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
# peptides in None	0 / 0
# calibrants in None	0 / 0

1) Order of Acquisition
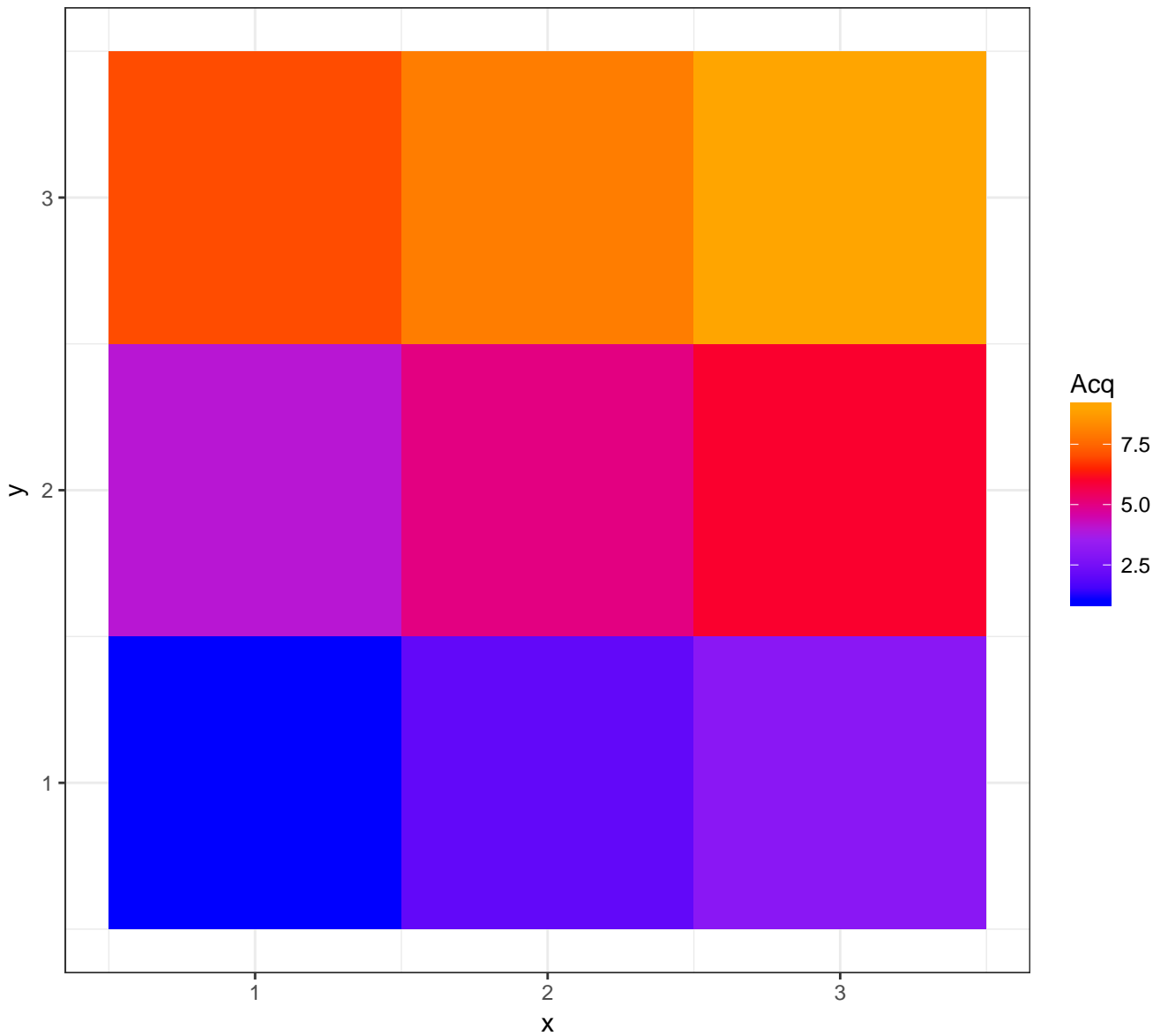
