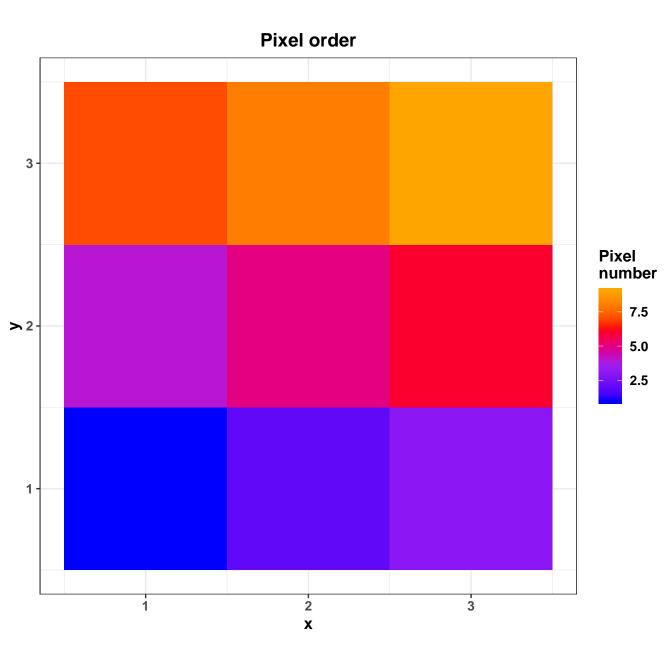
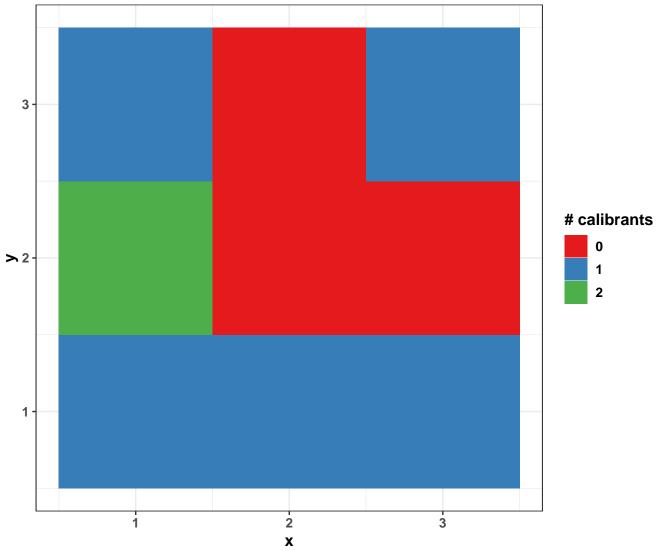
## Testfile\_imzml

properties	values
Number of m/z features	5199
Range of m/z values	100 – 799.81
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
Median of intensities	0
Intensities > 0	35.16 %
Number of empty spectra	0
Median TIC ± sd	161.8 ± 43
Median # peaks per spectrum ± sd	1961 ± 260
Centroided	FALSE
calibrants (#valid/#input) in inputcalibrantfile1.tabular	3/3

