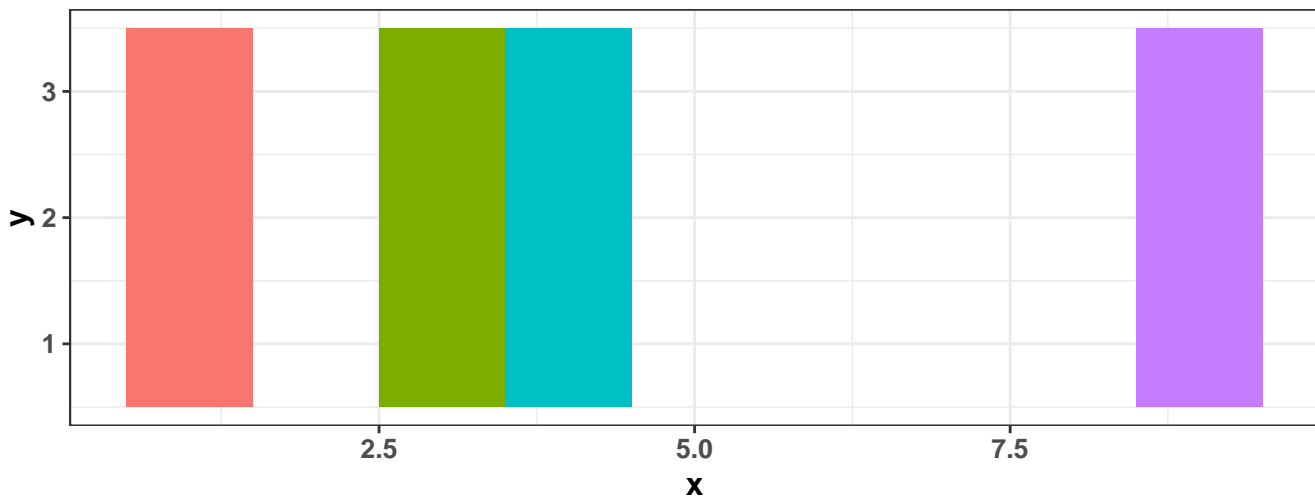


## Testfile\_rdata

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
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
calibrants (#valid/#input) in inputcalibrantfile1.tabular	3 / 3

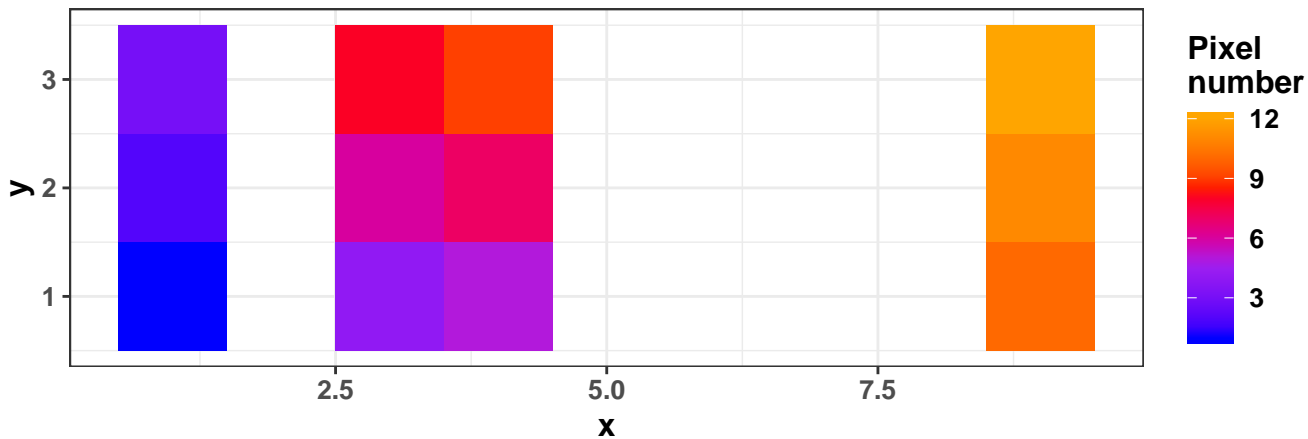
## Spatial orientation of pixel annotations



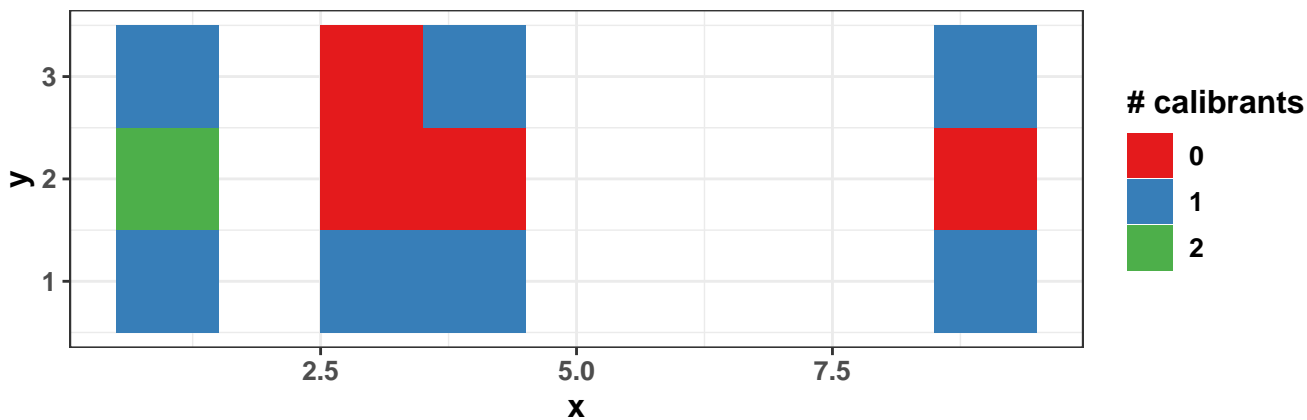
### annotation

column1 column2 column3 column4

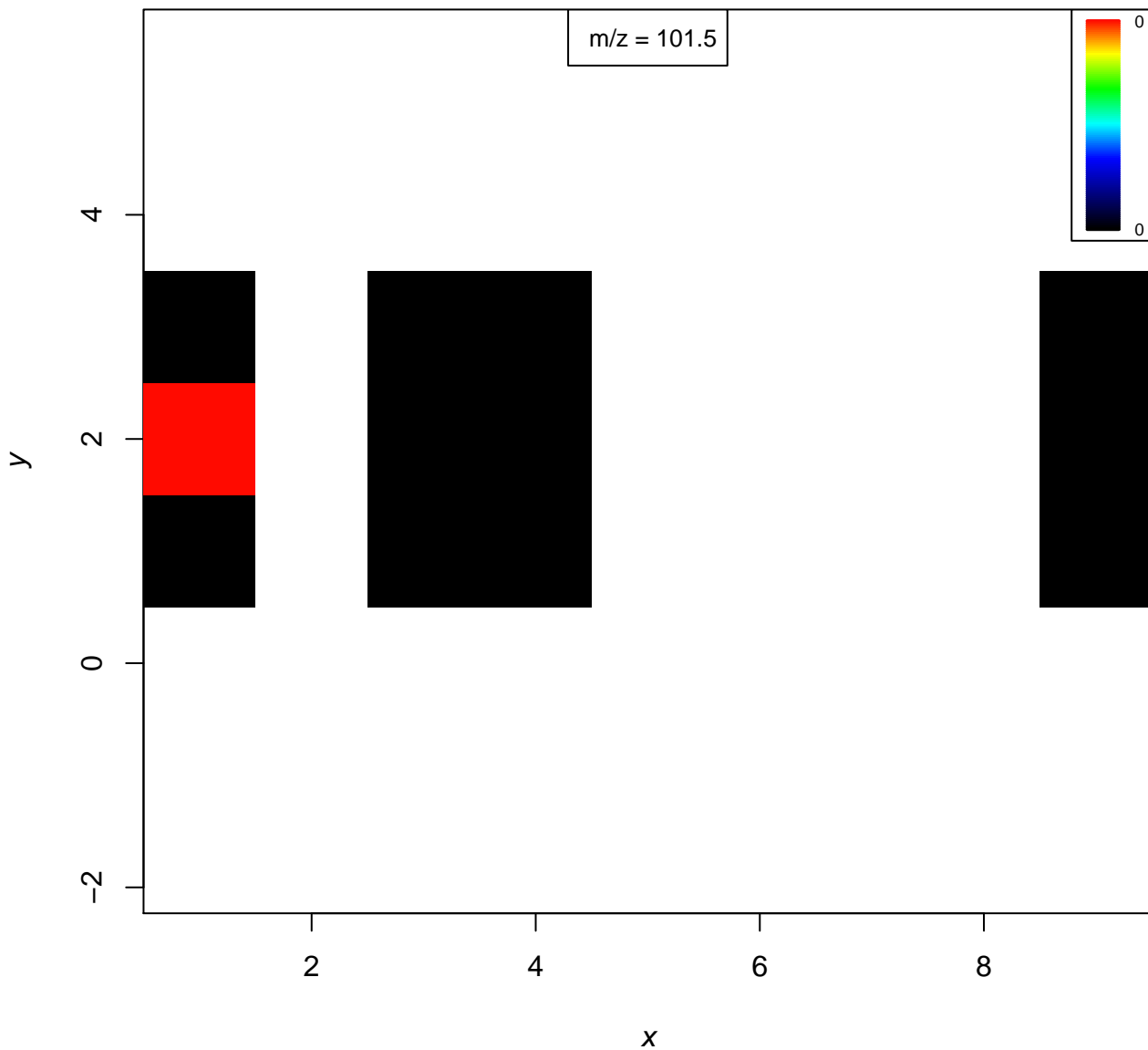
Pixel order



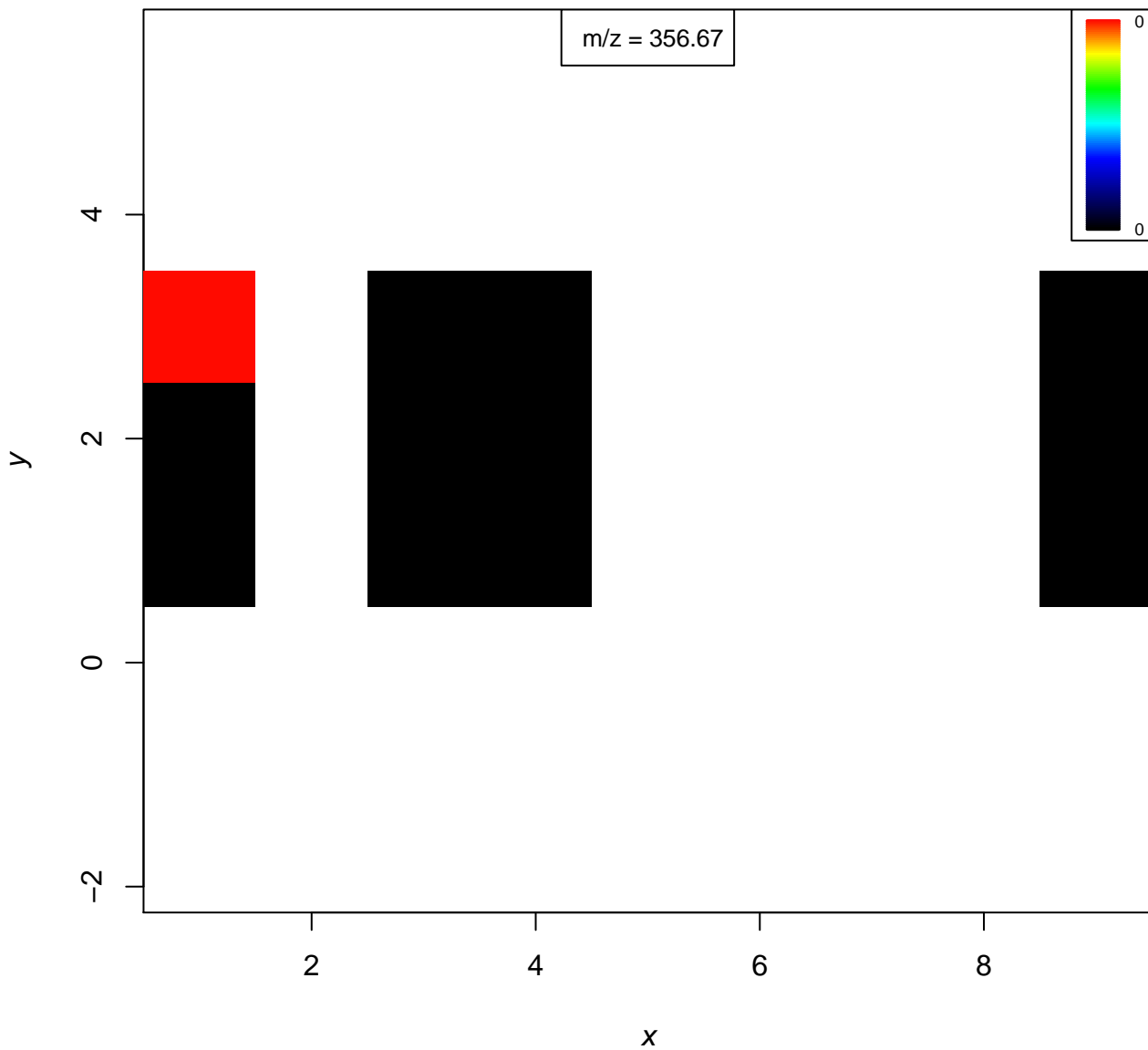
Number of calibrants per pixel ( $\pm 100$  ppm)