4) Number of peaks per pixel
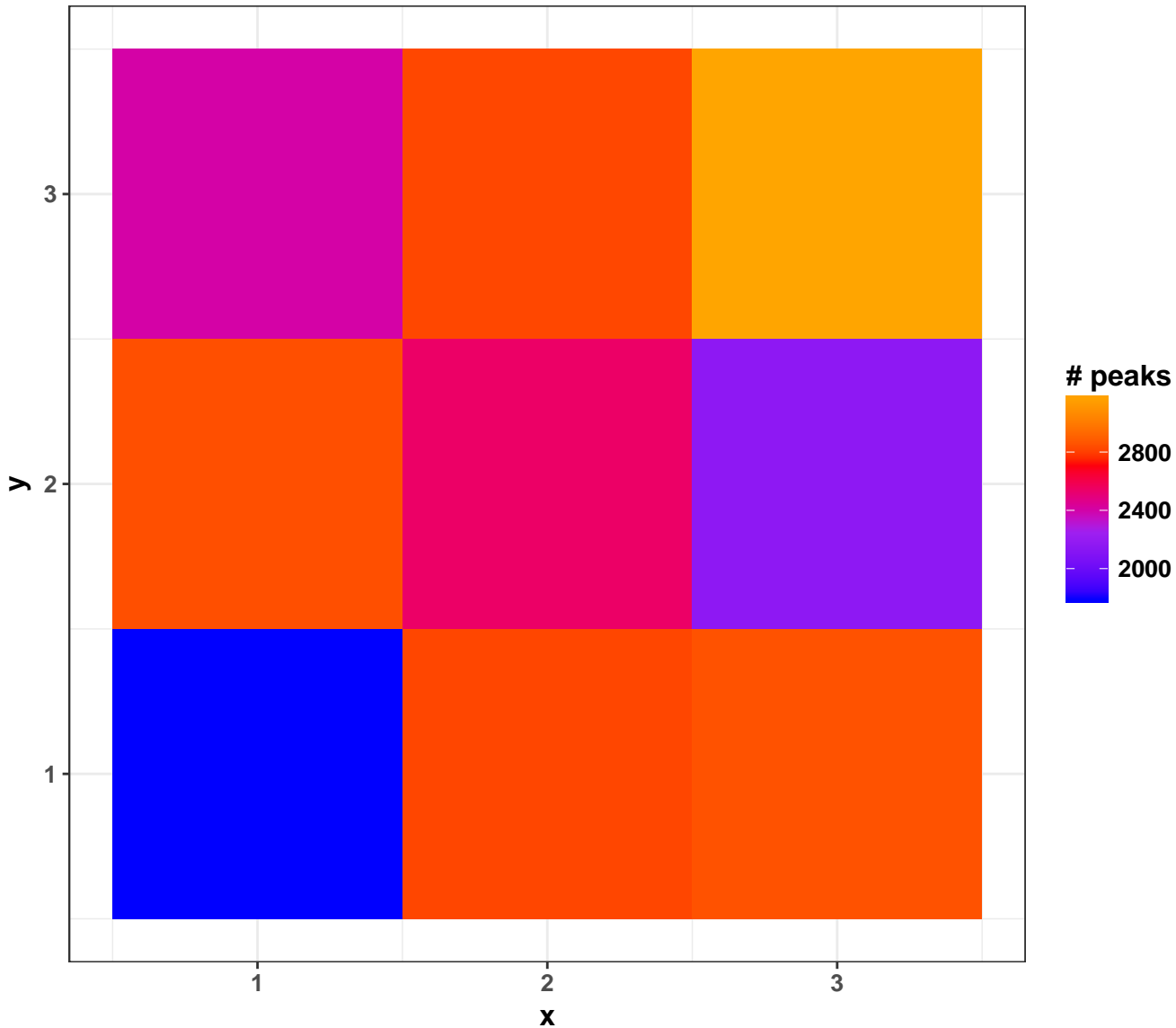
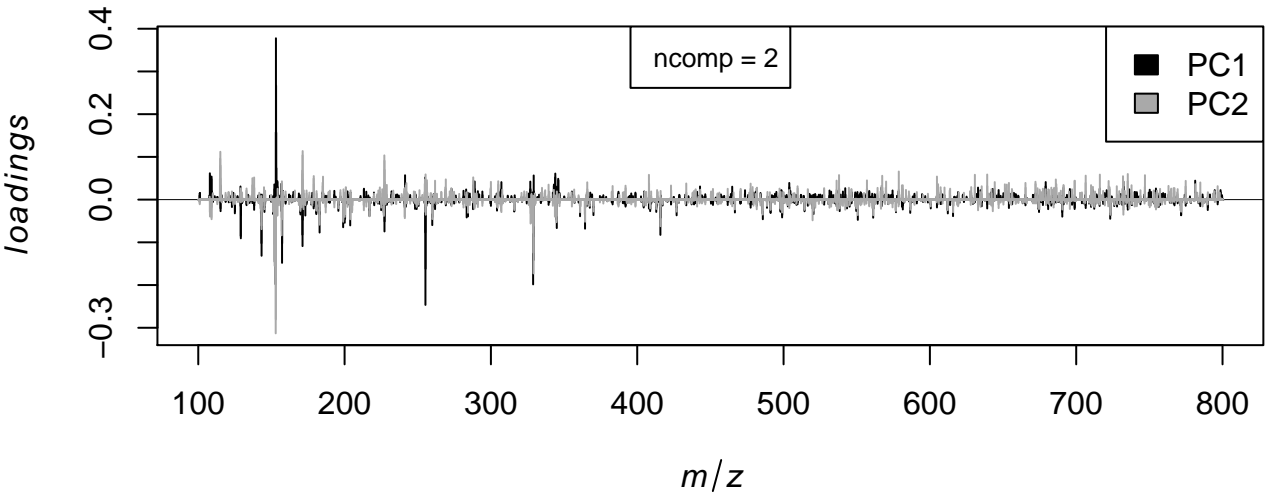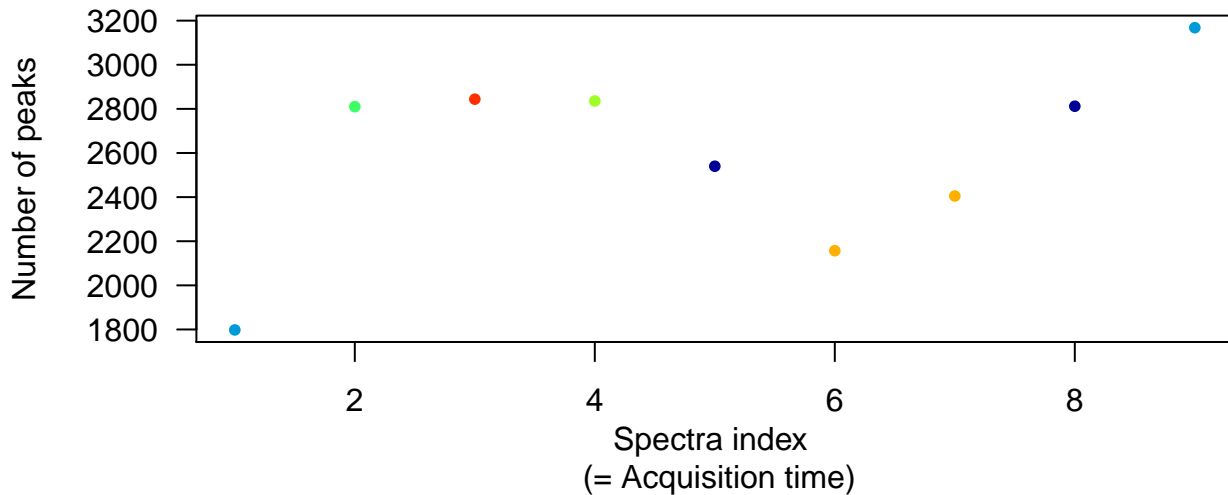