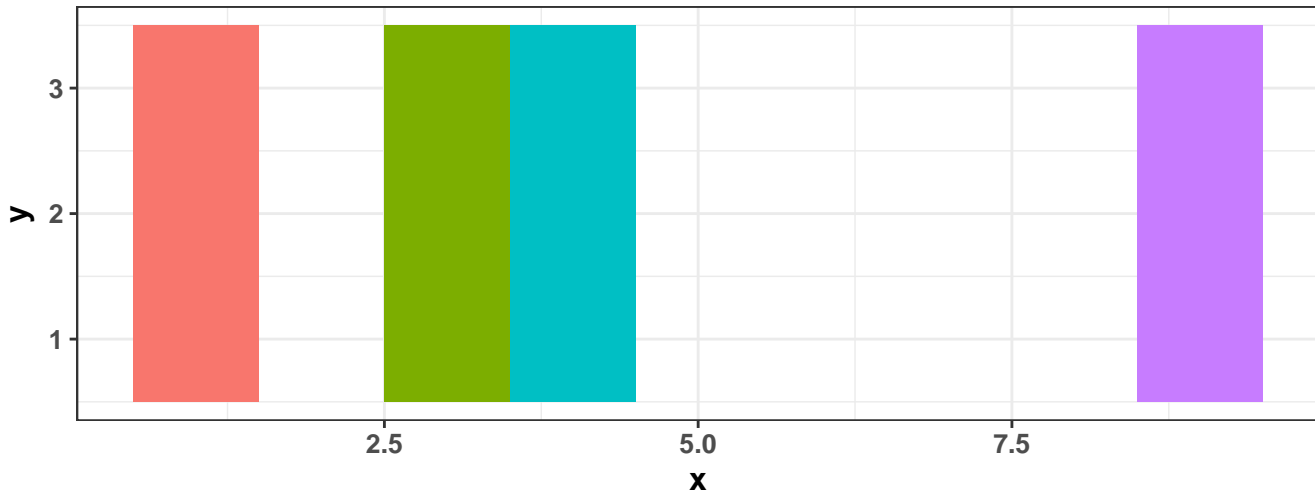


Testfile_rdata

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	161.81
Median # peaks per spectrum	2811
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.txt	3 / 3

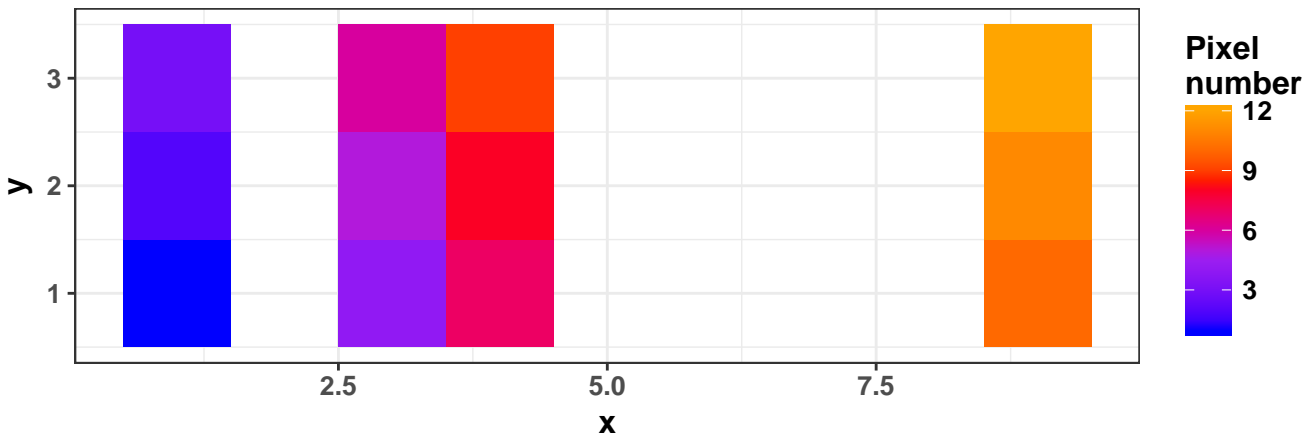
Spatial orientation of combined data



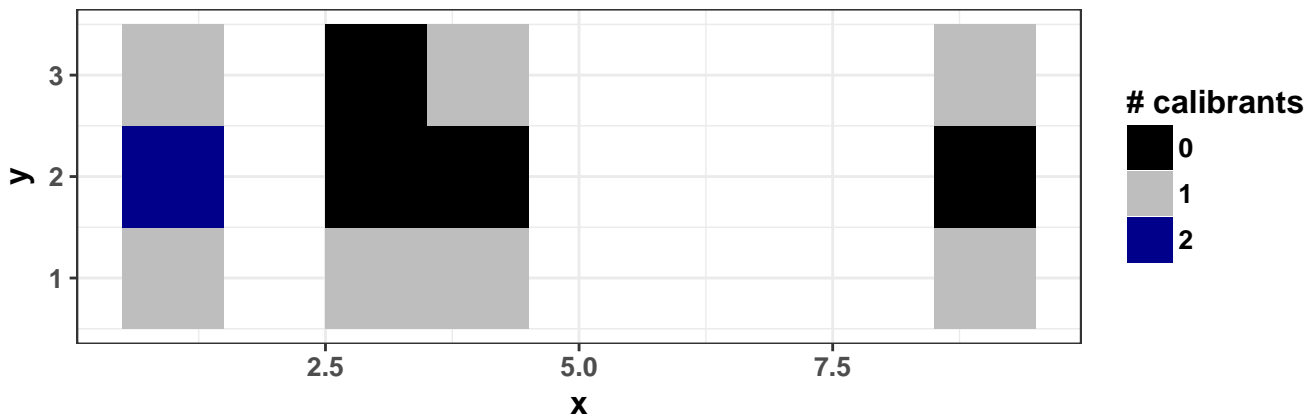
Annotation

column1 column2 column3 column4

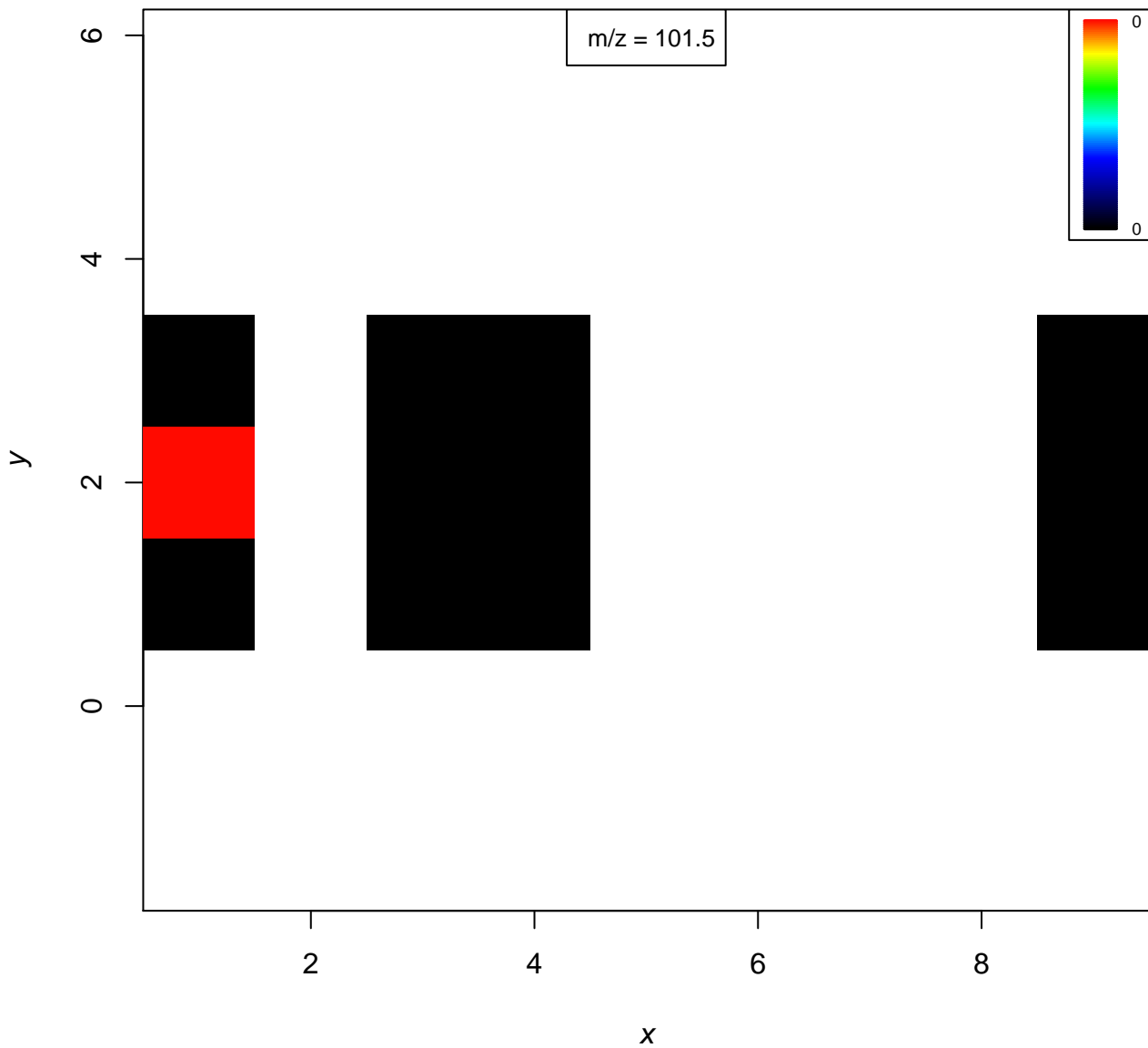
Pixel ordered for annotation groups



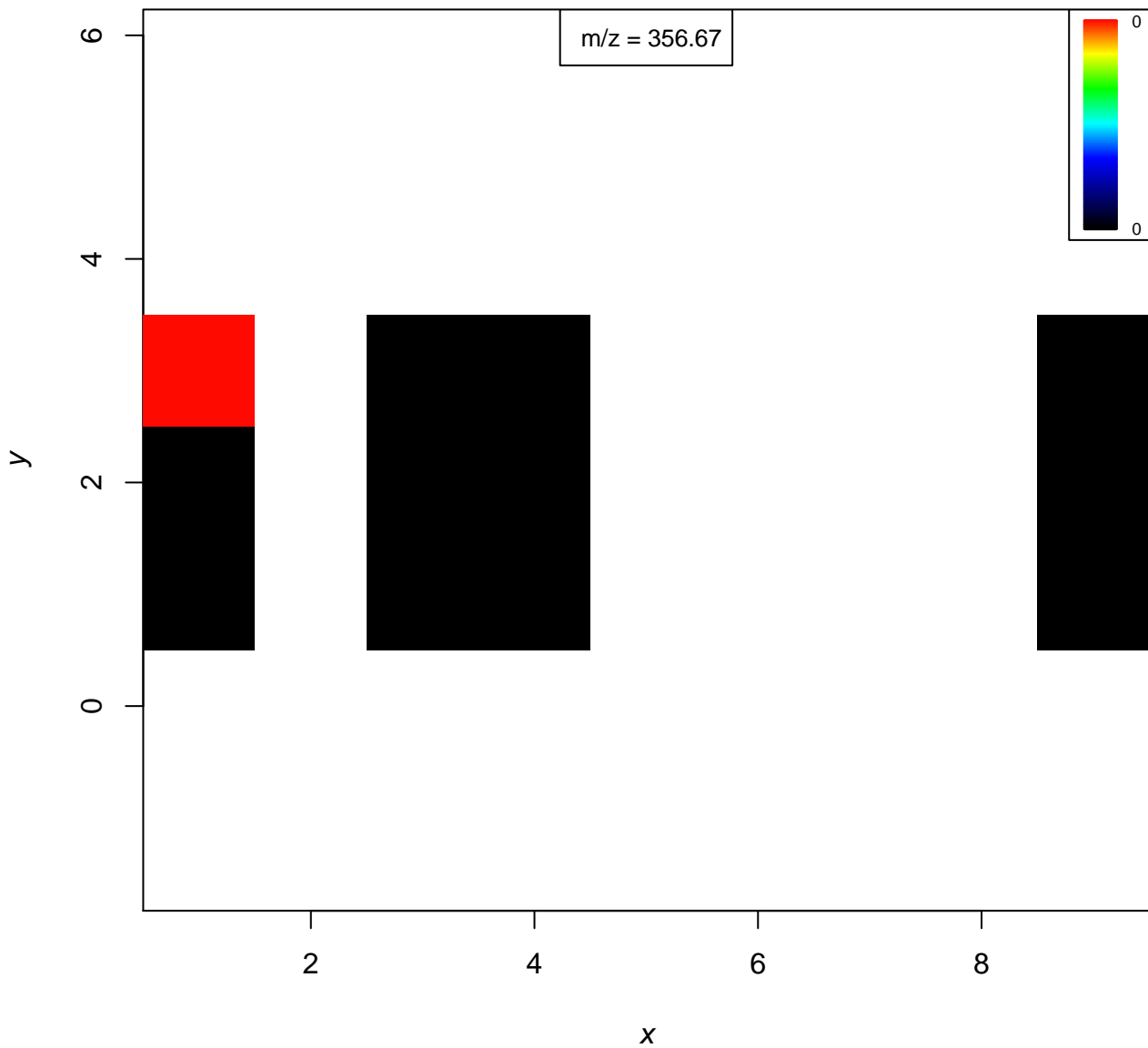
Number of calibrants per pixel (± 100 ppm)



