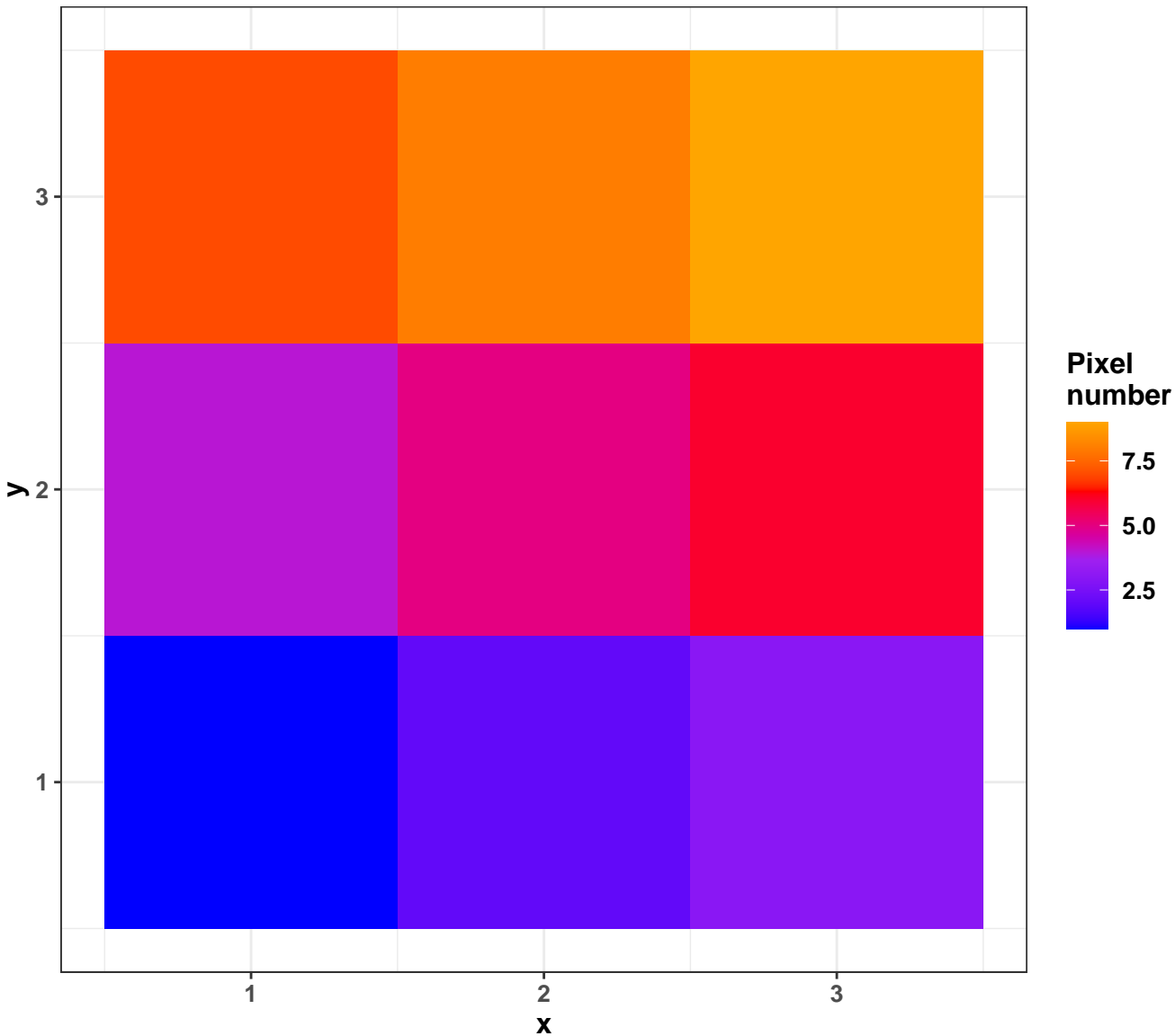


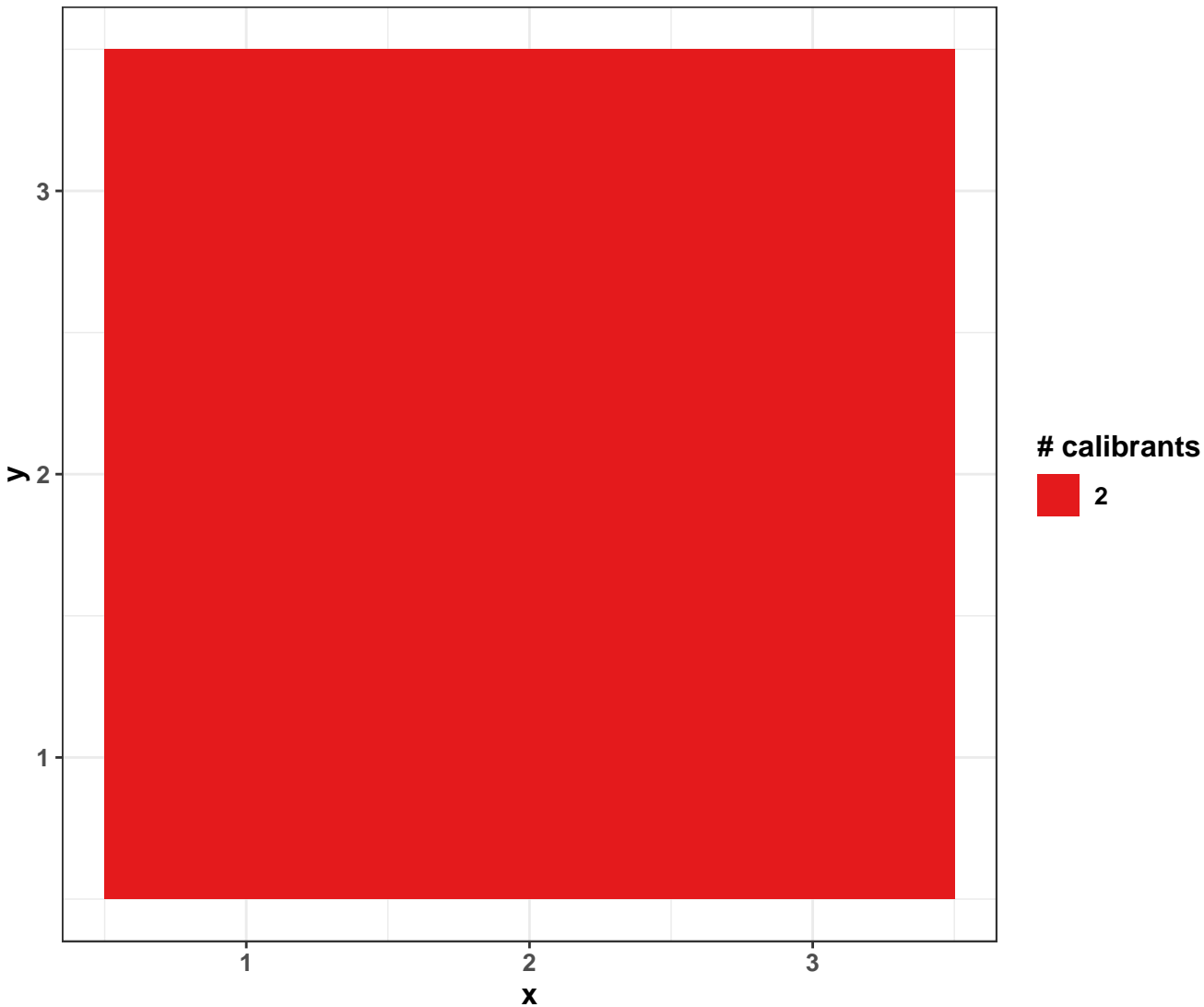
Composite Dataset

properties	values
Number of m/z features	10398
Range of m/z values	100 – 799.97
Number of pixels	9
Range of x coordinates	1 – 3
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	32.95 %
Number of empty spectra	0
Median TIC \pm sd	212.8 \pm 58
Median # peaks per spectrum \pm sd	3666 \pm 486
maximum m/z window size	0.16
Centroided	FALSE
input m/z (#valid/#input) in inputcalibrantfile1.tabular	3 / 3

