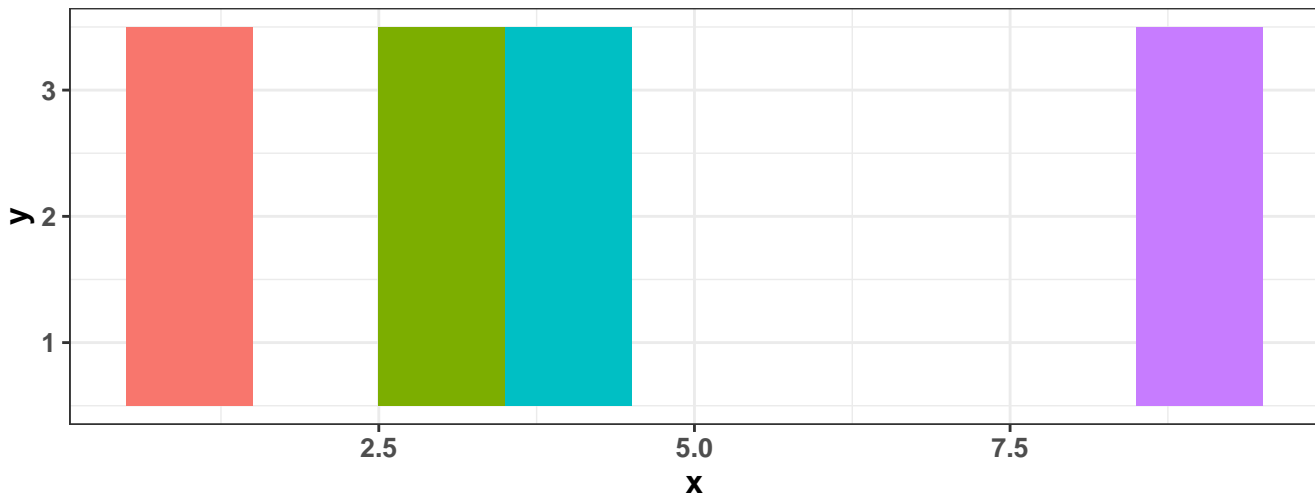


Testfile_rdata

properties	values
Number of m/z features	8399
Range of m/z values	100.08 – 799.92
Number of pixels	12
Range of x coordinates	1 – 9
Range of y coordinates	1 – 3
Range of intensities	0 – 9.24
Number of NA intensities	0
Number of Inf intensities	0
Number of duplicated coordinates	0
Median of intensities	0
Intensities > 0	31.29 %
Number of empty spectra	0
Median TIC \pm sd	161.8 \pm 47
Median # peaks per spectrum \pm sd	2811 \pm 424
Centroided	FALSE
input m/z (#valid/#input) in inputcalibrantfile1.tabular	3 / 3

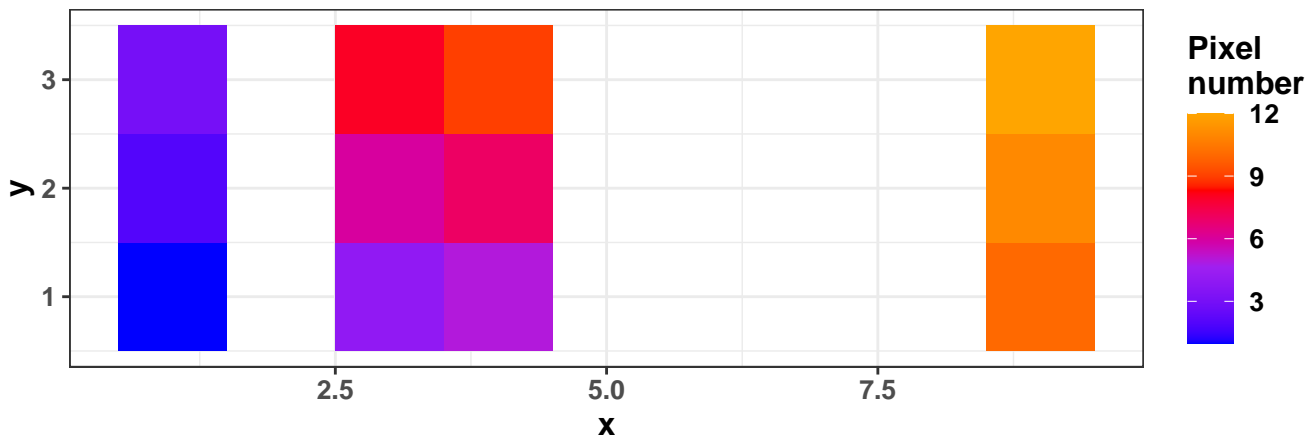
Spatial orientation of pixel annotations



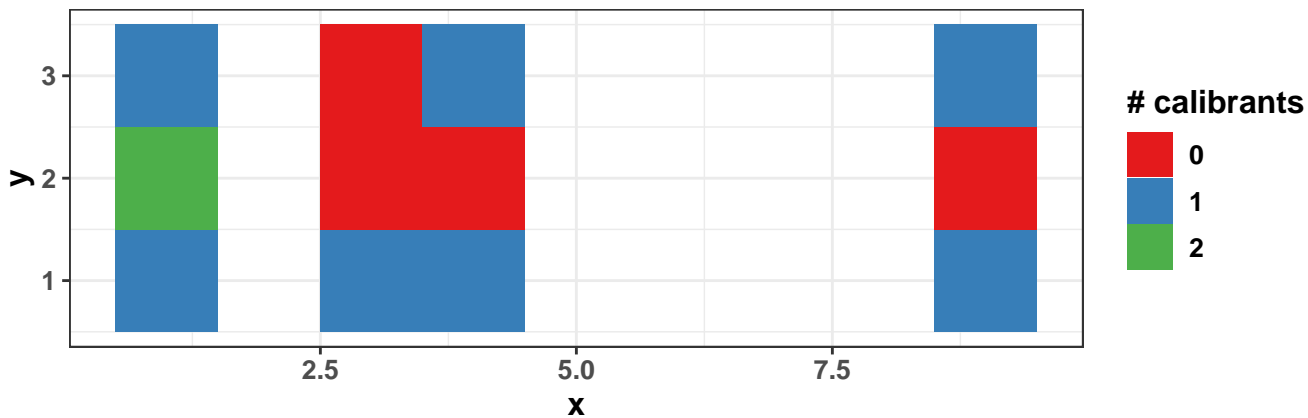
annotation

column1 column2 column3 column4

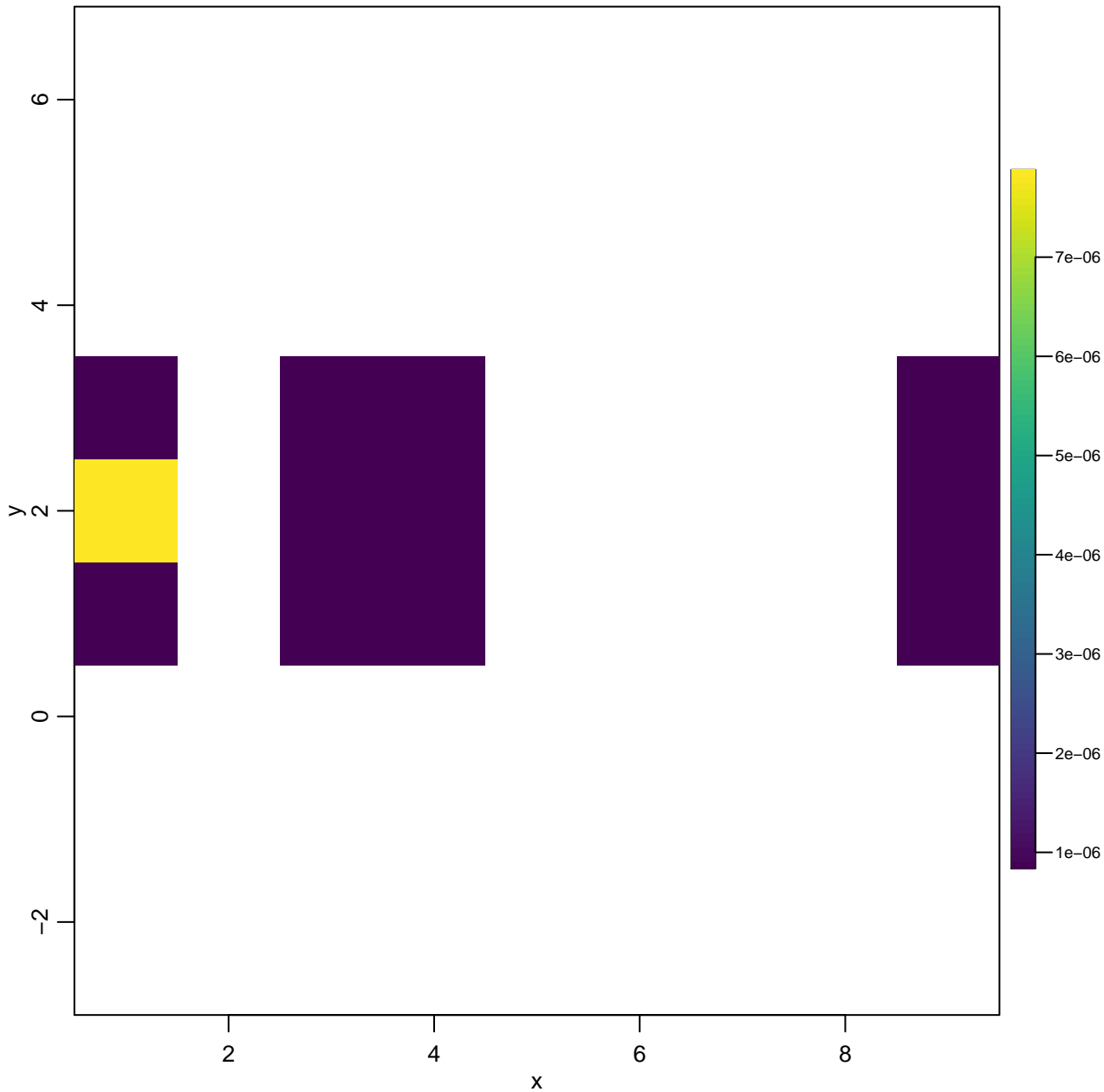
Pixel order



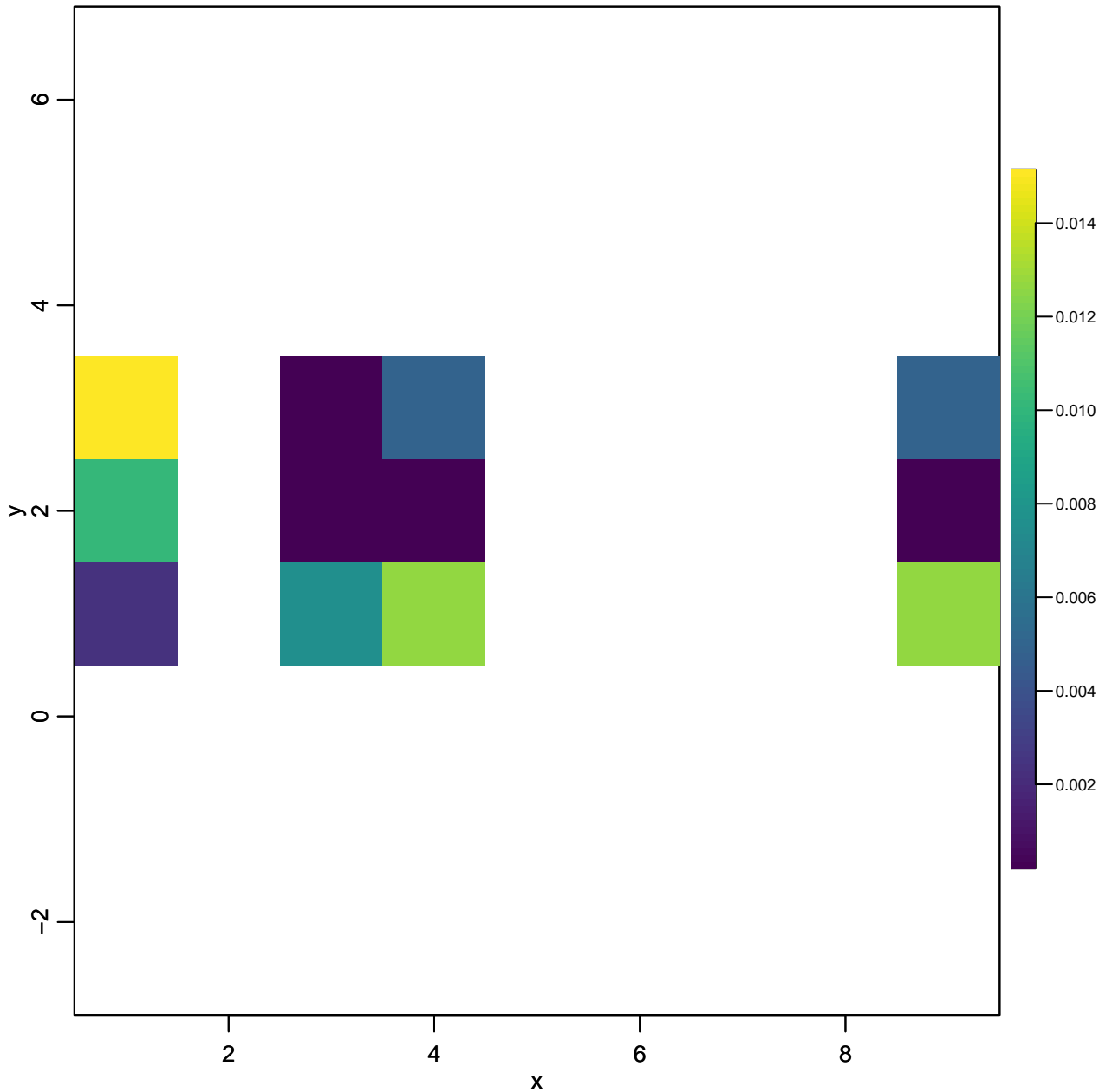
Number of calibrants per pixel (± 100 ppm)



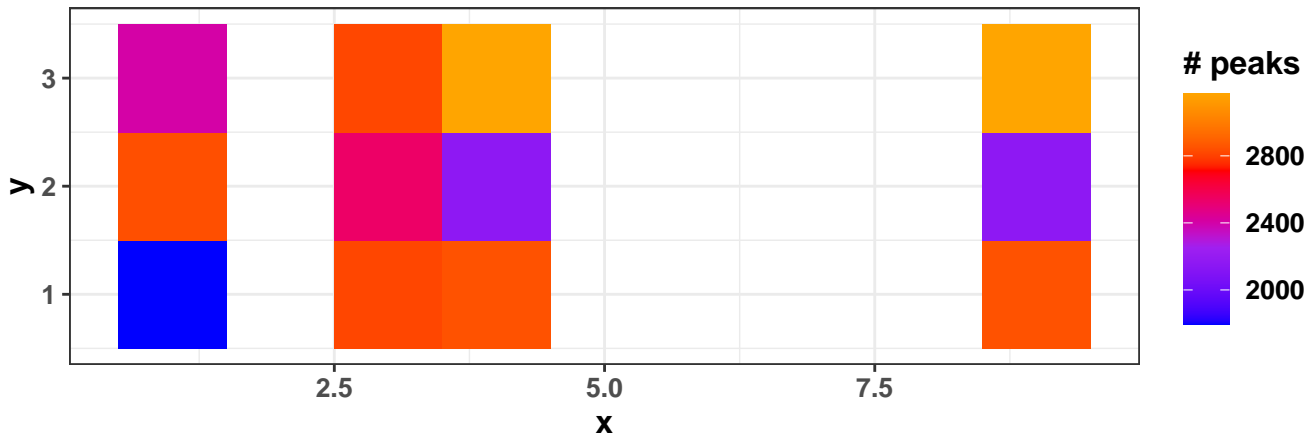
101.5: 101.5 (± 100 ppm)