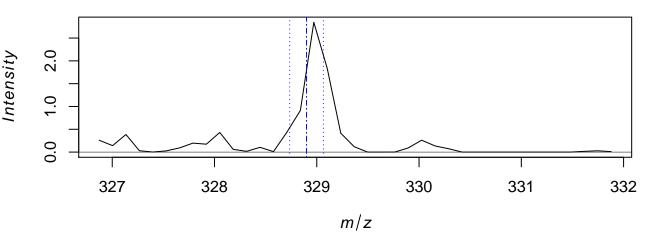


# Number of calibrants per pixel (±100 ppm)

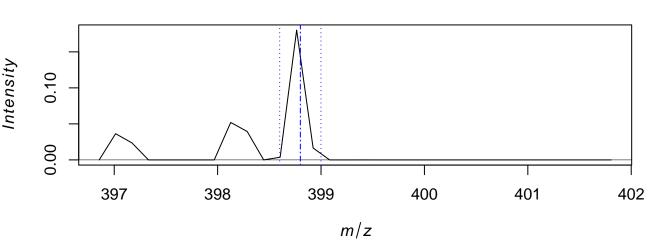


### Control of fold change plot

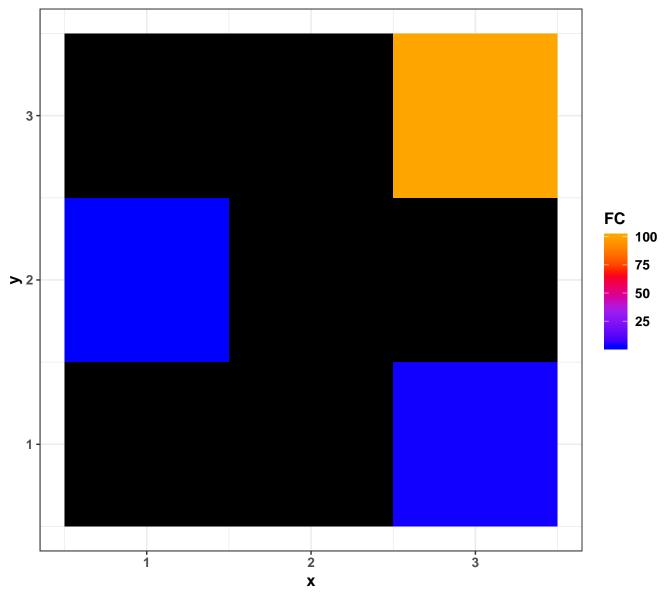
#### Average spectrum 328.9 Da



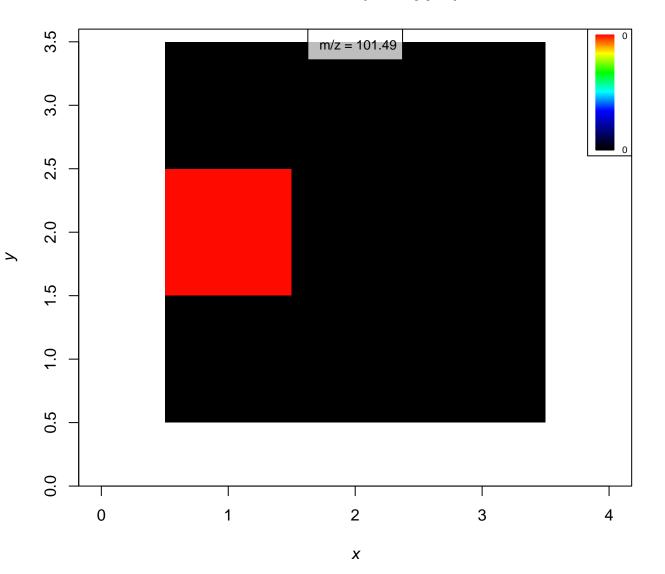
