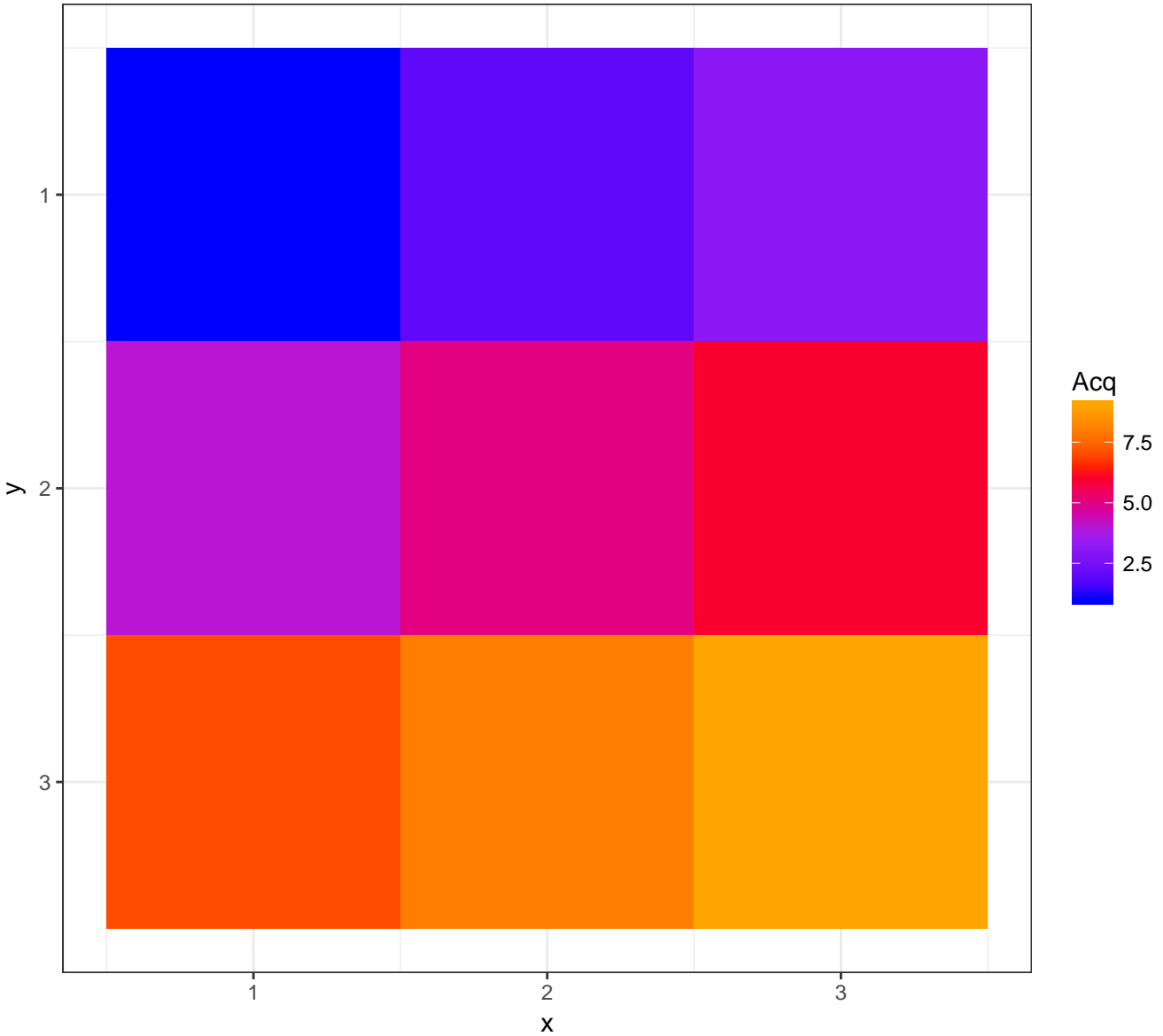


Quality control of MSI data

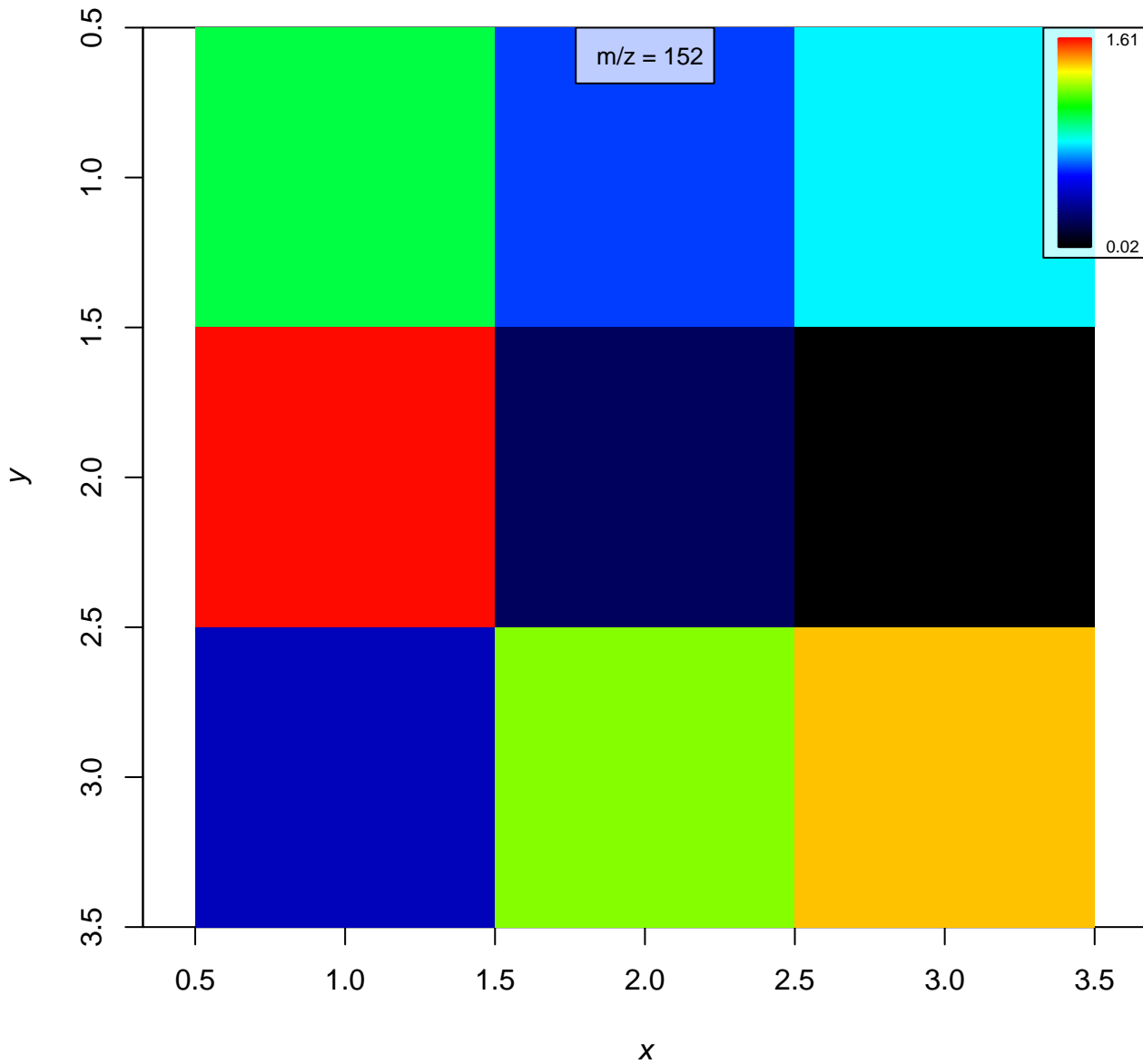
Filename: Testfile_imzml

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 