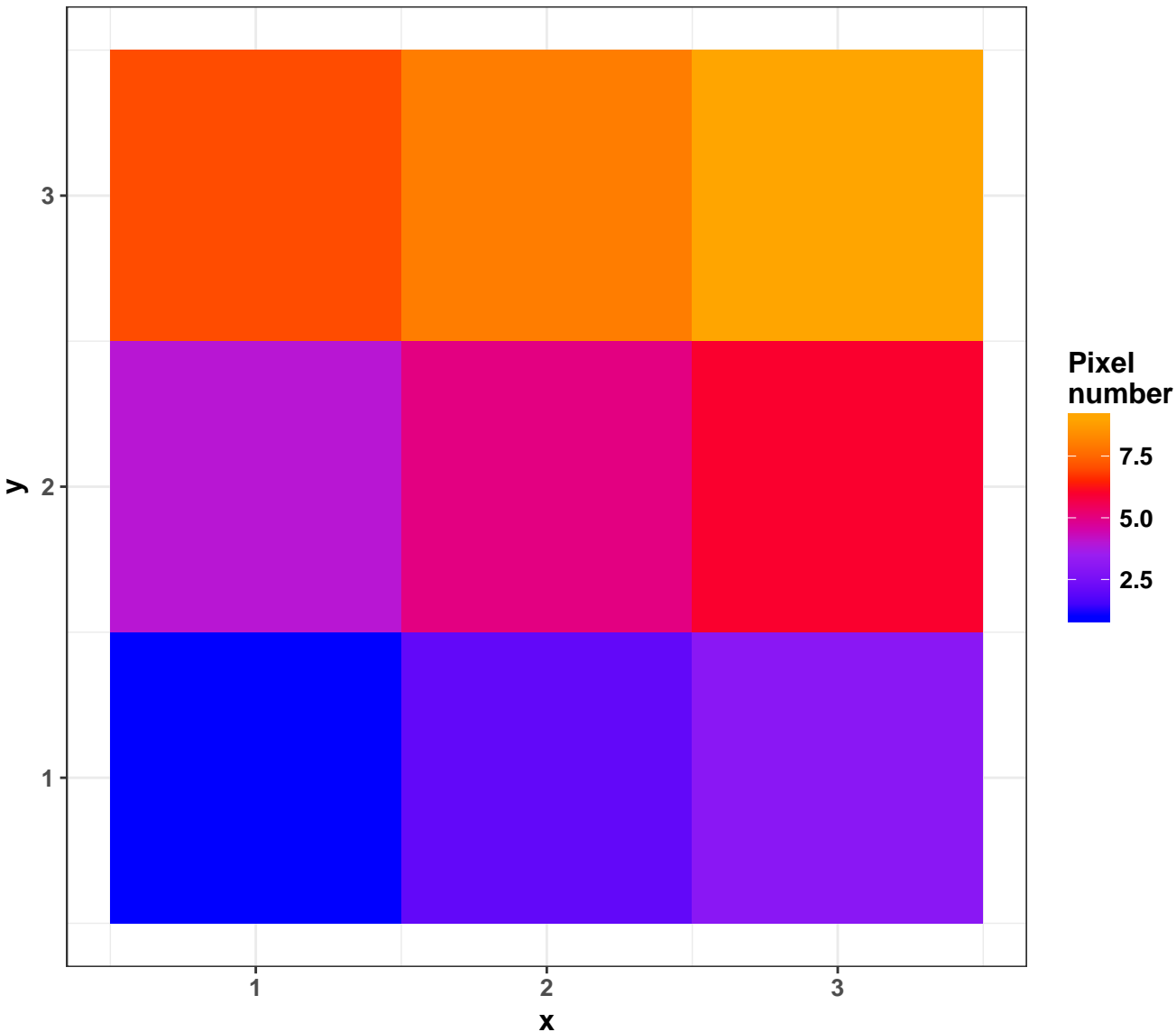


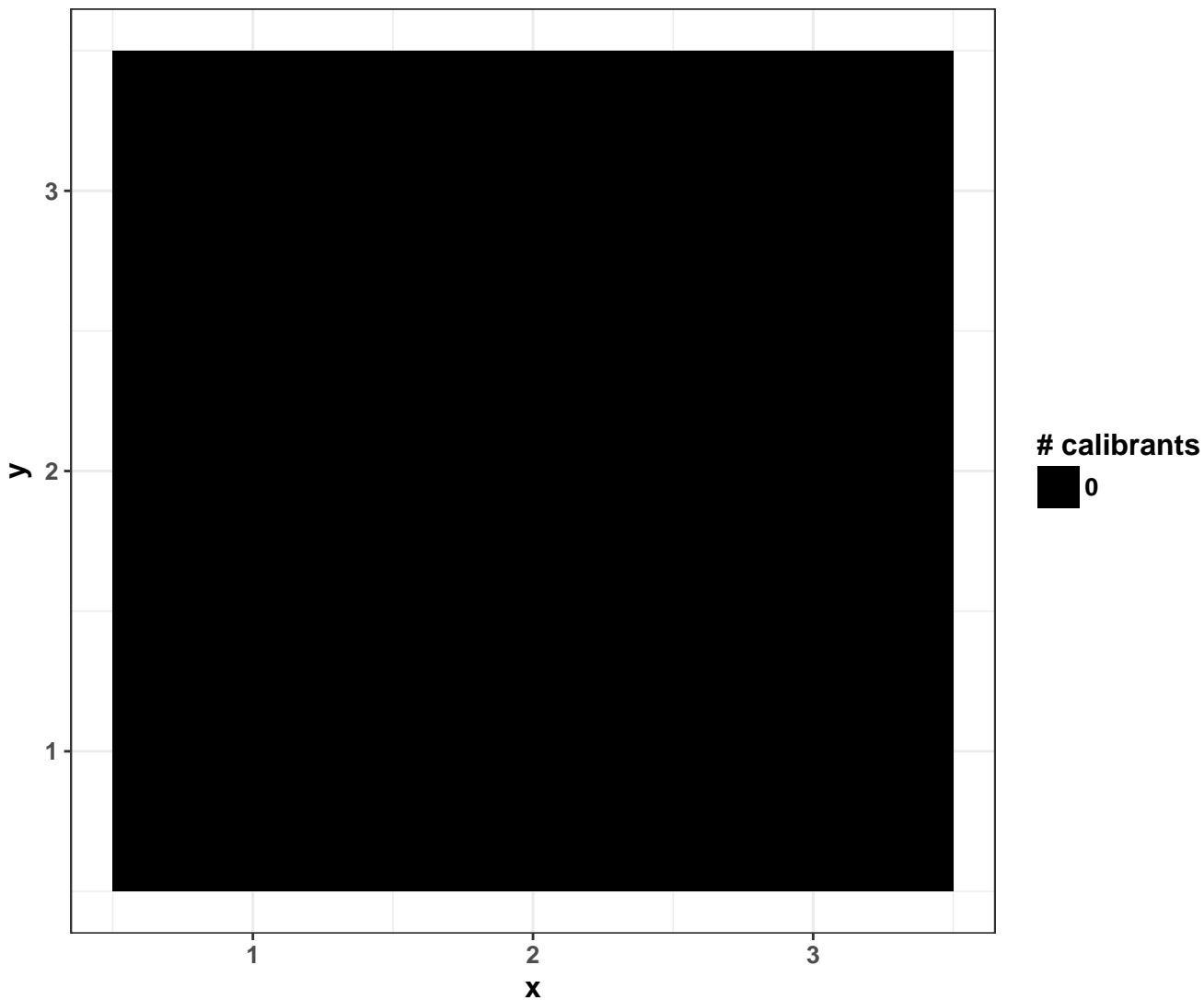
Testfile_imzml

properties	values
Number of m/z features	1199
Range of m/z values	300.08 – 399.92
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	0 – 2.59
Median of intensities	0
Intensities > 0	26.17 %
Number of empty spectra	0
Median TIC \pm sd	24.4 \pm 9
Median # peaks per spectrum \pm sd	323 \pm 65
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.txt	1 / 3