#### Average spectrum 398.8 Da



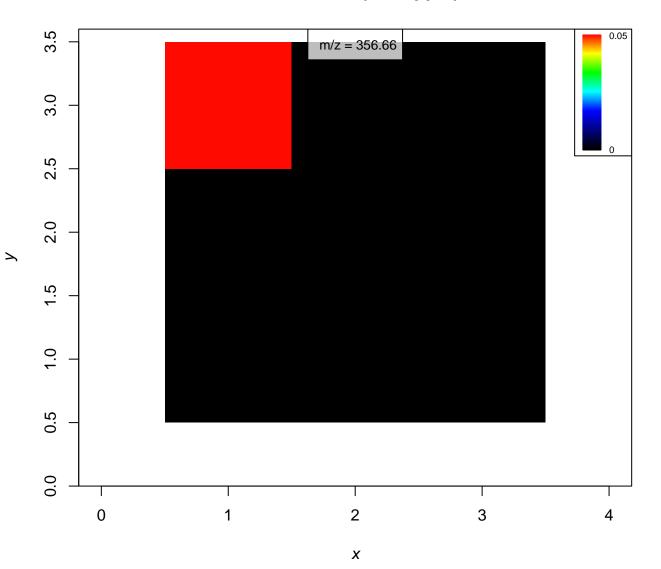




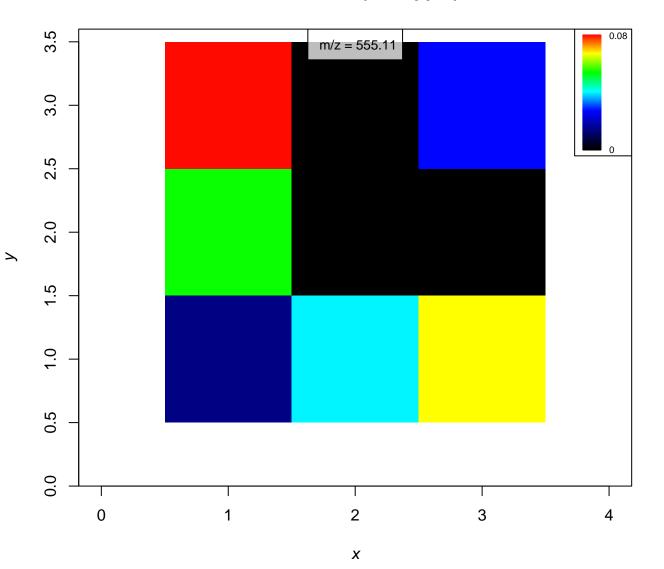
101.5: 101.5 (±100 ppm)



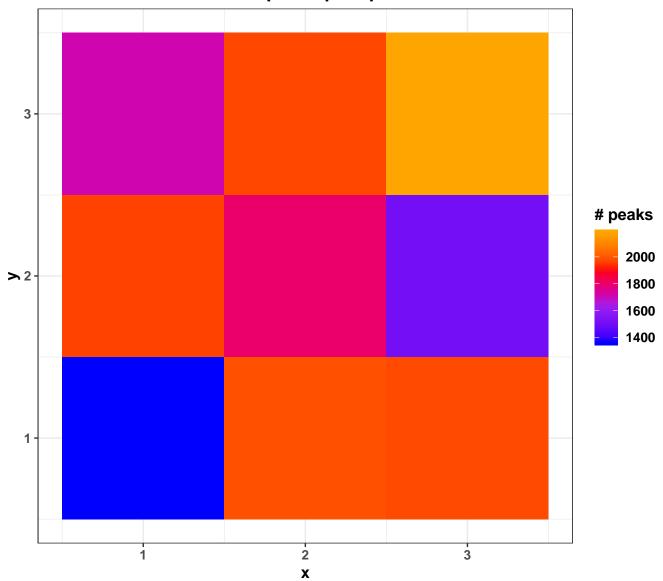
356.7: 356.7 (±100 ppm)