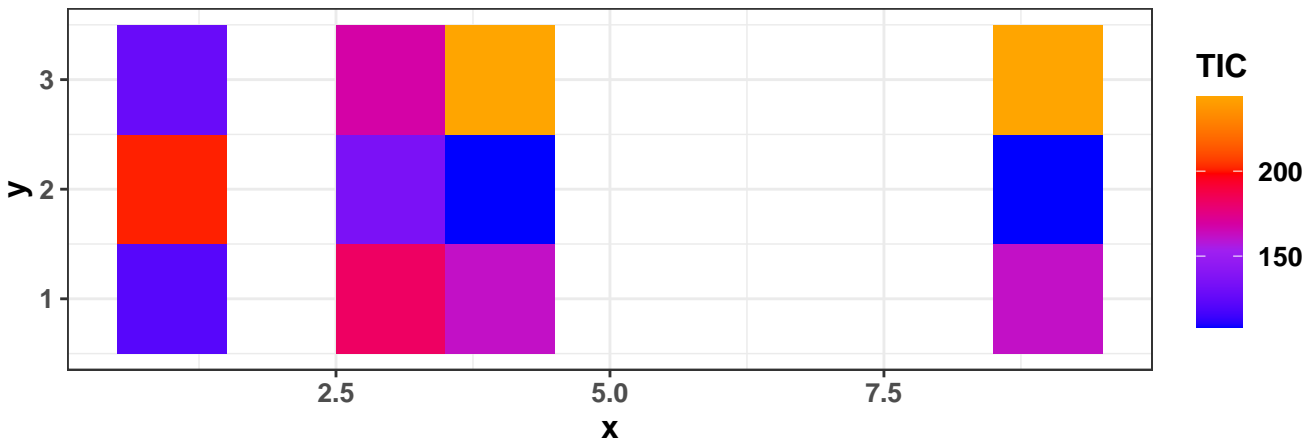
556.7: 556.7 (± 100 ppm)



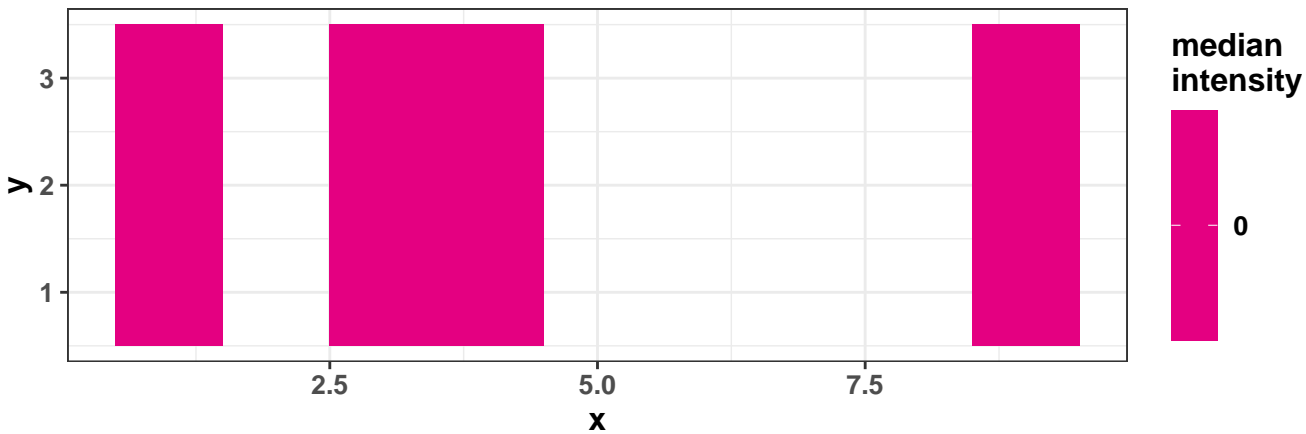
Number of peaks per spectrum



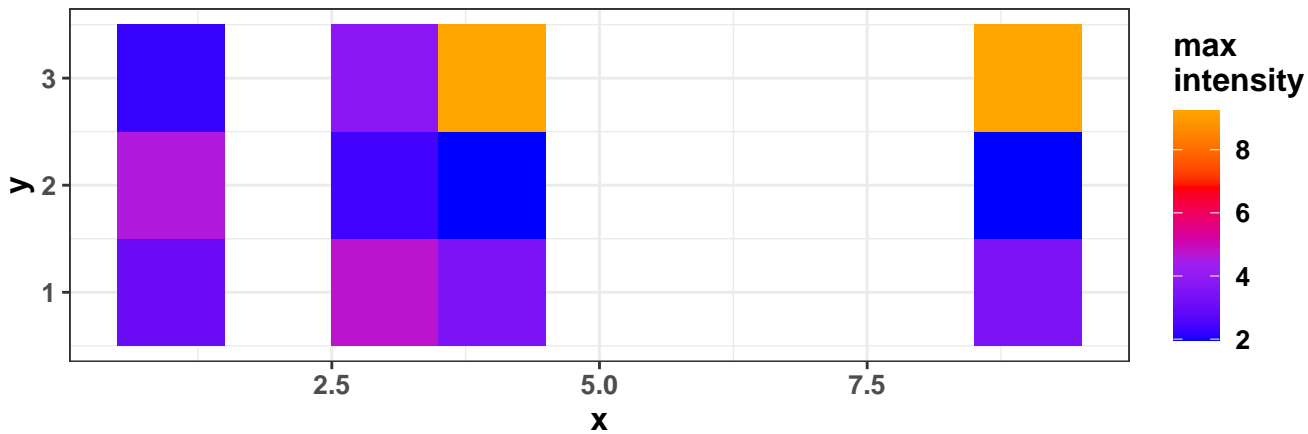
Total Ion Current



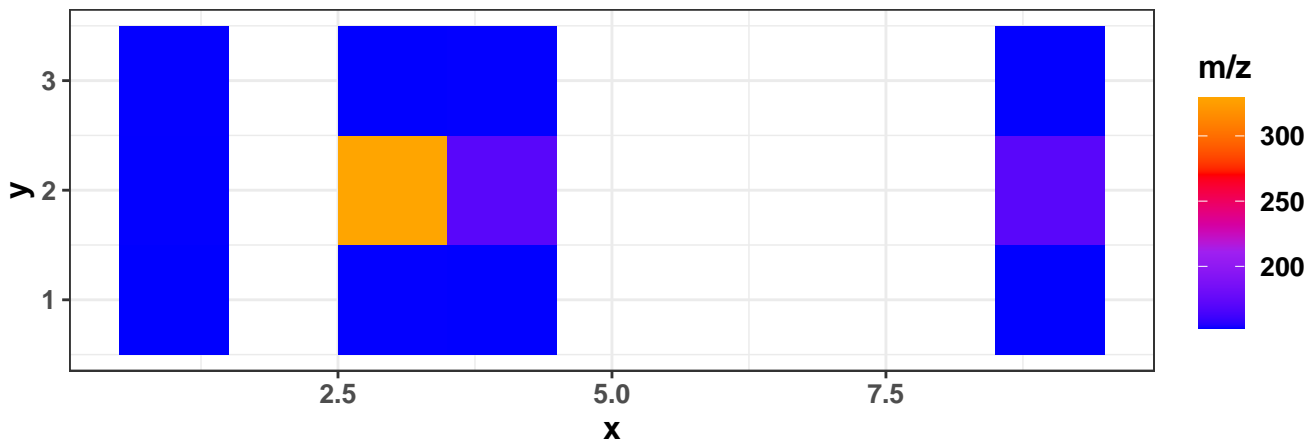
Median intensity per spectrum



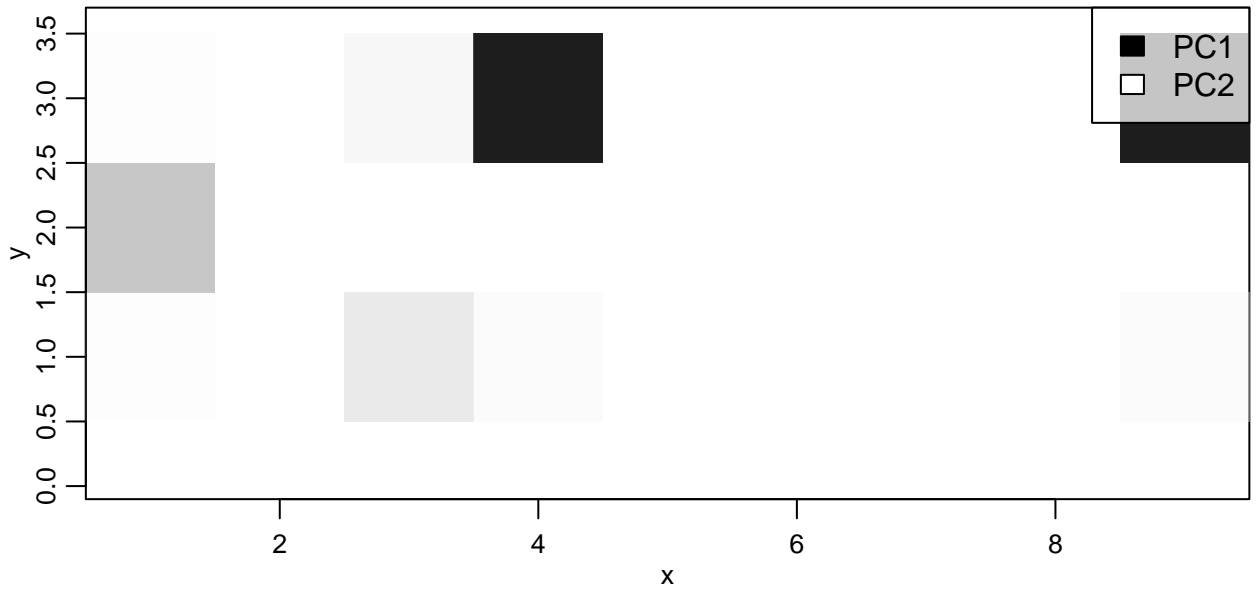
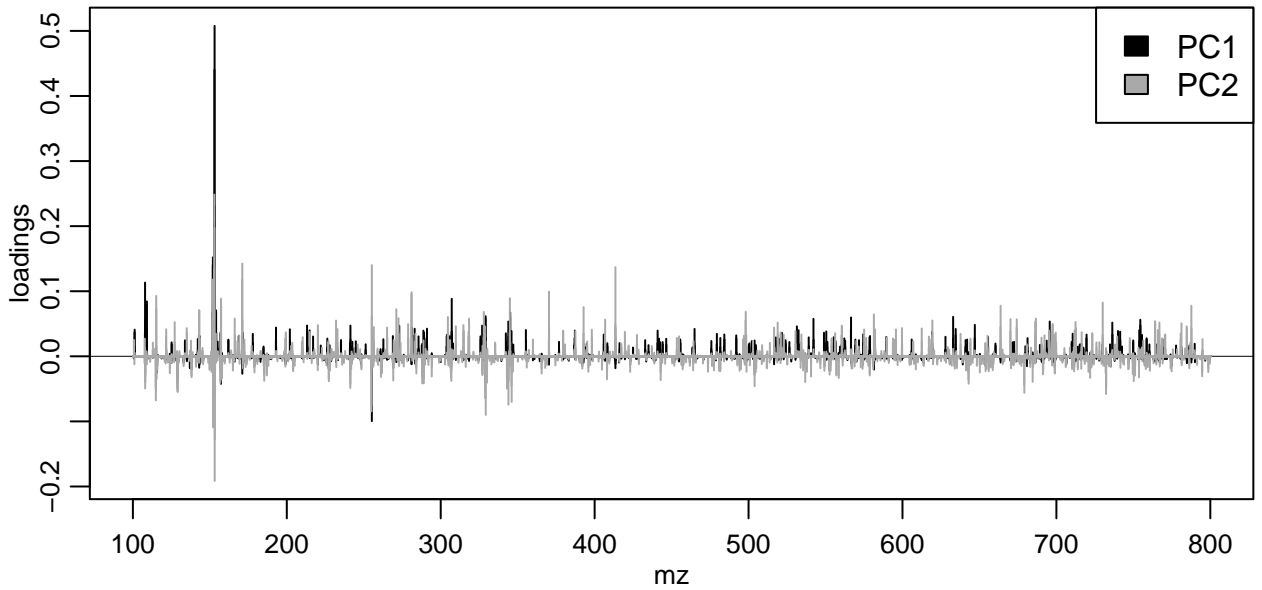
Maximum intensity per spectrum

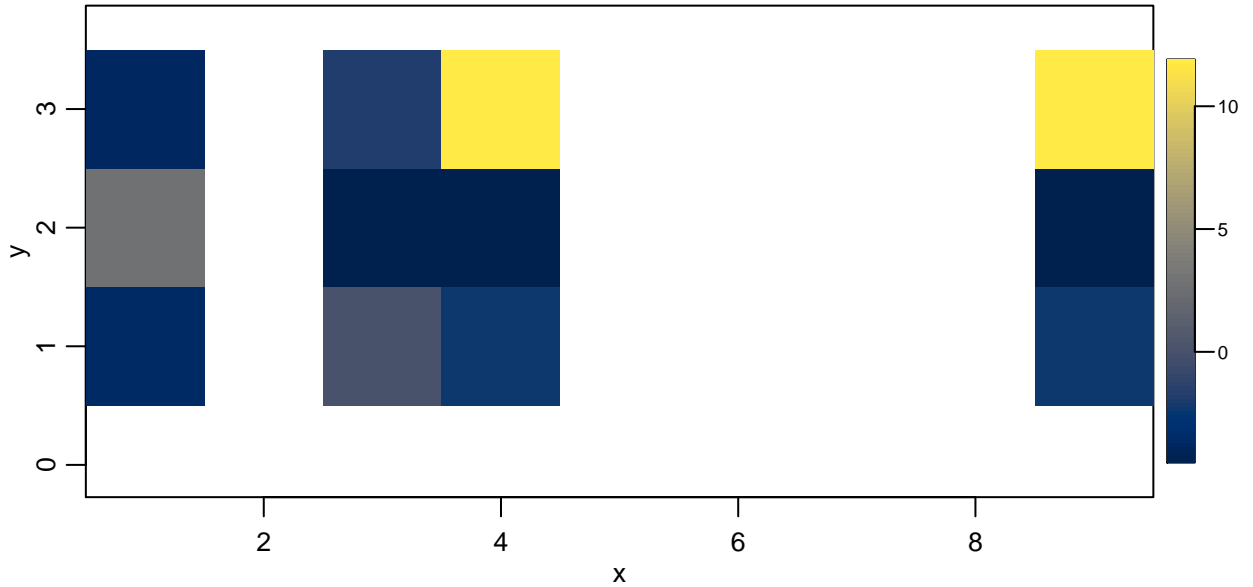
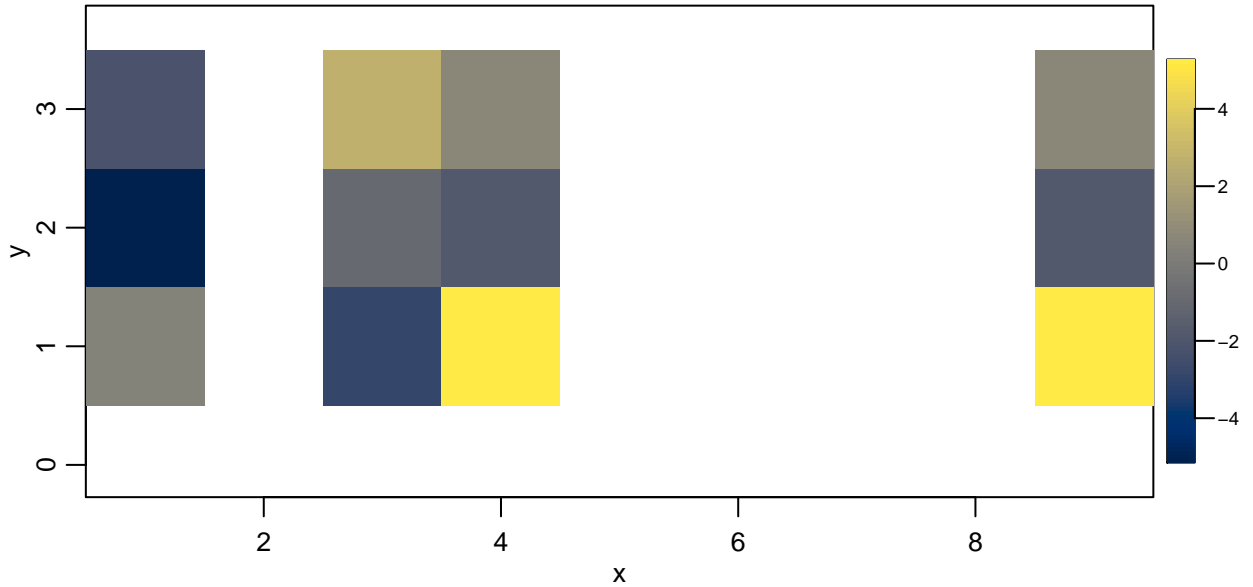