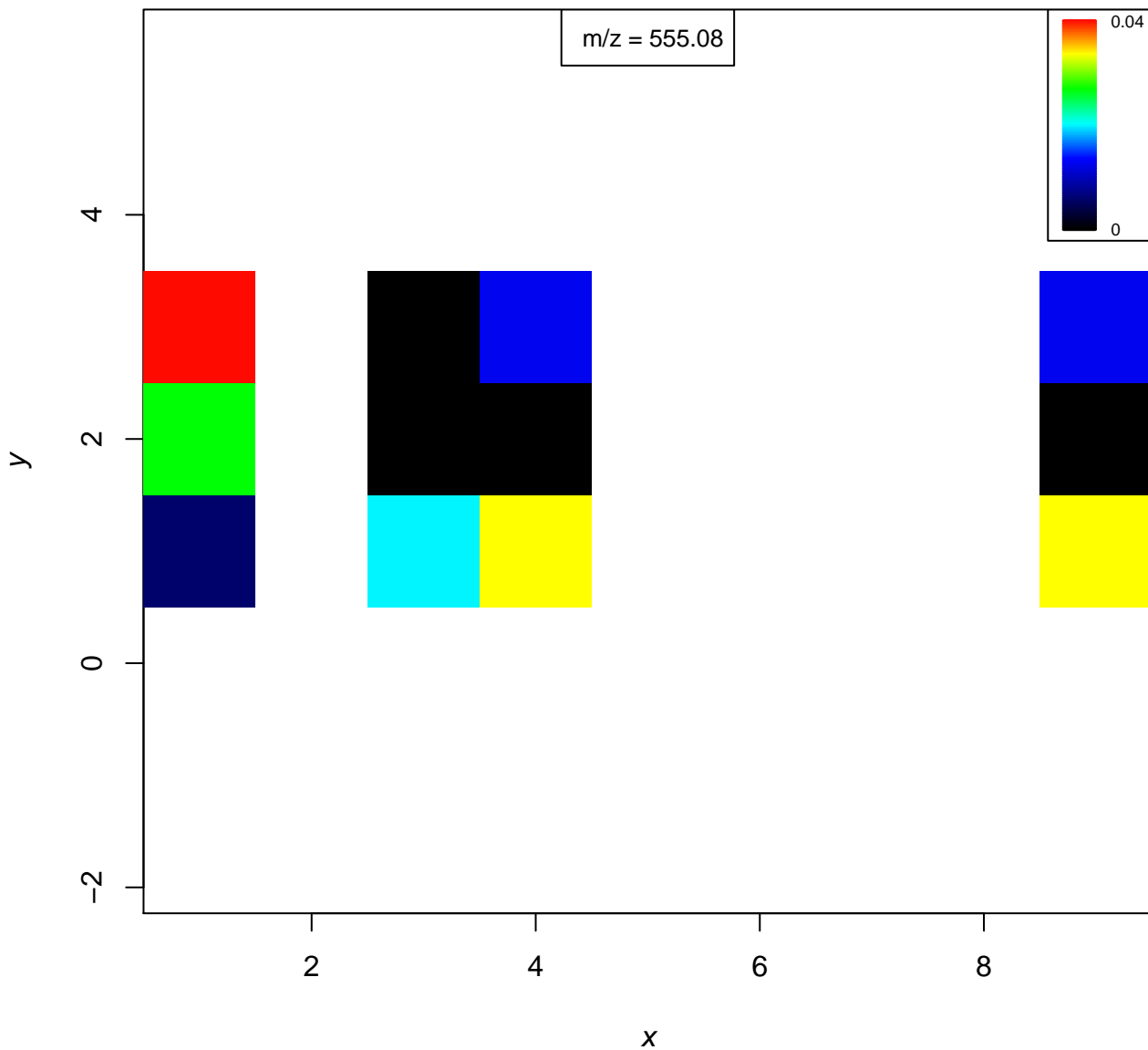
# 101.5: 101.5 ( $\pm 100$ ppm)



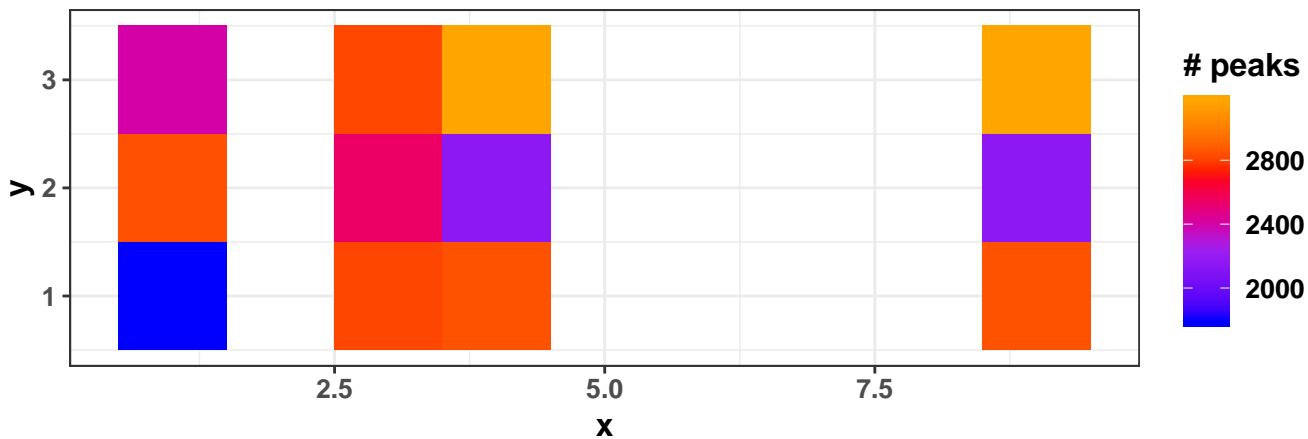
356.7: 356.7 ( $\pm 100$  ppm)



555.1: 555.1 ( $\pm 100$  ppm)

