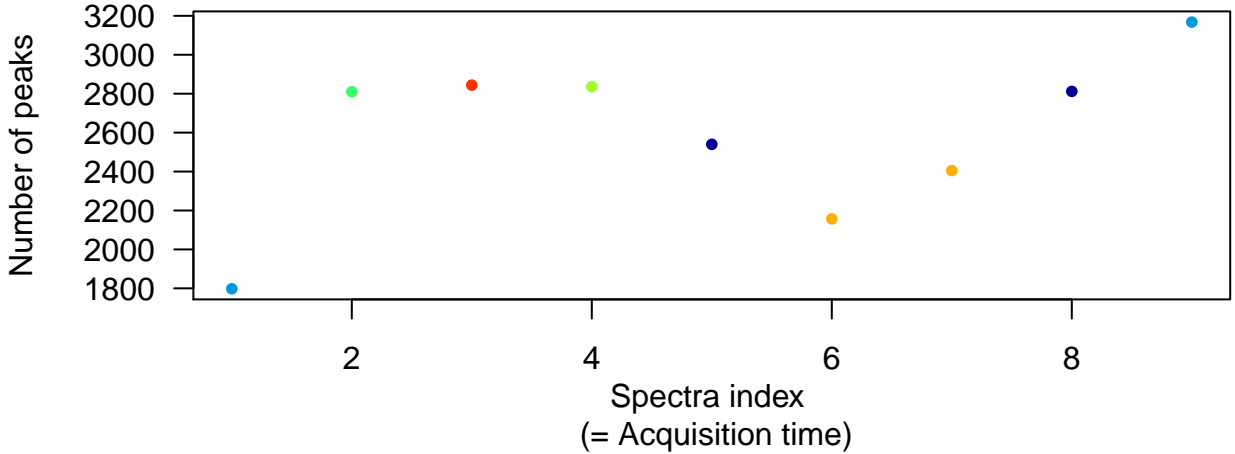
6) Most abundant m/z in each pixel



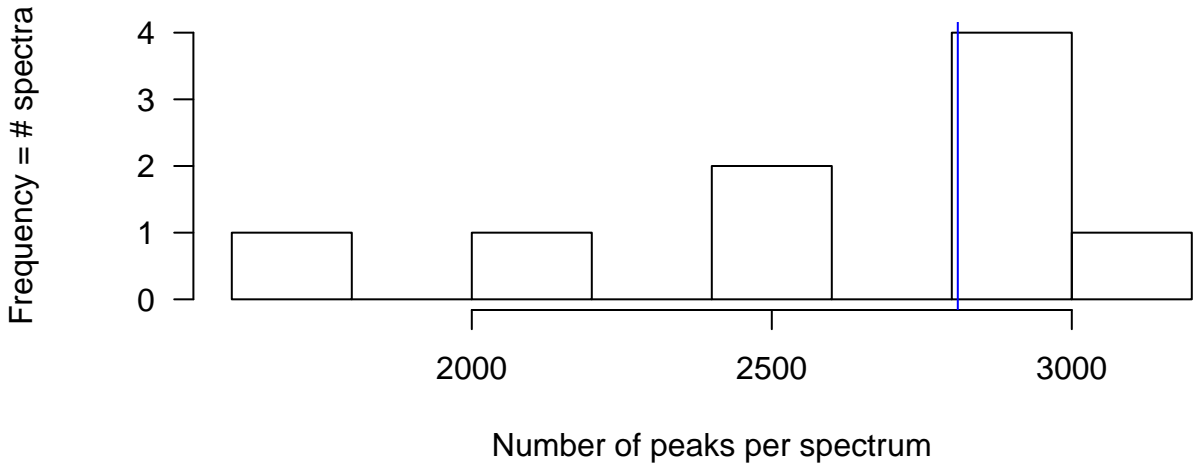
7) PCA for two components



8a) Number of peaks per spectrum

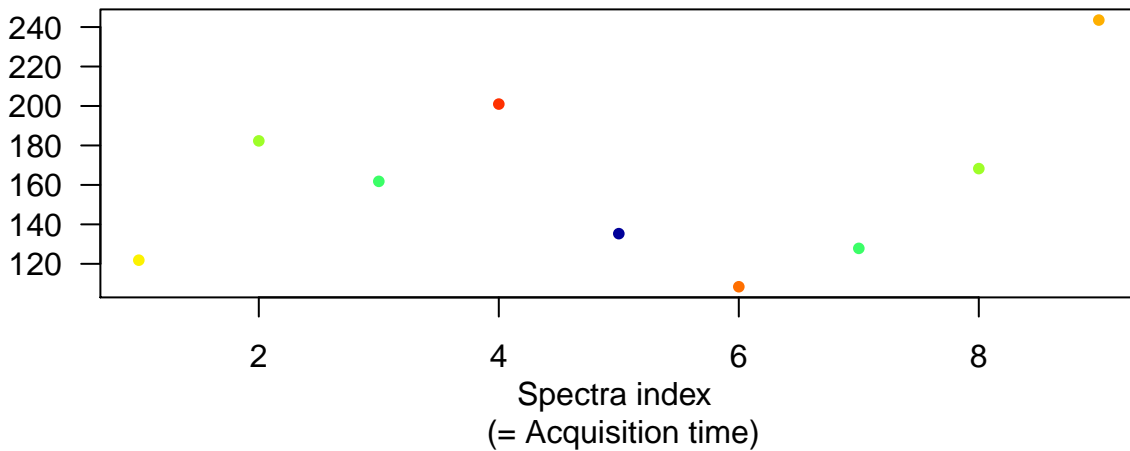


