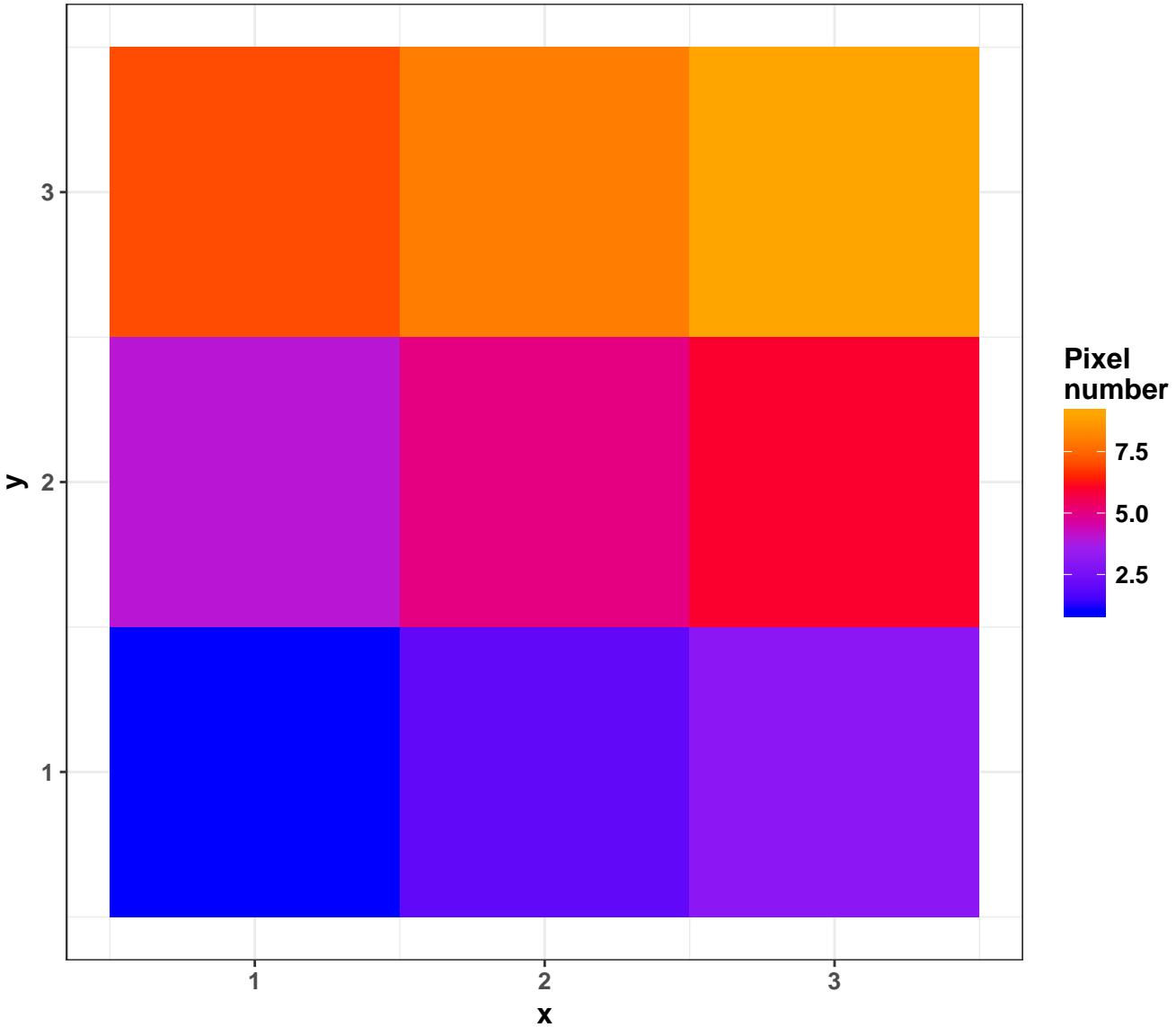


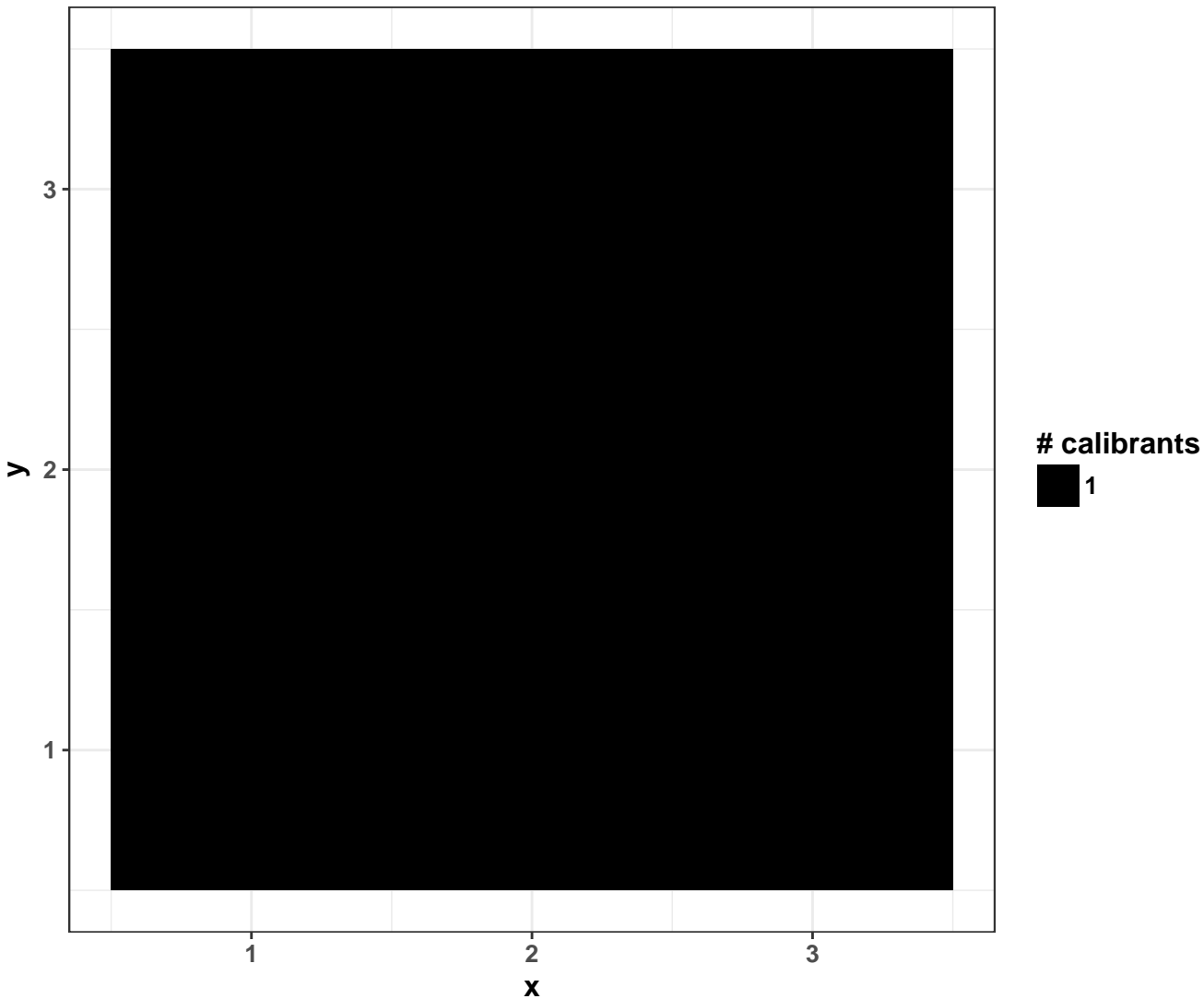
Testfile_analyze75

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	37005
Median # peaks per spectrum	3672
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile2.txt	1 / 3