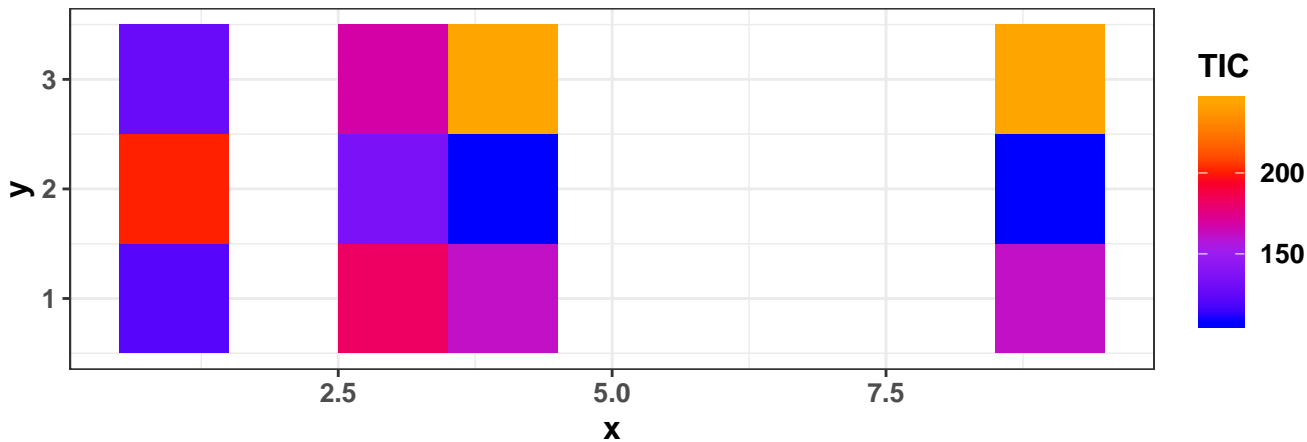


Number of peaks per spectrum

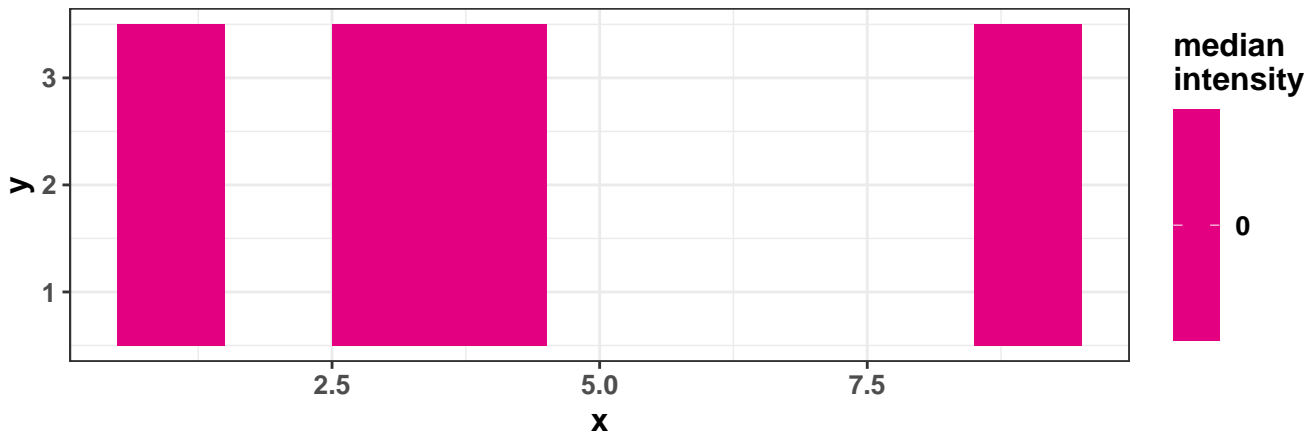




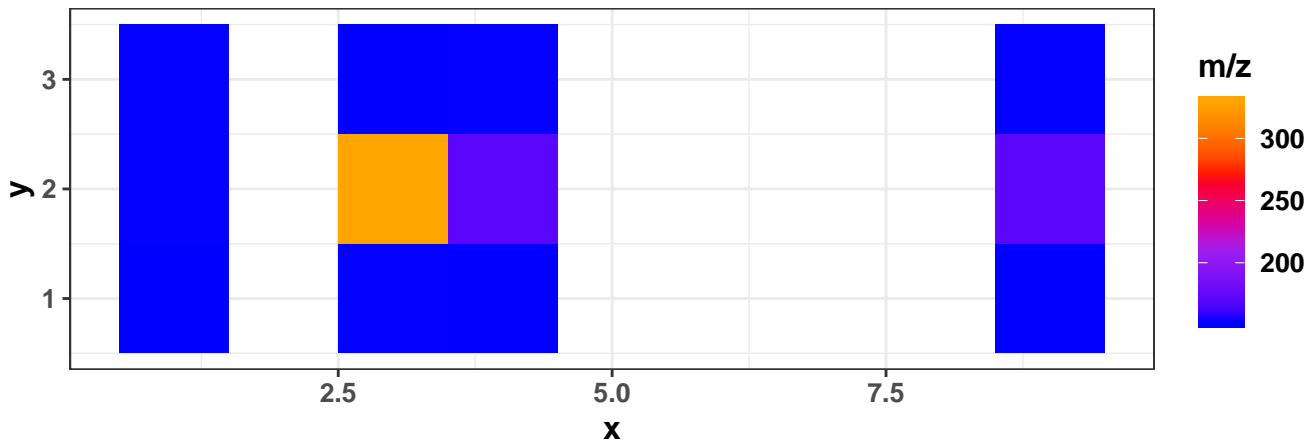
# Total Ion Chromatogram



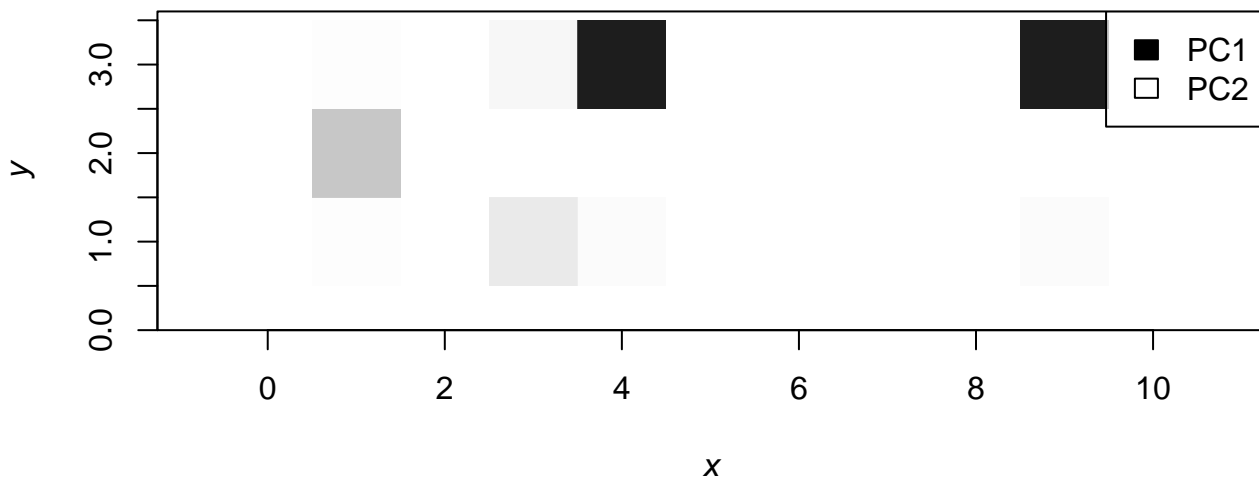
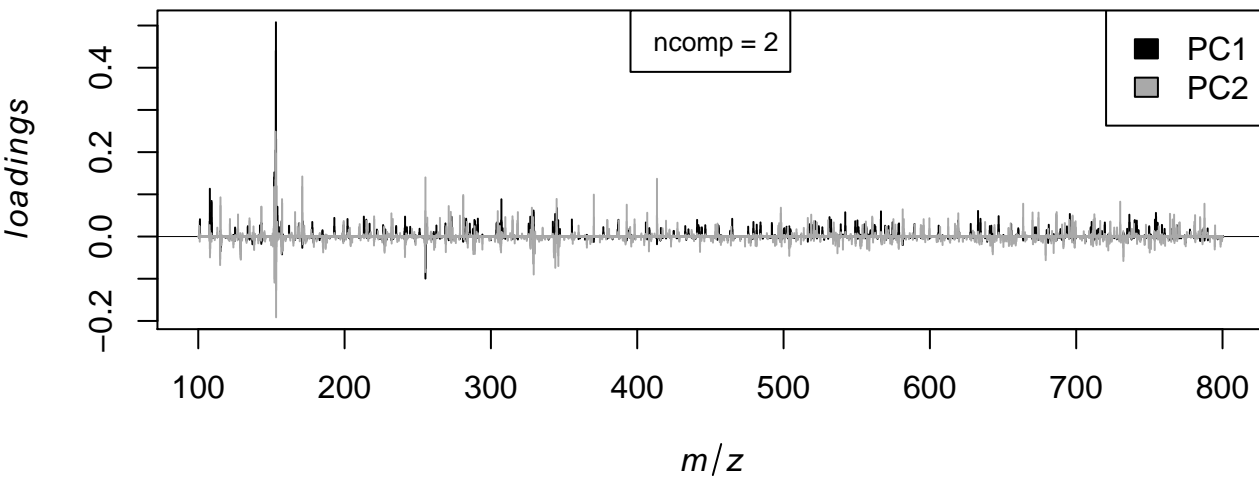
**Median intensity per pixel**