Pixel order

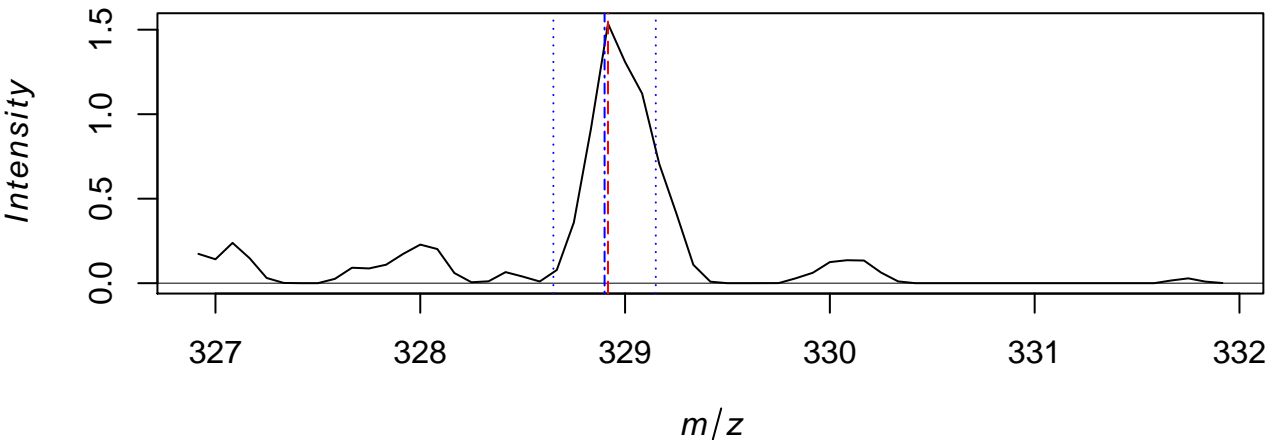


Number of calibrants per pixel (± 100 ppm)