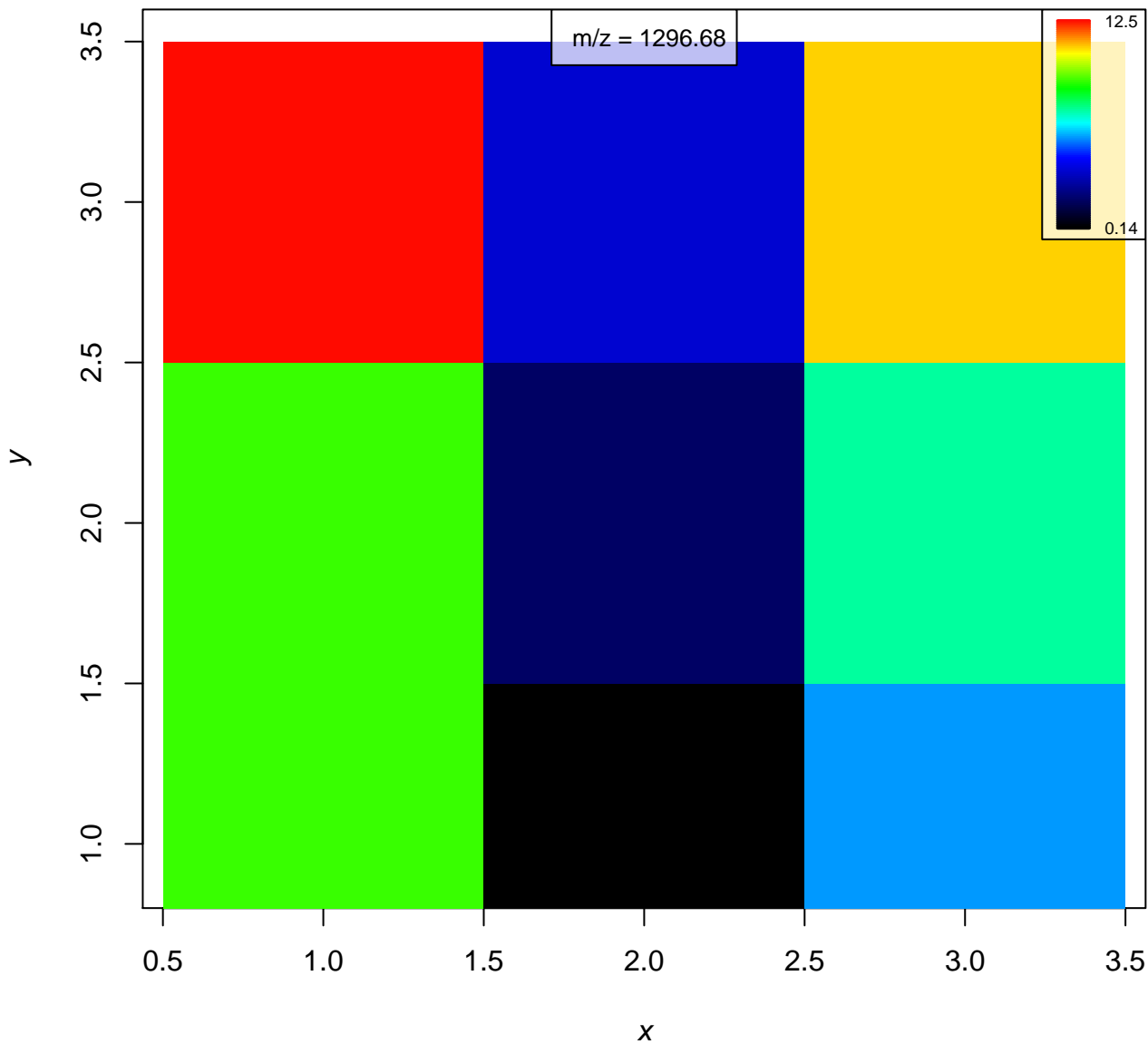
Pixel order



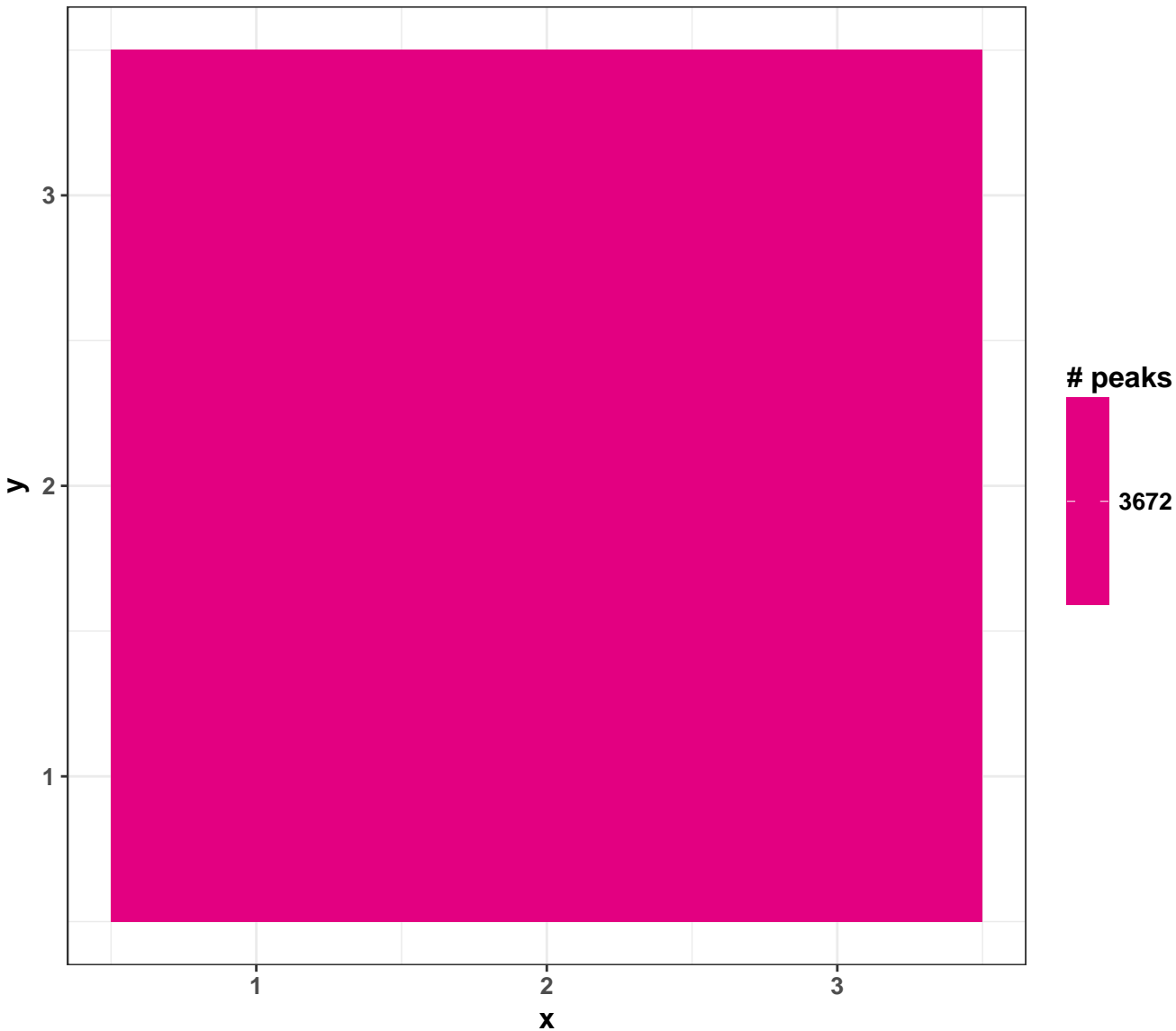
Number of calibrants per pixel (± 50 ppm)



