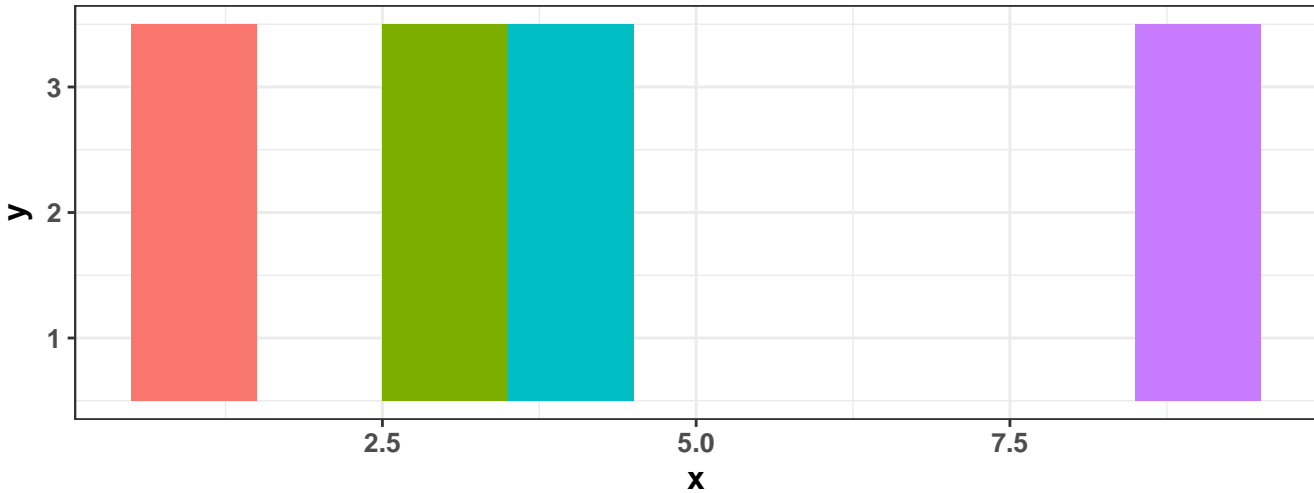


Testfile_rdata

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
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.txt	3 / 3

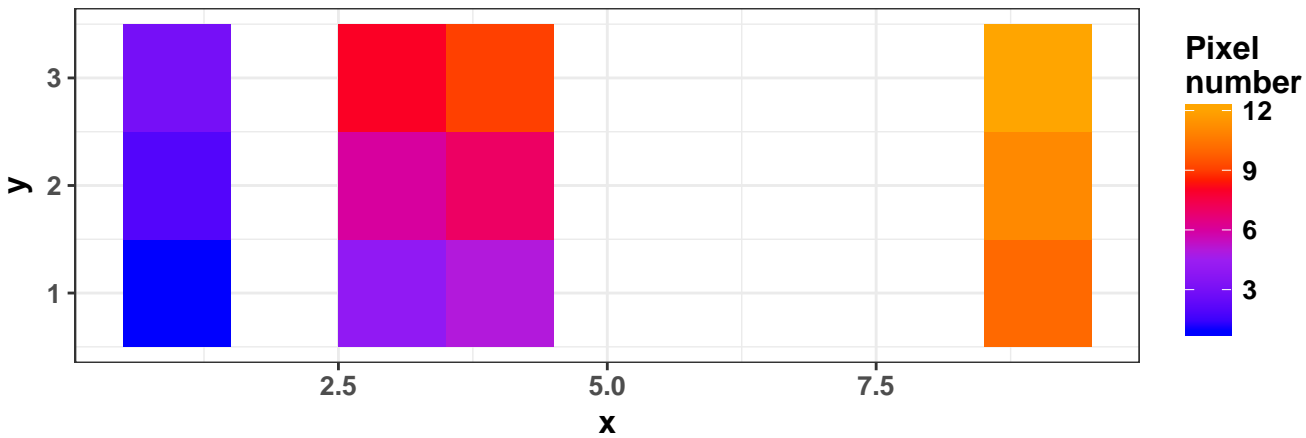
Spatial orientation of pixel annotations



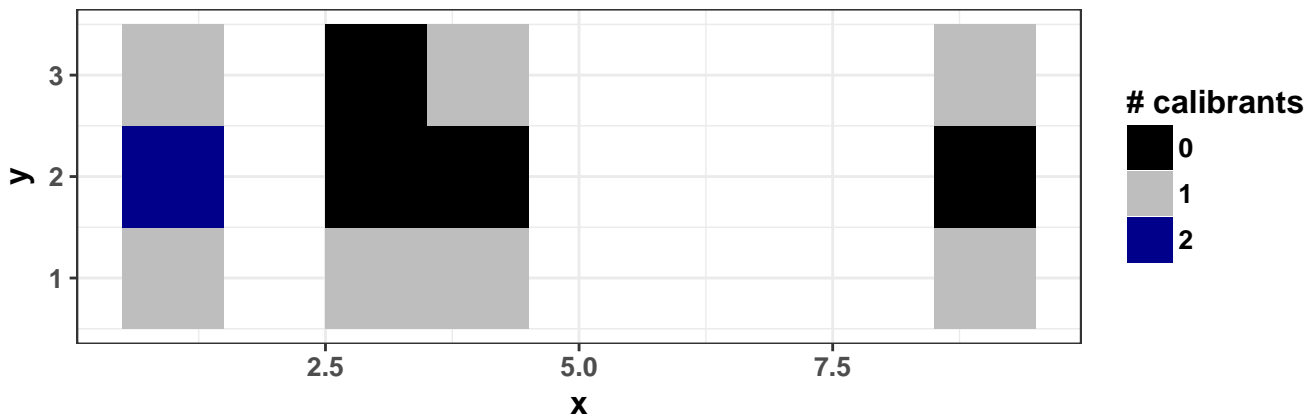
annotation

column1 column2 column3 column4

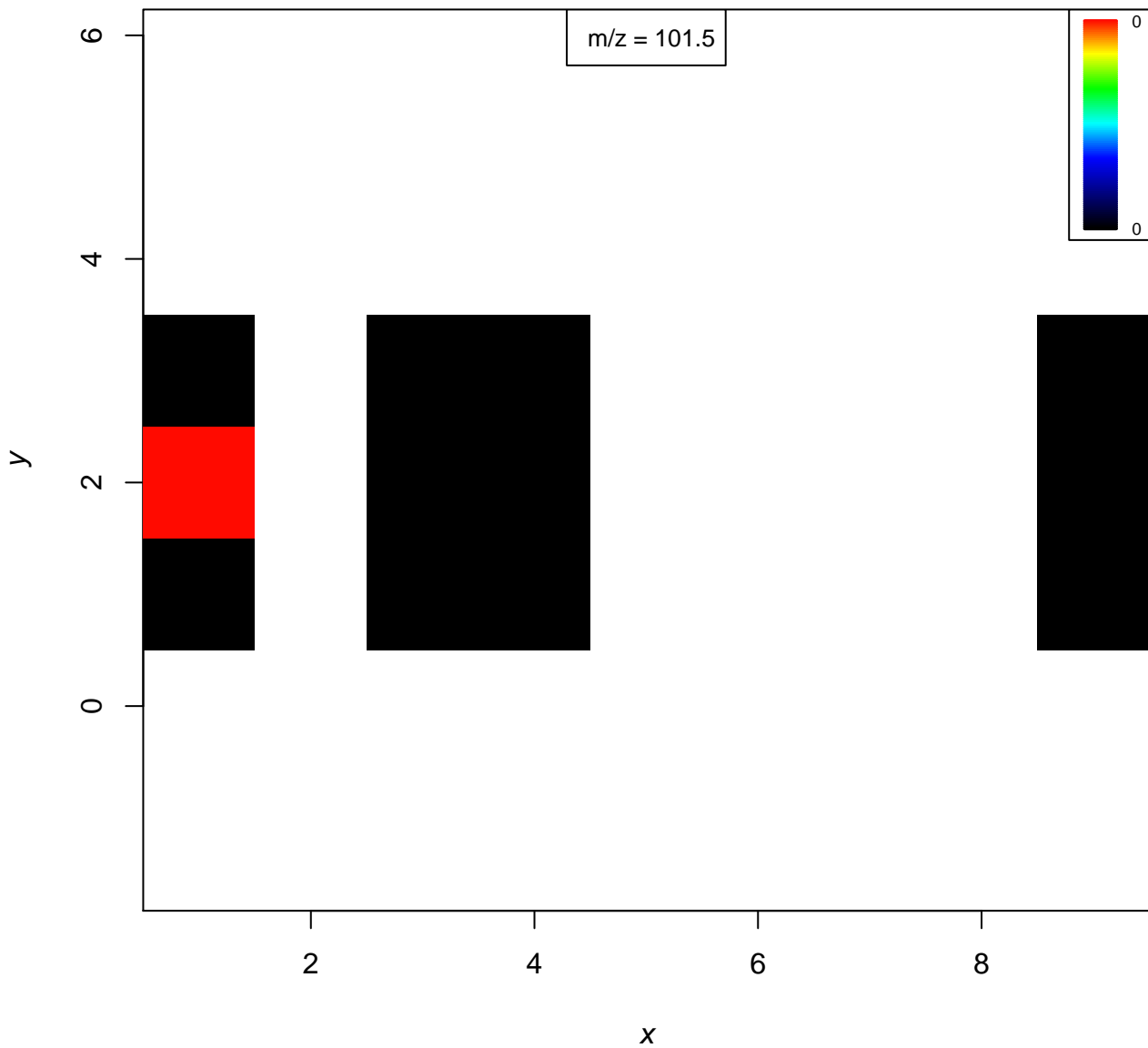
Pixel order



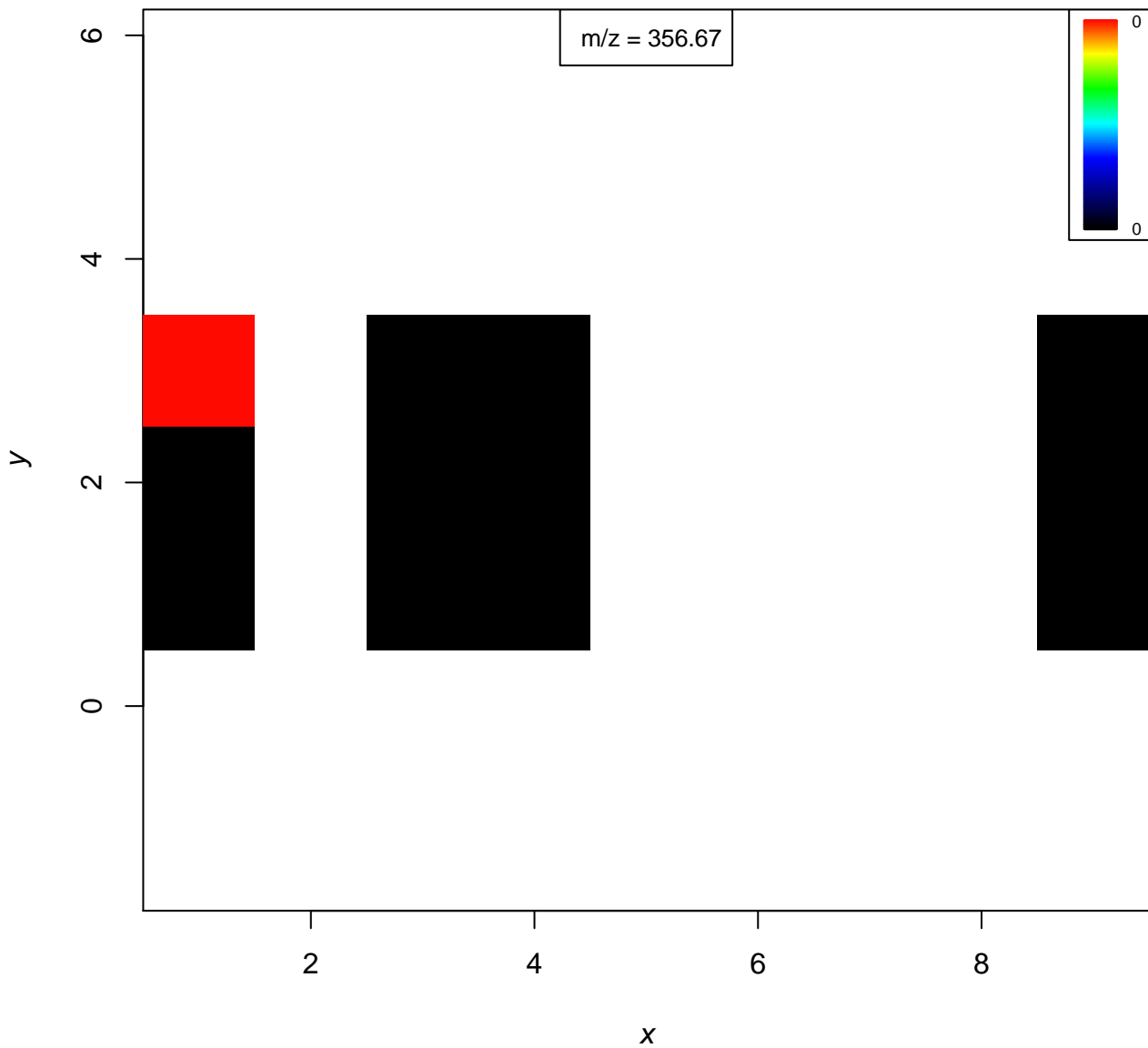
Number of calibrants per pixel (± 100 ppm)