8b) Number of peaks per spectrum



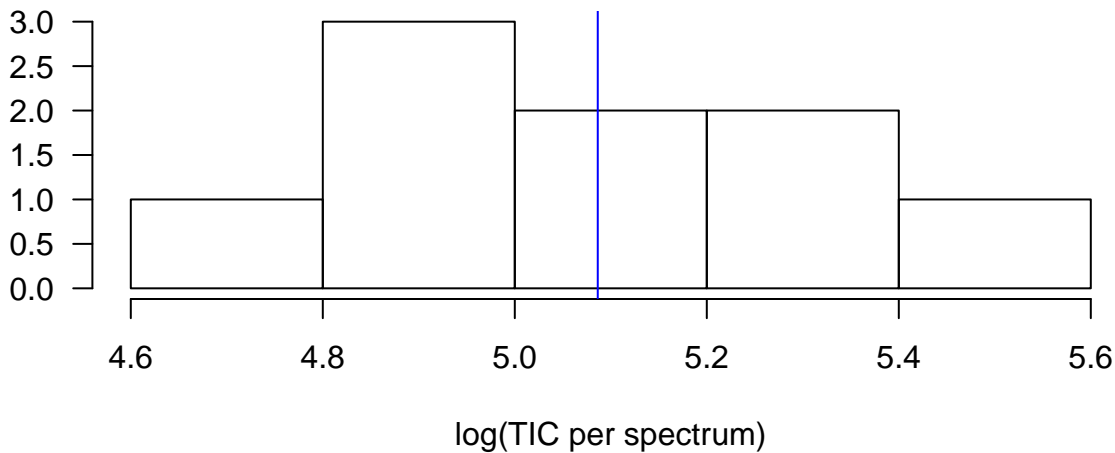
9a) TIC per pixel

Total ion chromatogram intensity



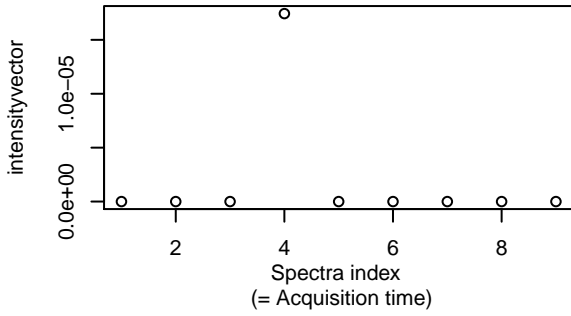
9b) TIC per spectrum

Frequency = # spectra

