Testfile_analyze75

| properties	values
Number of m/z features	3672
Range of m/z values	1199.47 – 1356.08
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	3 – 84
Median of intensities	9
Intensities > 0	100 %
Number of empty spectra	0
Median TIC ± sd	37005 ± 5329
Median # peaks per spectrum ± sd	3672 ± 0
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile2.txt	1 / 3

Pixel order
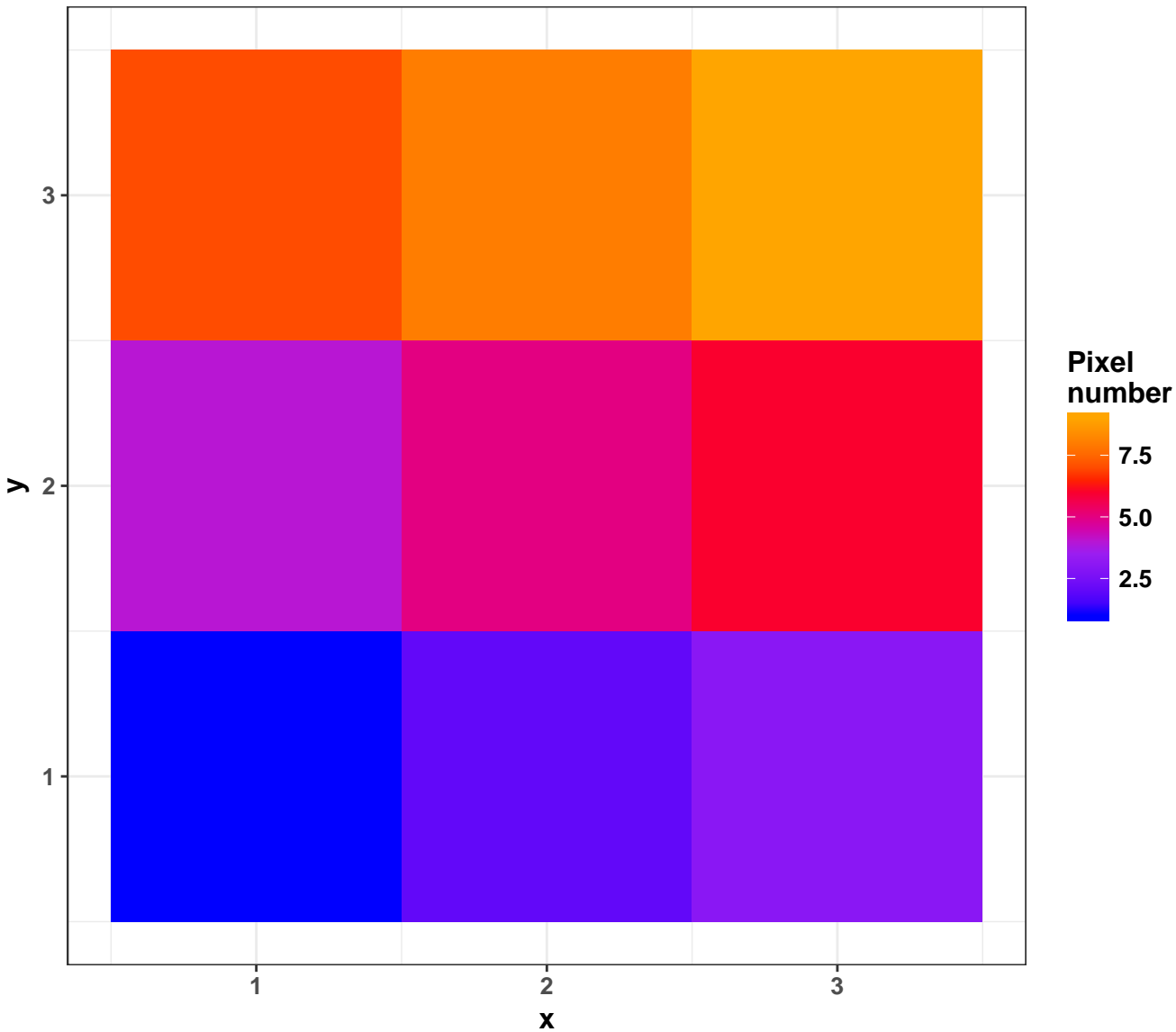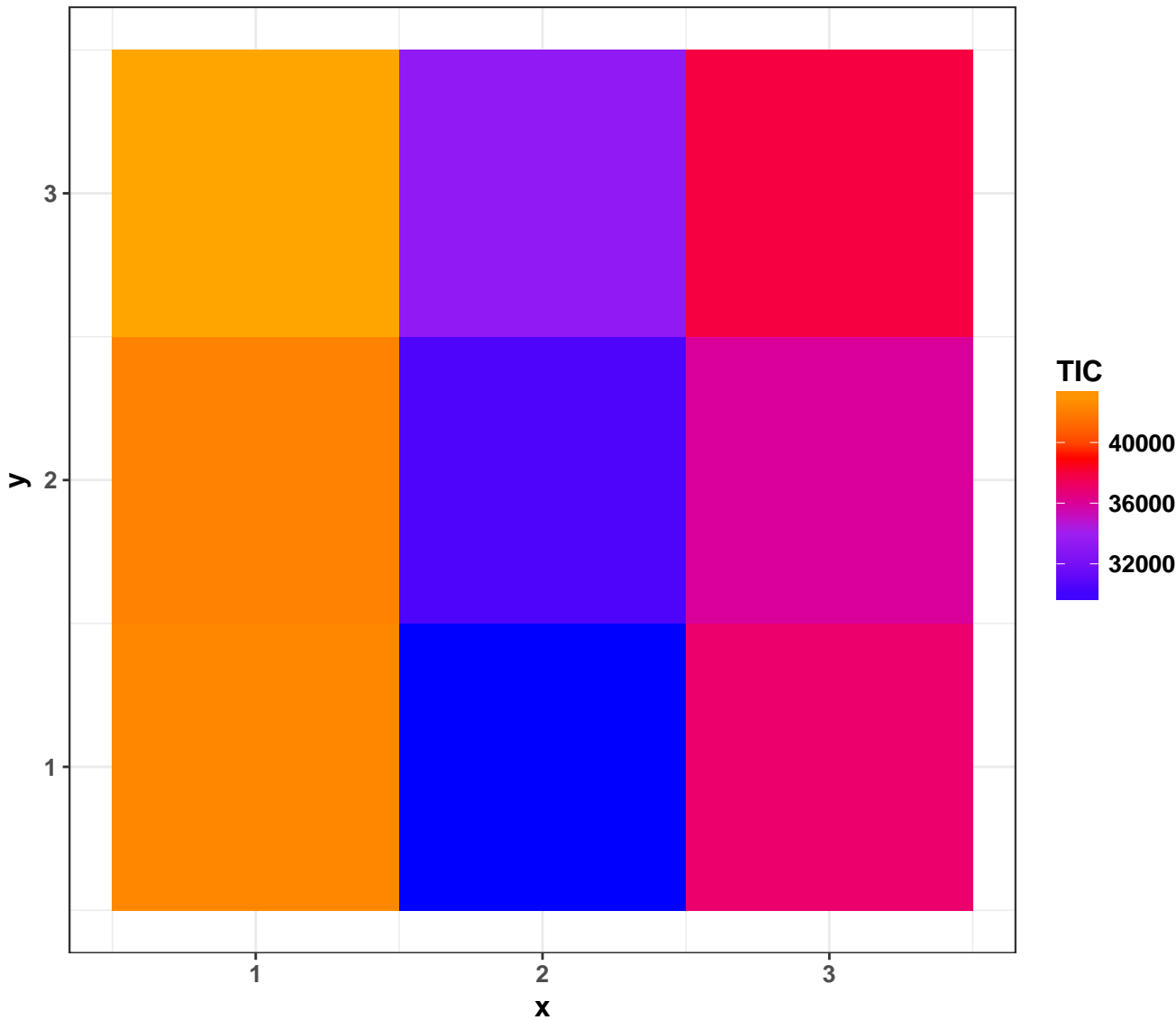