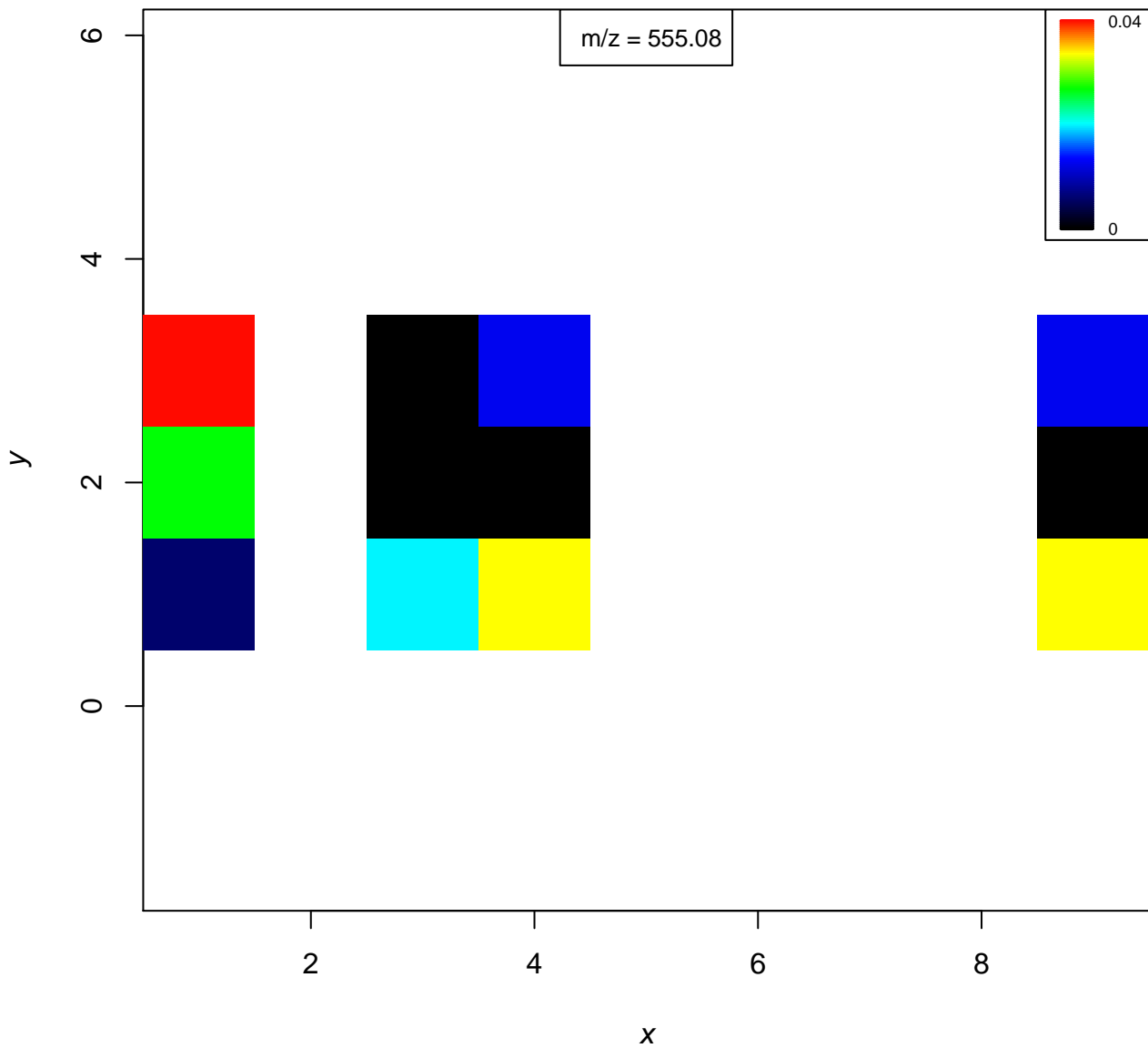
101.5: 101.5 (± 100 ppm)



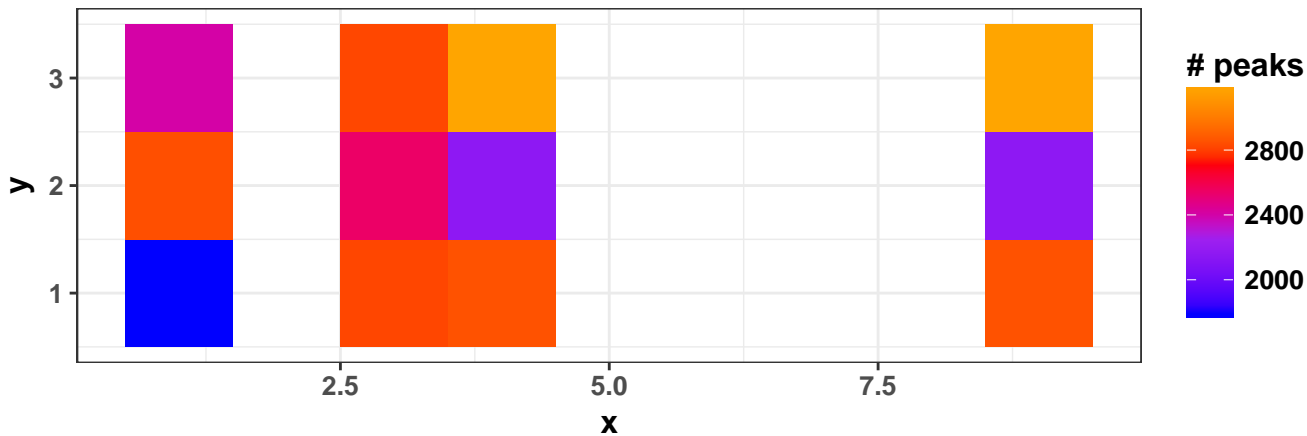
356.7: 356.7 (± 100 ppm)



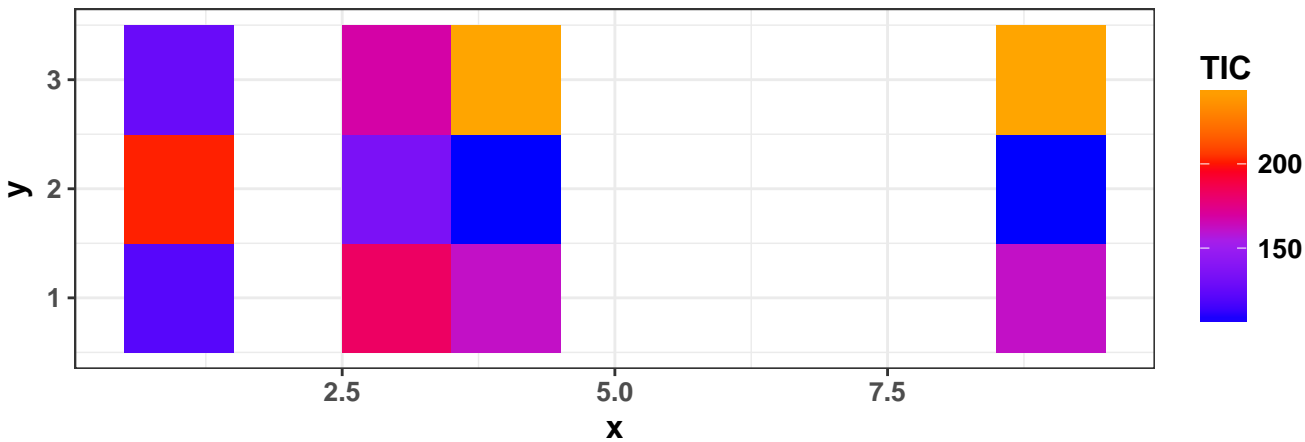
555.1: 555.1 (± 100 ppm)



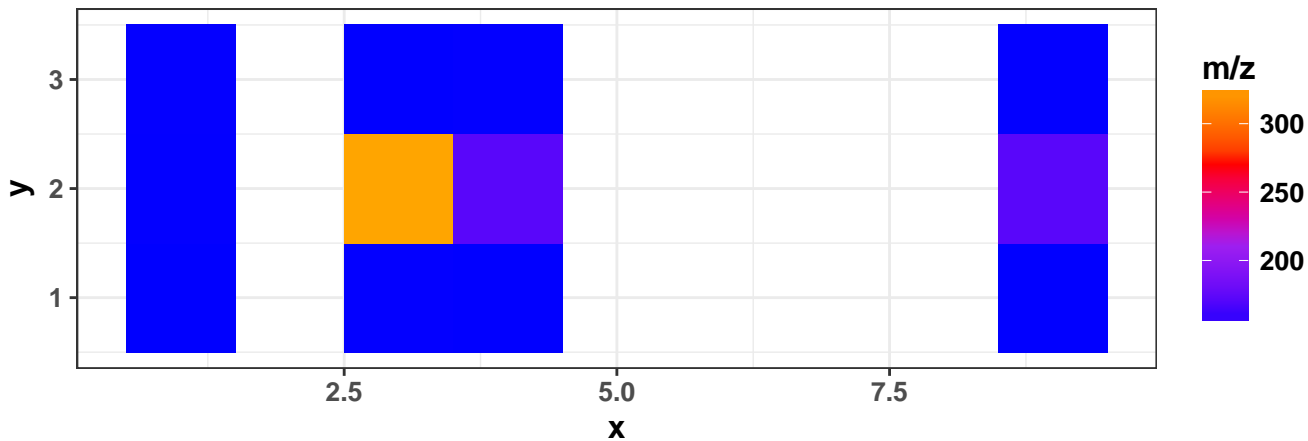
Number of peaks per spectrum



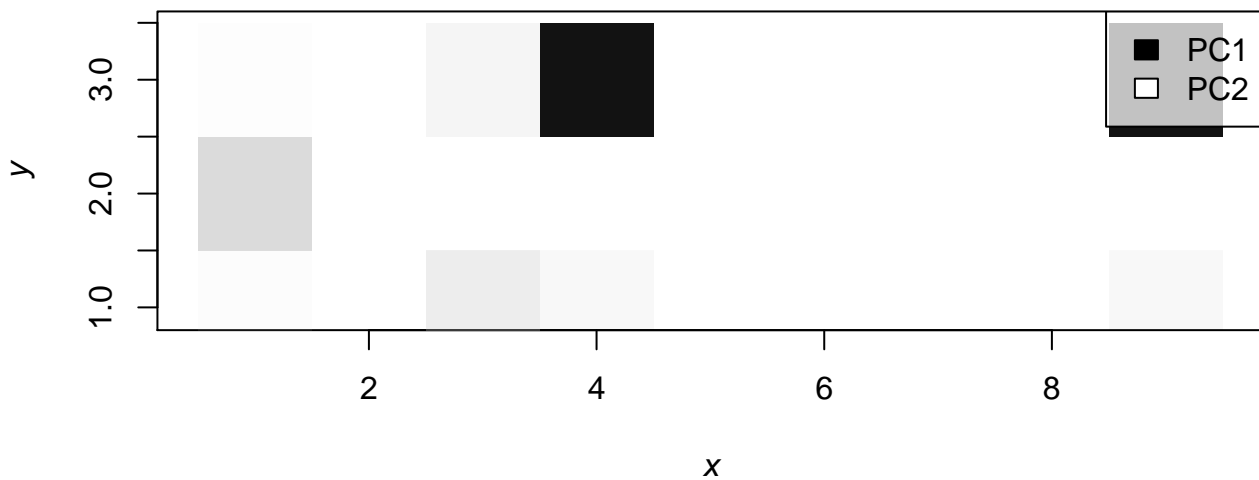
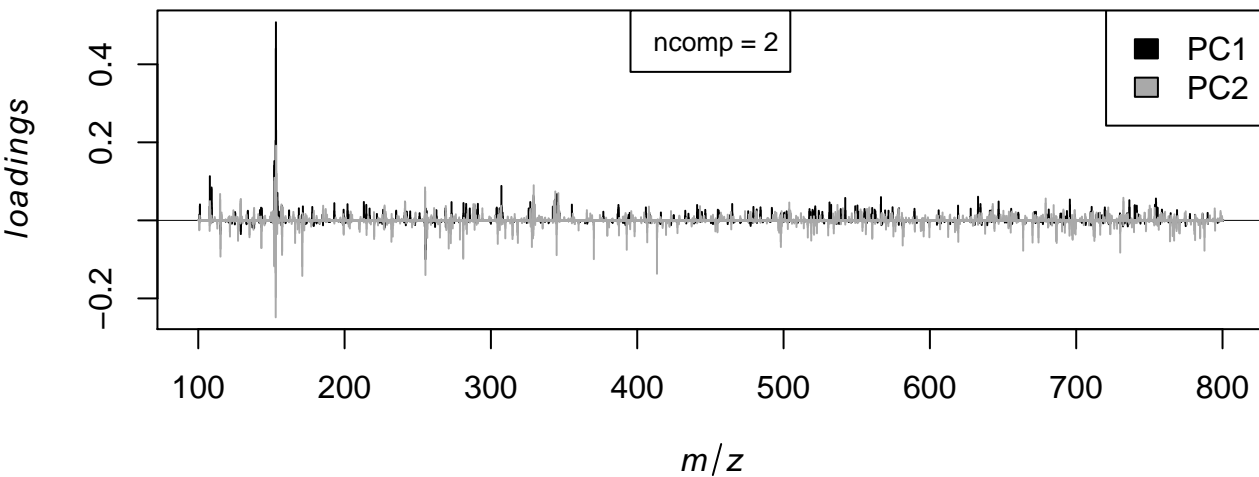
Total Ion Chromatogram