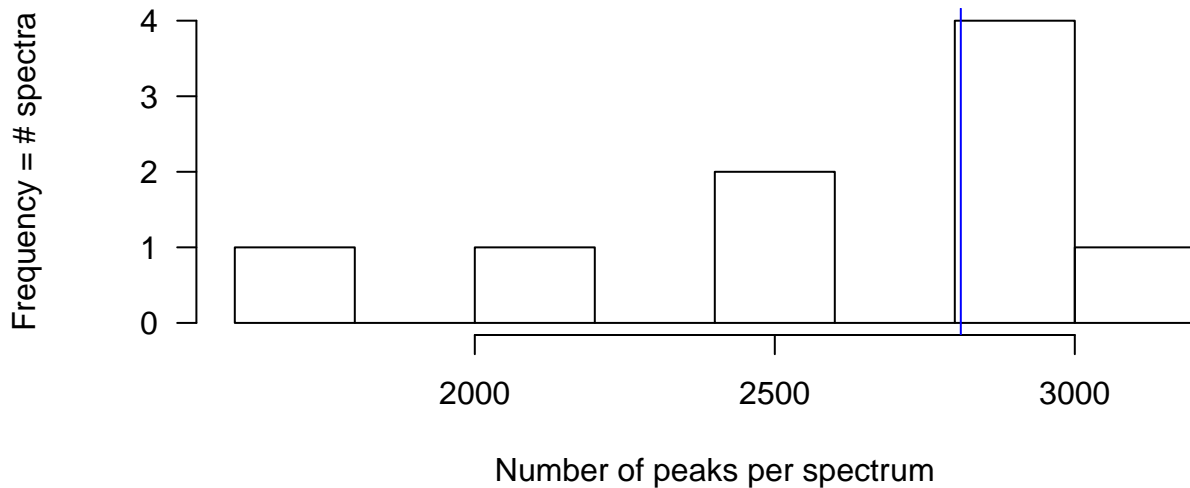**5) Total Ion Chromatogram**
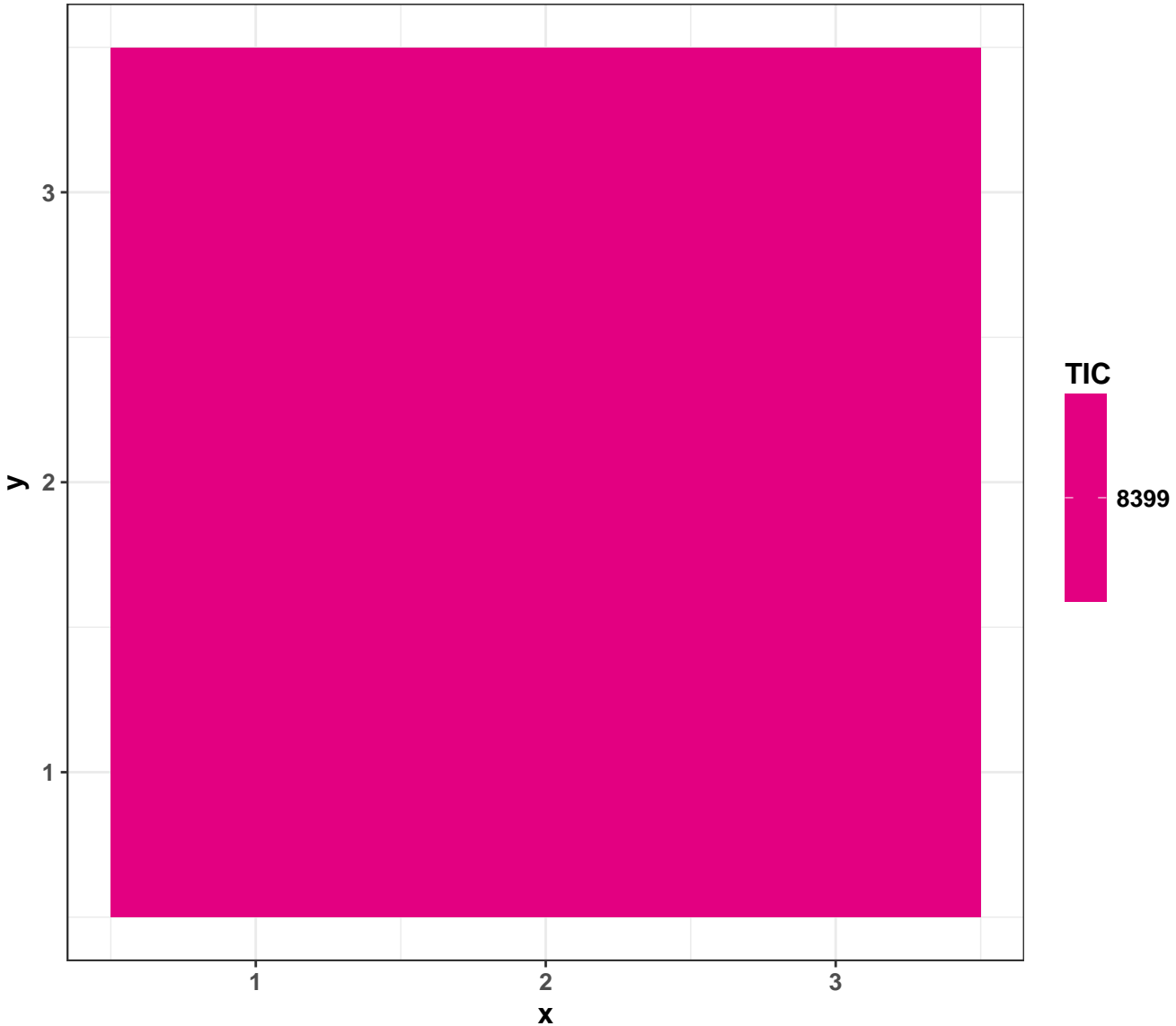
6) Most abundant m/z in each pixel
