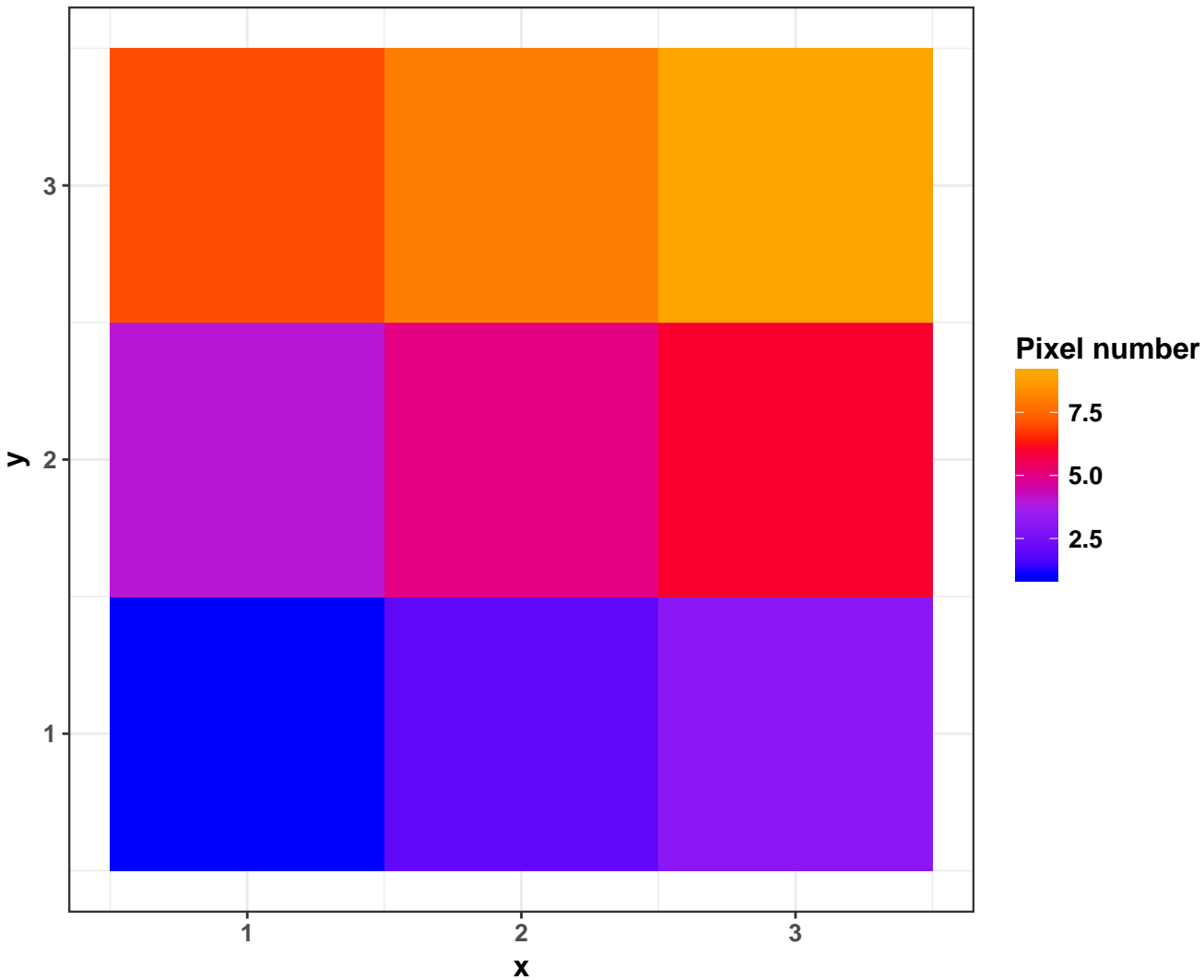


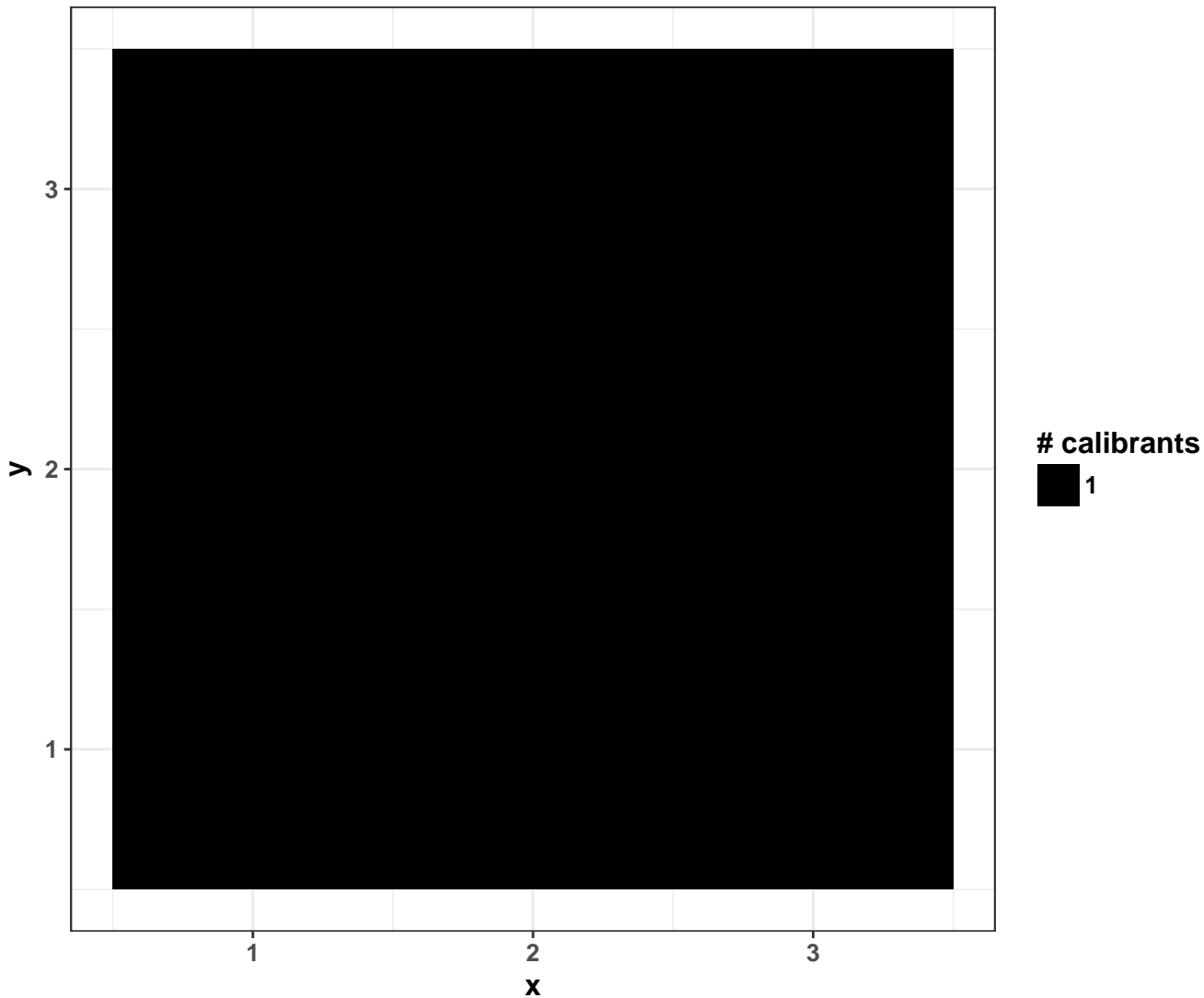
Testfile_analyze75

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 zero TICs	0
Median TIC	37005
Median # peaks per spectrum	3672
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in inputpeptides.txt	1 / 6
# calibrants in inputcalibrantfile2.txt	1 / 3