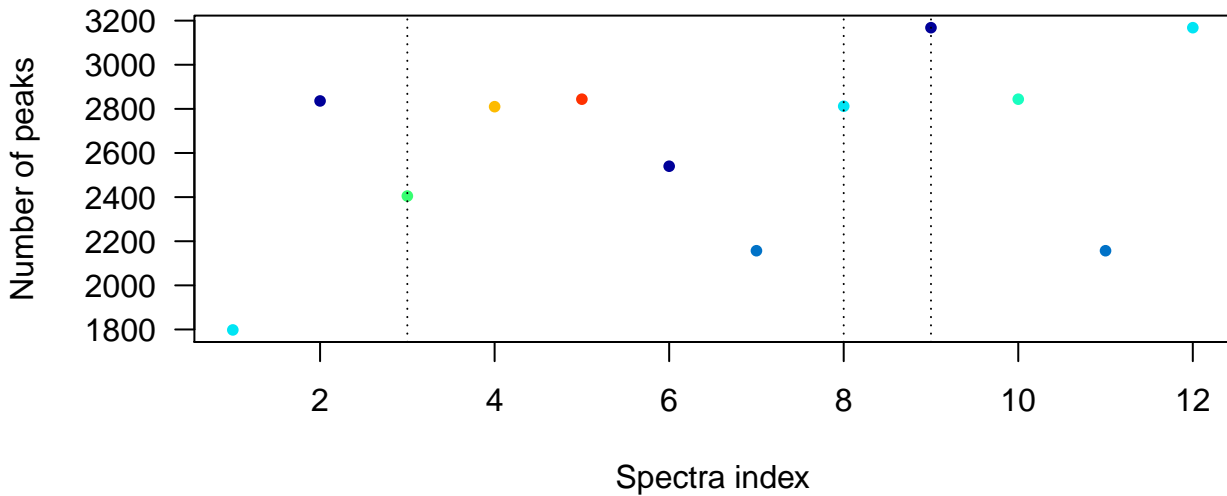
Most abundant m/z in each spectrum



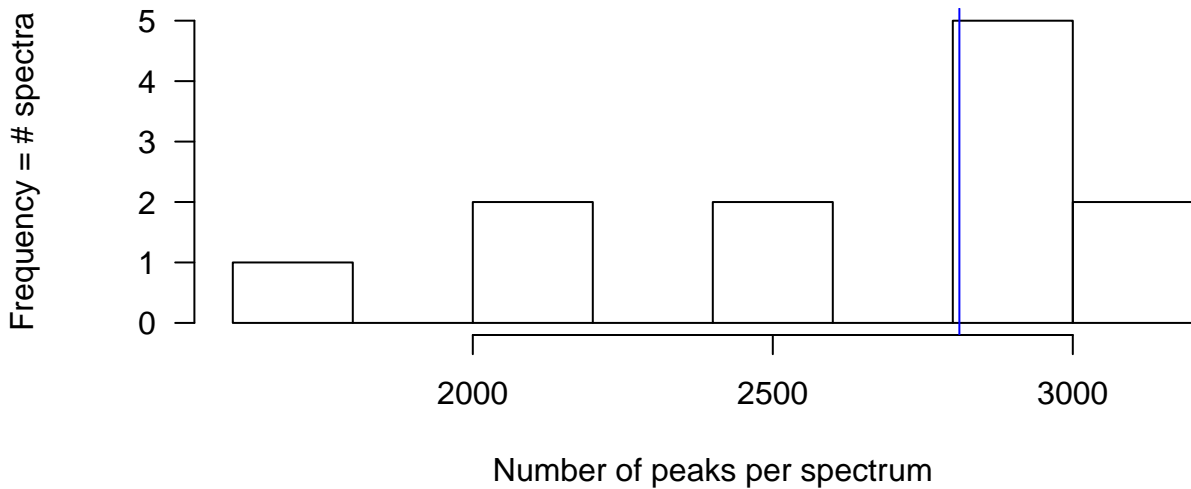
PCA for two components



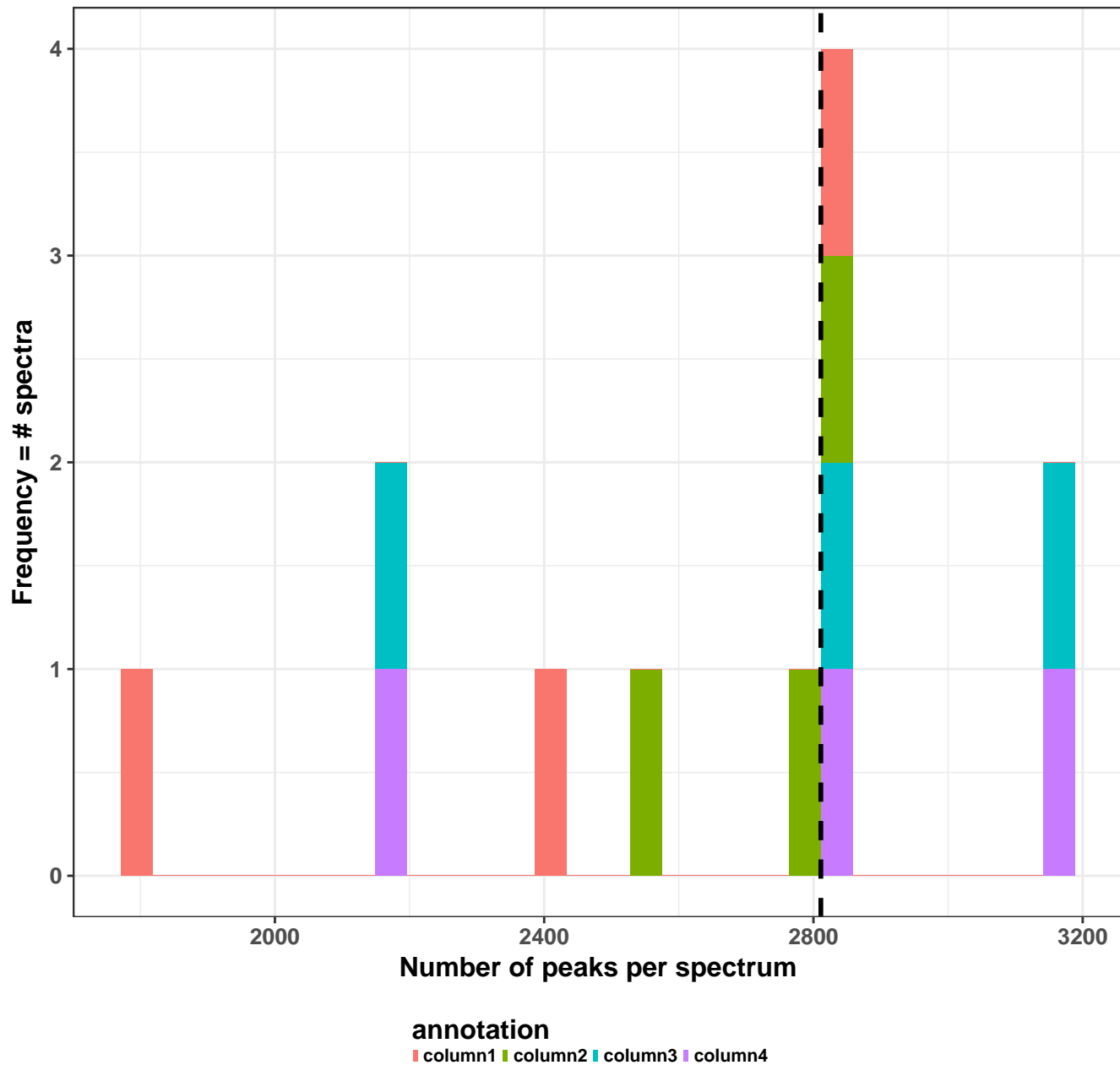
Number of peaks per spectrum



Number of peaks per spectrum

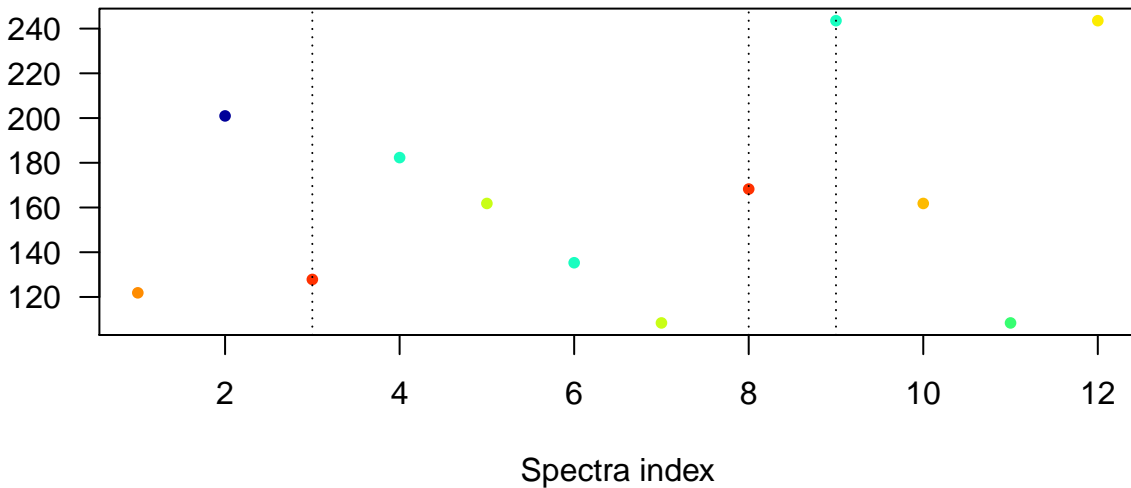


Number of peaks per spectrum and annotation group



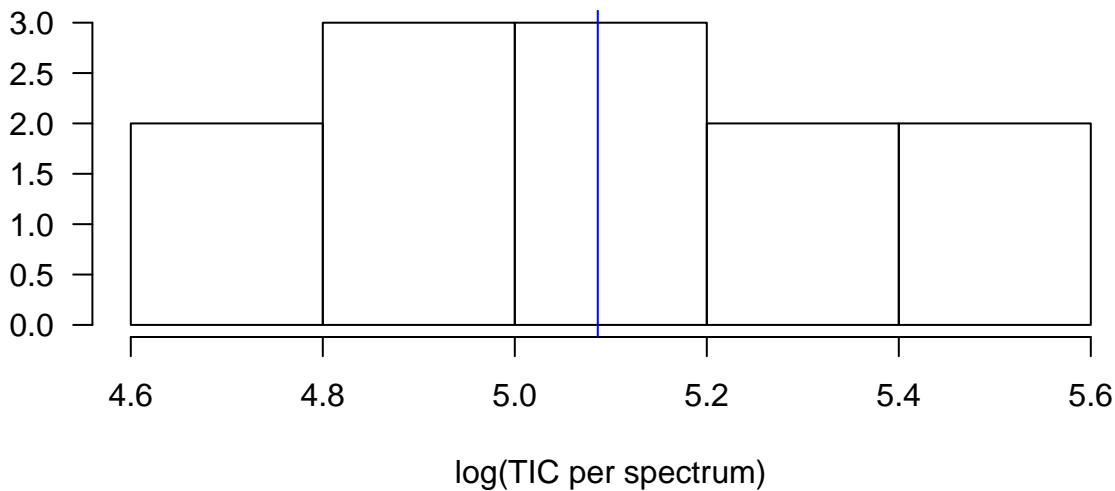
TIC per spectrum

Total ion chromatogram intensity

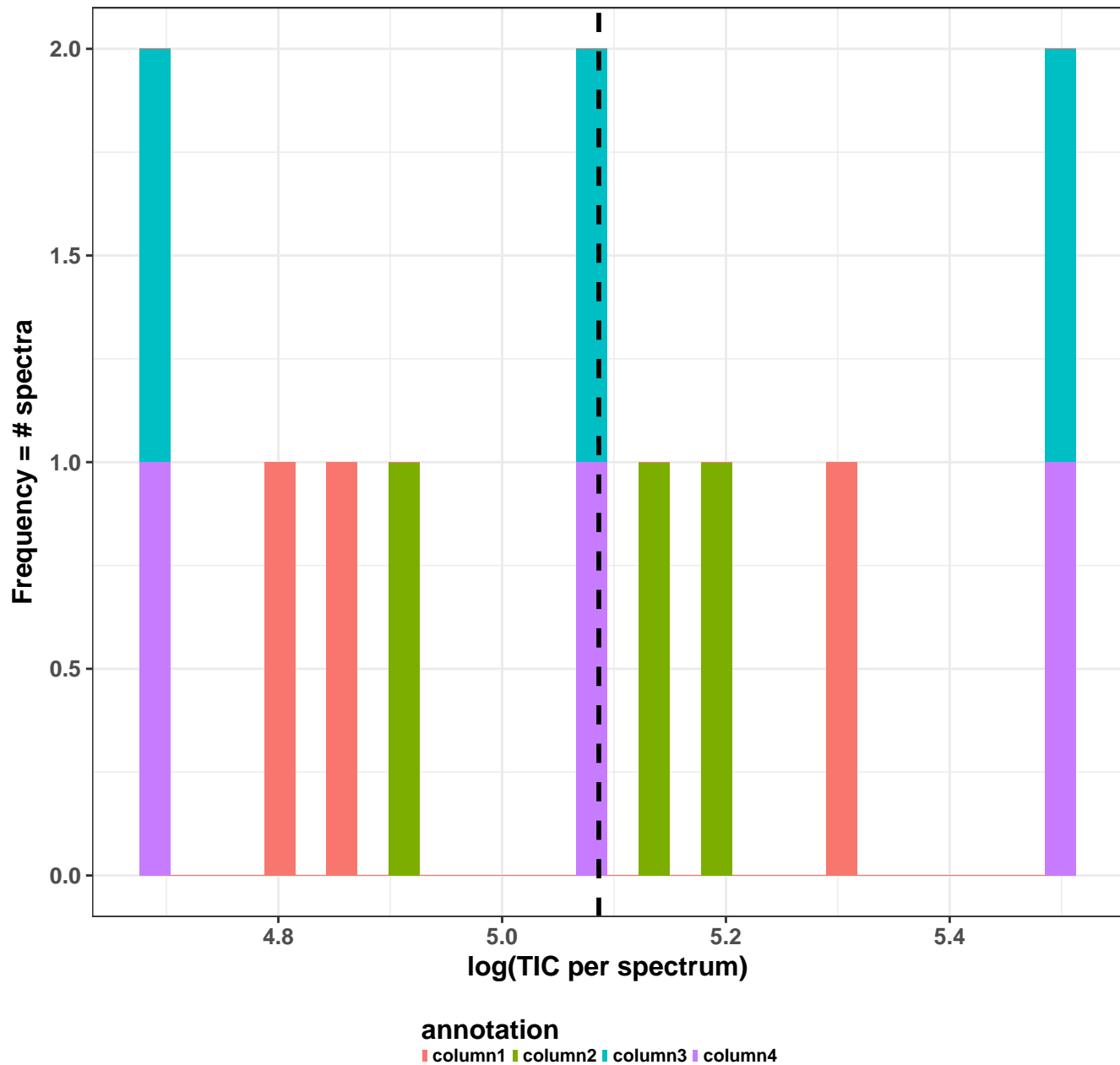