Number of calibrants per pixel (±200 ppm)
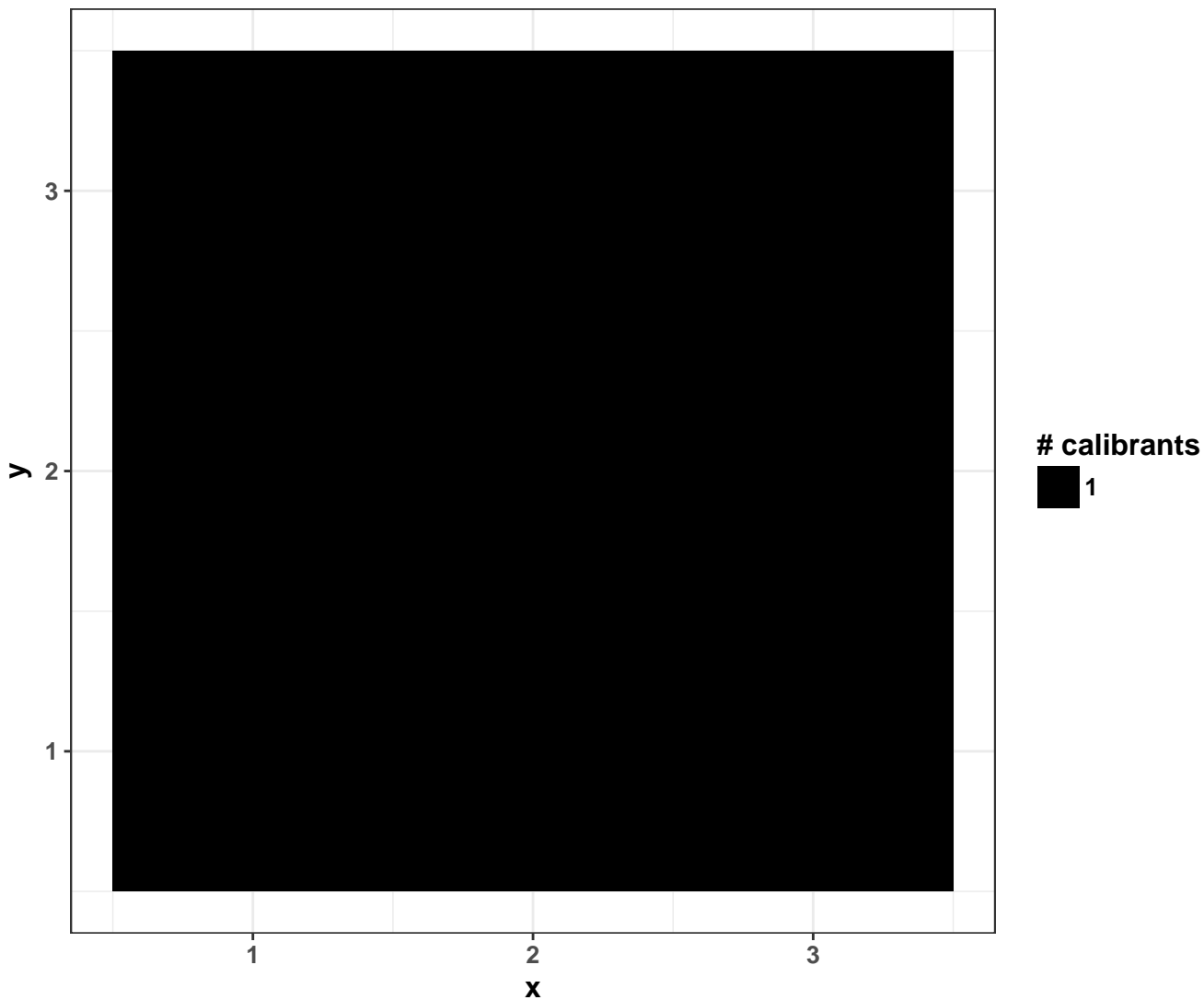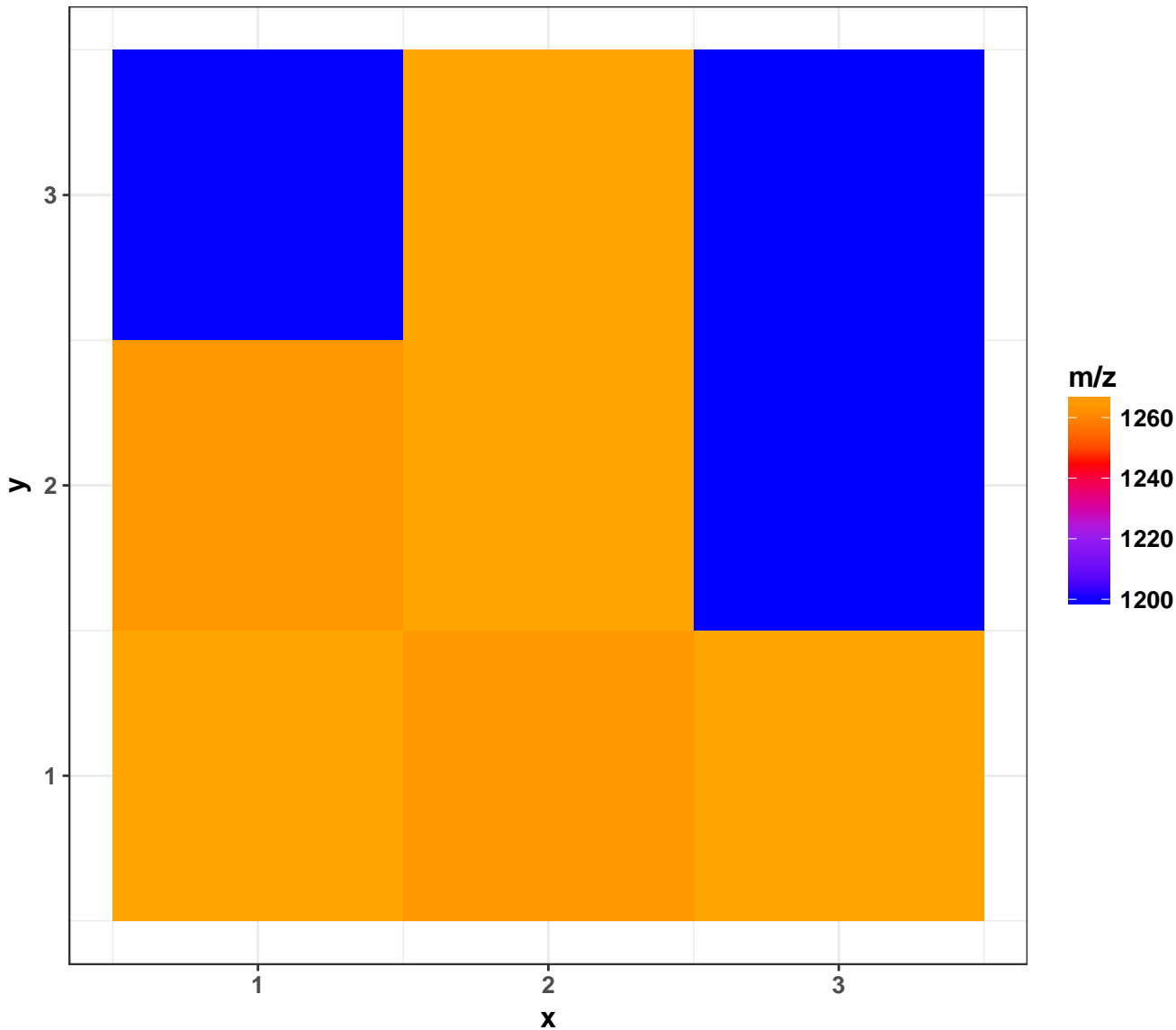
mass3: 1296.7 (±200 ppm)
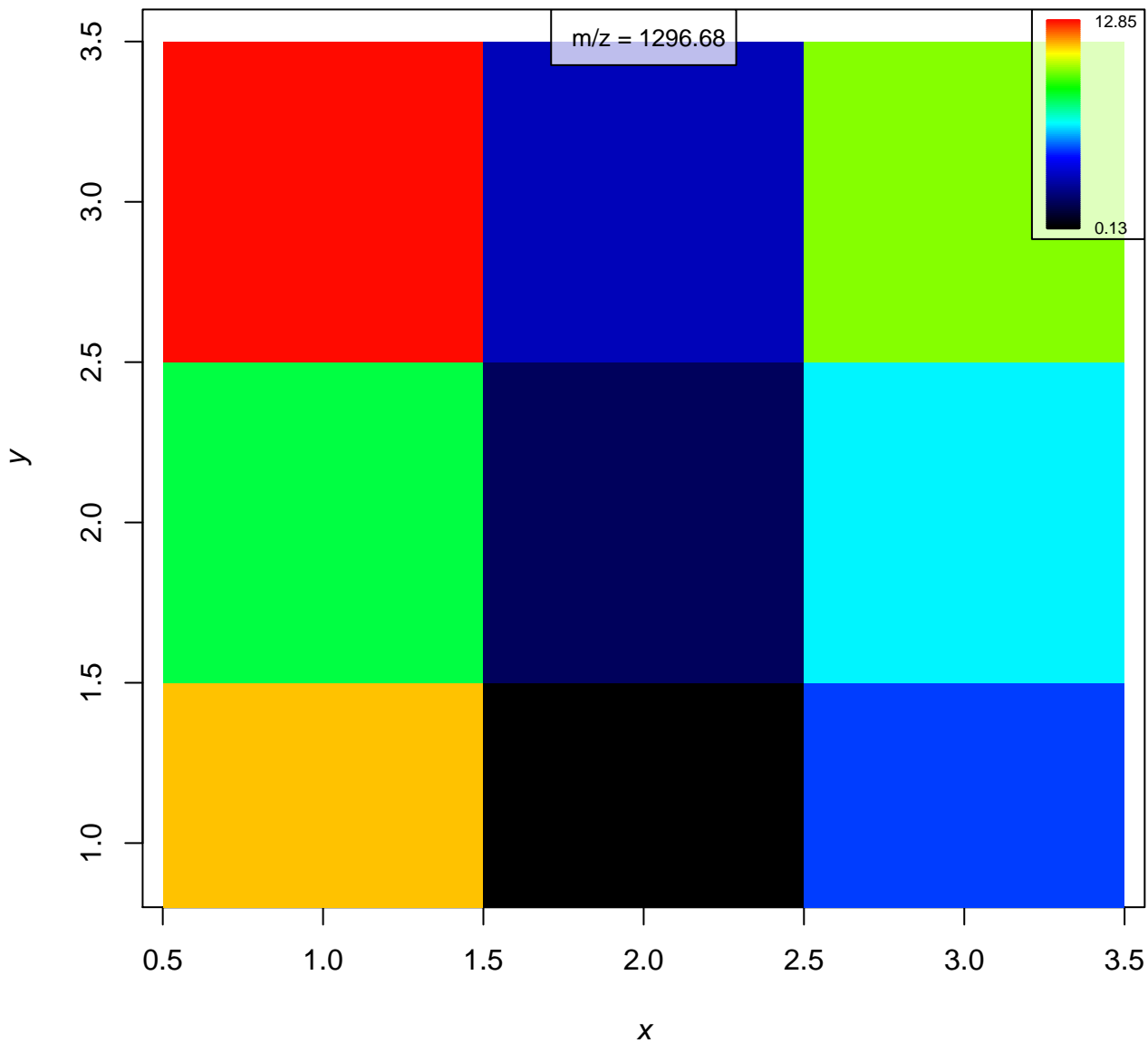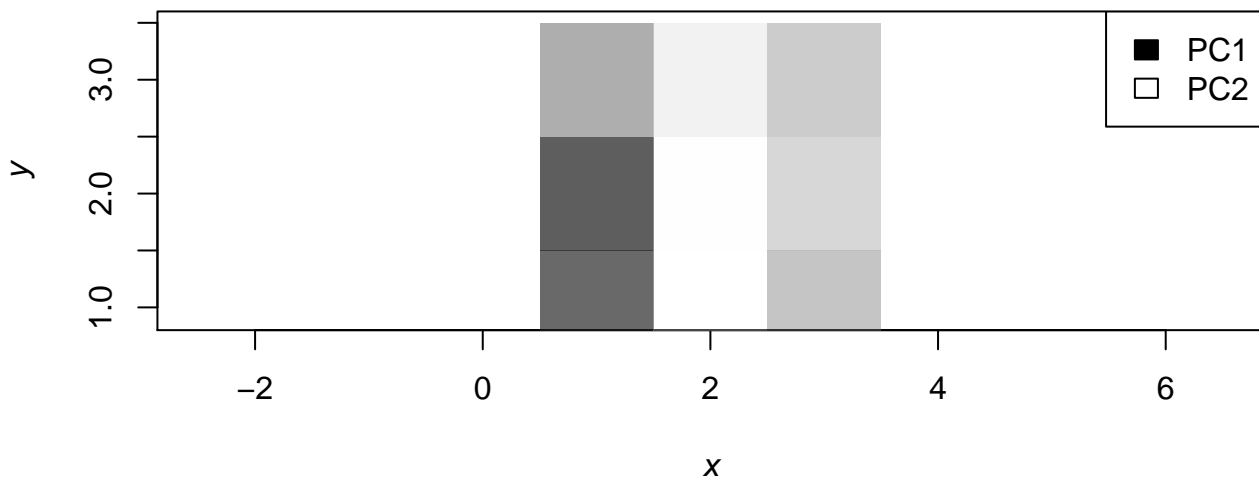