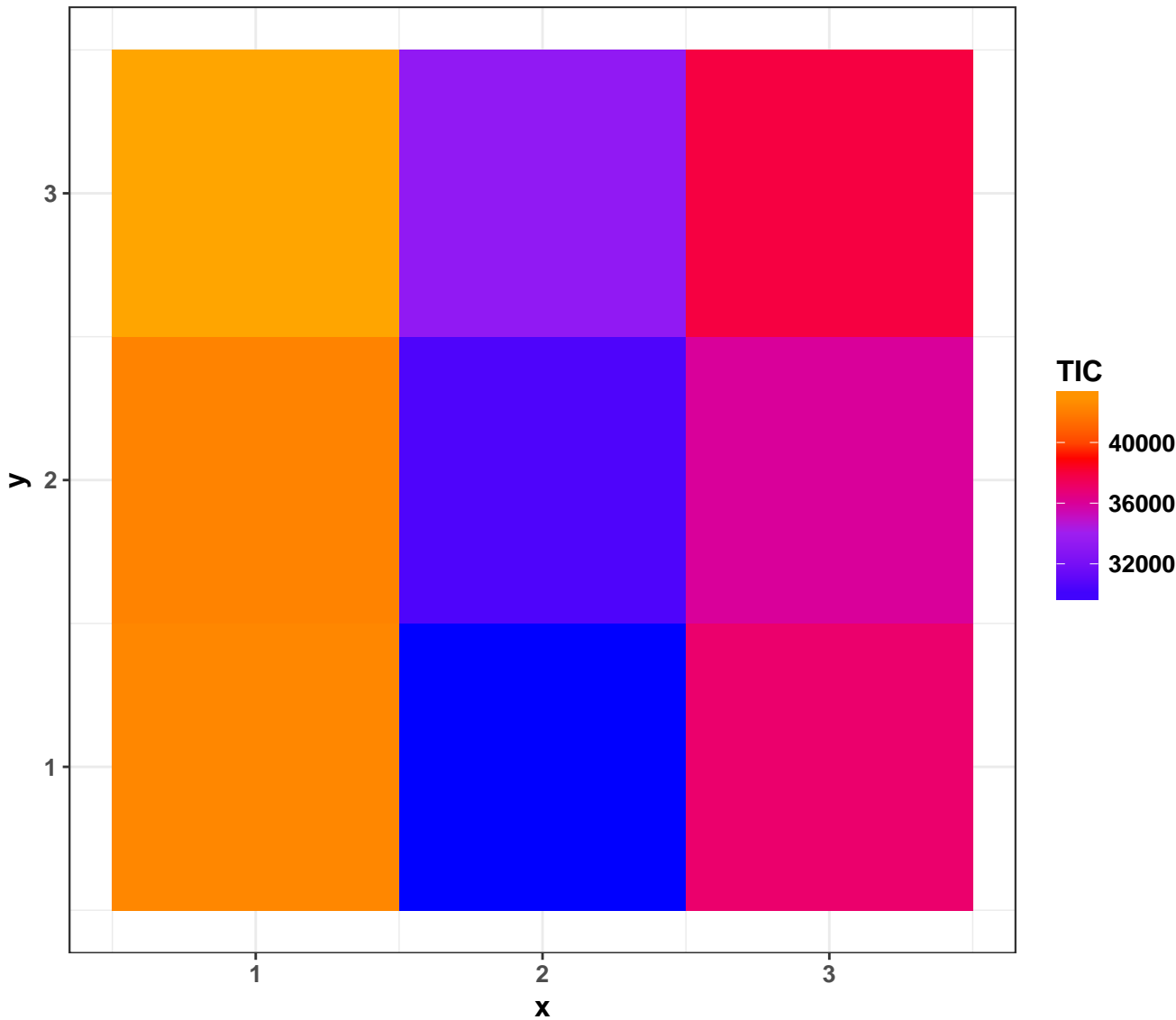
mass3: 1296.7 (± 50 ppm)