TIC per spectrum

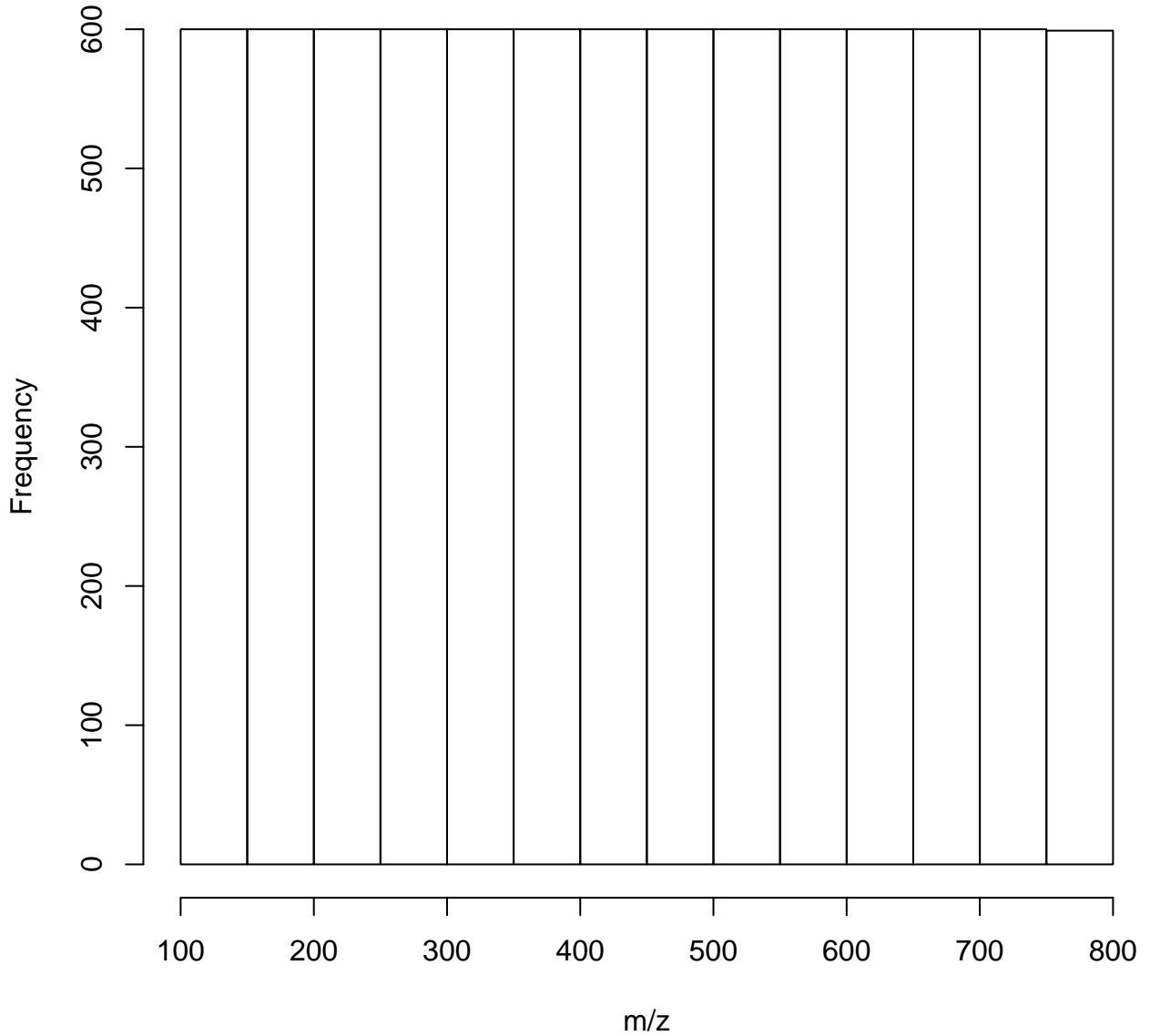
Frequency = # spectra



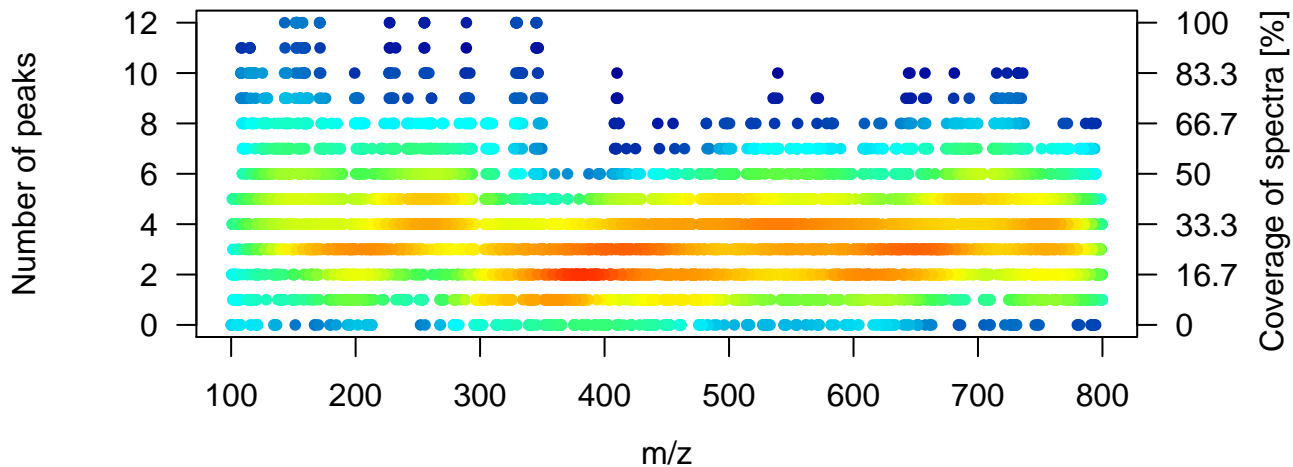
TIC per spectrum and annotation group



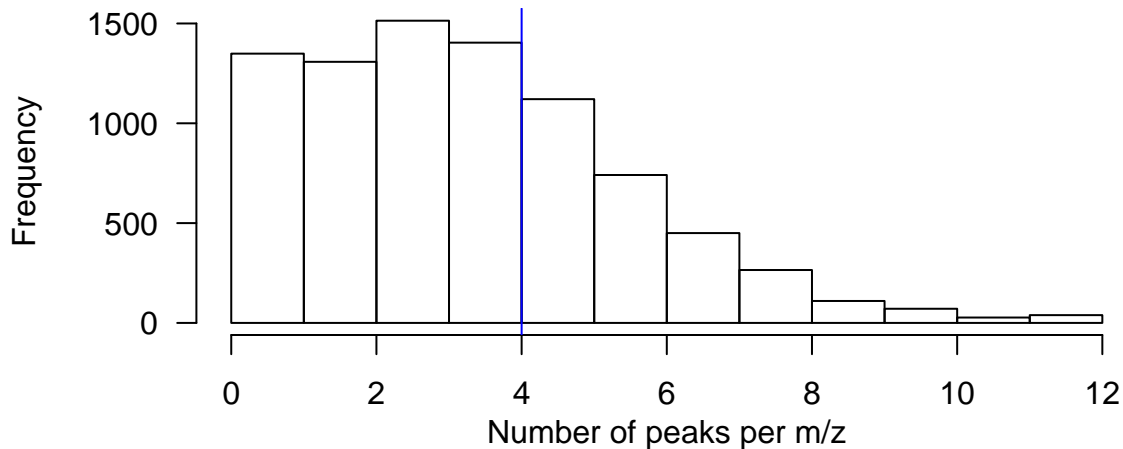
Histogram of m/z values



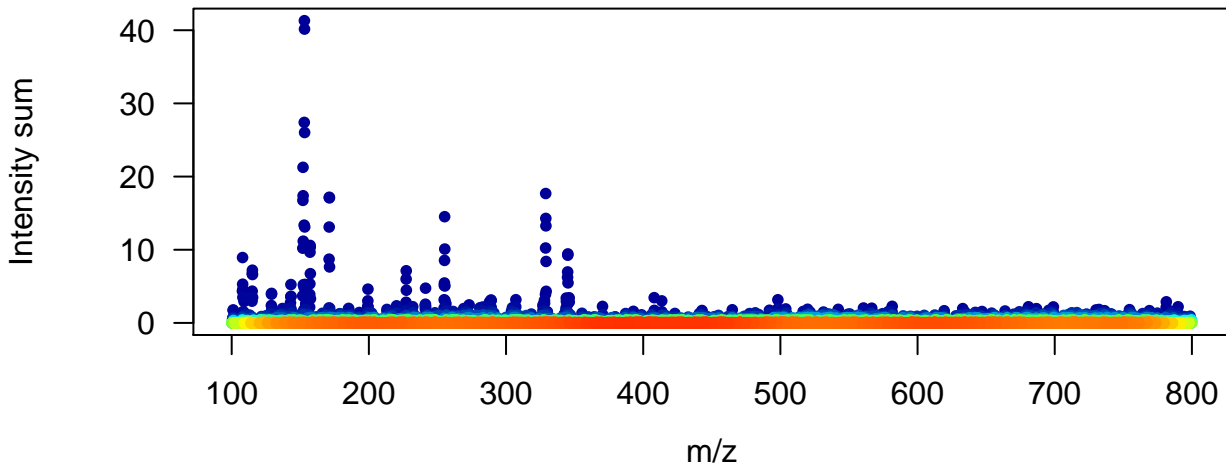
Number of peaks per m/z



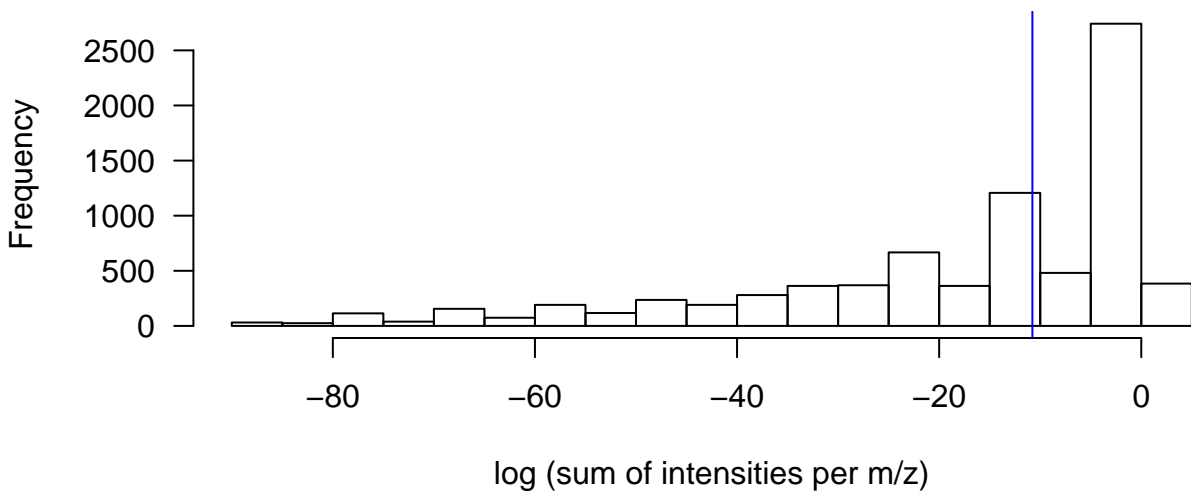
Number of peaks per m/z



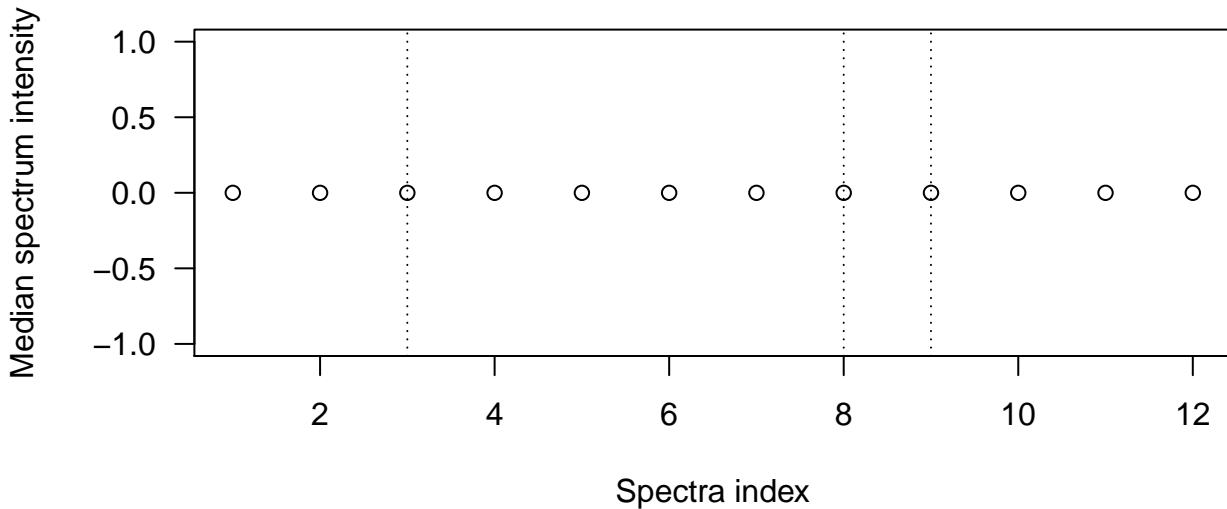
Sum of intensities per m/z



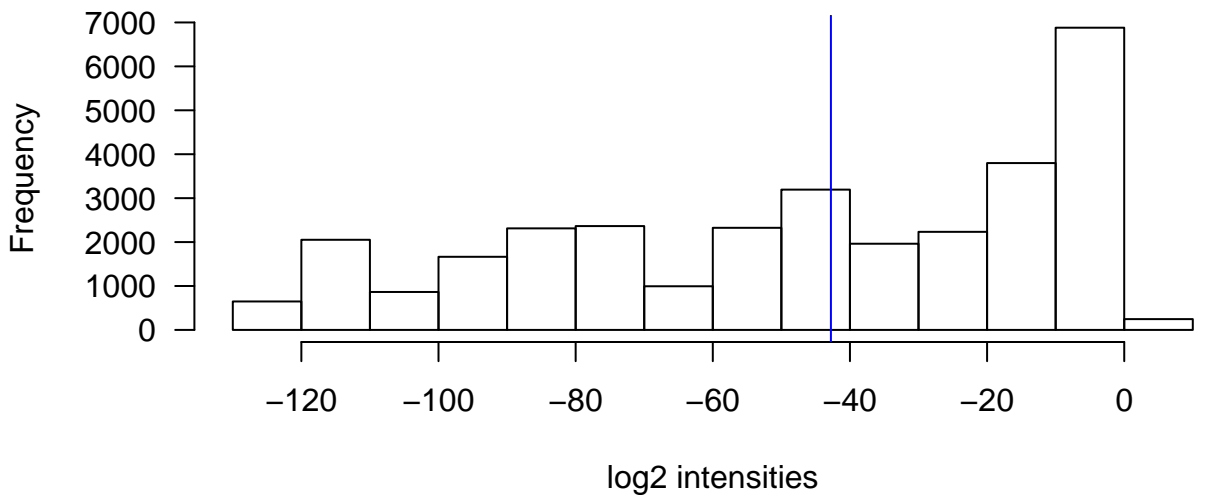