Most abundant m/z in each spectrum

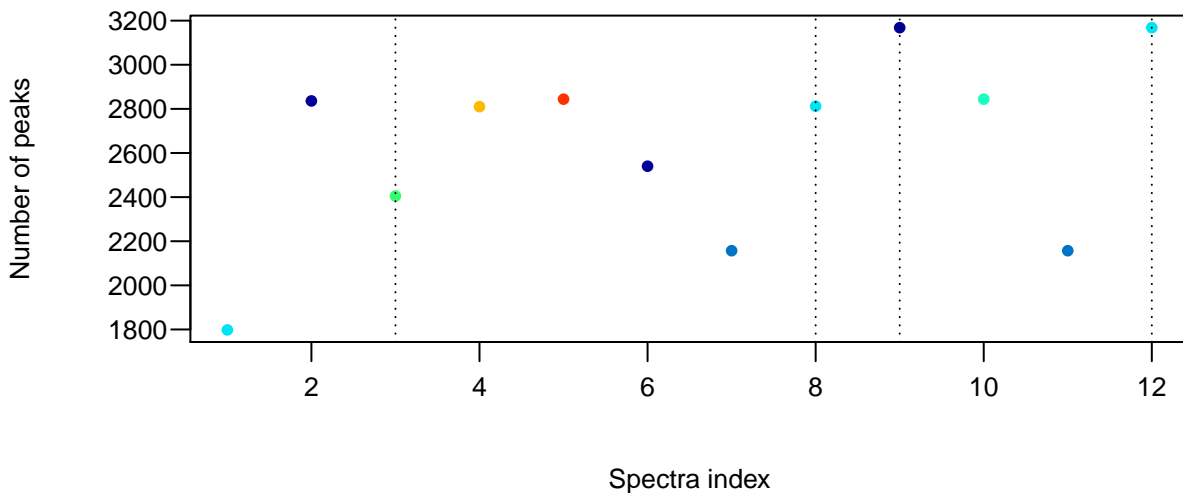


PCA for two components

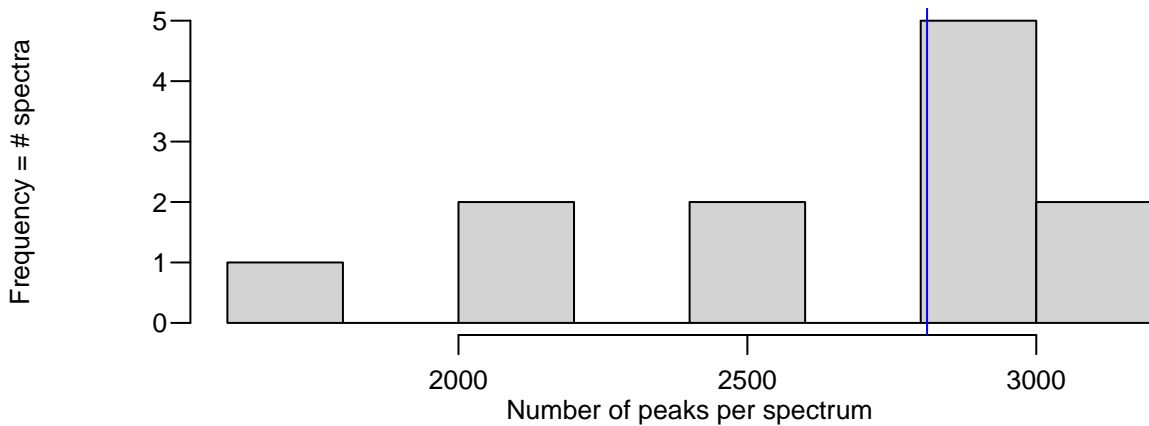


PC1**PC2**

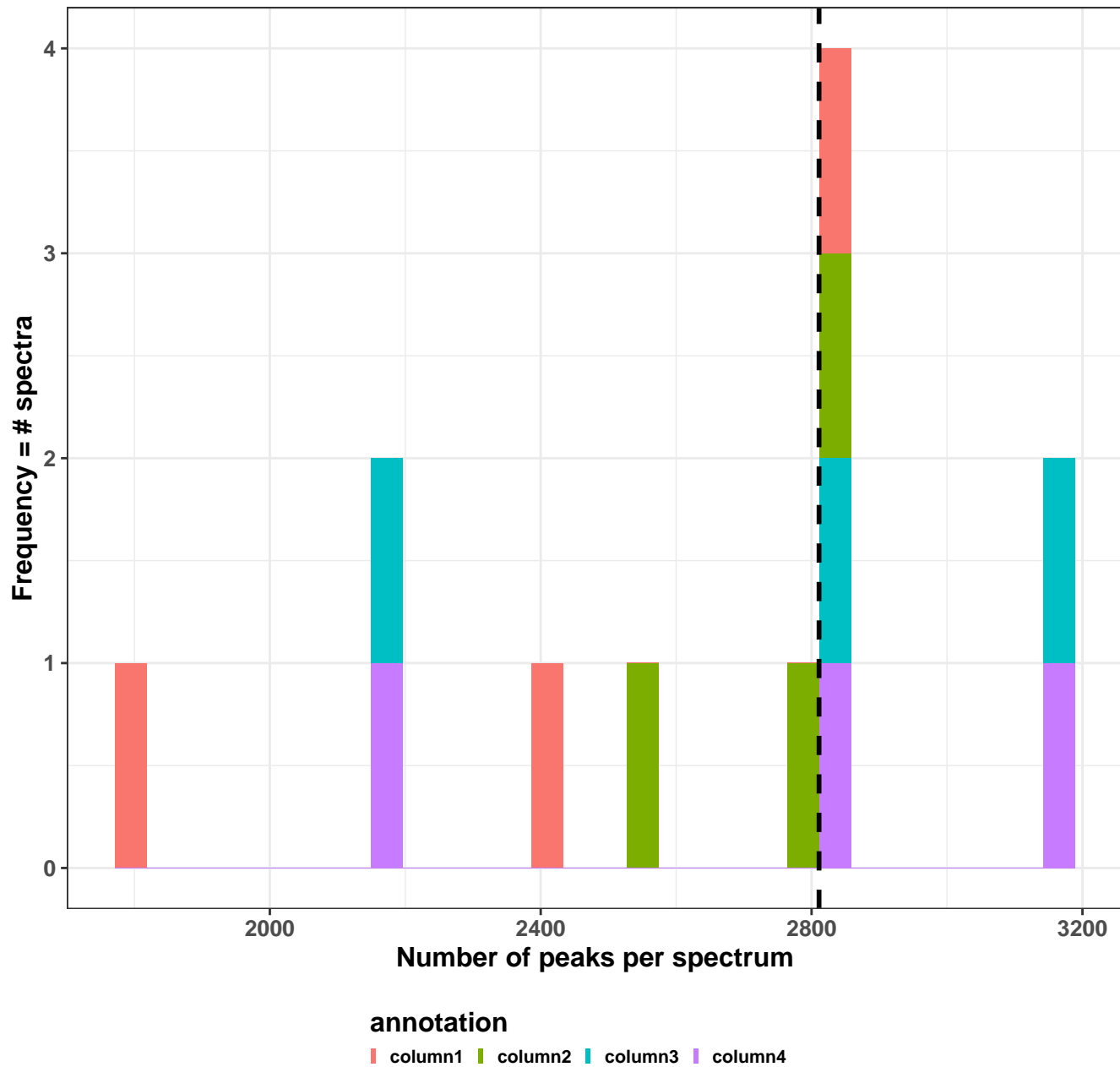
Number of peaks per spectrum



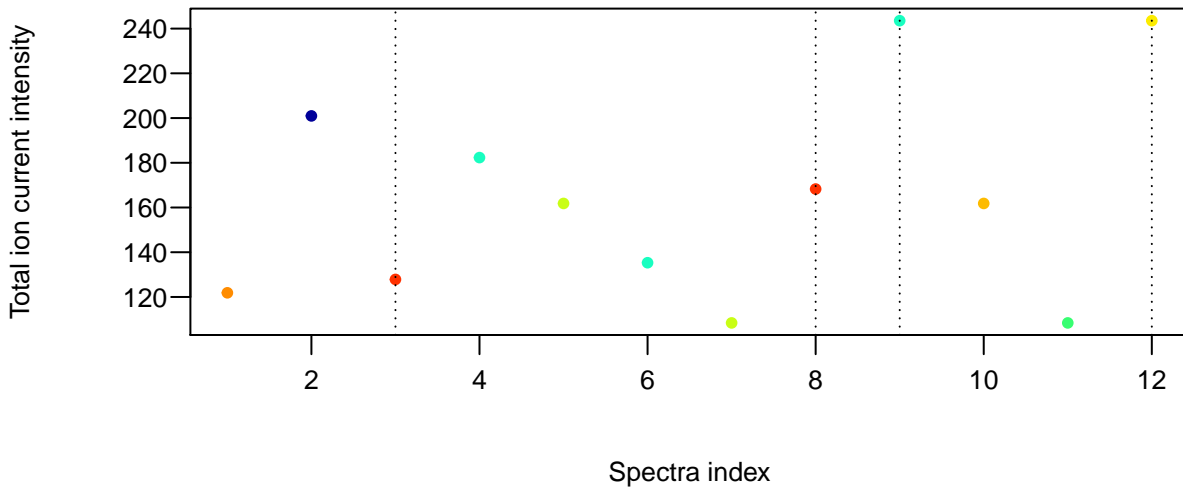
Number of peaks per spectrum



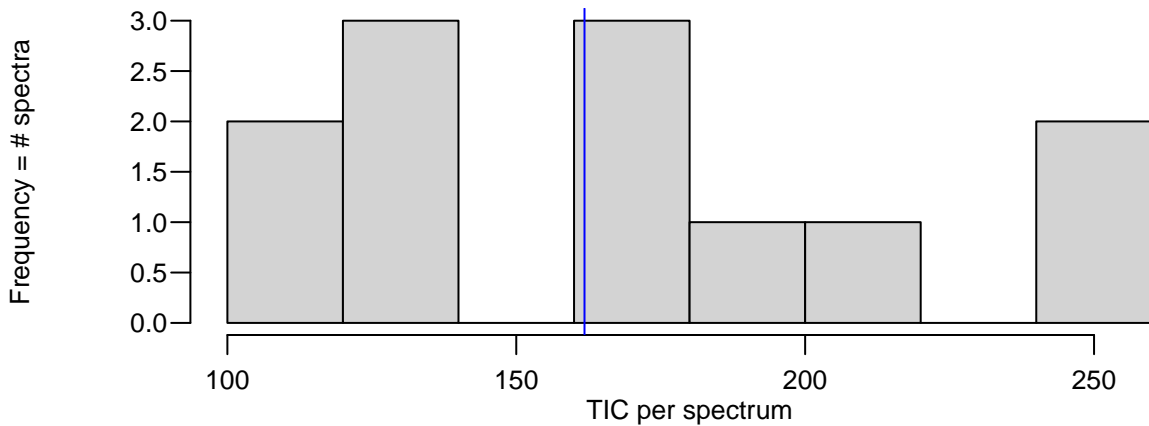
Number of peaks per spectrum and annotation group