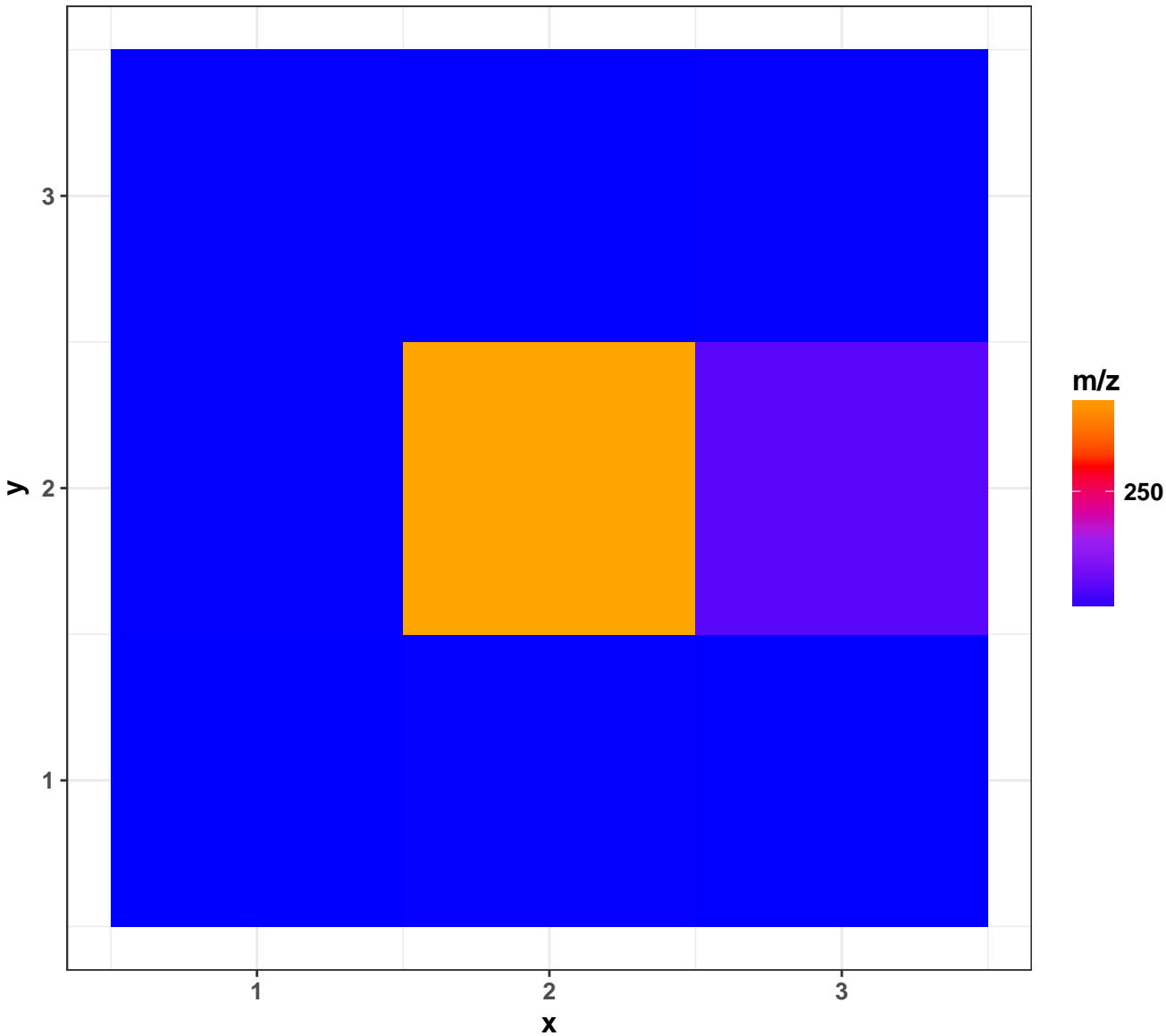
7) PCA for two components
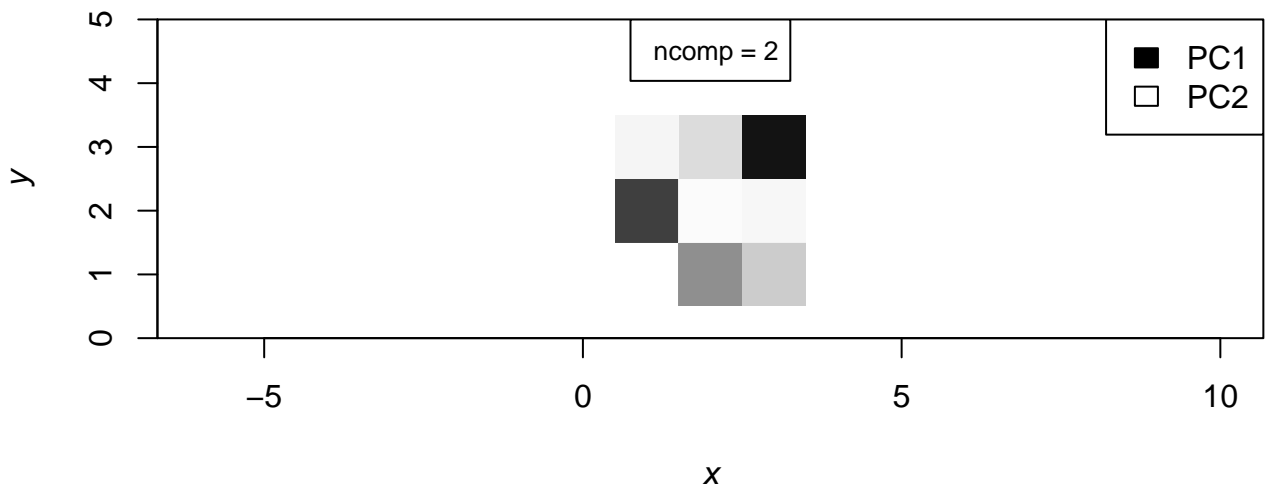
8a) Number of peaks per spectrum