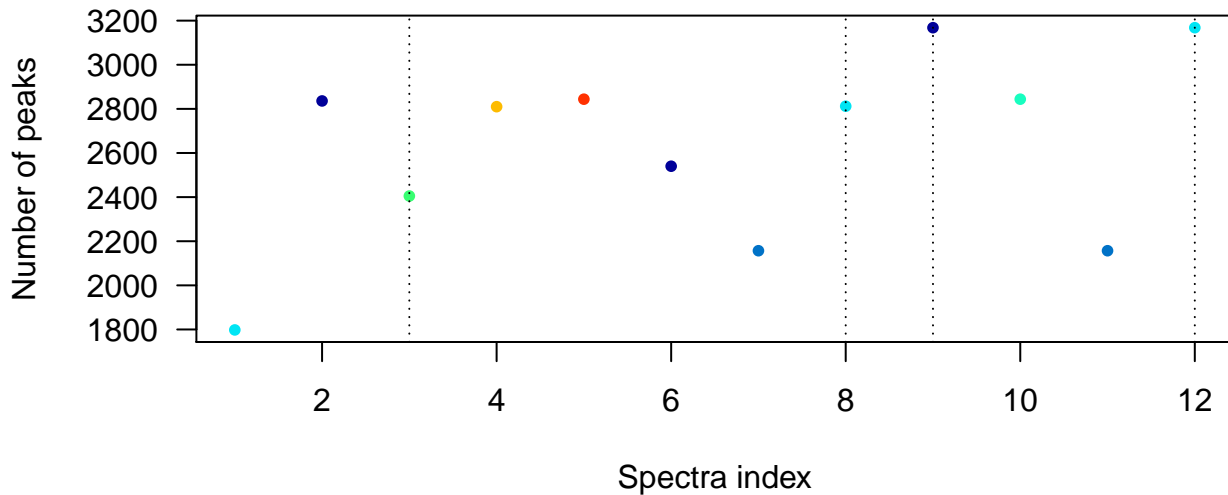
Most abundant m/z in each spectrum



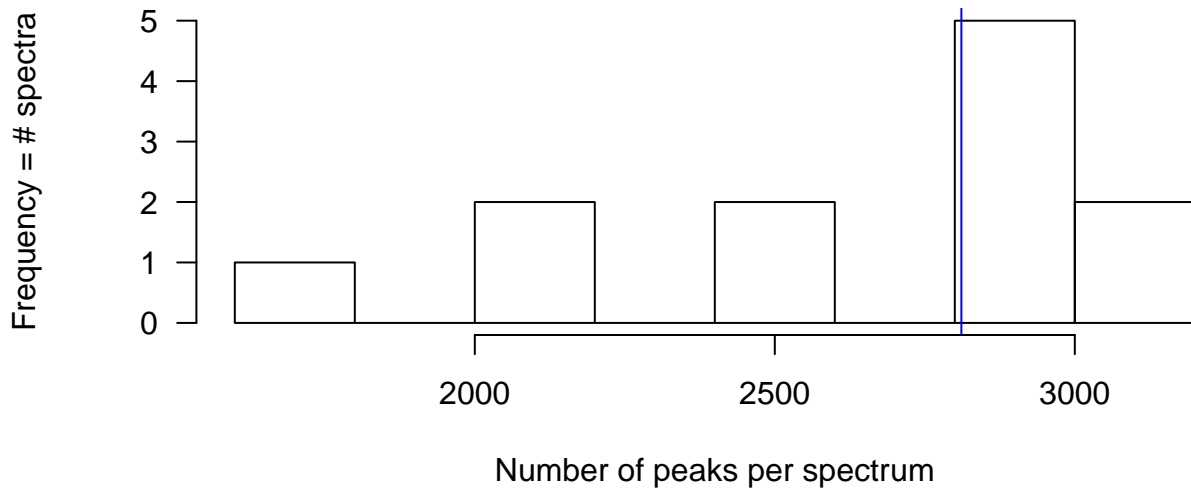
# PCA for two components



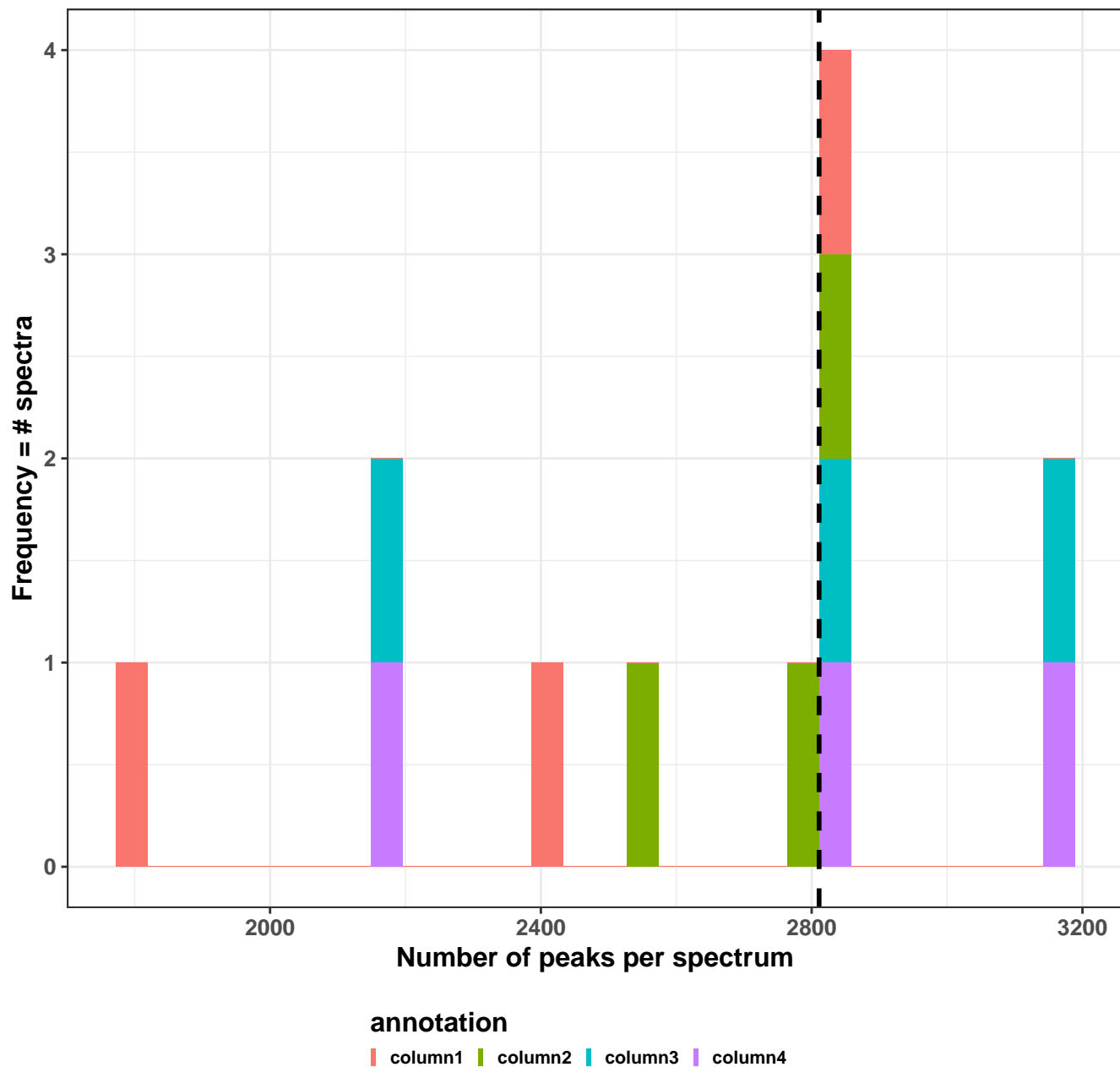
**Number of peaks per spectrum**

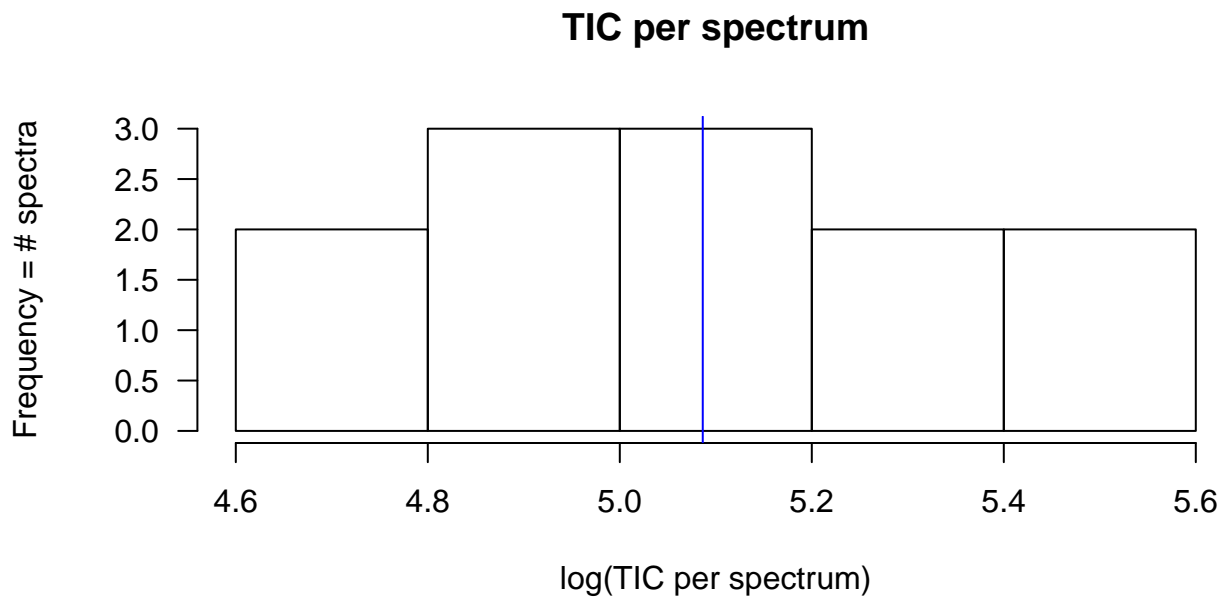
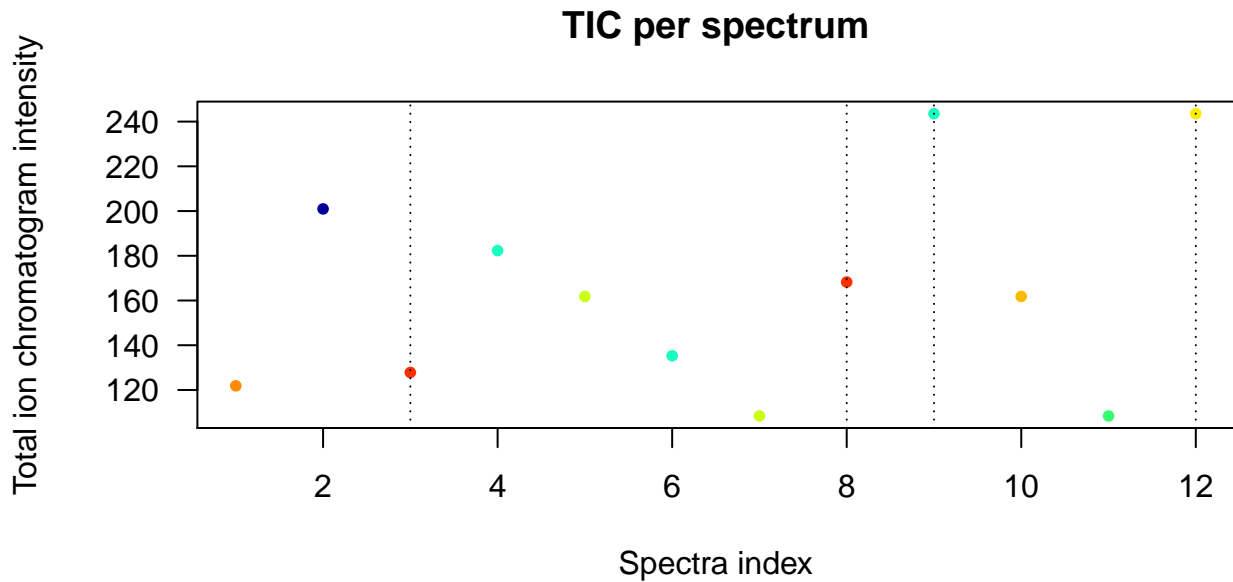