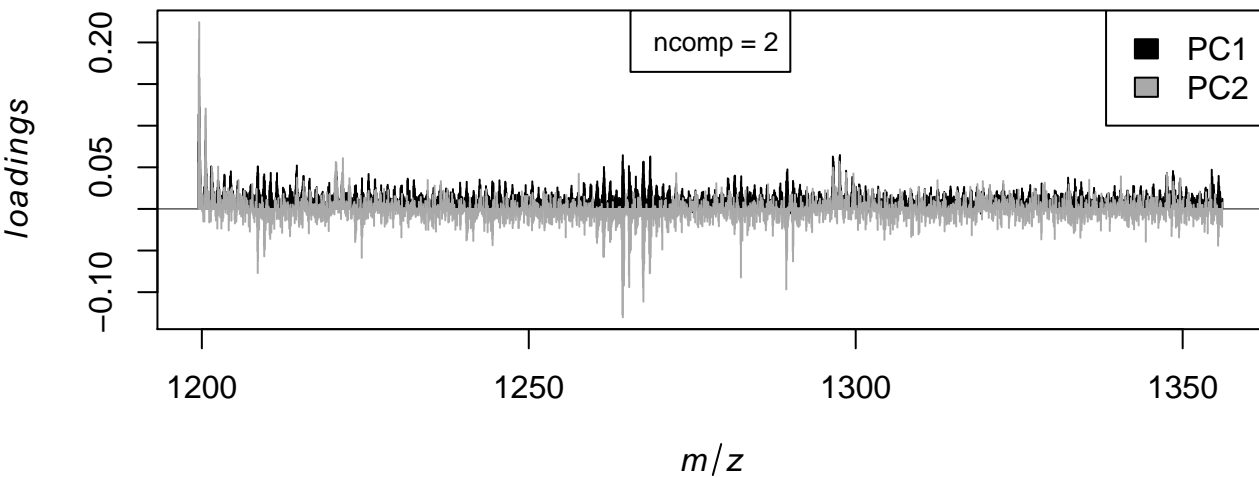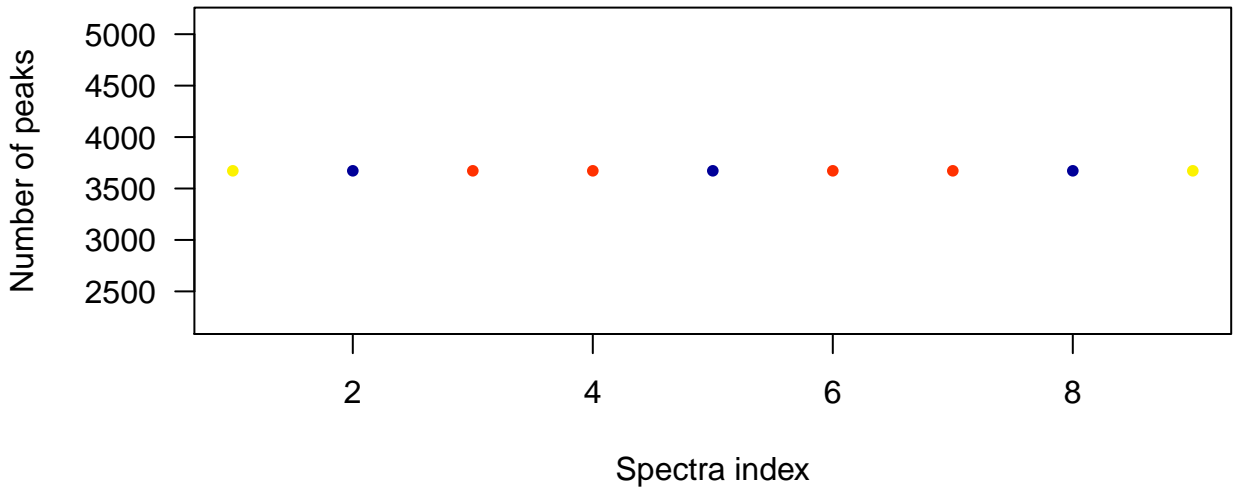
Number of peaks per spectrum
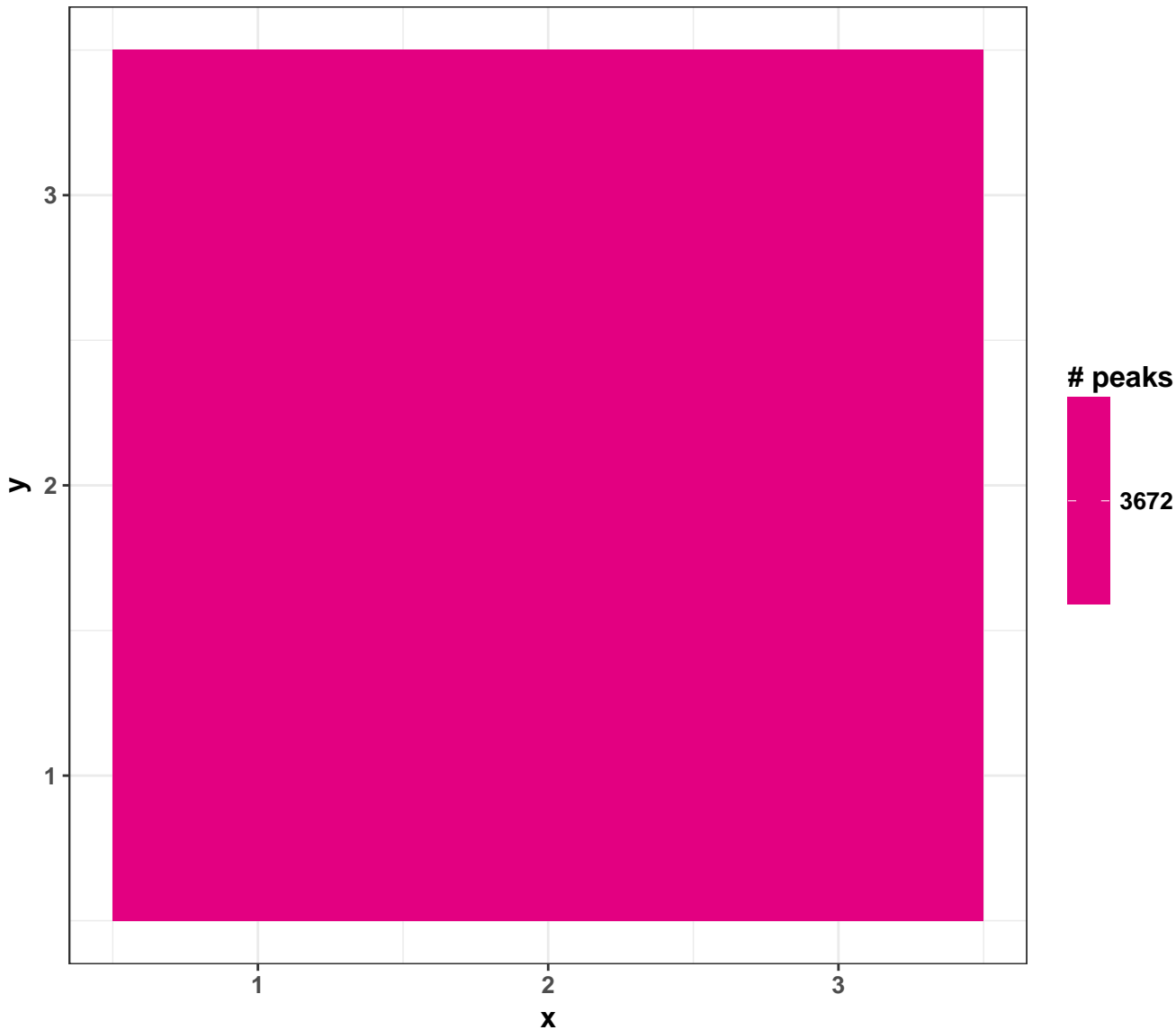
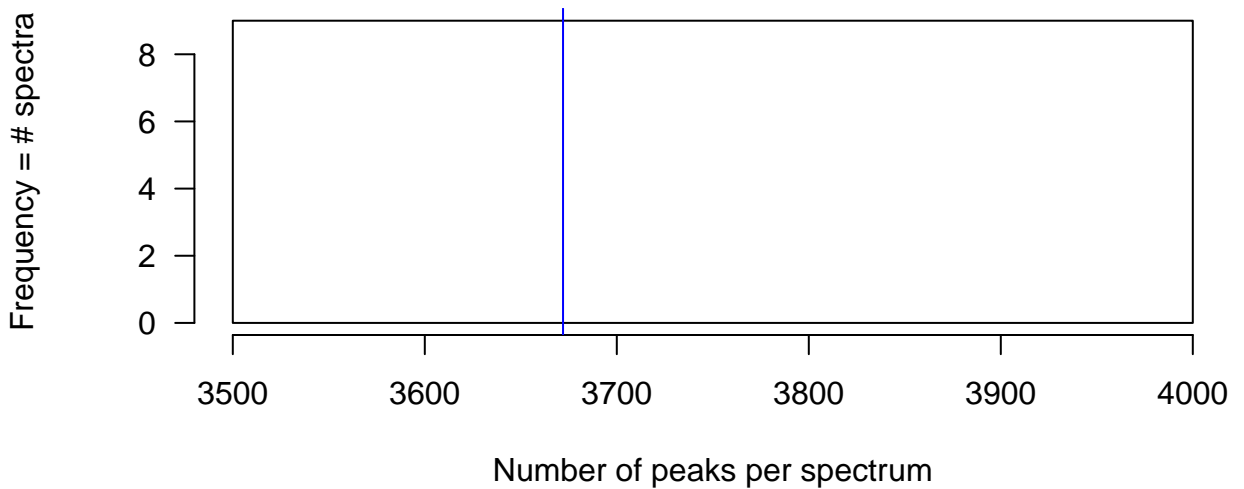**Total Ion Chromatogram**