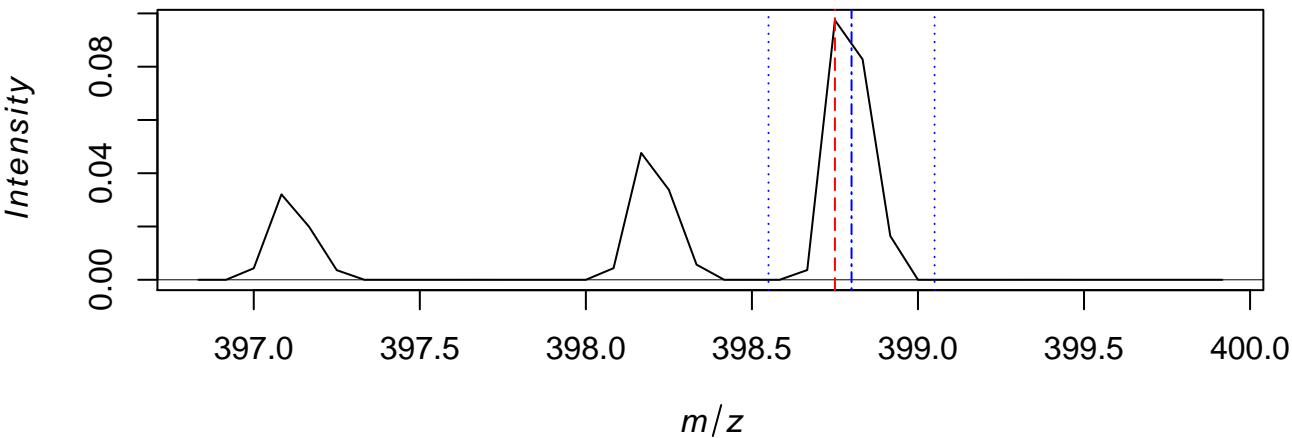


Control of fold change plot

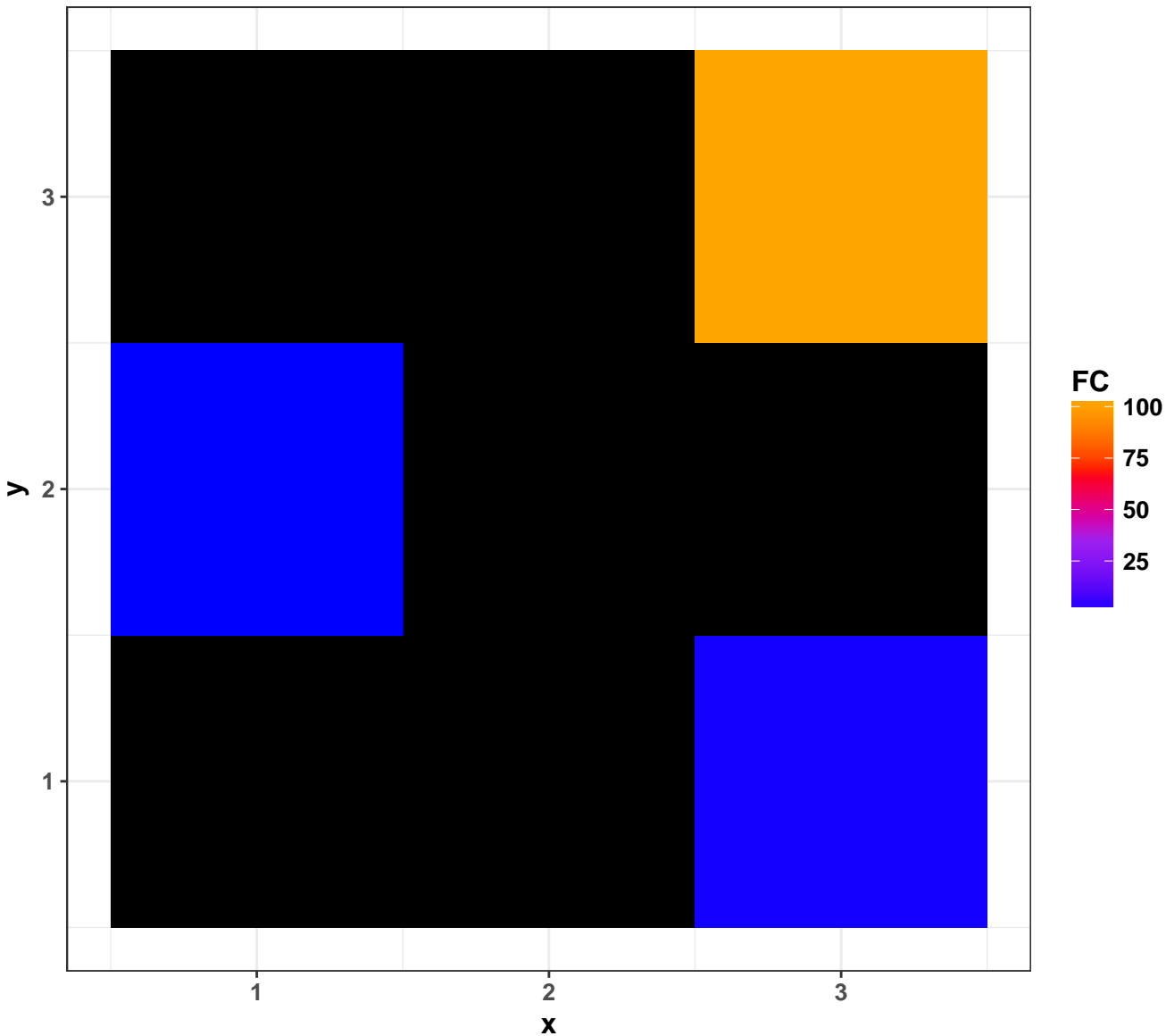
Average spectrum 328.9 Da



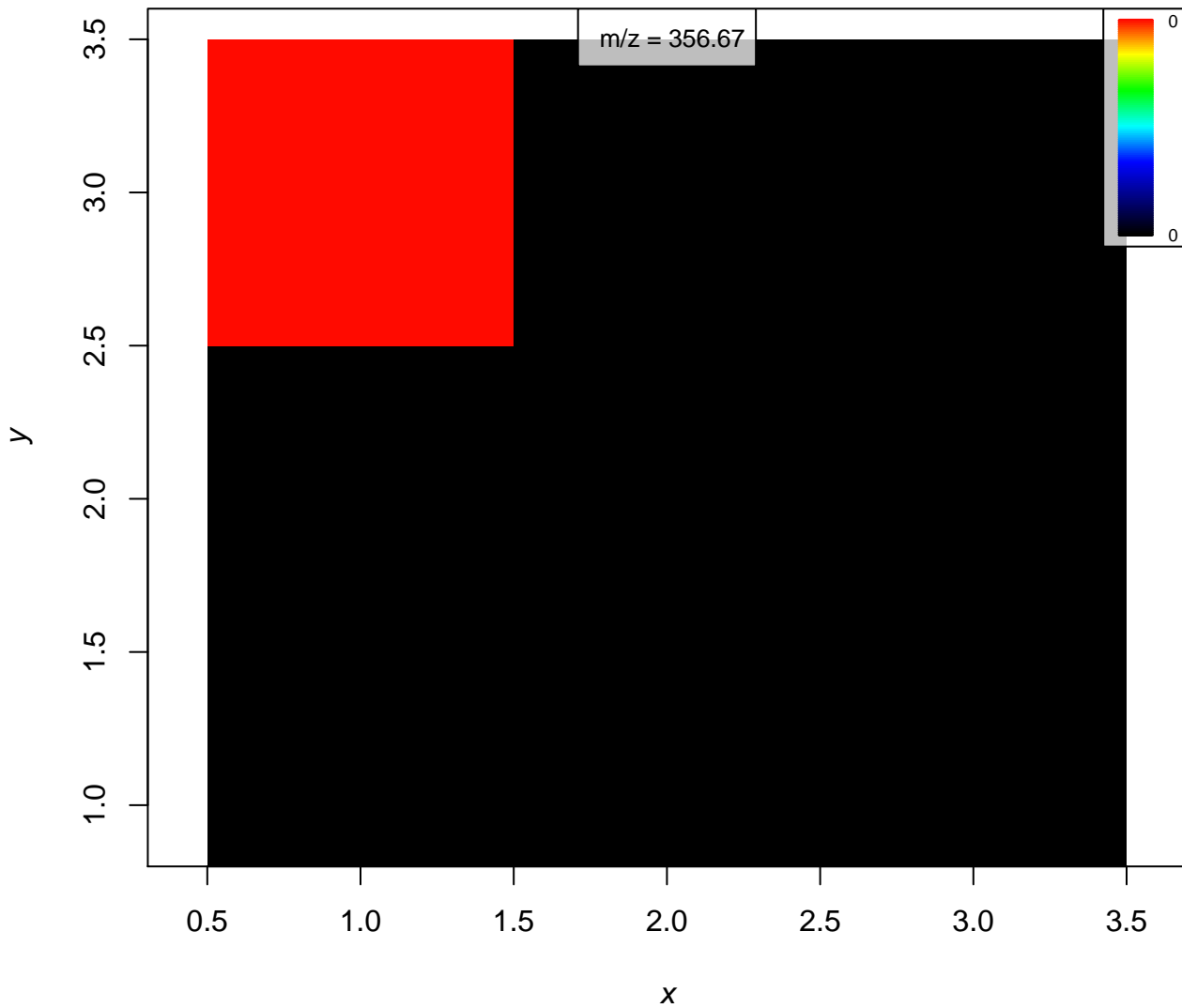
Average spectrum 398.8 Da



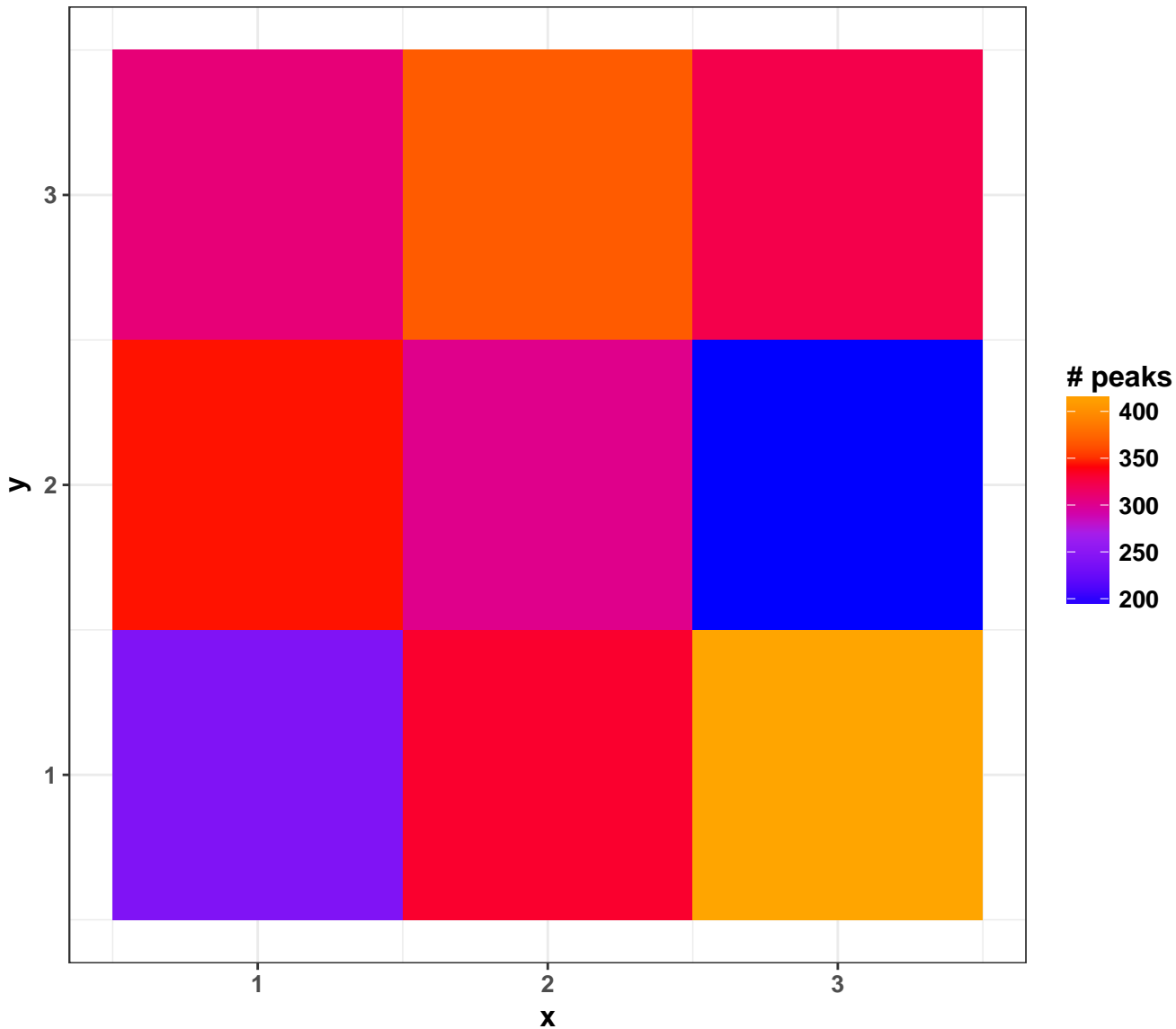
Ratio of mass1 (328.9) / mass2 (398.8)



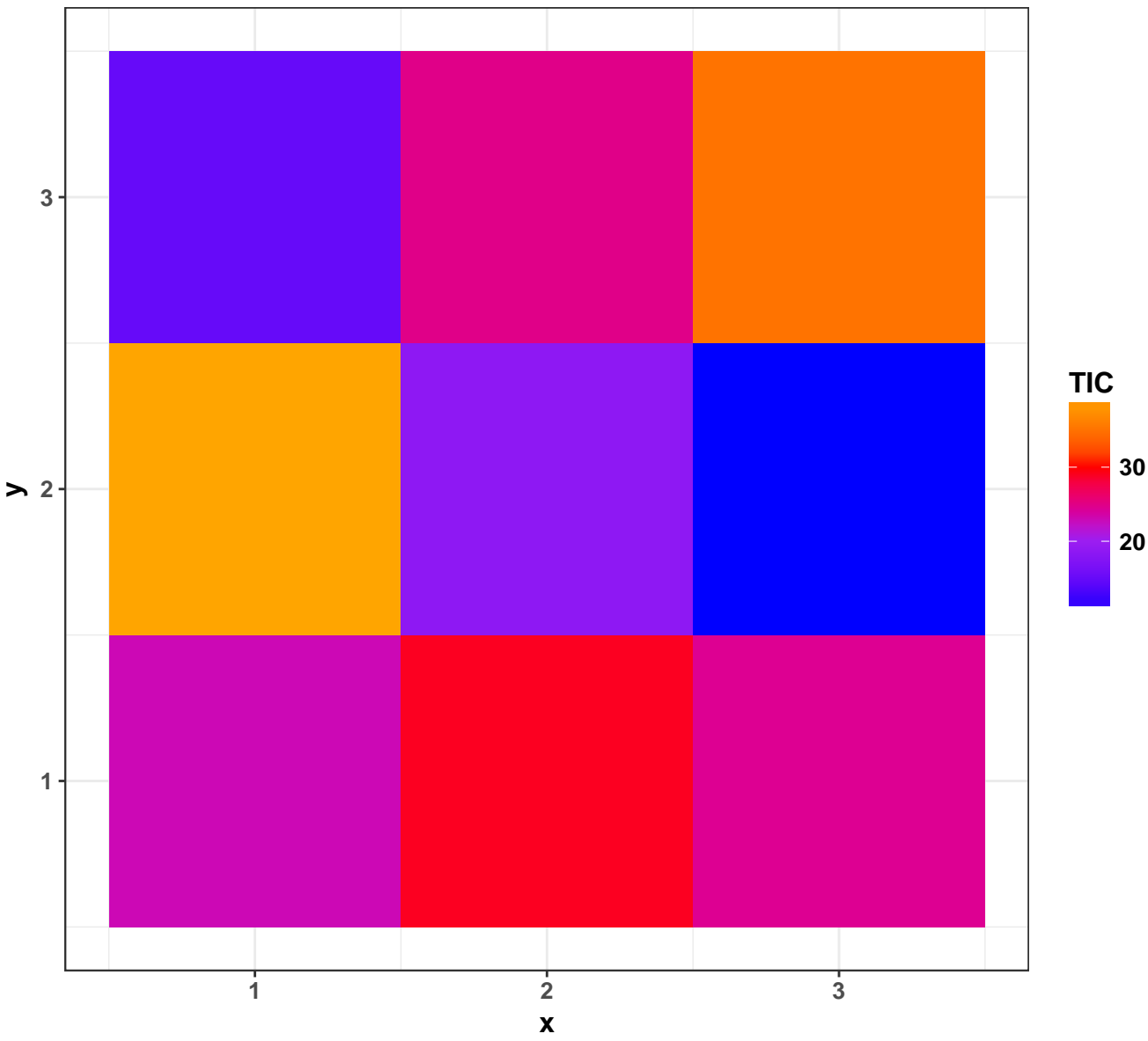
356.7: 356.7 (± 100 ppm)