Sum of intensities per m/z



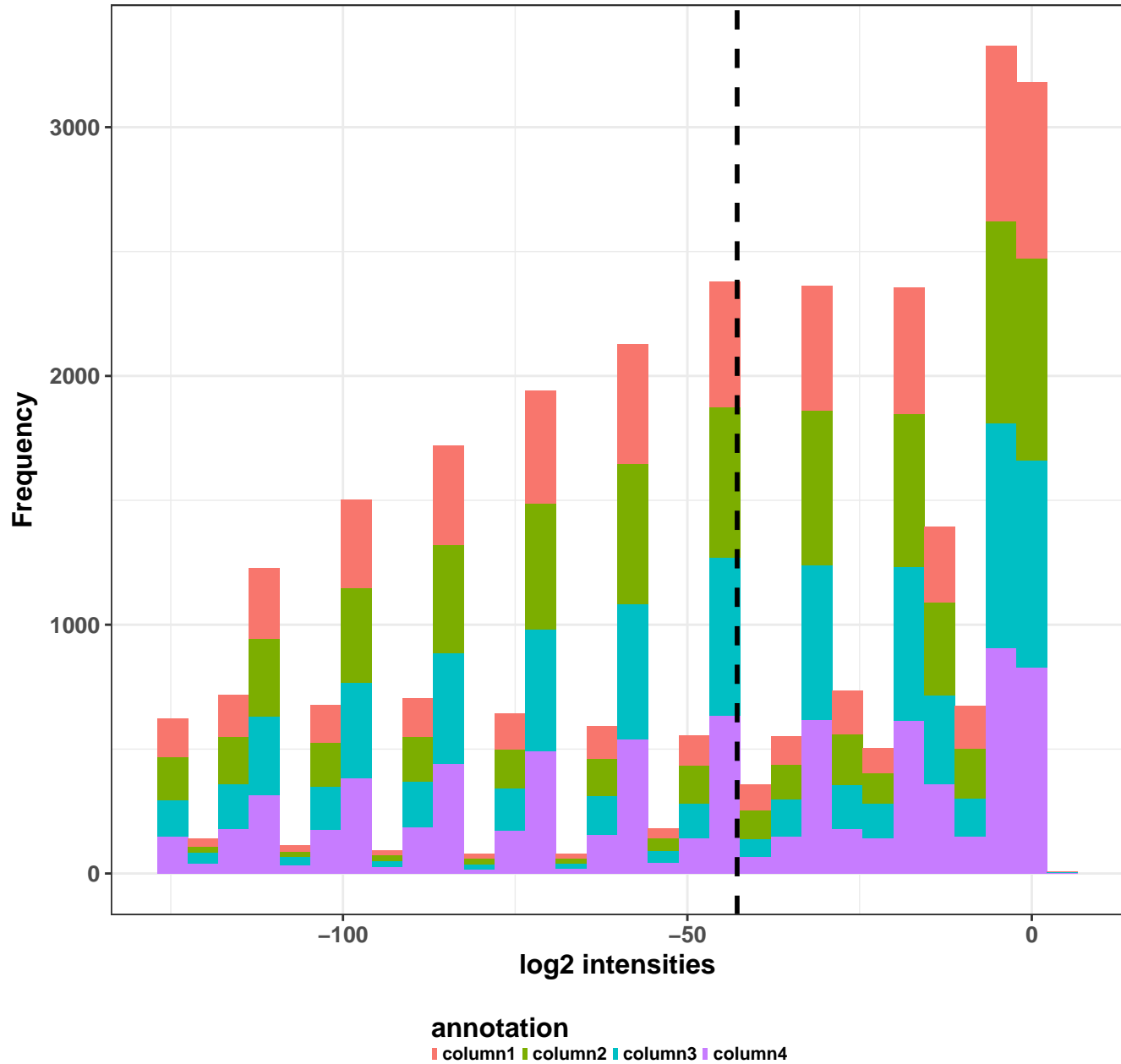
Median intensity per spectrum



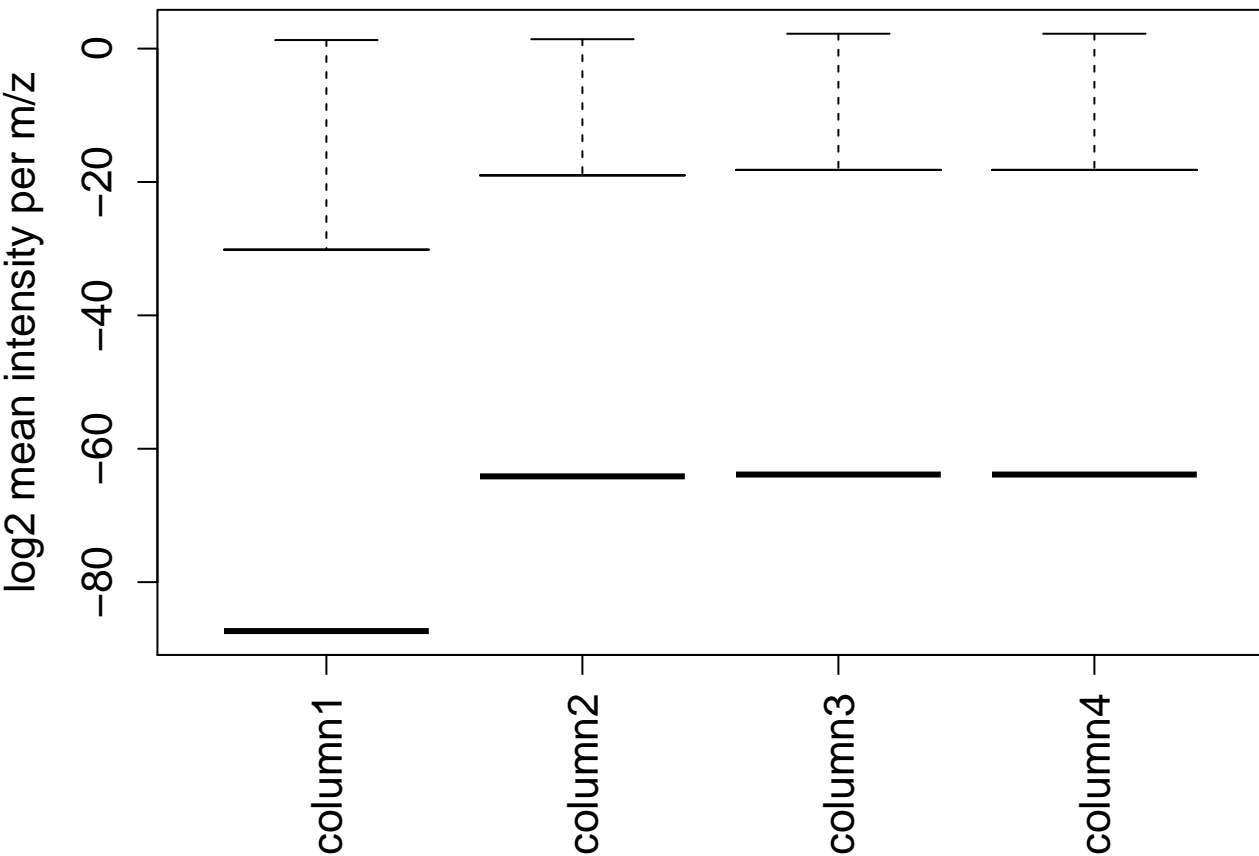
Log2-transformed intensities



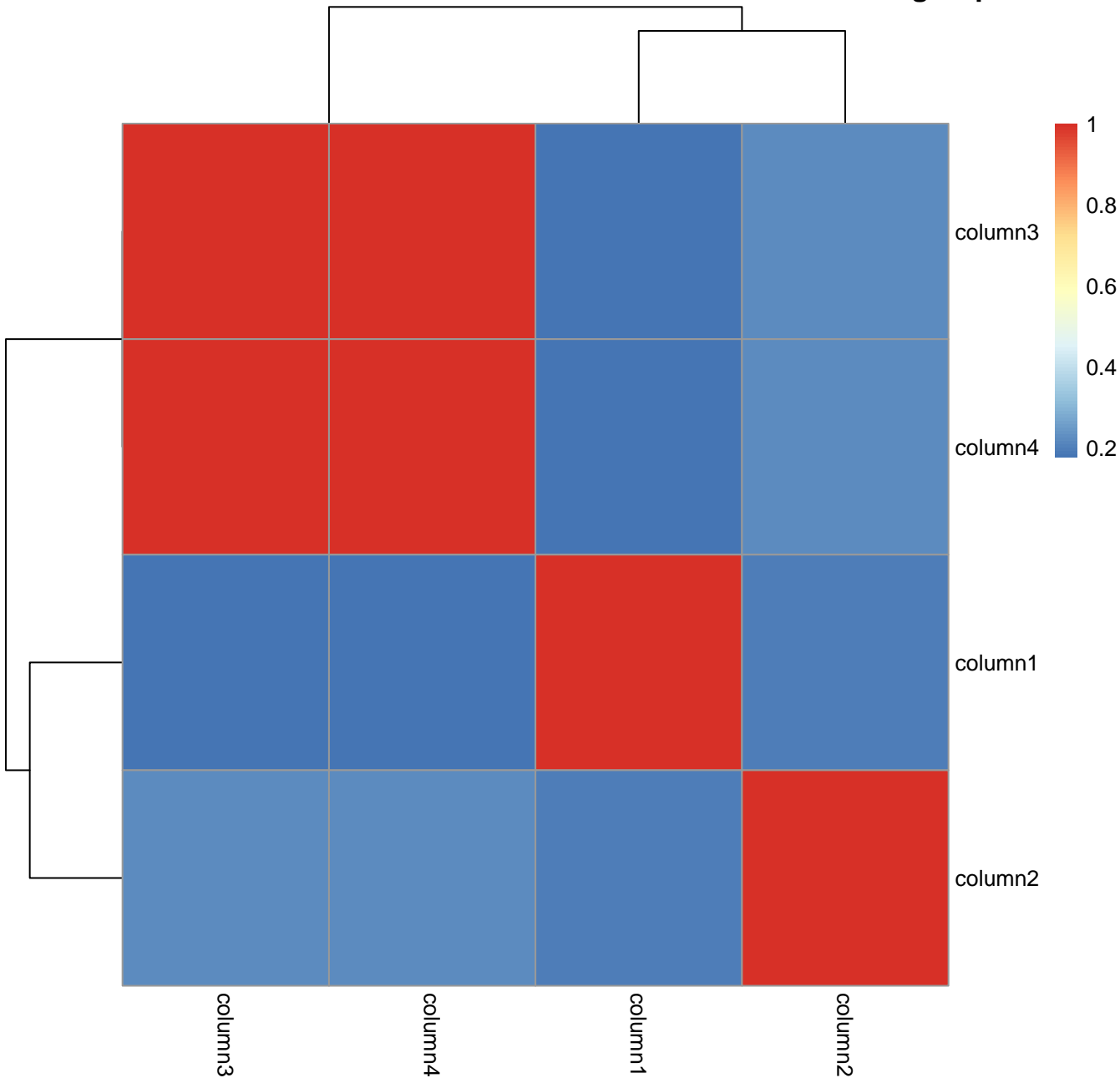
Log2-transformed intensities per sample



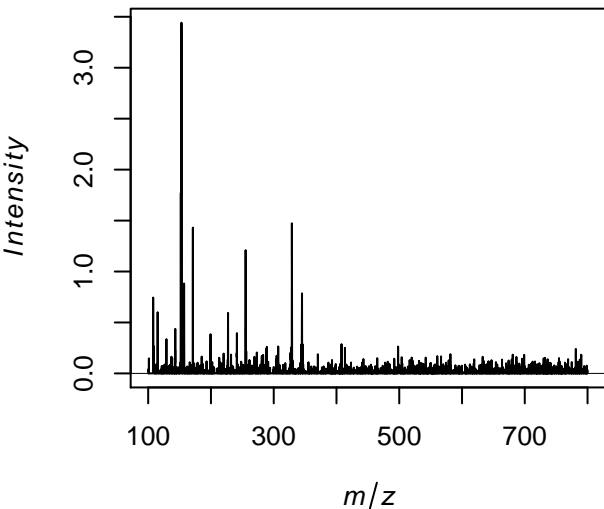
Mean m/z intensities per annotation group



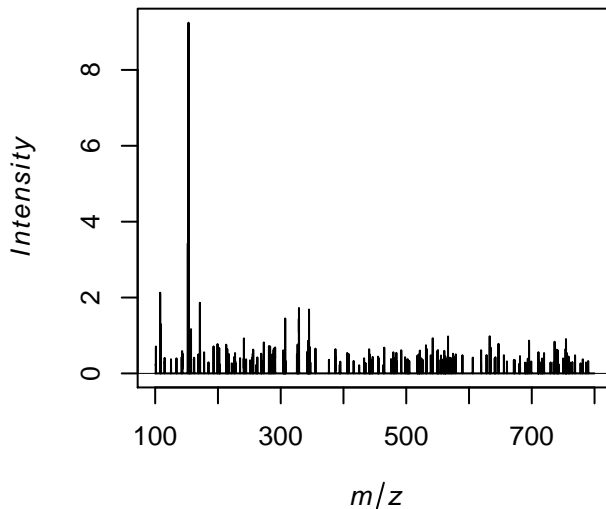
Pearson correlation on mean intensities for each annotation group