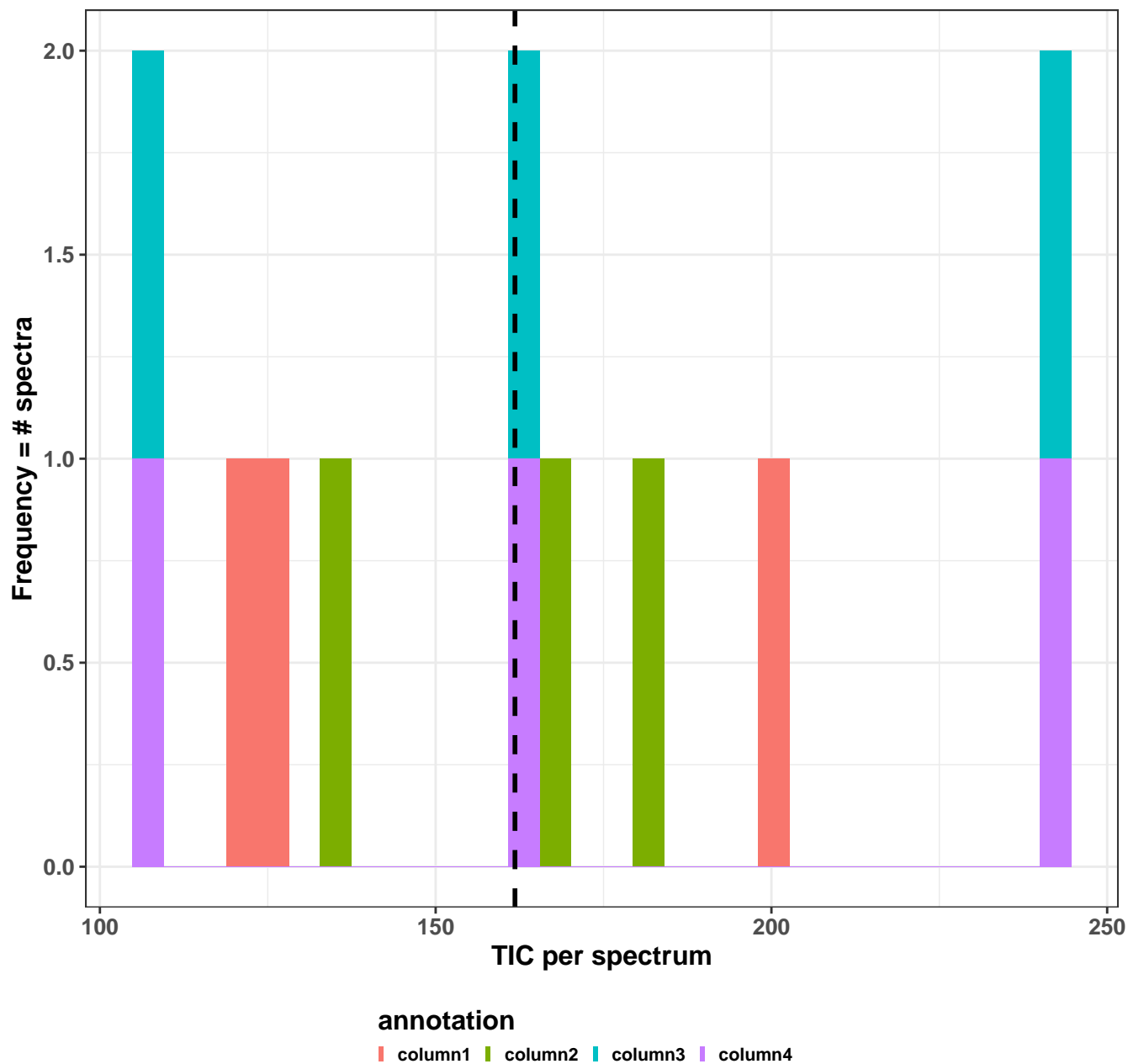
TIC per spectrum



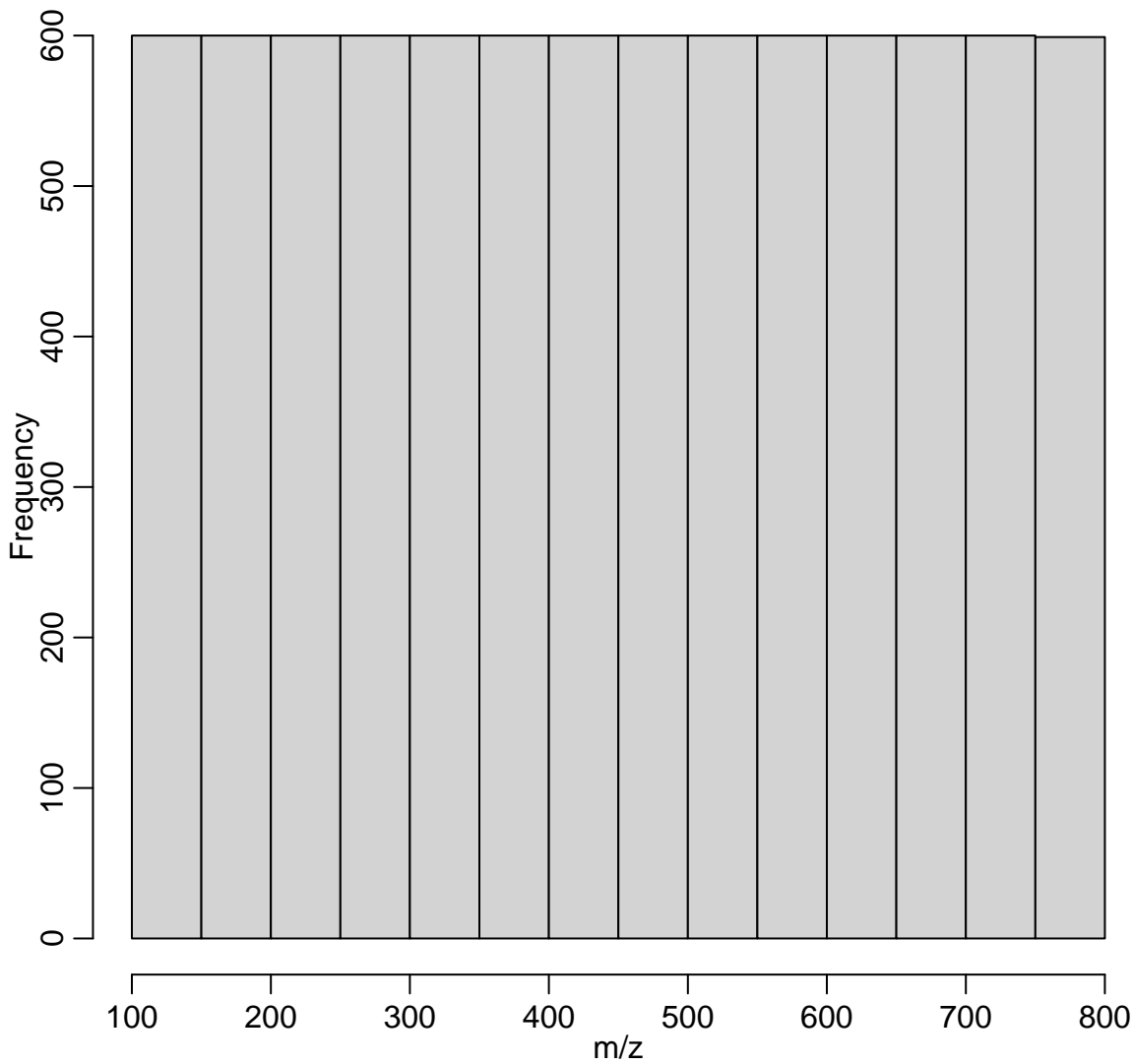
TIC per spectrum



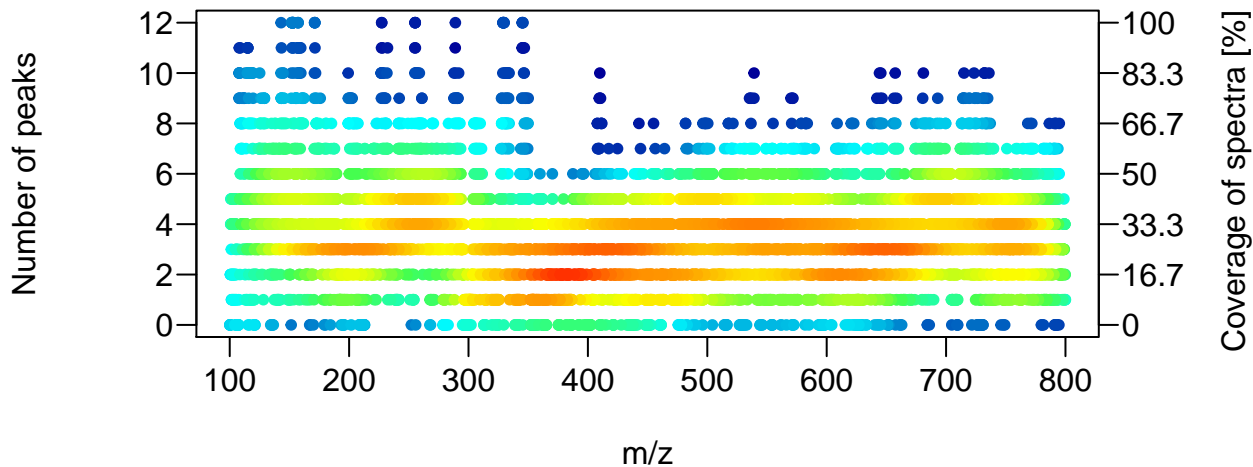
TIC per spectrum and annotation group



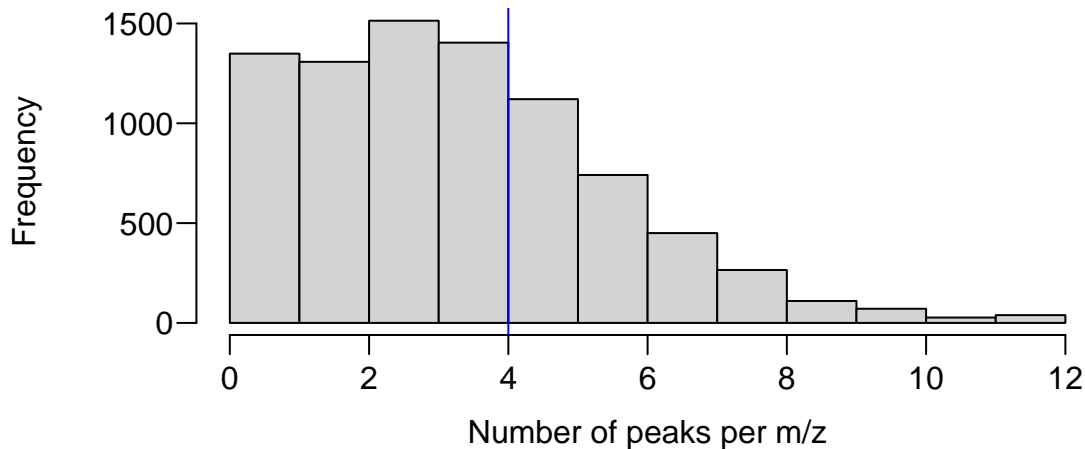
Histogram of m/z values



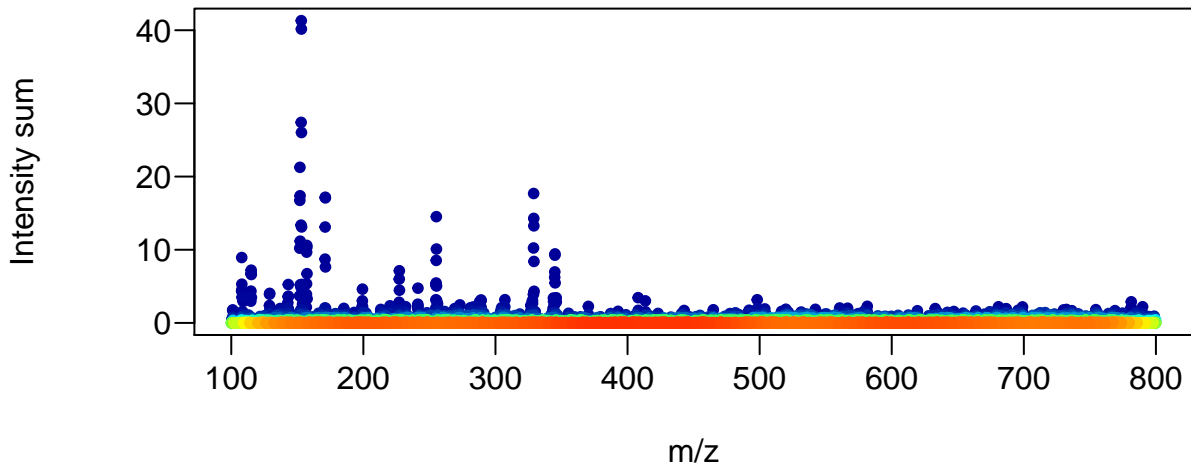
Number of peaks per m/z



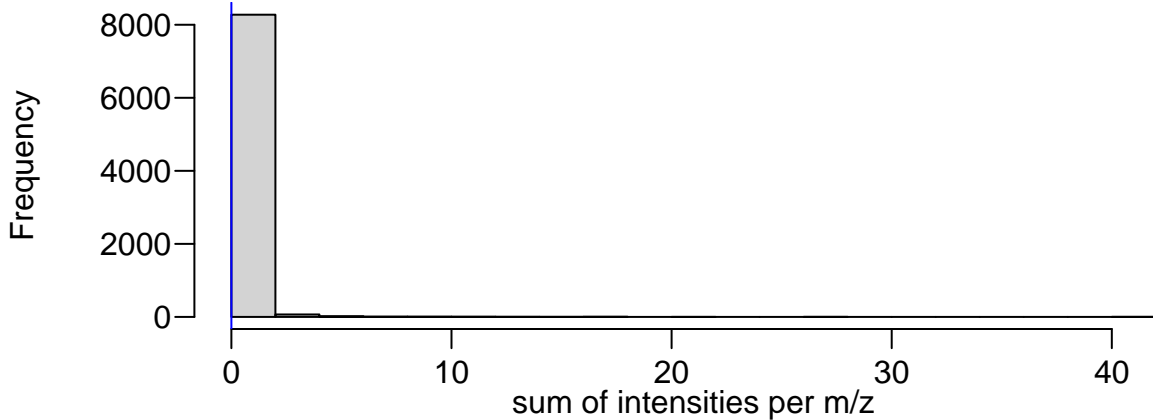
Number of peaks per m/z



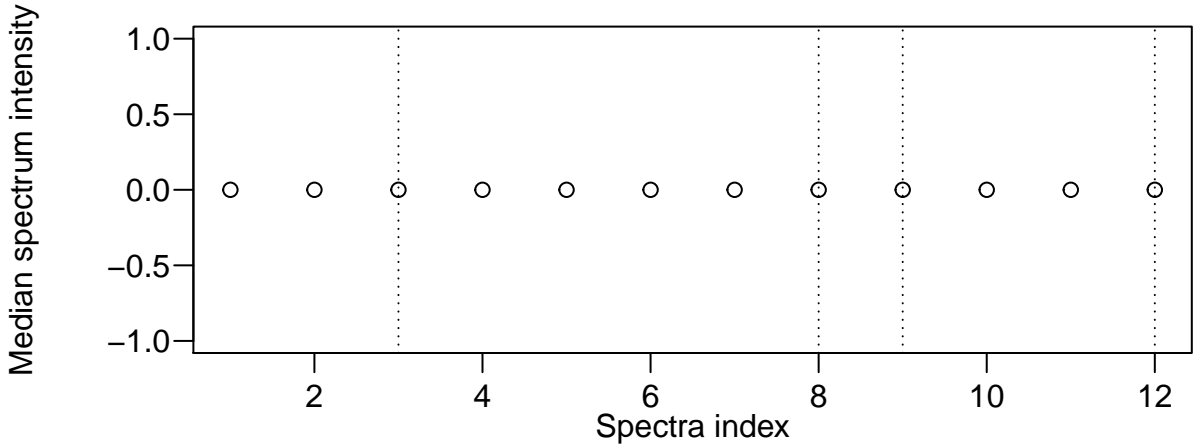