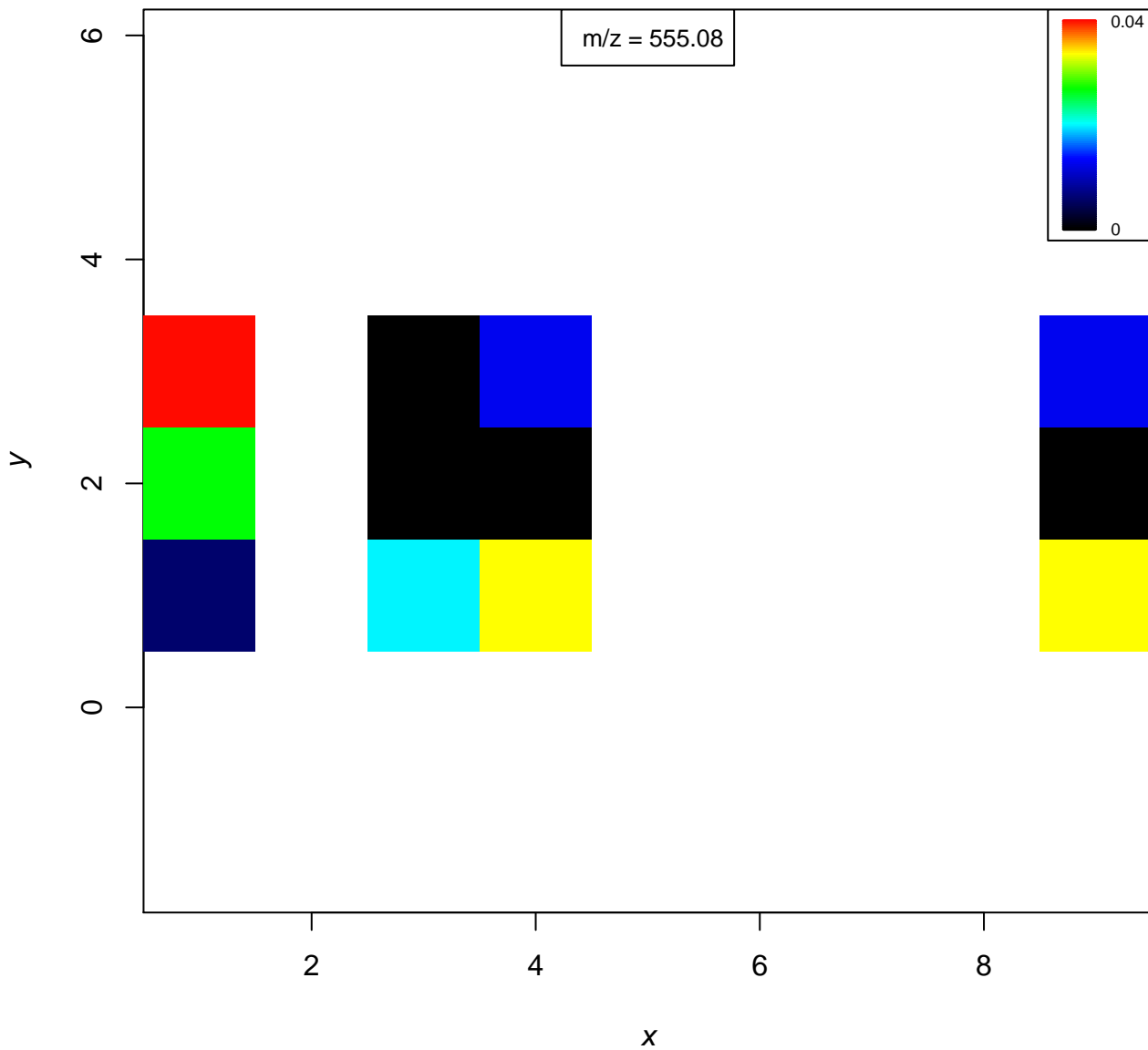
101.5: 101.5 (± 100 ppm)



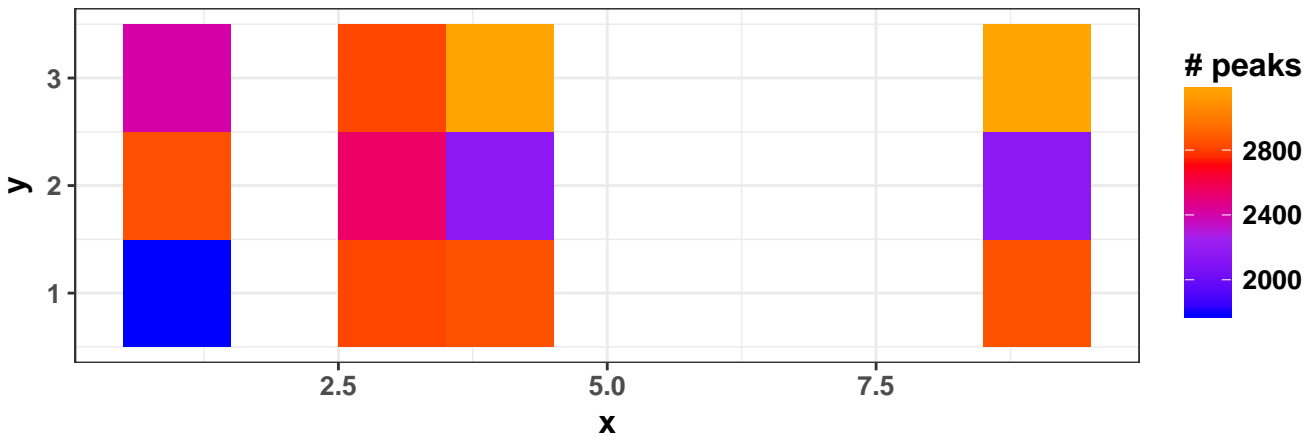
356.7: 356.7 (± 100 ppm)



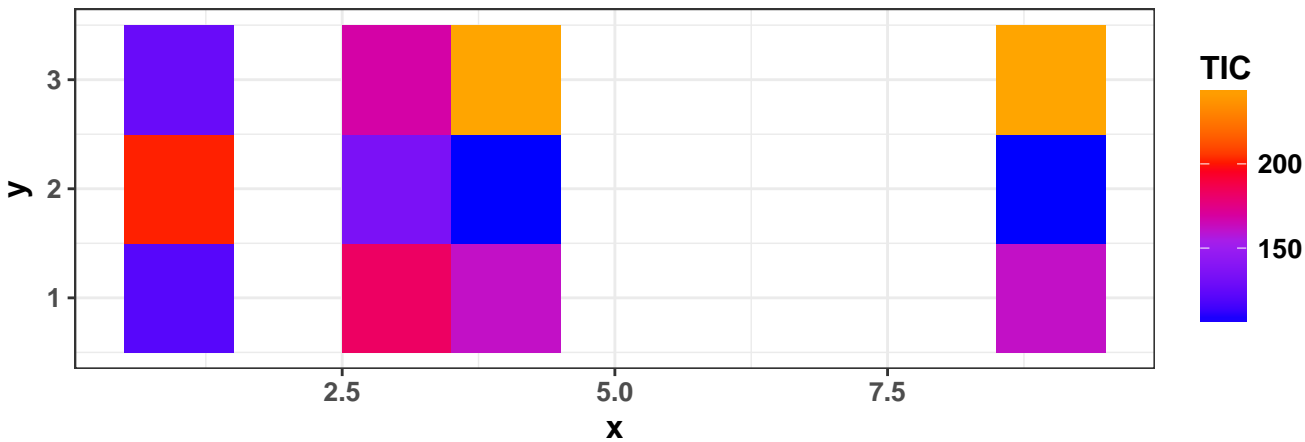
555.1: 555.1 (± 100 ppm)