8b) Number of peaks per spectrum

9a) TIC per pixel

Total ion chromatogram intensity

Spectra index
(= Acquisition time)

9b) TIC per spectrum

Frequency = # spectra
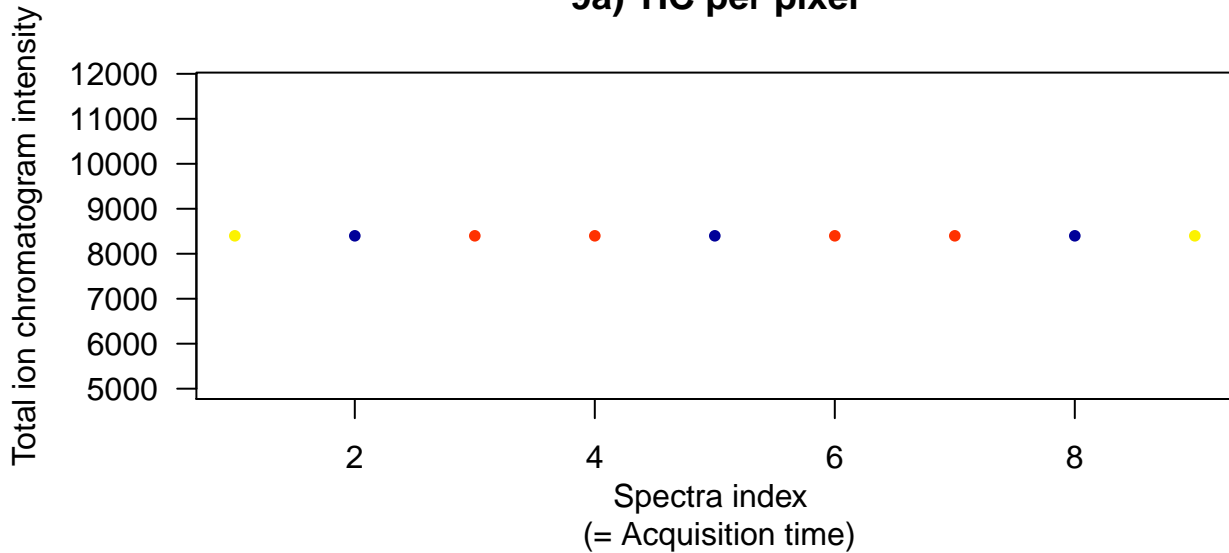