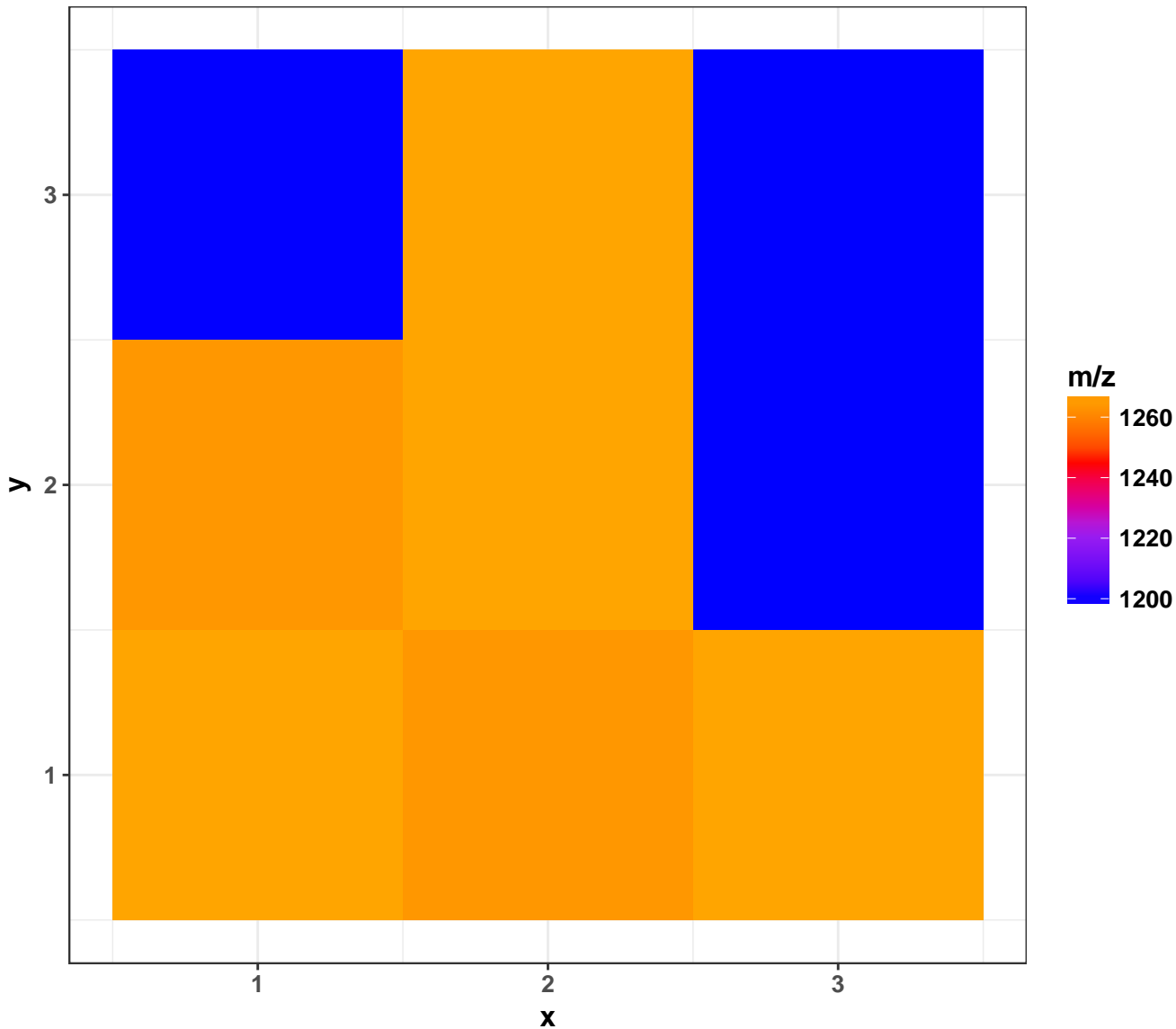
Number of peaks per spectrum



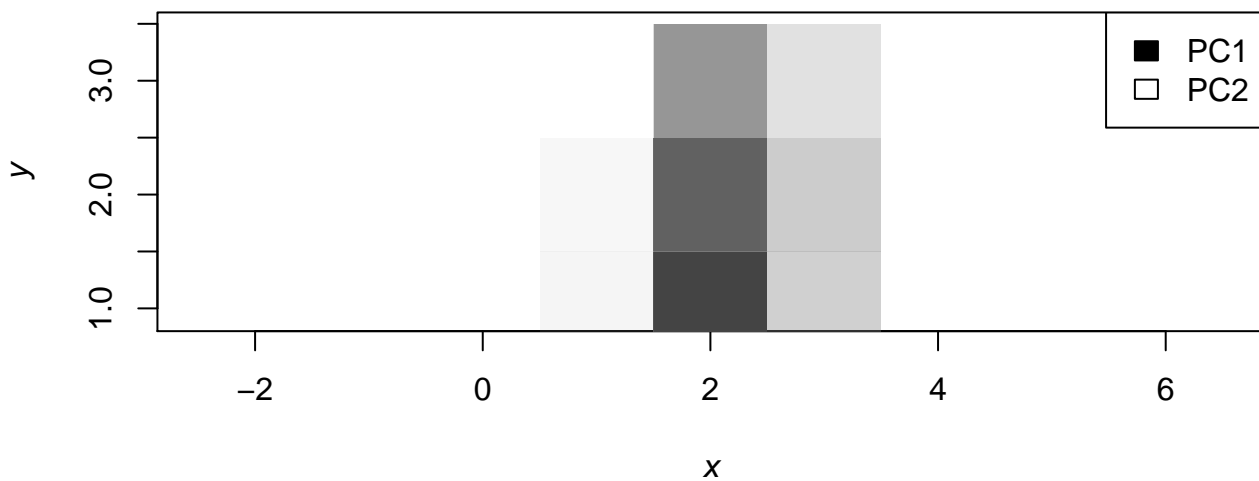
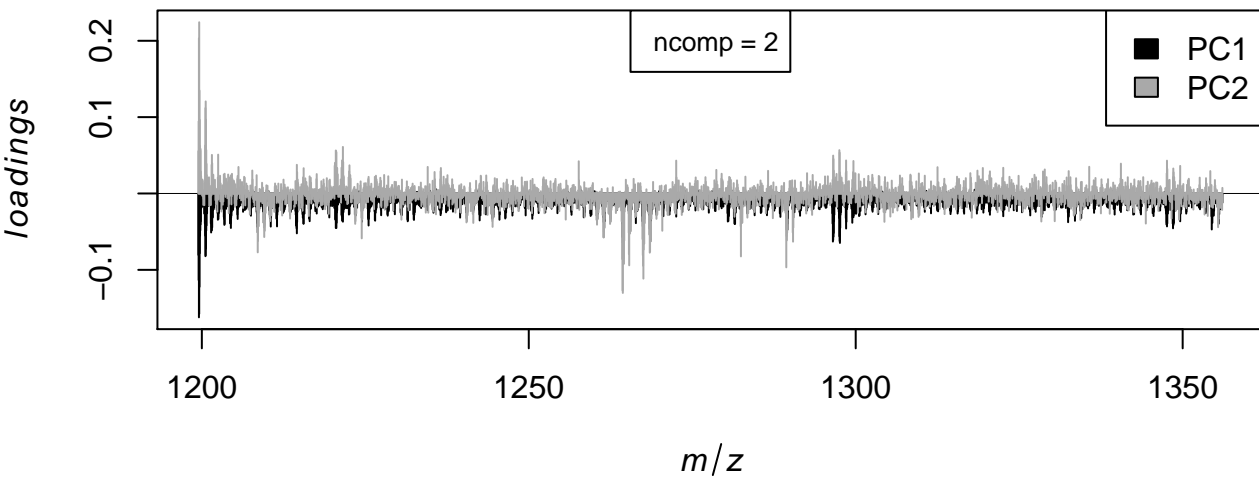
Total Ion Chromatogram