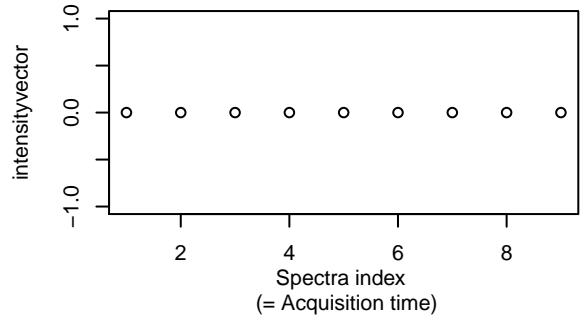


10) intensity of calibrants over acquisition

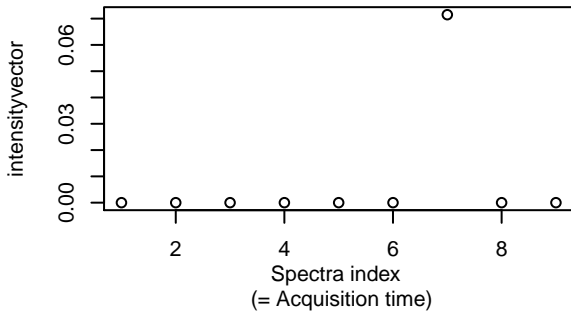
101.5



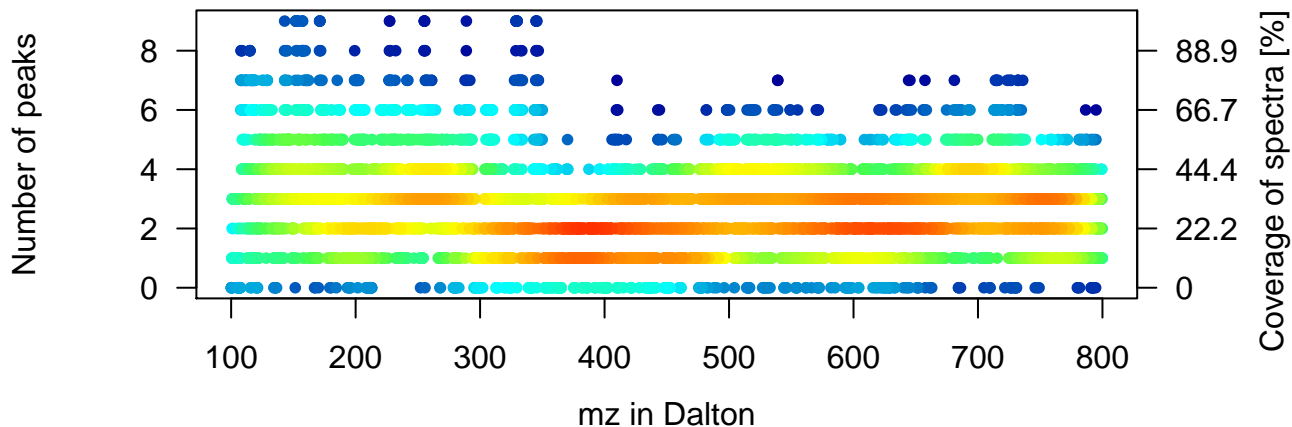
356.7



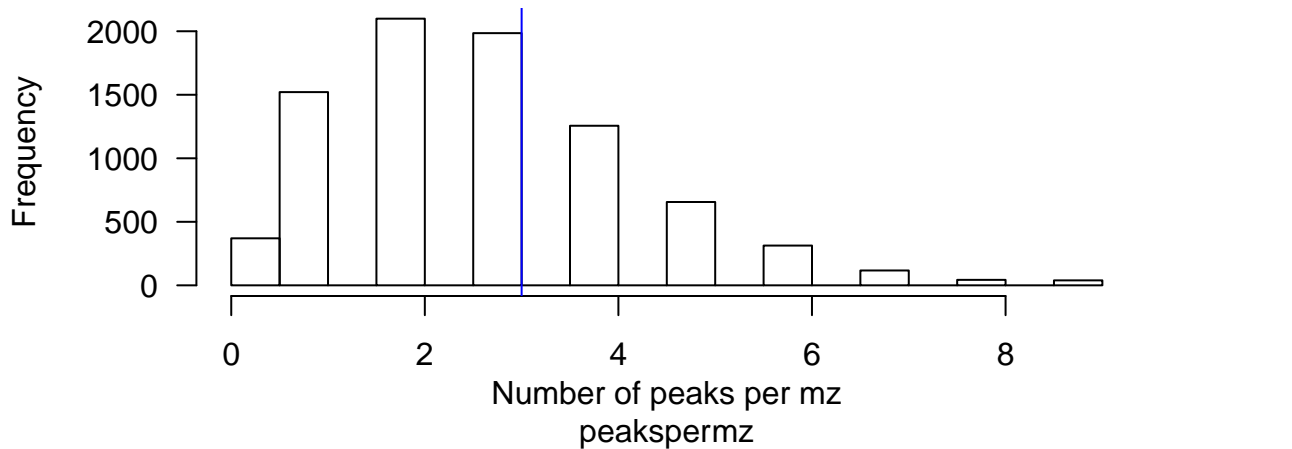
555.1