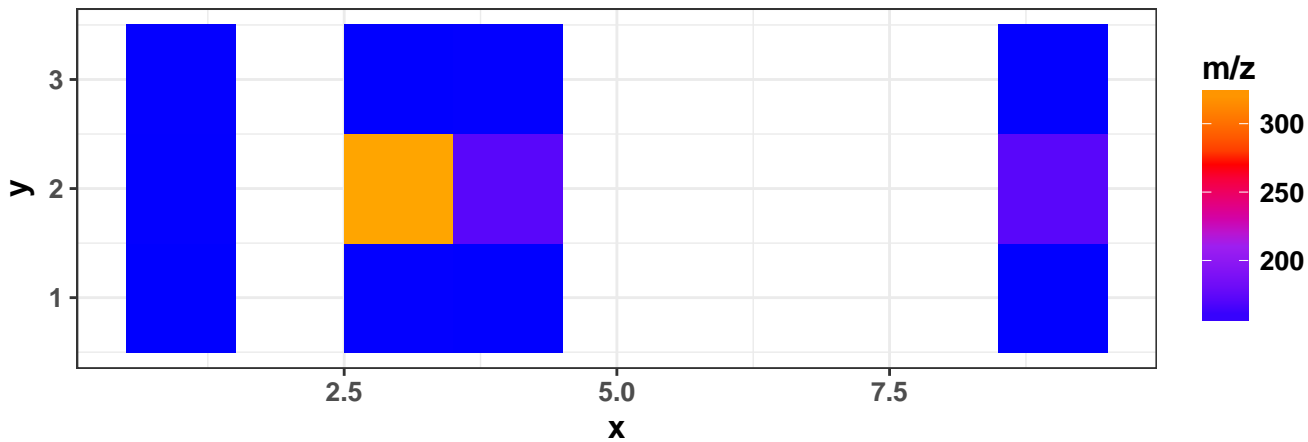
Number of peaks per spectrum



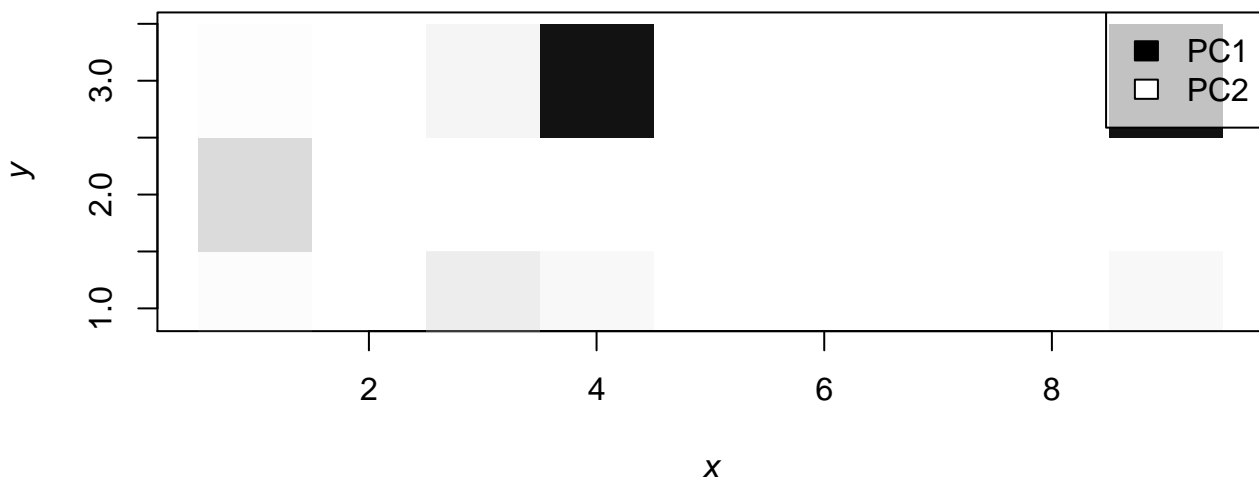
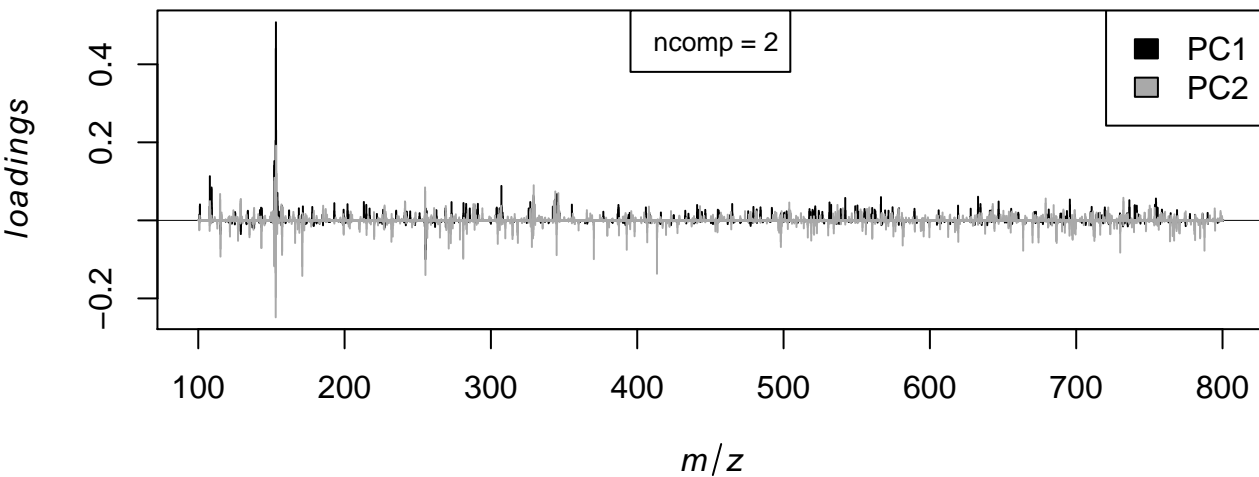
Total Ion Chromatogram