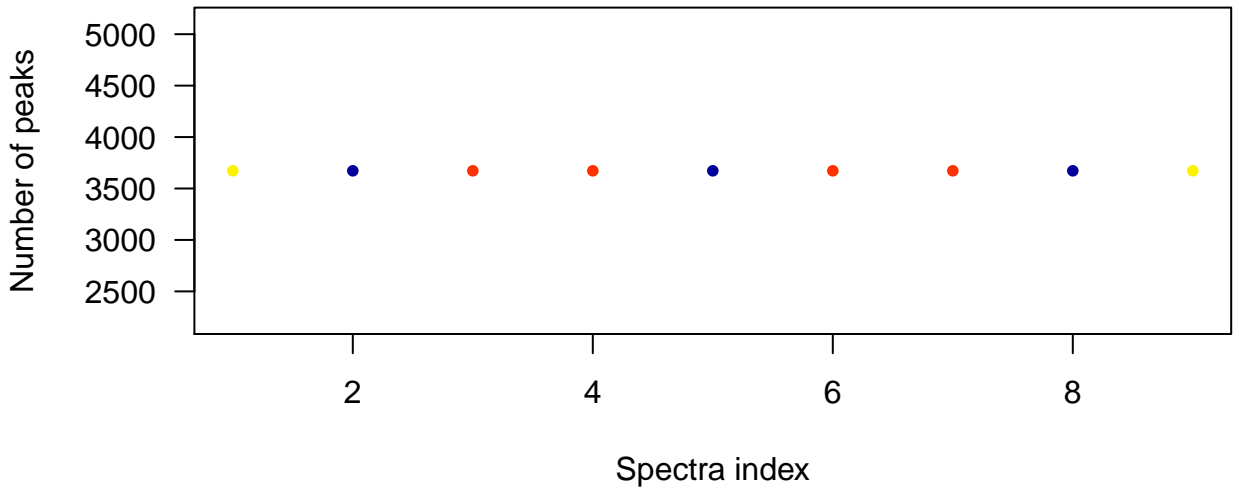
Most abundant m/z in each spectrum



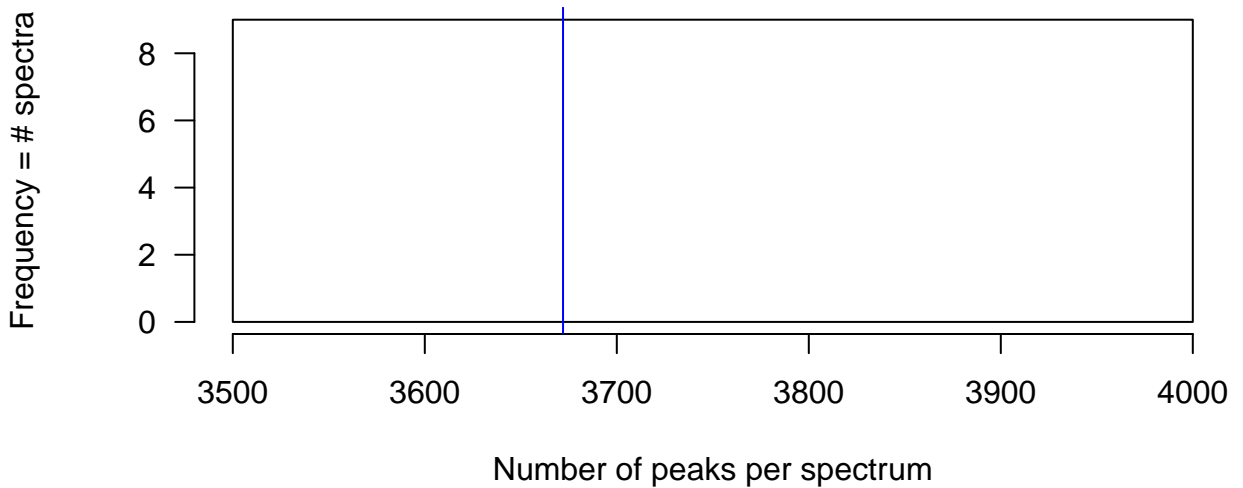
PCA for two components



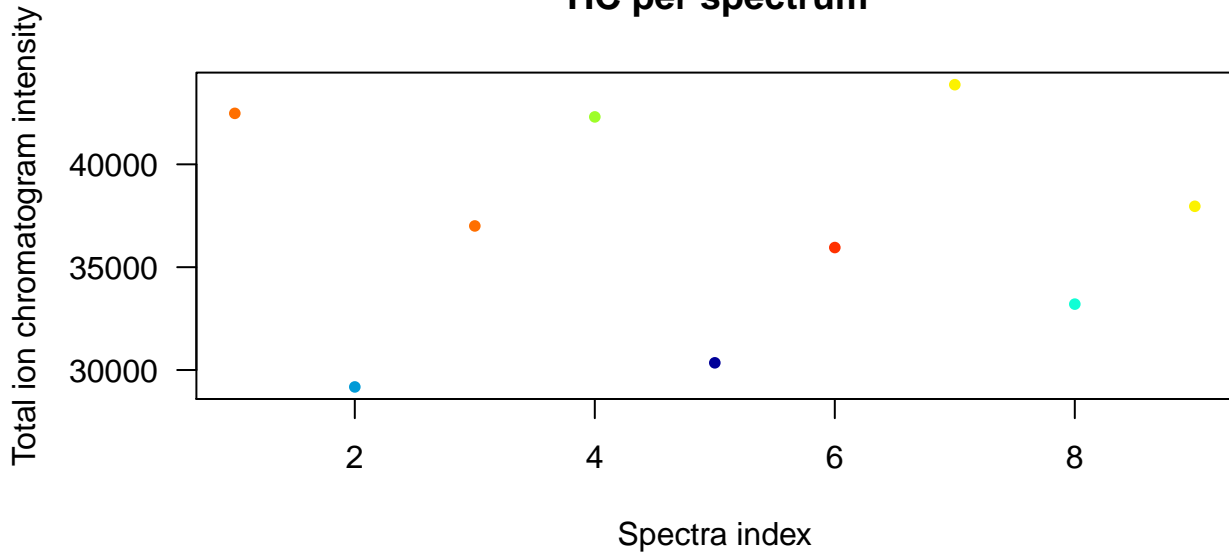
Number of peaks per spectrum



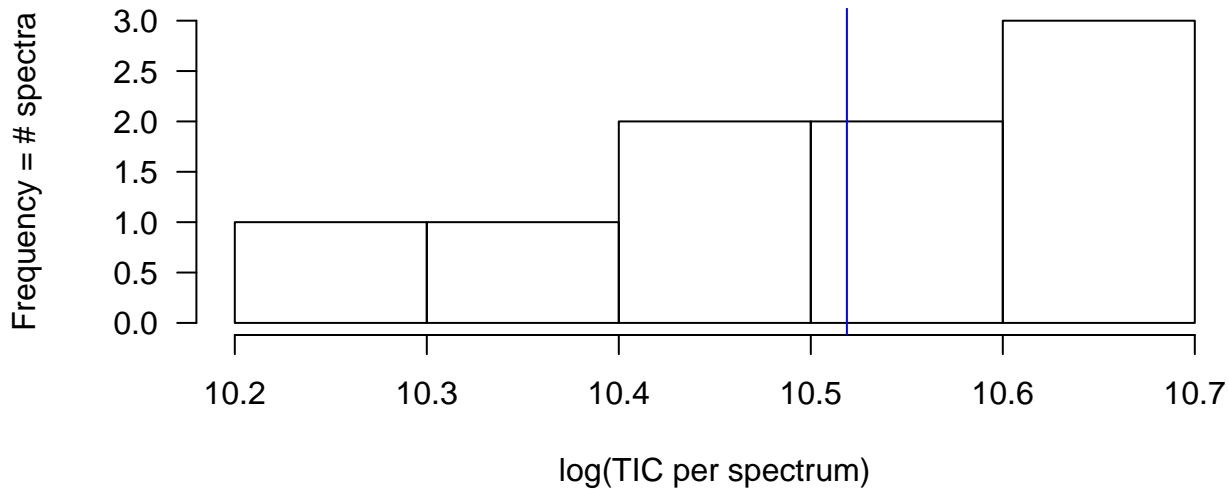
Number of peaks per spectrum



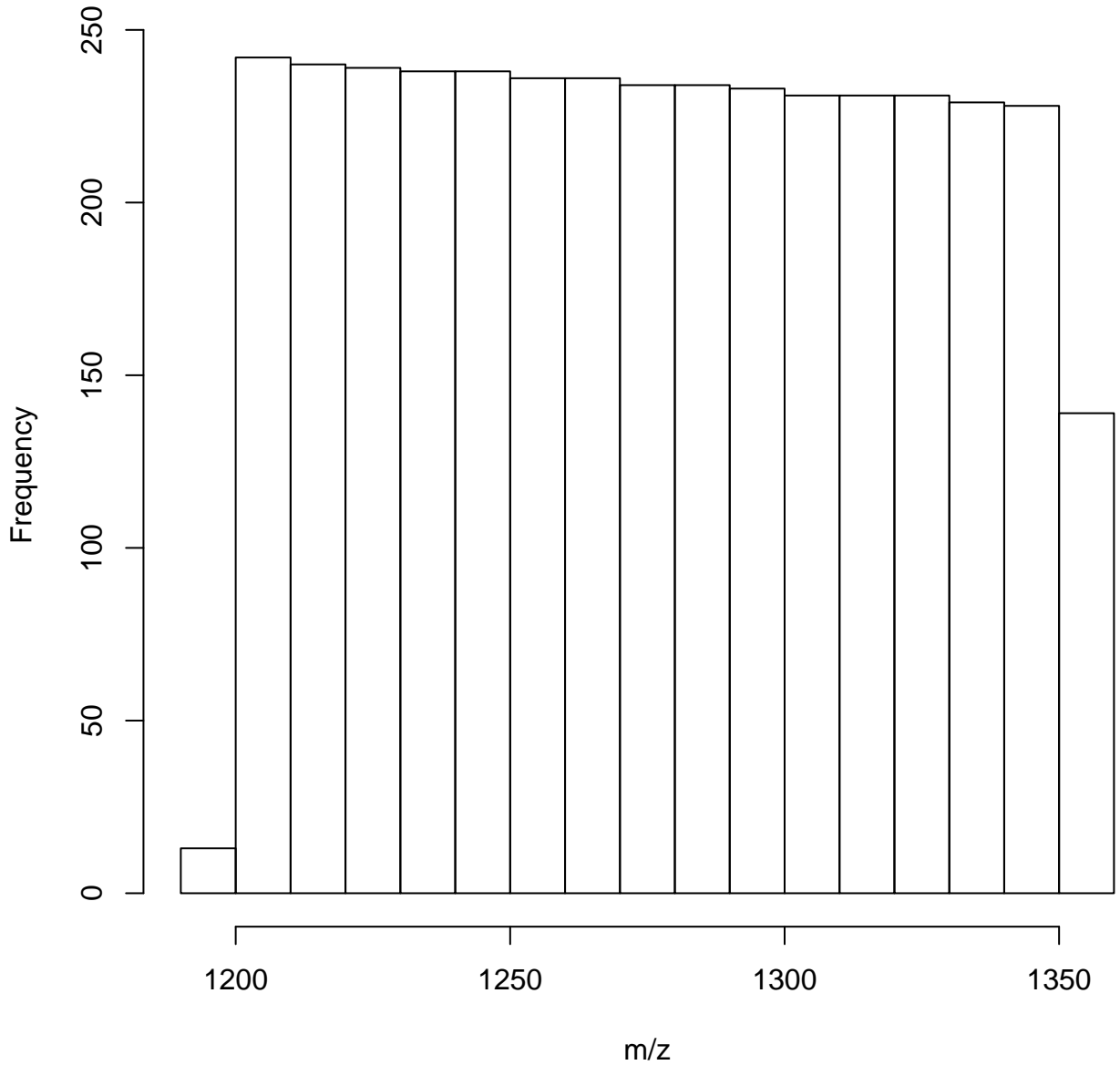
TIC per spectrum



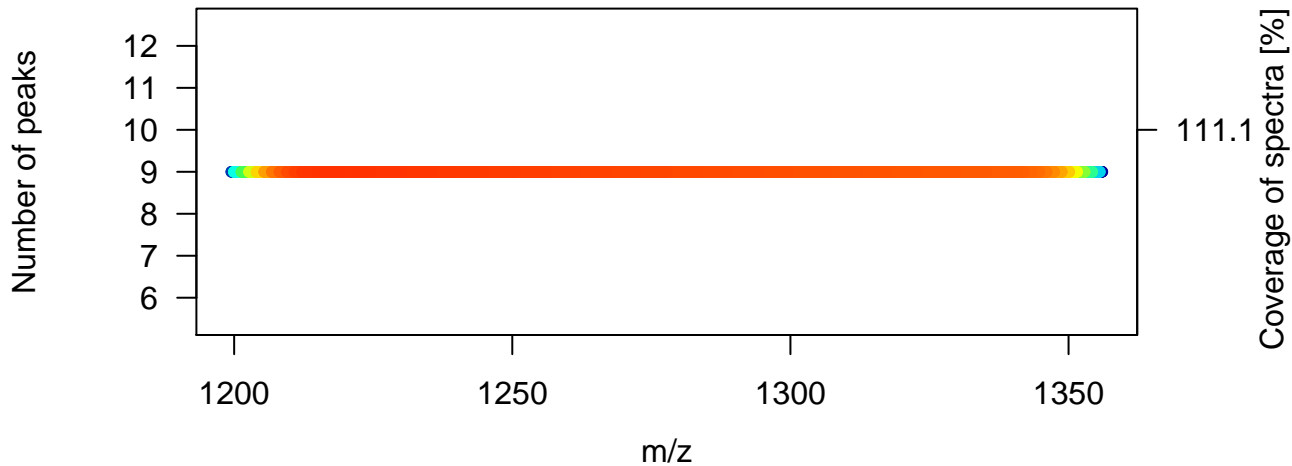