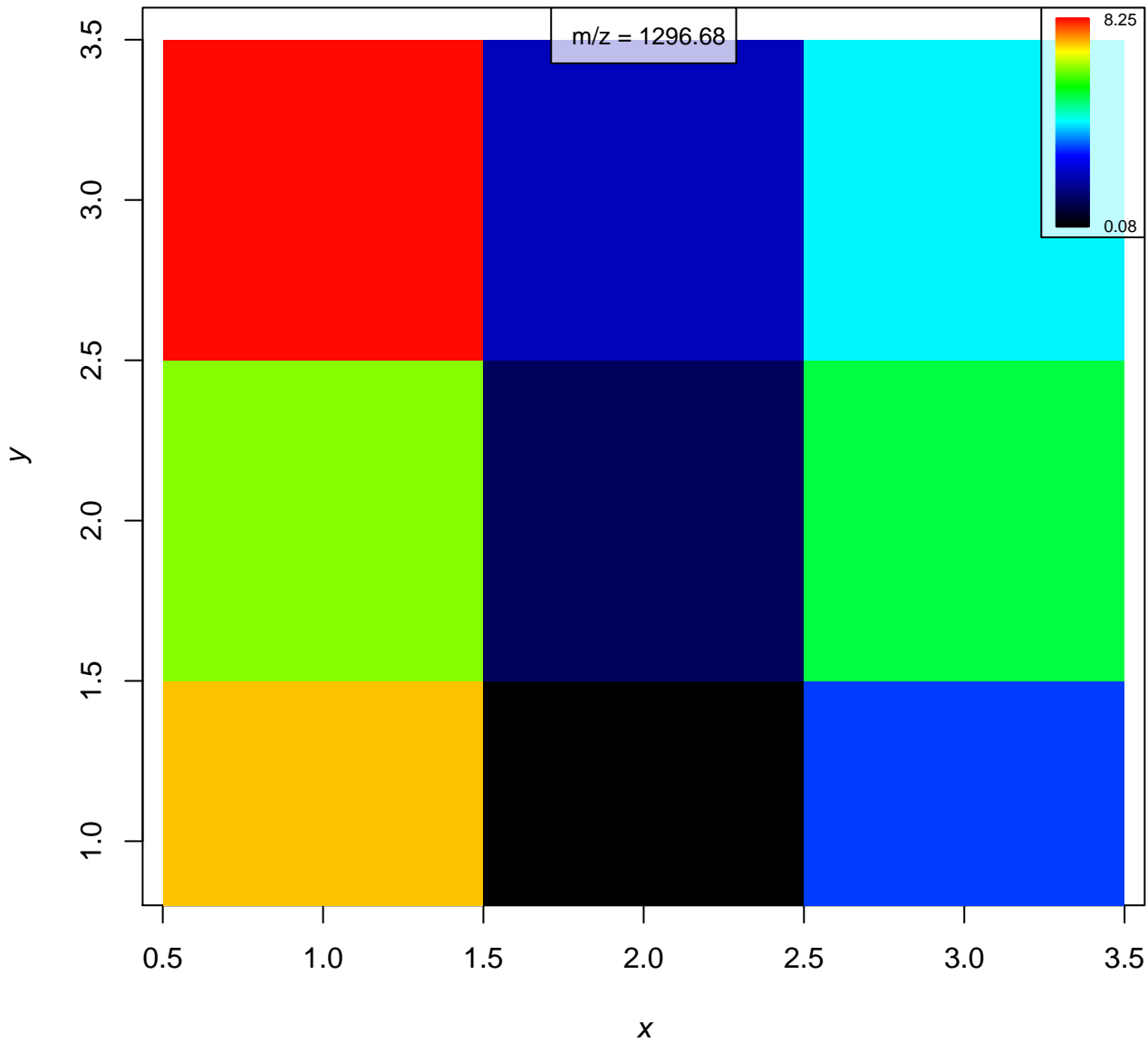
Pixel order



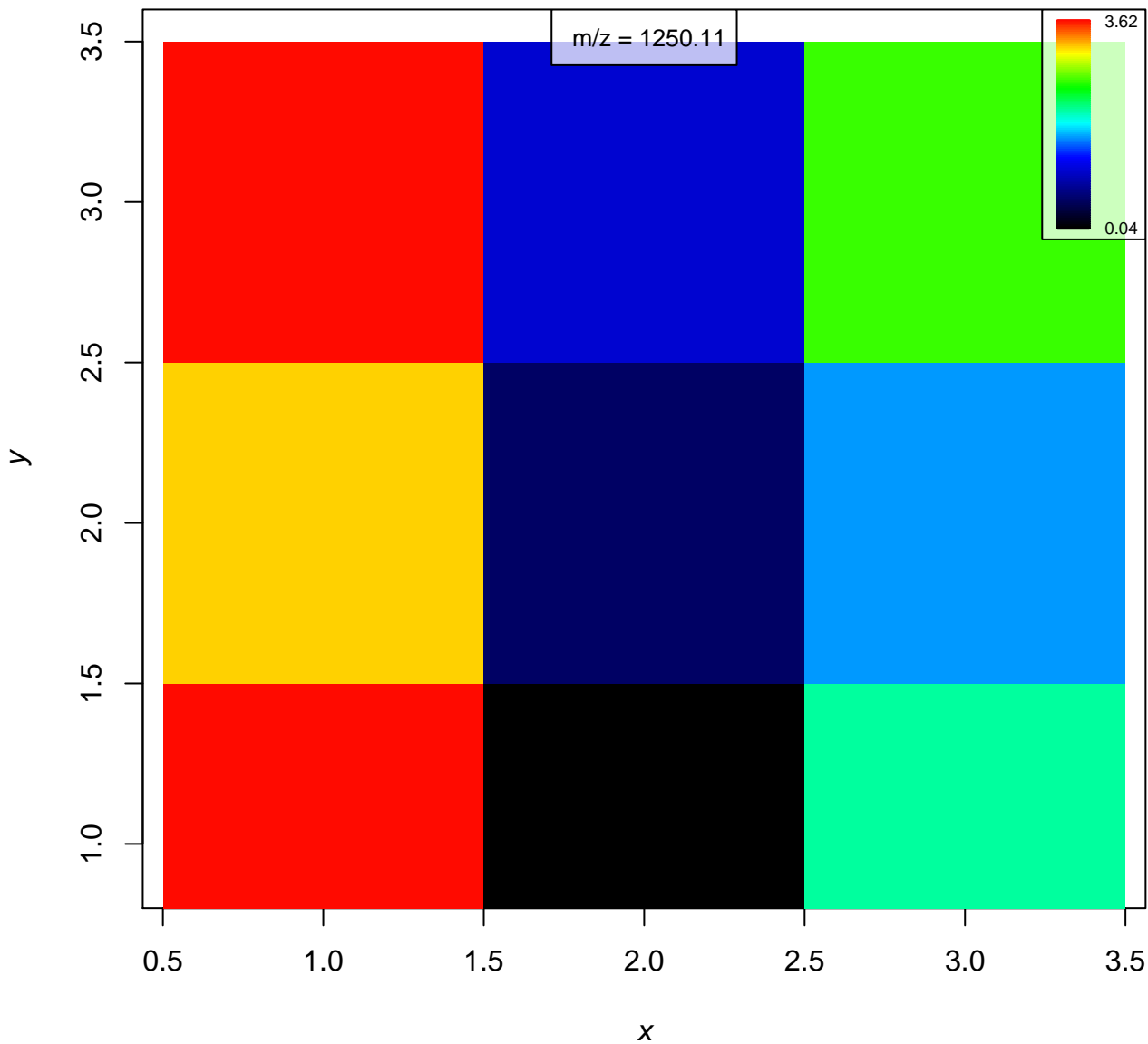
Number of calibrants per pixel



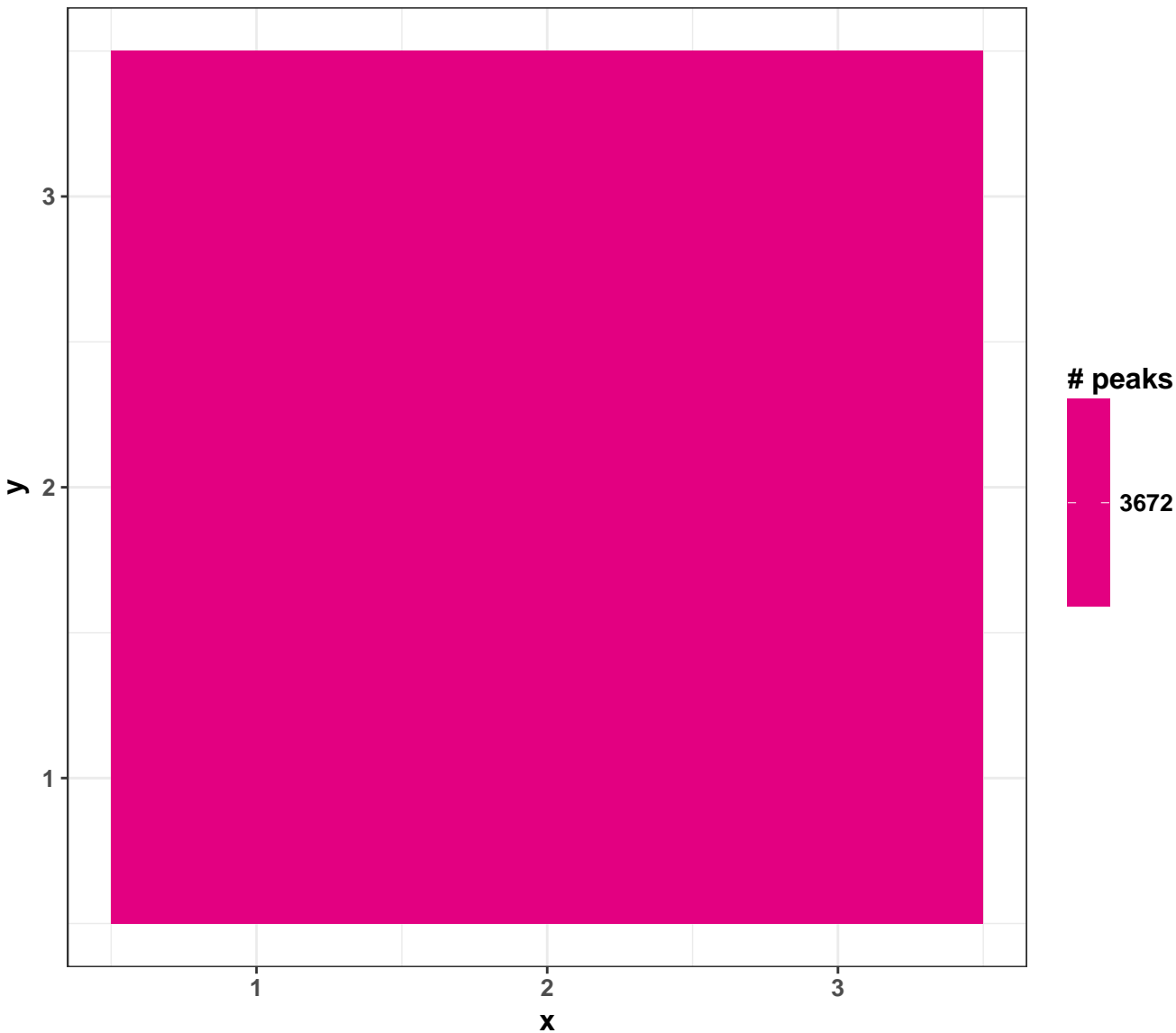
mass3 (1296.7 ± 0.5 Da)