**Number of peaks per spectrum**

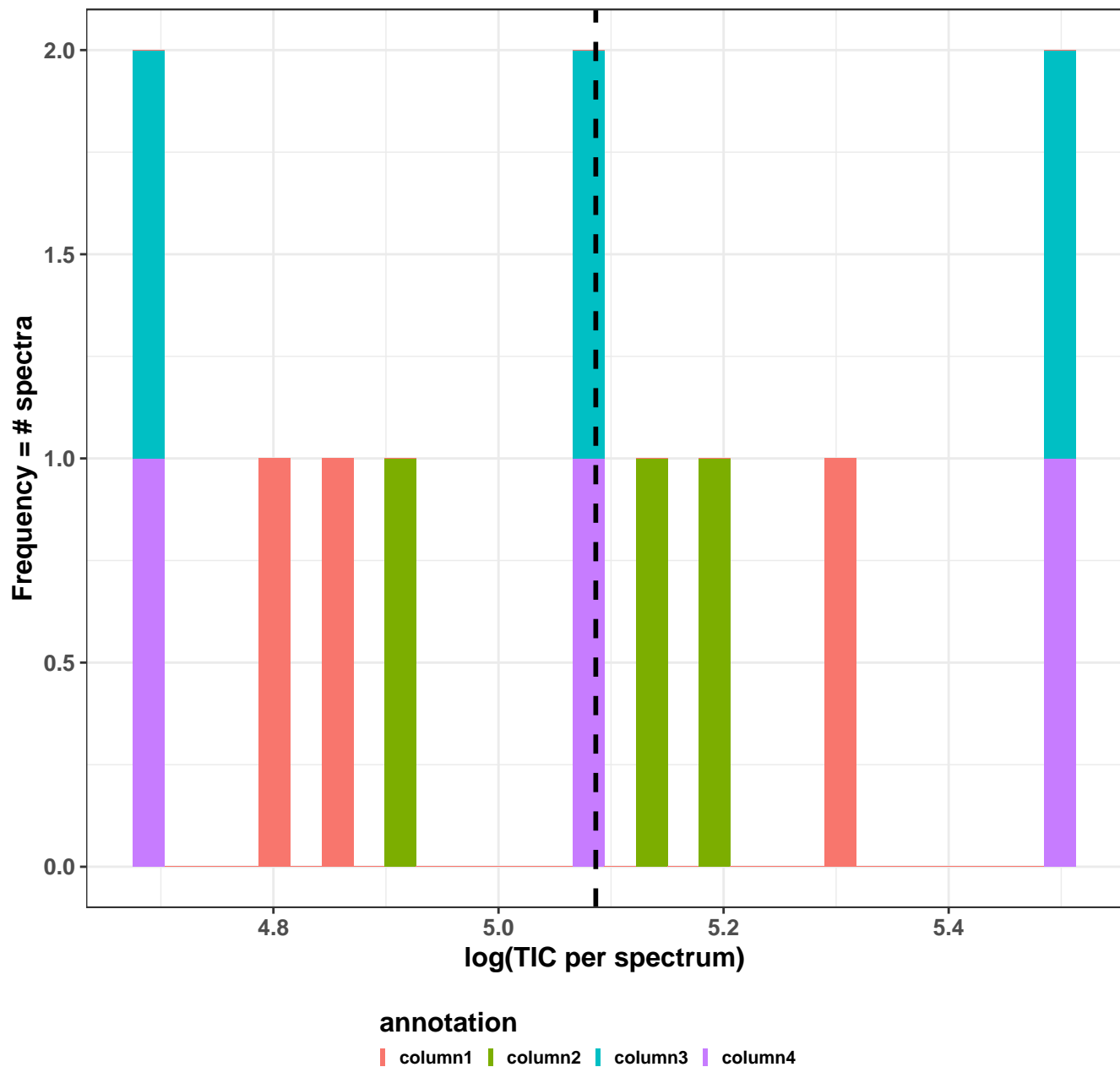


Number of peaks per spectrum and annotation group



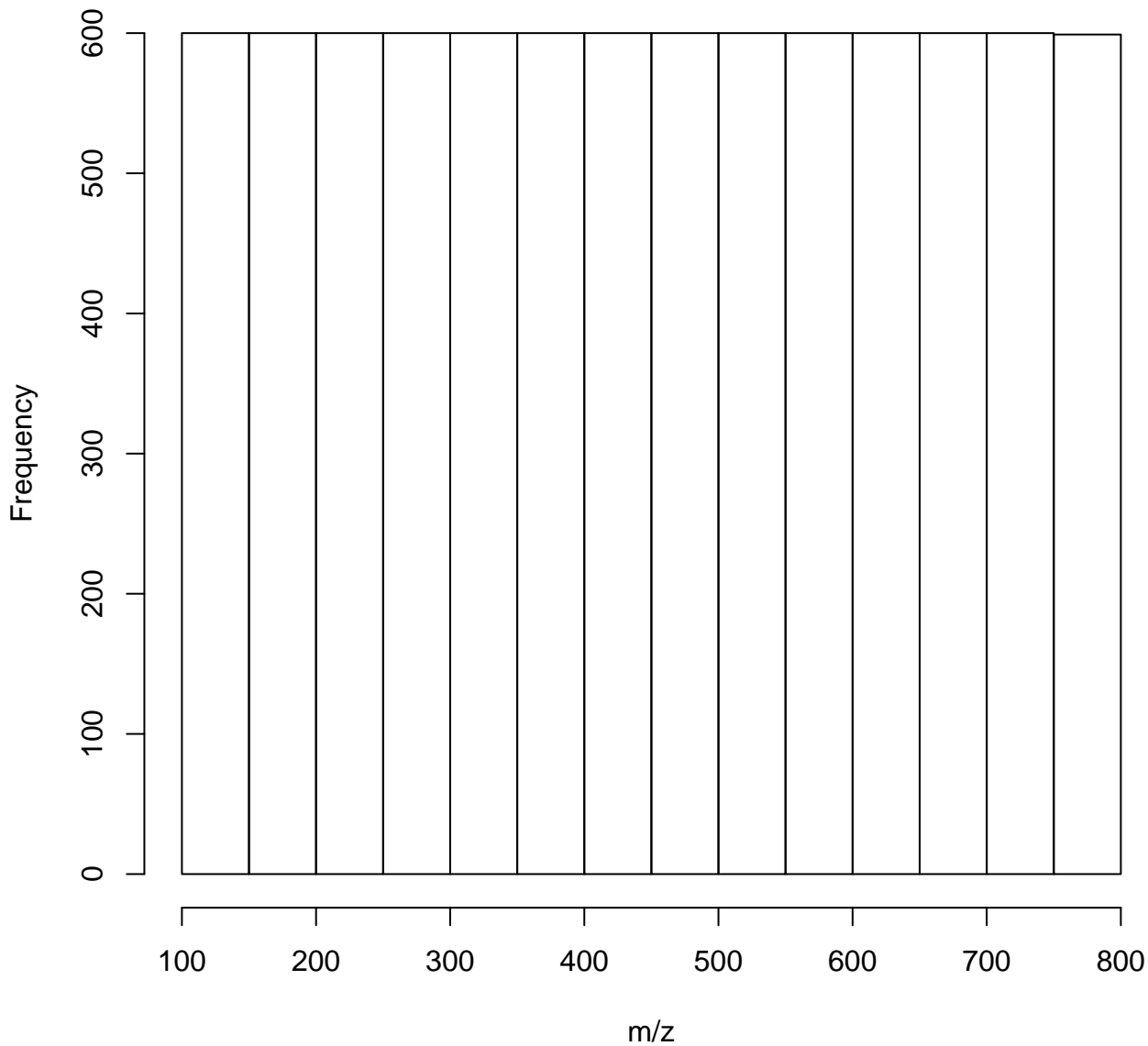


TIC per spectrum and annotation group

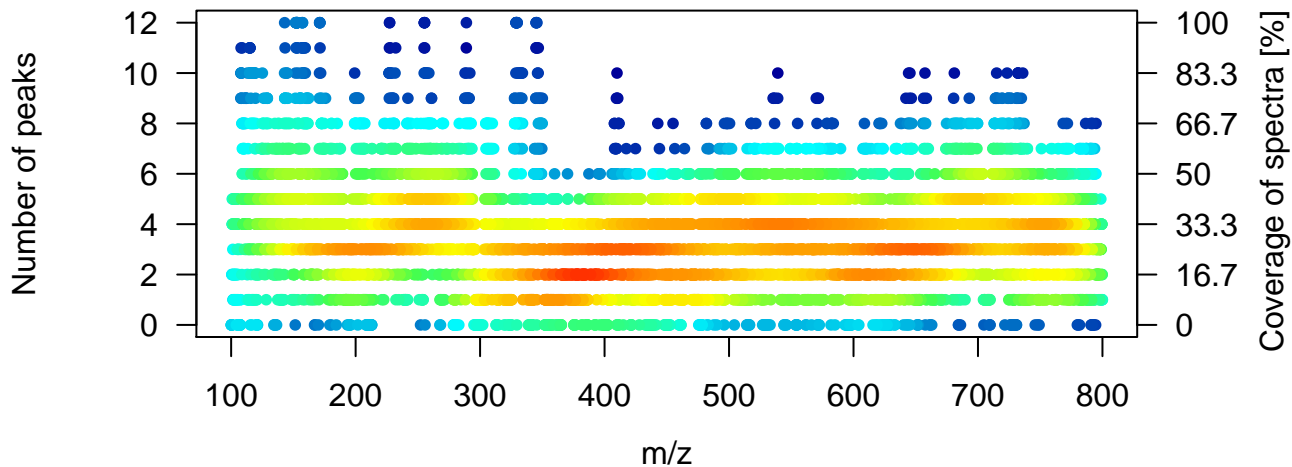




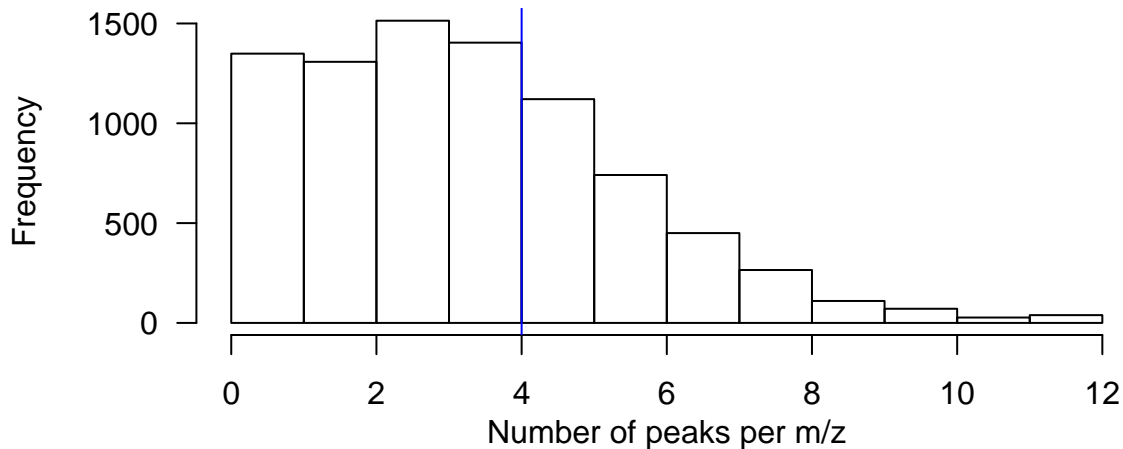
**Histogram of m/z values**



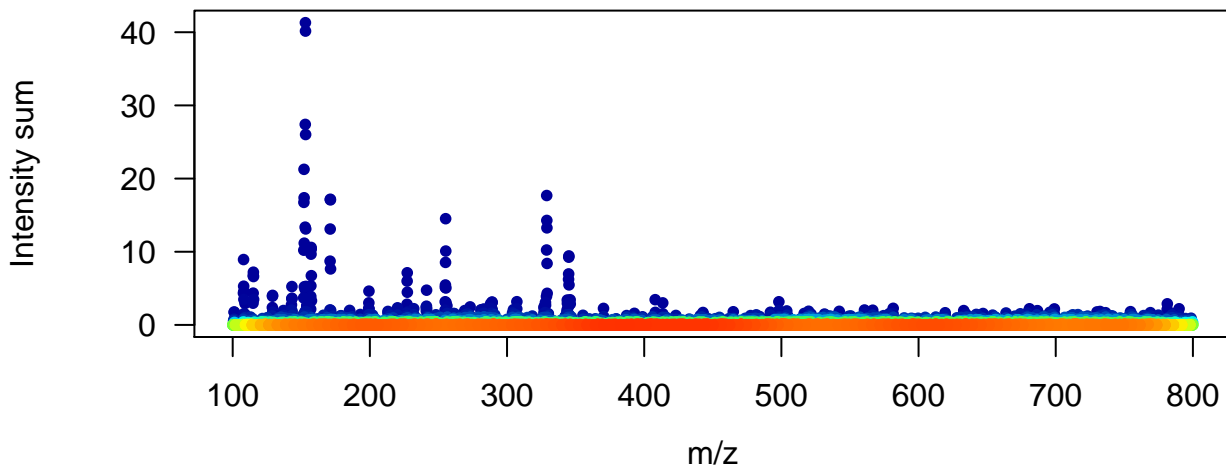
Number of peaks per m/z



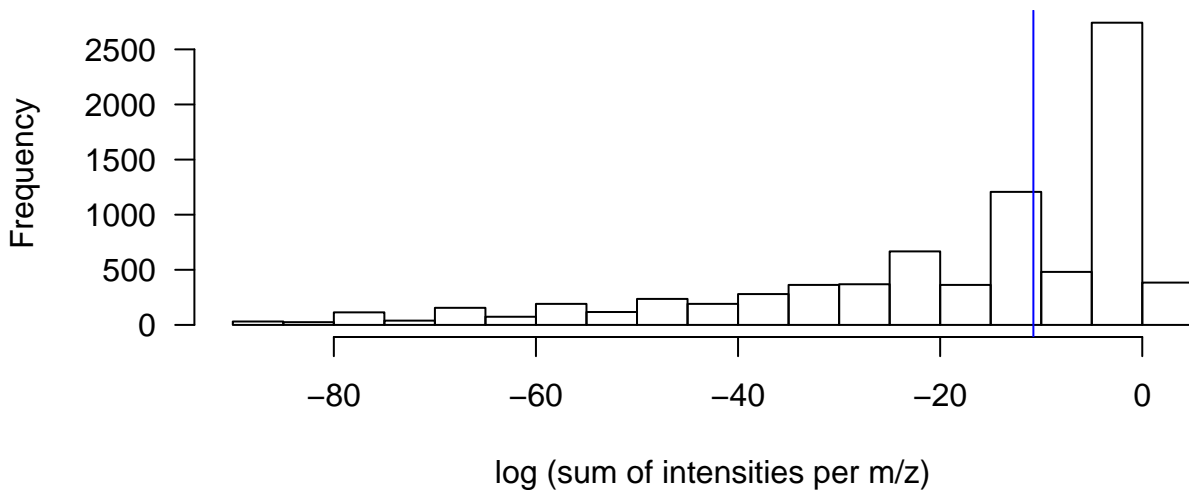
Number of peaks per m/z