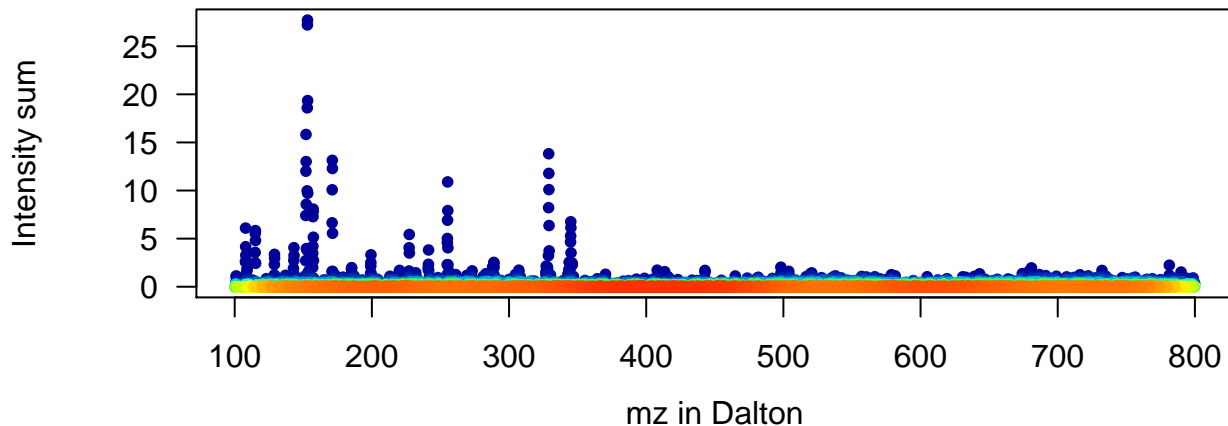
11a) Number of peaks for each mz



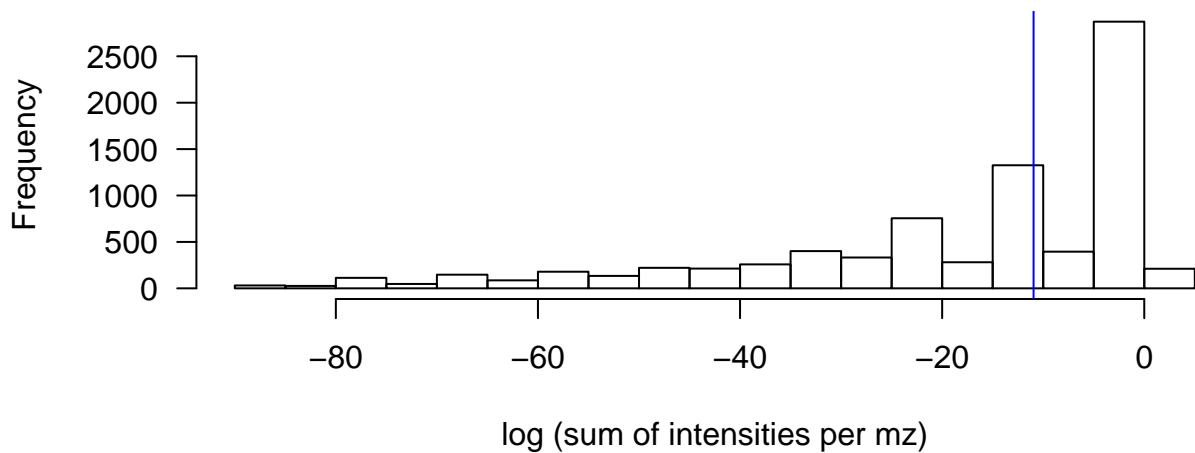
11b) Number of peaks per mz



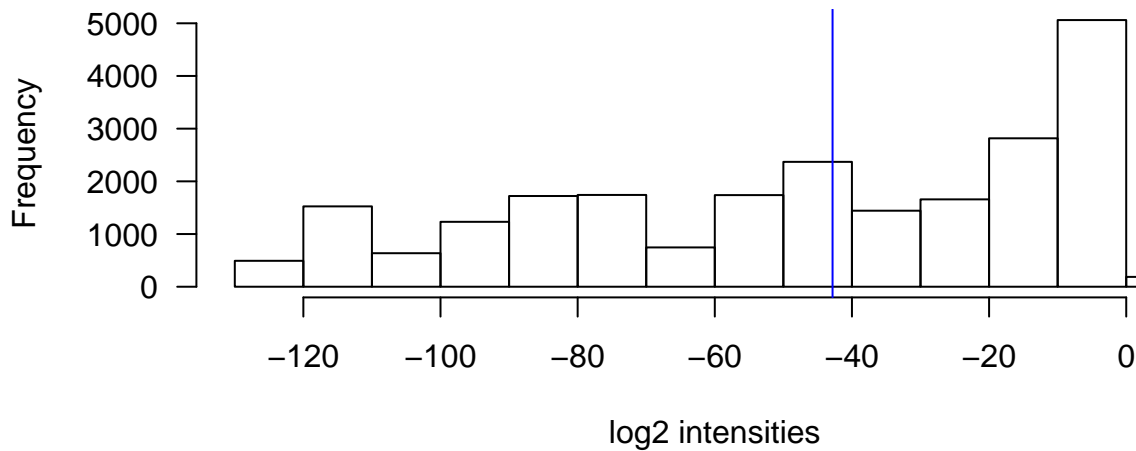
12a) Sum of all peak intensities for each mz