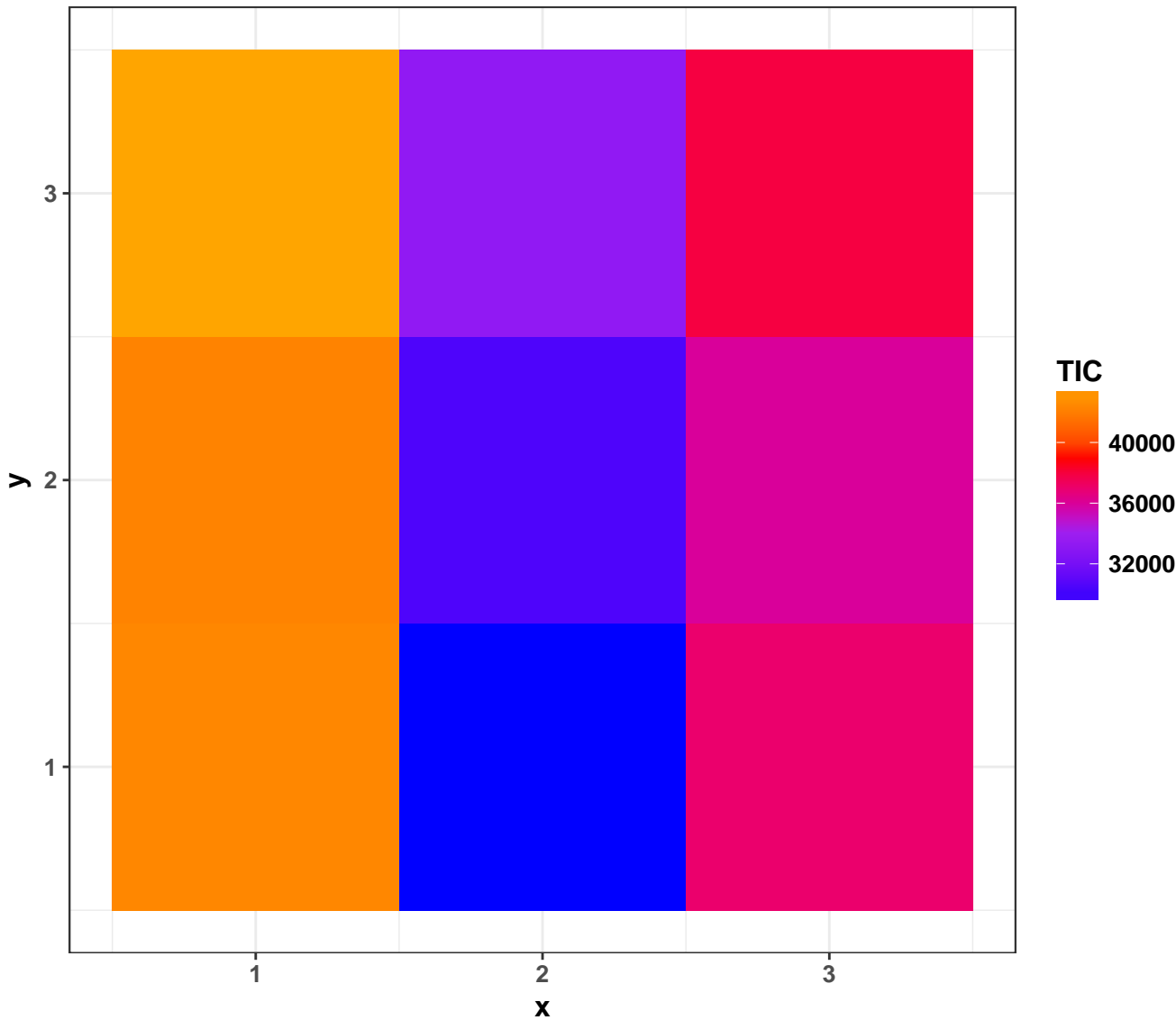
1250.1 (1250.1 ± 0.5 Da)