peptidemasses	3

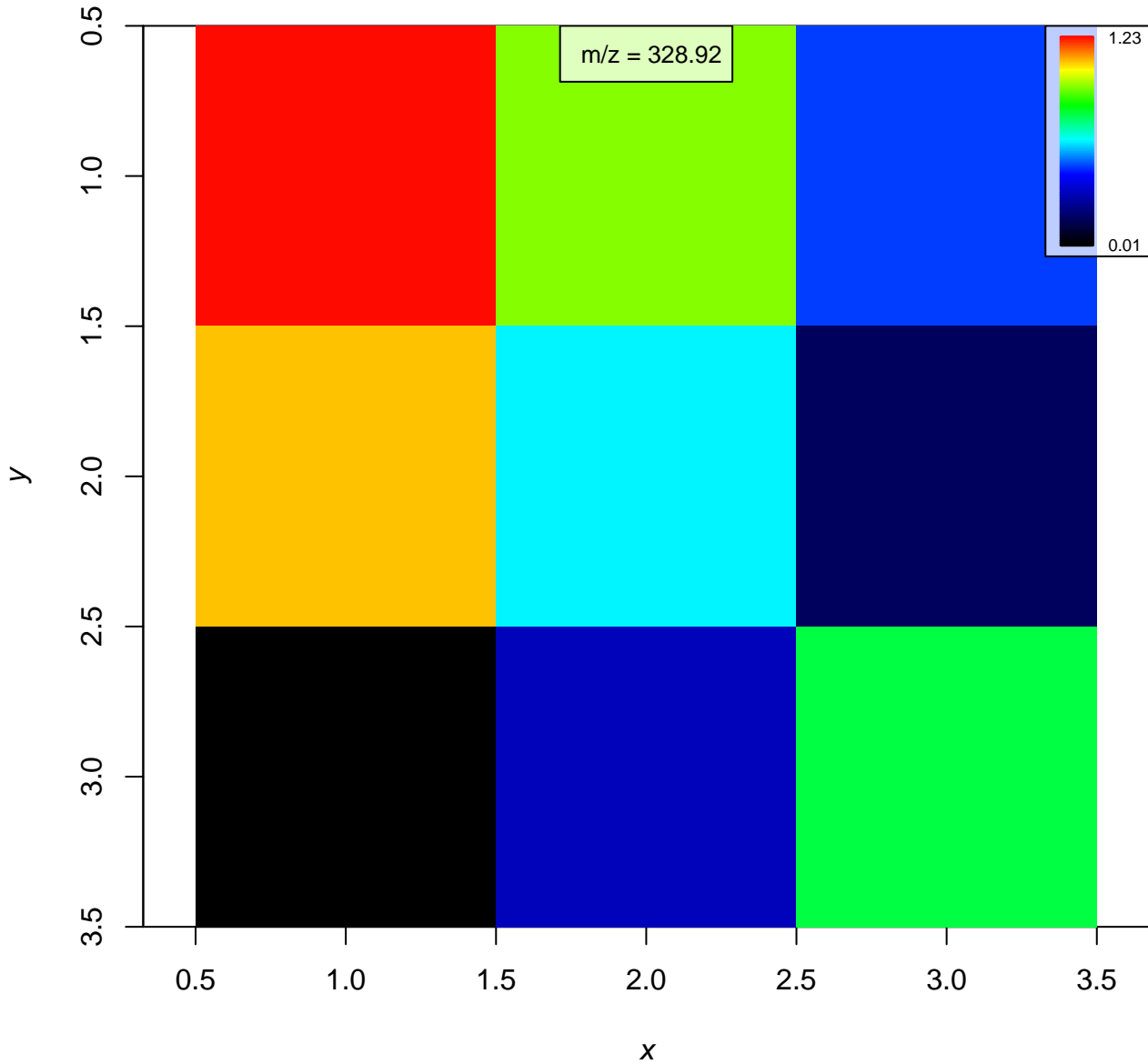
1) Order of Acquisition



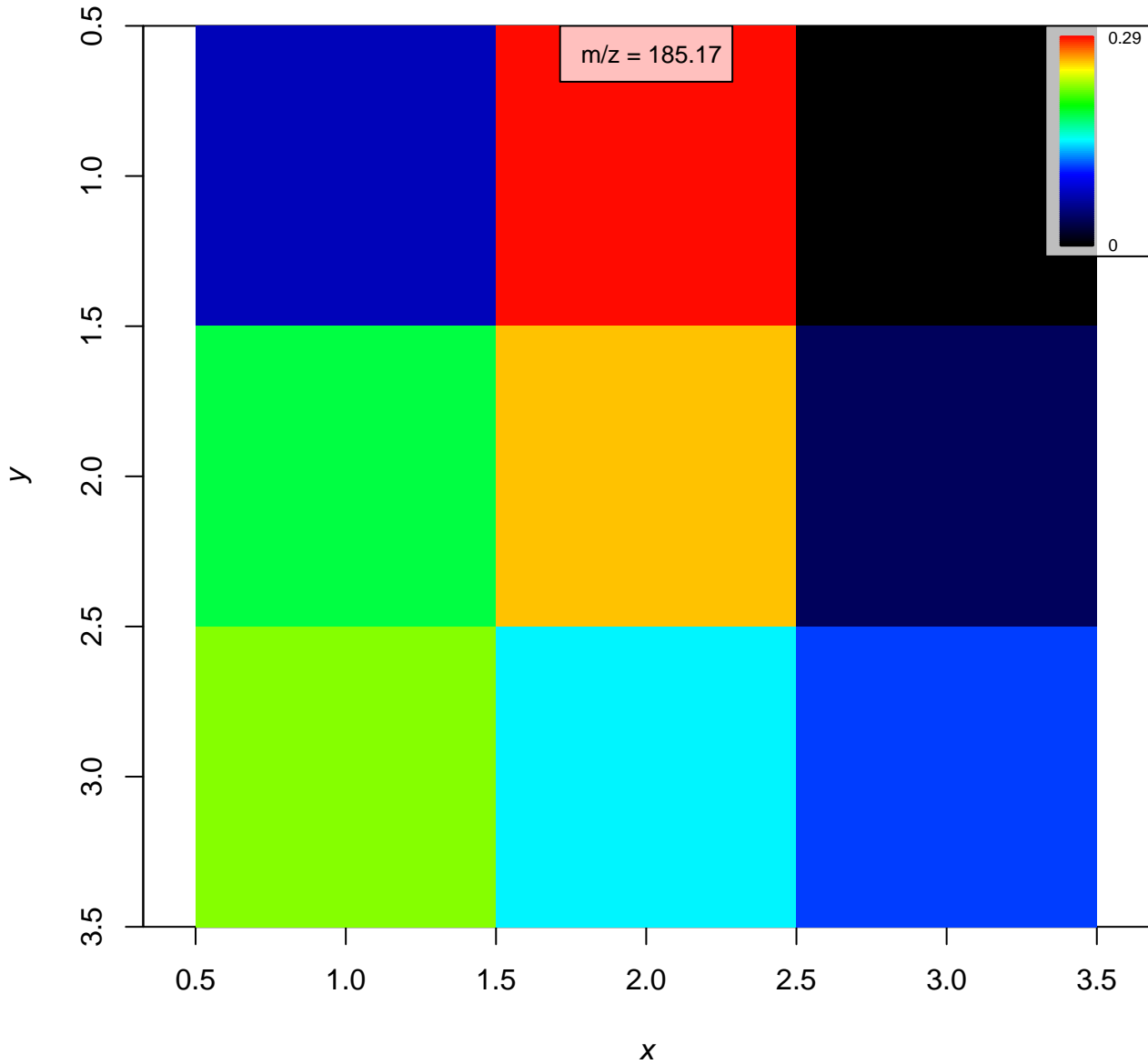
2A) mass1 (152 Da)