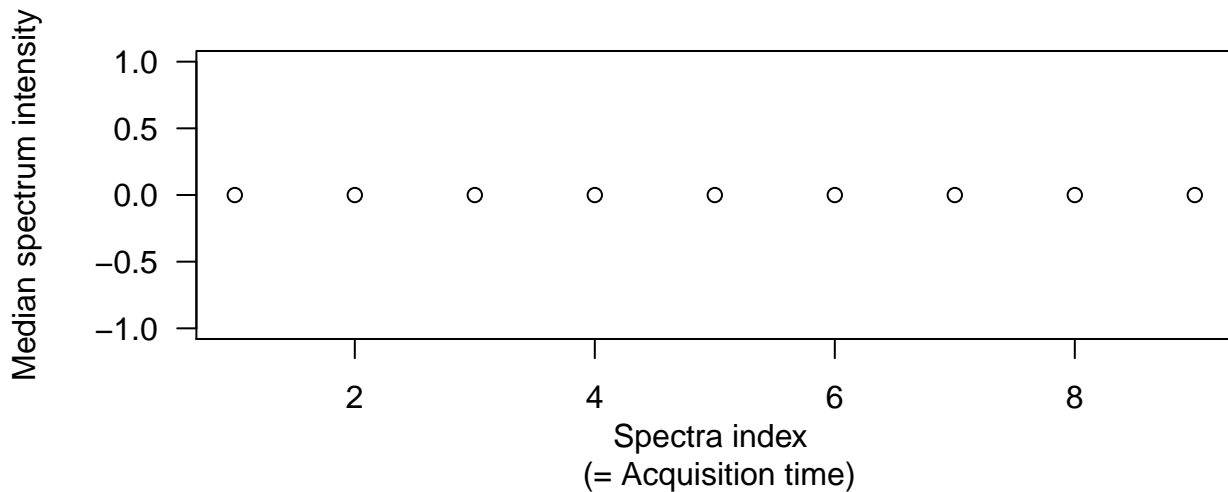
12b) Sum of intensities per mz



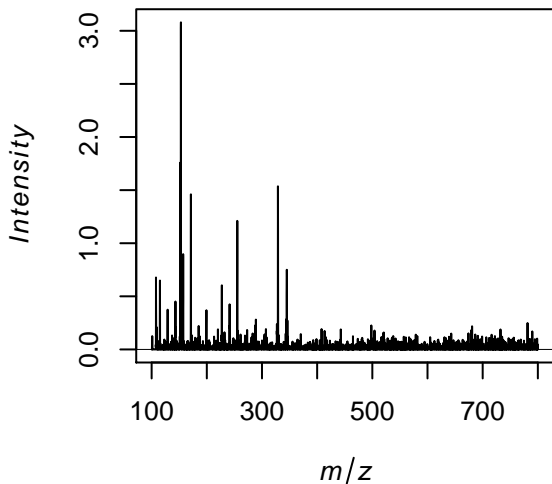
13a) Log2-transformed intensities



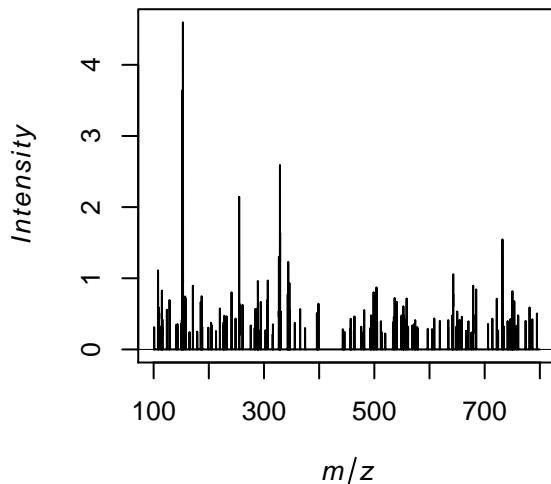
13b) Median intensity per spectrum



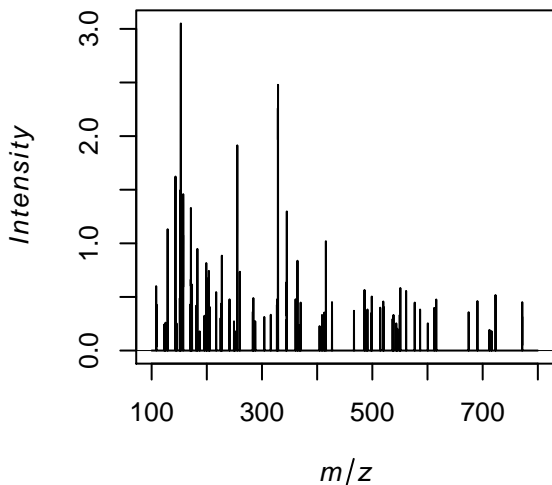
Average spectrum