TIC per spectrum



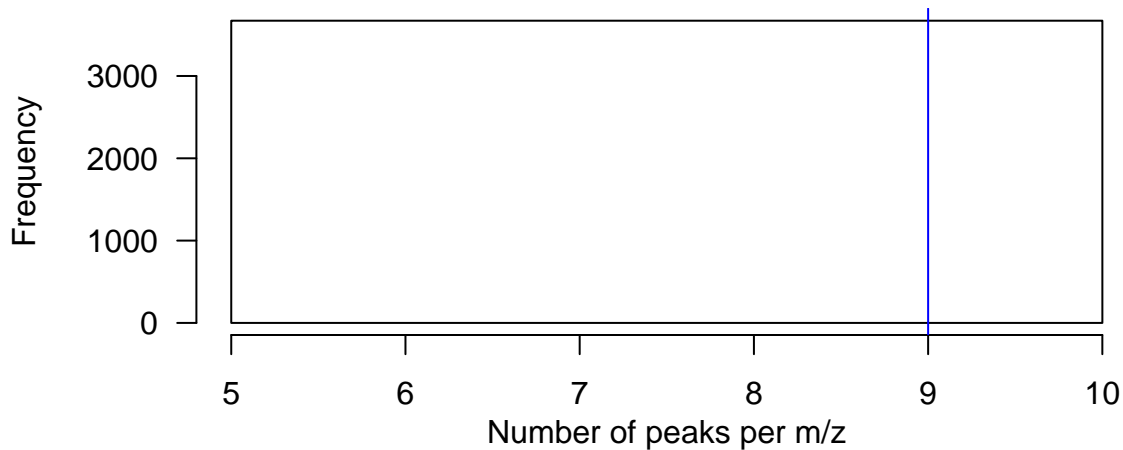
Histogram of m/z values



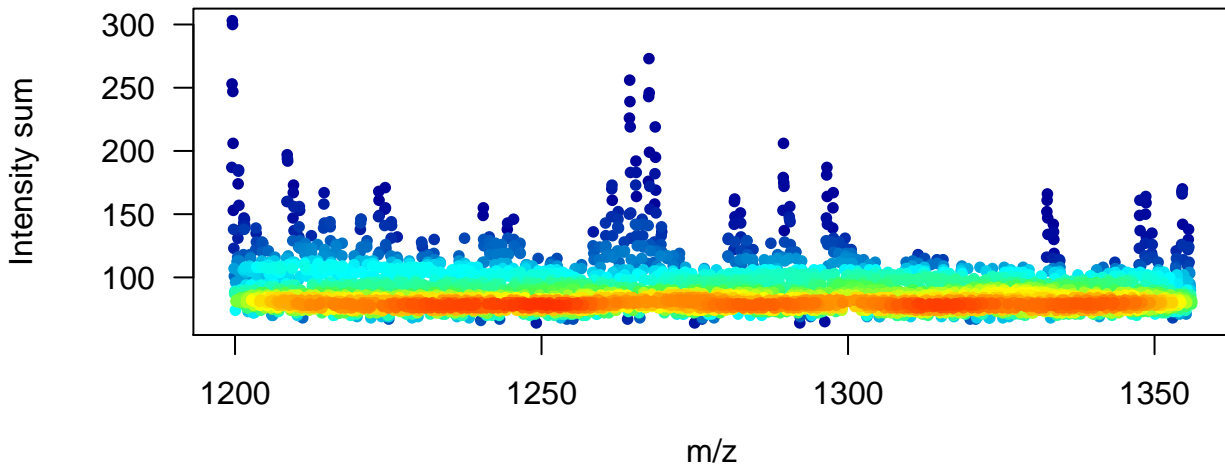
Number of peaks per m/z



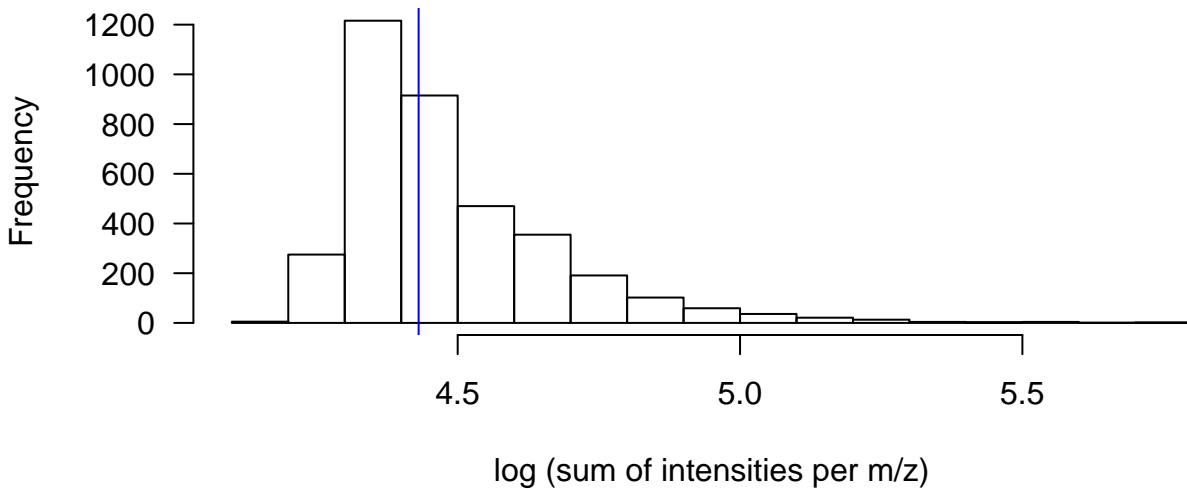
Number of peaks per m/z



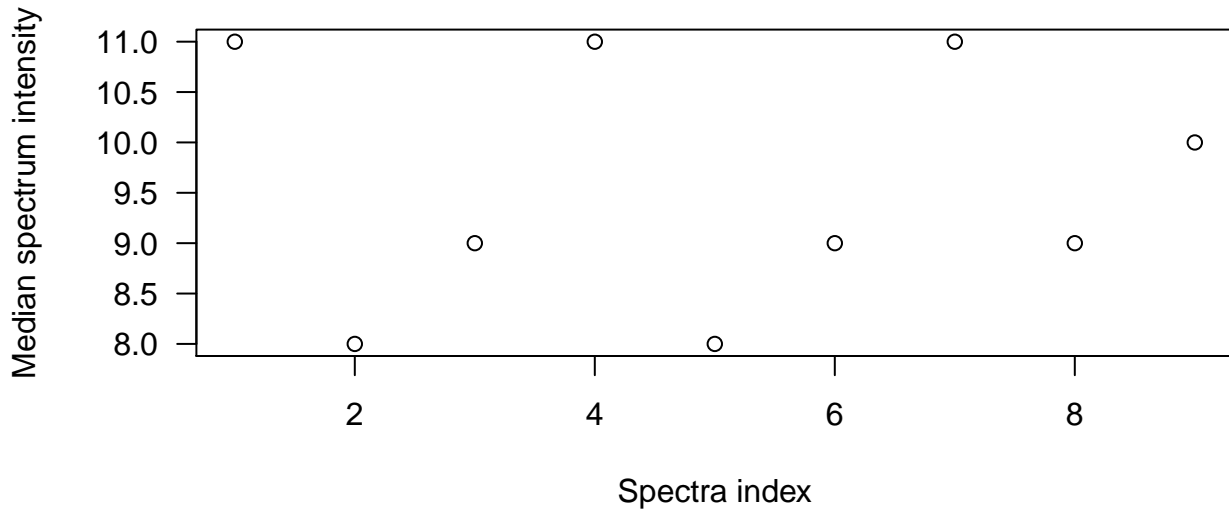
Sum of intensities per m/z



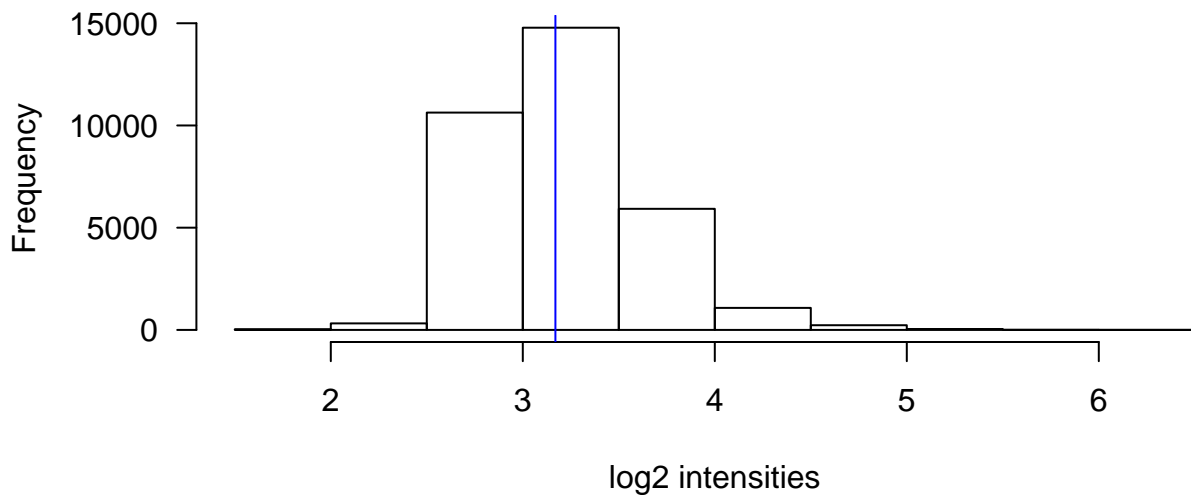
Sum of intensities per m/z



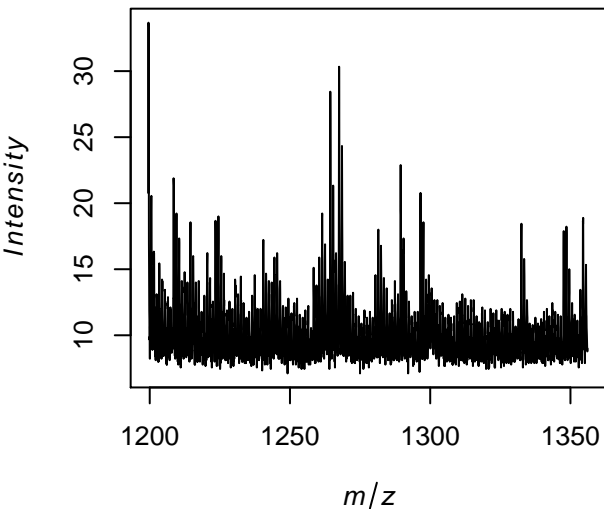