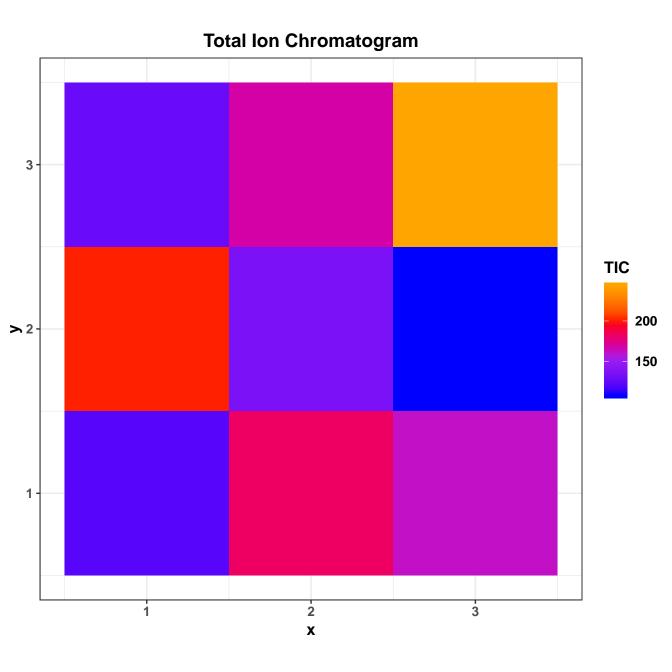


555.1: 555.1 (±100 ppm)