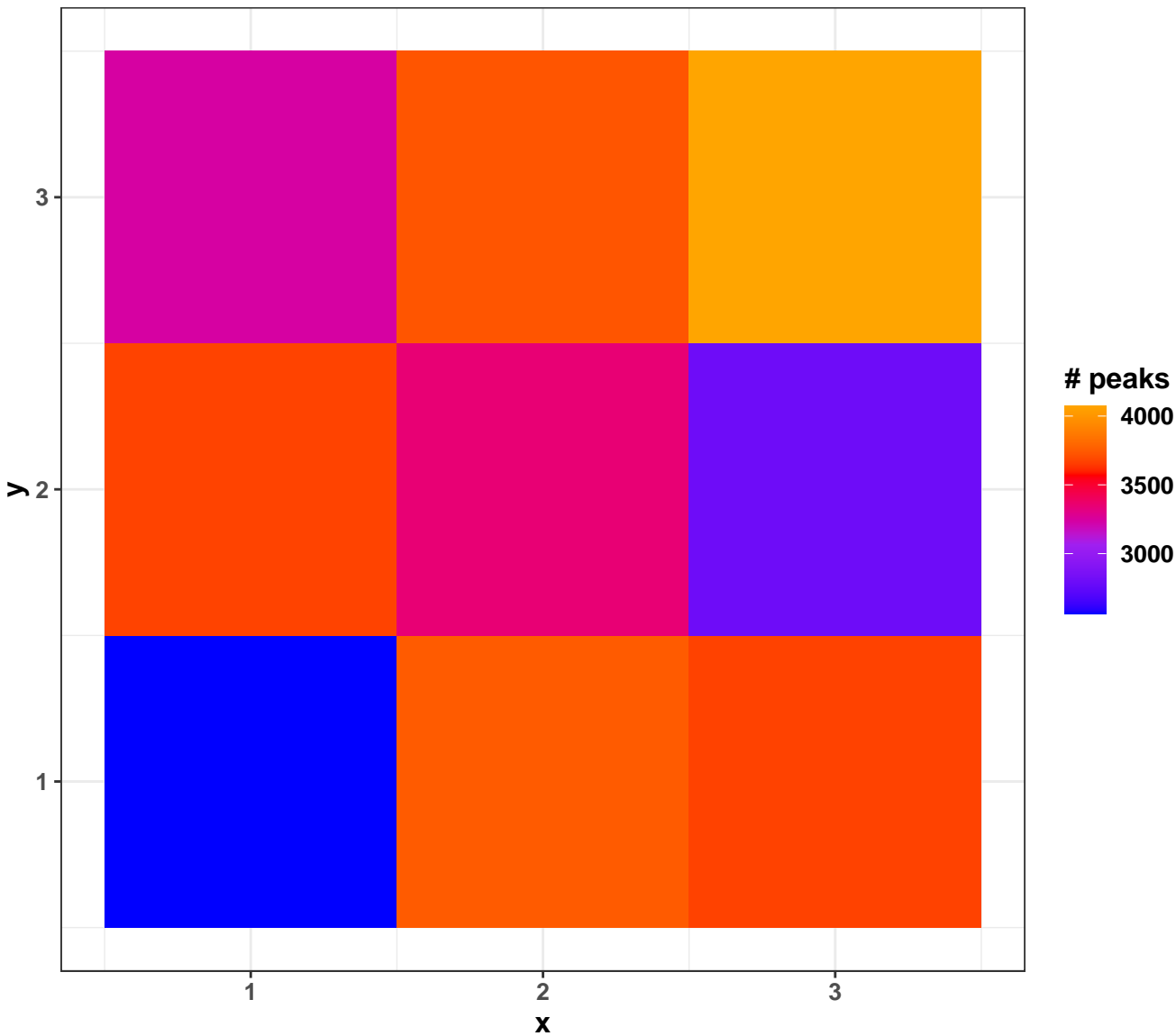
Pixel order



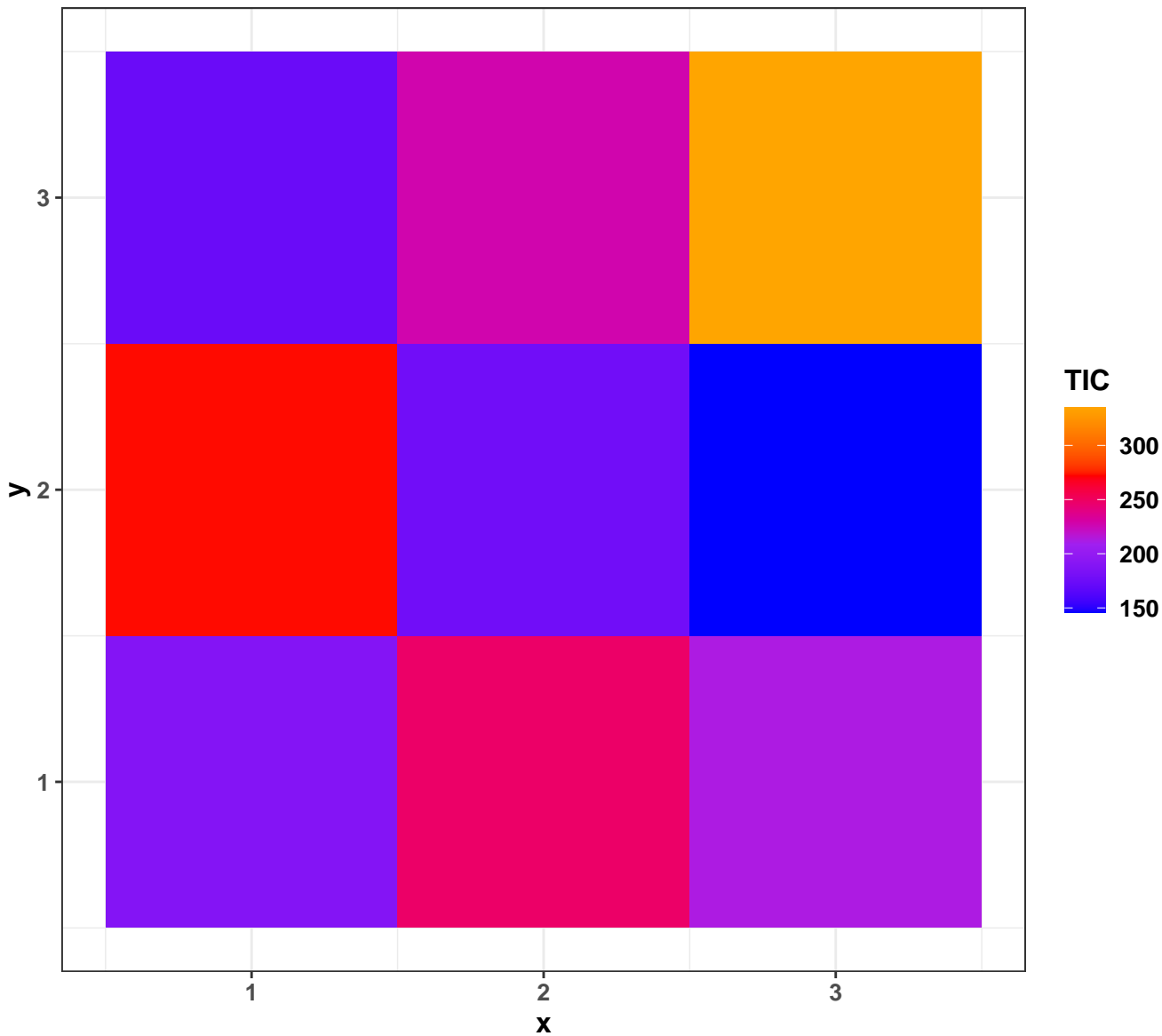
Number of calibrants per pixel (± 200 ppm)