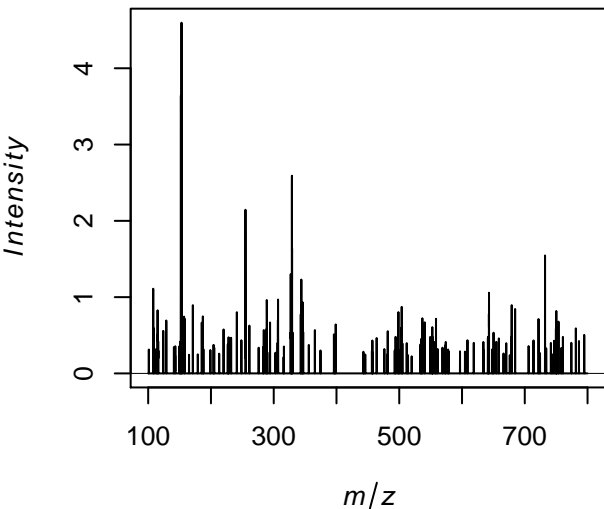
Average spectrum



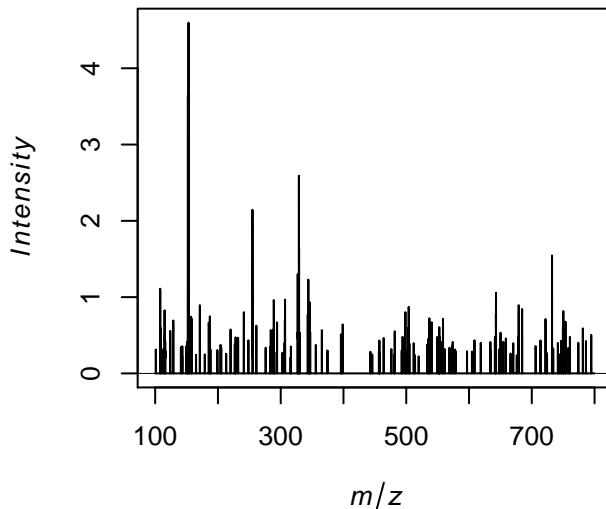
Spectrum at x = 4, y = 3



Spectrum at x = 1, y = 2



Spectrum at x = 1, y = 2

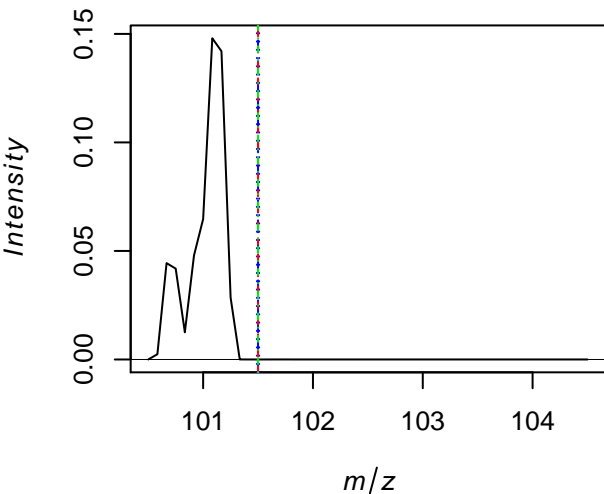


theor. m/z: 101.5

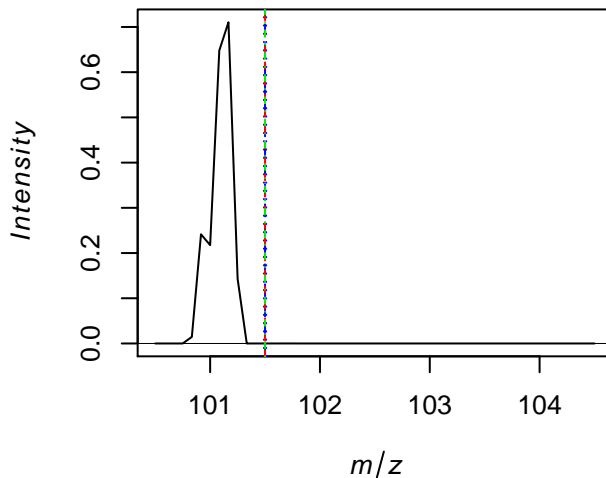
most abundant m/z: 101.5

closest m/z: 101.5

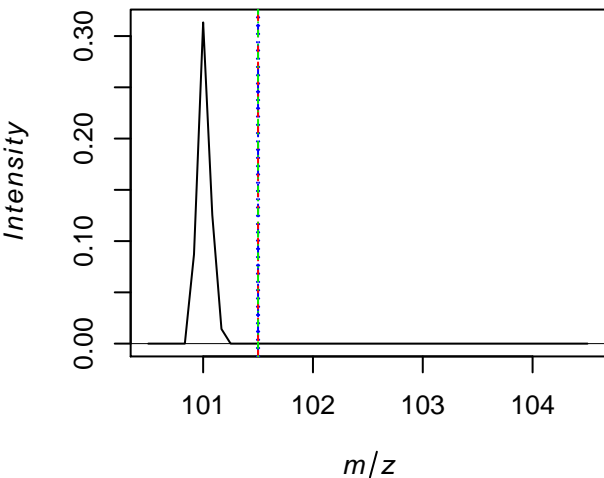
Average spectrum



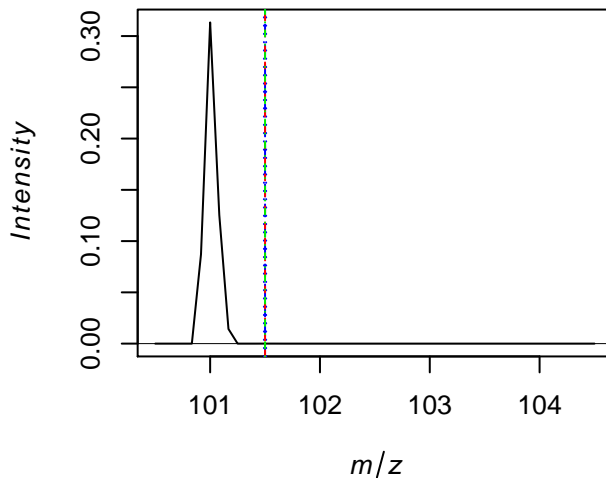
Spectrum at x = 4, y = 3



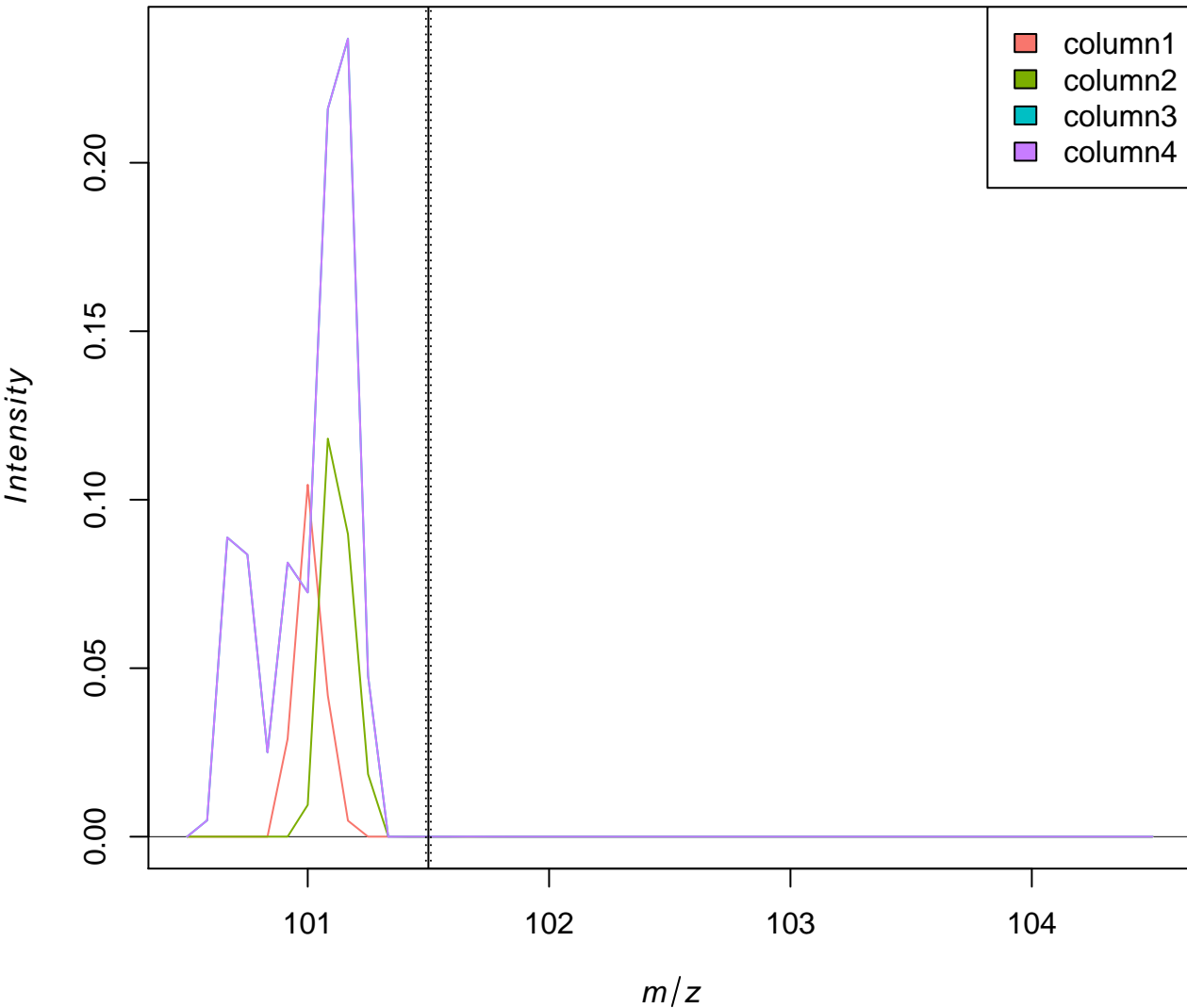
Spectrum at x = 1, y = 2