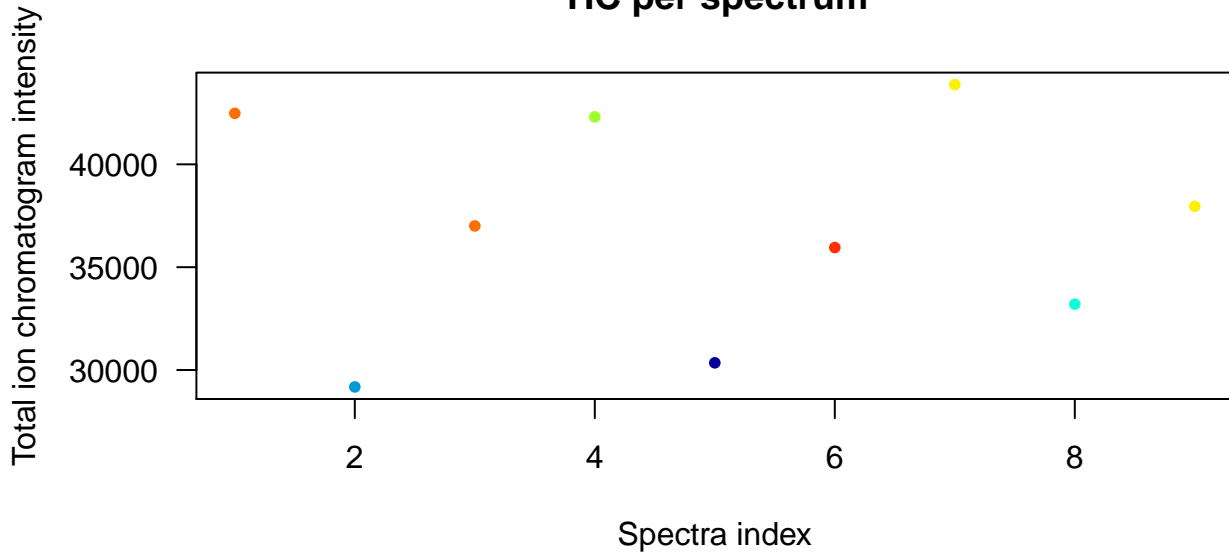**Most abundant m/z in each spectrum**
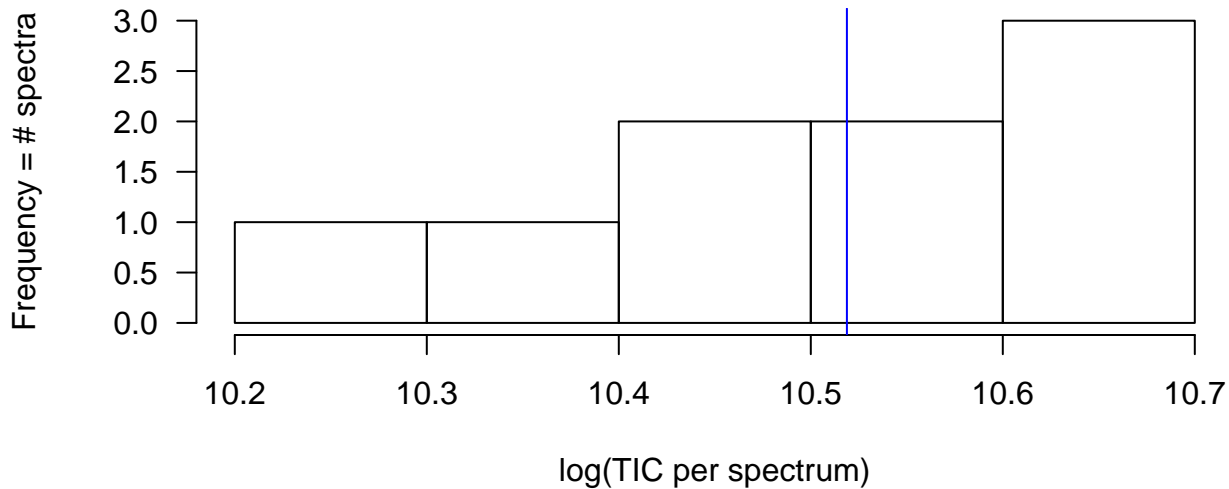
PCA for two components

