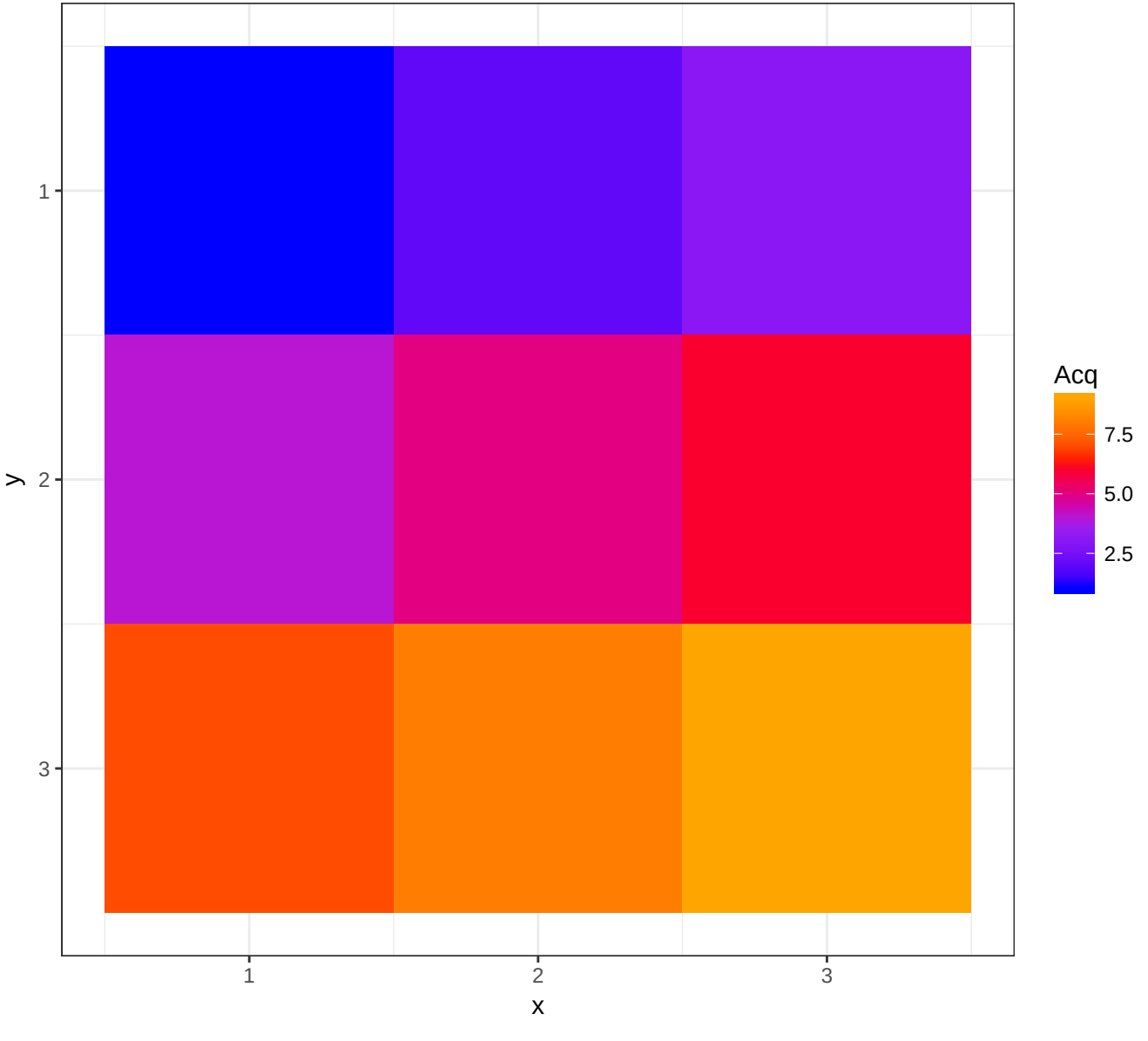