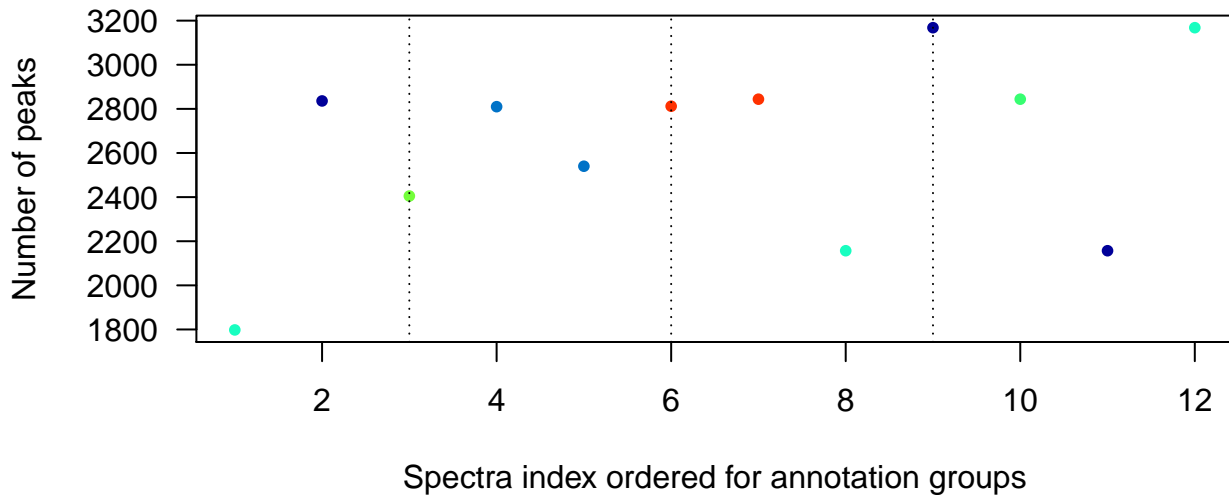
Most abundant m/z in each spectrum



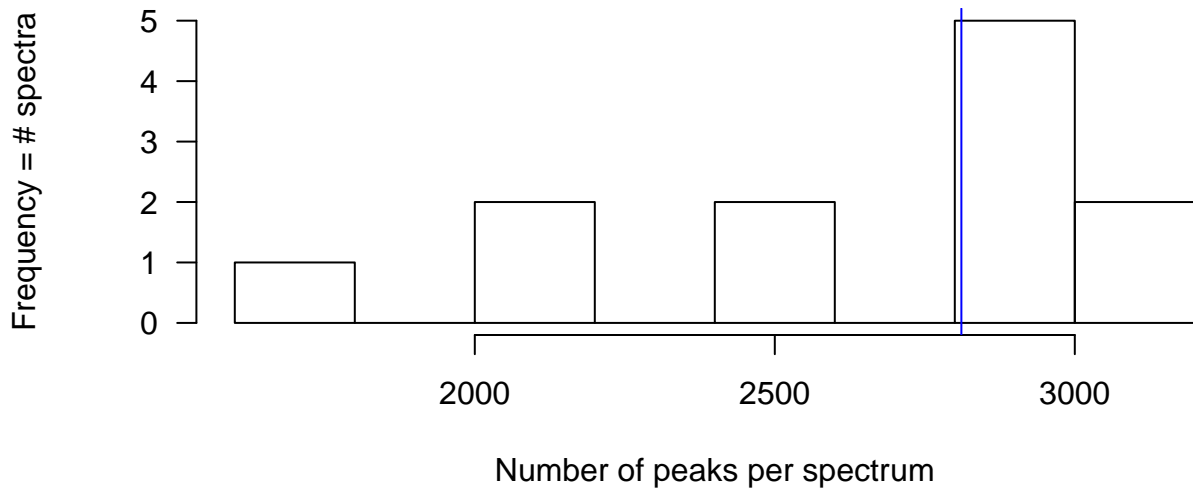
PCA for two components



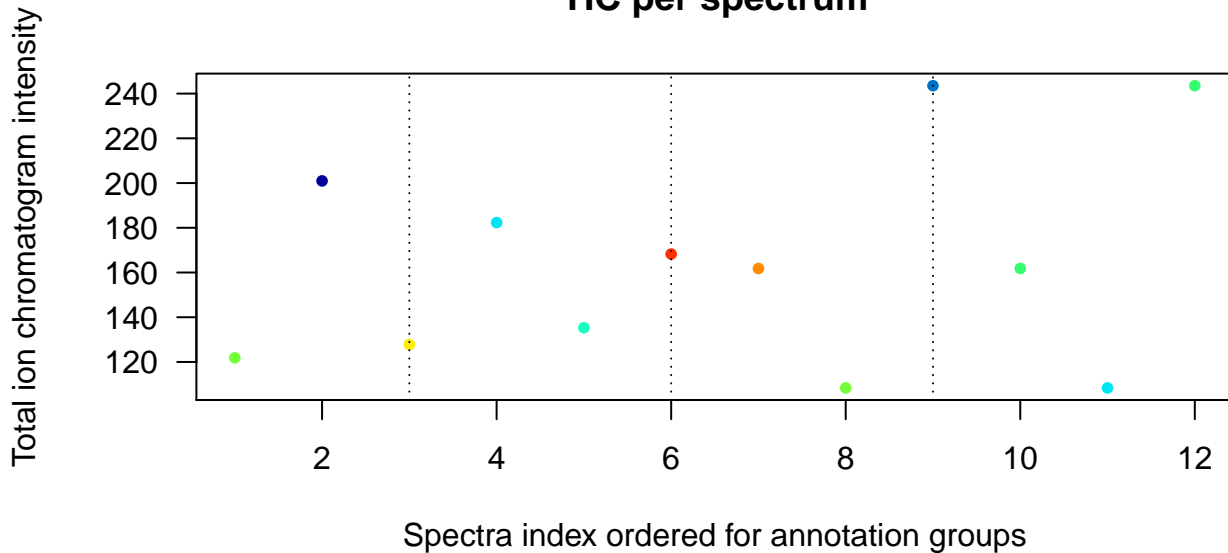
Number of peaks per spectrum



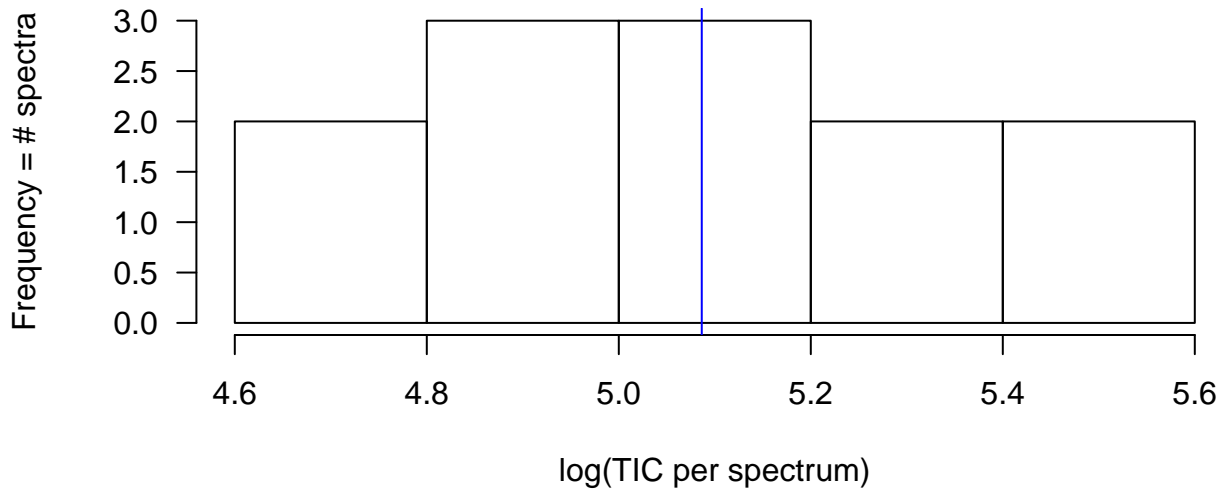
Number of peaks per spectrum



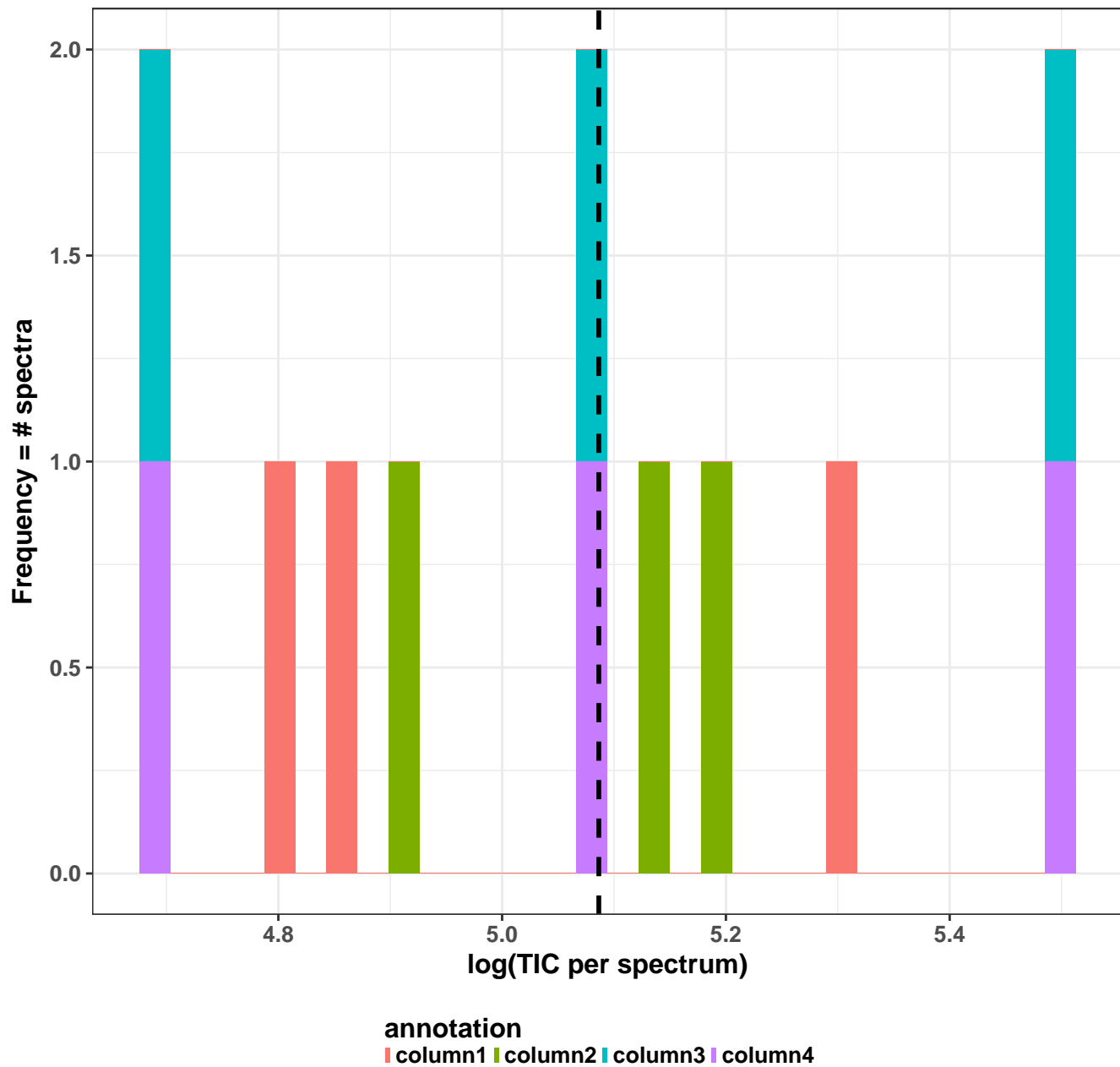
TIC per spectrum



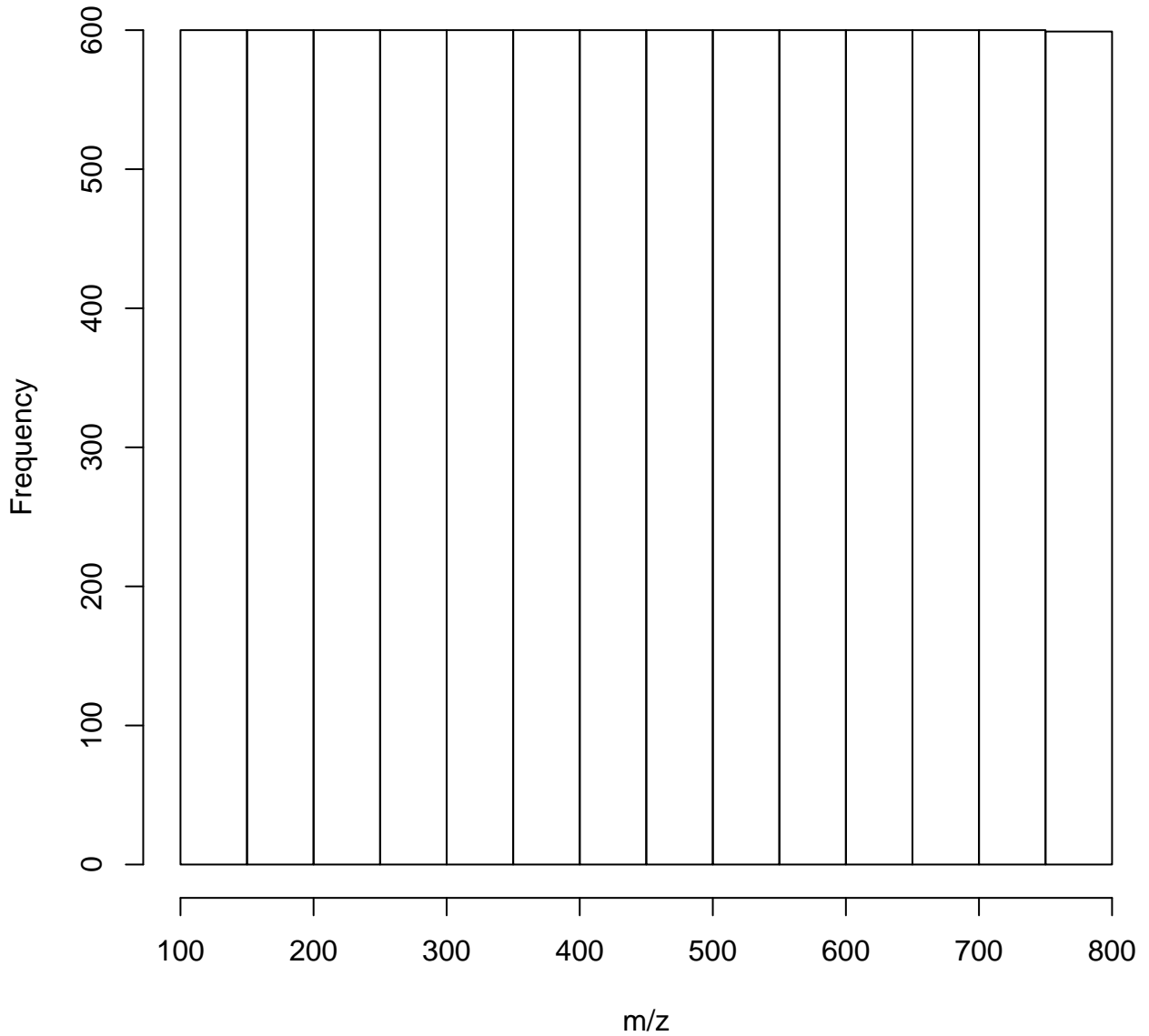