Median intensity per spectrum



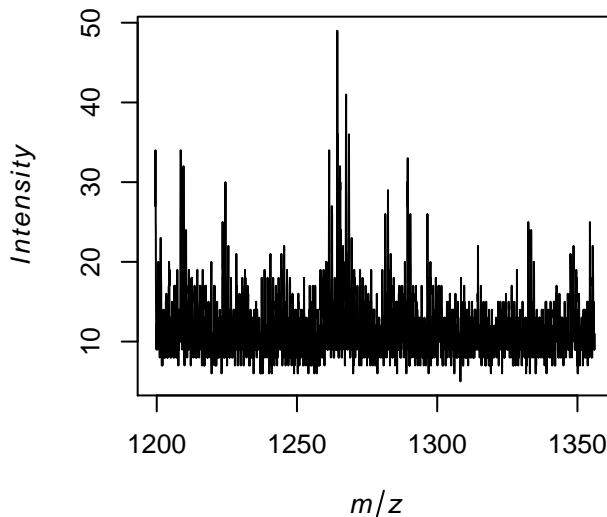
Log2-transformed intensities



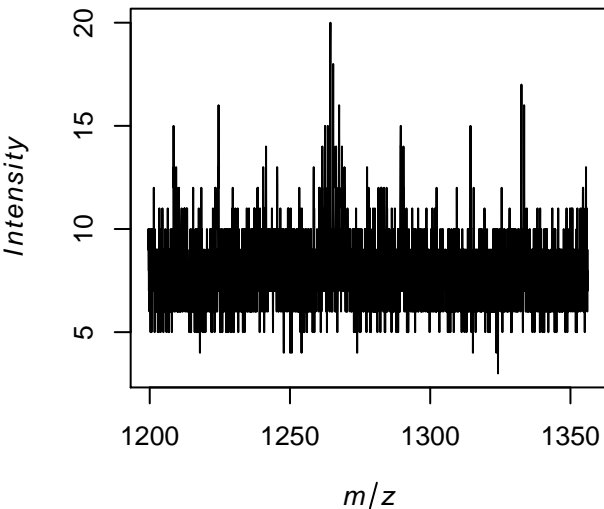
Average spectrum



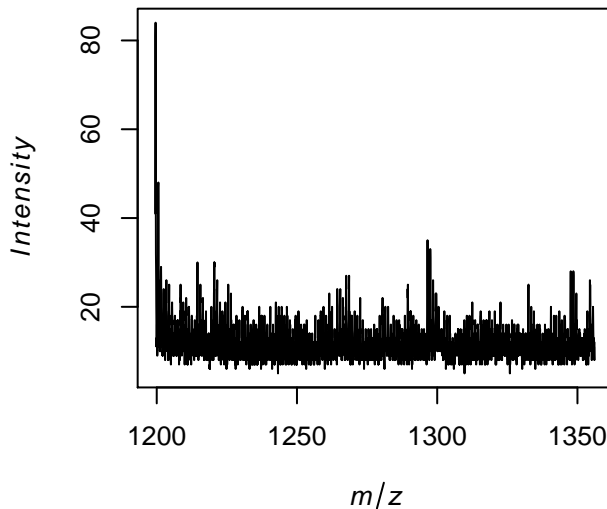
Spectrum at $x = 1, y = 2$



Spectrum at $x = 2, y = 1$



Spectrum at $x = 1, y = 3$

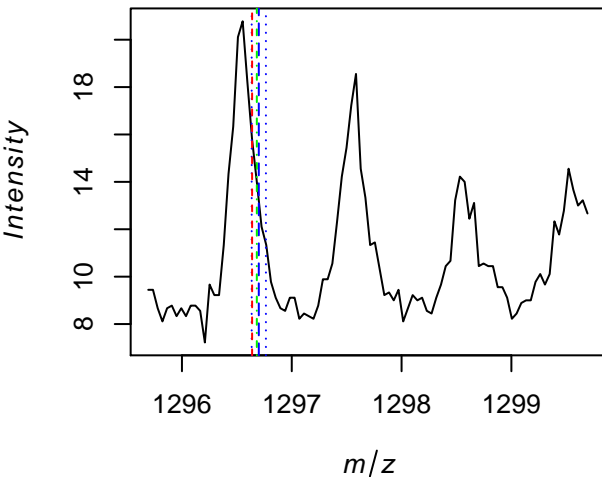


theor. m/z: 1296.7

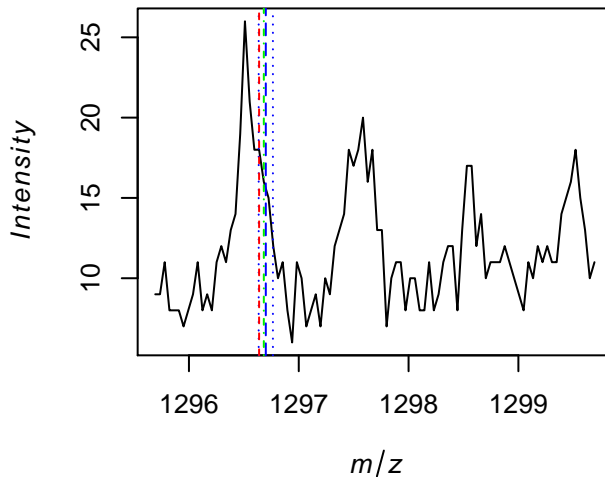