Sum of intensities per m/z



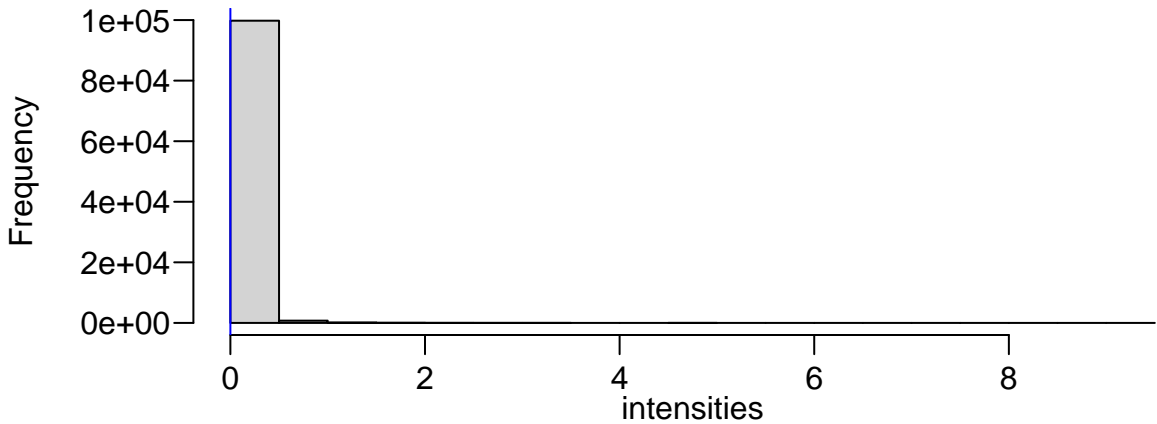
Sum of intensities per m/z



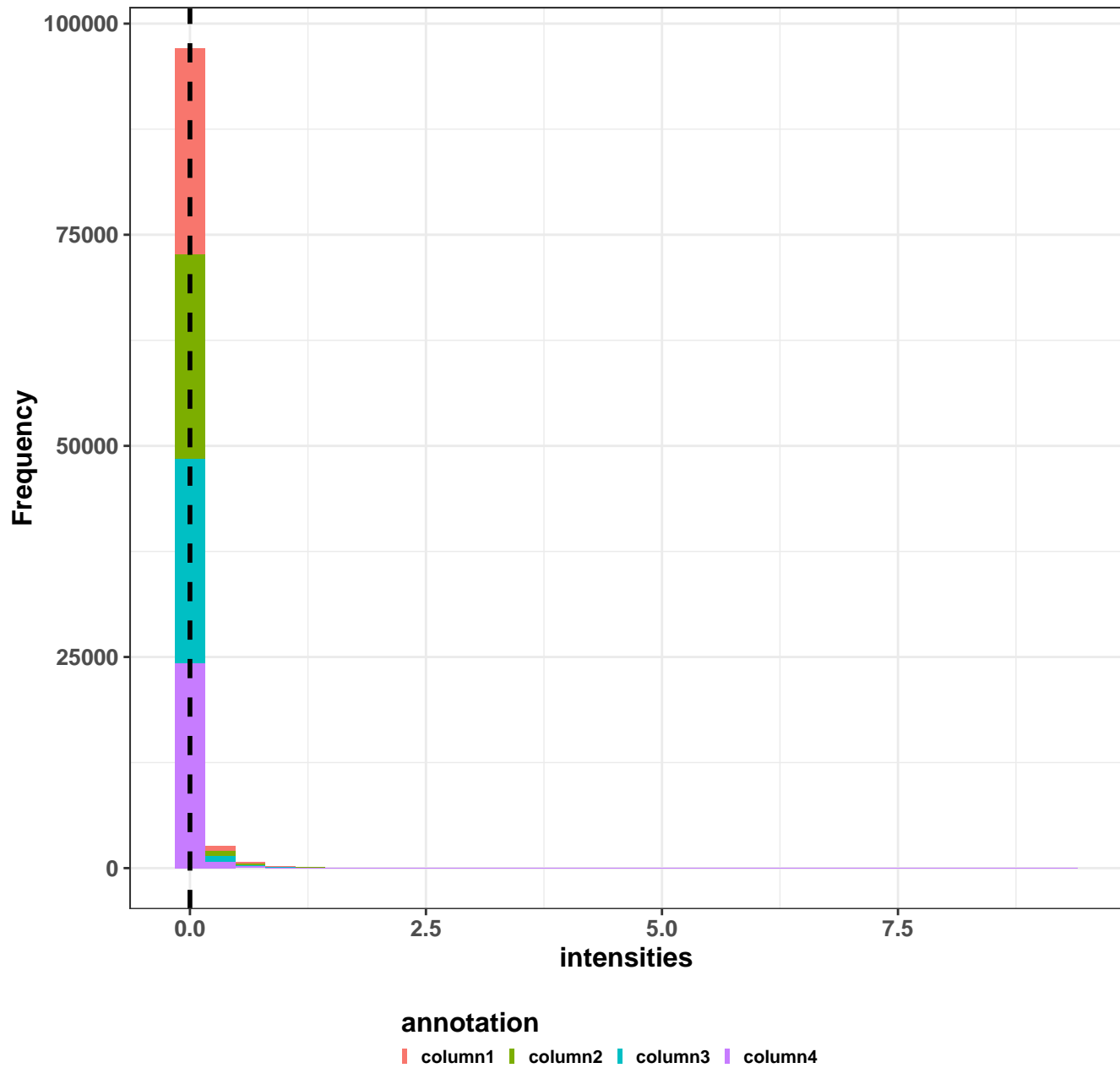
Median intensity per spectrum



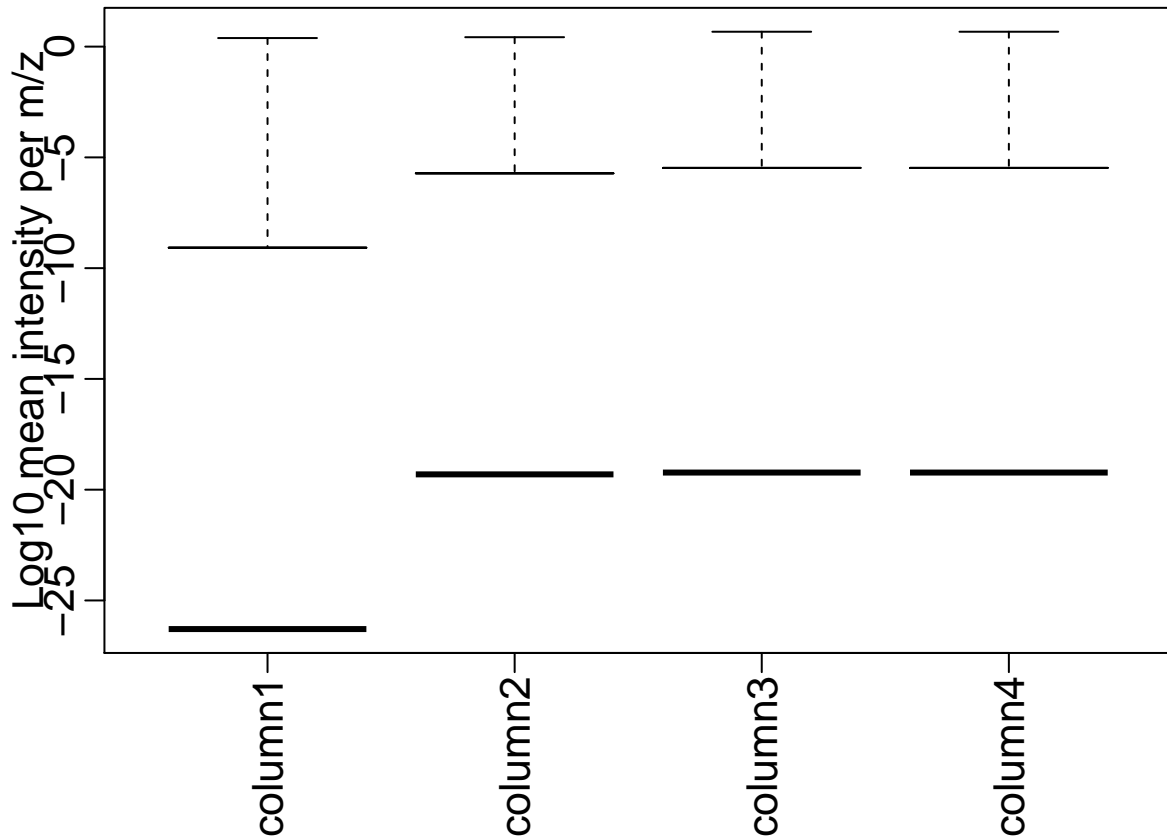
Intensity histogram

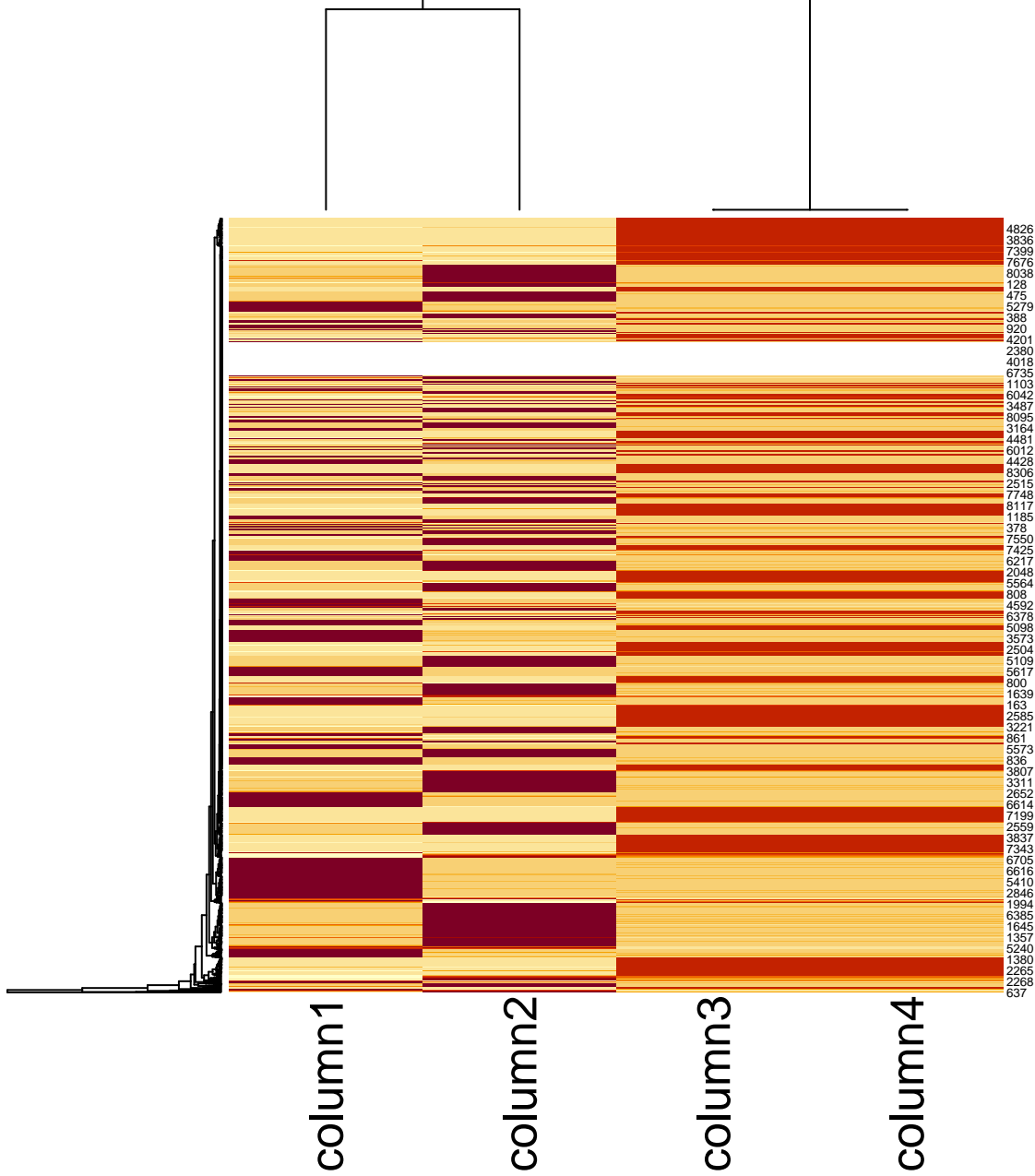


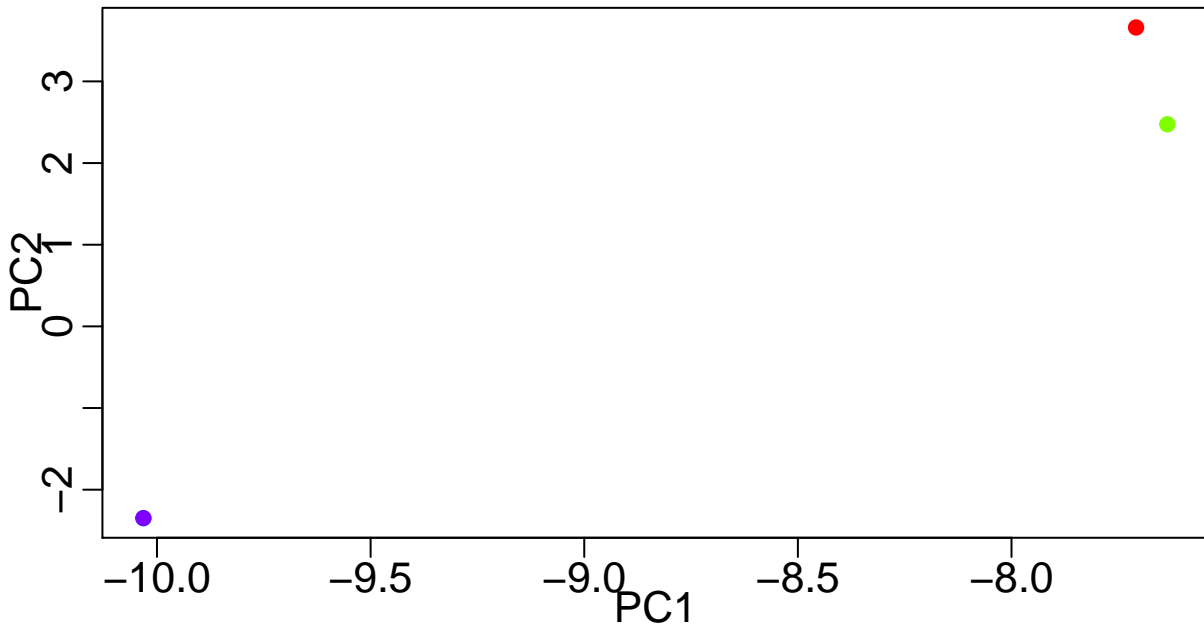
Intensities per sample

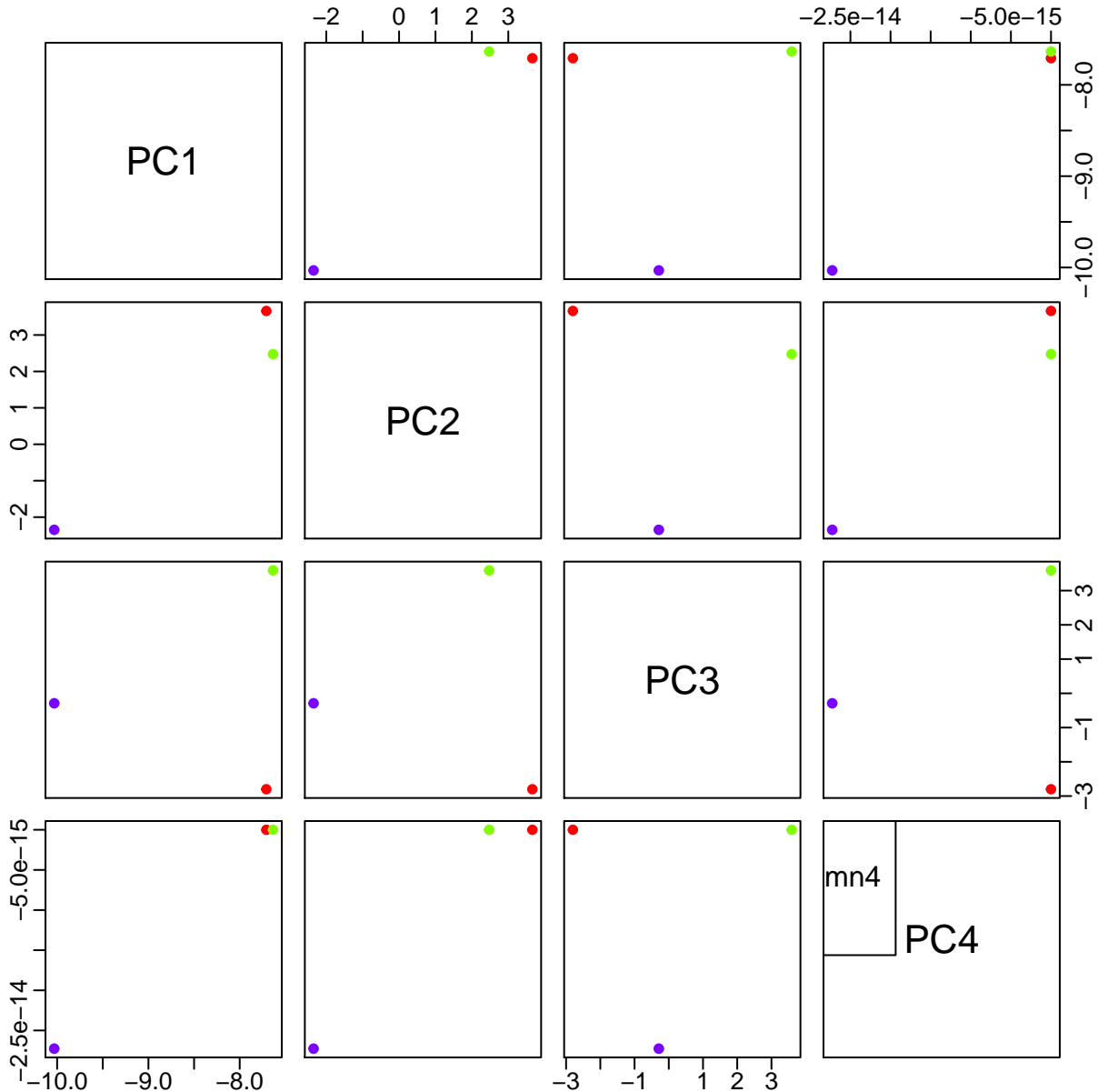


Log10 mean m/z intensities per annotation group