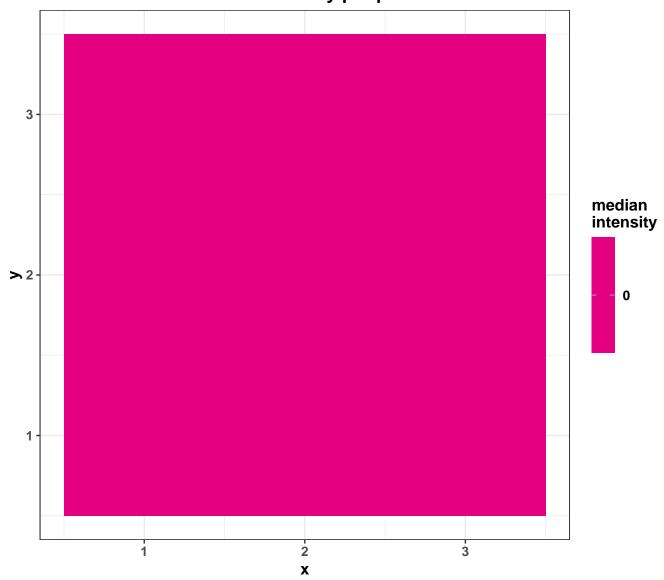


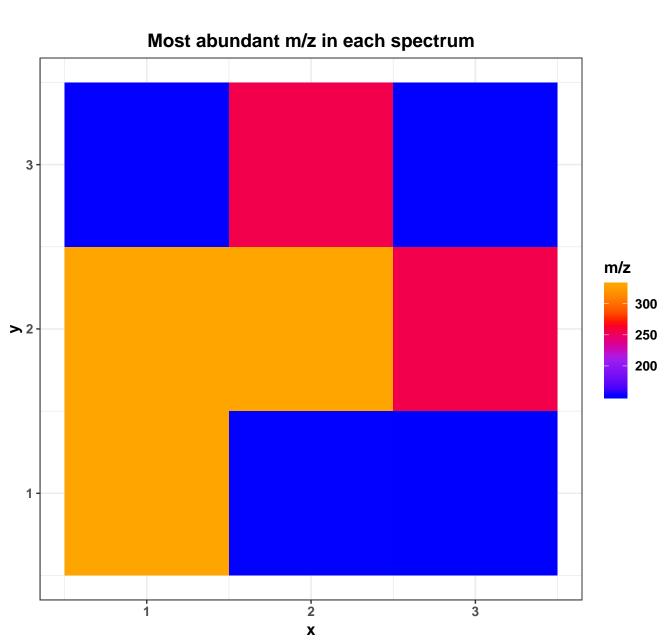




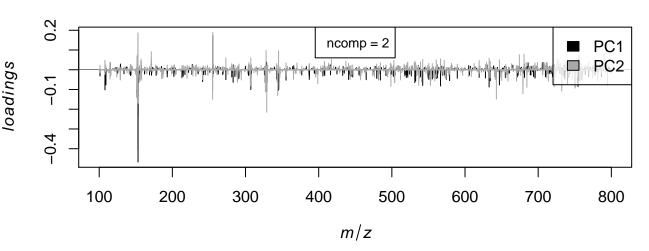


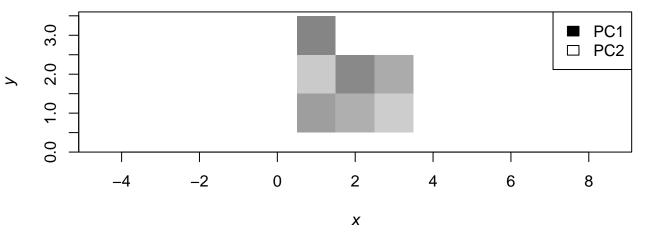
# **Median intensity per pixel**

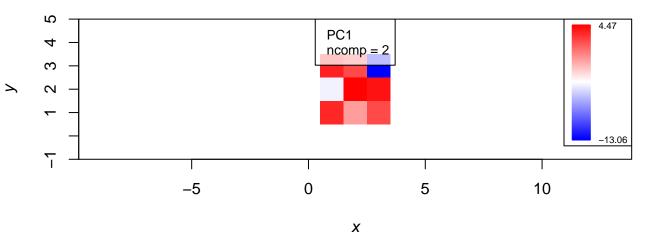


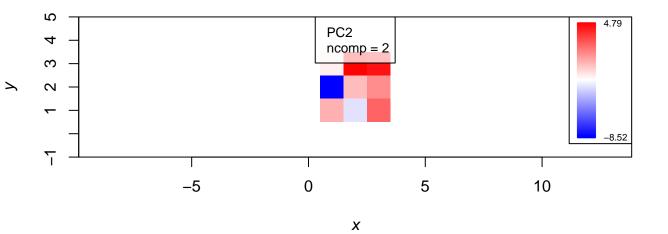