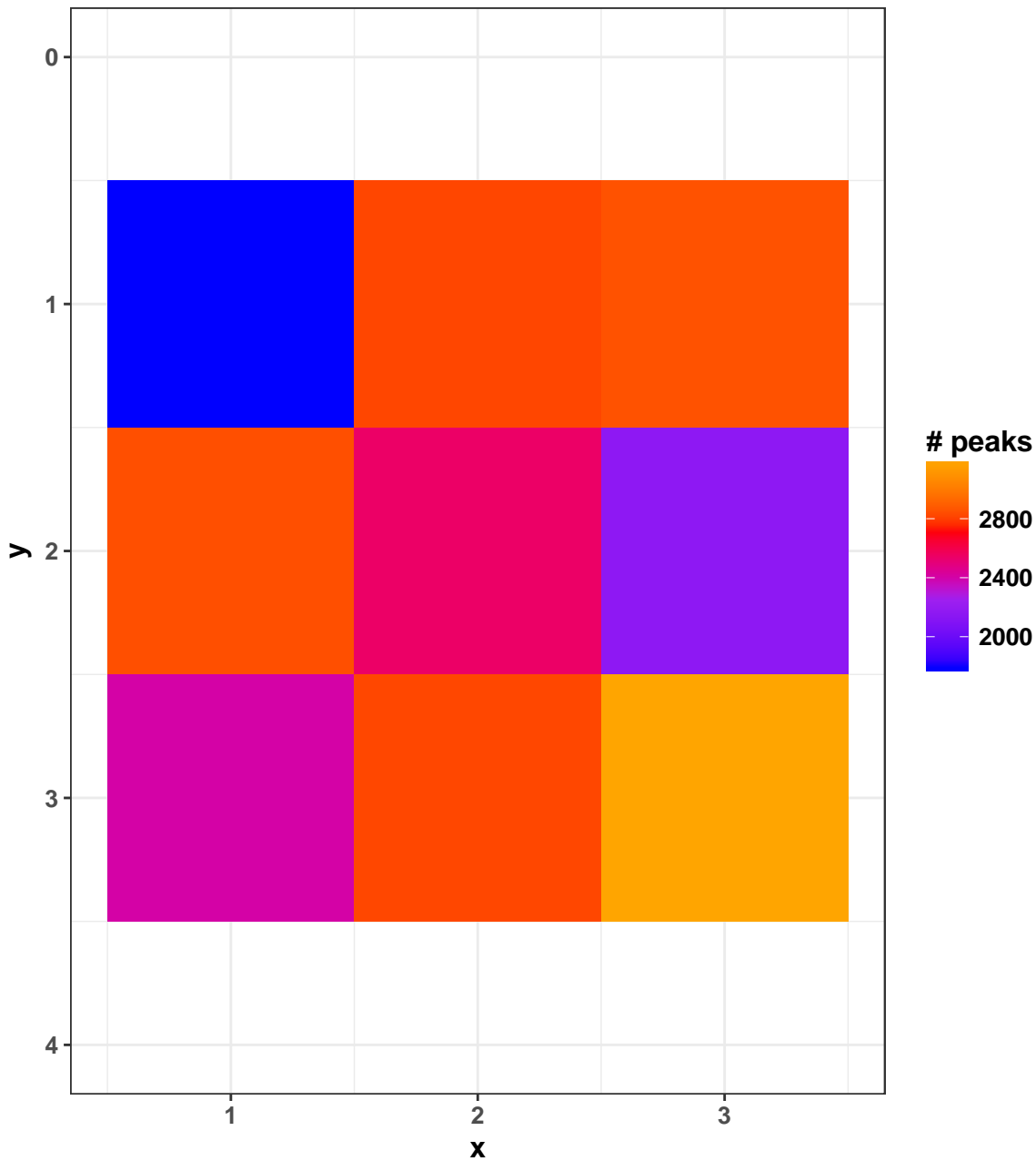
2B) mass2 (328.9 Da)