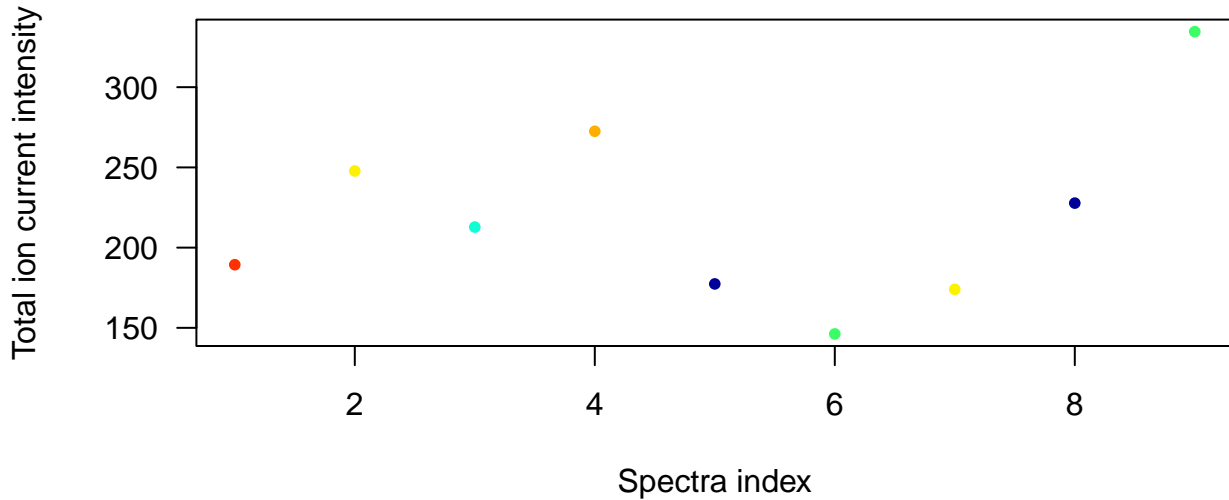
Number of peaks per spectrum



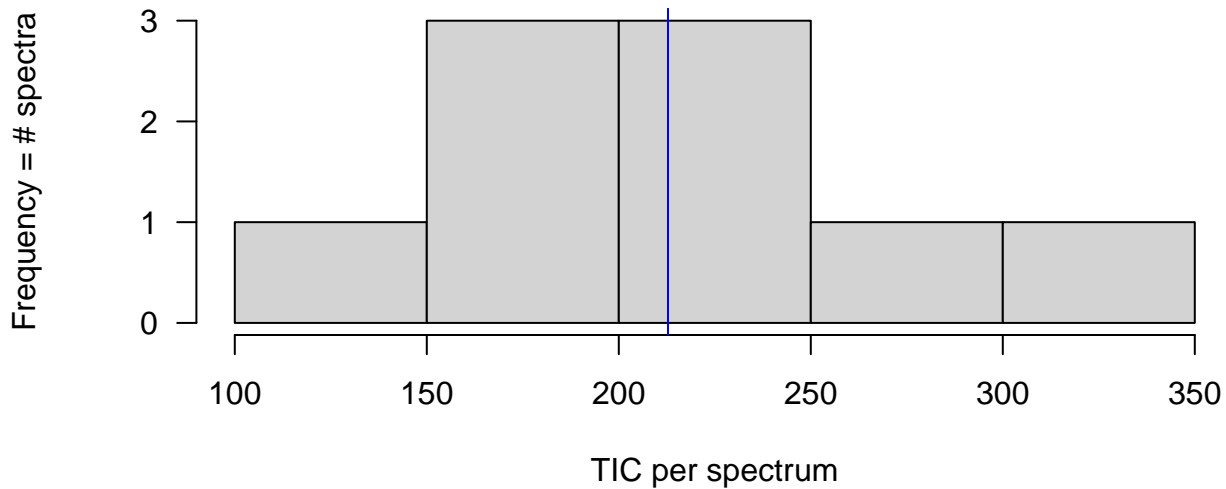
Total Ion Current



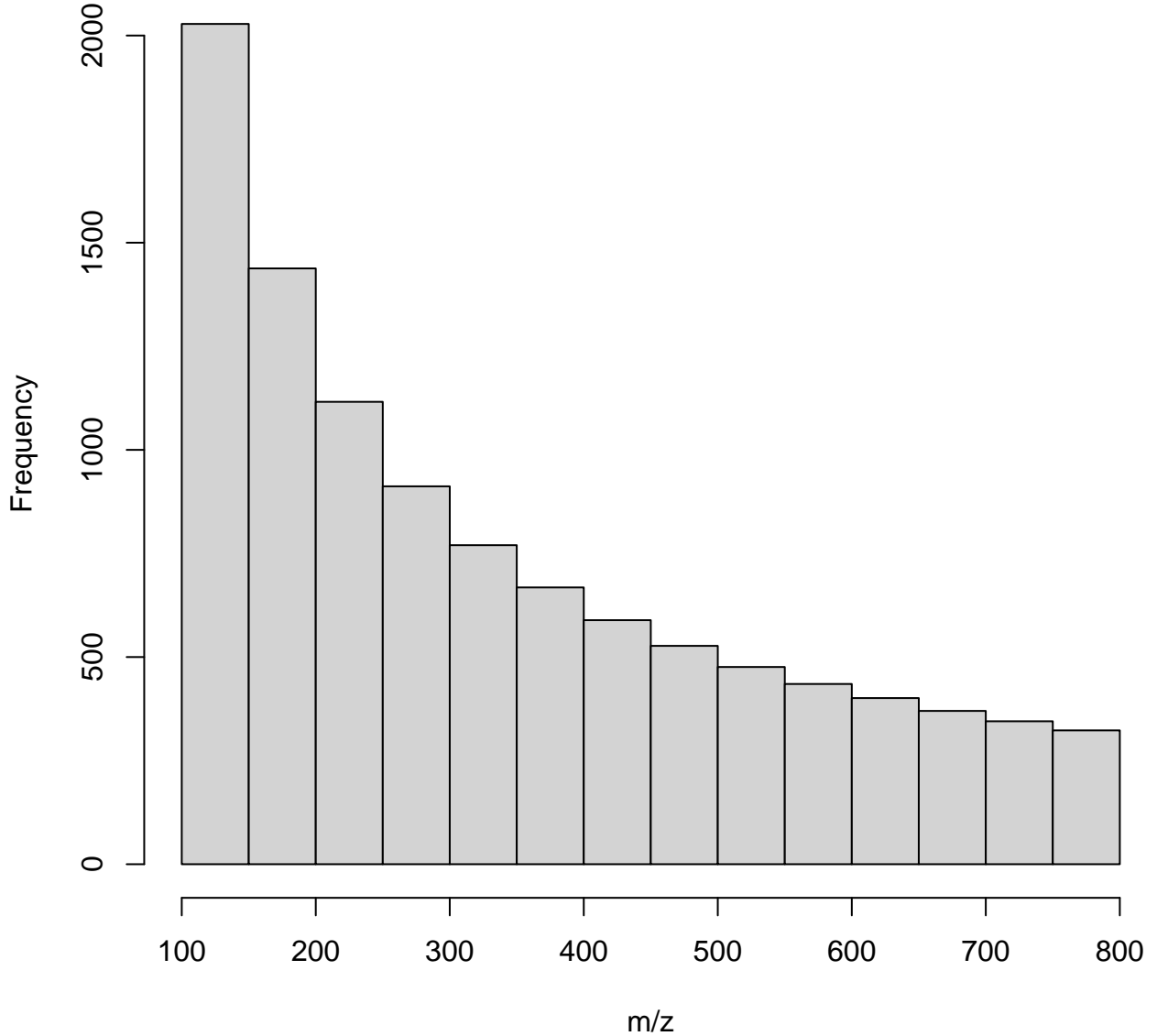
TIC per spectrum



TIC per spectrum



Histogram of m/z values