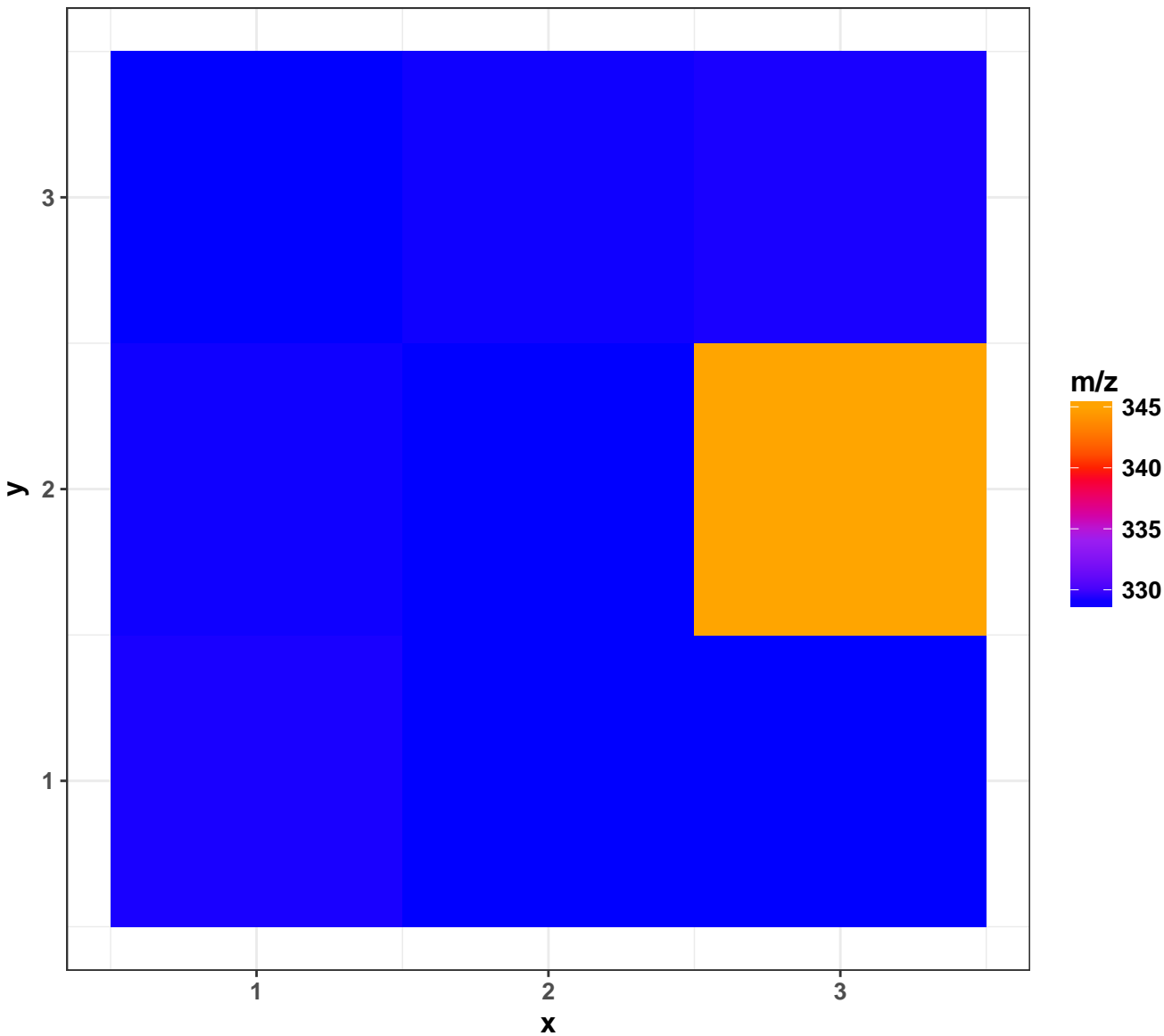
Number of peaks per spectrum



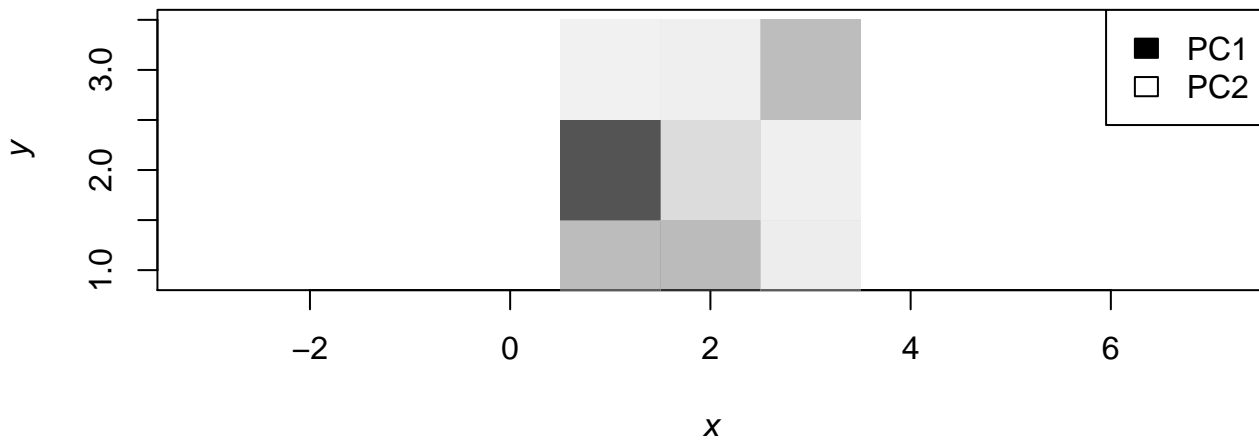
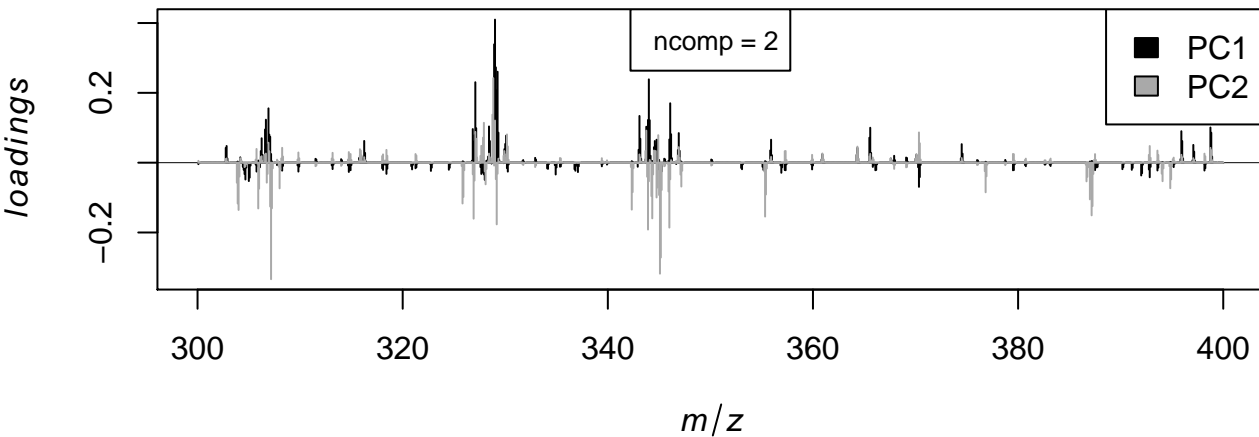
Total Ion Chromatogram