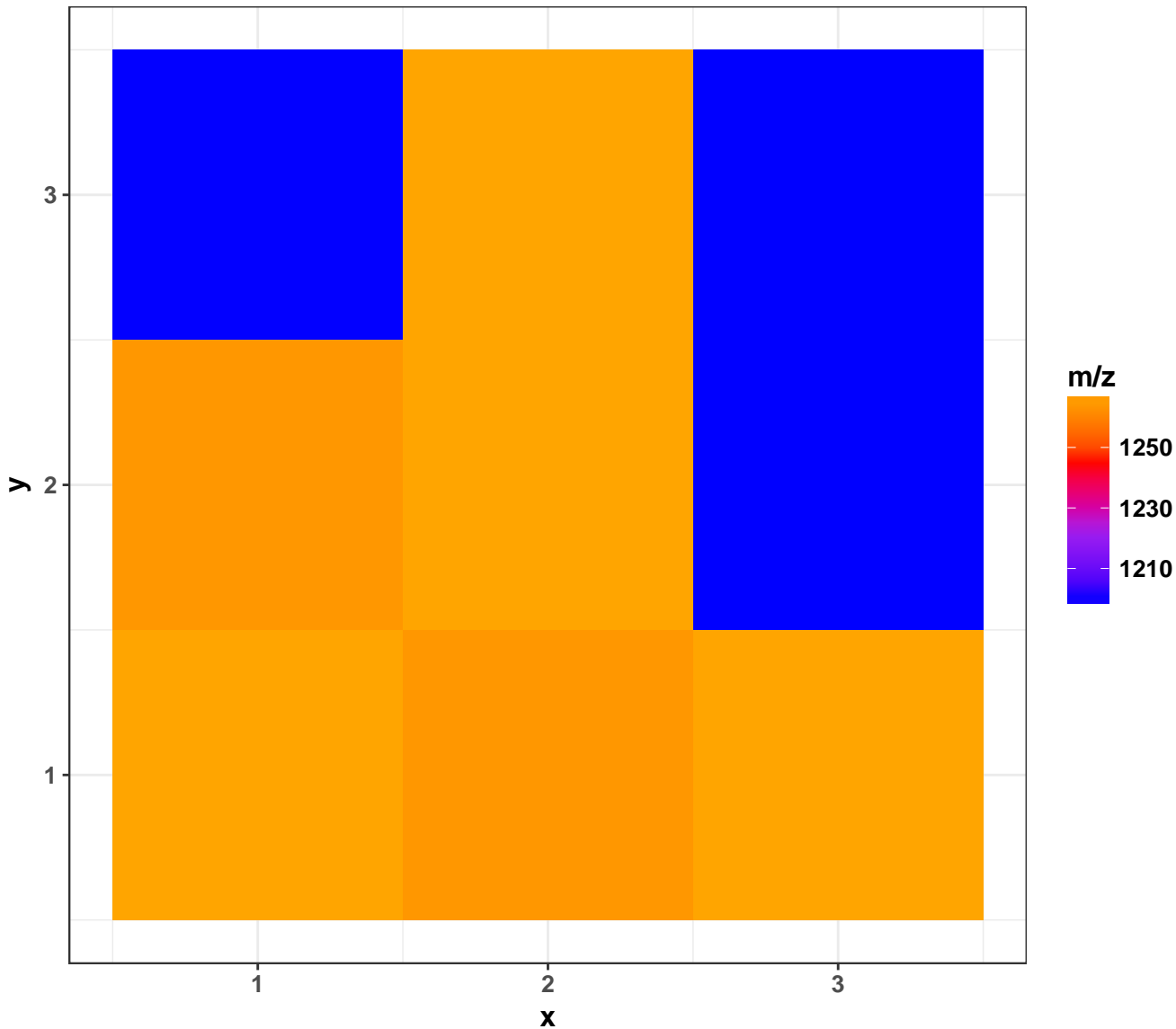
Number of peaks per spectrum



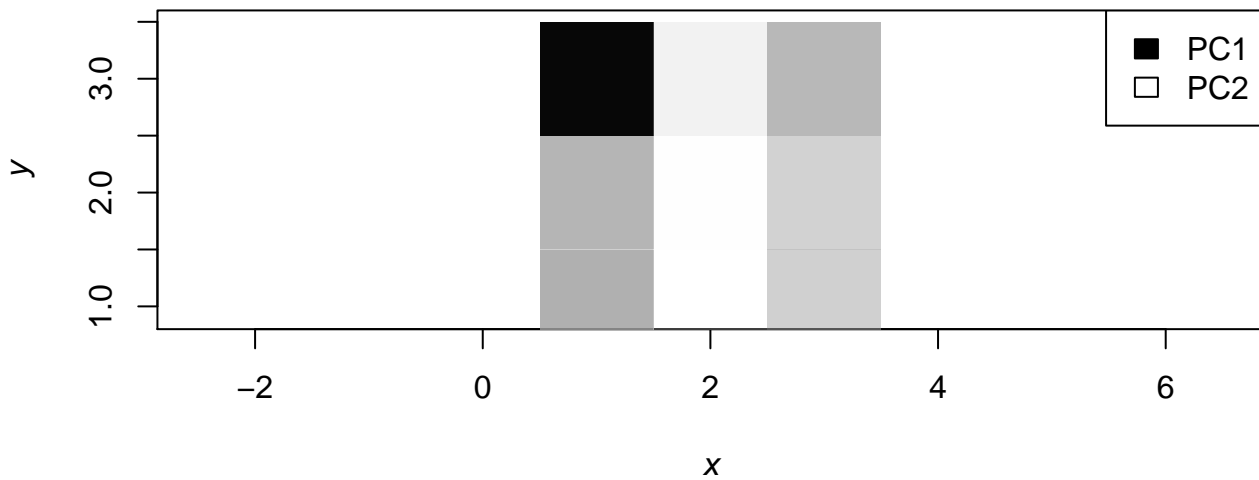
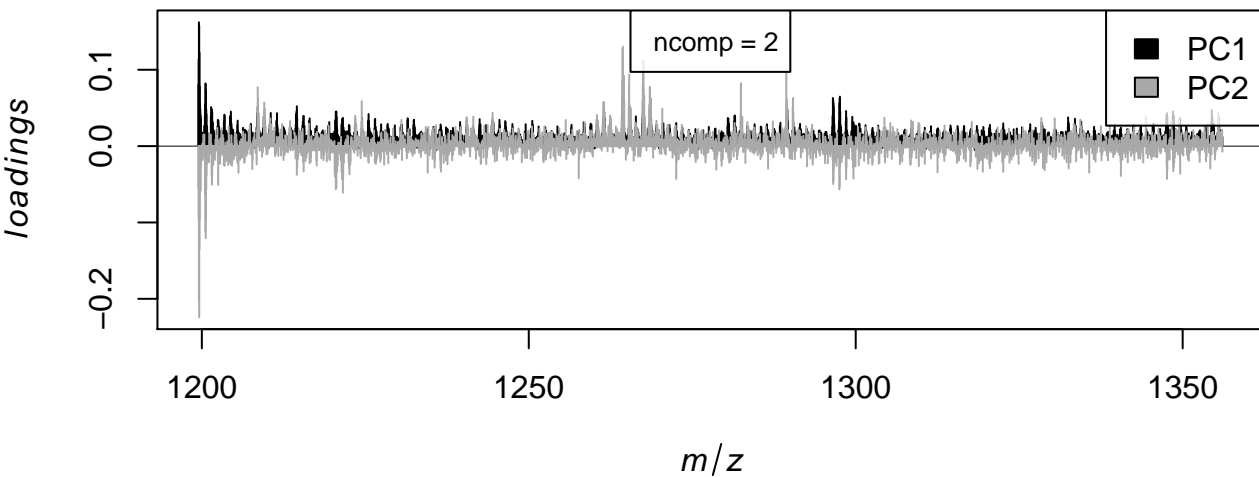
Total Ion Chromatogram