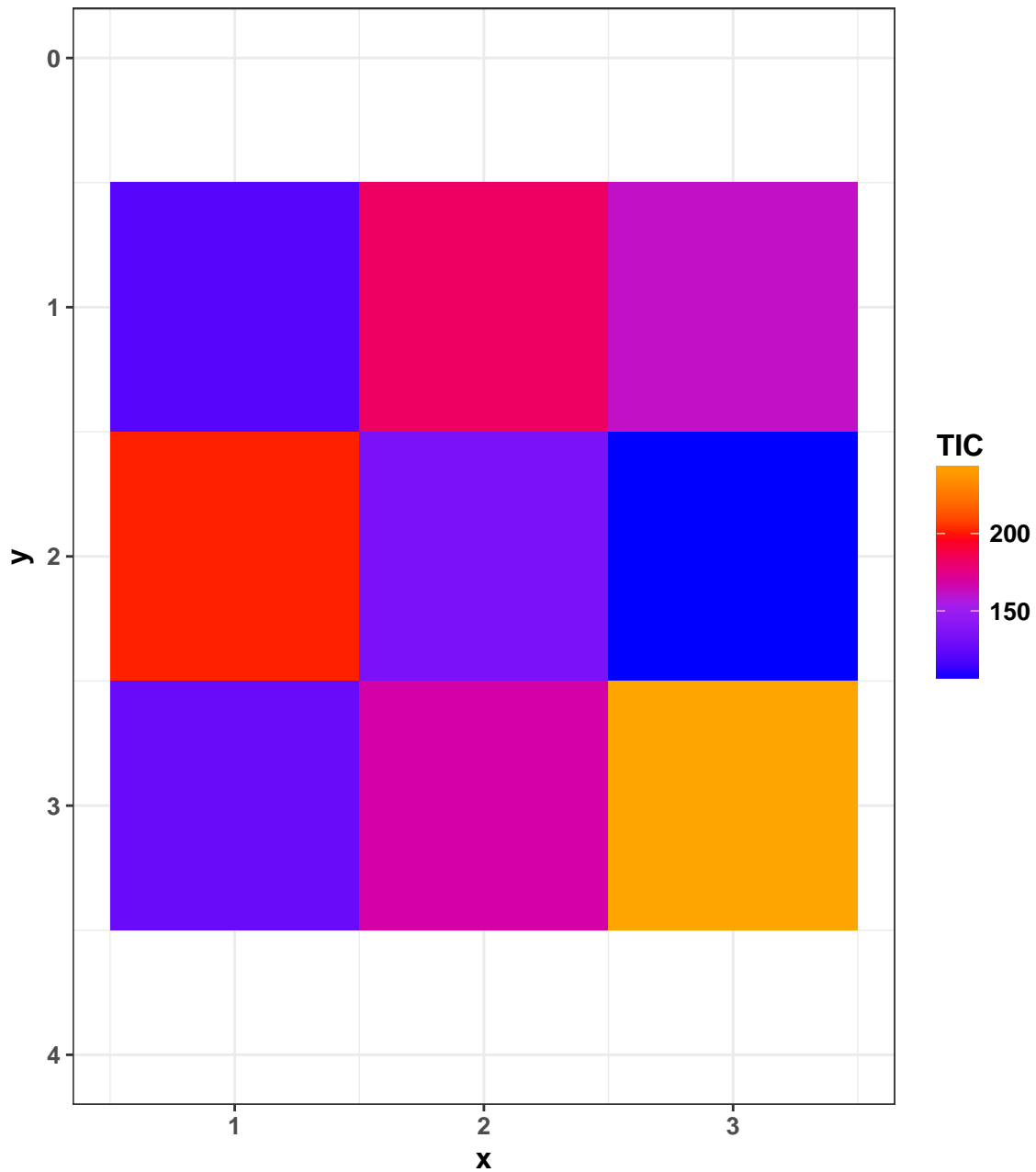
2C) mass3 (185.2 Da)