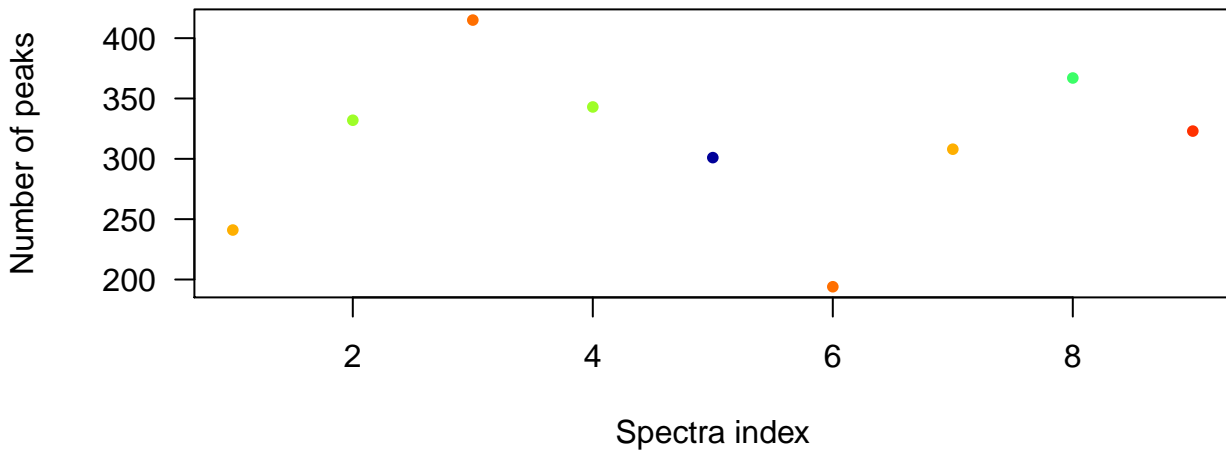
Most abundant m/z in each spectrum



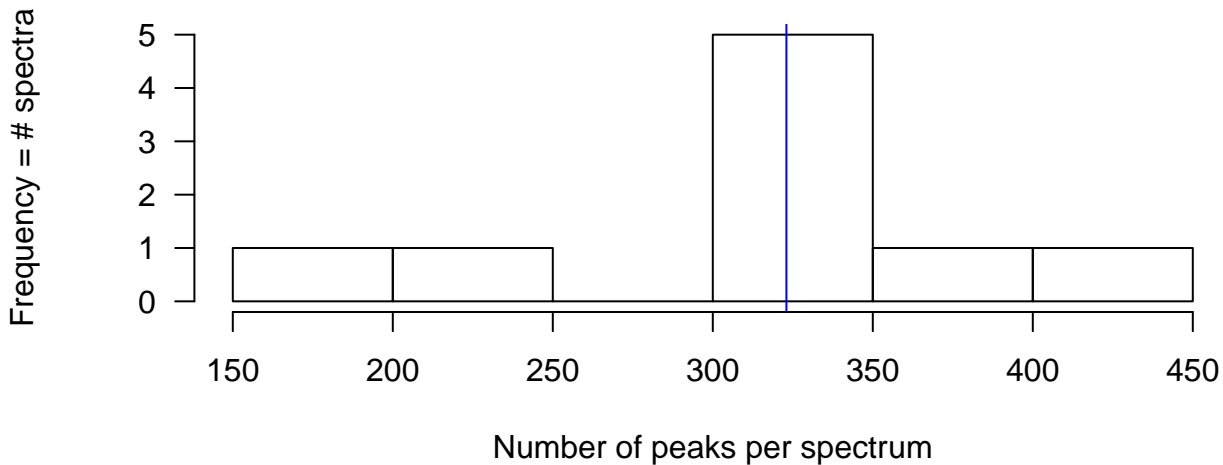
PCA for two components

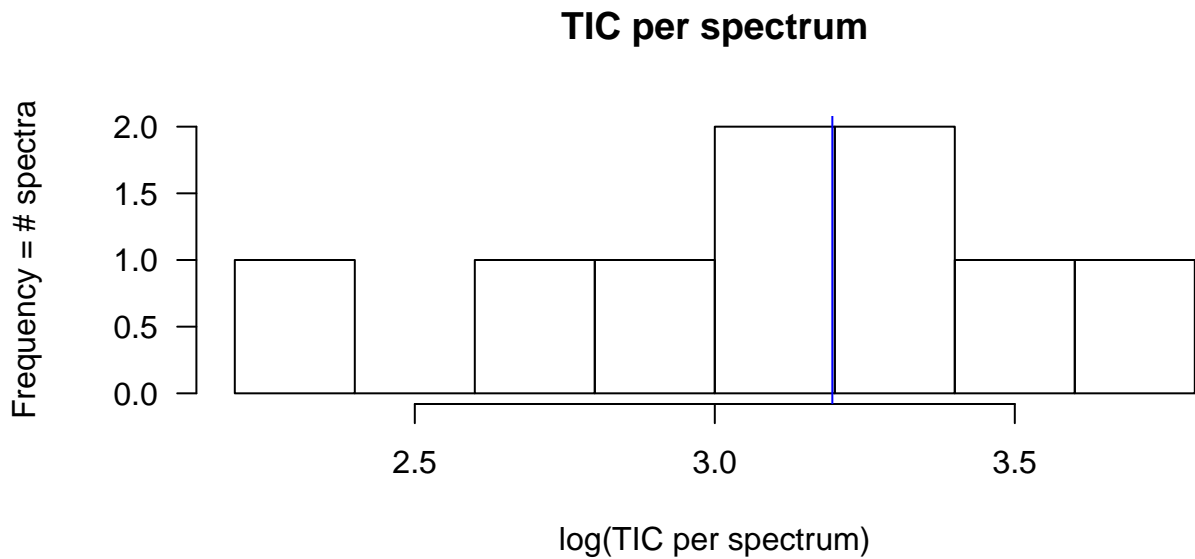
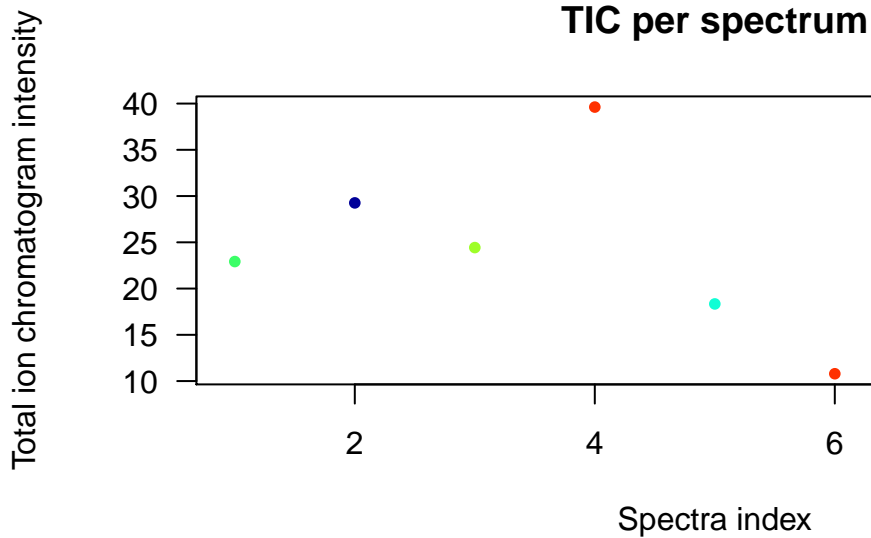