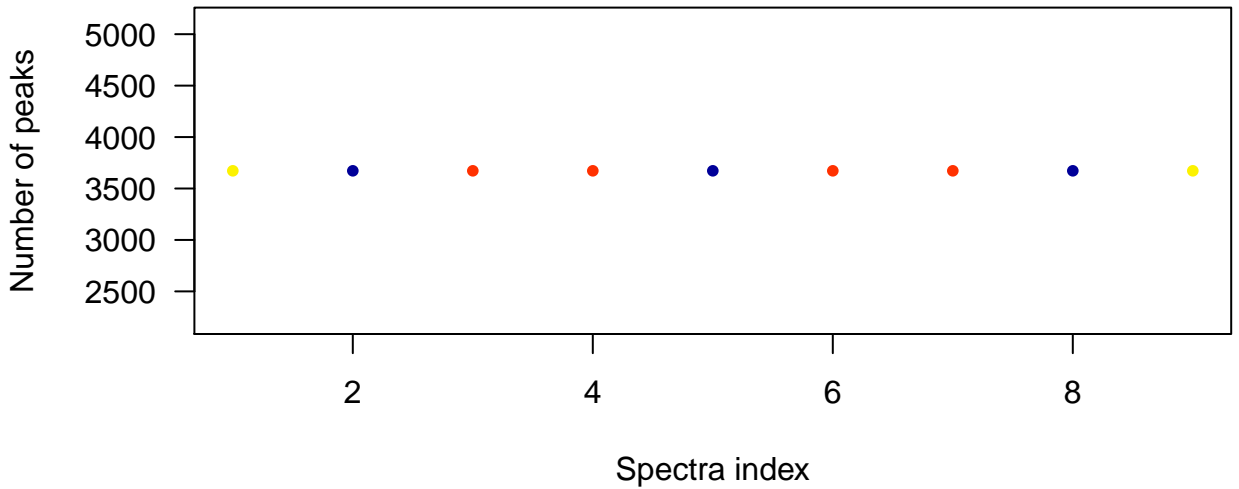
Most abundant m/z in each spectrum



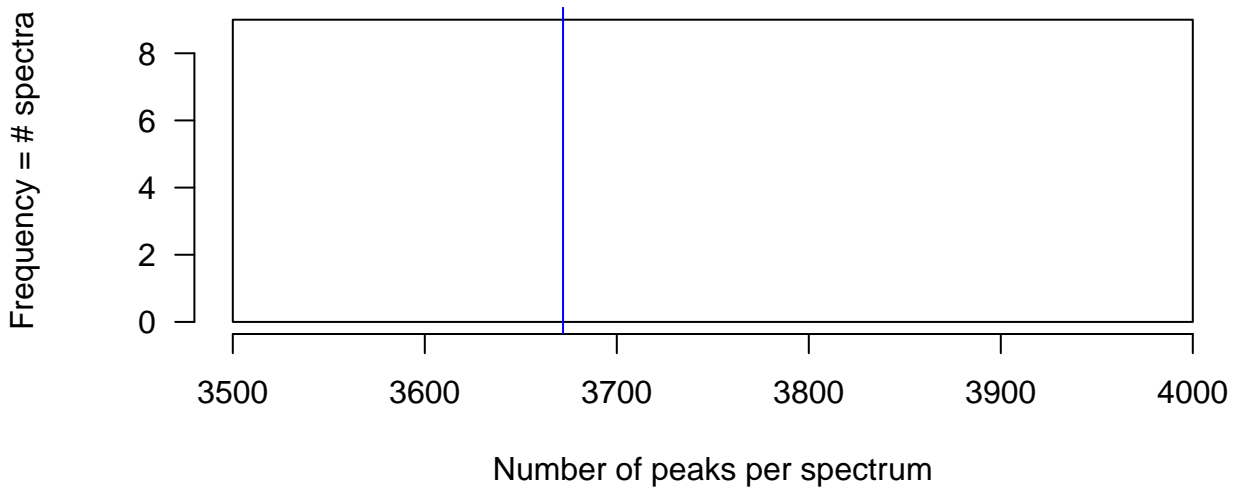
PCA for two components



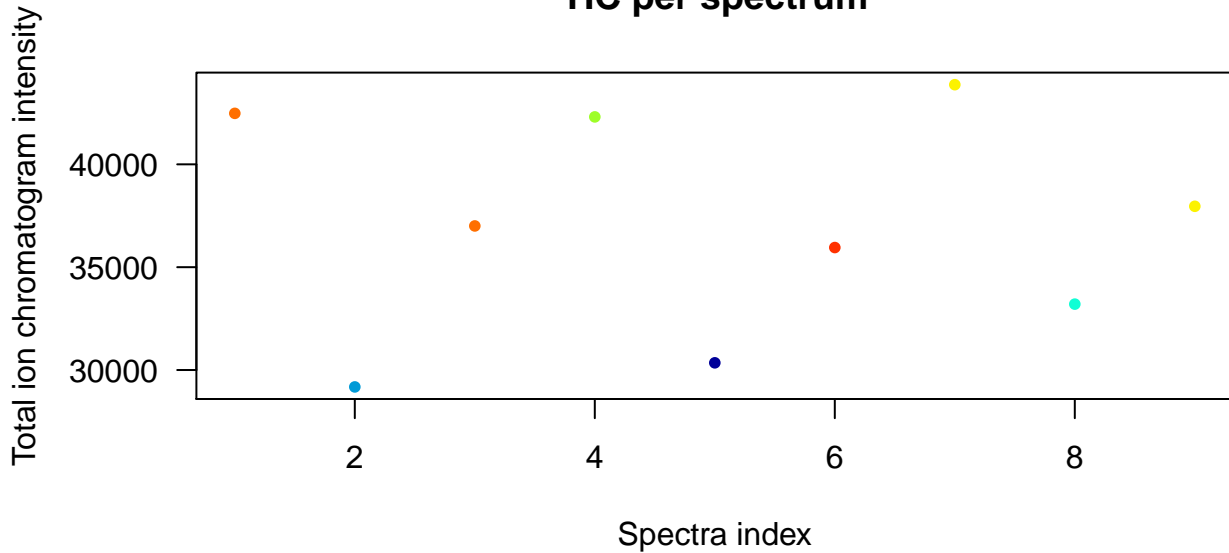
Number of peaks per spectrum



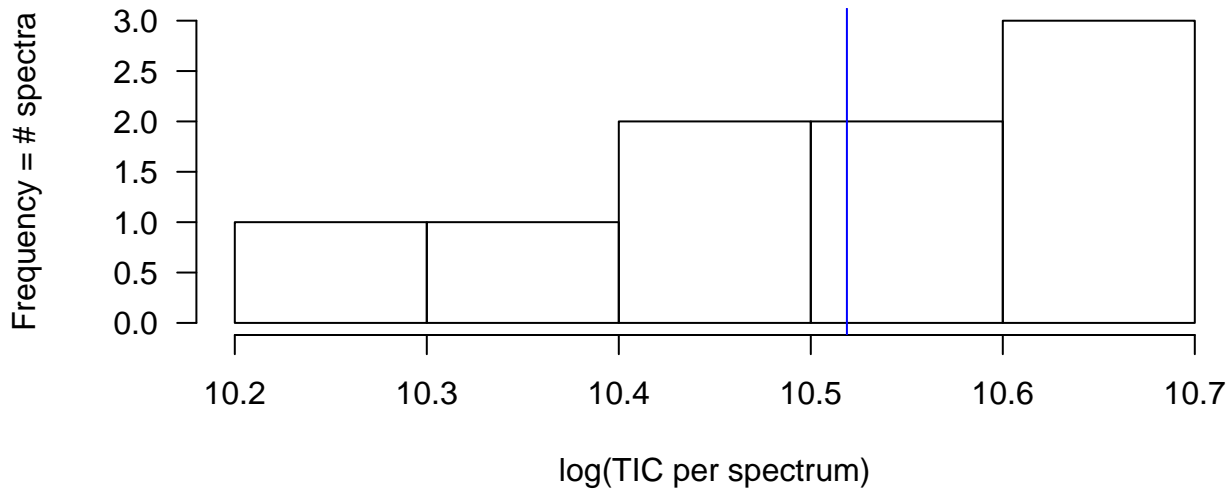
Number of peaks per spectrum



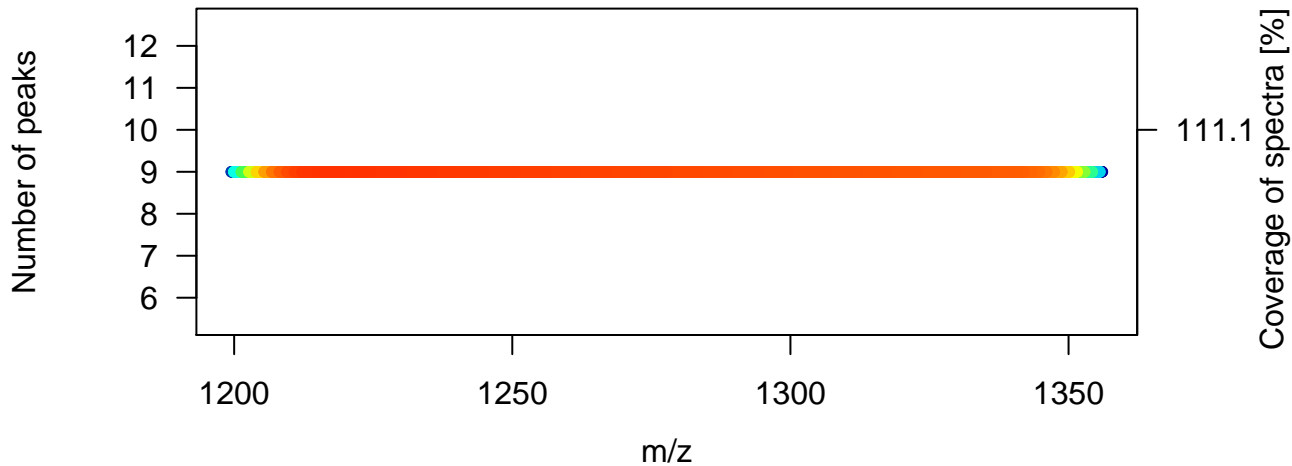
TIC per spectrum



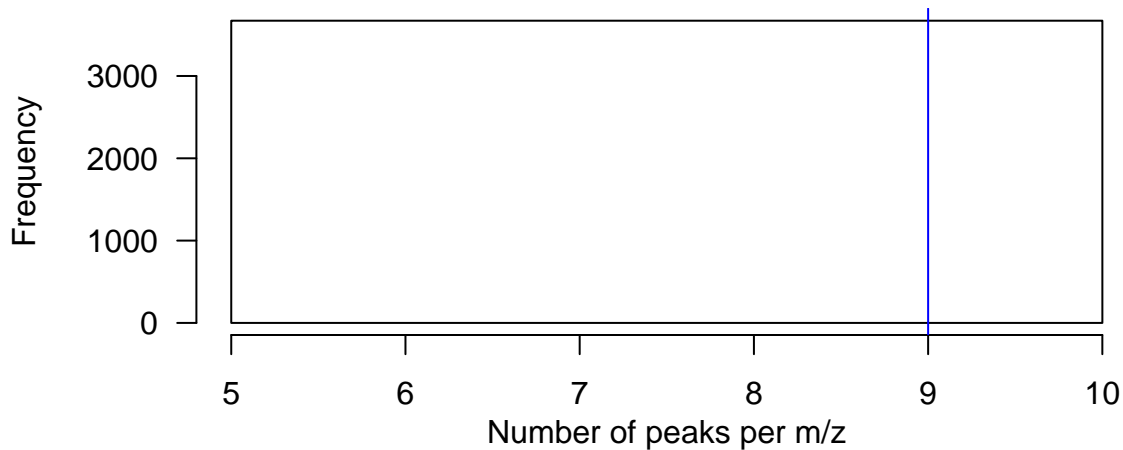
TIC per spectrum



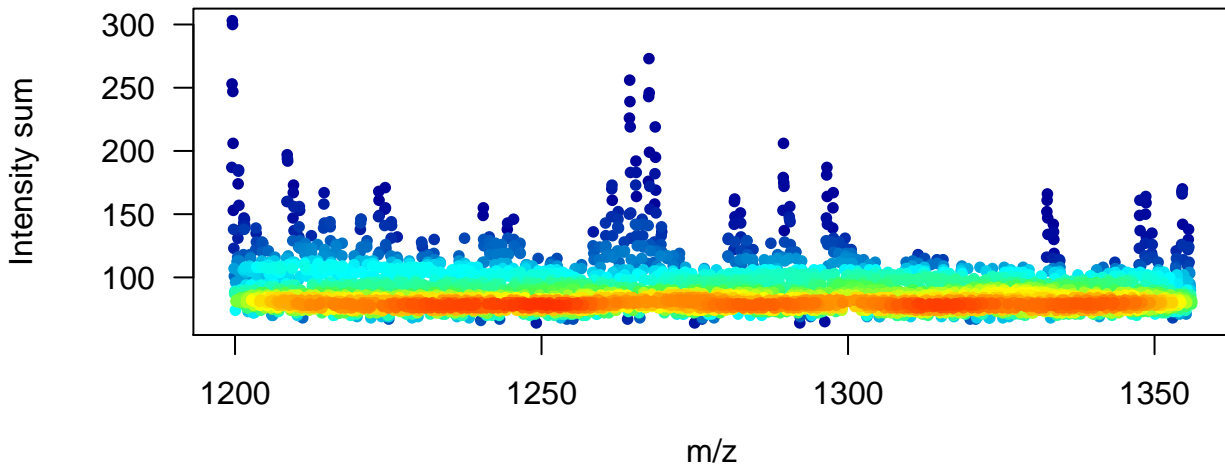