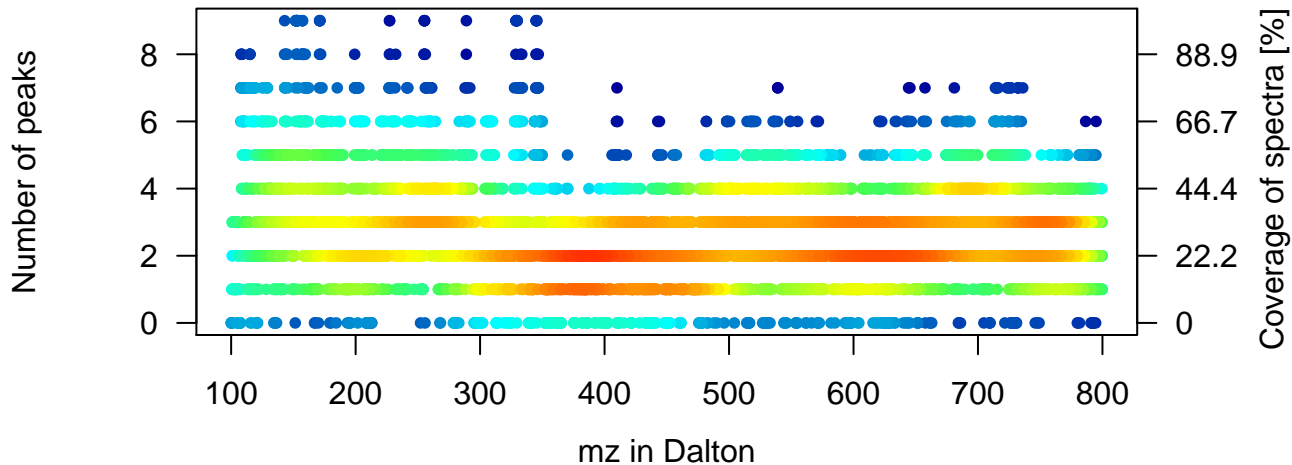log(TIC per spectrum)
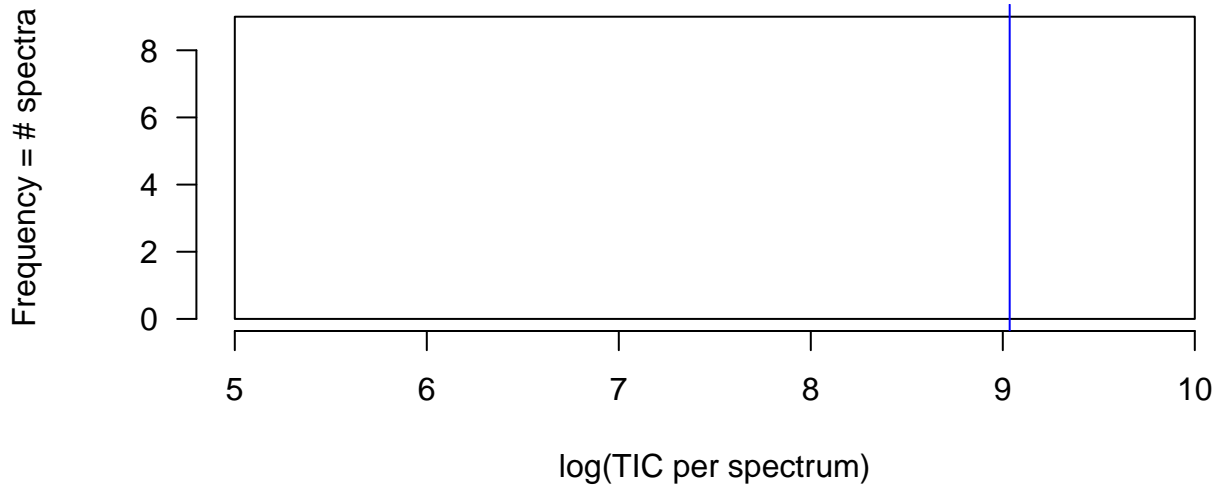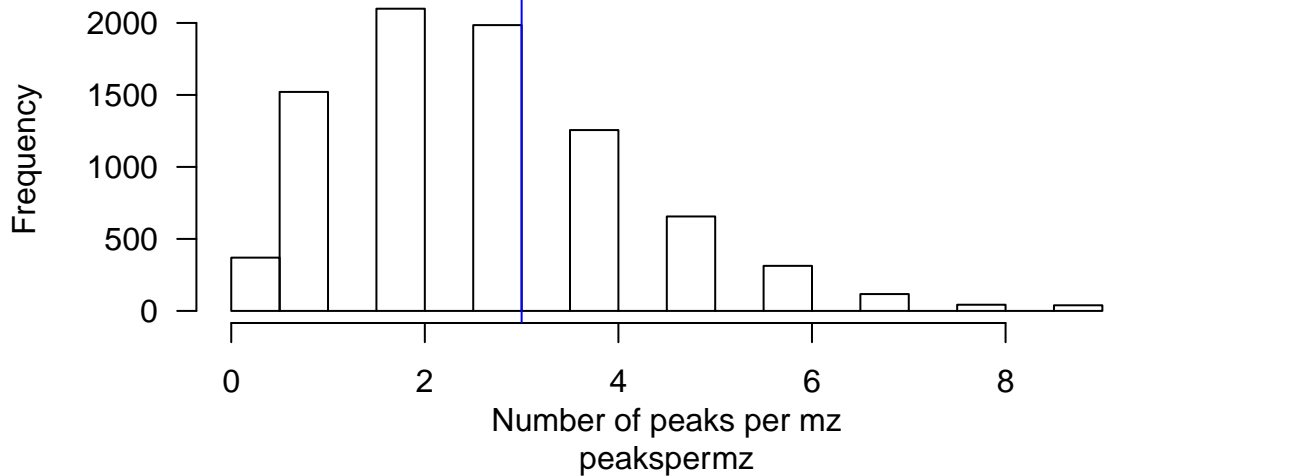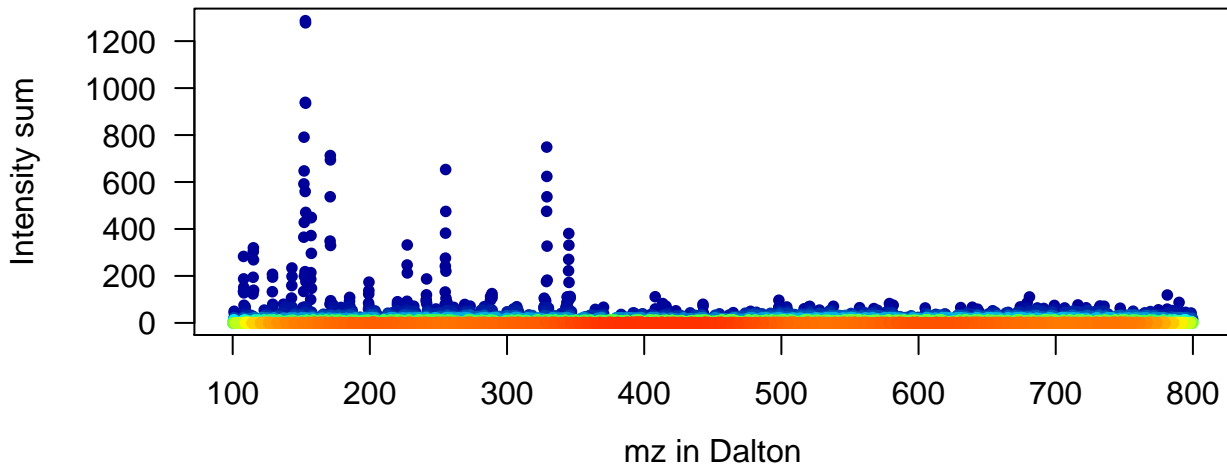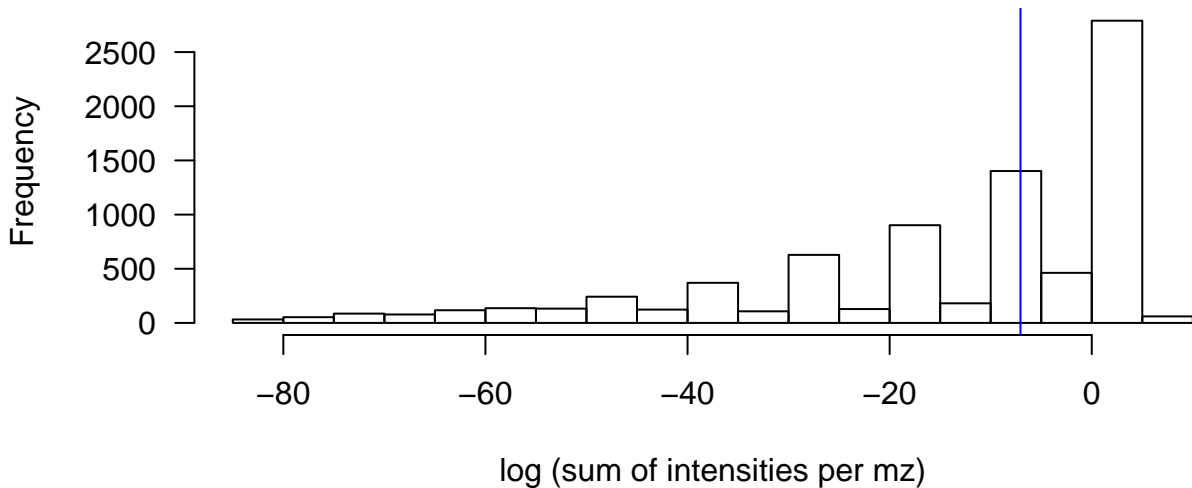
11a) Number of peaks for each mz