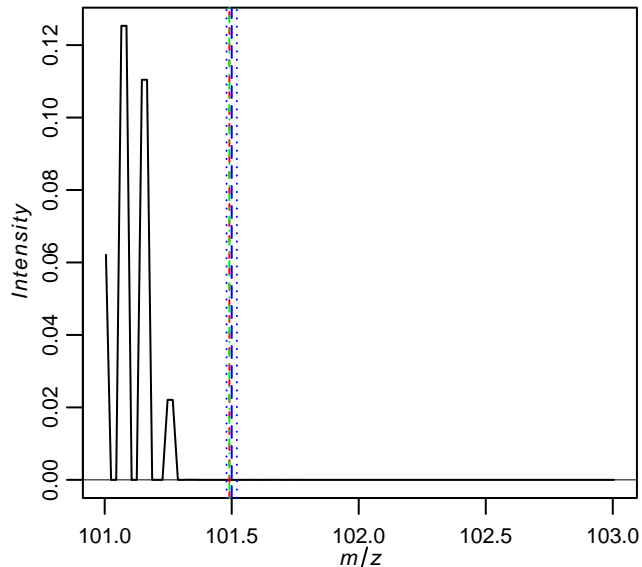


theor. m/z: 101.5

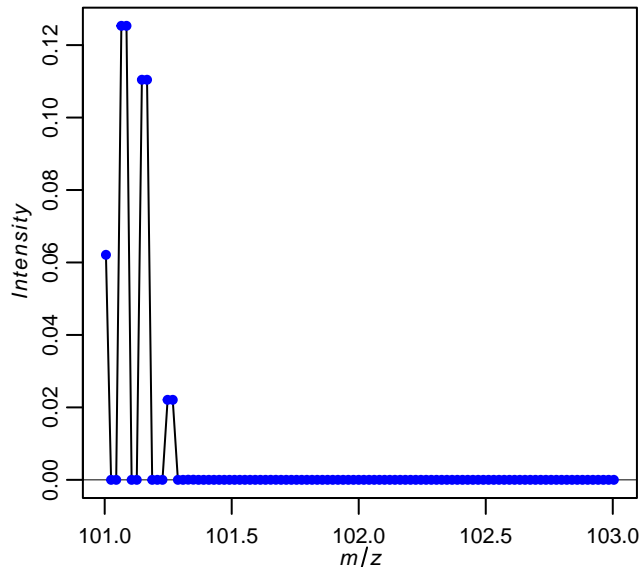
most abundant m/z: 101.491

closest m/z: 101.491

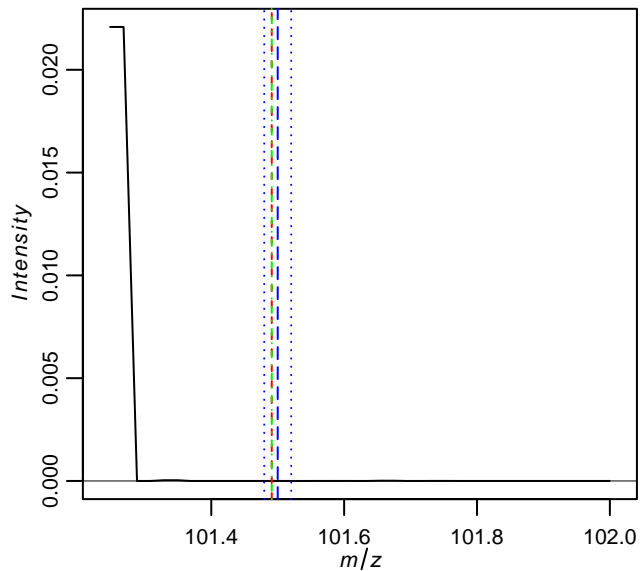
Average spectrum



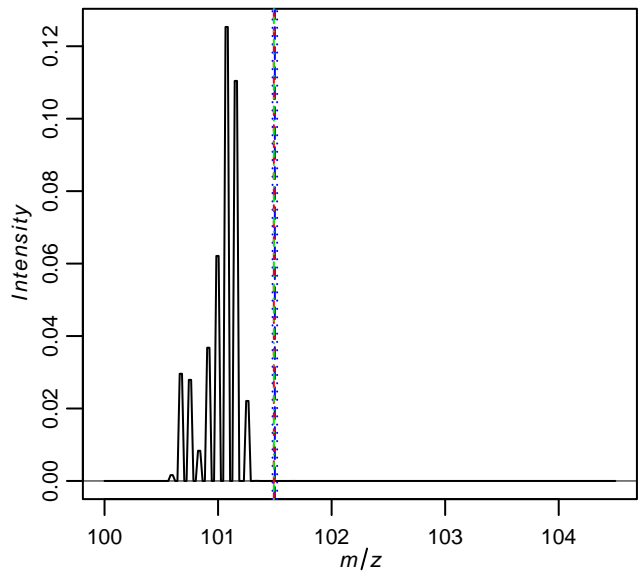
Average spectrum with data points