Number of peaks per m/z



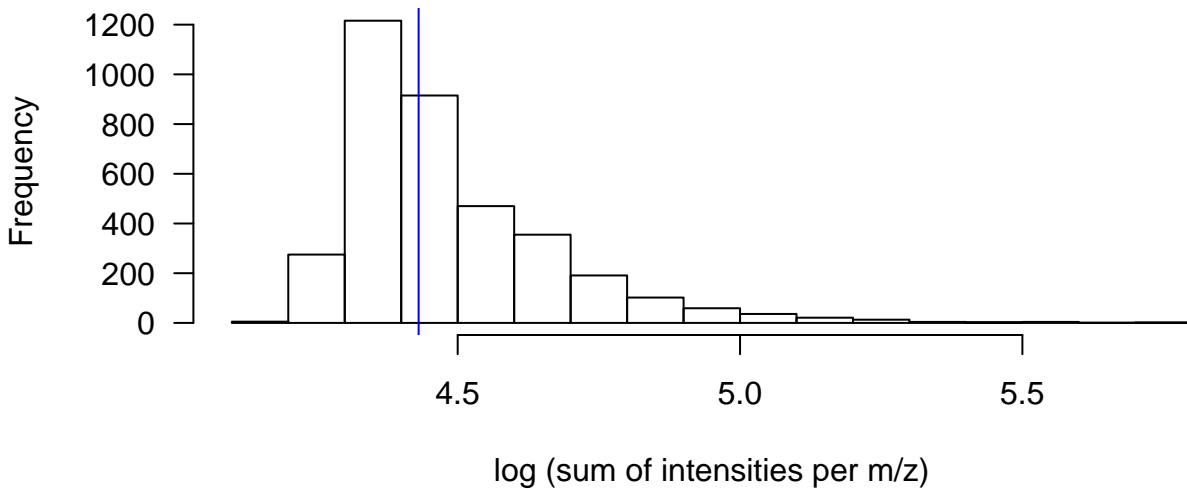
Number of peaks per m/z



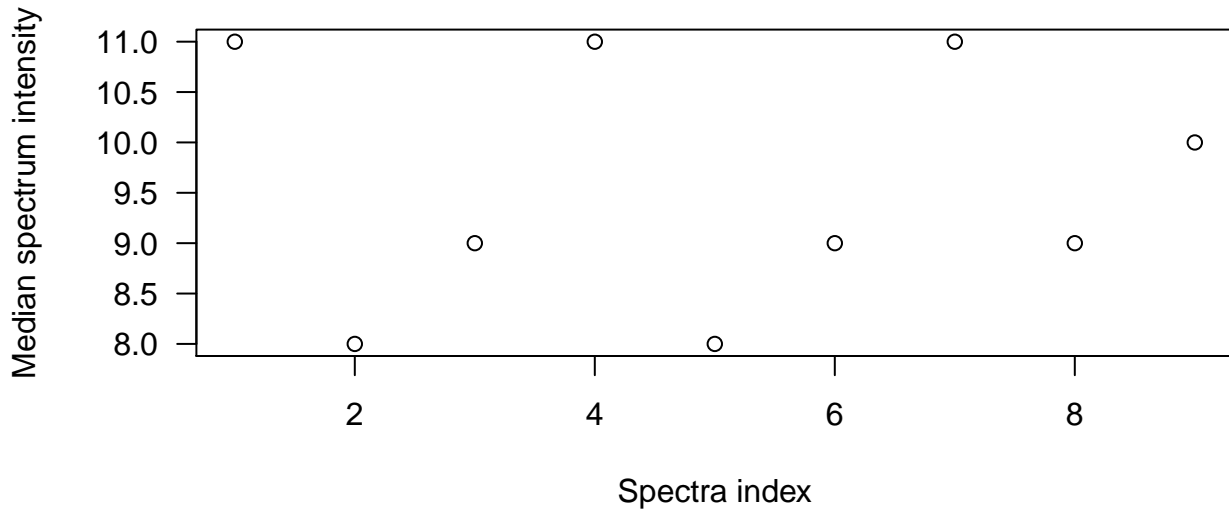
Sum of intensities per m/z



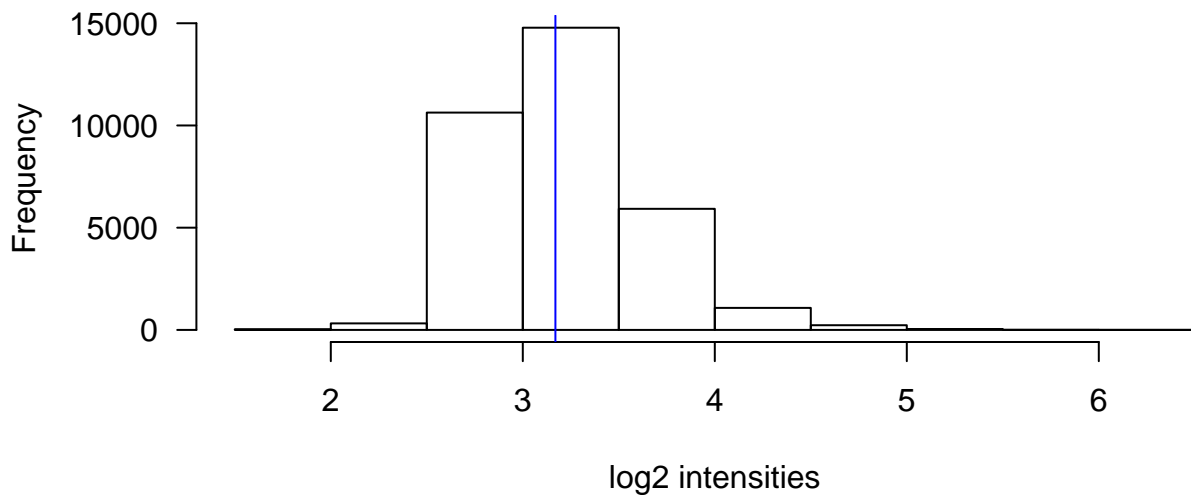
Sum of intensities per m/z



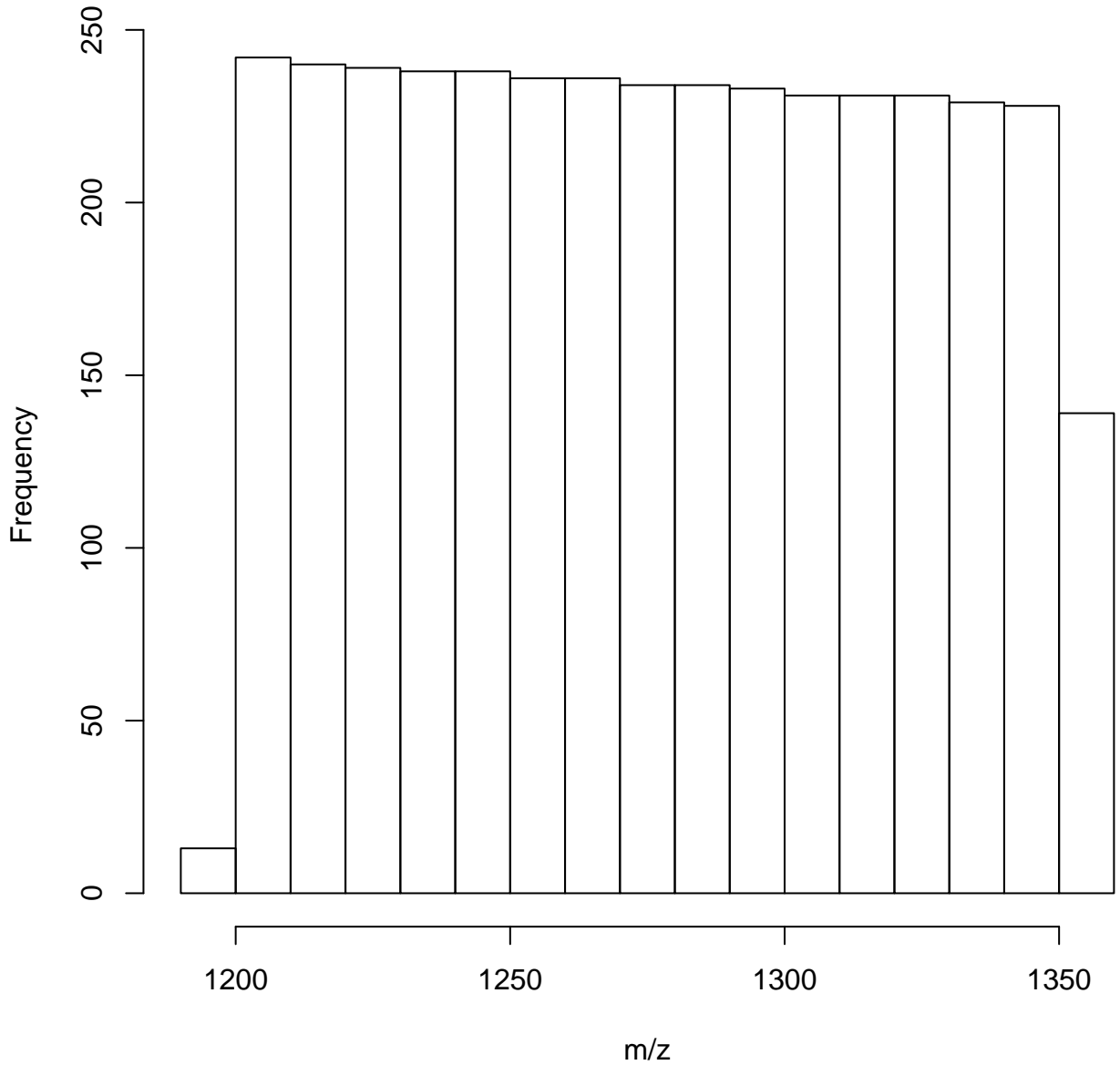
Median intensity per spectrum



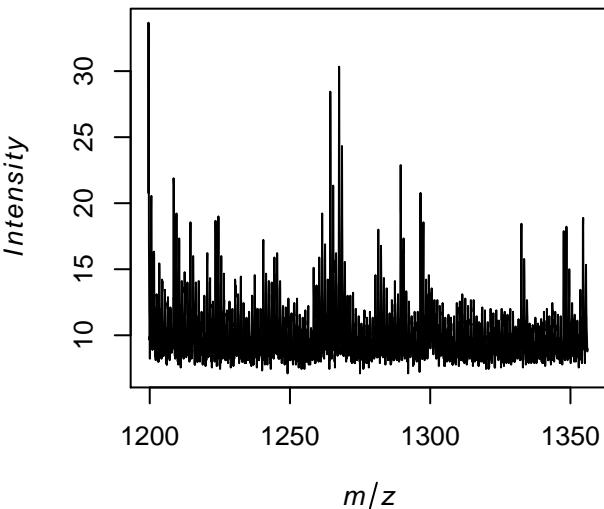
Log2-transformed intensities



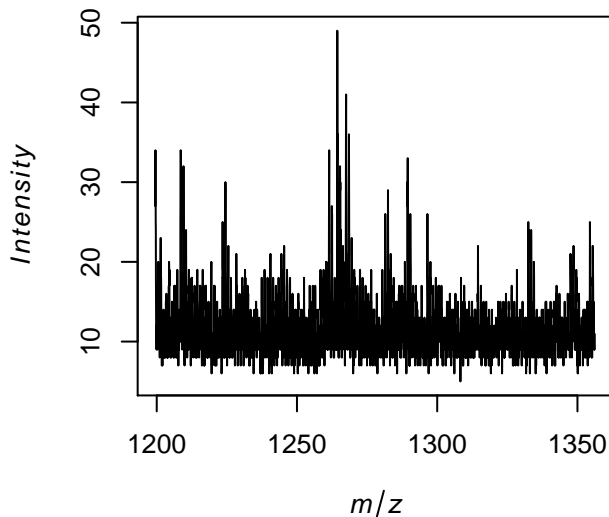