TIC per spectrum



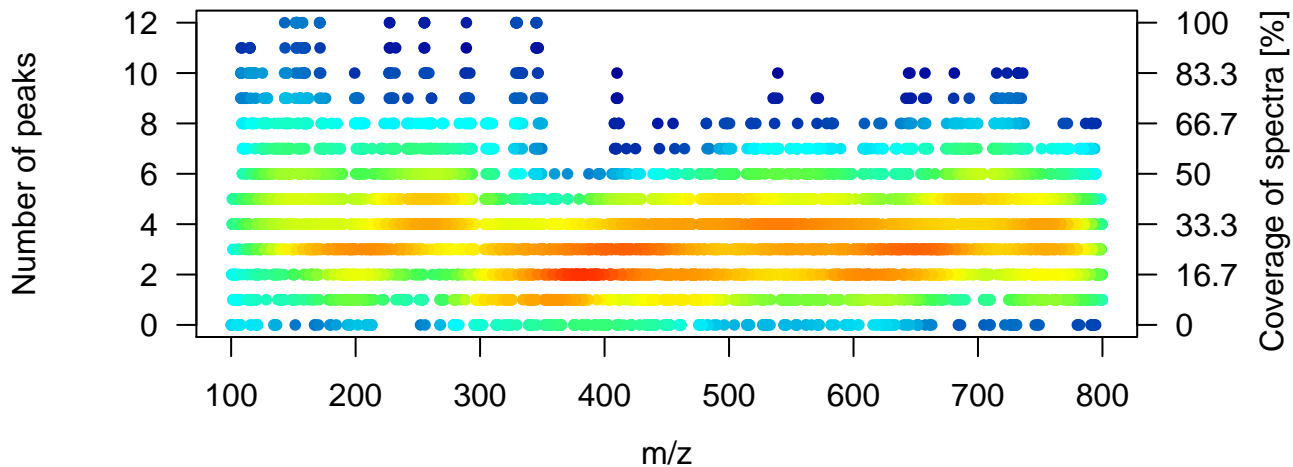
TIC per spectrum and annotation group



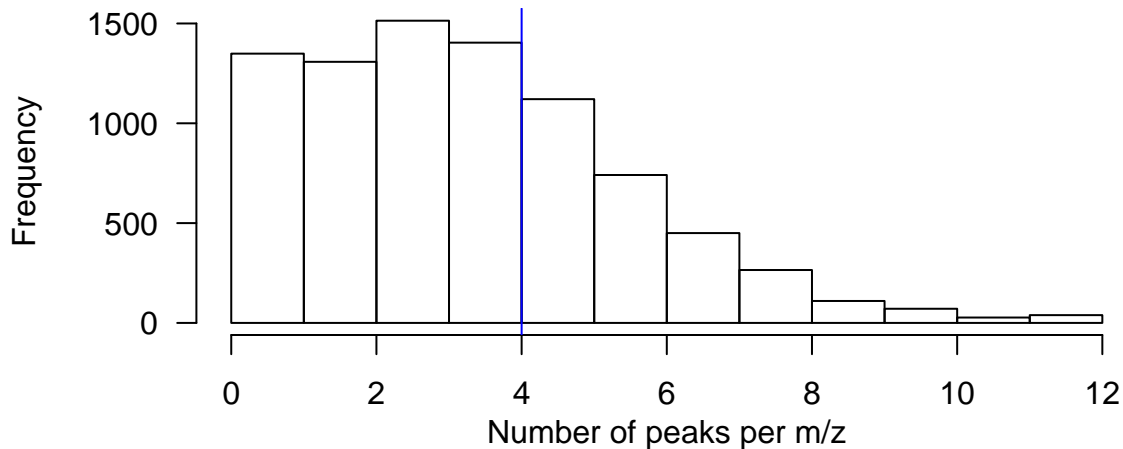
Histogram of m/z values



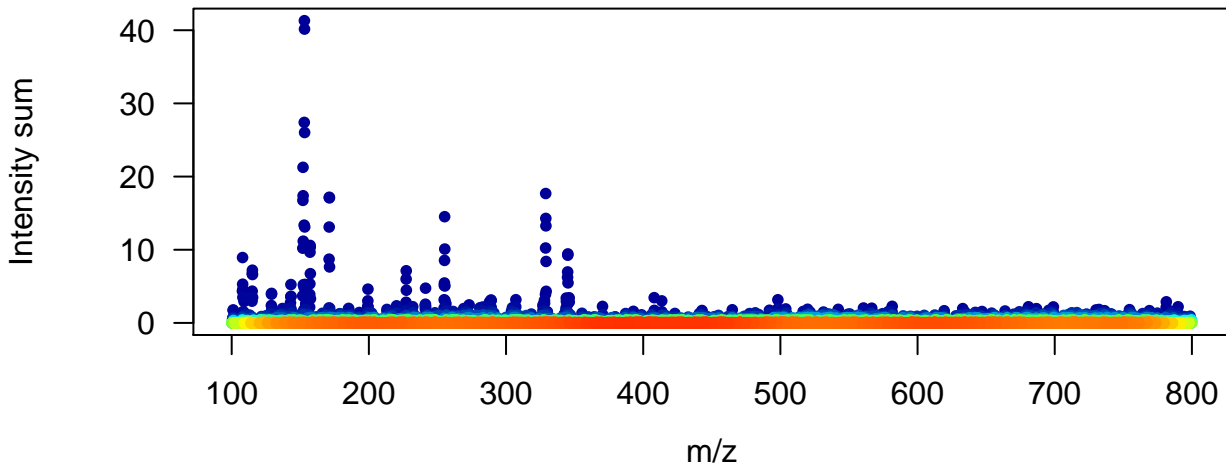
Number of peaks per m/z



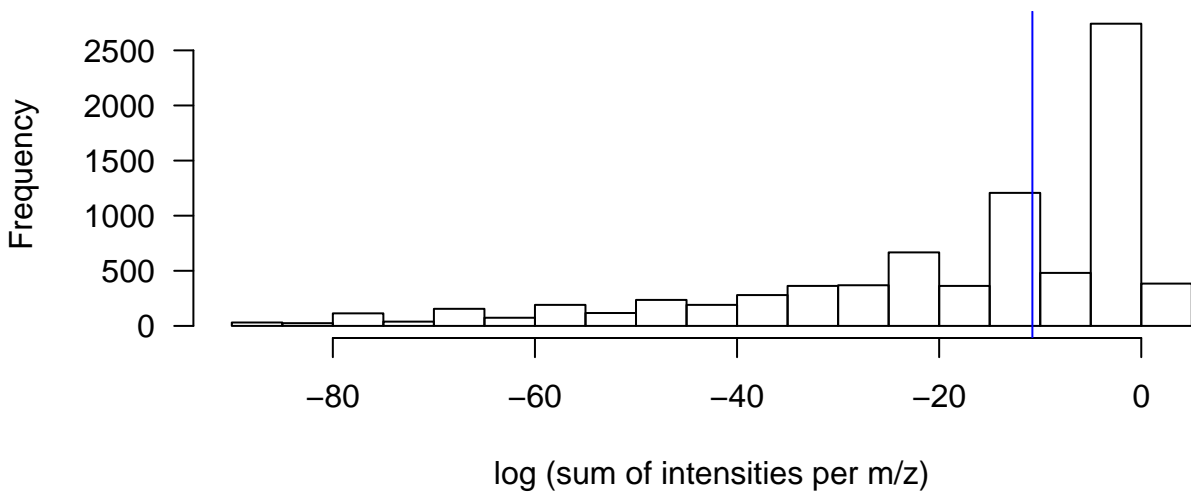
Number of peaks per m/z



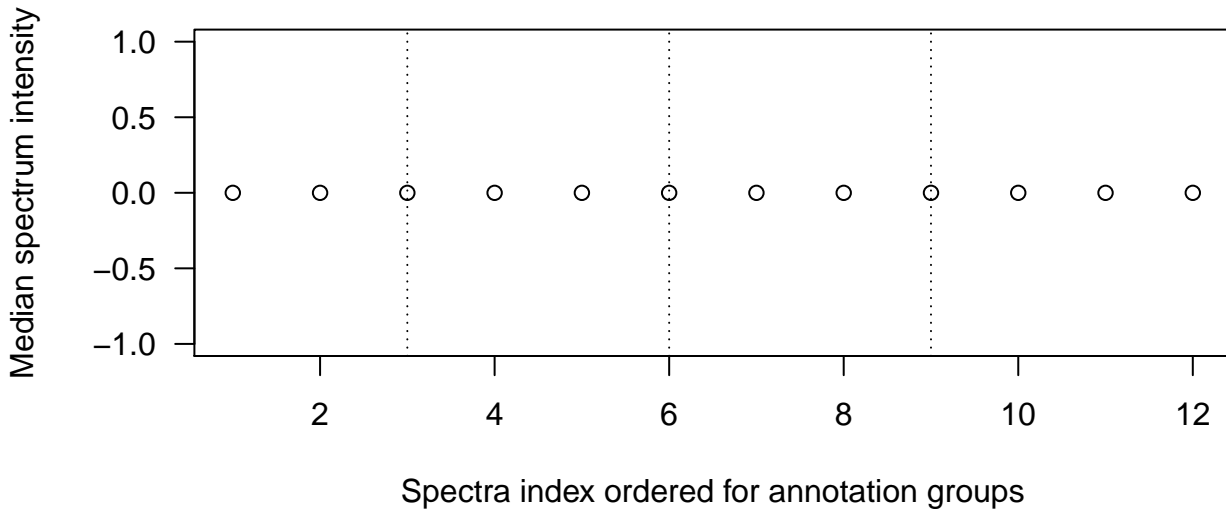
Sum of intensities per m/z



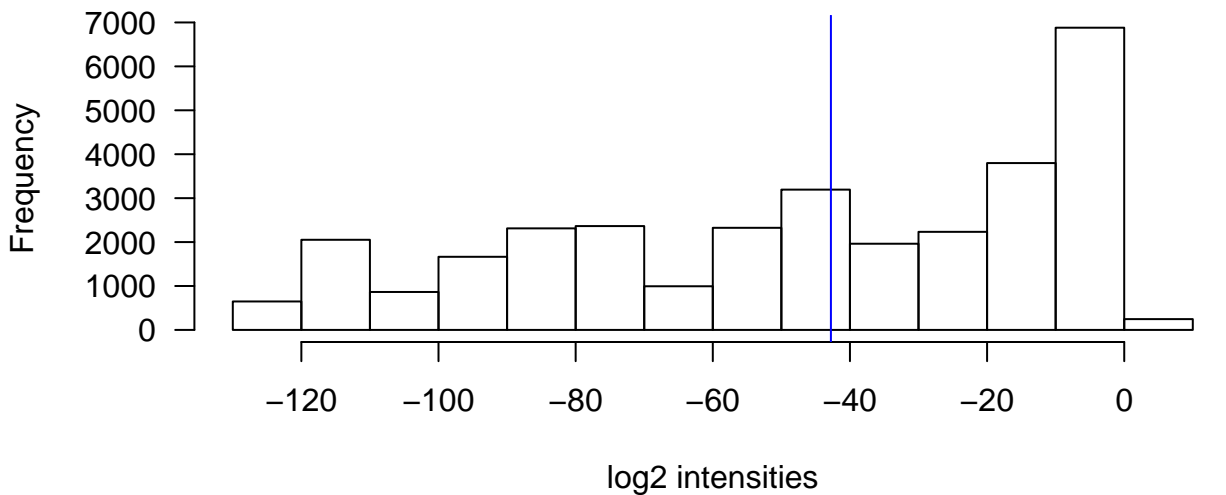