most abundant m/z: 1296.6389

closest m/z: 1296.6819

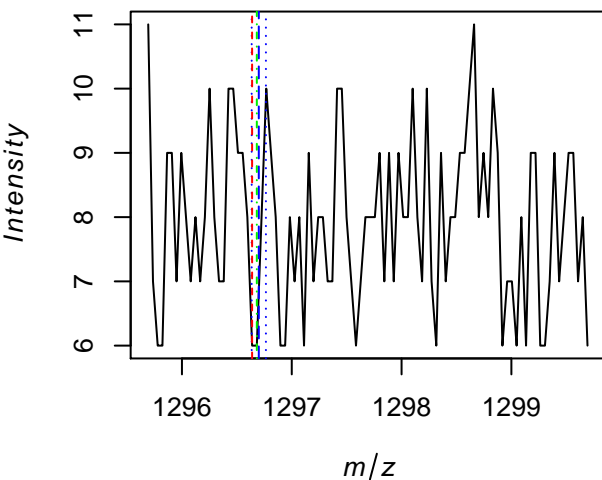
average spectrum



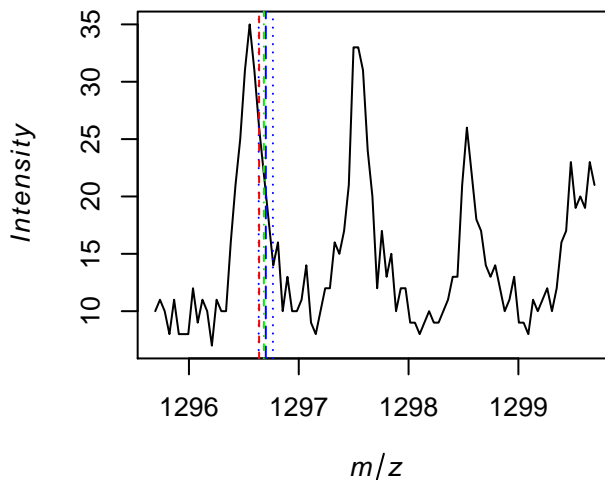
Spectrum at $x = 1, y = 2$



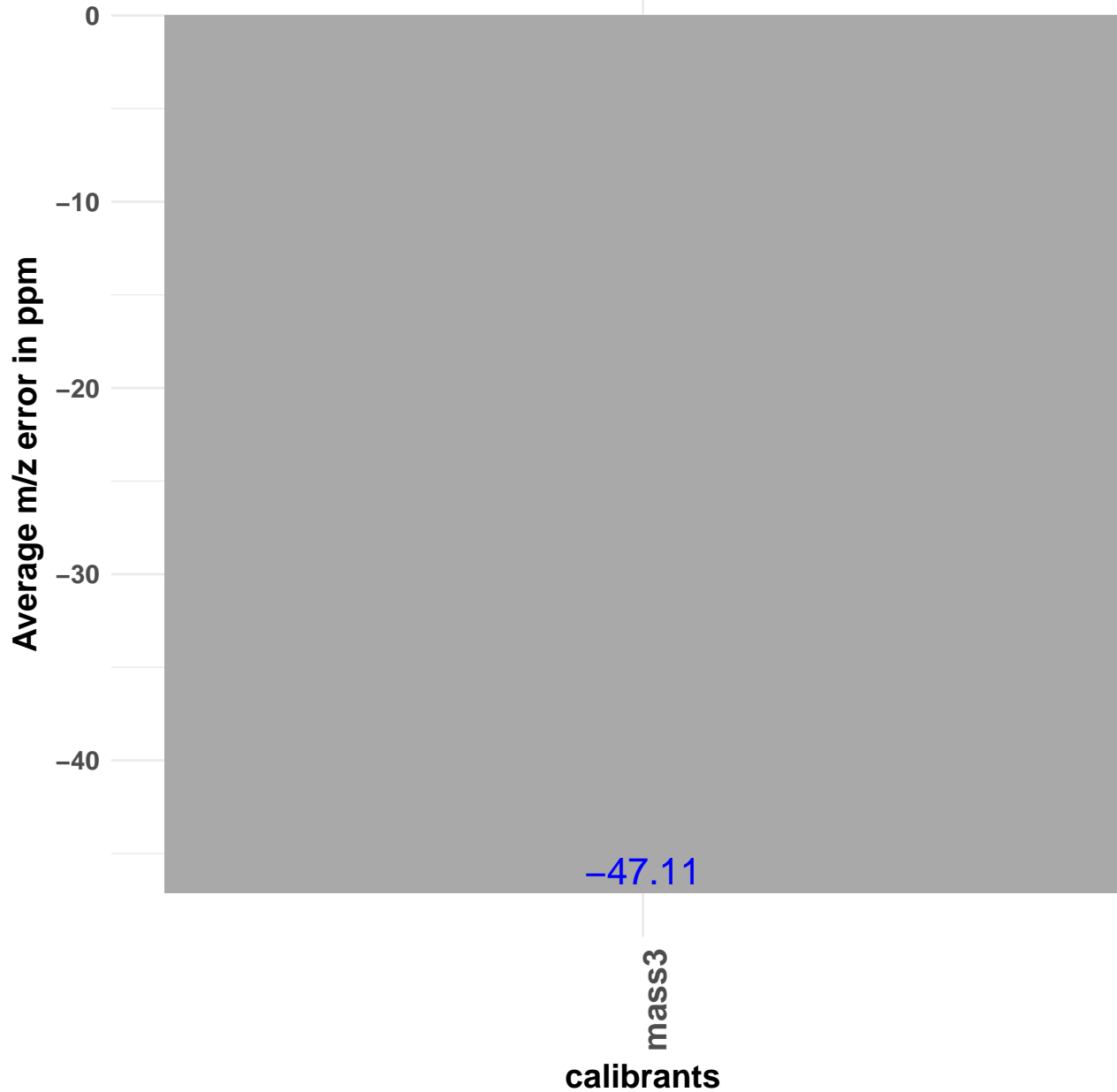
Spectrum at $x = 2, y = 1$



Spectrum at $x = 1, y = 3$



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



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)