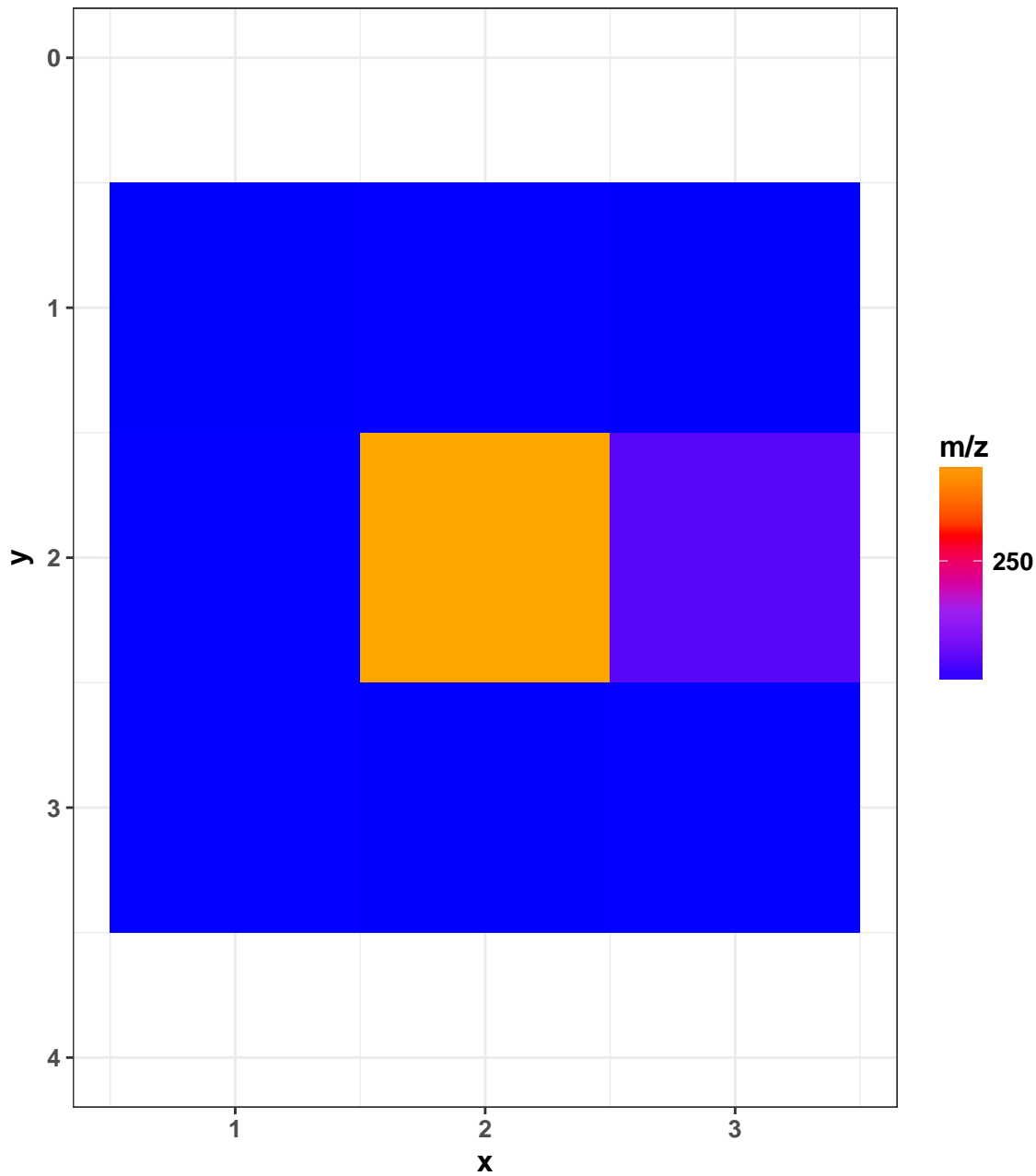
3) Number of peaks per pixel



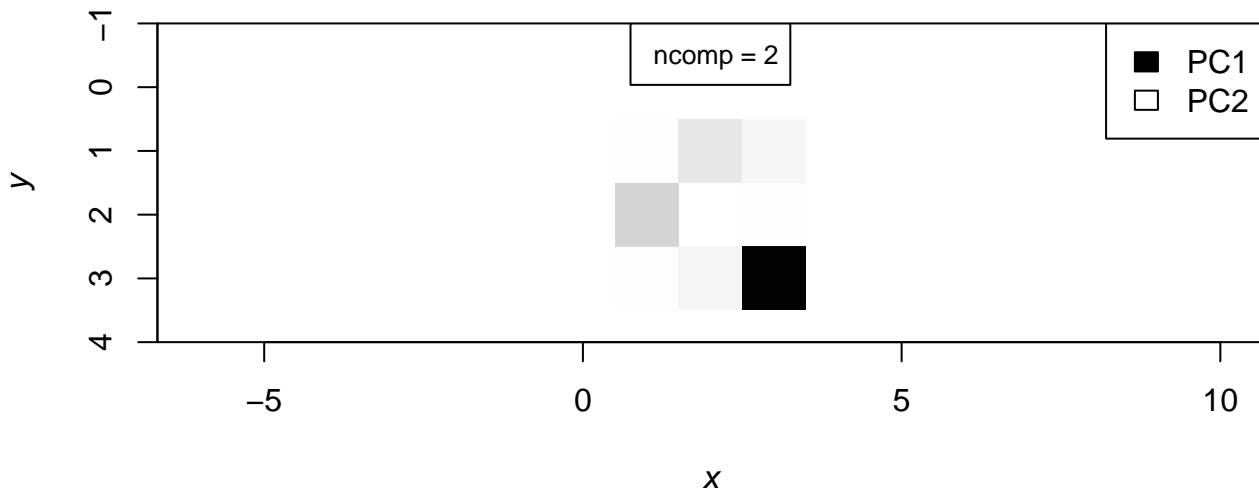
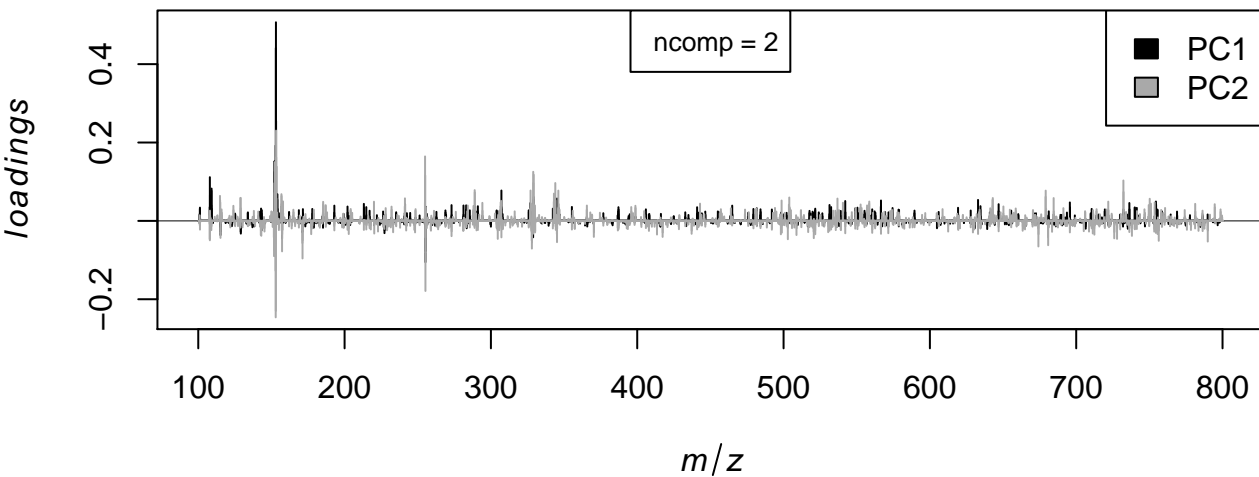
4) Total Ion Chromatogram



