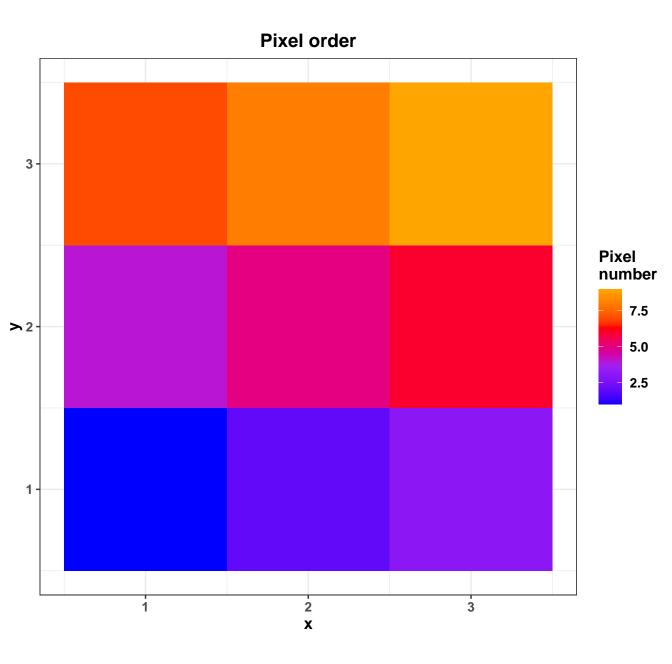
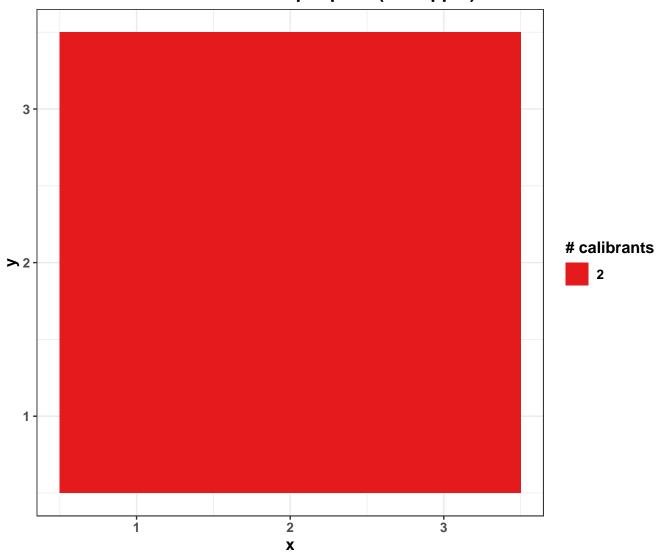
# **Composite Dataset**

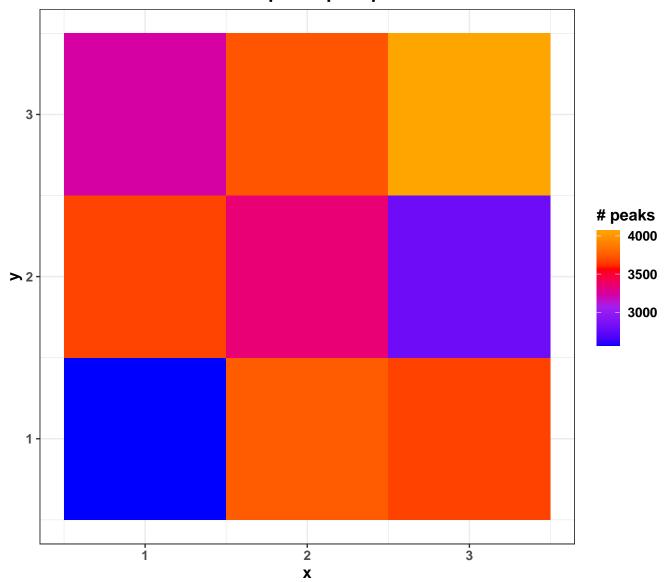
properties	values
Number of m/z features	10398
Range of m/z values	100 – 799.97
Number of pixels	9
Range of x coordinates	1 – 3
Range of y coordinates	1 – 3
Range of intensities	0 – 9.24
Number of NA intensities	0
Number of Inf intensities	0
Number of duplicated coordinates	0
Median of intensities	0
Intensities > 0	32.95 %
Number of empty spectra	0
Median TIC ± sd	212.8 ± 58
Median # peaks per spectrum ± sd	3666 ± 486
maximum m/z window size	0.16
Centroided	FALSE
input m/z (#valid/#input) in inputcalibrantfile1.tabular	3/3