Average spectrum



Average spectrum

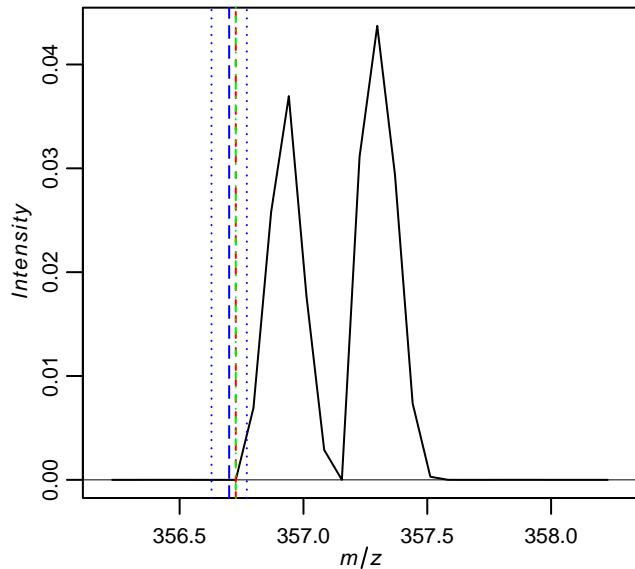


theor. m/z: 356.7

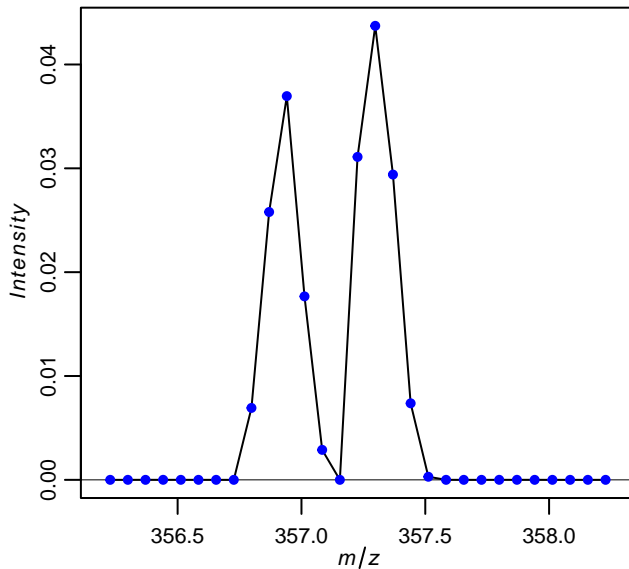
most abundant m/z: 356.7268

closest m/z: 356.7268

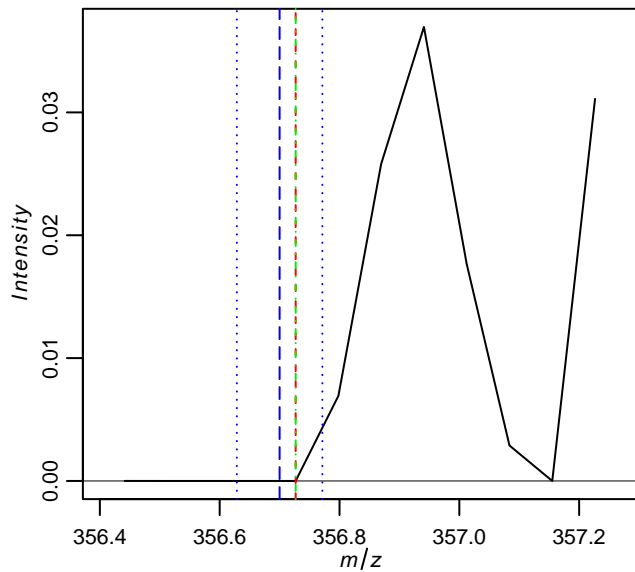