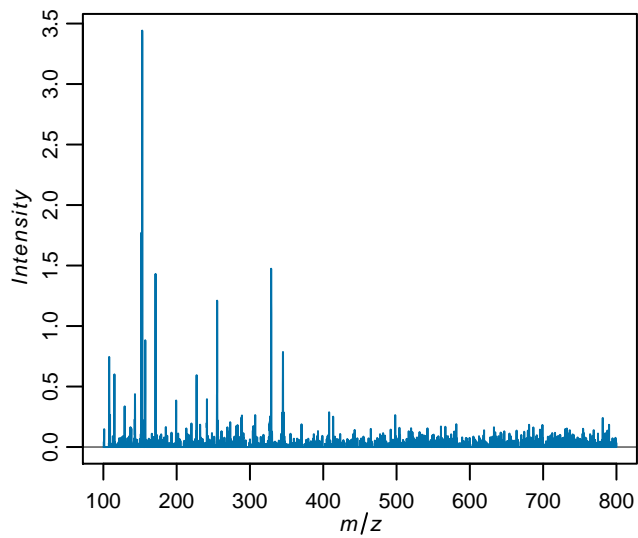




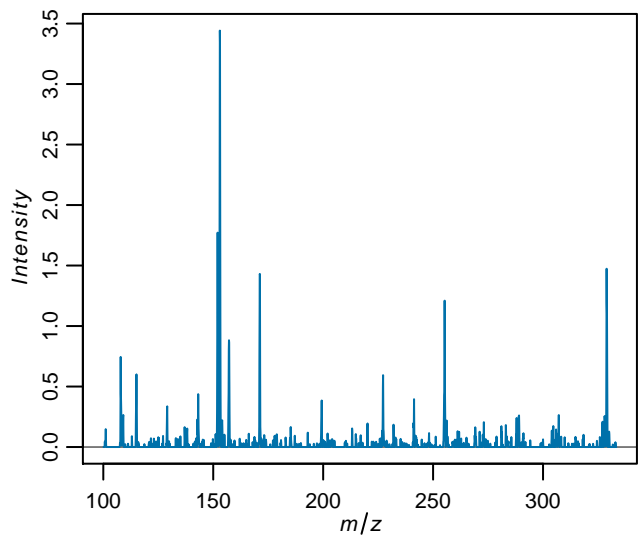




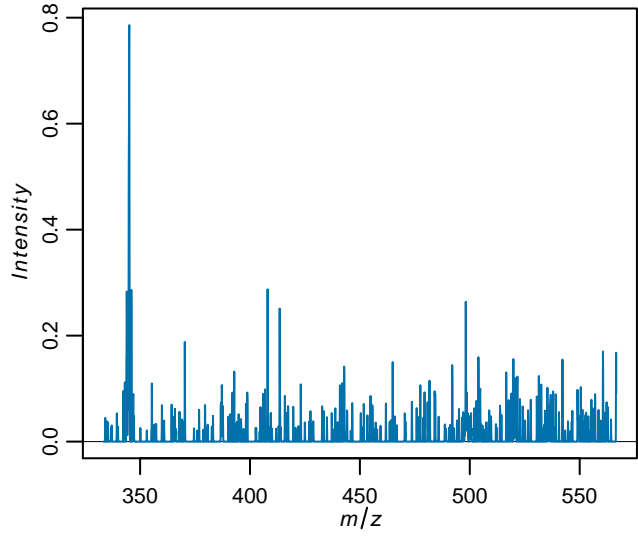
Average spectrum



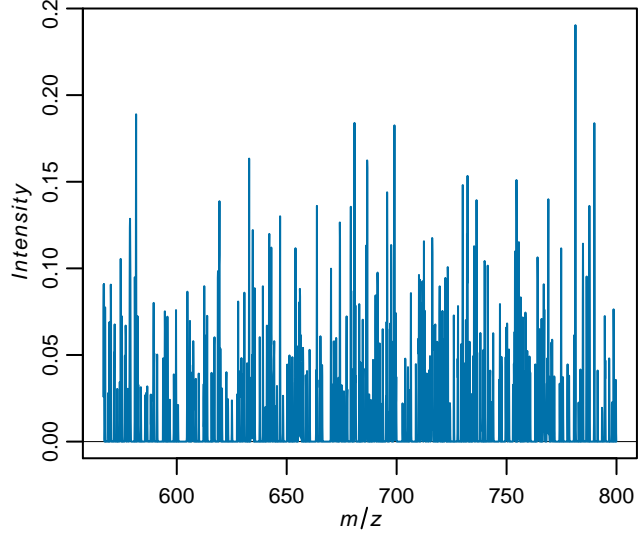
Zoomed average spectrum



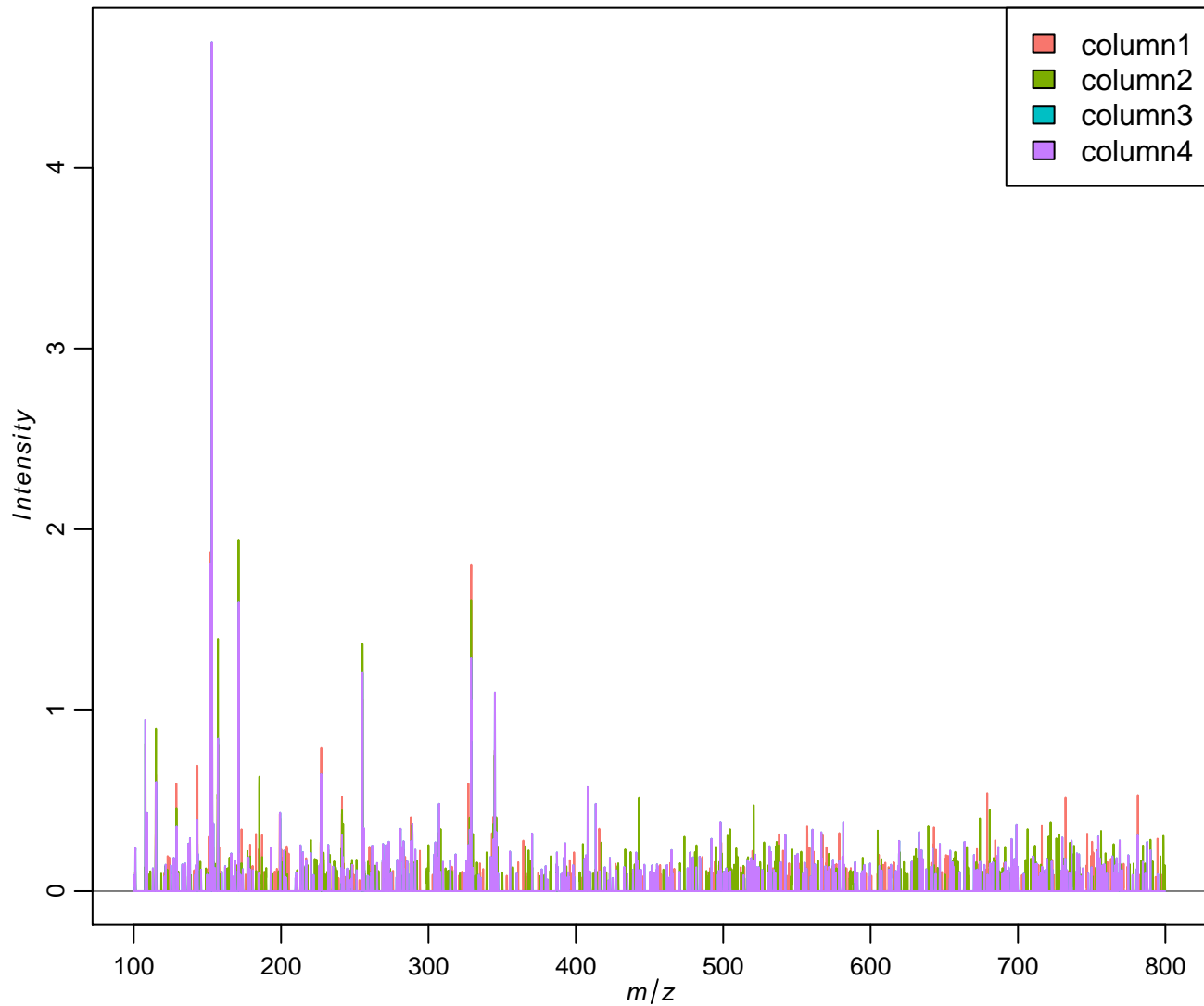
Zoomed average spectrum



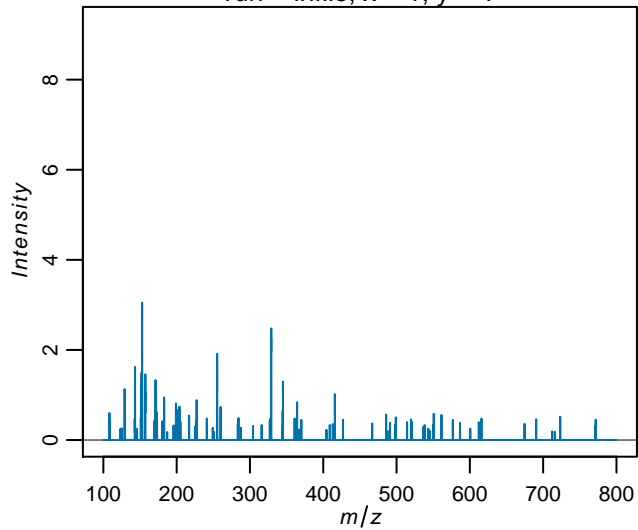
Zoomed average spectrum



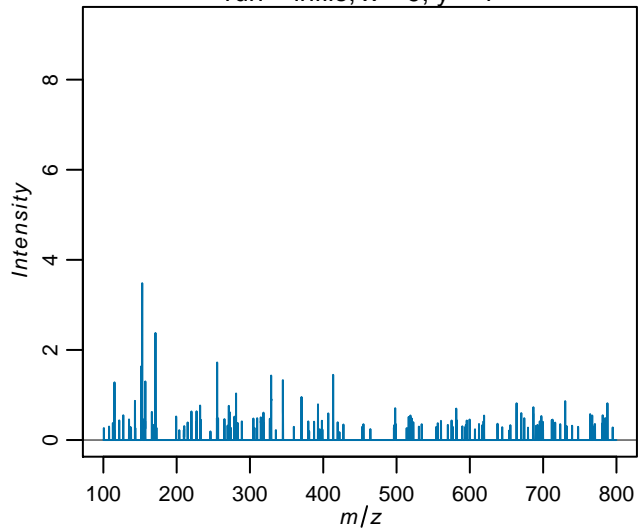
Average mass spectra for annotation groups