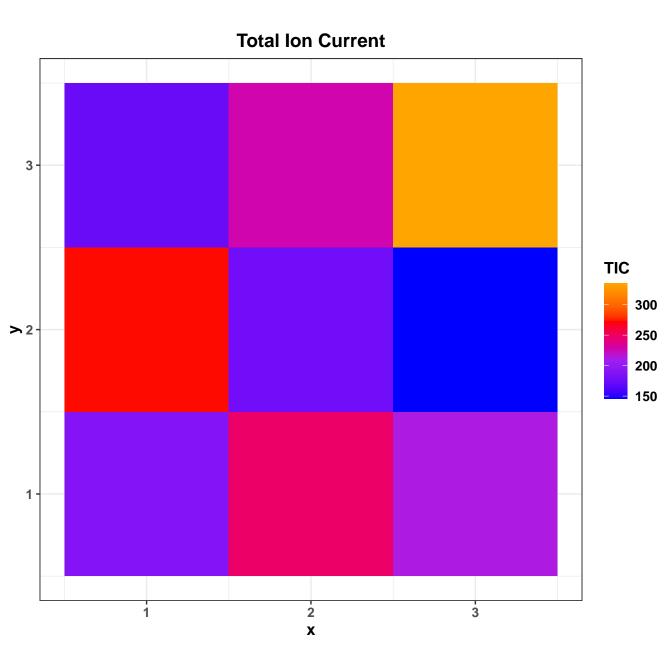




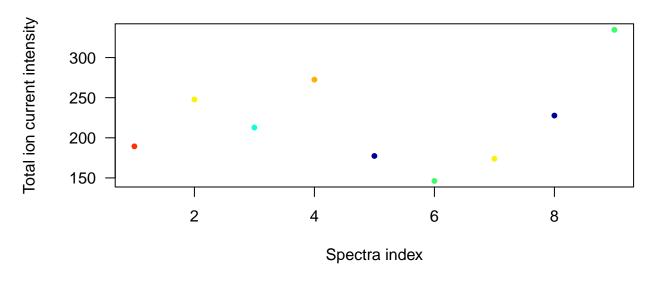


# Number of peaks per spectrum

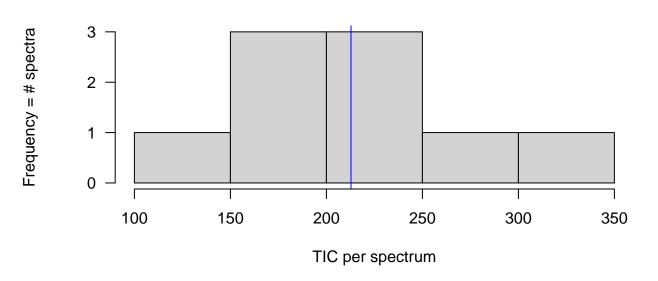




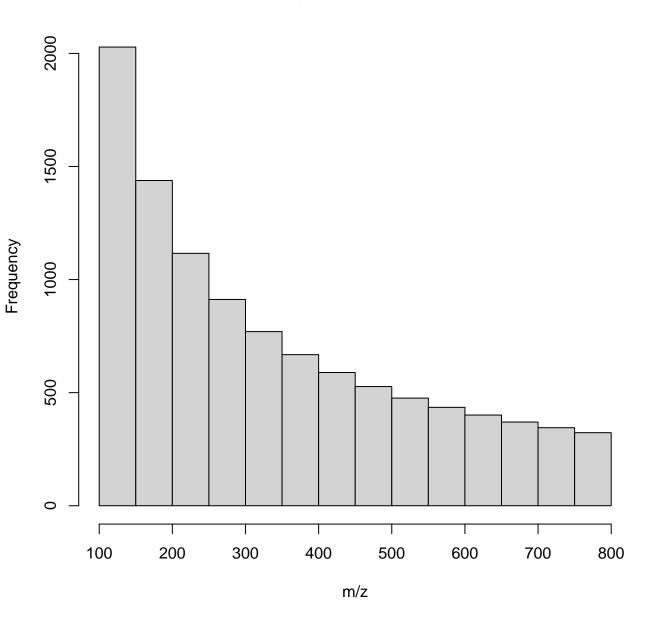
### **TIC** per spectrum

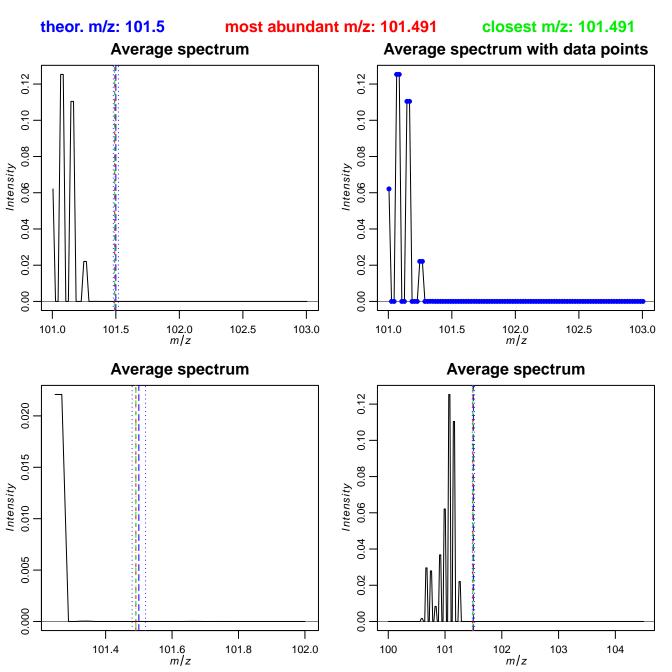


### **TIC** per spectrum



### Histogram of m/z values





theor. m/z: 356.7 most abundant m/z: 356.7268 closest m/z: 356.7268 Average spectrum with data points Average spectrum 0.04 0.04 0.03 0.03 Intensity 0.02 Intensity 0.02 0.01 0.01 0.00 0.00 356.5 357.0 357.5 358.0 356.5 357.0 357.5 358.0 m/z m/z Average spectrum Average spectrum 90.0 0.05 0.03 0.04 Intensity 0.02 Intensity 0.03 0.02 0.01 0.01 0.00 0.00 356.8 m/z 356.6 357.0 357.2 356 357 358 359 356.4 m/z

theor. m/z: 555.1 most abundant m/z: 555.0012 closest m/z: 555.1122 Average spectrum with data points Average spectrum 0.05 0.05 0.04 0.04 0.03 0.03 Intensity Intensity 0.02 0.01 0.01 0.00 0.00 555.5 m/z 555.5 m/z 556.0 556.5 555.0 556.0 556.5 554.5 555.0 554.5 Average spectrum Average spectrum 0.12 0.05 0.10 0.04 0.08 0.03 Intensity 90.0 0.04 0.01 0.02 0.00 0.00 555.2 m/z 556 m/z 555.0 555.4 554 558 555.6 555 557

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