11b) Number of peaks per mz

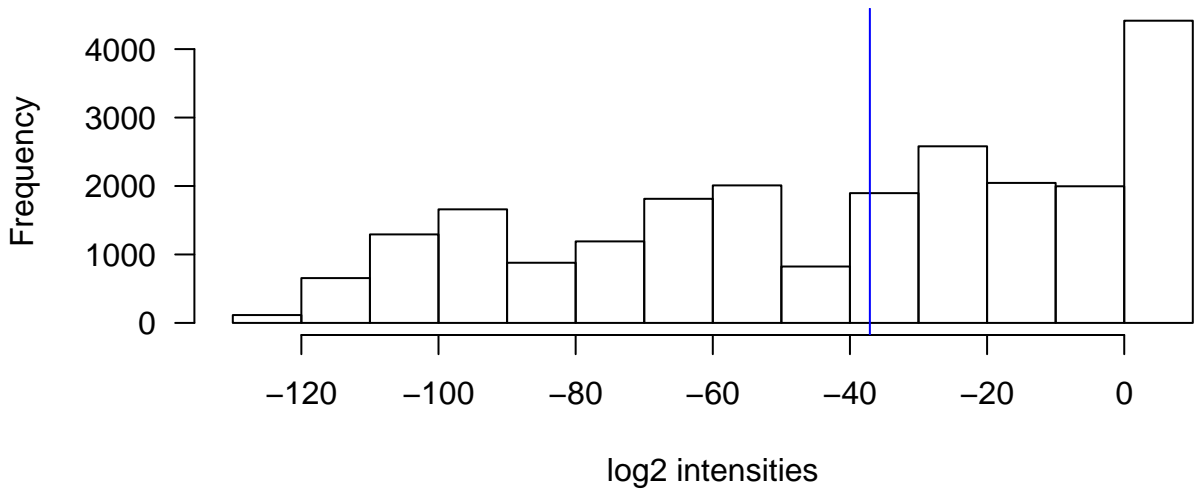**12a) Sum of all peak intensities for each mz**