Spectrum at x = 1, y = 2



Average spectrum per annotation group

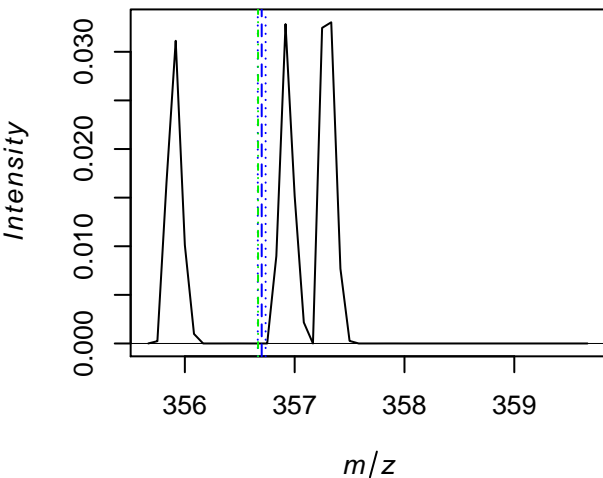


theor. m/z: 356.7

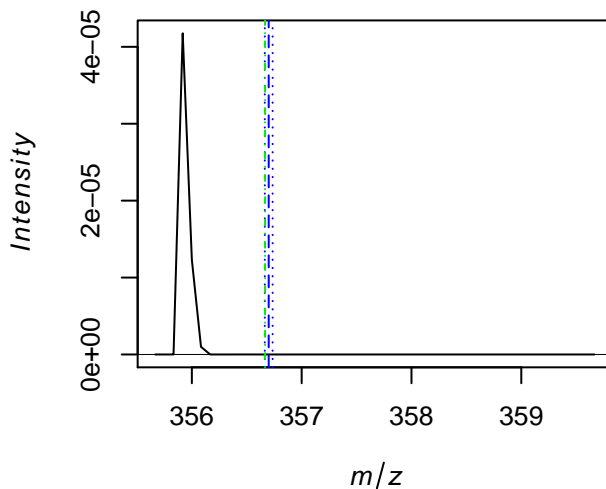
most abundant m/z: NA

closest m/z: 356.6667

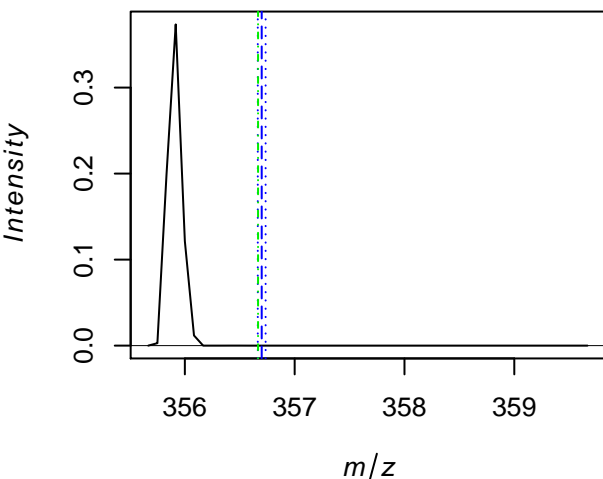
Average spectrum



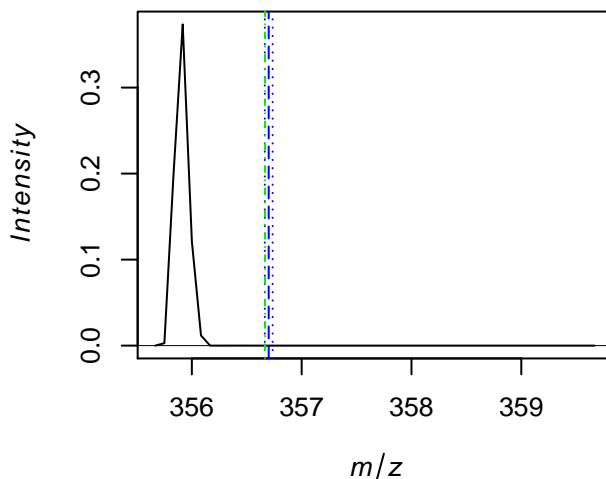
Spectrum at x = 4, y = 3



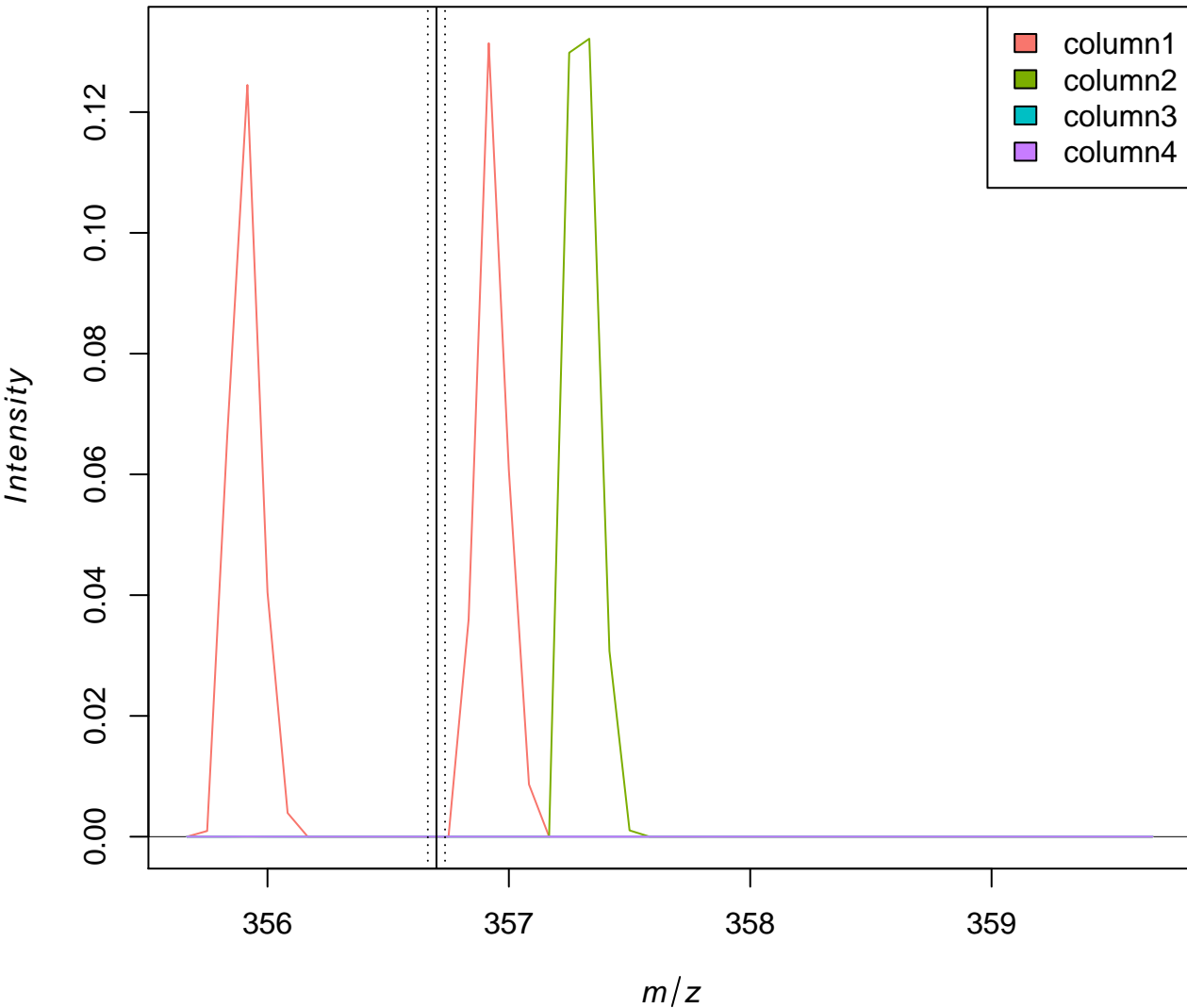
Spectrum at x = 1, y = 2



Spectrum at x = 1, y = 2



Average spectrum per annotation group

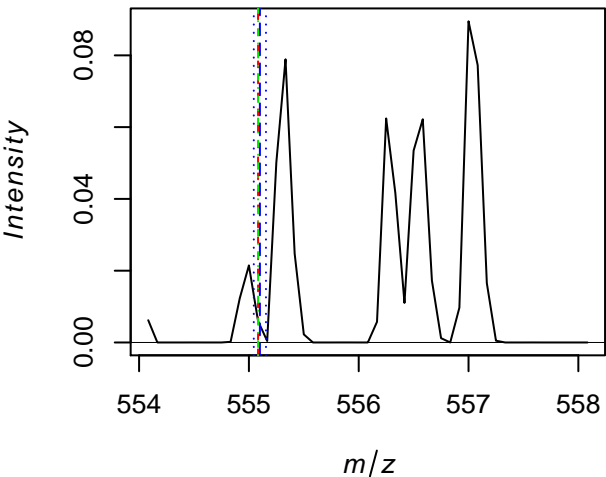