Number of peaks per spectrum
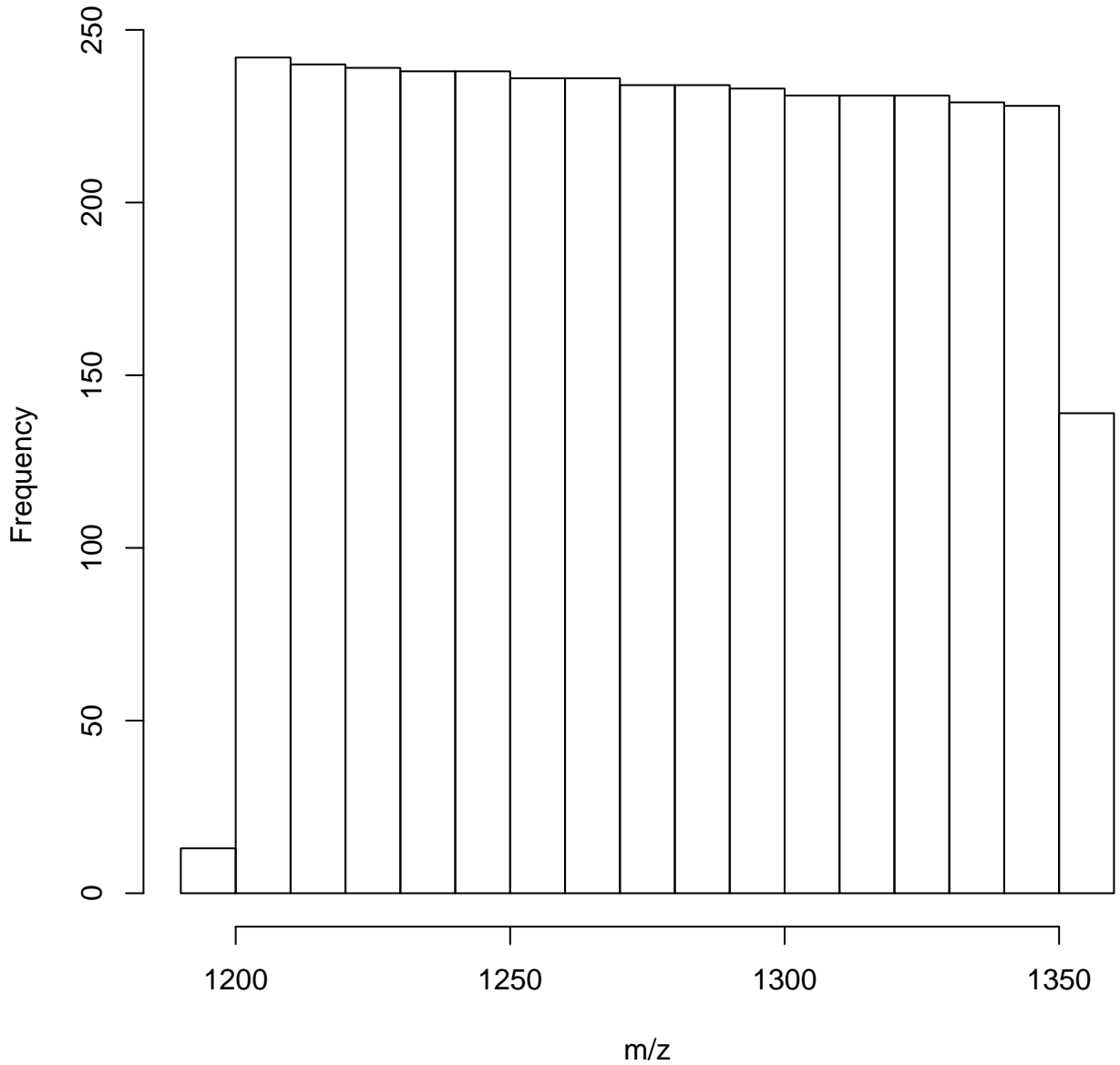
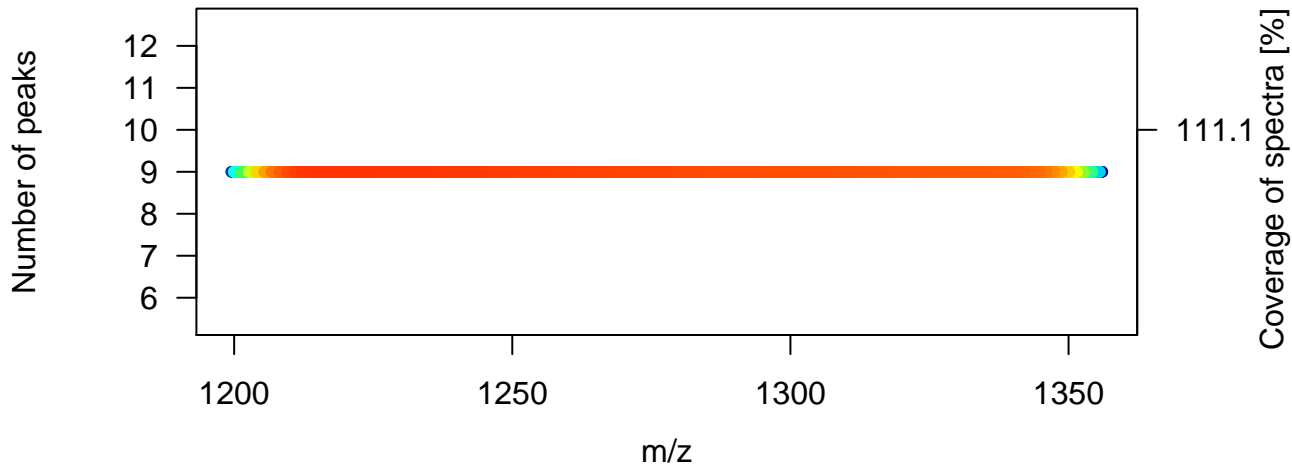**Number of peaks per spectrum**