Sum of intensities per m/z



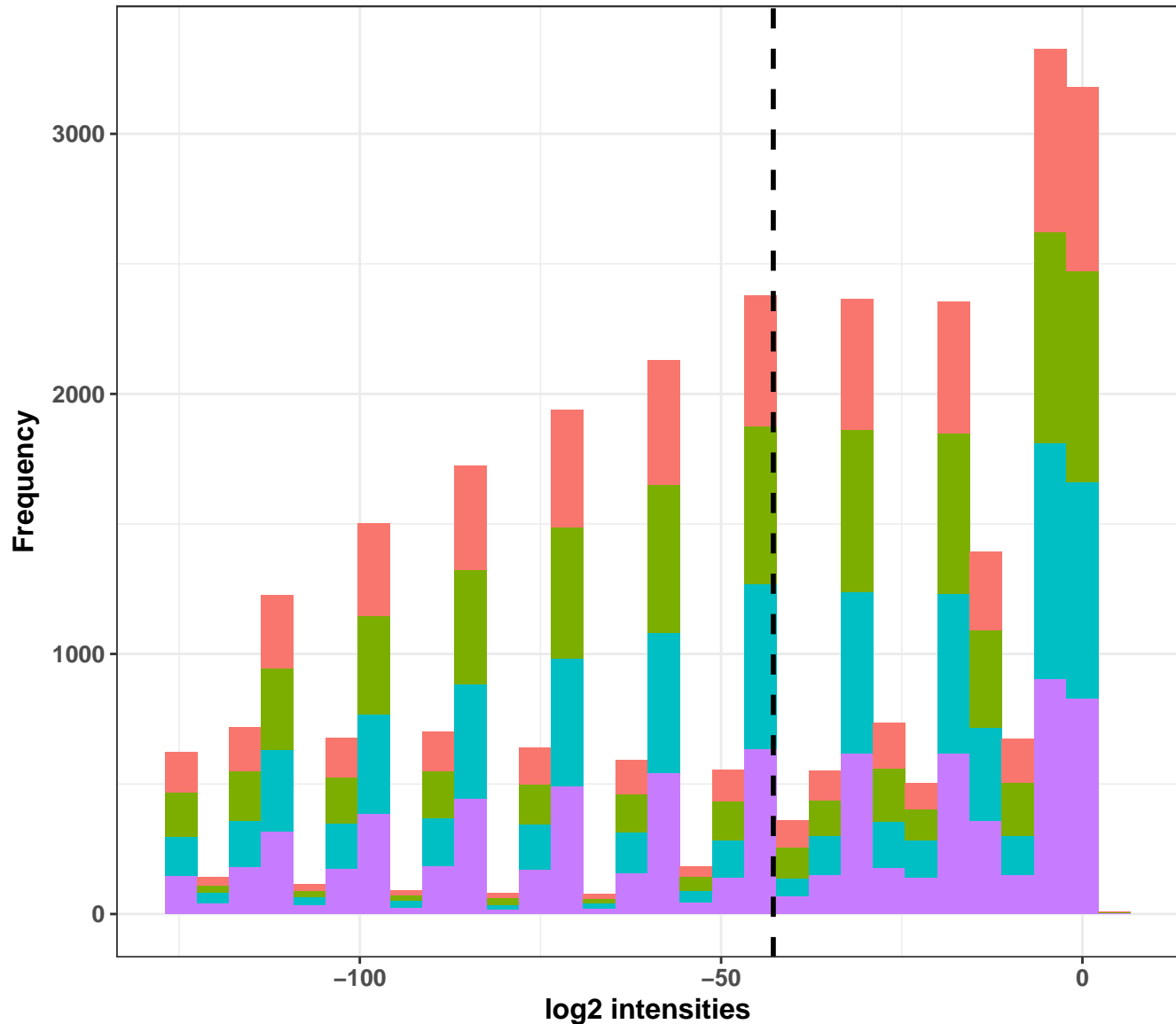
Median intensity per spectrum



Log2-transformed intensities



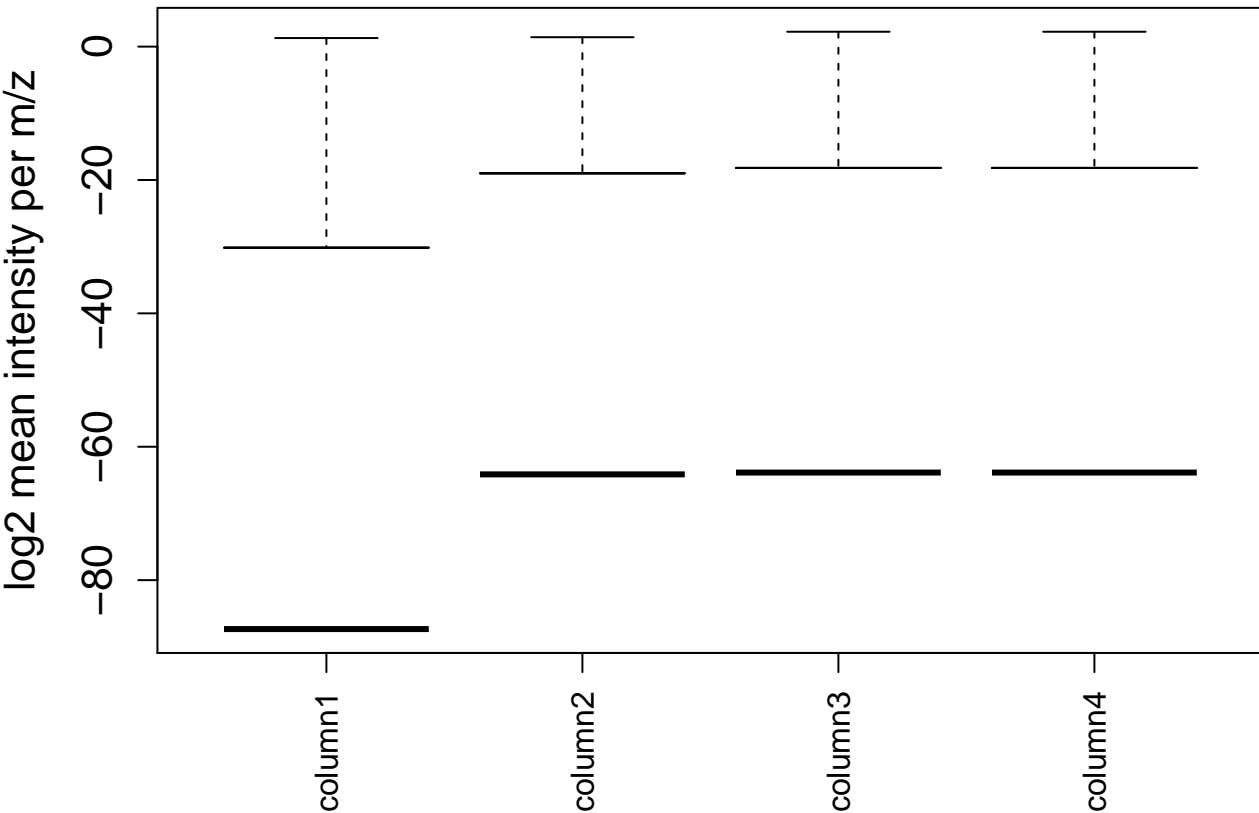
Log2-transformed intensities per sample



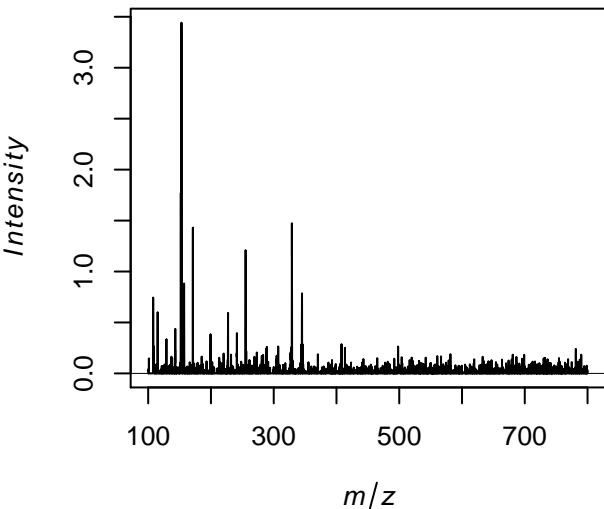
annotation

column1 column2 column3 column4

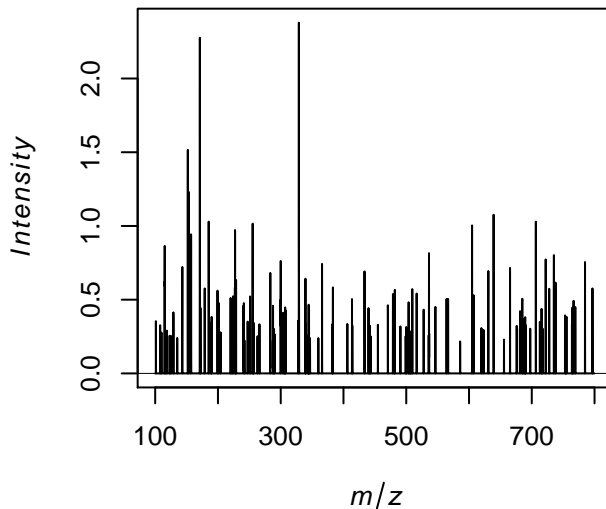
Mean intensities per m/z and annotation group