#### **PCA** for two components

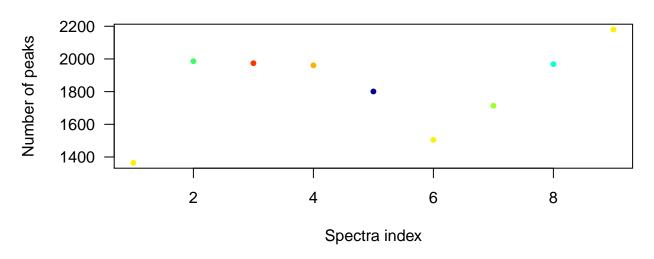




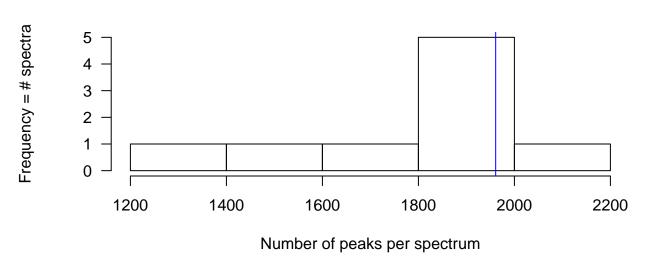


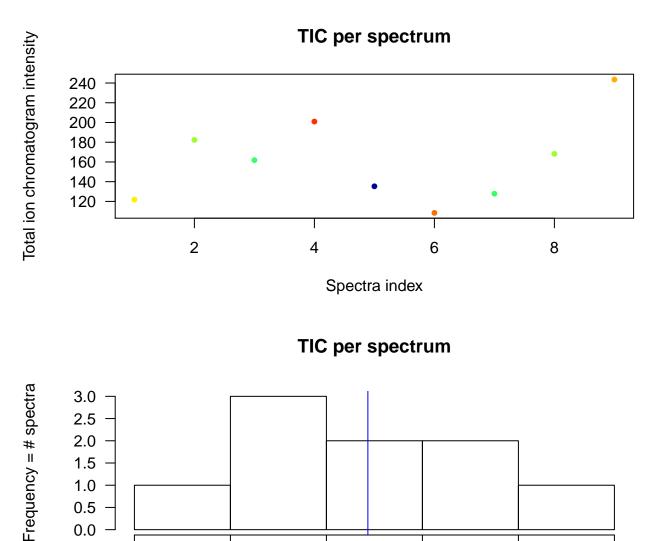


#### Number of peaks per spectrum



#### Number of peaks per spectrum





0.5 0.0

4.6

4.8

log(TIC per spectrum)