Average spectrum



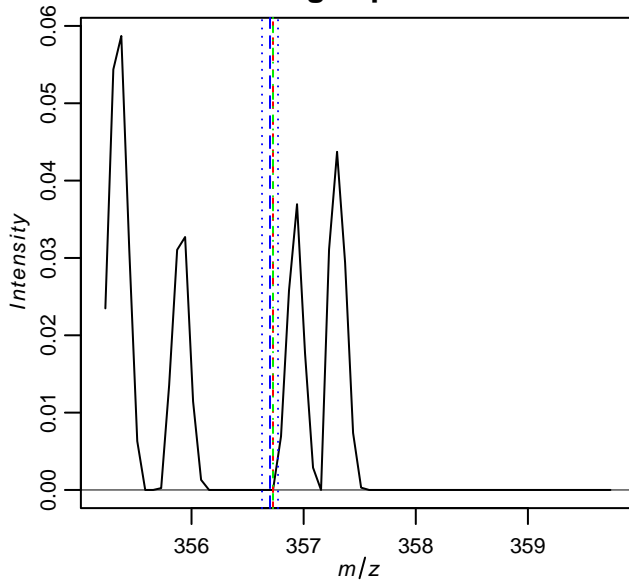
Average spectrum with data points



Average spectrum



Average spectrum

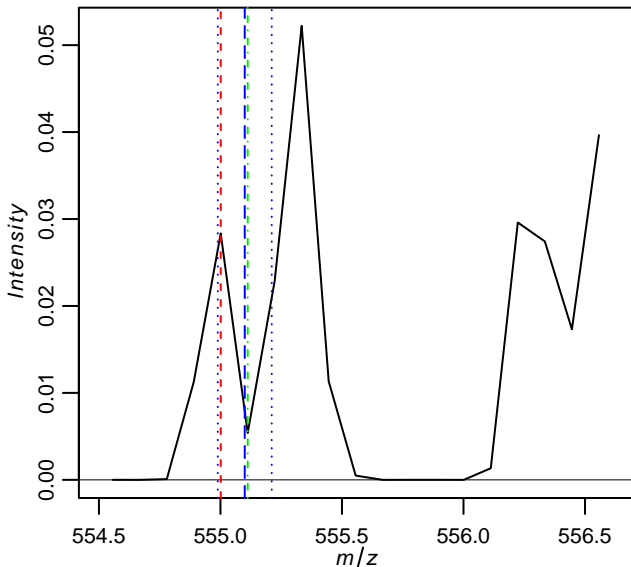


theor. m/z: 555.1

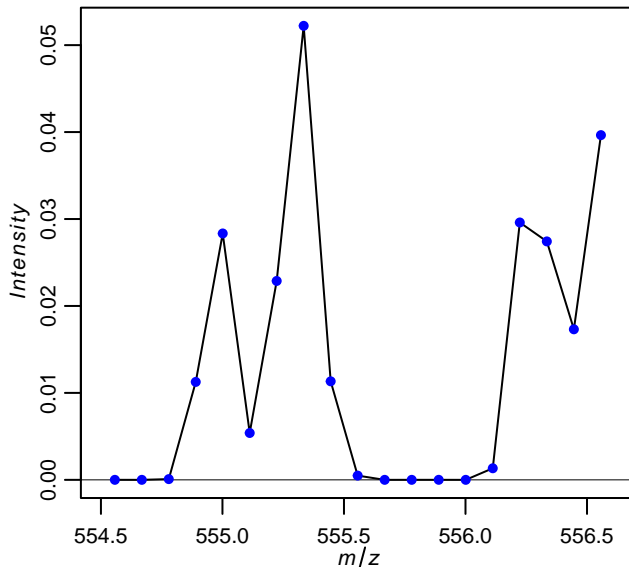
most abundant m/z: 555.012