Number of peaks per spectrum

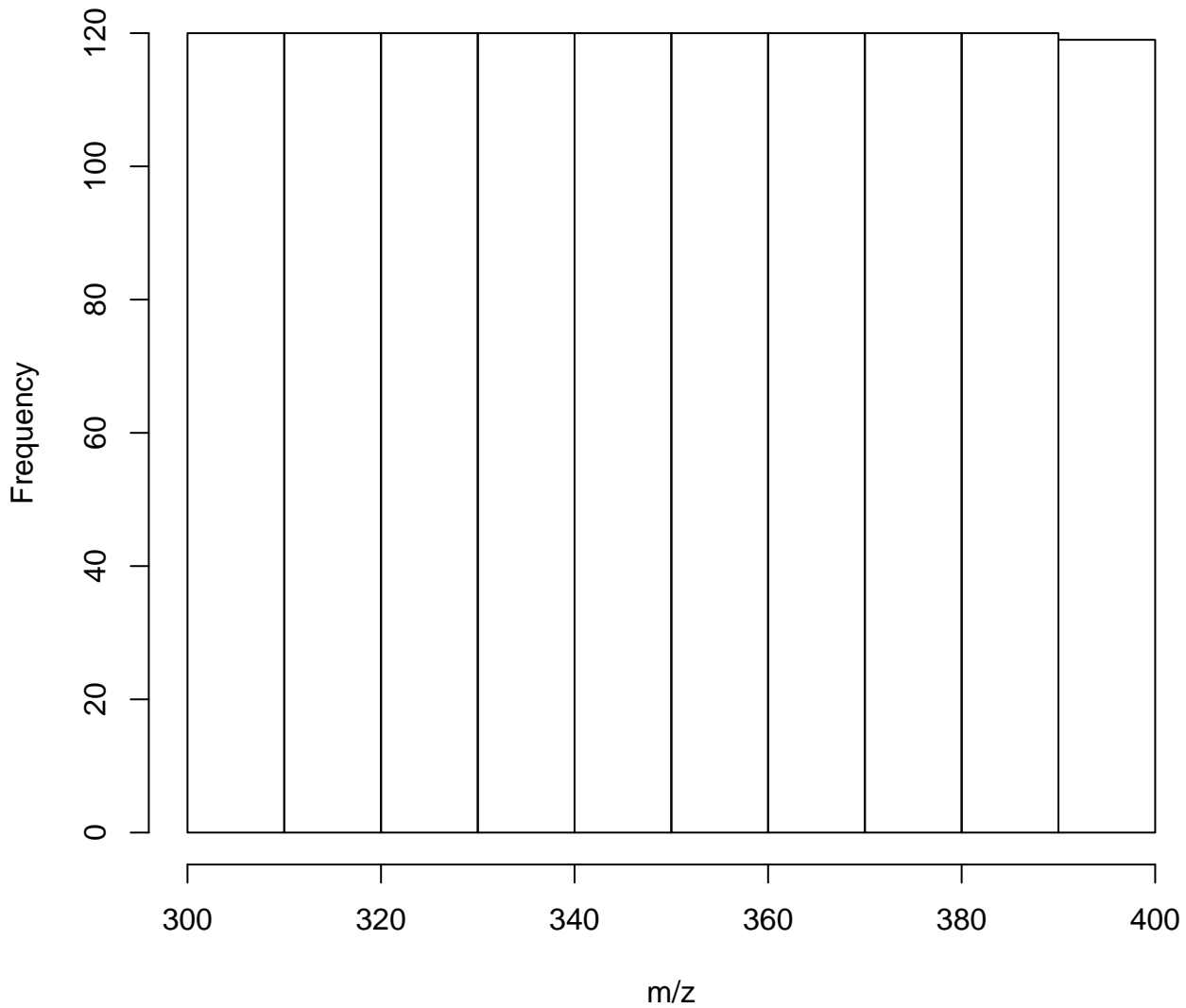


Number of peaks per spectrum

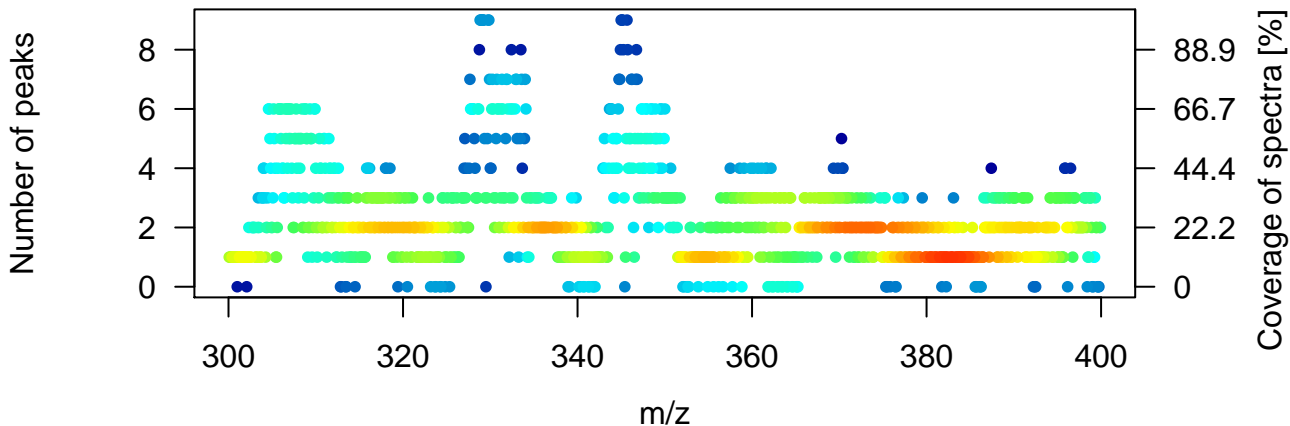




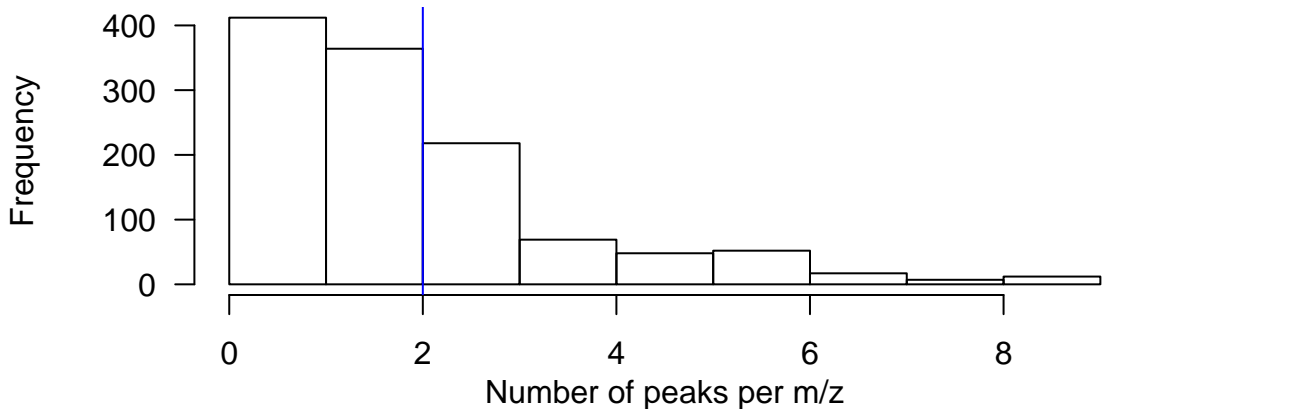
Histogram of m/z values



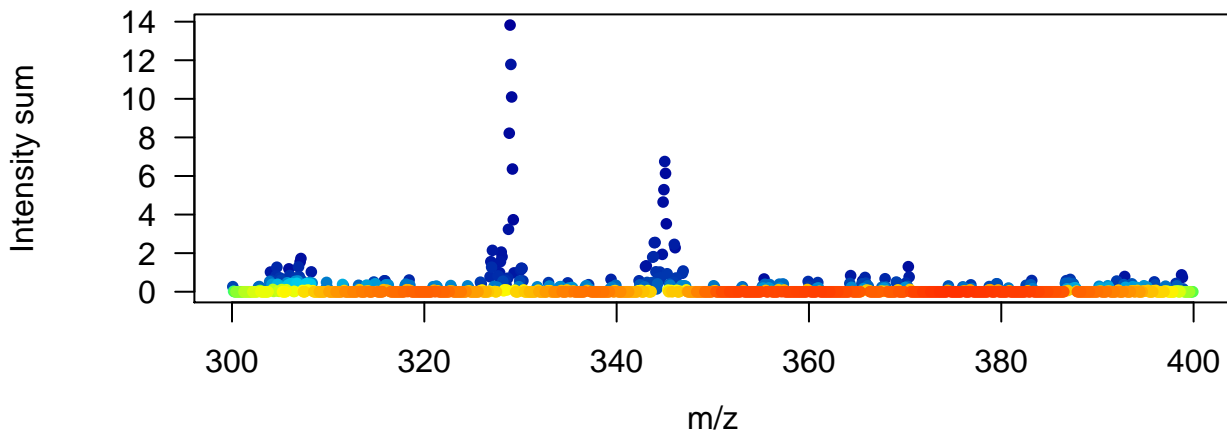
Number of peaks per m/z



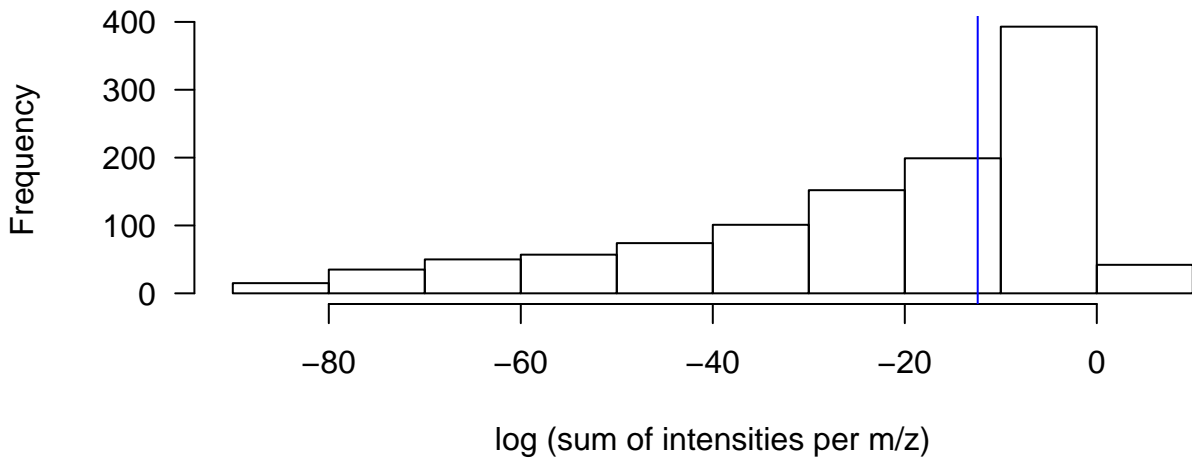
Number of peaks per m/z



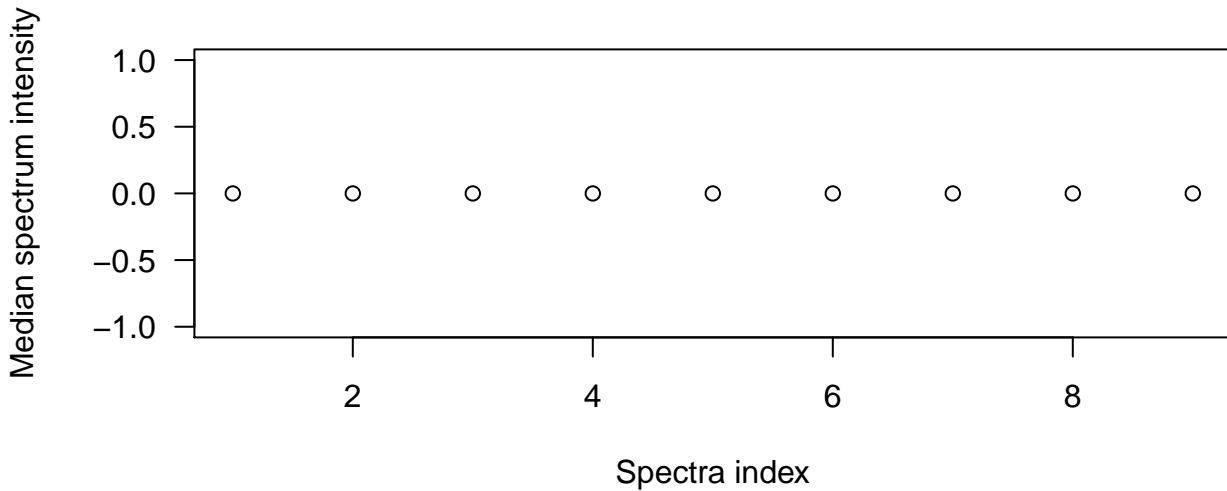
Sum of intensities per m/z



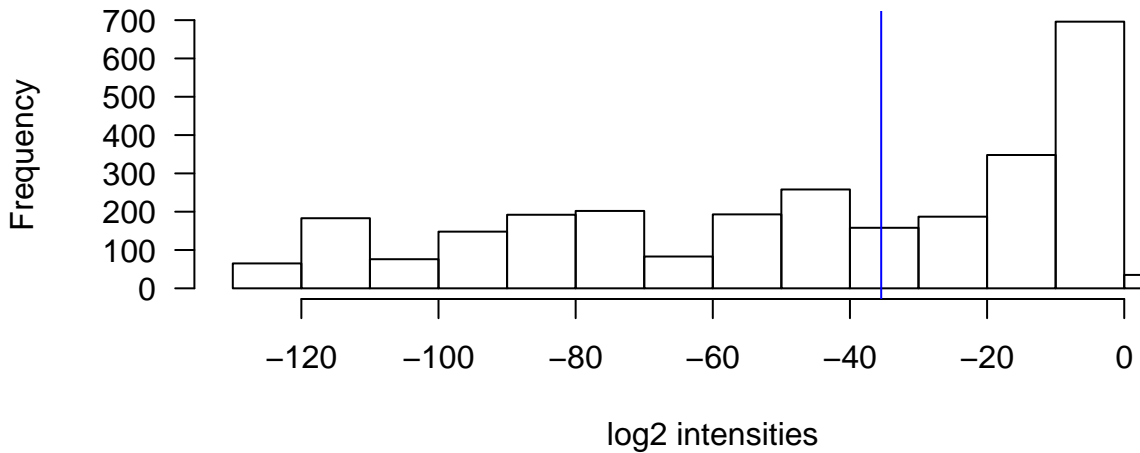