TIC per spectrum

Total ion chromatogram intensity vs Spectra index

TIC per spectrum

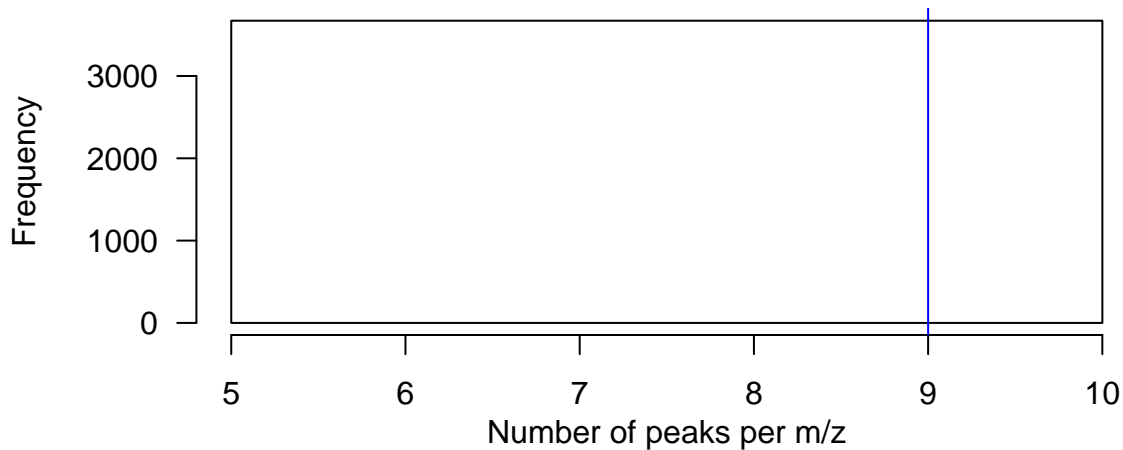Frequency = # spectra vs log(TIC per spectrum)
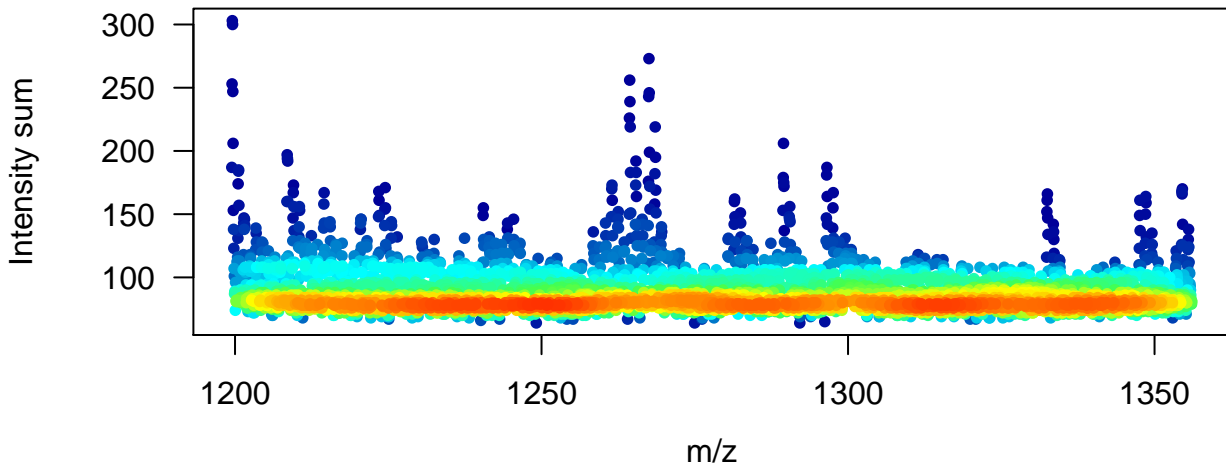
Histogram of m/z values
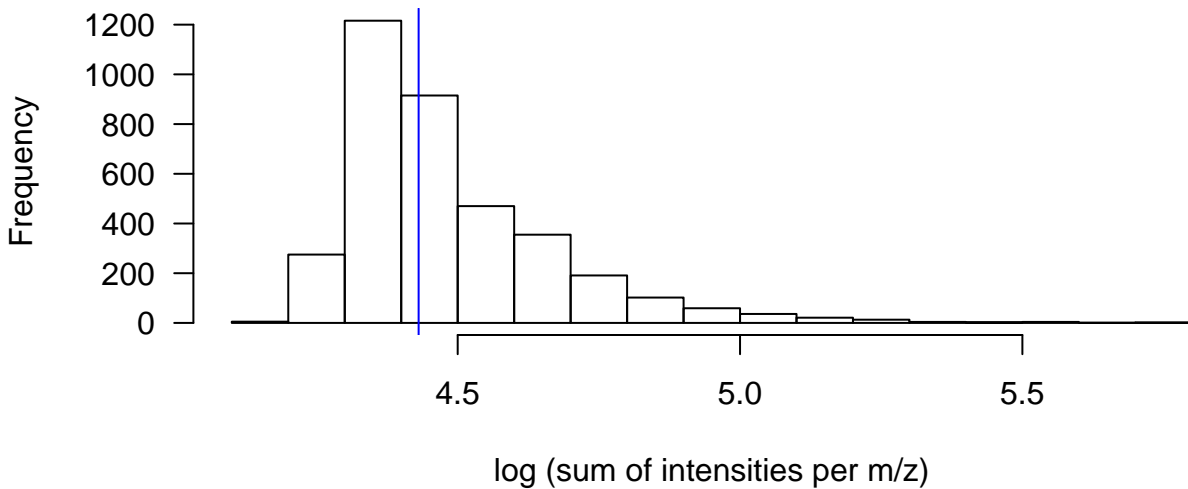
Number of peaks per m/z
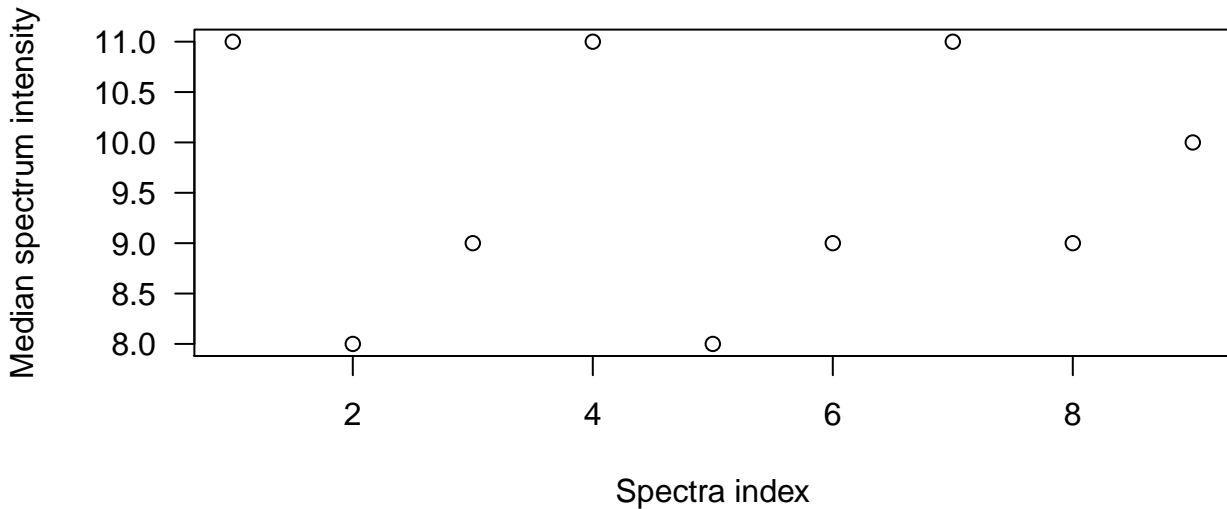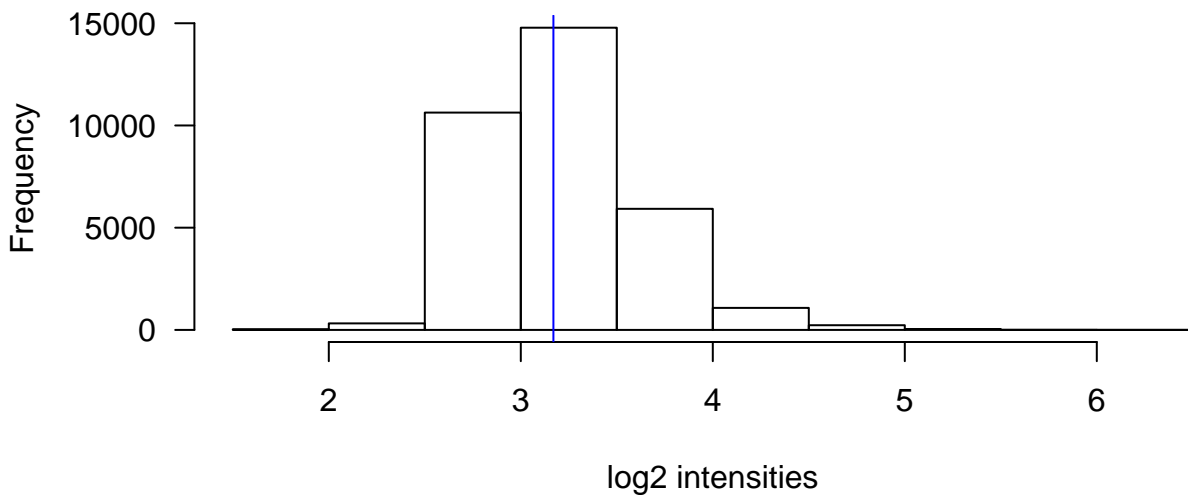