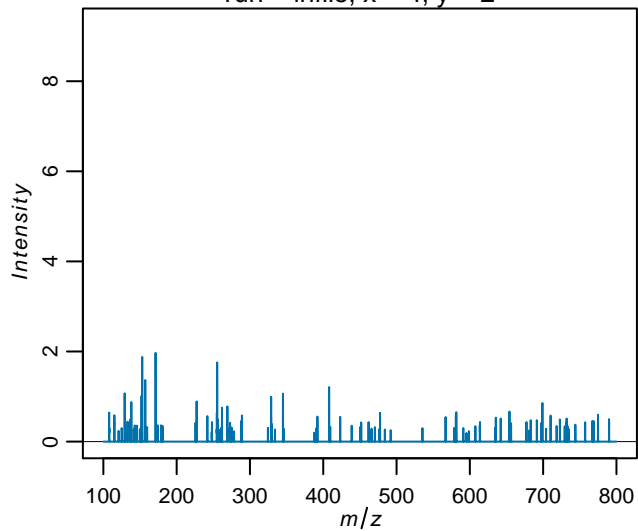
run = infile, x = 1, y = 1



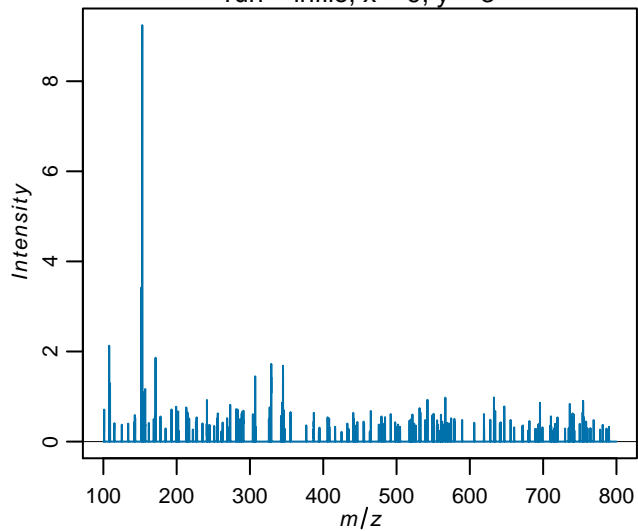
run = infile, x = 9, y = 1



run = infile, x = 4, y = 2



run = infile, x = 9, y = 3

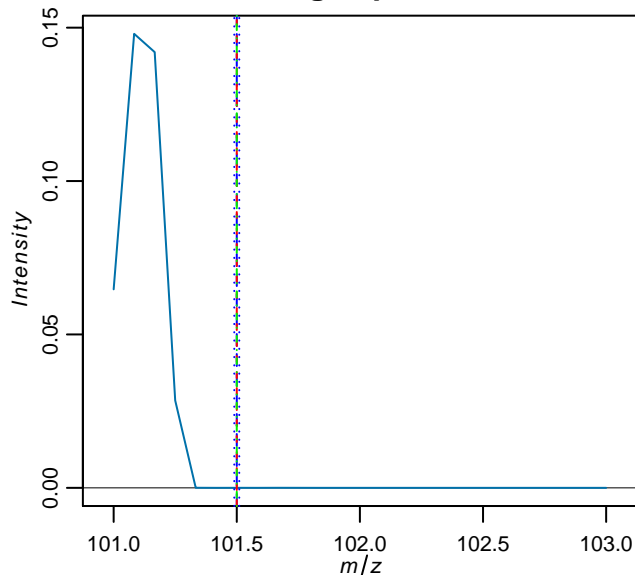


theor. m/z: 101.5

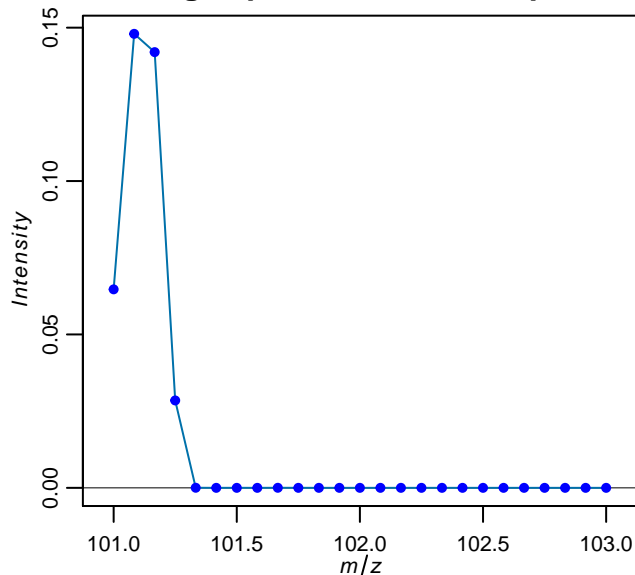
most abundant m/z: 101.5

closest m/z: 101.5

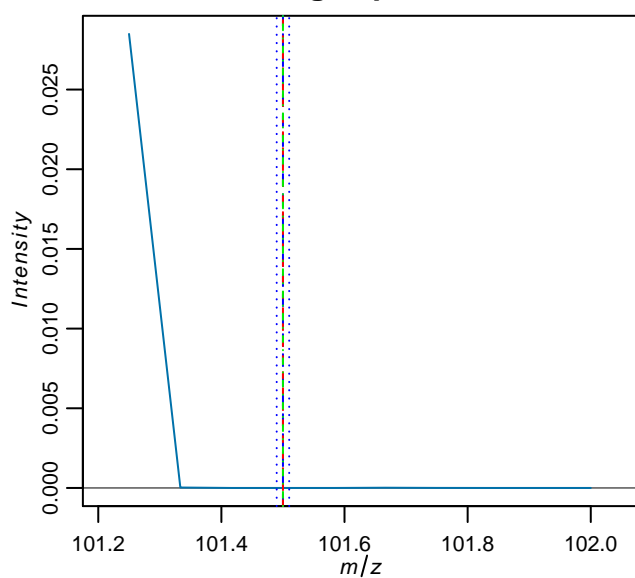
Average spectrum



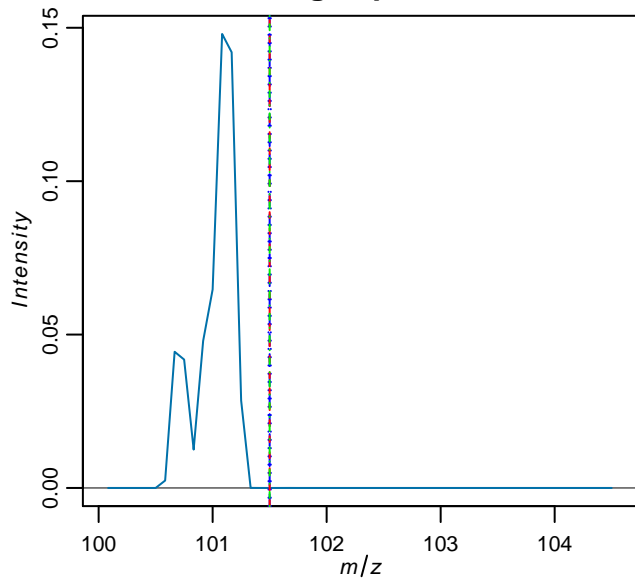
Average spectrum with data points



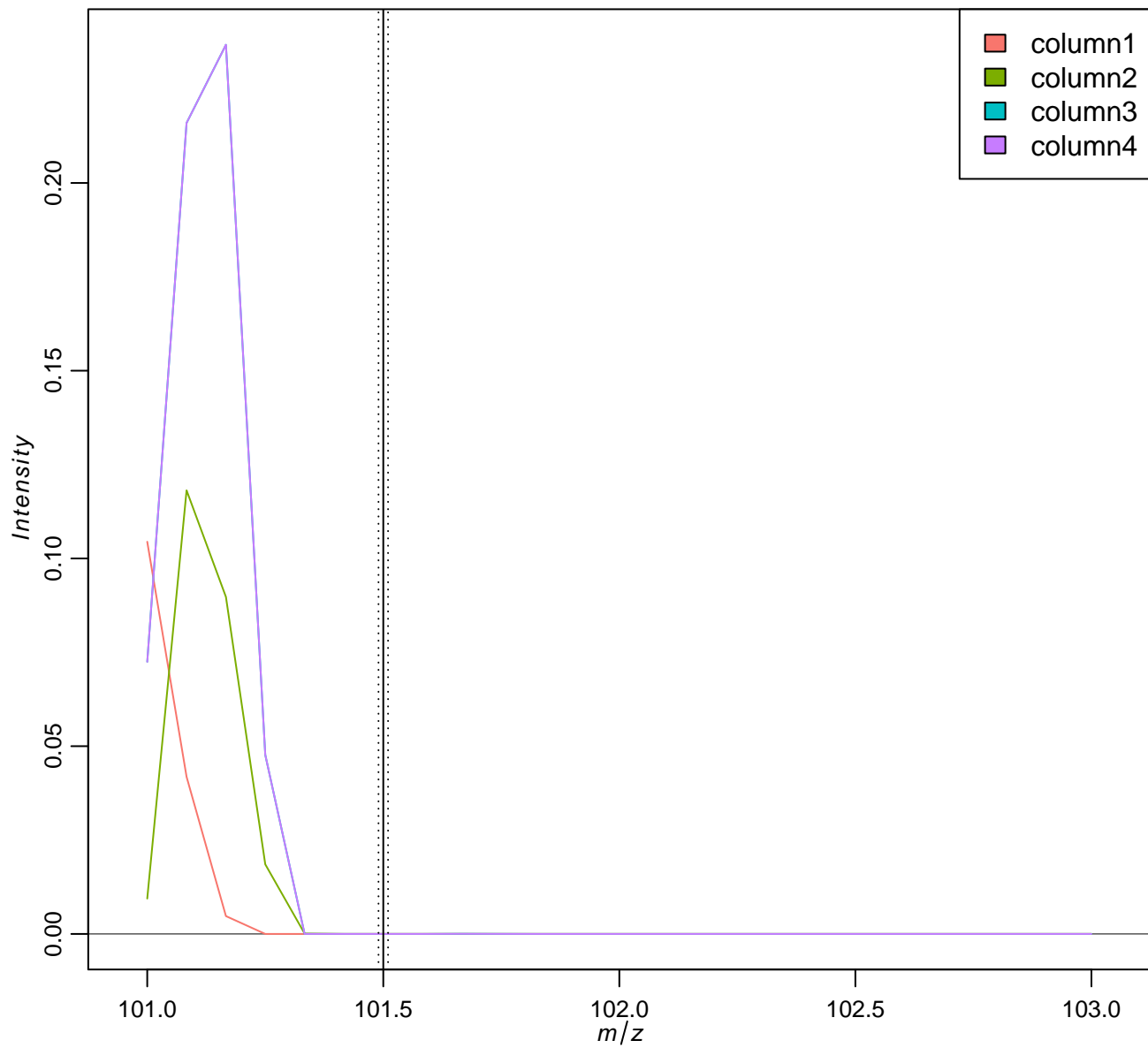
Average spectrum



Average spectrum



Average spectrum per annotation group

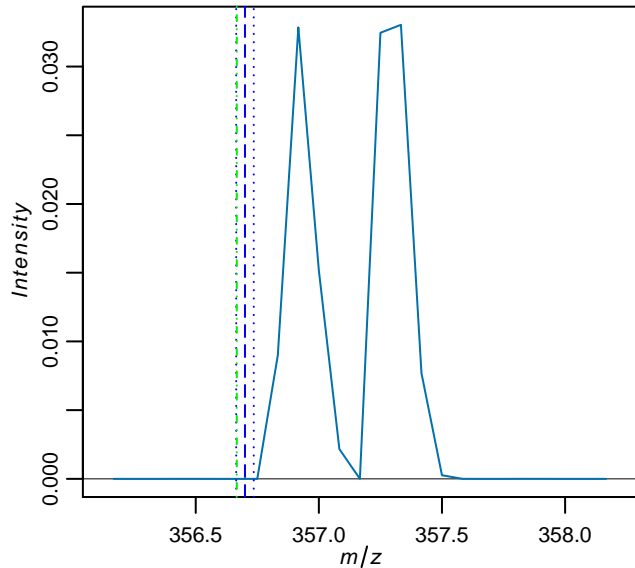


theor. m/z: 356.7

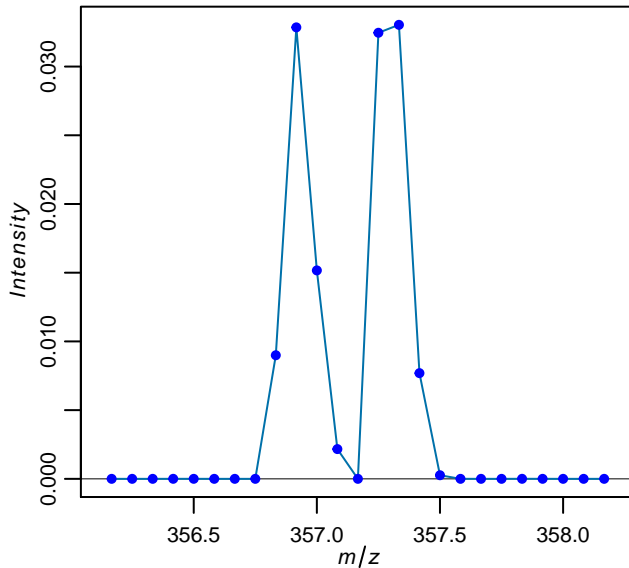
most abundant m/z: NA

closest m/z: 356.667

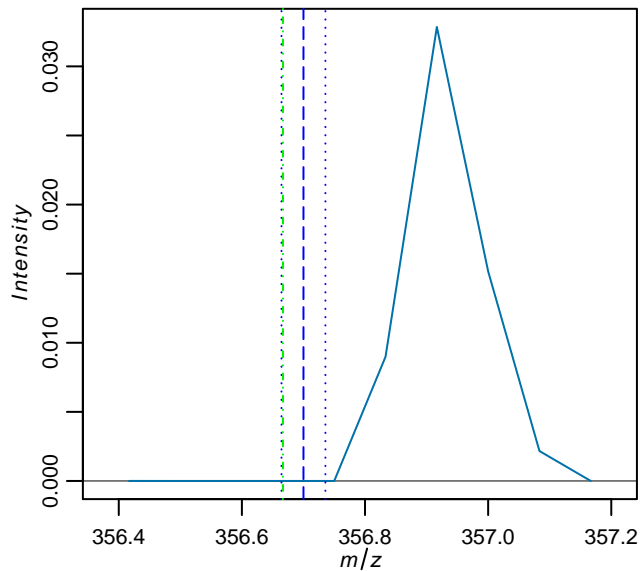
Average spectrum



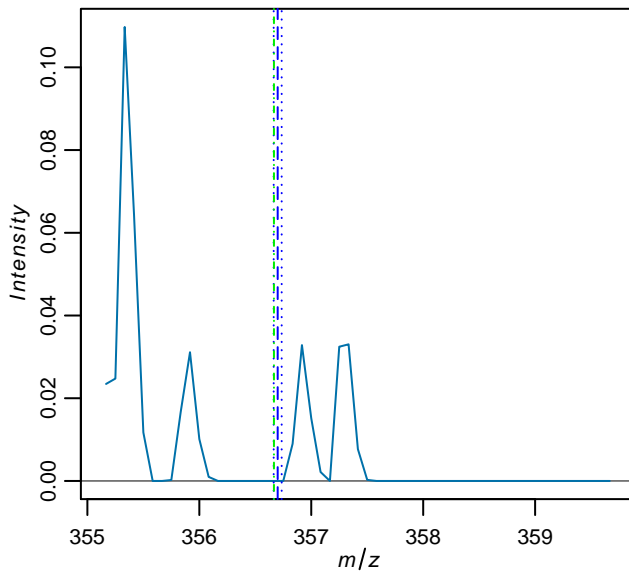
Average spectrum with data points



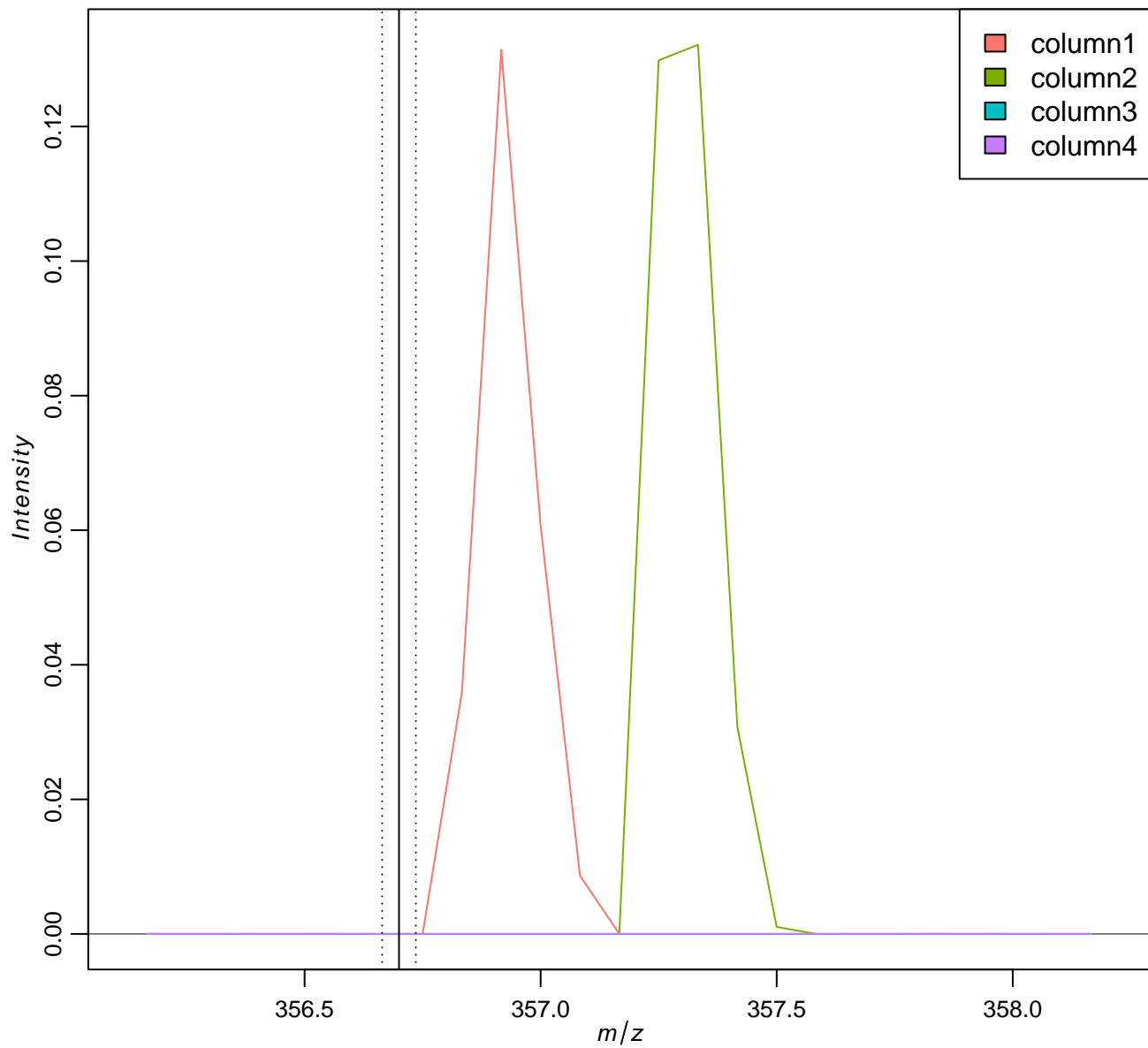
Average spectrum