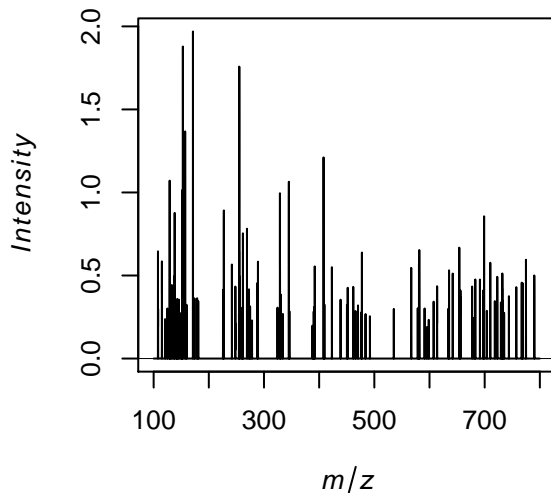
Spectrum in middle of acquisition



Spectrum at x = 1, y = 1

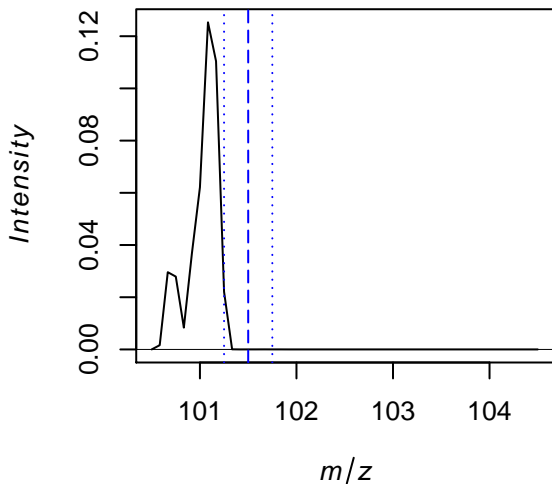


Spectrum at x = 3, y = 2

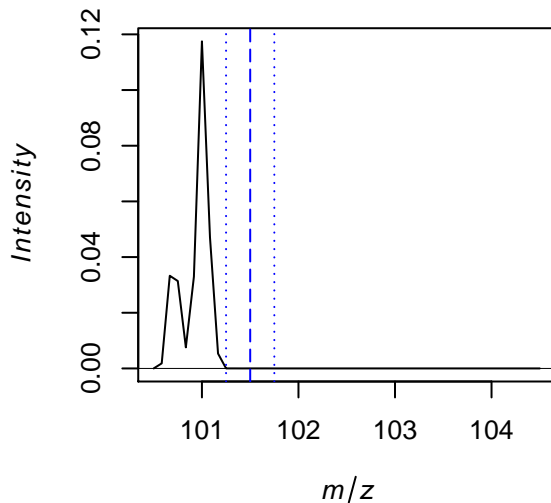


101.5

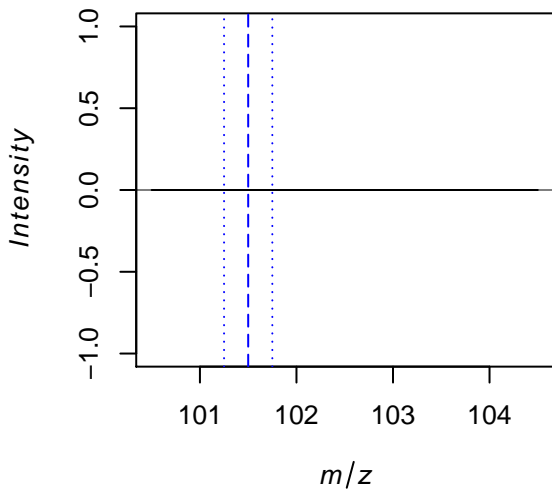
average spectrum



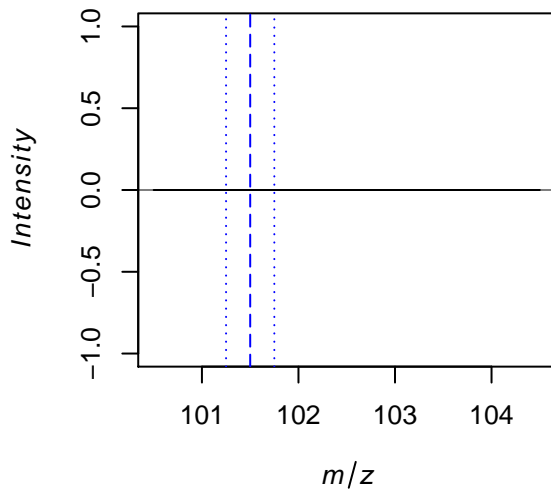