Intensity sum
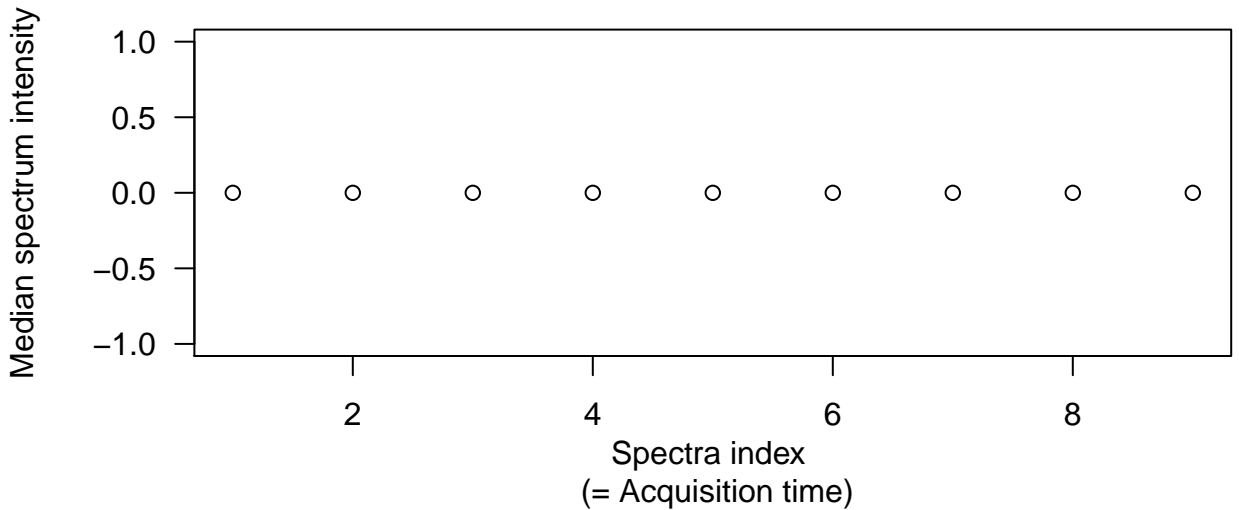
mz in Dalton

12b) Sum of intensities per mz
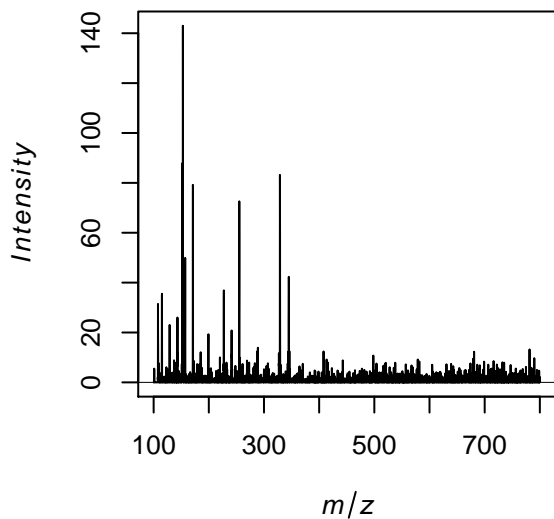
Frequency

log (sum of intensities per mz)
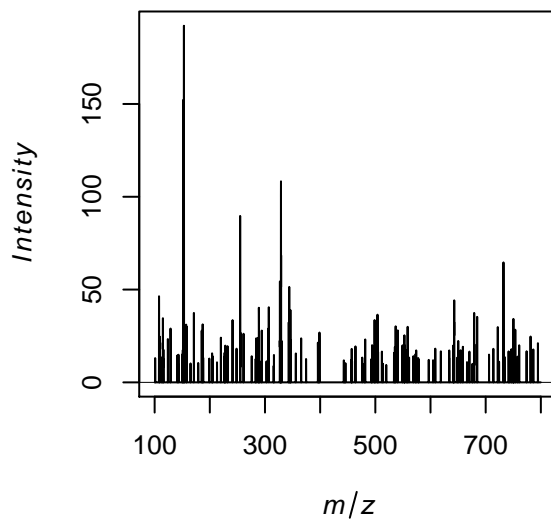
13a) Log2–transformed intensities

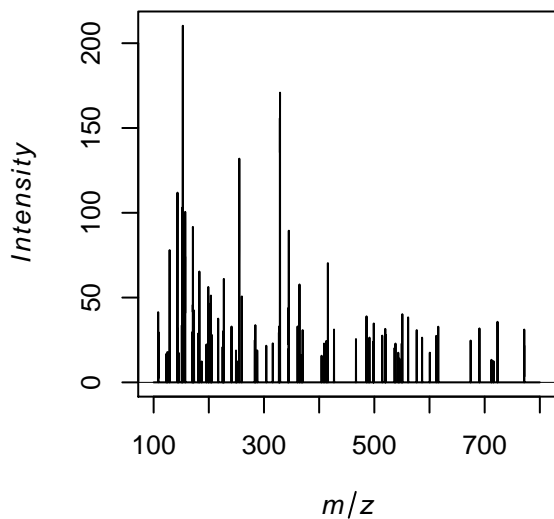**13b) Median intensity per spectrum**

Average spectrum

Spectrum in middle of acquisition

Spectrum at x = 1, y = 1

Spectrum at x = 3, y = 2