Sum of intensities per m/z



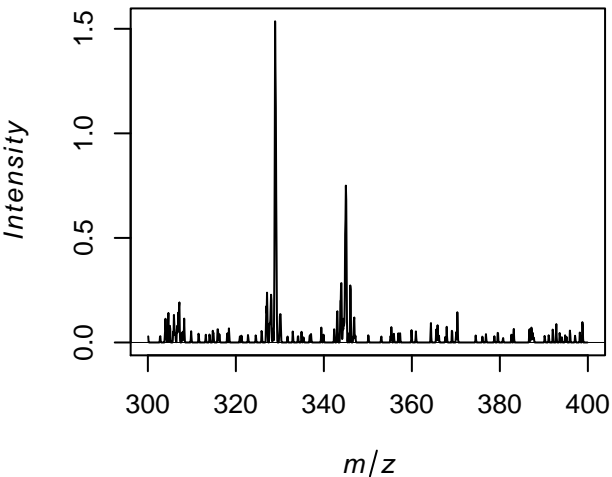
Median intensity per spectrum



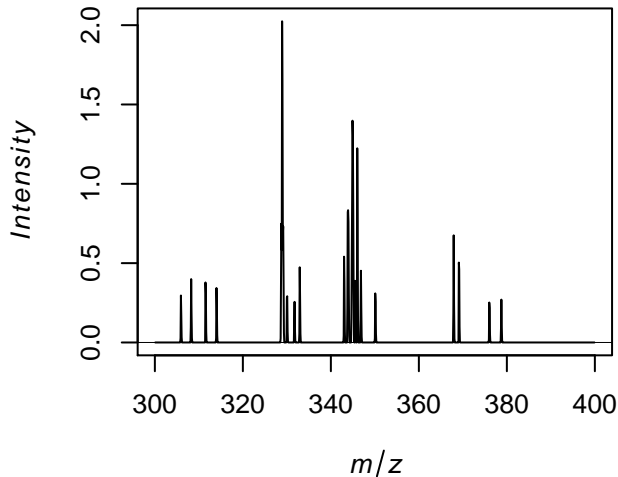
Log2-transformed intensities



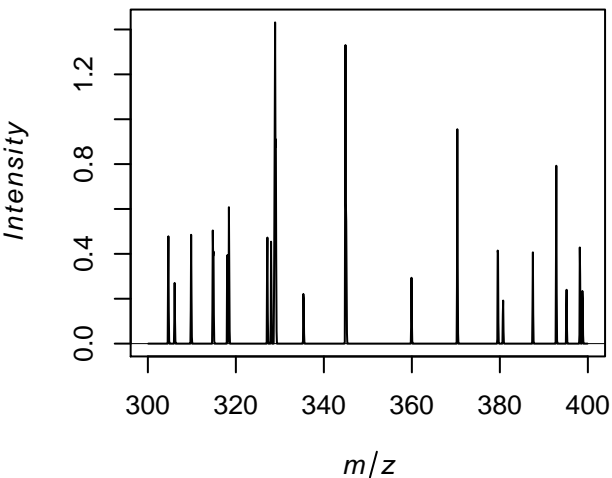
Average spectrum



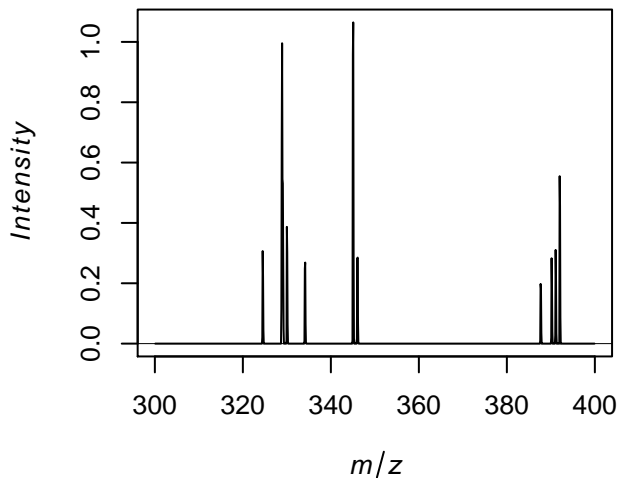
Spectrum at x = 2, y = 1



Spectrum at x = 3, y = 1



Spectrum at x = 3, y = 2

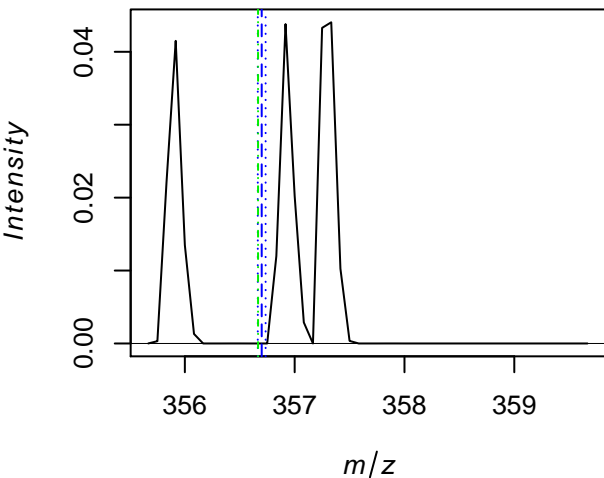


theor. m/z: 356.7

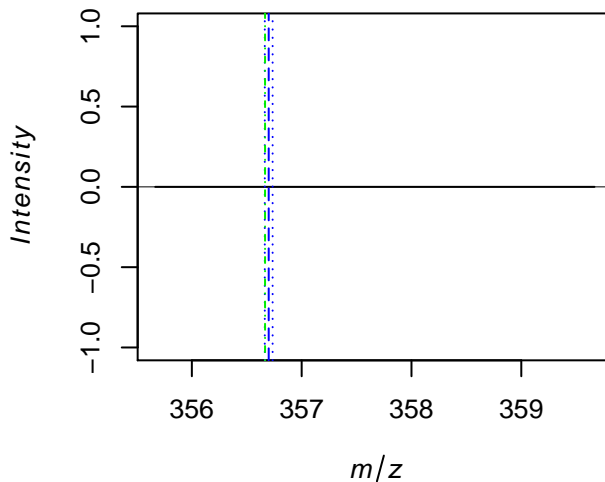