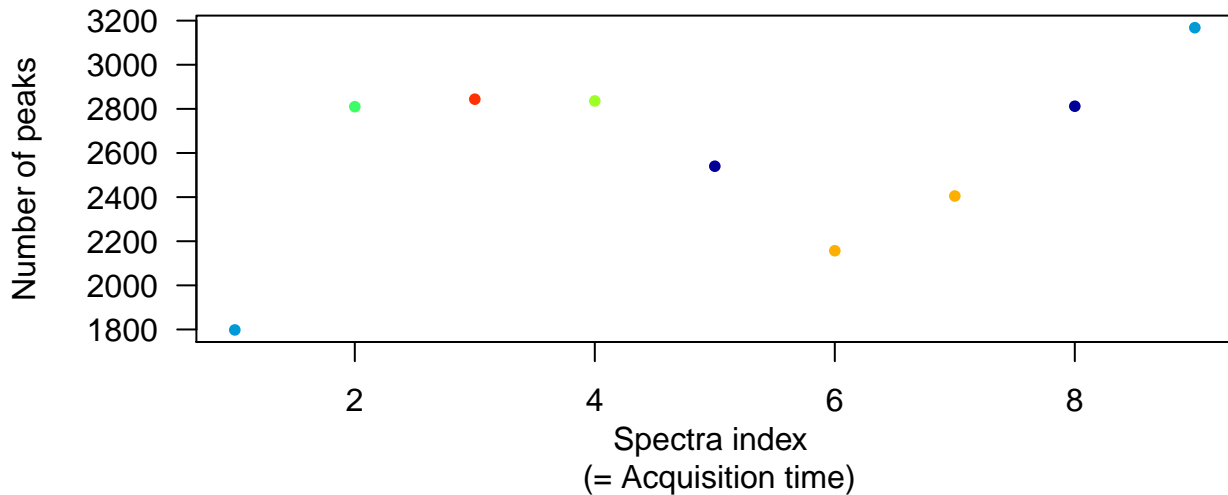
5) Most abundant m/z in each pixel



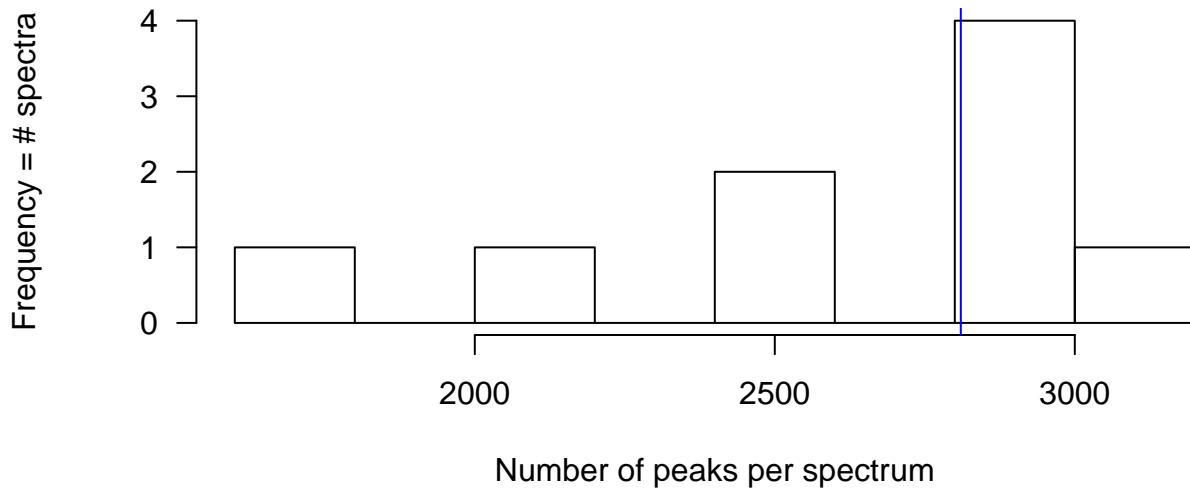
6) PCA for two components



7a) Number of peaks per spectrum

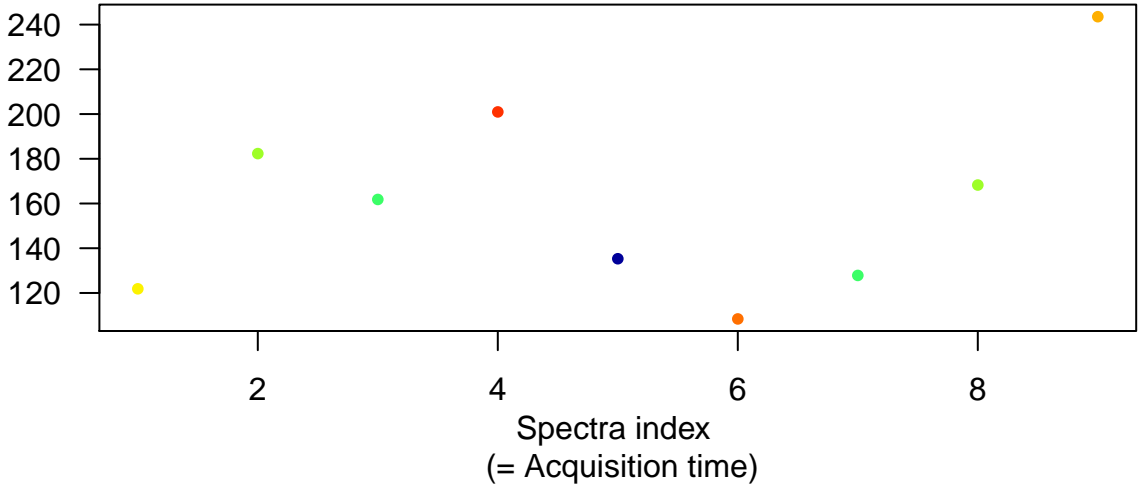


7b) Number of peaks per spectrum



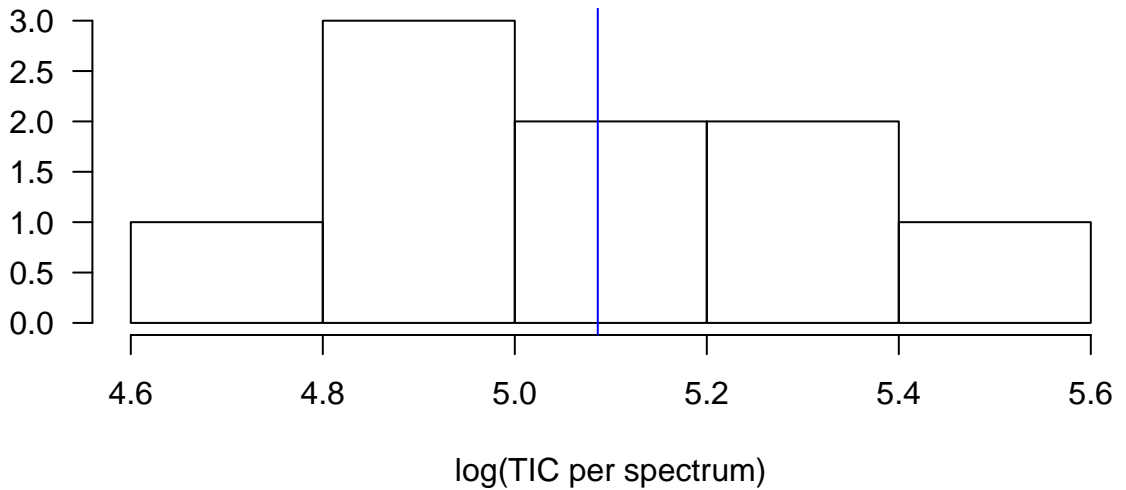
8a) TIC per pixel

Total ion chromatogram intensity

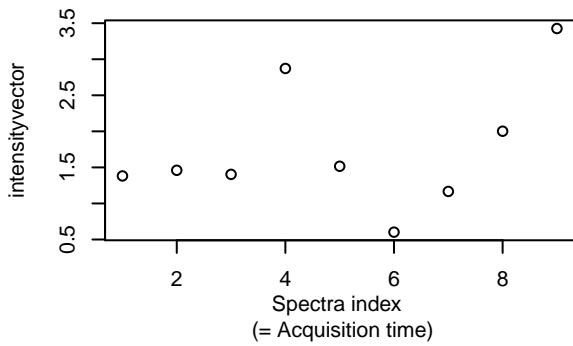


8b) TIC per spectrum