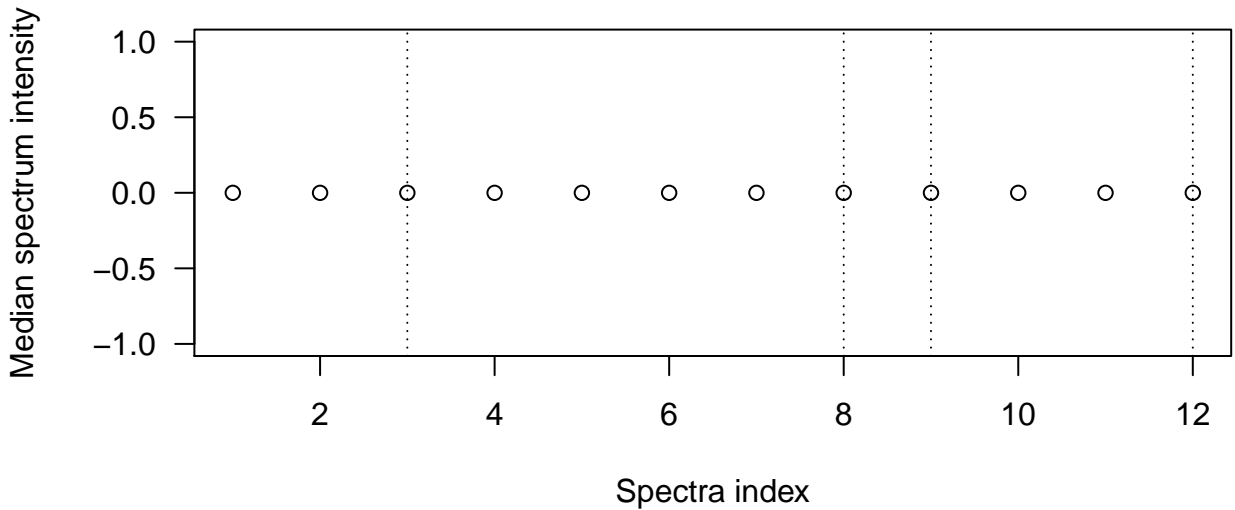
Sum of intensities per m/z



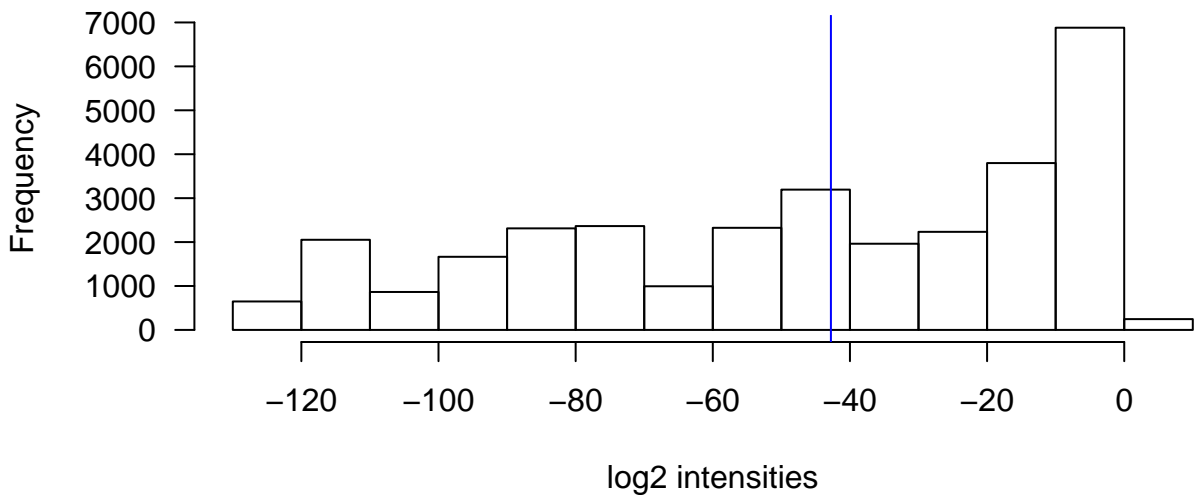
Sum of intensities per m/z



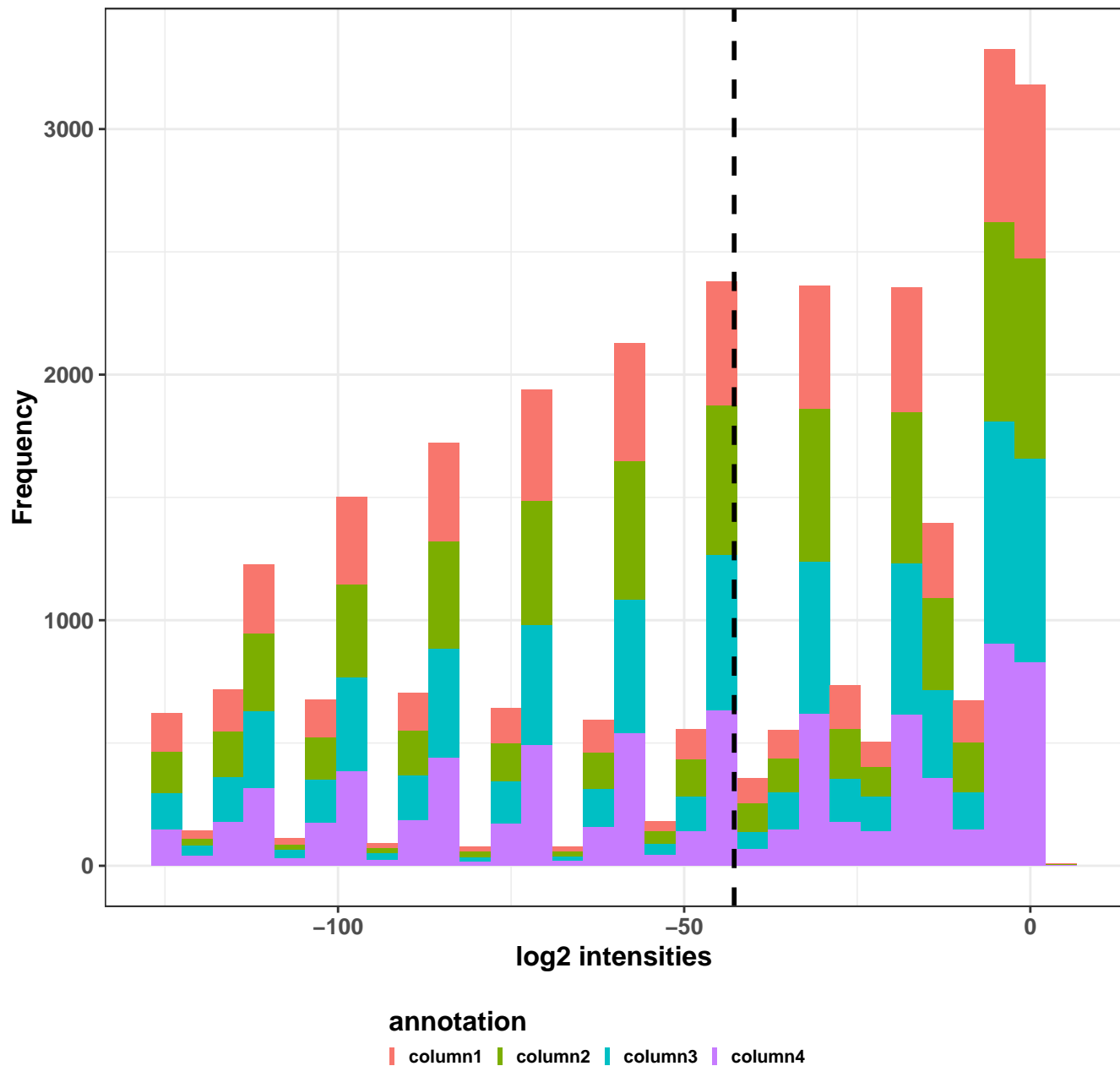
**Median intensity per spectrum**



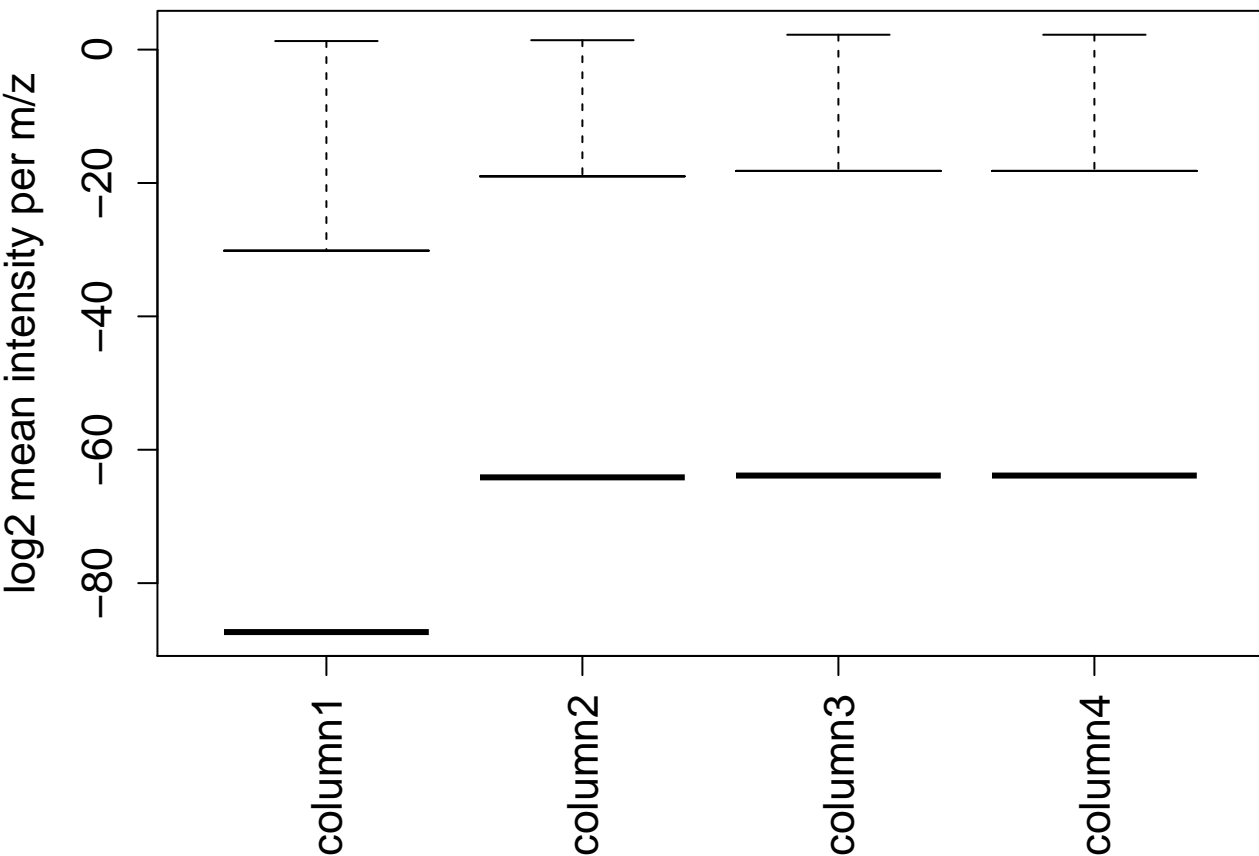
**Log2-transformed intensities**



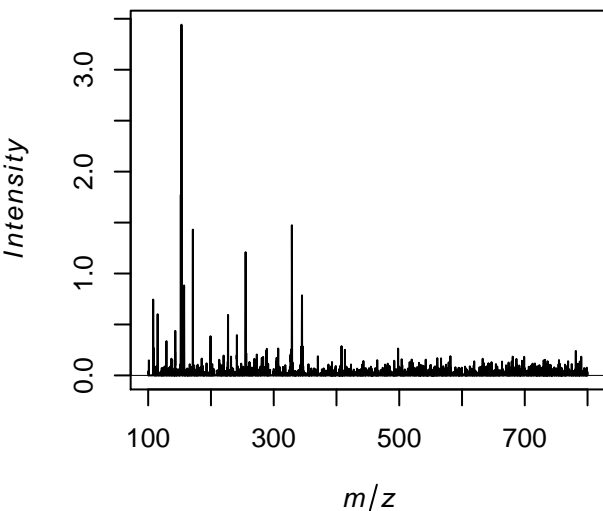
Log2-transformed intensities per sample



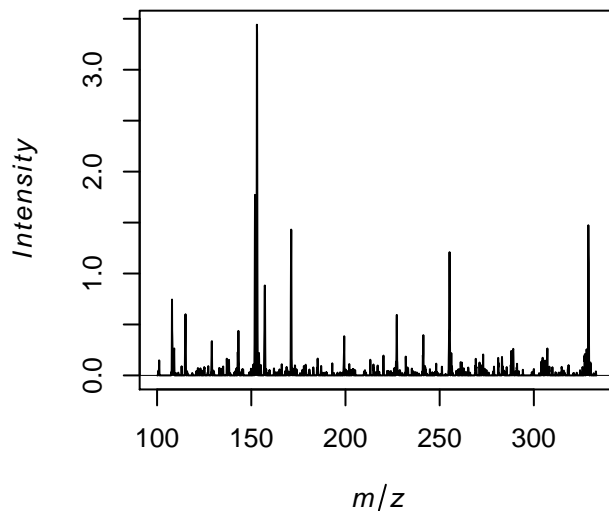
Mean m/z intensities per annotation group