pixel in middle of acquisition



Spectrum at x = 1, y = 1

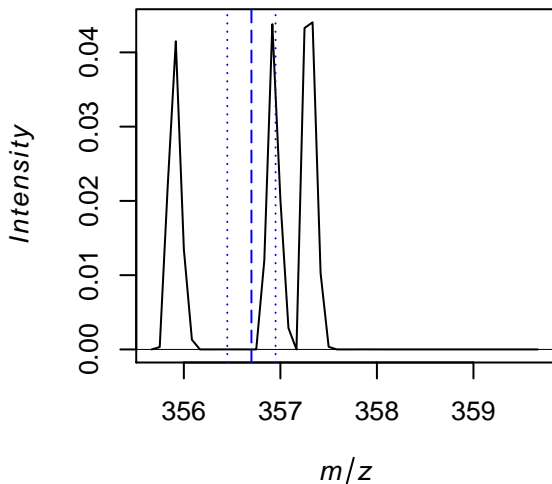


Spectrum at x = 3, y = 2

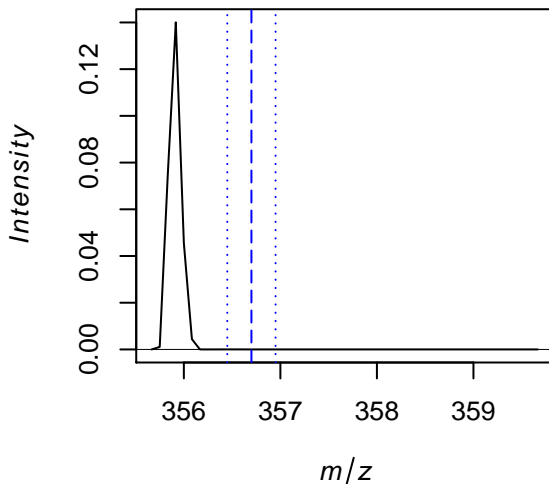


356.7

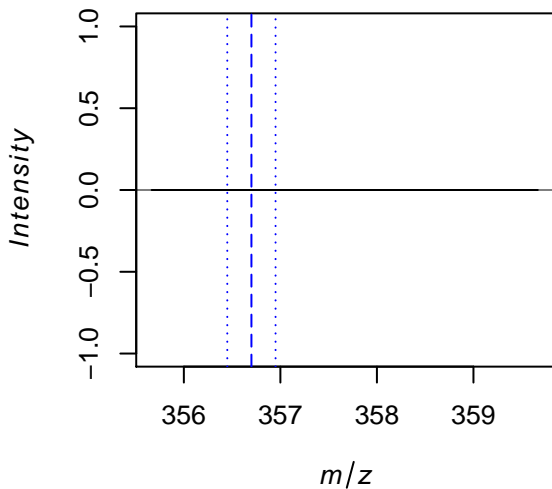
average spectrum



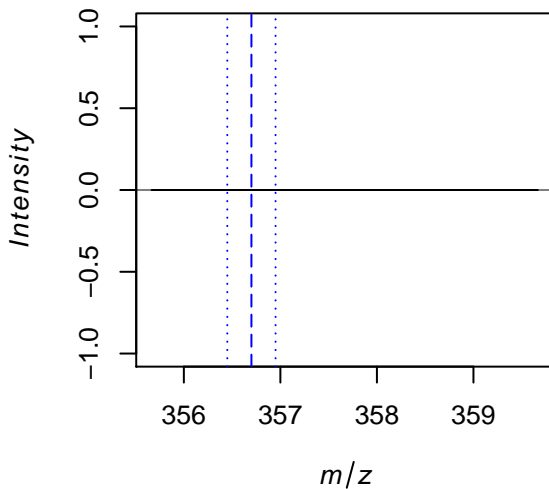
pixel in middle of acquisition