Histogram of m/z values



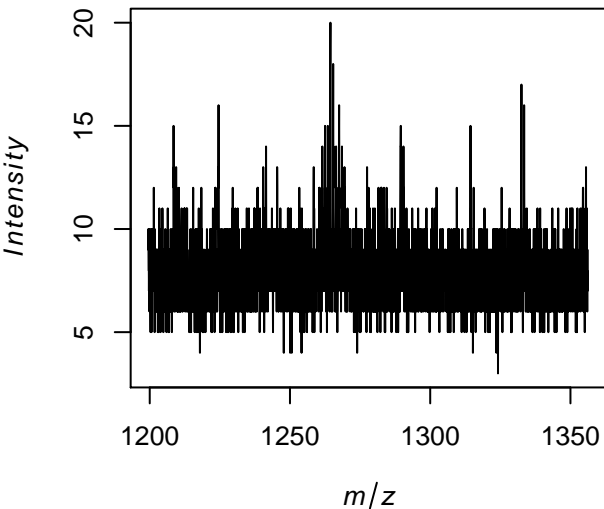
Average spectrum



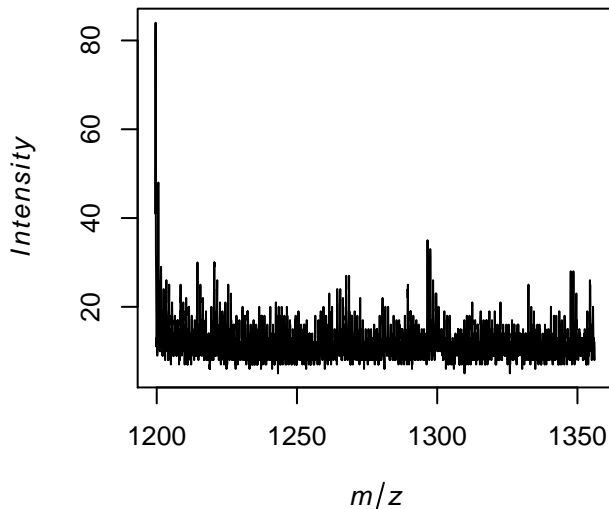
Spectrum at x = 1, y = 2



Spectrum at x = 2, y = 1



Spectrum at x = 1, y = 3

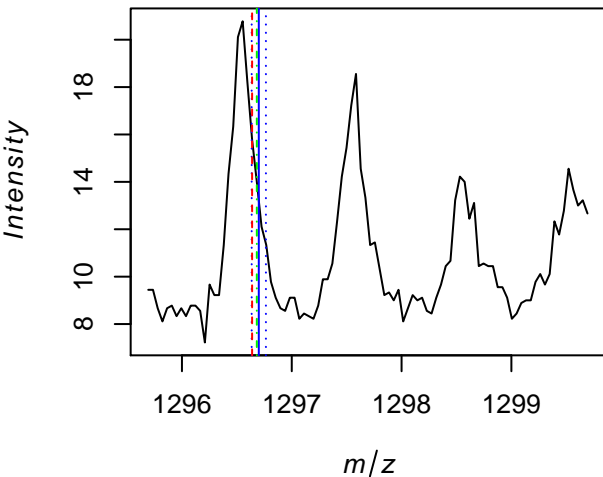


theor. m/z: 1296.7

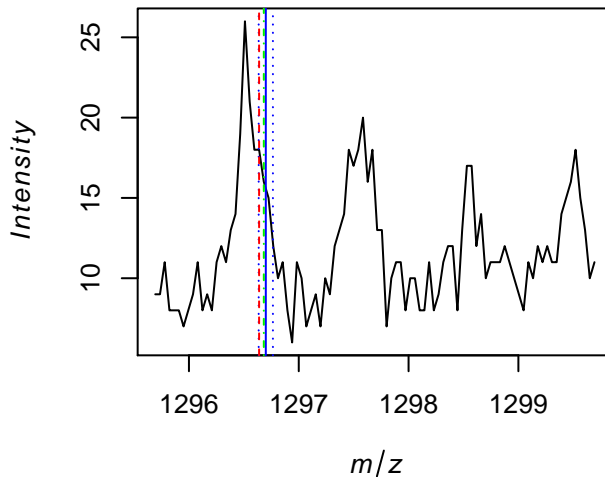
most abundant m/z: 1296.6389

closest m/z: 1296.6819

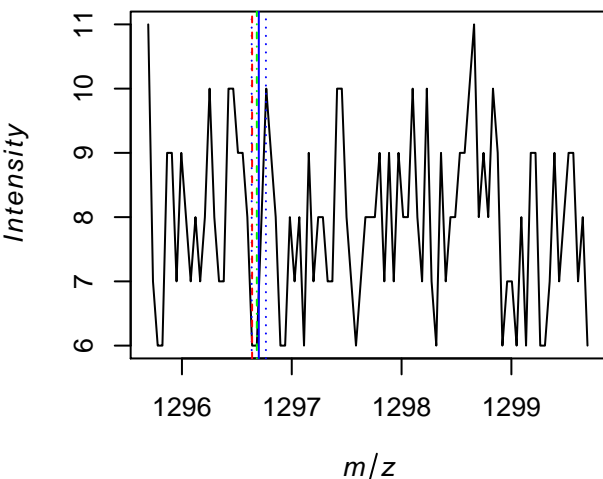
average spectrum



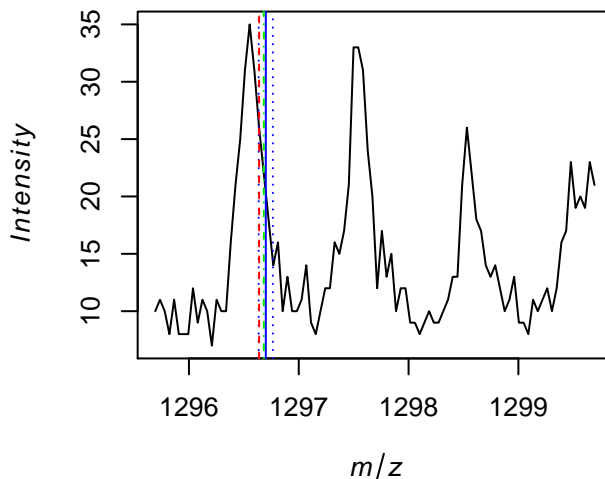