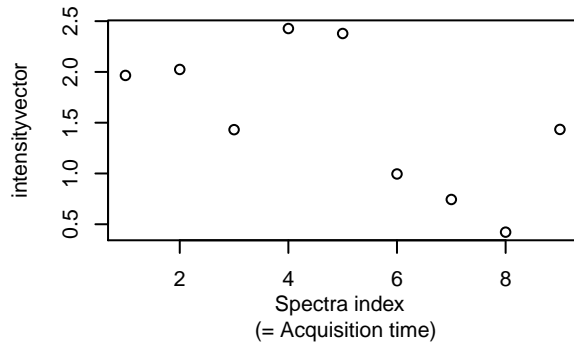
Frequency = # spectra



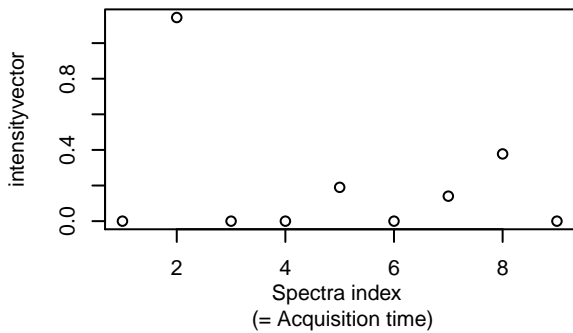
mass1



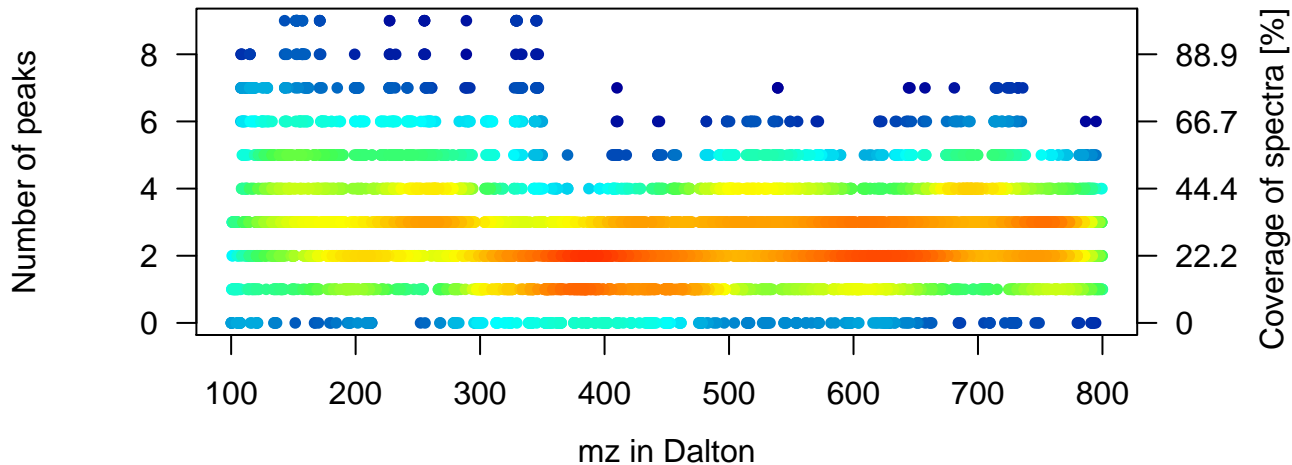
mass2



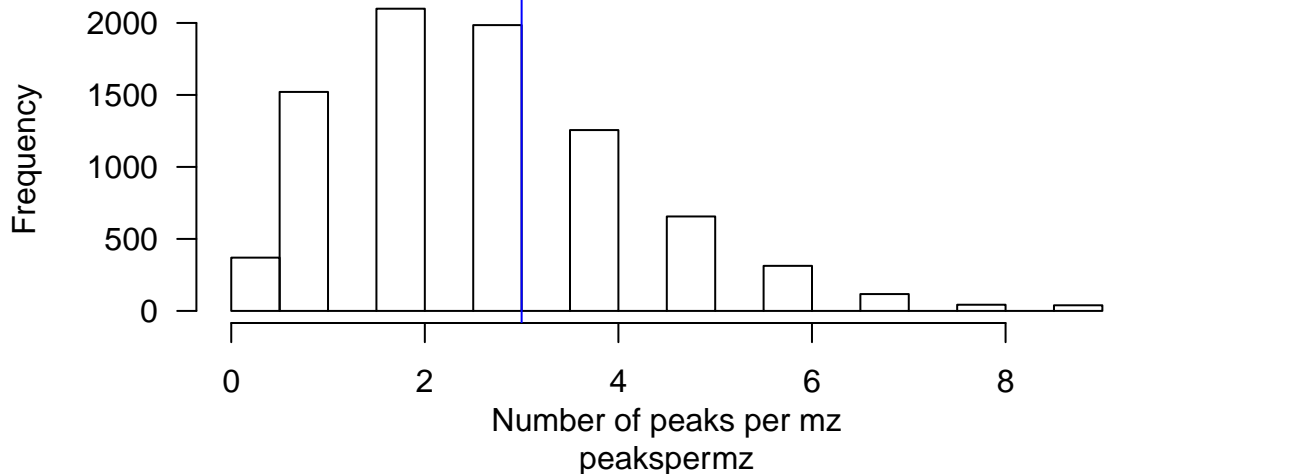
mass3



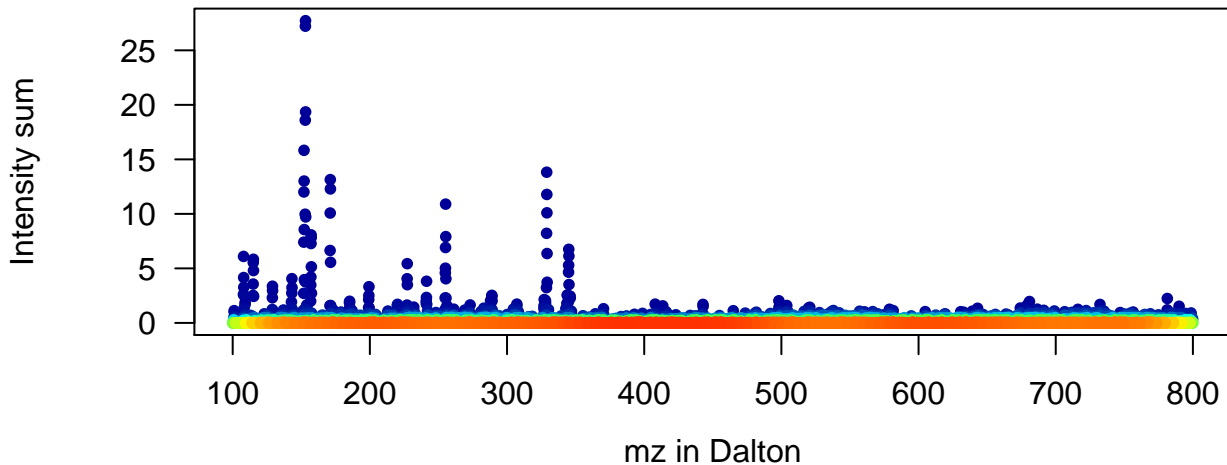
10a) Number of peaks for each mz



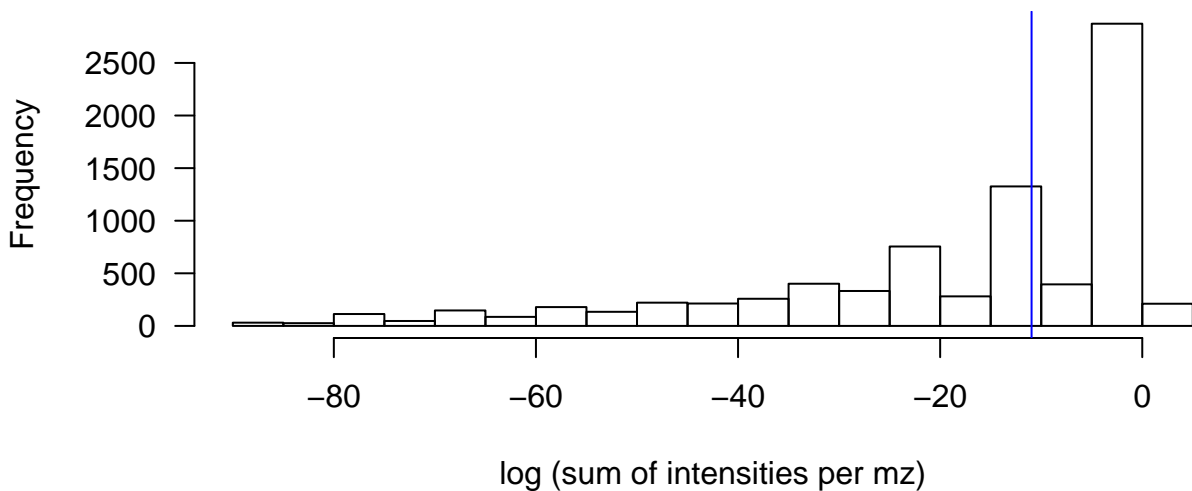
10b) Number of peaks per mz



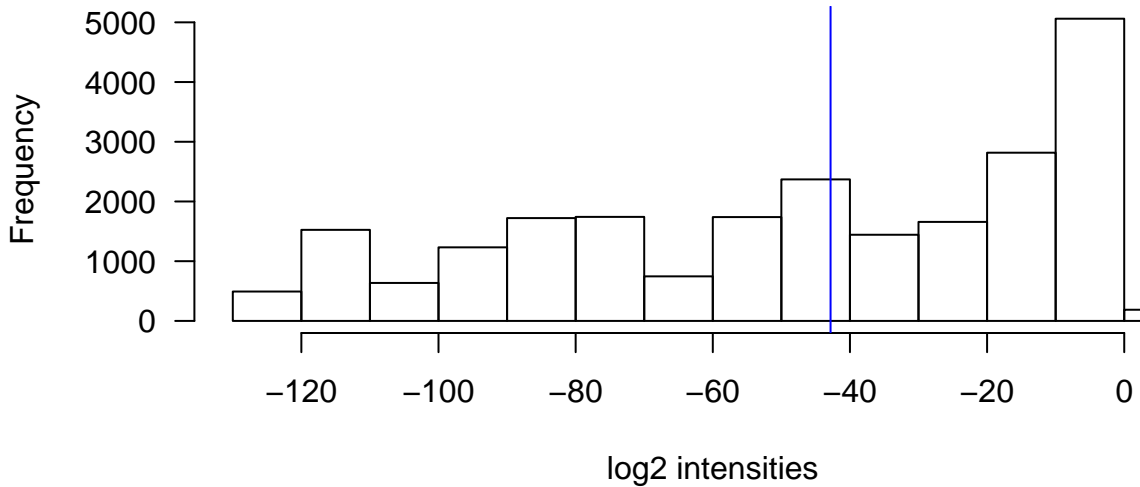