Spectrum at $x = 1, y = 1$

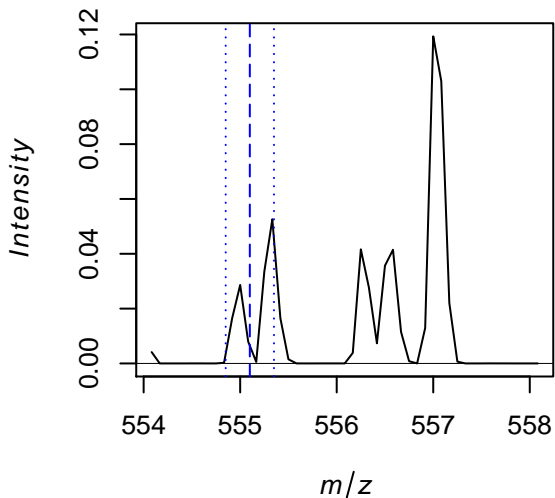


Spectrum at $x = 3, y = 2$

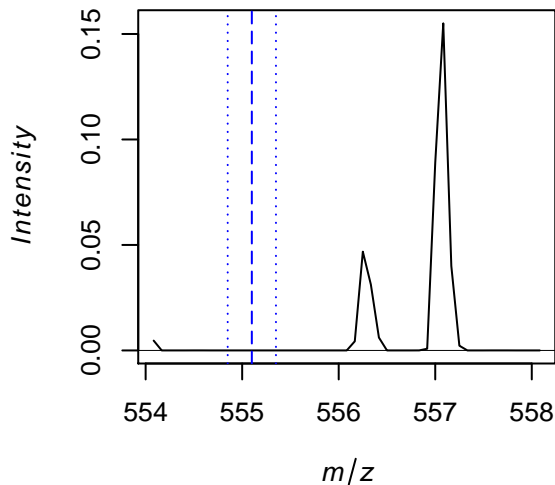


555.1

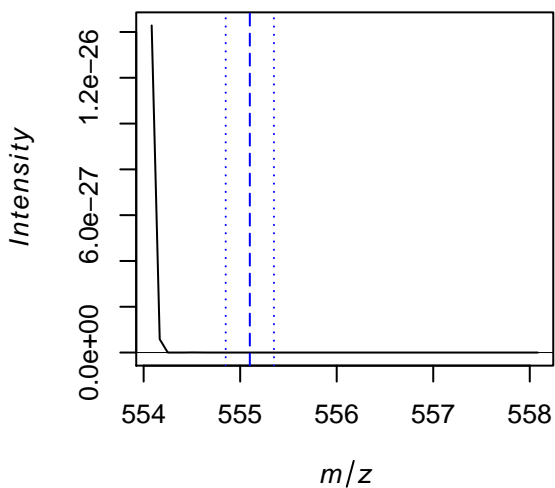
average spectrum



pixel in middle of acquisition



Spectrum at x = 1, y = 1



Spectrum at x = 3, y = 2