Spectrum at $x = 1, y = 2$



Spectrum at $x = 2, y = 1$



Spectrum at $x = 1, y = 3$



Difference m/z with max. average intensity vs. theor. calibrant m/z

Difference in ppm

0

-10

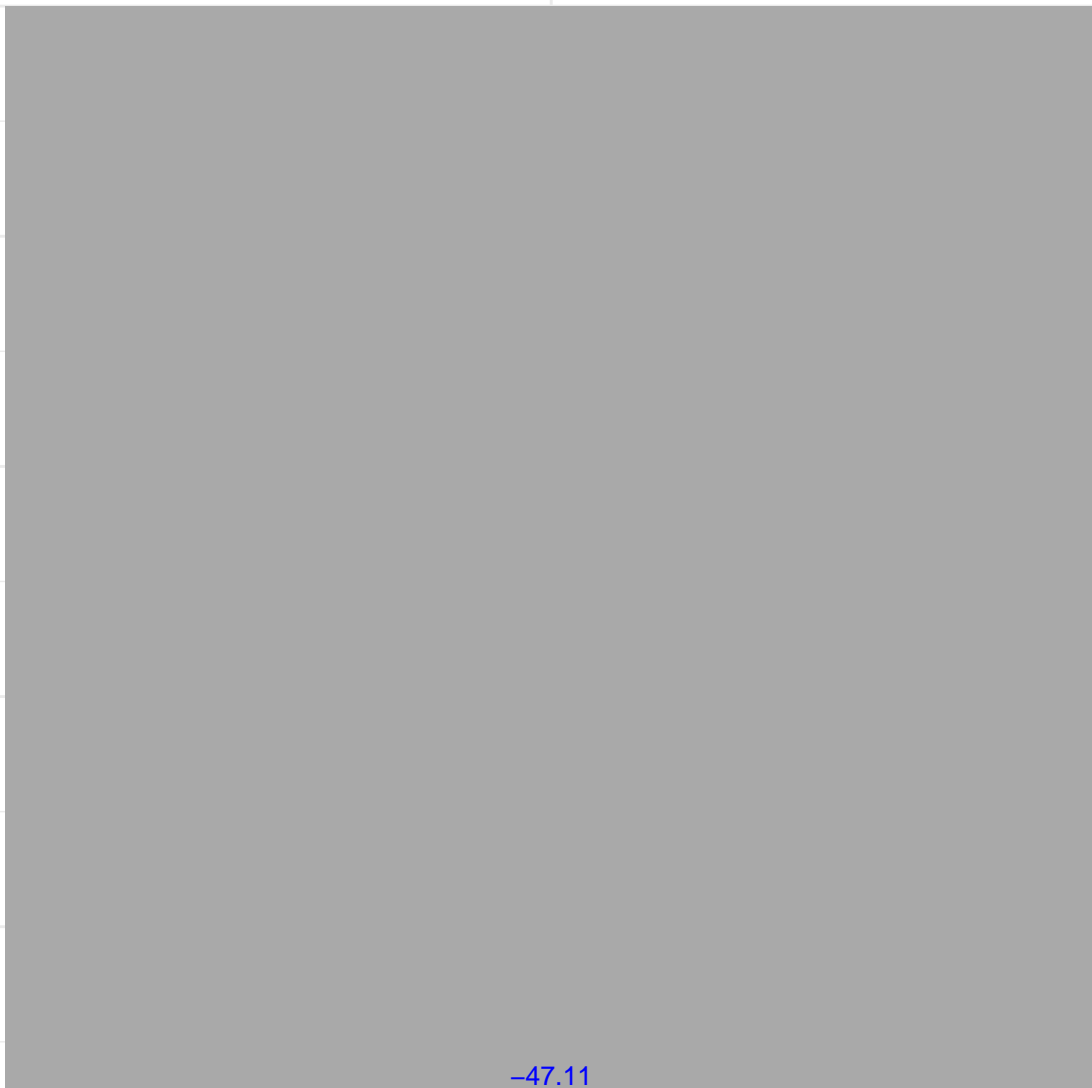
-20

-30

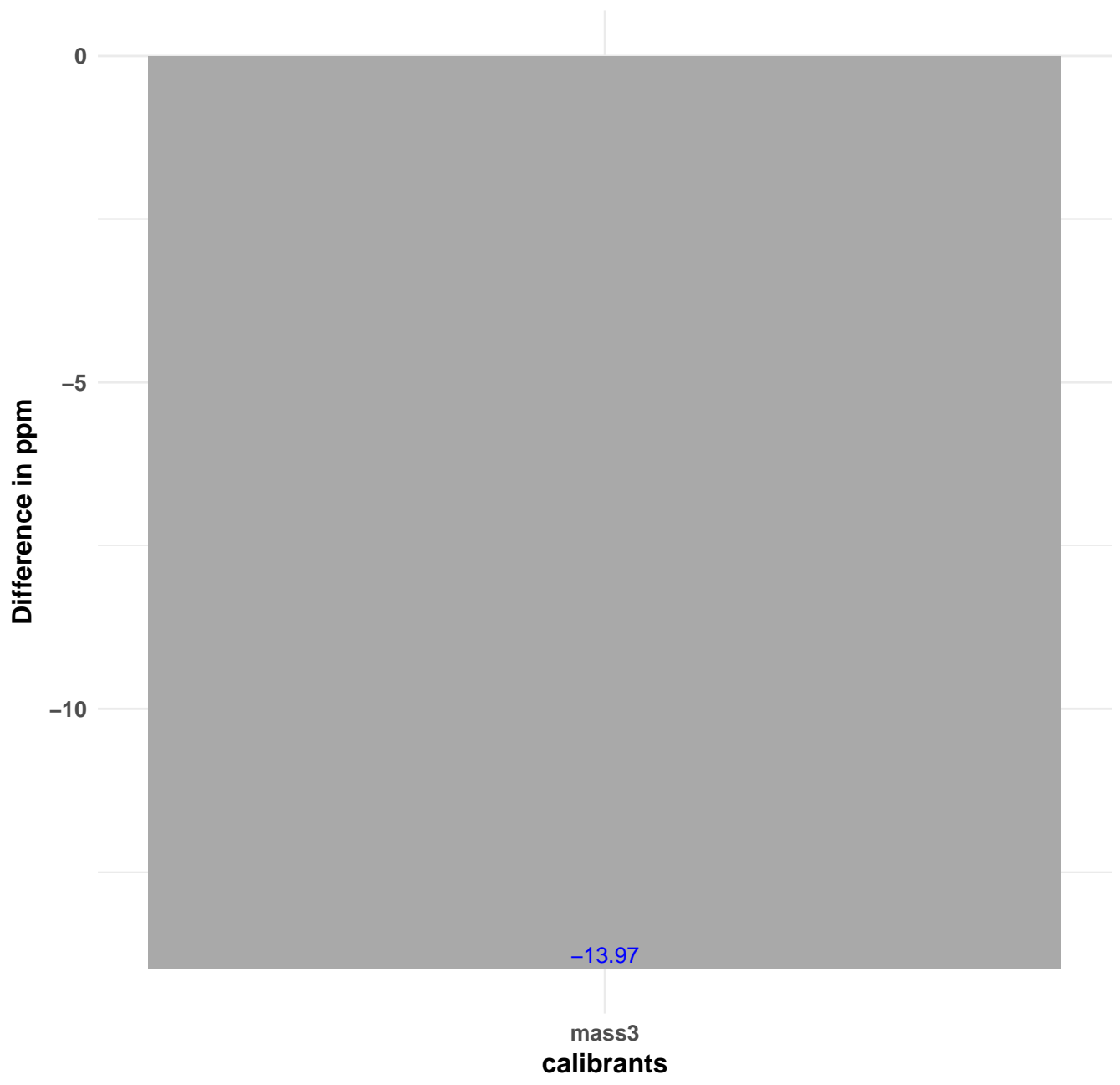
-40

-47.11

mass3
calibrants



Difference closest measured m/z vs. theor. calibrant m/z



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