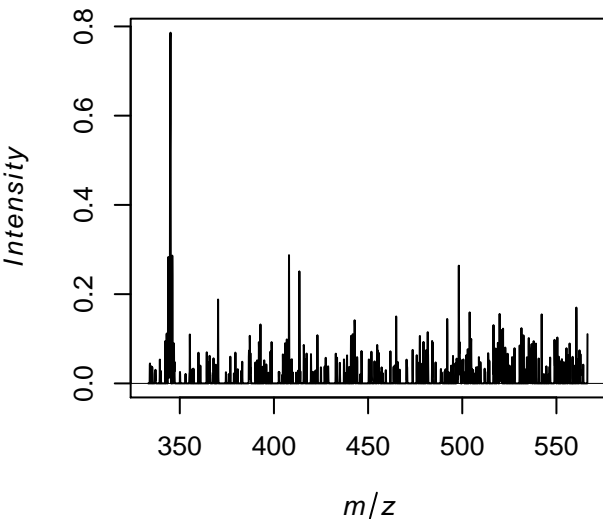
**Average spectrum**



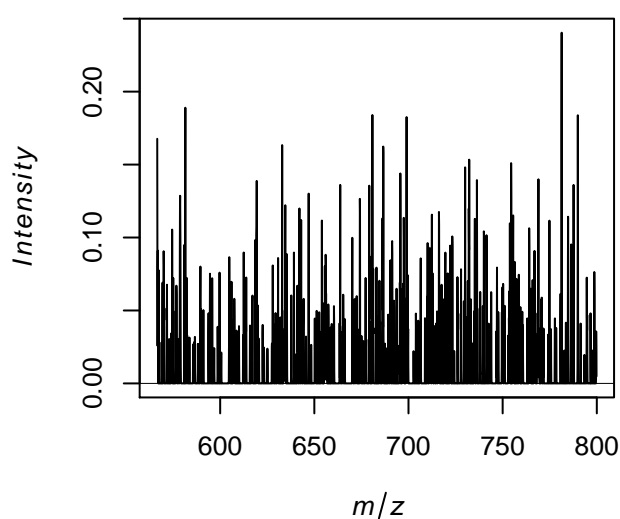
**Zoomed average spectrum**



**Zoomed average spectrum**



**Zoomed average spectrum**

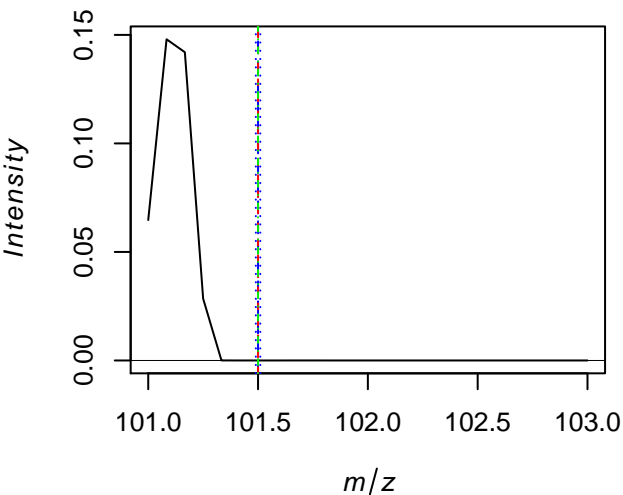


theor. m/z: 101.5

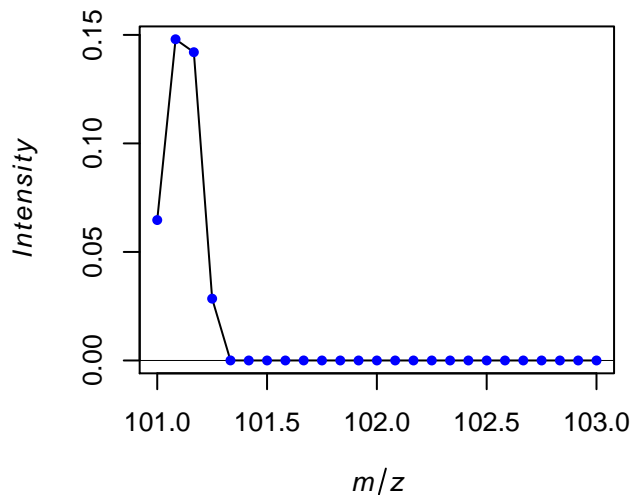
most abundant m/z: 101.5

closest m/z: 101.5

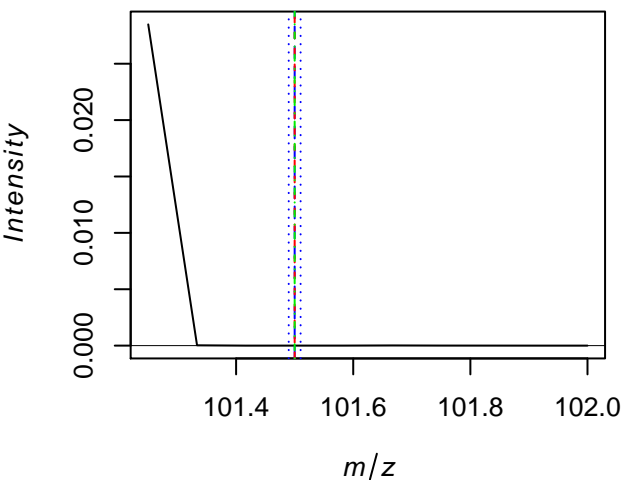
Average spectrum



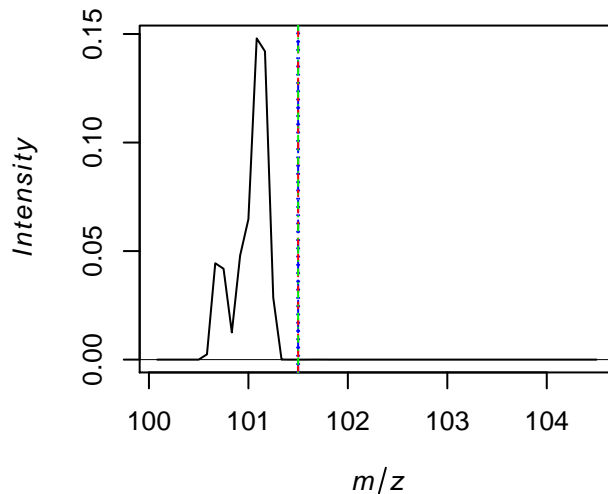
Average spectrum with data points



Average spectrum

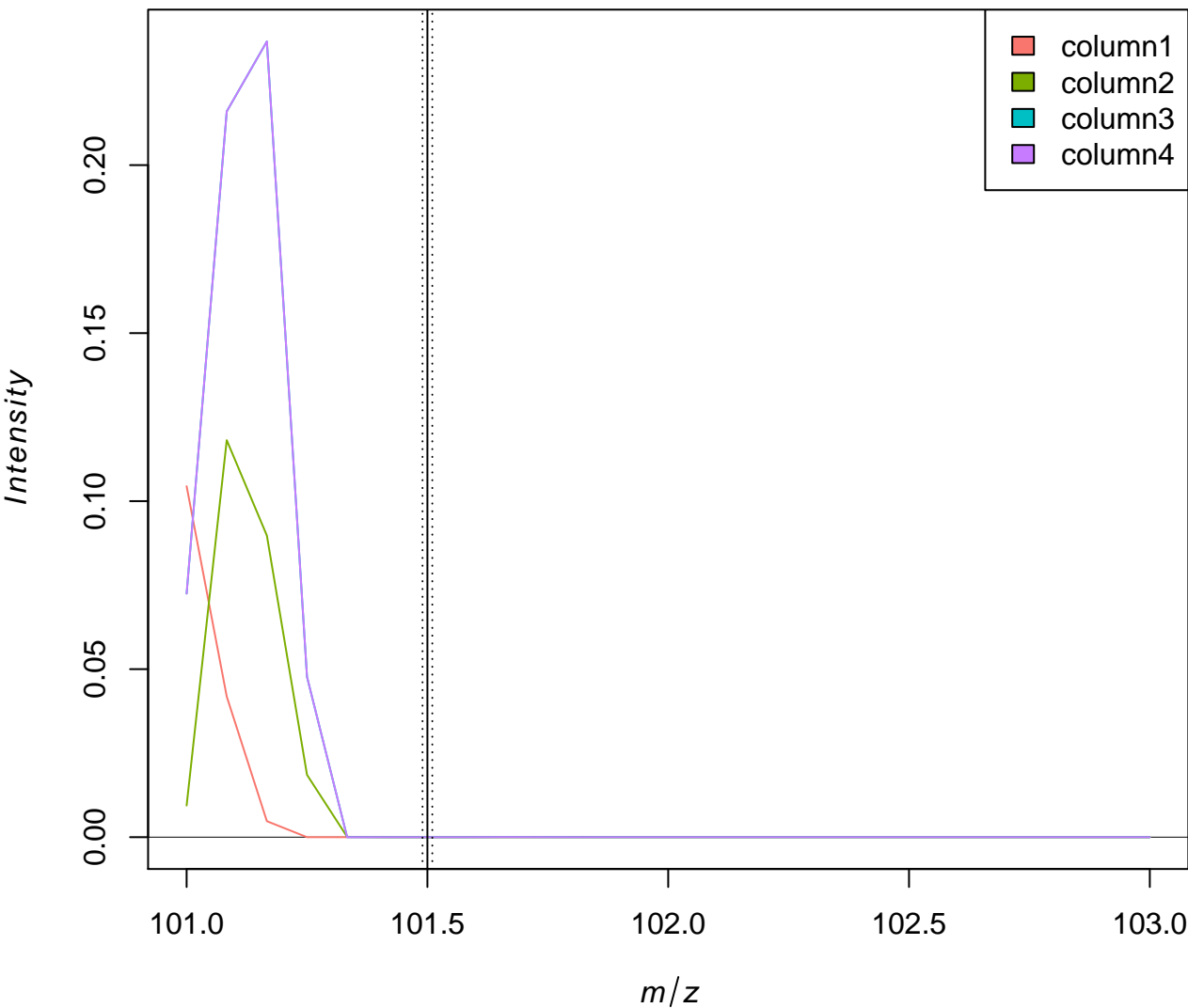


Average spectrum





Average spectrum per annotation group

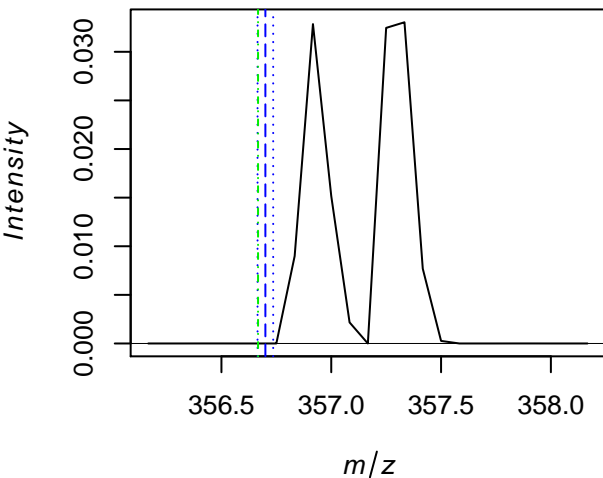


theor. m/z: 356.7

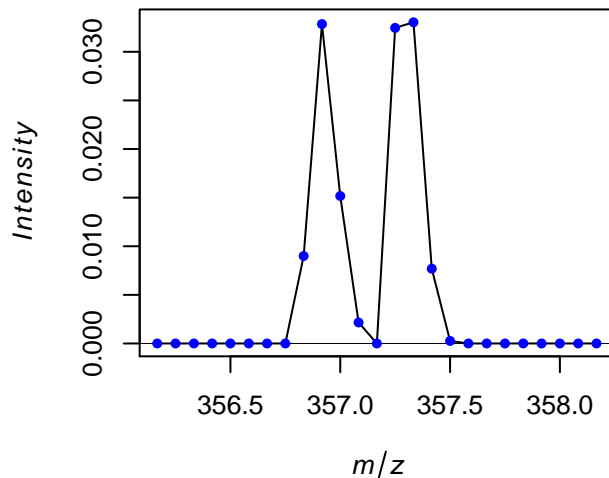
most abundant m/z: NA

closest m/z: 356.6667

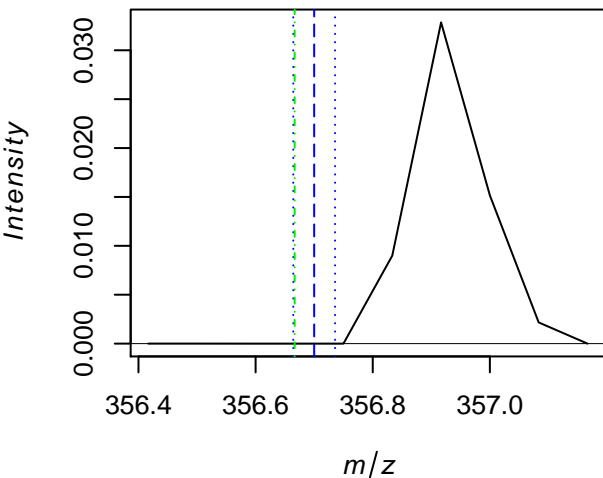
Average spectrum