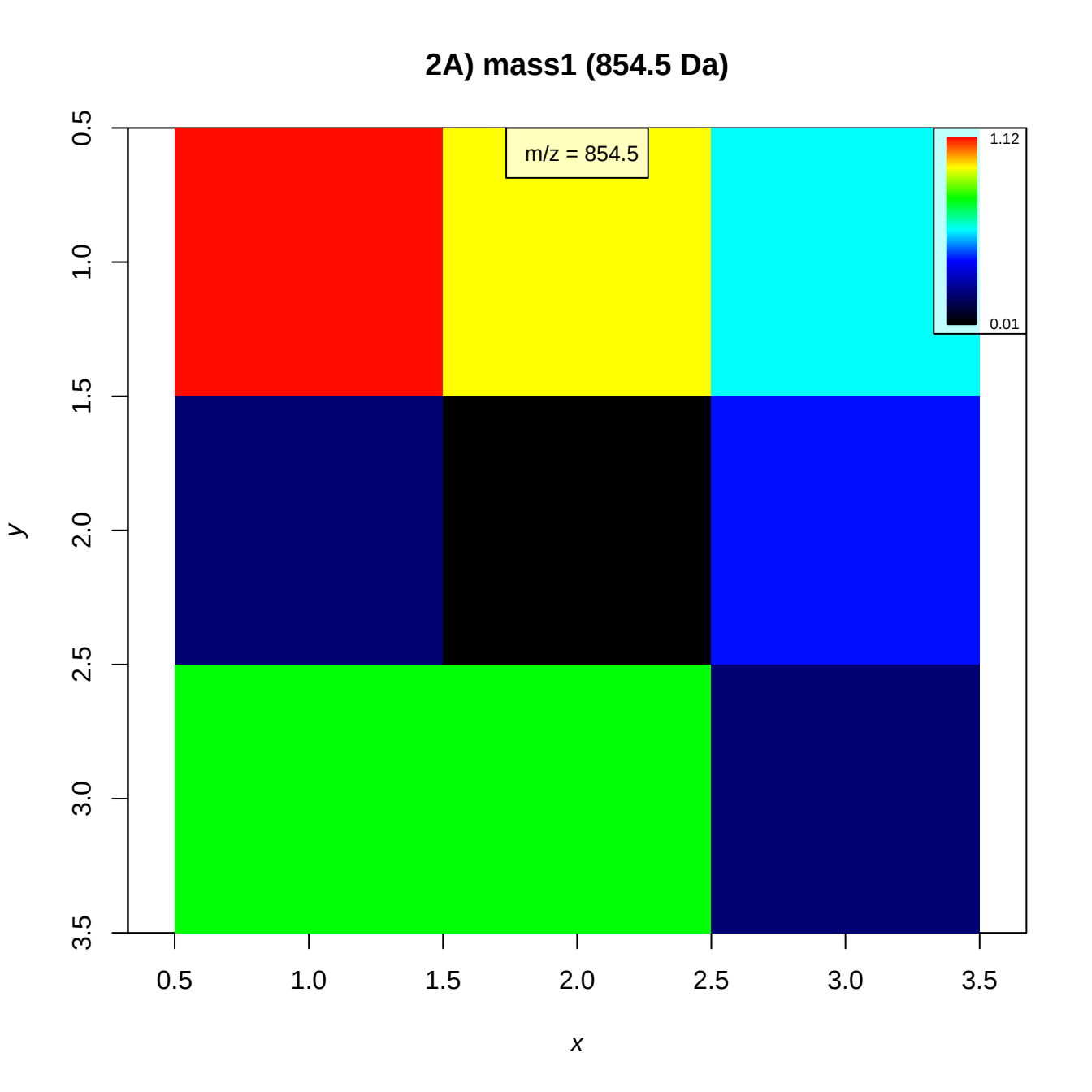
Quality control of MSI data