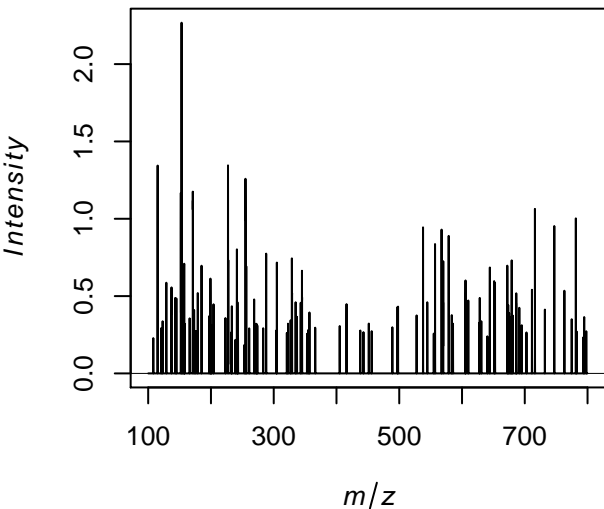
Average spectrum



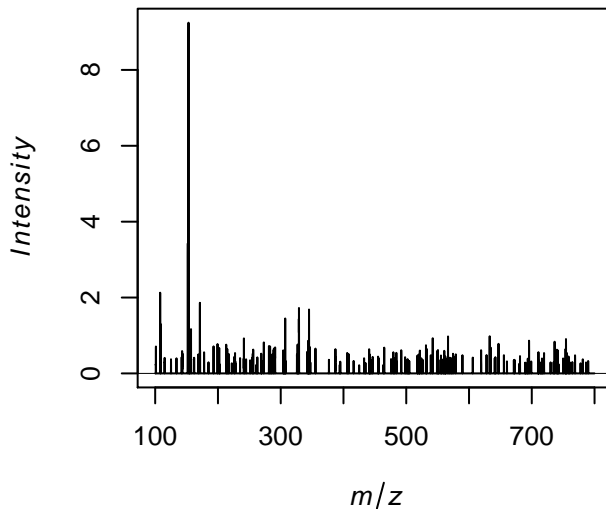
Spectrum at x = 3, y = 2



Spectrum at x = 1, y = 3



Spectrum at x = 4, y = 3

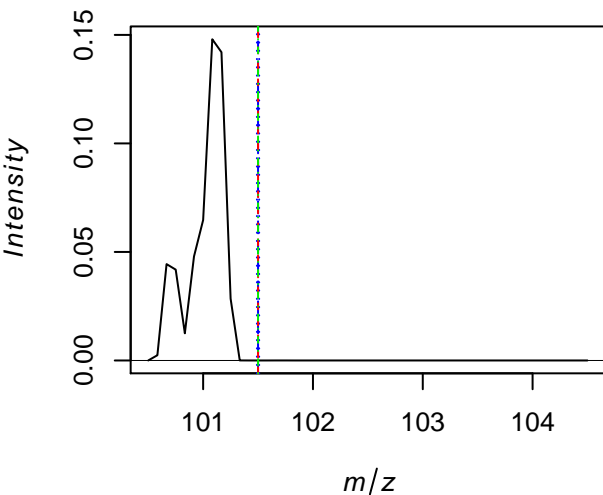


theor. m/z: 101.5

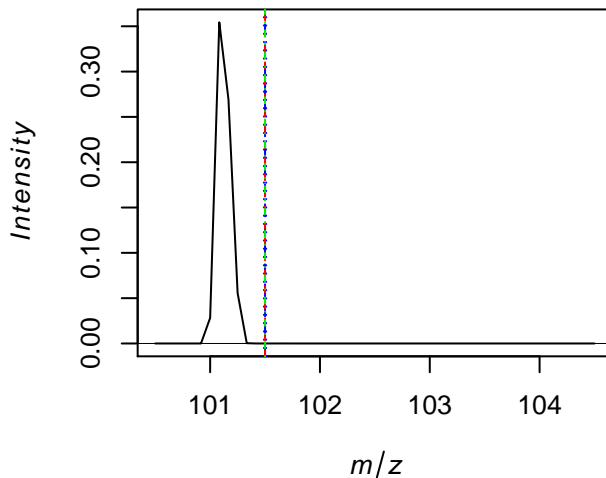
most abundant m/z: 101.5

closest m/z: 101.5

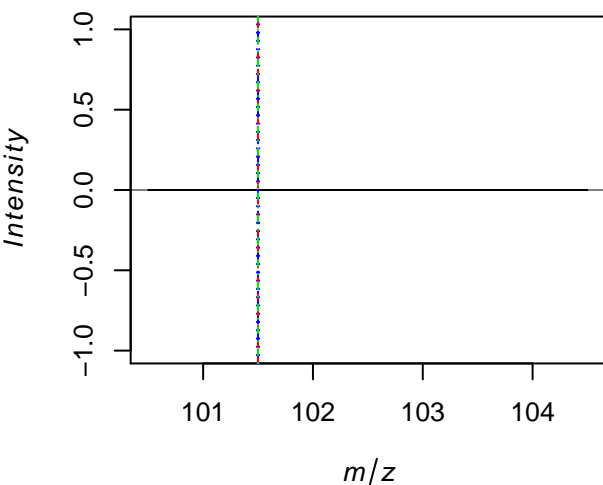
average spectrum



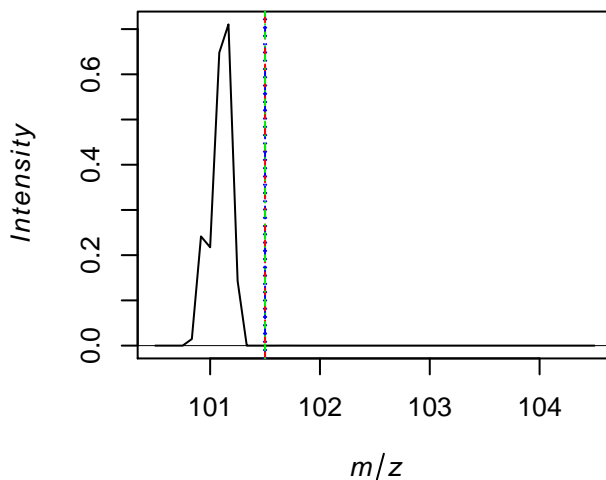
Spectrum at x = 3, y = 2



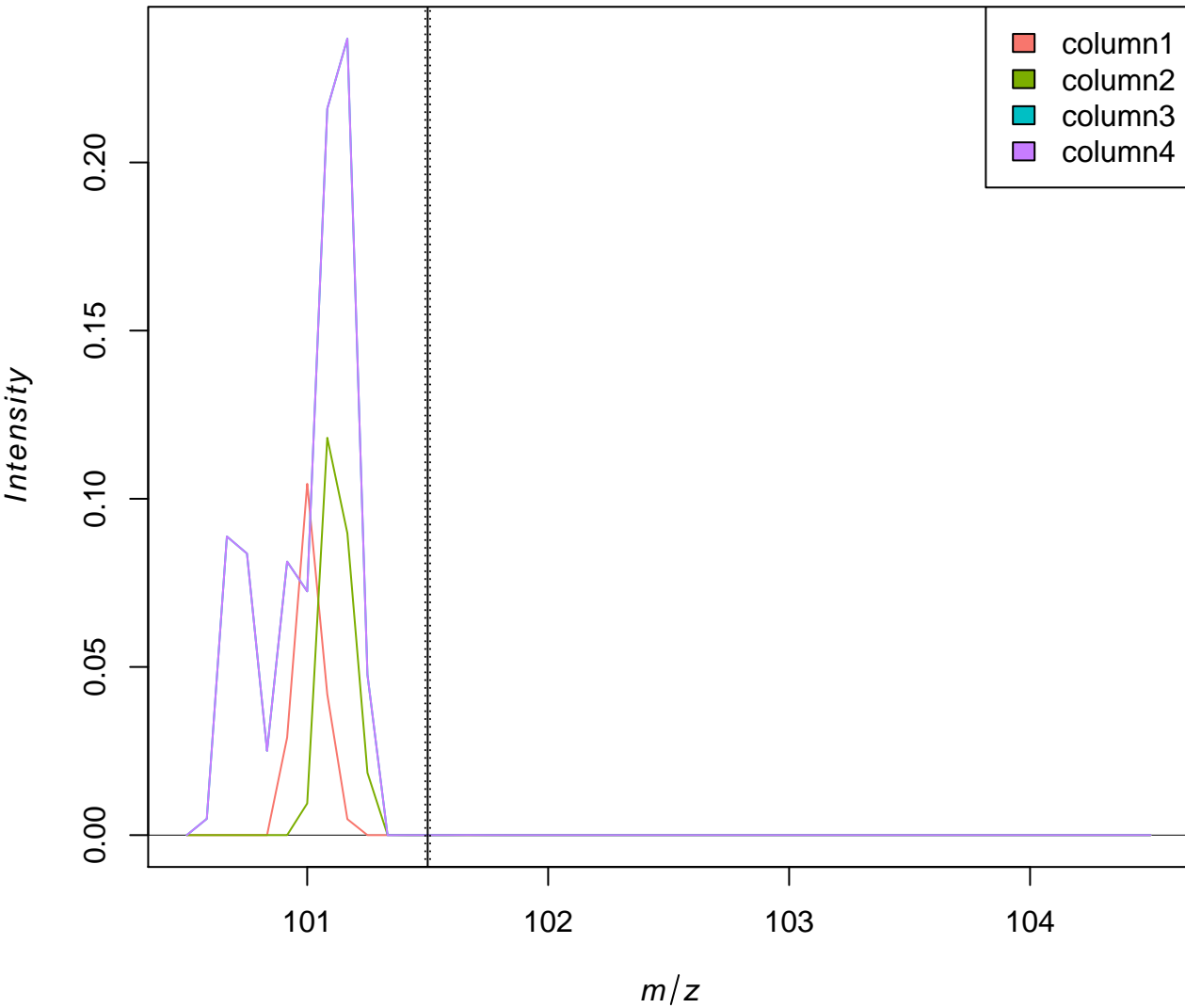
Spectrum at x = 1, y = 3



Spectrum at x = 4, y = 3



Average spectrum per annotation group

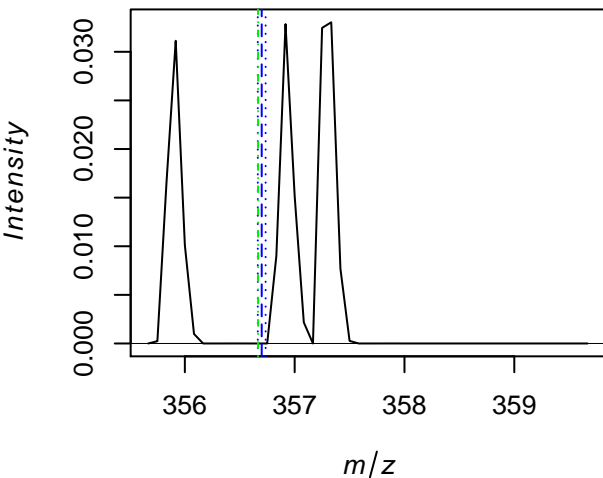


theor. m/z: 356.7

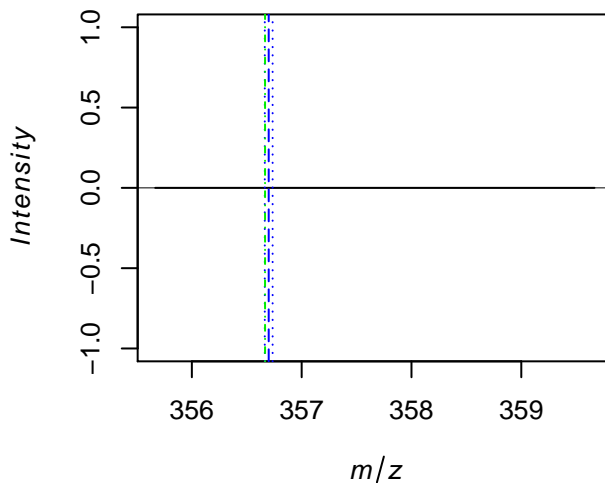
most abundant m/z: NA

closest m/z: 356.6667

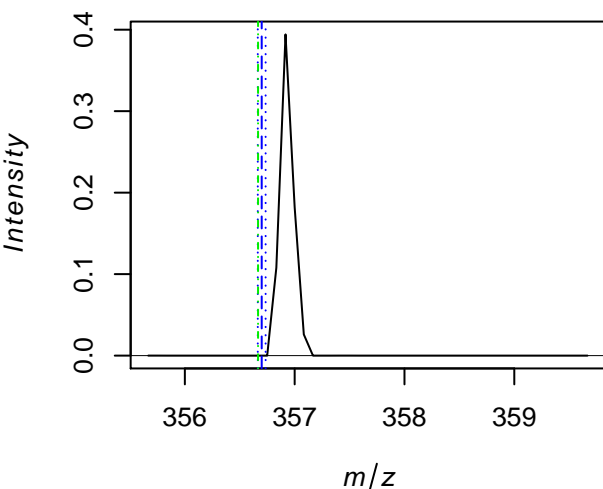