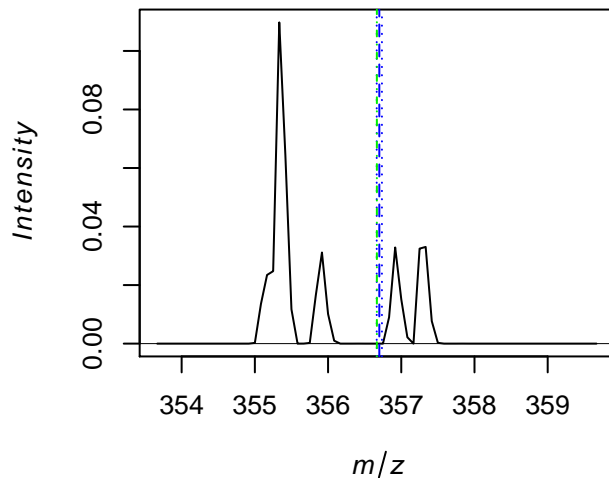
Average spectrum with data points



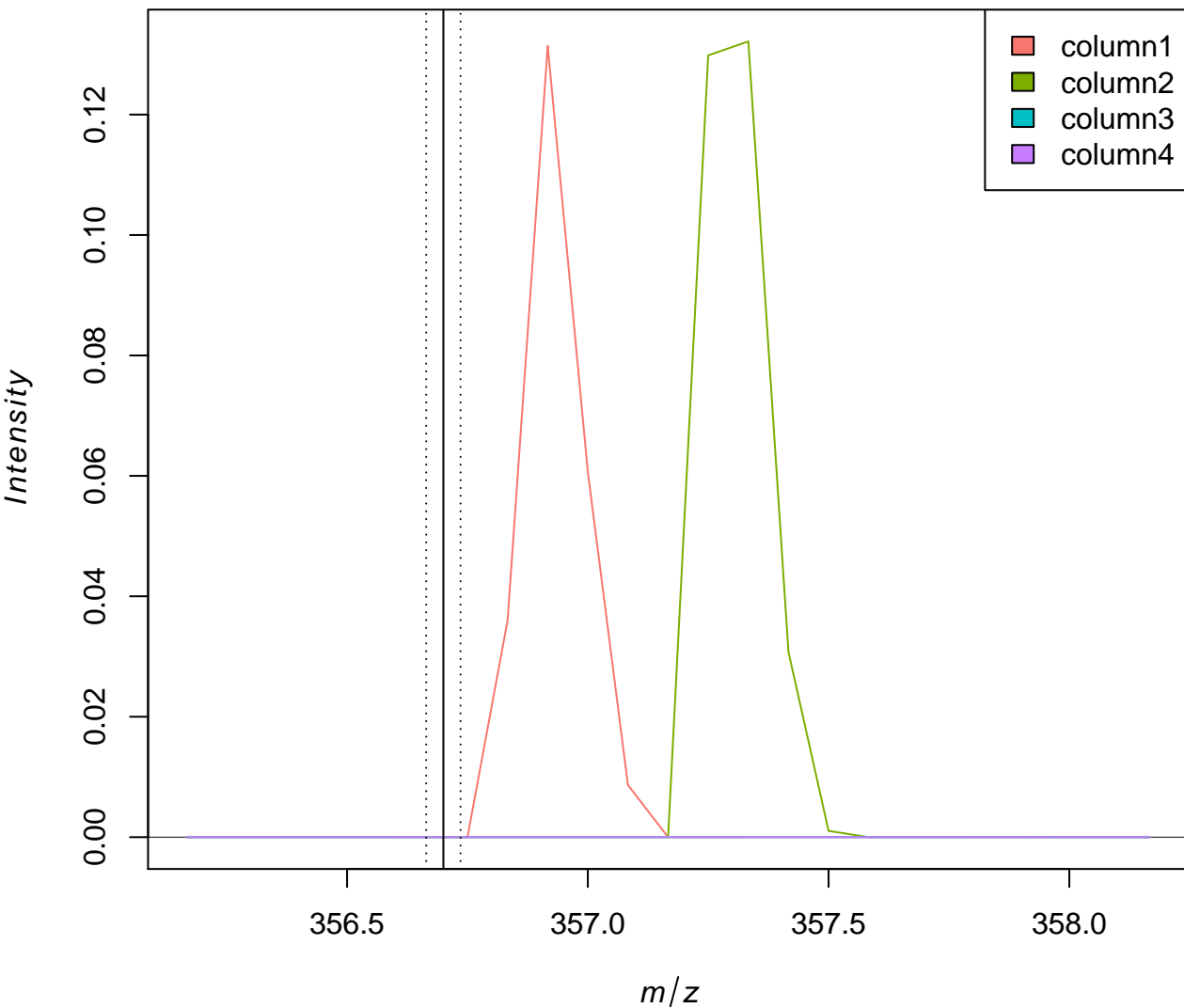
Average spectrum



Average spectrum



# Average spectrum per annotation group

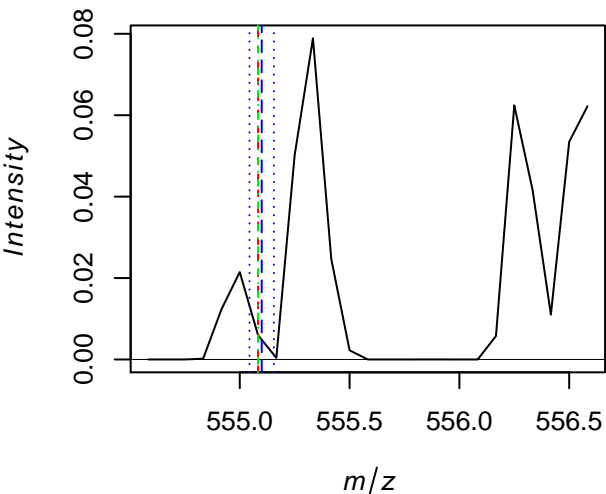


theor. m/z: 555.1

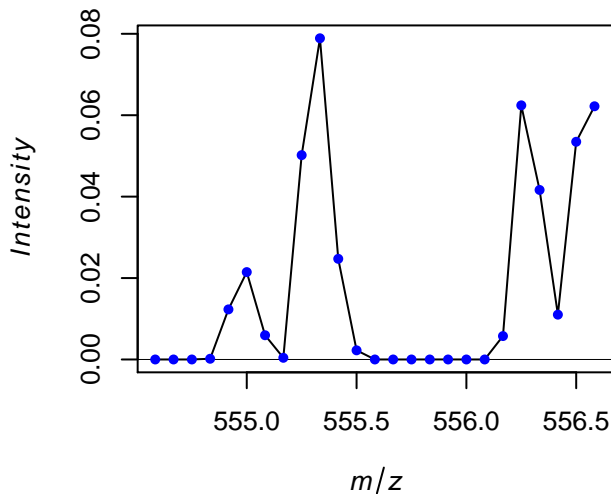
most abundant m/z: 555.0834

closest m/z: 555.0834

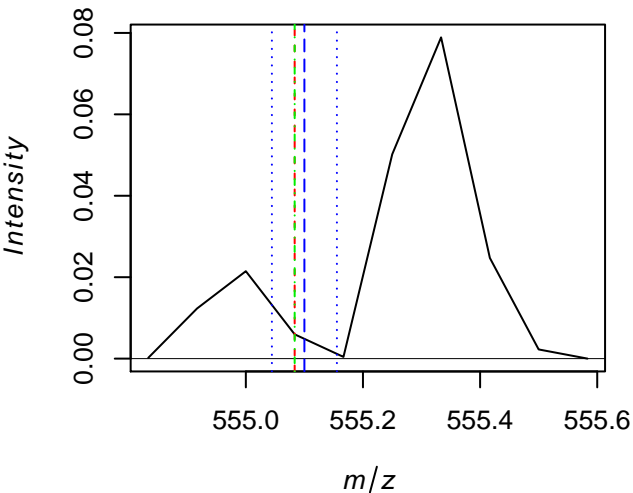
Average spectrum



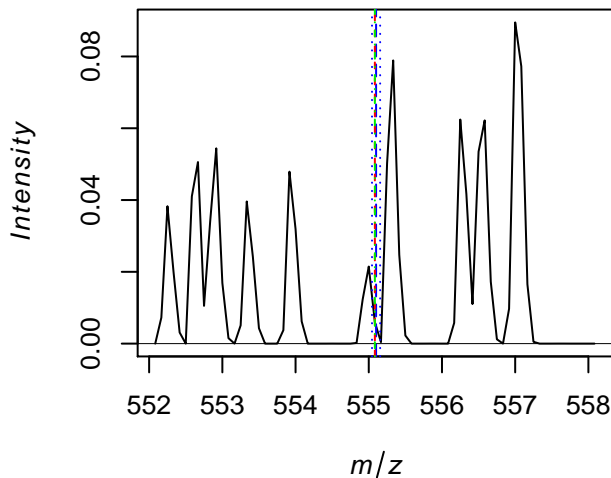
Average spectrum with data points



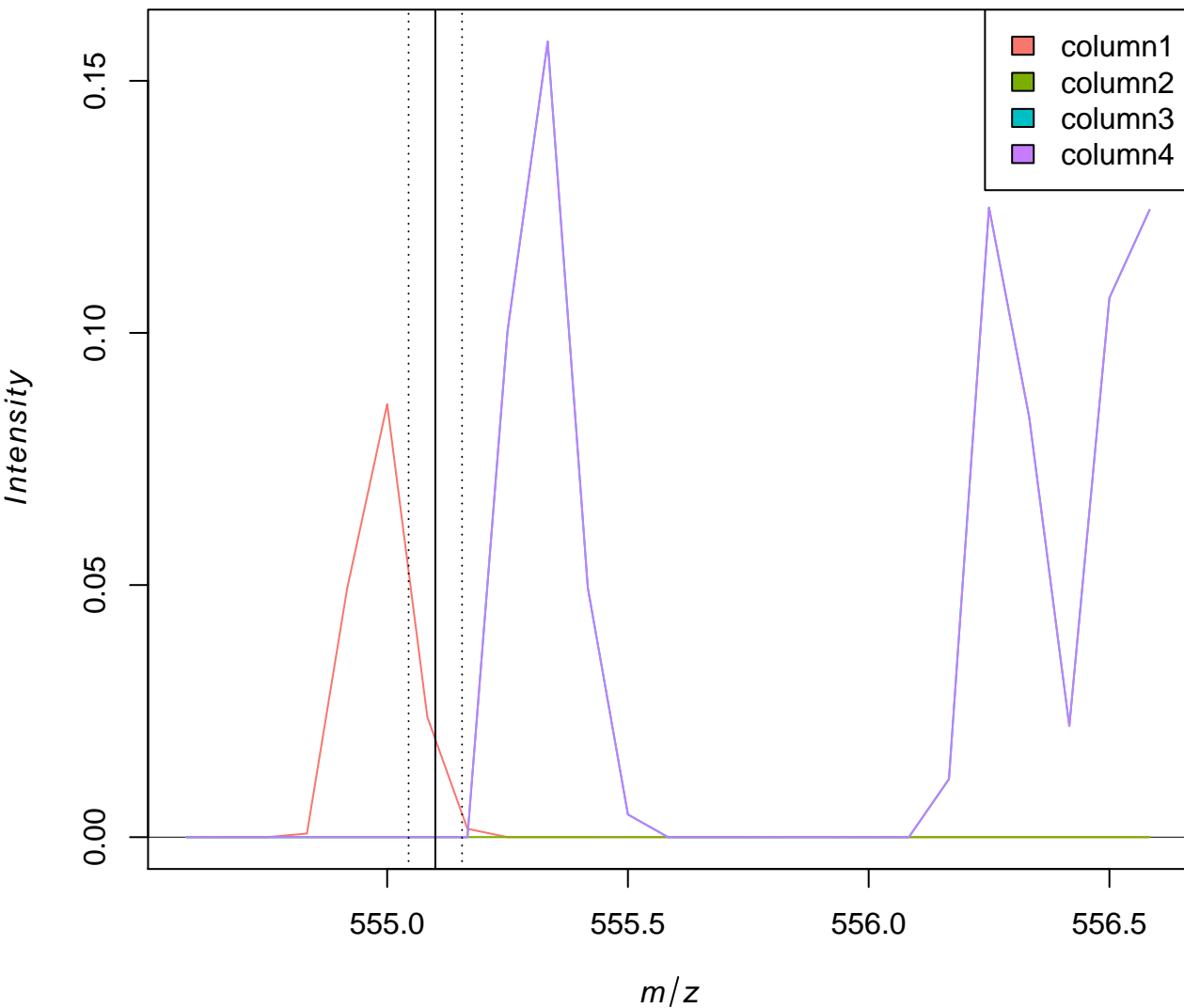
Average spectrum



Average spectrum

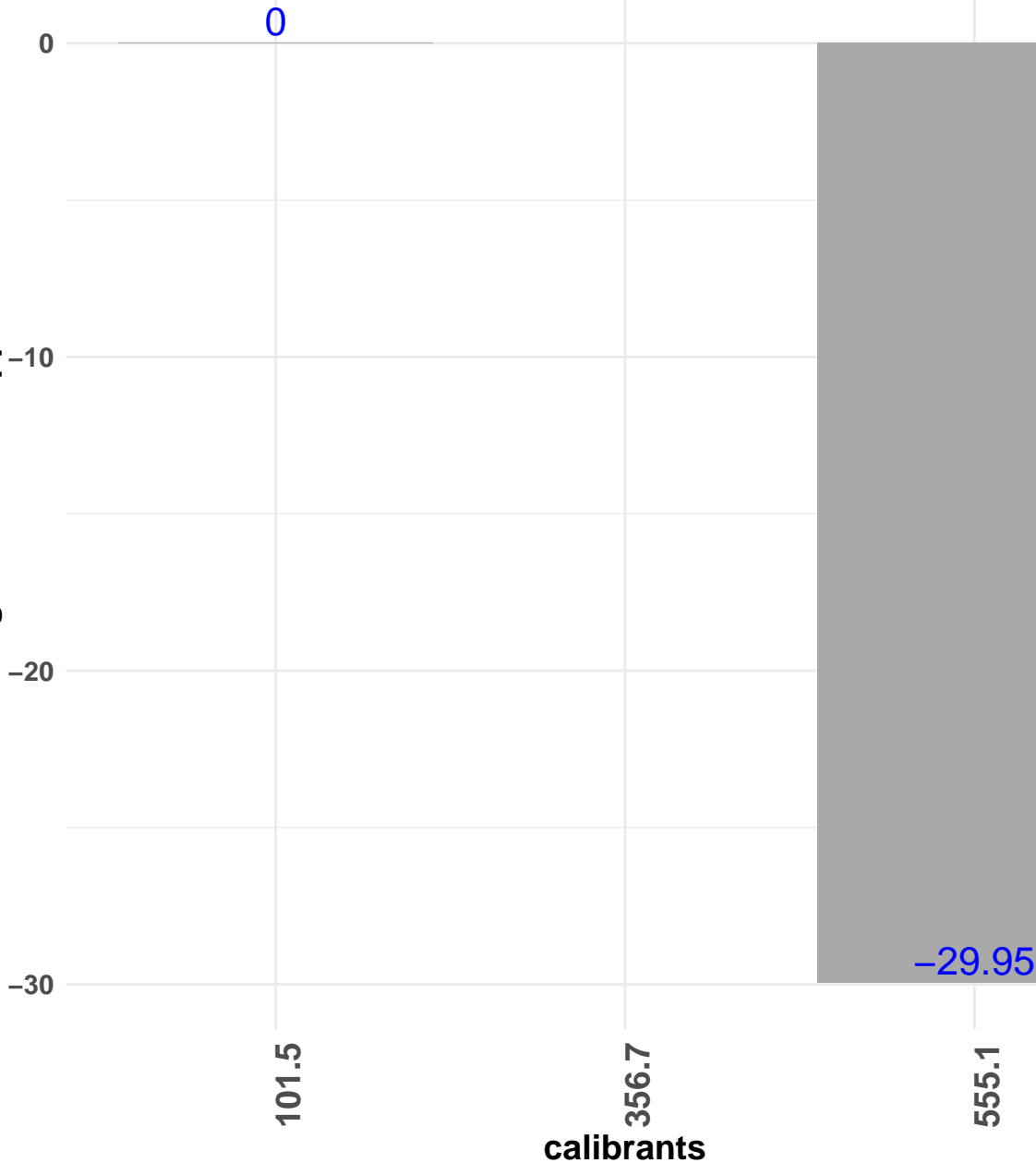


# Average spectrum per annotation group

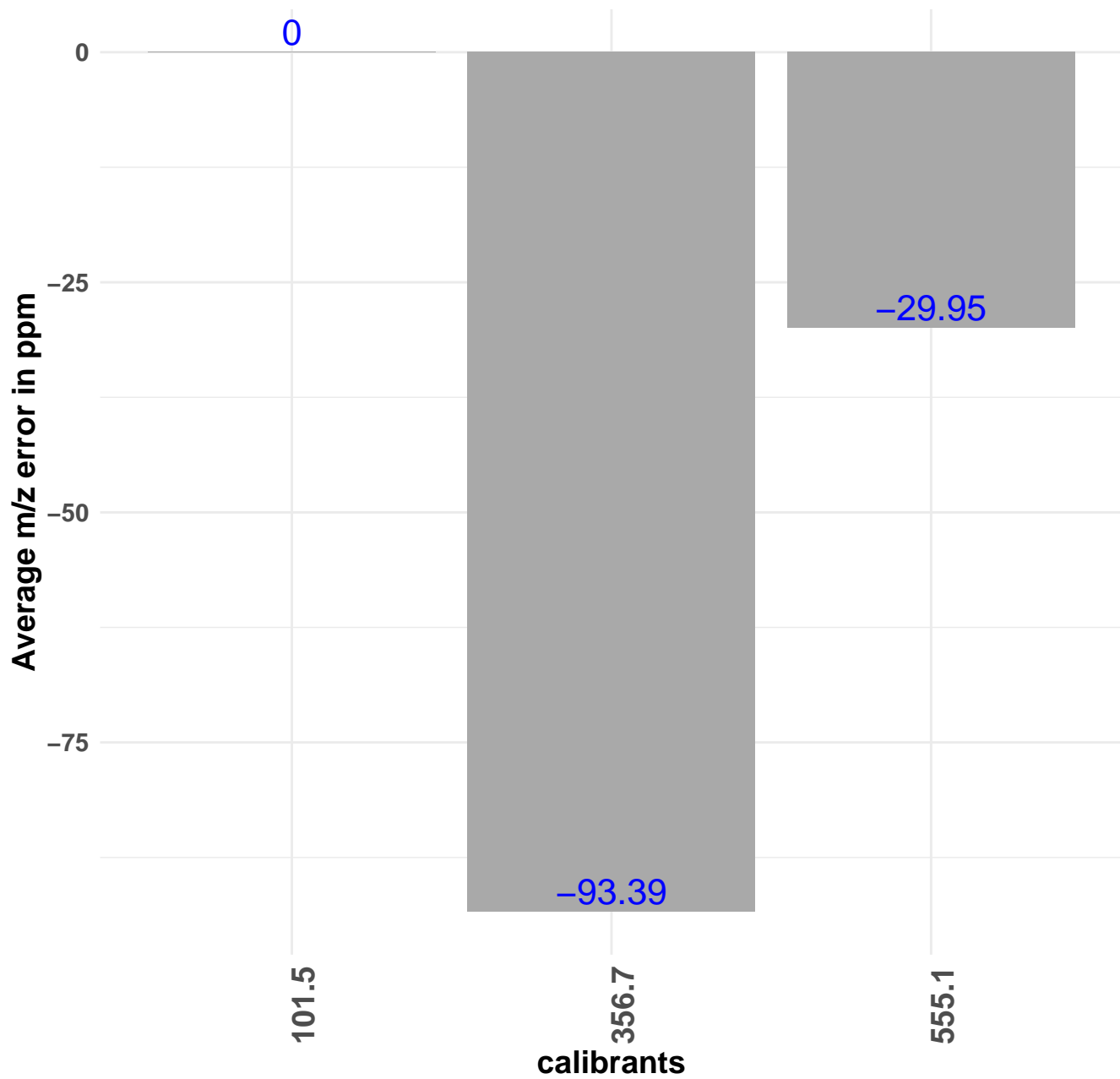


Average m/z error (max. average intensity vs. theor. calibrant m/z)

Average m/z error in ppm



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)**