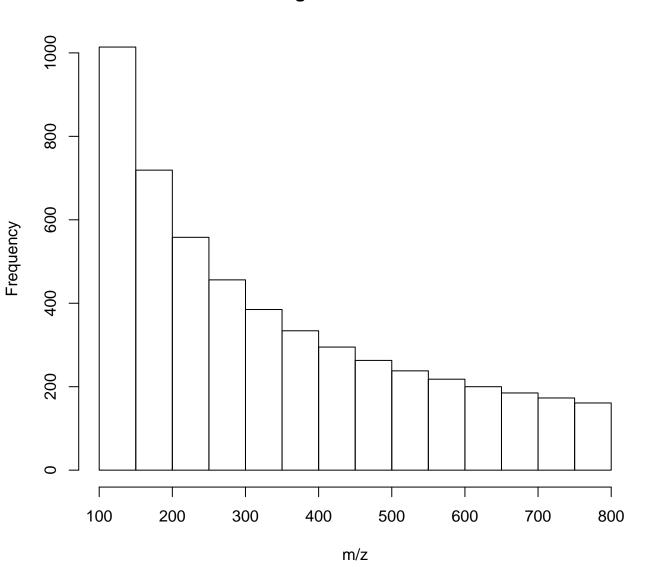
5.2

5.4

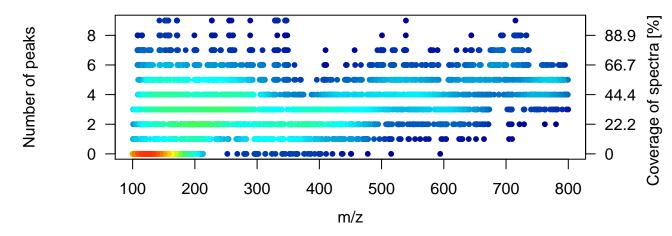
5.6

5.0

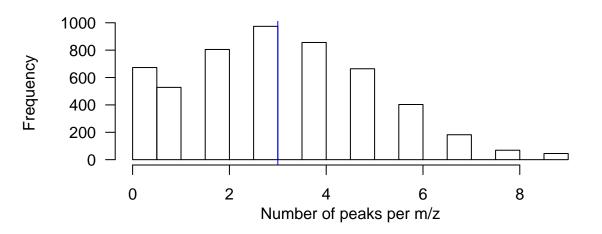
## Histogram of m/z values



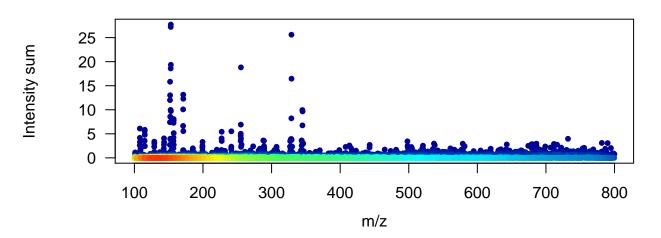
#### Number of peaks per m/z



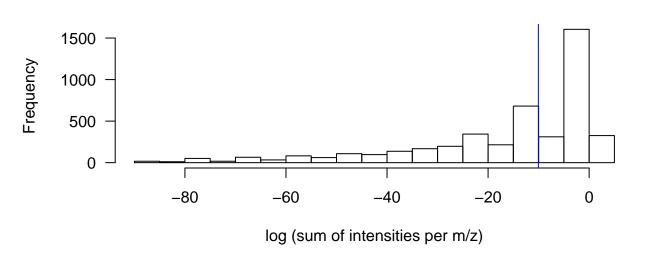
#### Number of peaks per m/z



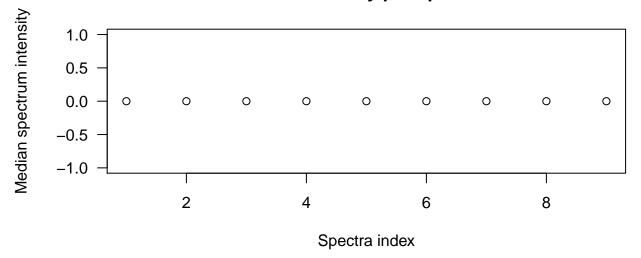
#### Sum of intensities per m/z



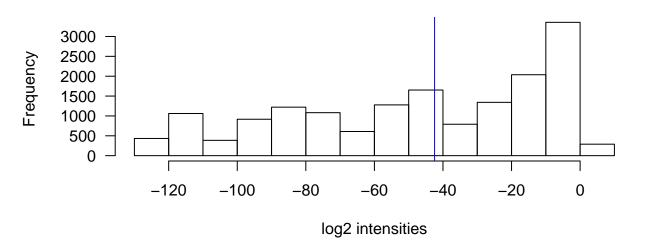
# Sum of intensities per m/z

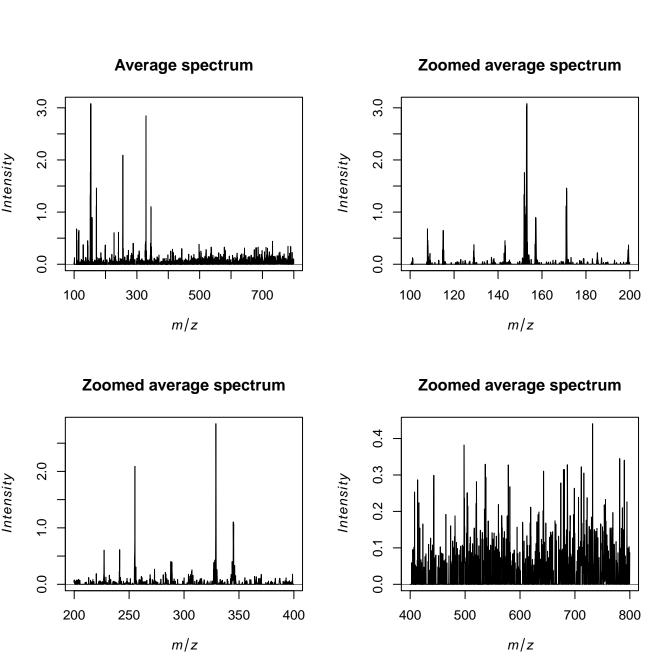


#### Median intensity per spectrum



#### Log2-transformed intensities





theor. m/z: 101.5 most abundant m/z: 101.491 closest m/z: 101.491 Average spectrum with data points Average spectrum 0.12 0.12 0.08 0.08 Intensity 0.04 0.04 0.00 0.00 101.0 101.5 102.0 102.5 103.0 101.0 101.5 102.0 102.5 103.0 m/zm/zAverage spectrum Average spectrum 0.020 0.08 Intensity 0.010 0.04 0.000 0.00 101.4 101.6 101.8 102.0 100 101 102 103 104 m/zm/z

Intensity

Intensity

Intensity

Intensity

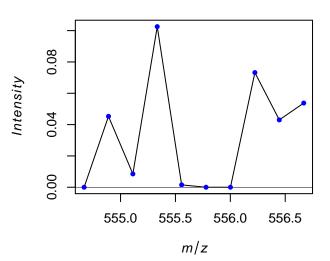
theor. m/z: 555.1 most abundant m/z: 555.1122 closest m/z: 555.1122