11a) Sum of all peak intensities for each mz



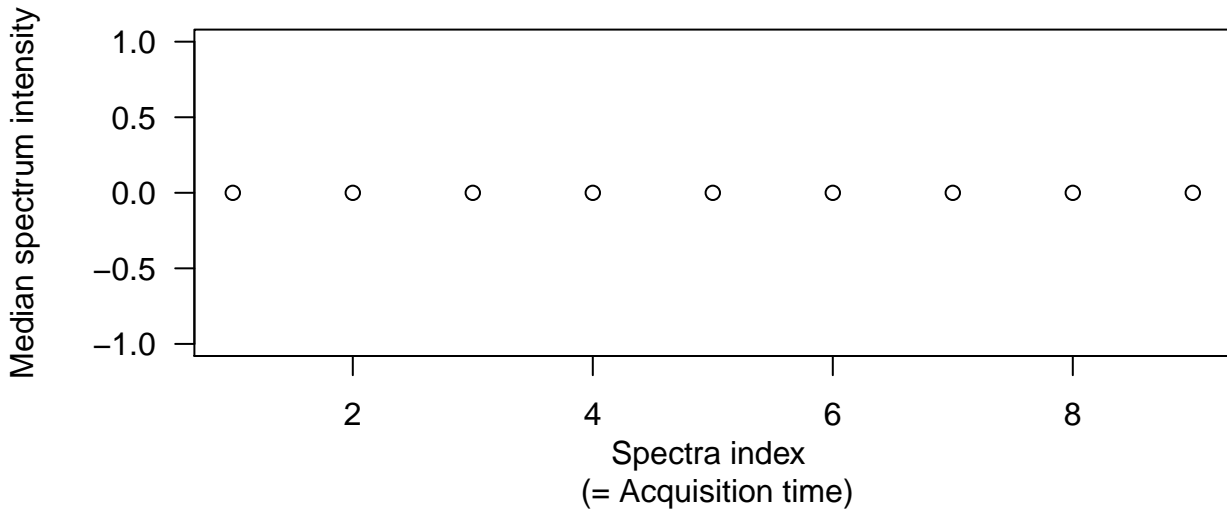
11b) Sum of intensities per mz



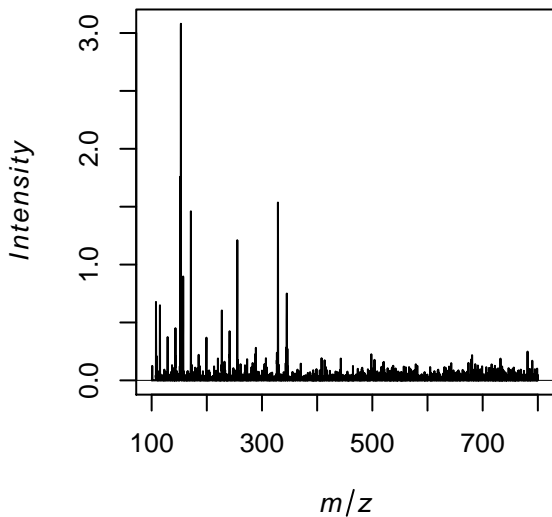
12a) Log2-transformed intensities



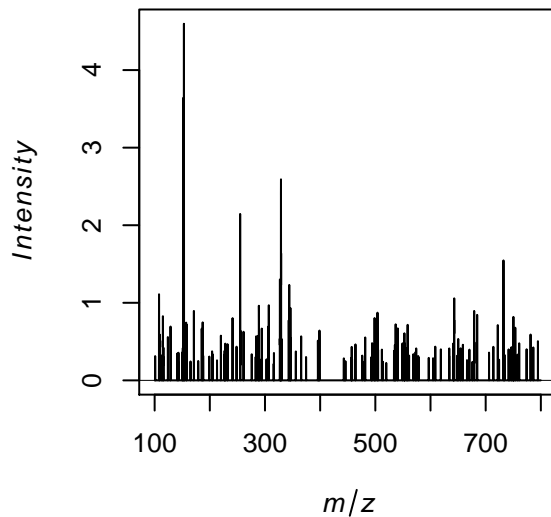
12b) Median intensity per spectrum



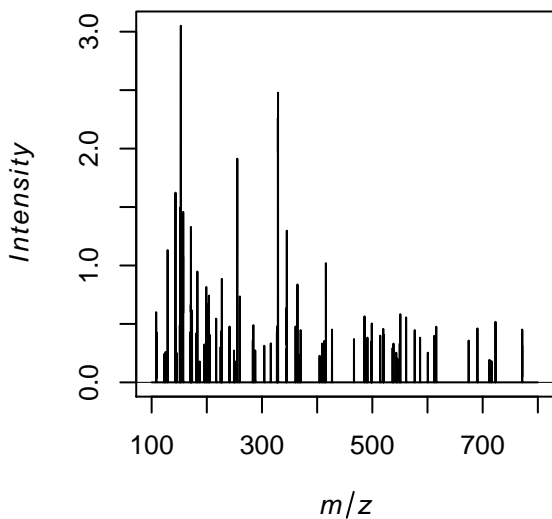
Average spectrum



Spectrum in middle of acquisition



Spectrum at x = 1, y = 1



Spectrum at x = 3, y = 2