Number of peaks per m/z

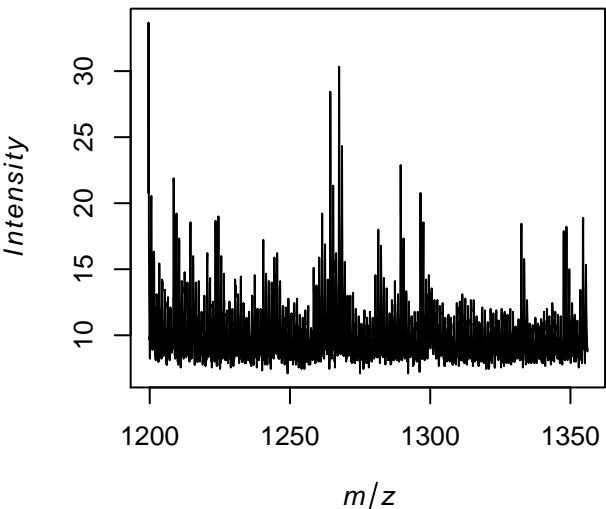# Sum of intensities per m/z

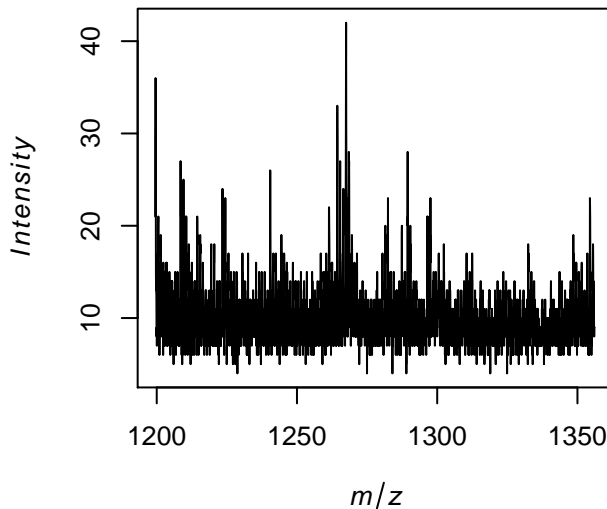# Sum of intensities per m/z

Median intensity per spectrum

Median spectrum intensity

Spectra index

Log2−transformed intensities

Frequency

log2 intensities

Average spectrum — *Intensity* vs *m/z*

Spectrum at x = 3, y = 1 — *Intensity* vs *m/z*

Spectrum at x = 1, y = 2 — *Intensity* vs *m/z*

Spectrum at x = 3, y = 3 — *Intensity* vs *m/z*

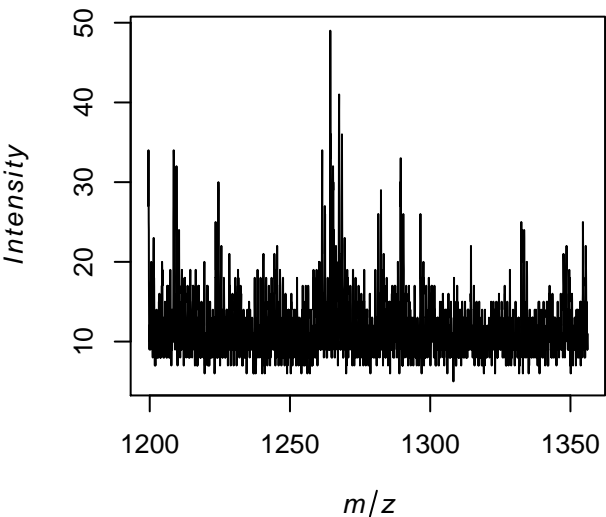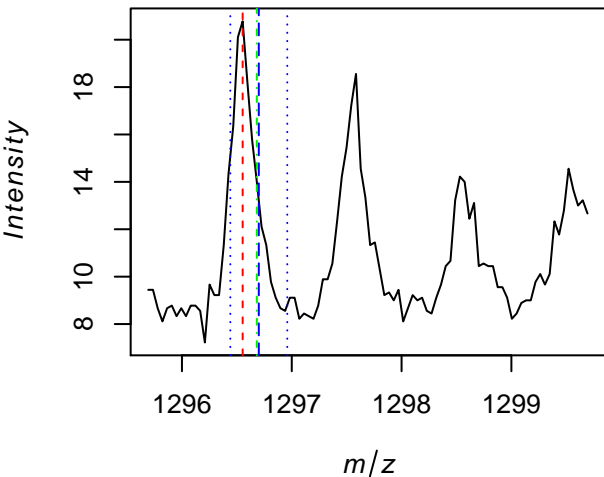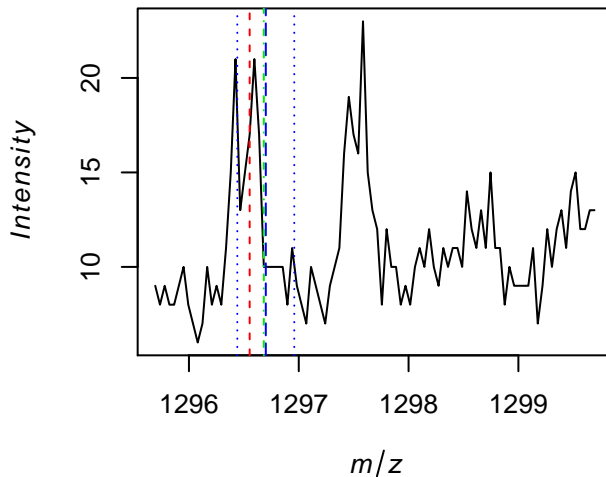theor. m/z: 1296.7   most abundant m/z: 1296.5529   closest m/z: 1296.6819
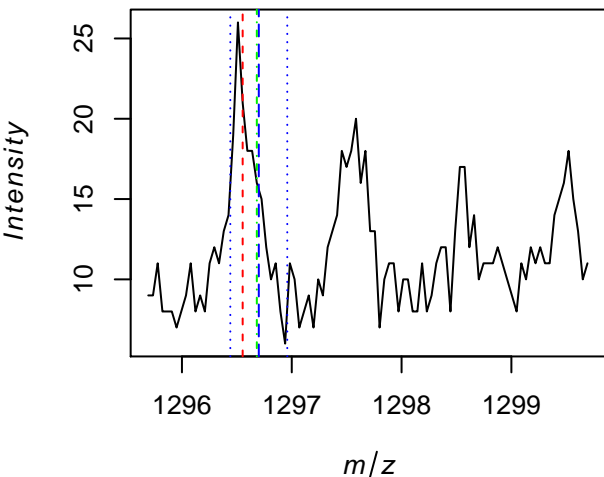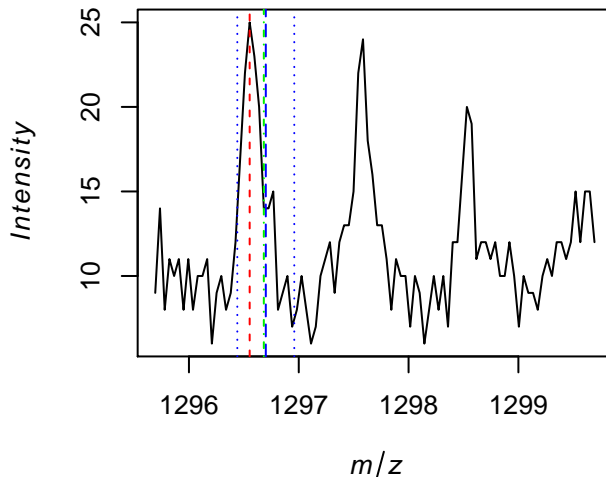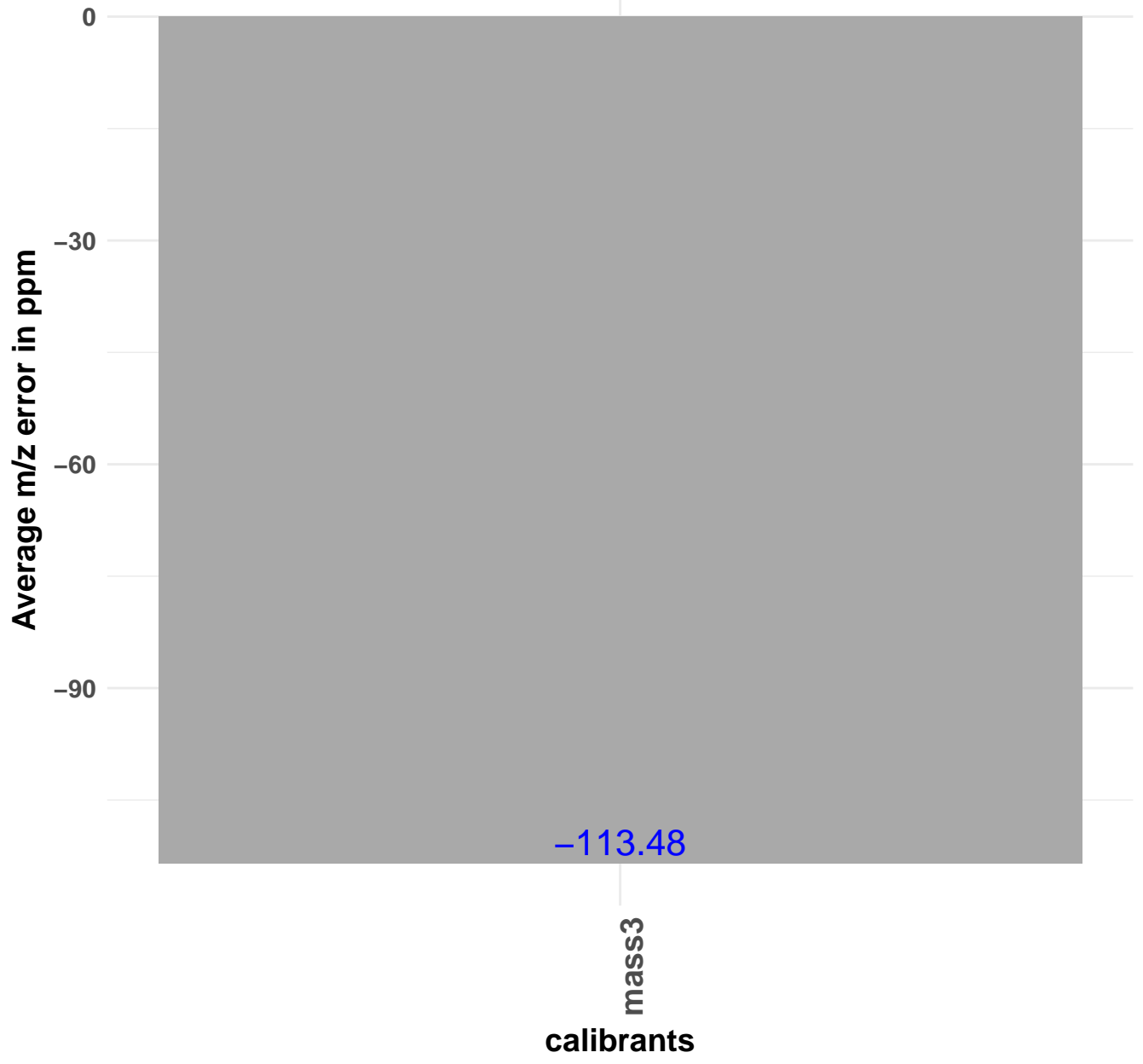
Average spectrum

Spectrum at x = 3, y = 1

Spectrum at x = 1, y = 2

Spectrum at x = 3, y = 3

Average m/z error (max. average intensity vs. theor. calibrant m/z)

Average m/z error in ppm

0

−30

−60

−90

−113.48

mass3

calibrants

Average m/z error (closest measured m/z vs. theor. calibrant m/z)

Average m/z error in ppm

0

−5

−10

−13.97

mass3

calibrants

Difference m/z with max. average intensity vs. theor. m/z (per spectrum)