Average spectrum



Average spectrum per annotation group

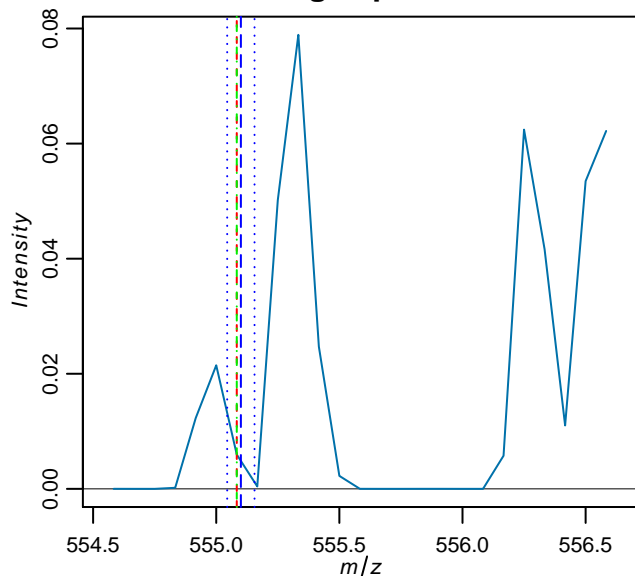


theor. m/z: 555.1

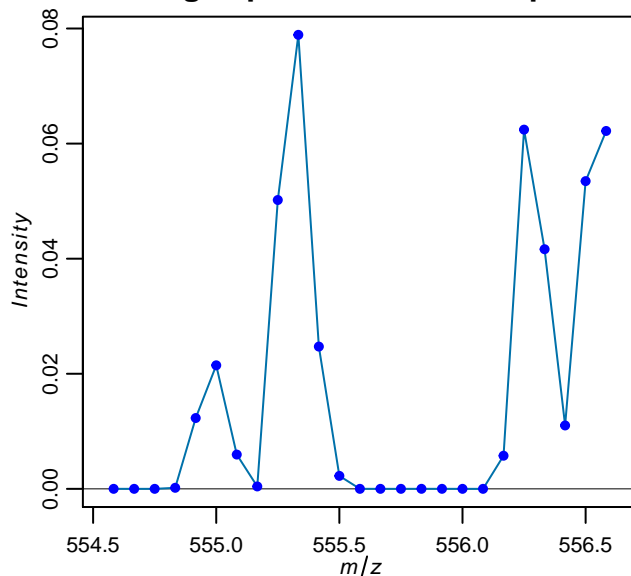
most abundant m/z: 555.0834

closest m/z: 555.0834

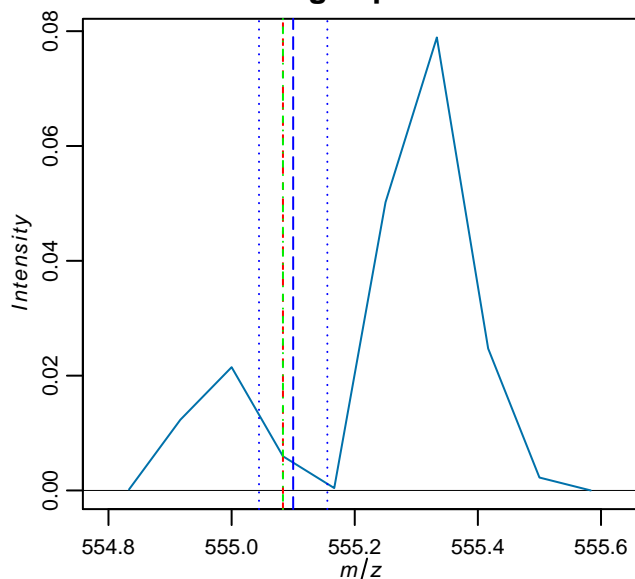
Average spectrum



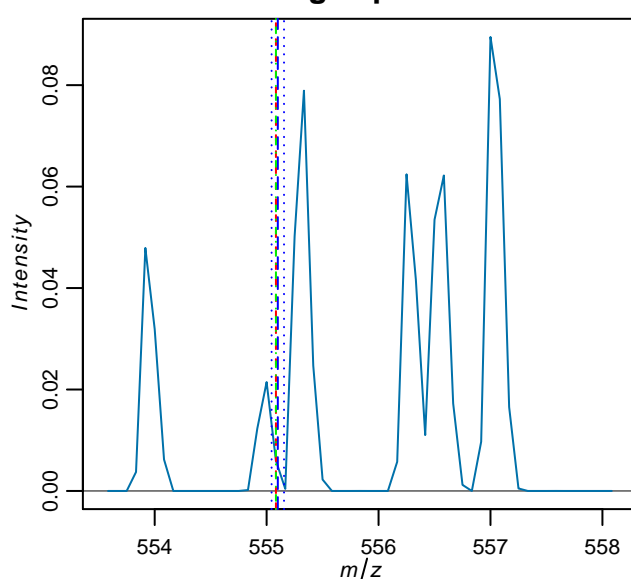
Average spectrum with data points



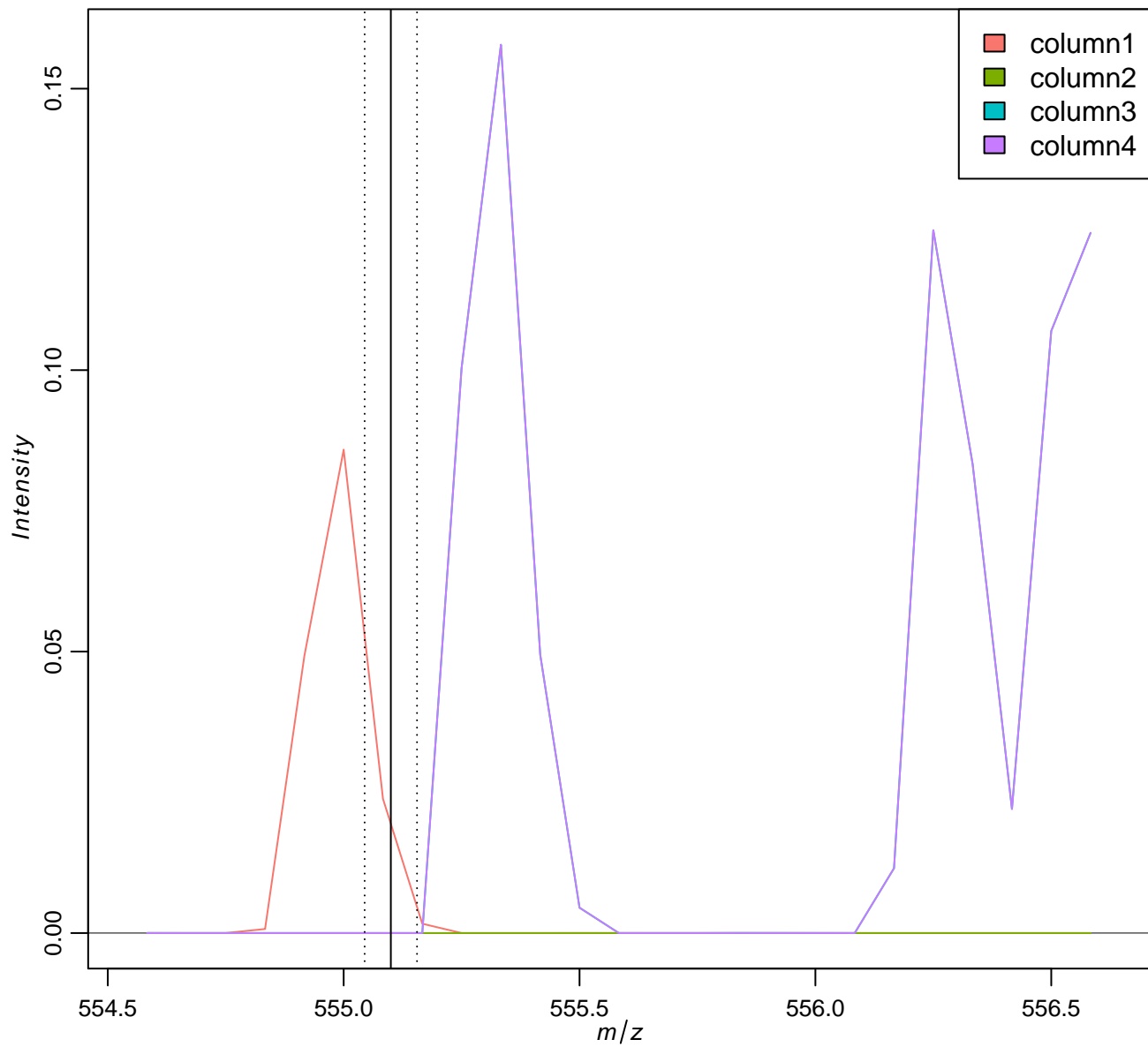
Average spectrum



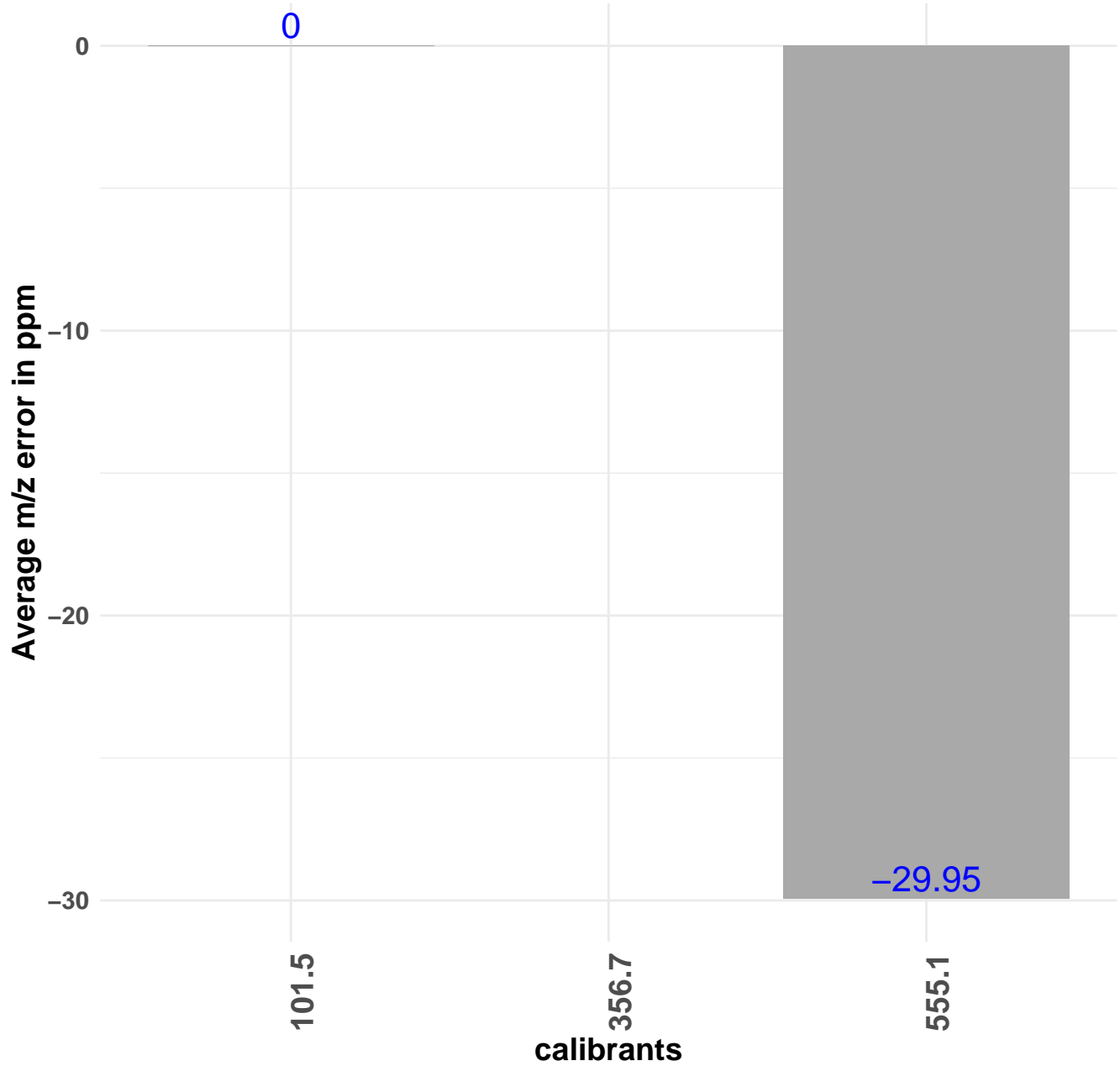
Average spectrum



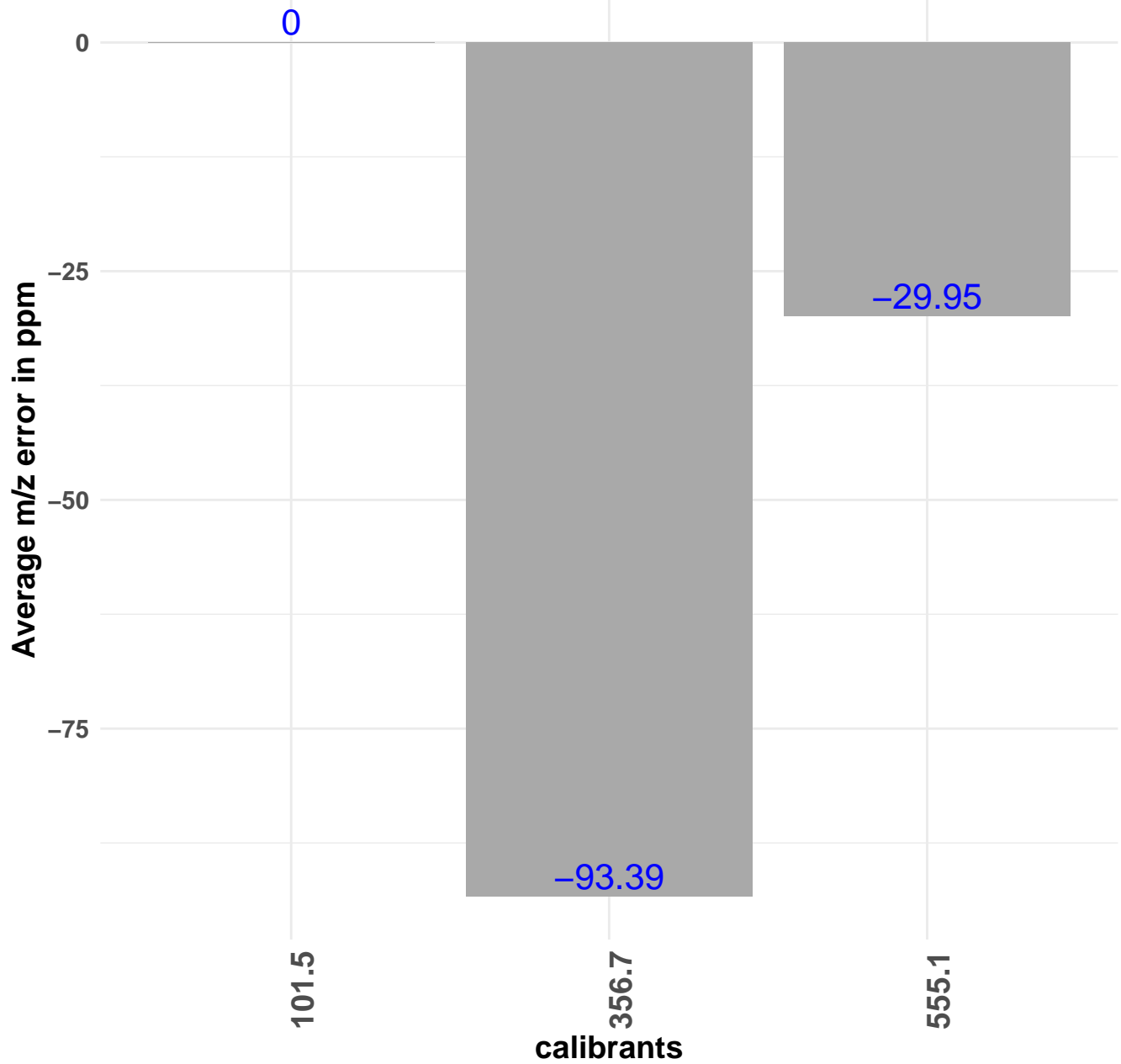
Average spectrum per annotation group



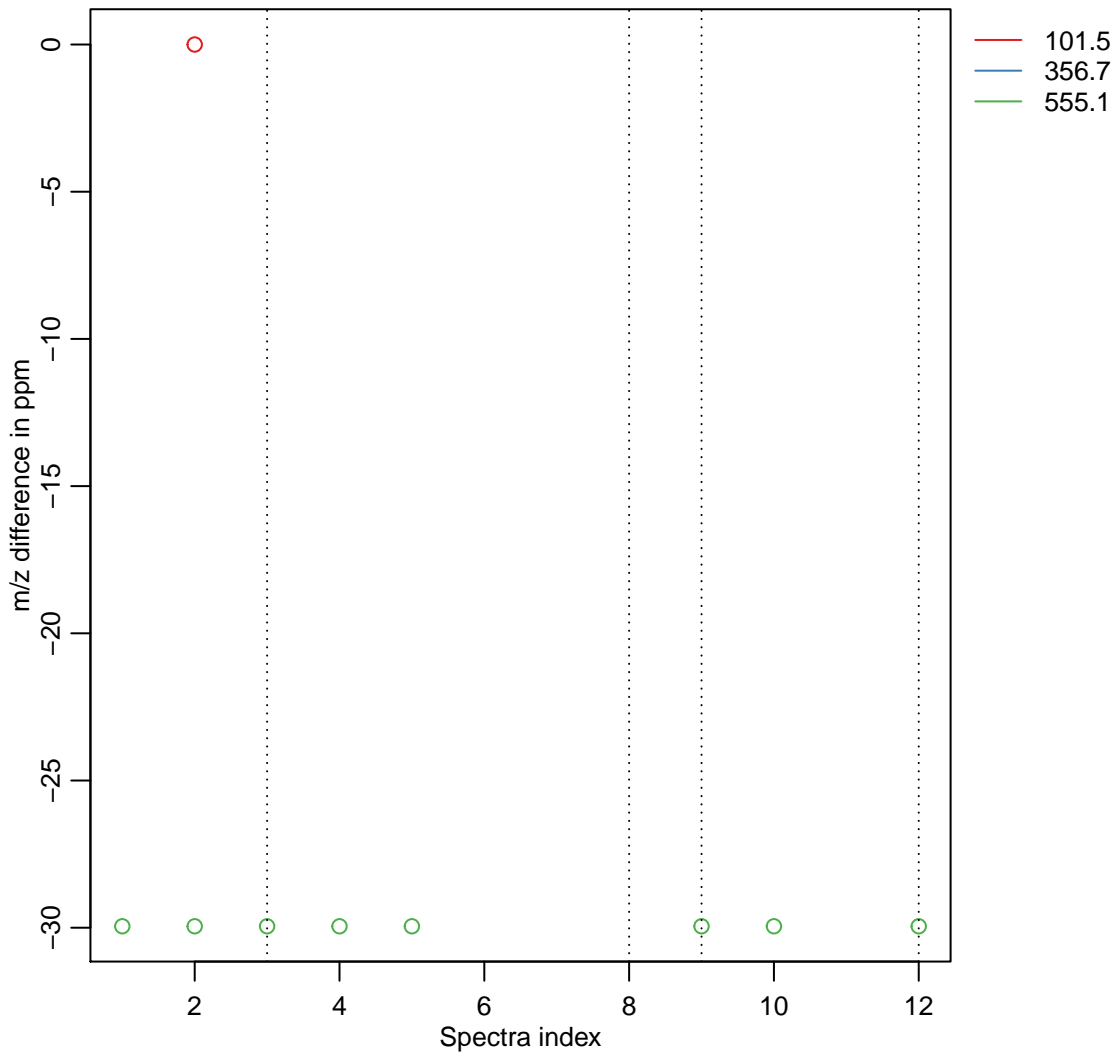
Average m/z error (max. average intensity vs. theor. calibrant m/z)



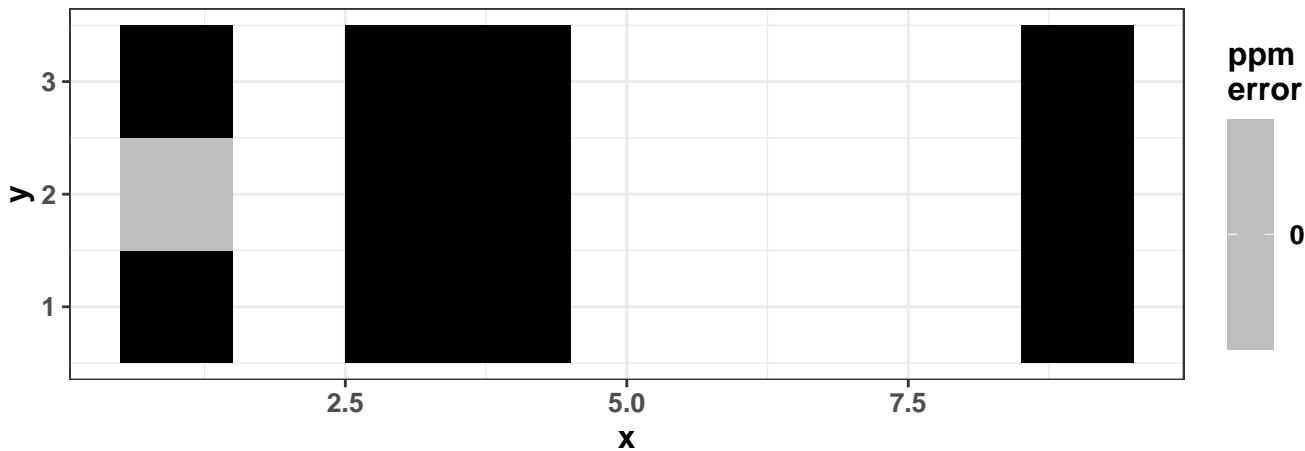
Average m/z error (closest measured m/z vs. theor. calibrant m/z)



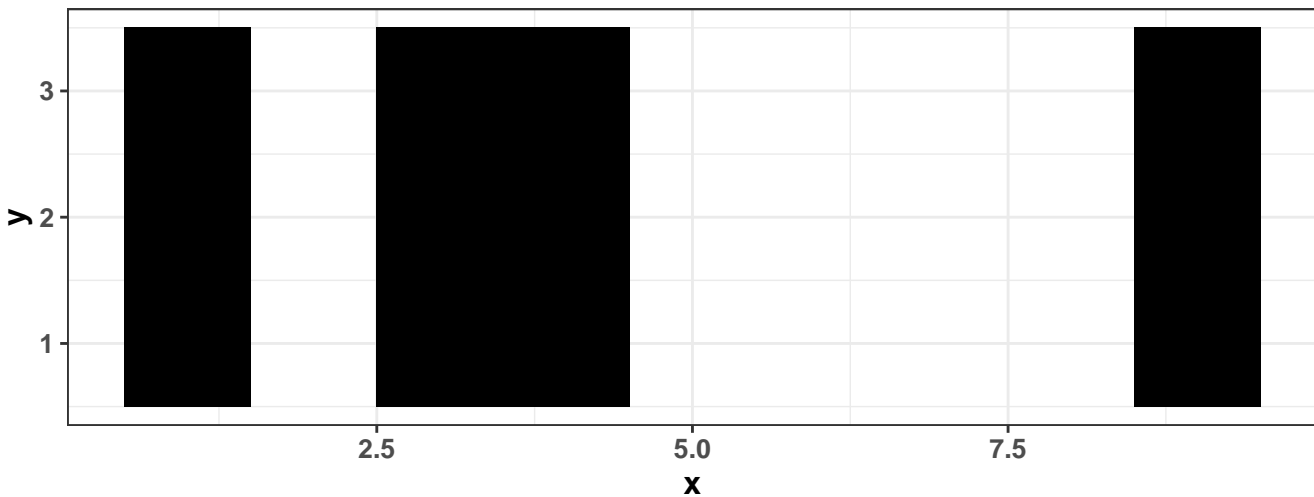
Difference m/z with max. average intensity vs. theor. m/z (per spectrum)



m/z accuracy for 101.5



m/z accuracy for 356.7



m/z accuracy for 555.1