#### Average spectrum

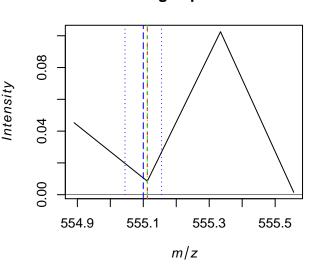
# 555.0 555.5 556.0 556.5 m/z

Intensity

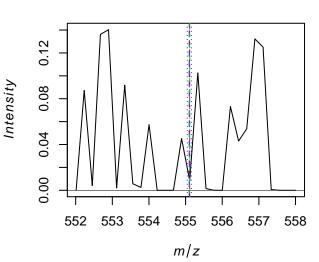
#### Average spectrum with data points

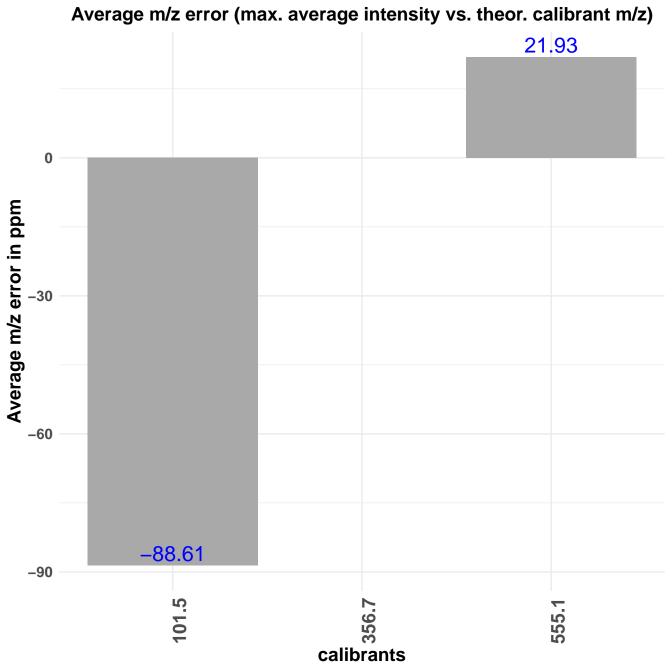


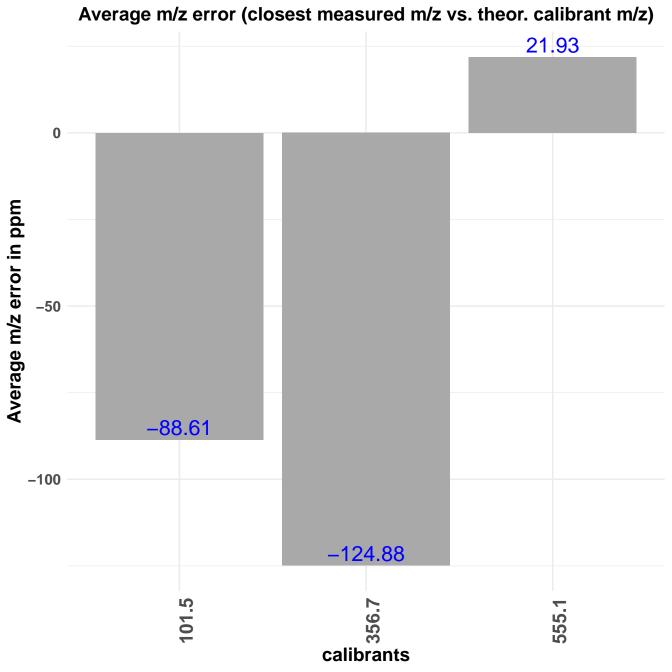
Average spectrum



Average spectrum







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