closest m/z: 555.1122

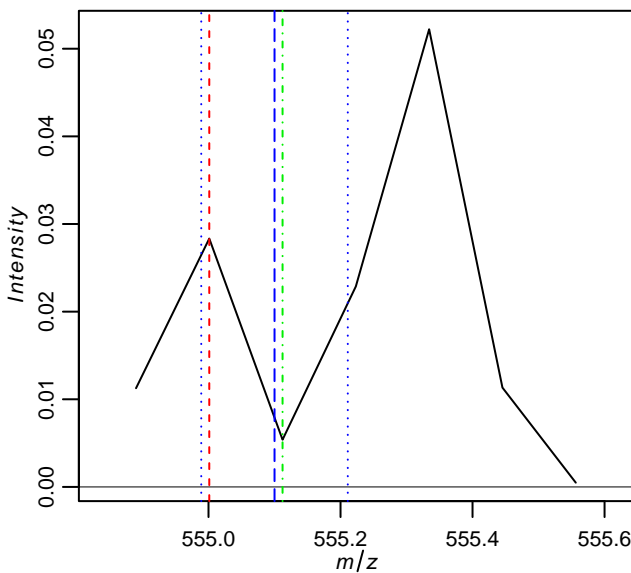
Average spectrum



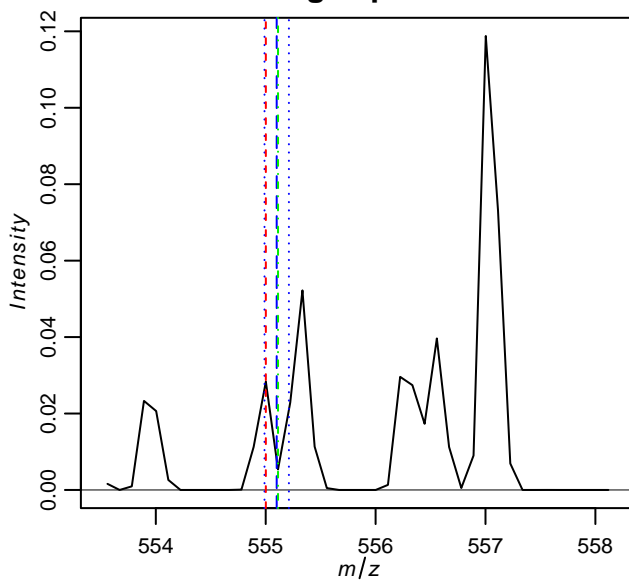
Average spectrum with data points



Average spectrum



Average spectrum



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