average spectrum



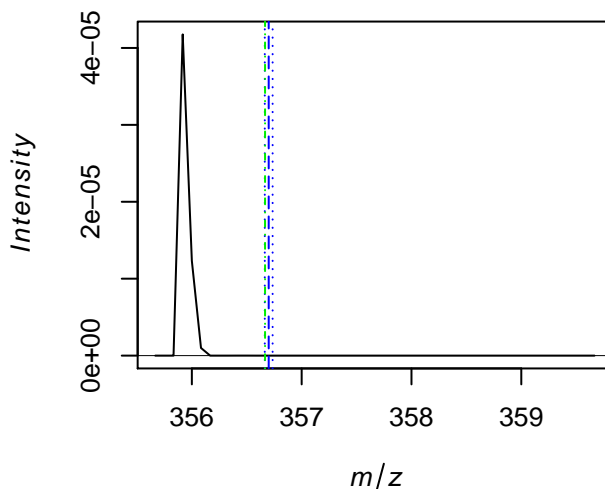
Spectrum at x = 3, y = 2



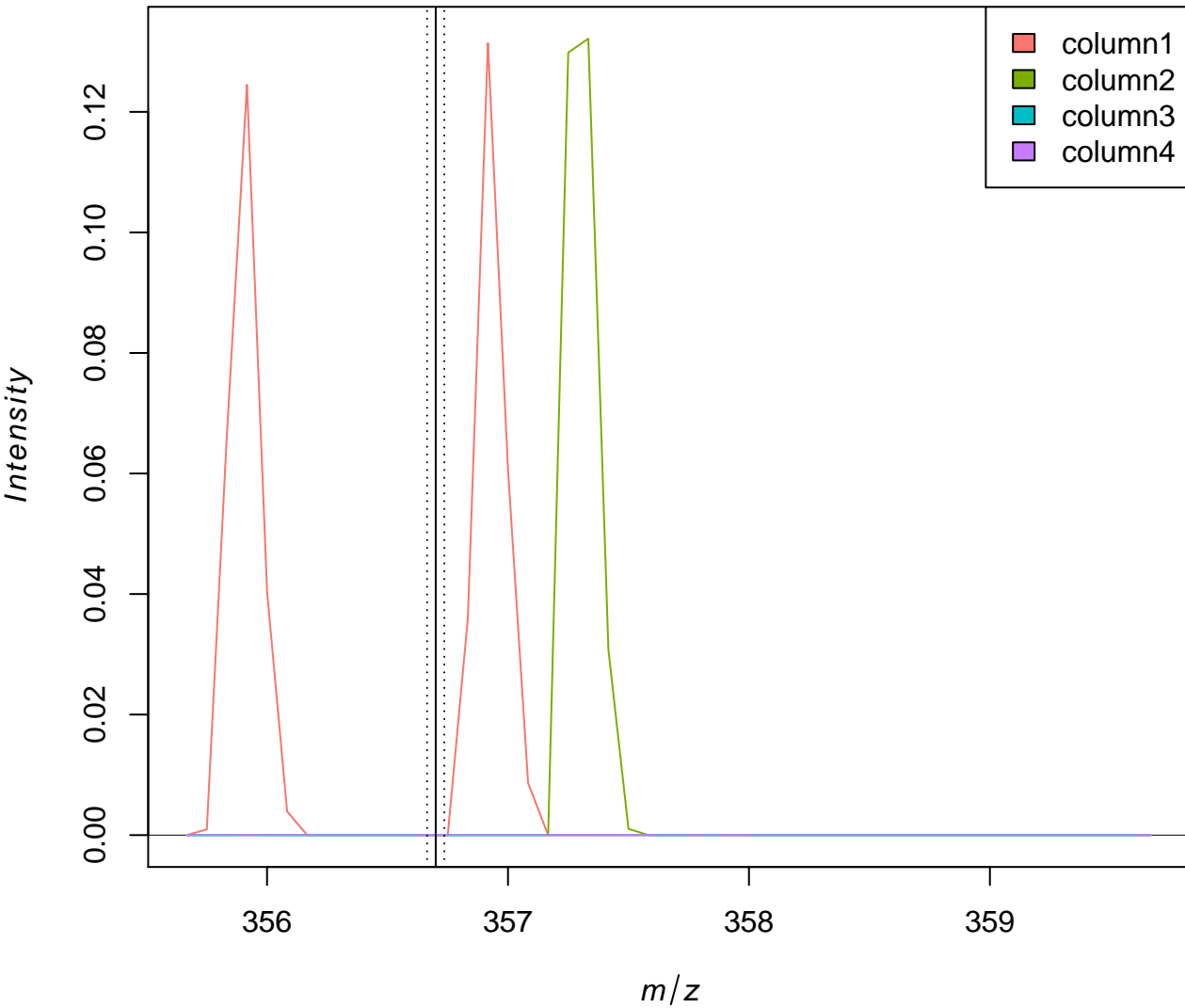
Spectrum at x = 1, y = 3



Spectrum at x = 4, y = 3



Average spectrum per annotation group

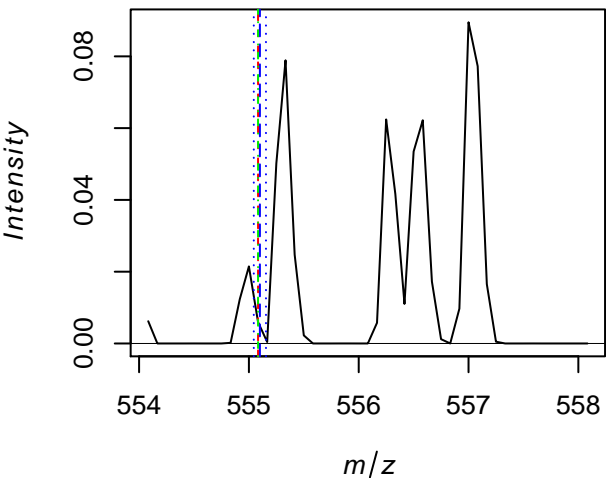


theor. m/z: 555.1

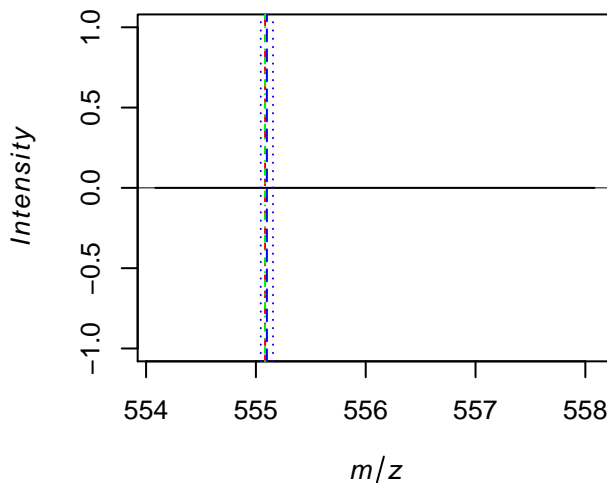
most abundant m/z: 555.0834

closest m/z: 555.0834

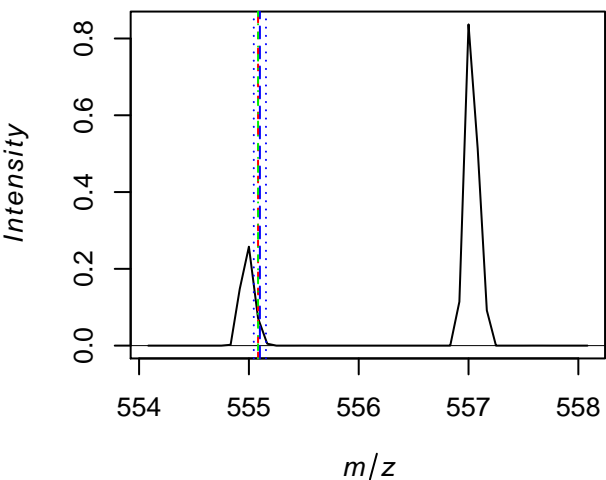
average spectrum



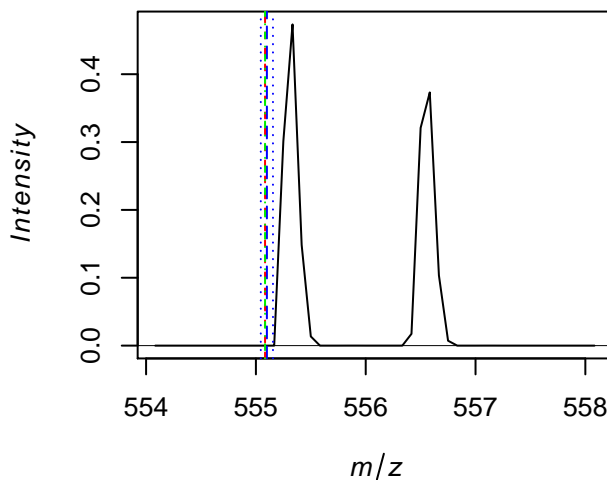
Spectrum at x = 3, y = 2



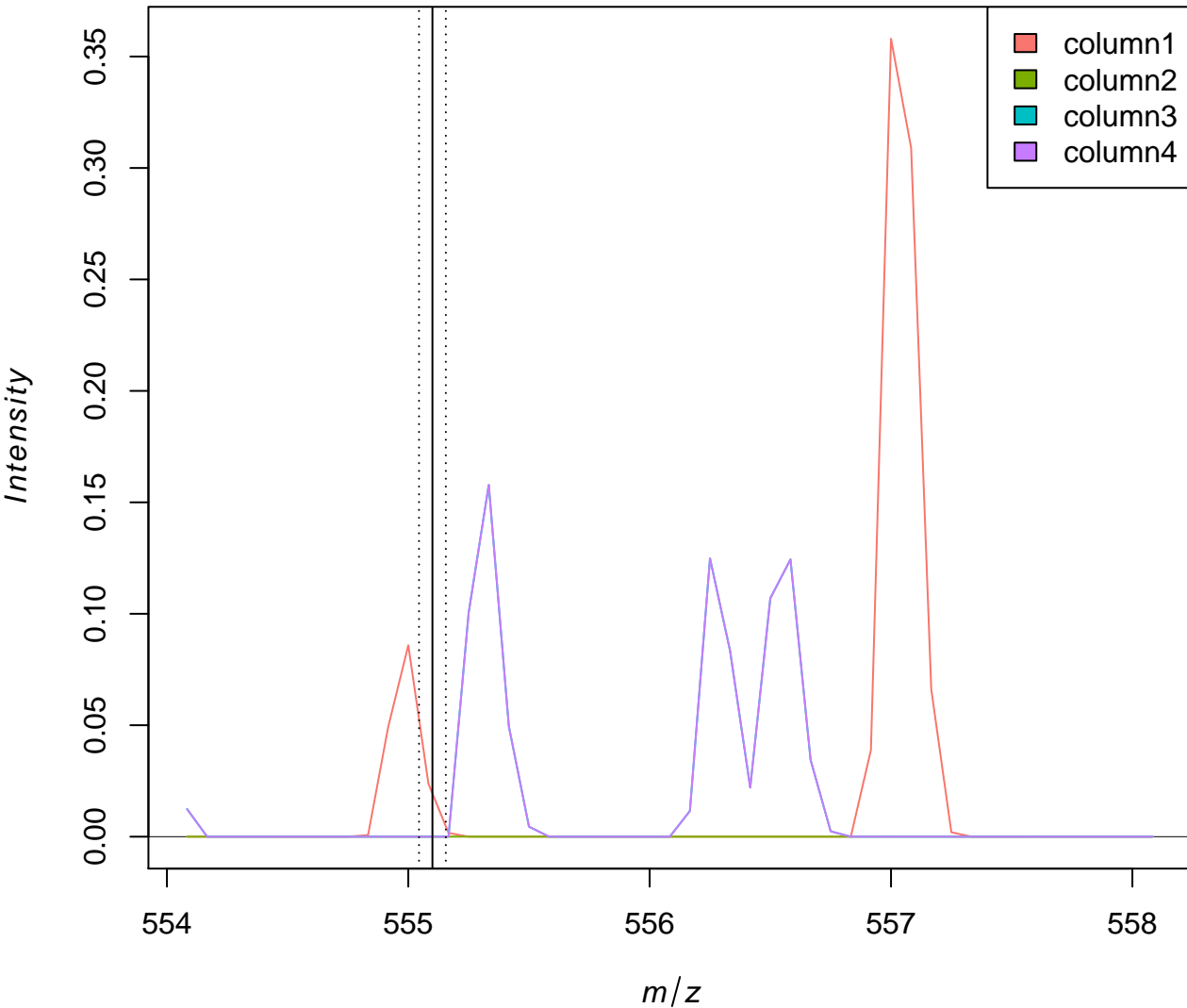
Spectrum at x = 1, y = 3



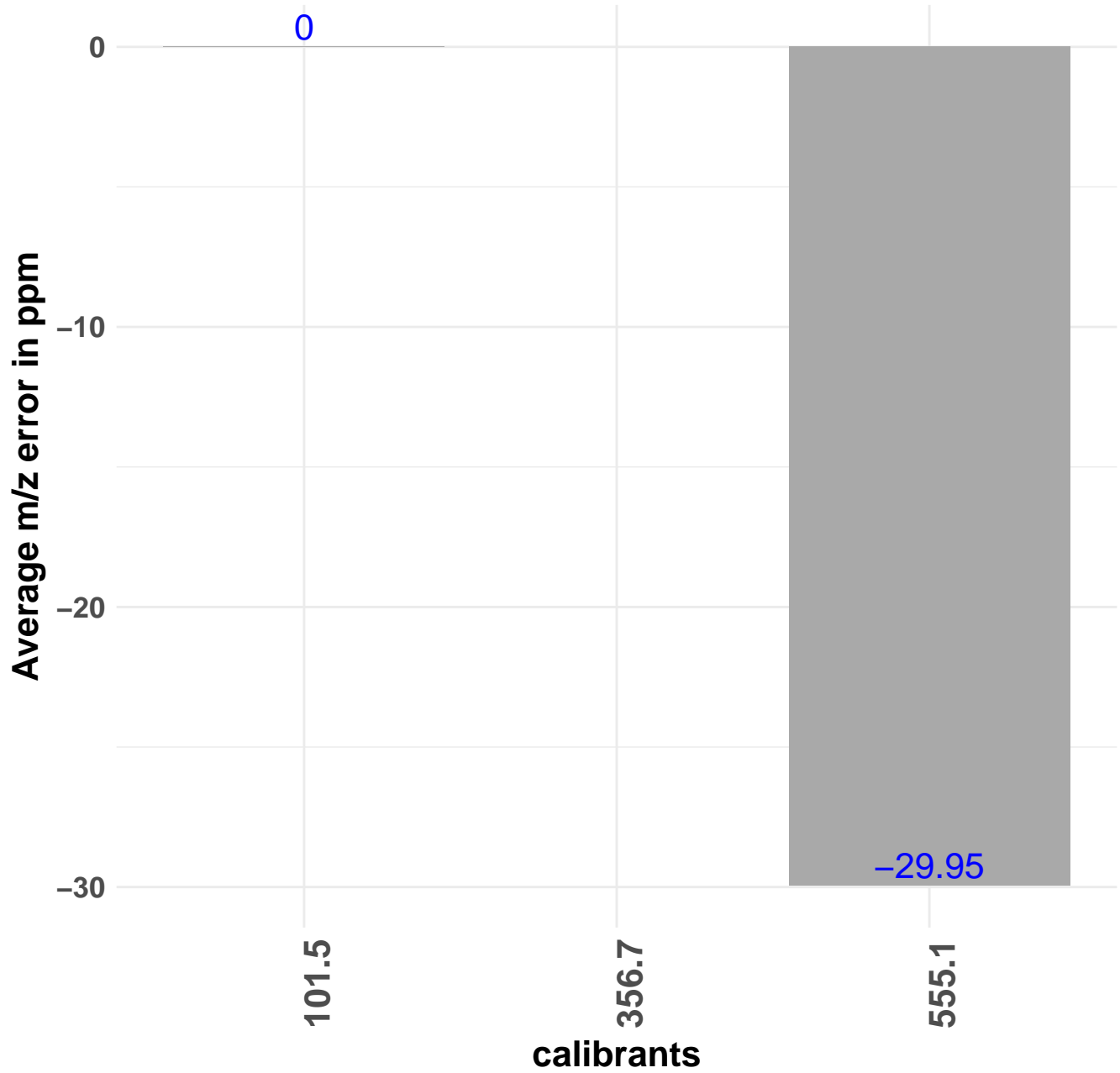
Spectrum at x = 4, y = 3



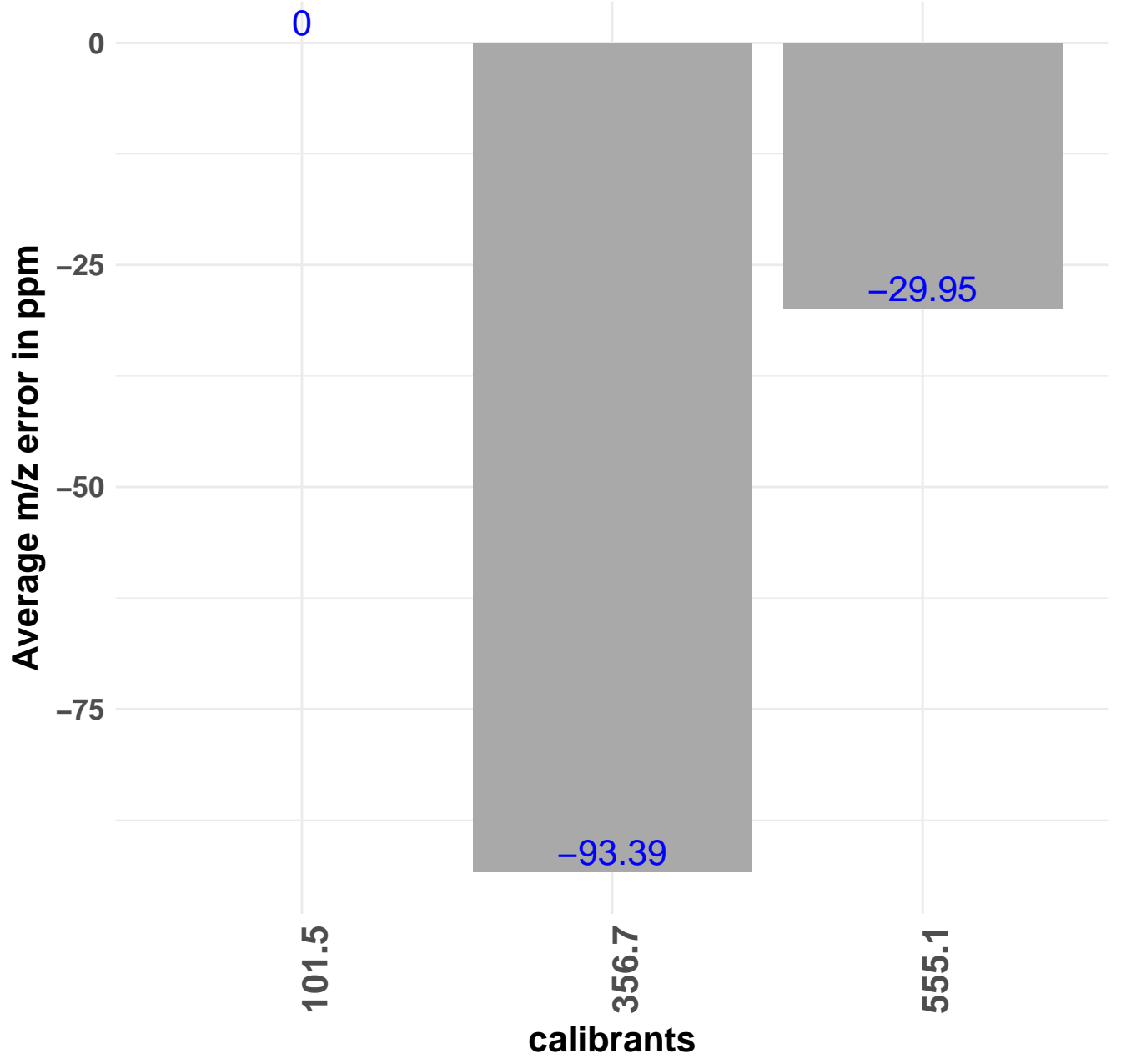
Average spectrum per annotation group



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)