most abundant m/z: NA

closest m/z: 356.6667

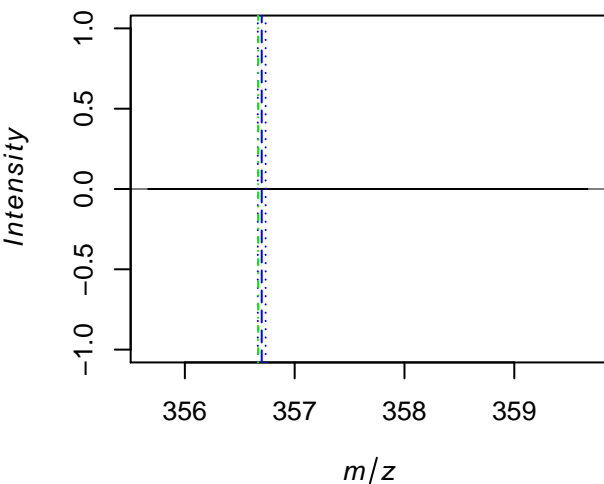
Average spectrum



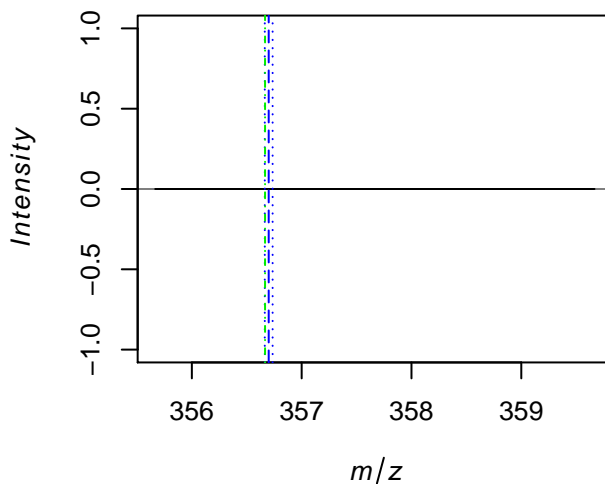
Spectrum at x = 2, y = 1



Spectrum at x = 3, y = 1

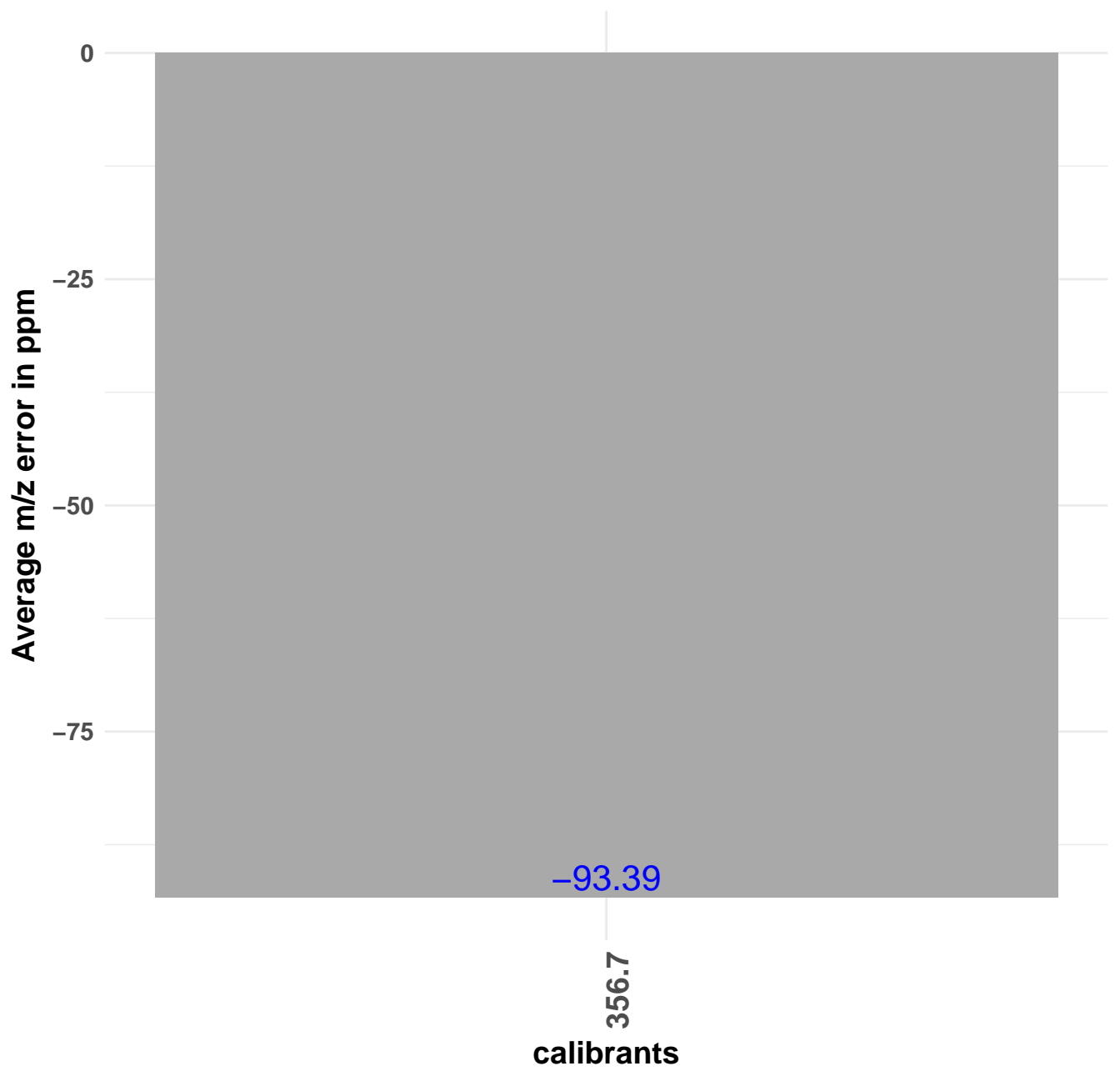


Spectrum at x = 3, y = 2



plot 17: no peaks in the chosen region, repeat with higher ppm range

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



plot 19: no peaks in the chosen region, repeat with higher ppm range