theor. m/z: 555.1

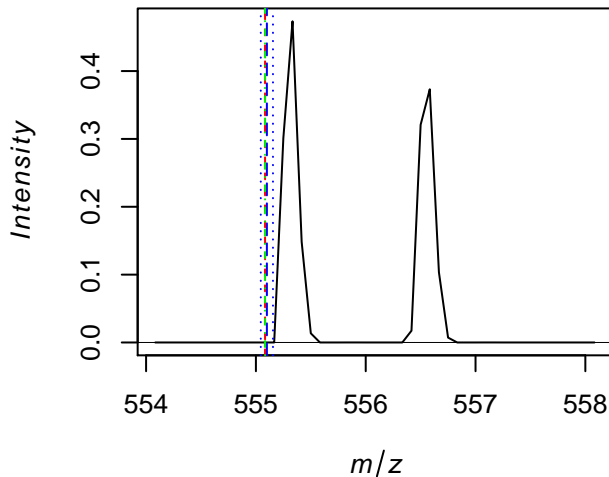
most abundant m/z: 555.0834

closest m/z: 555.0834

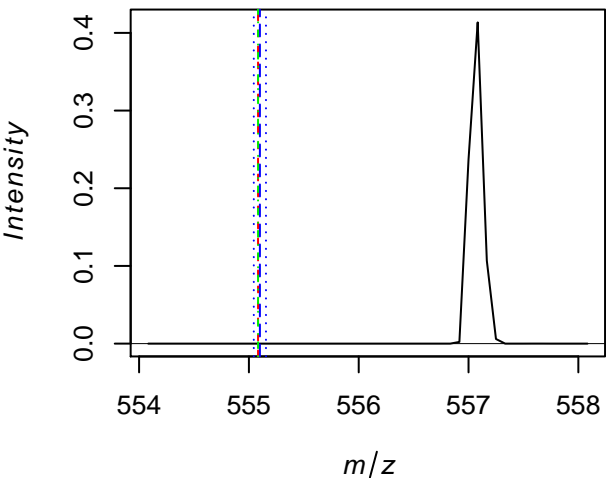
Average spectrum



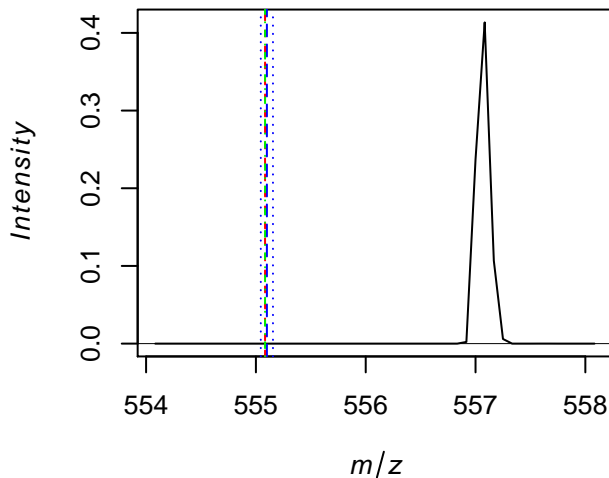
Spectrum at x = 4, y = 3



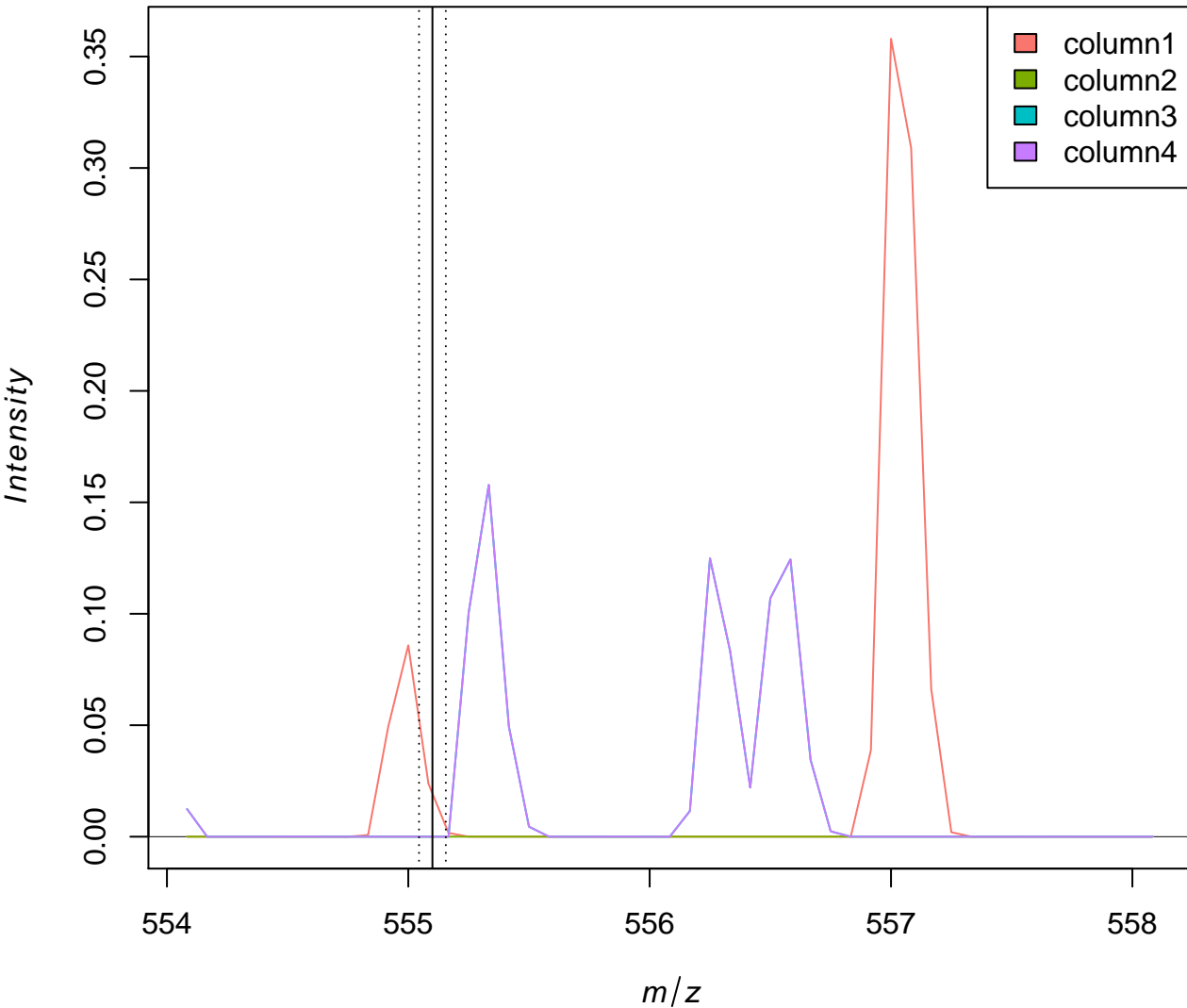
Spectrum at x = 1, y = 2



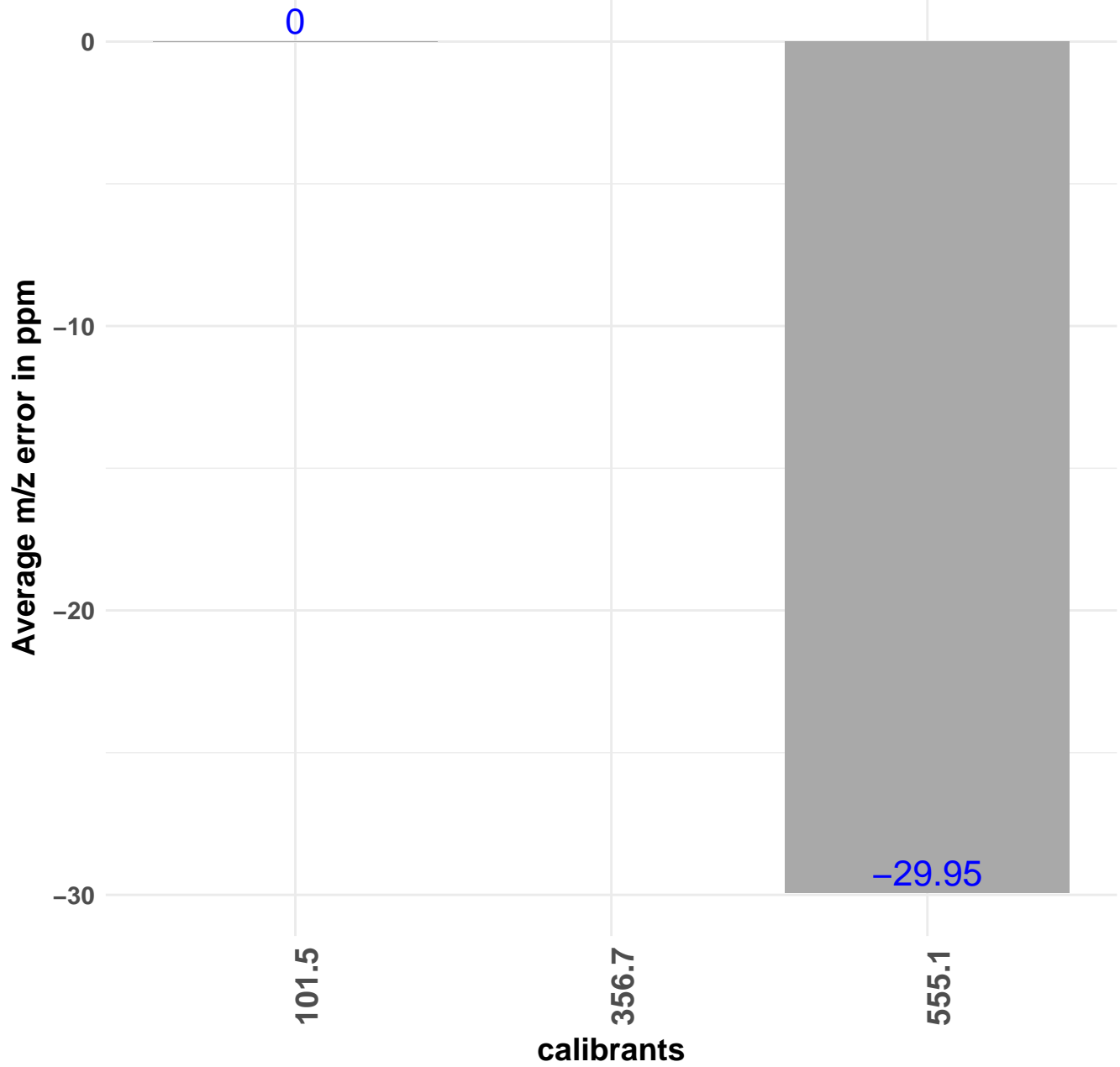
Spectrum at x = 1, y = 2



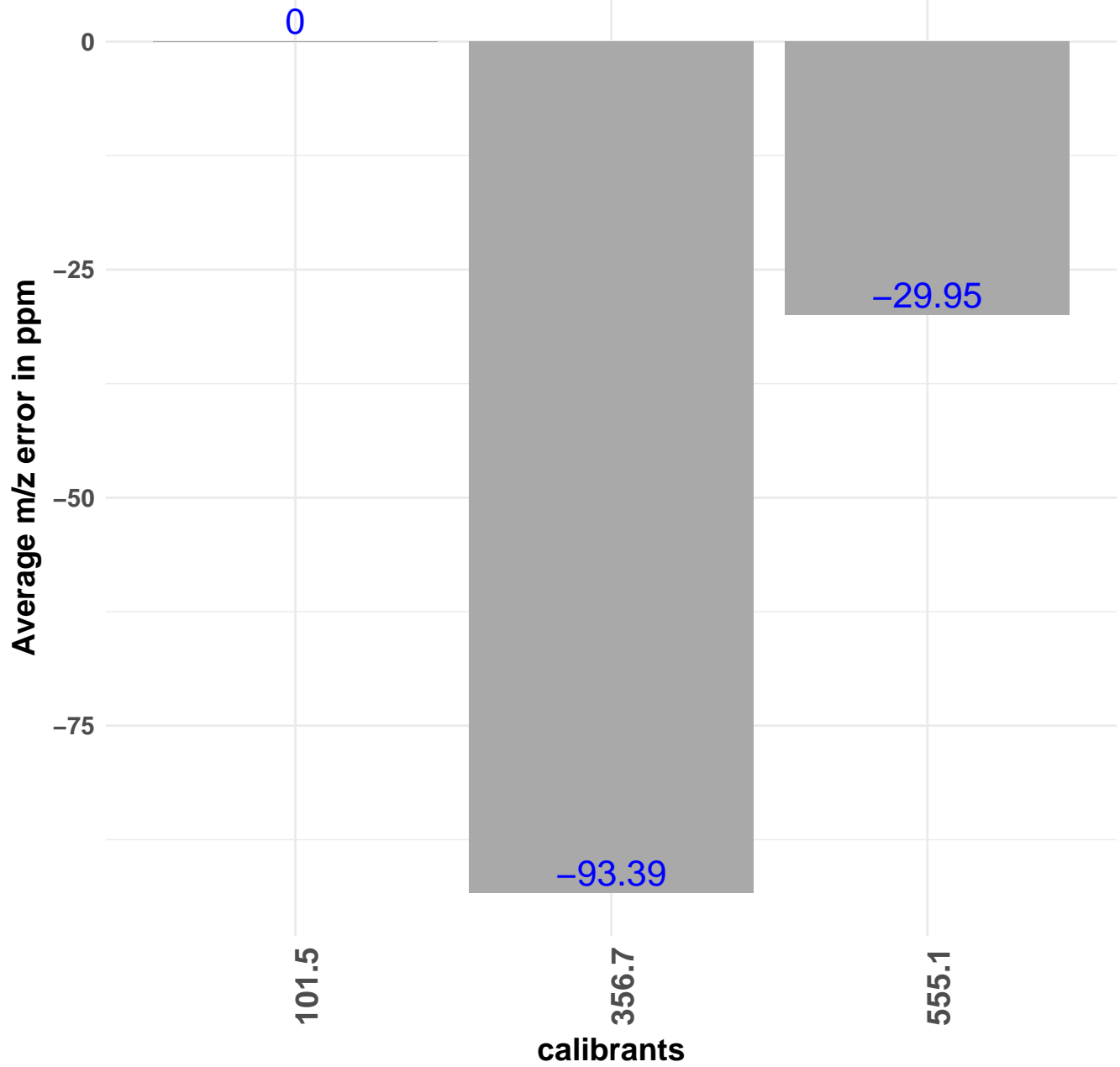
Average spectrum per annotation group



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)