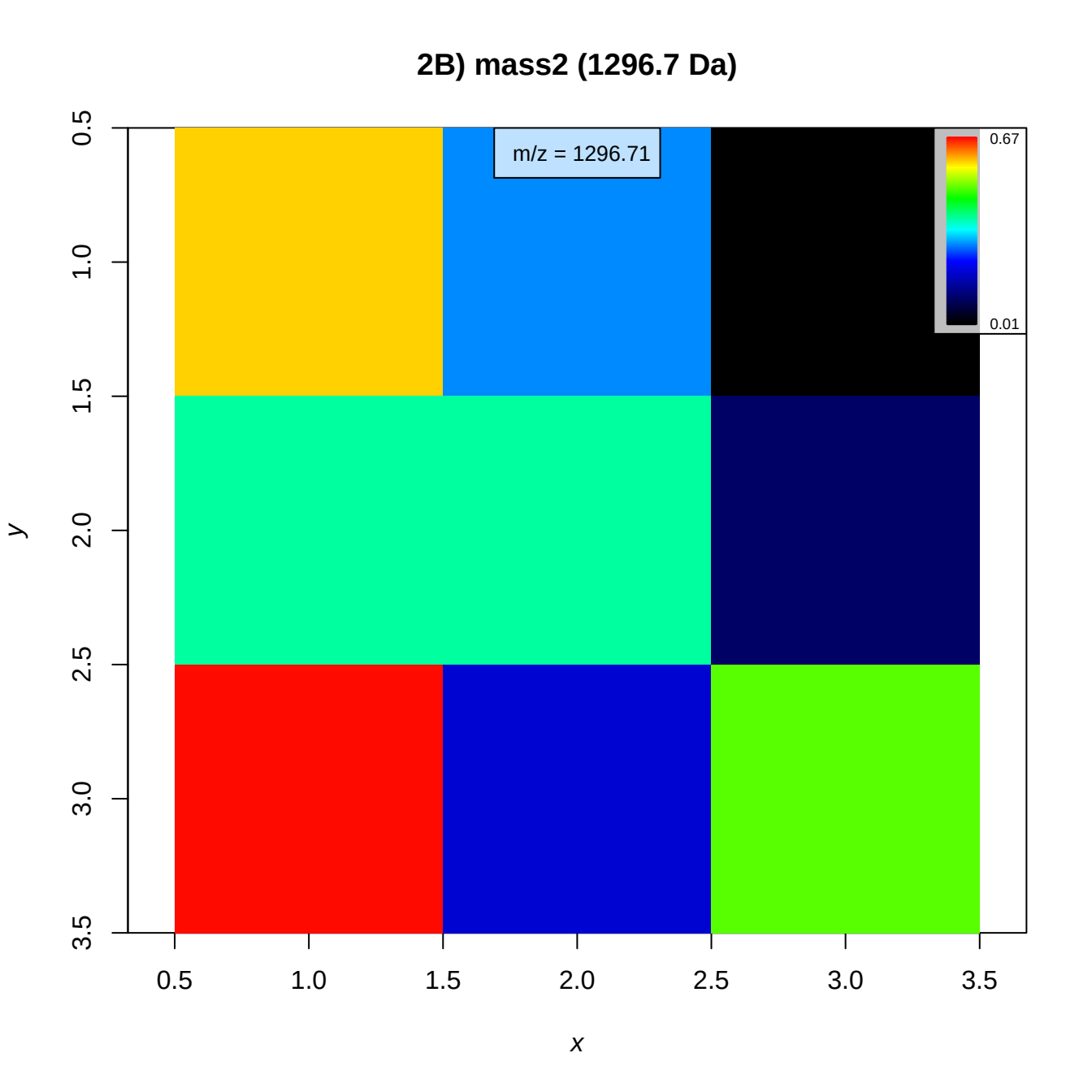
Filename: Testfile_analyze75

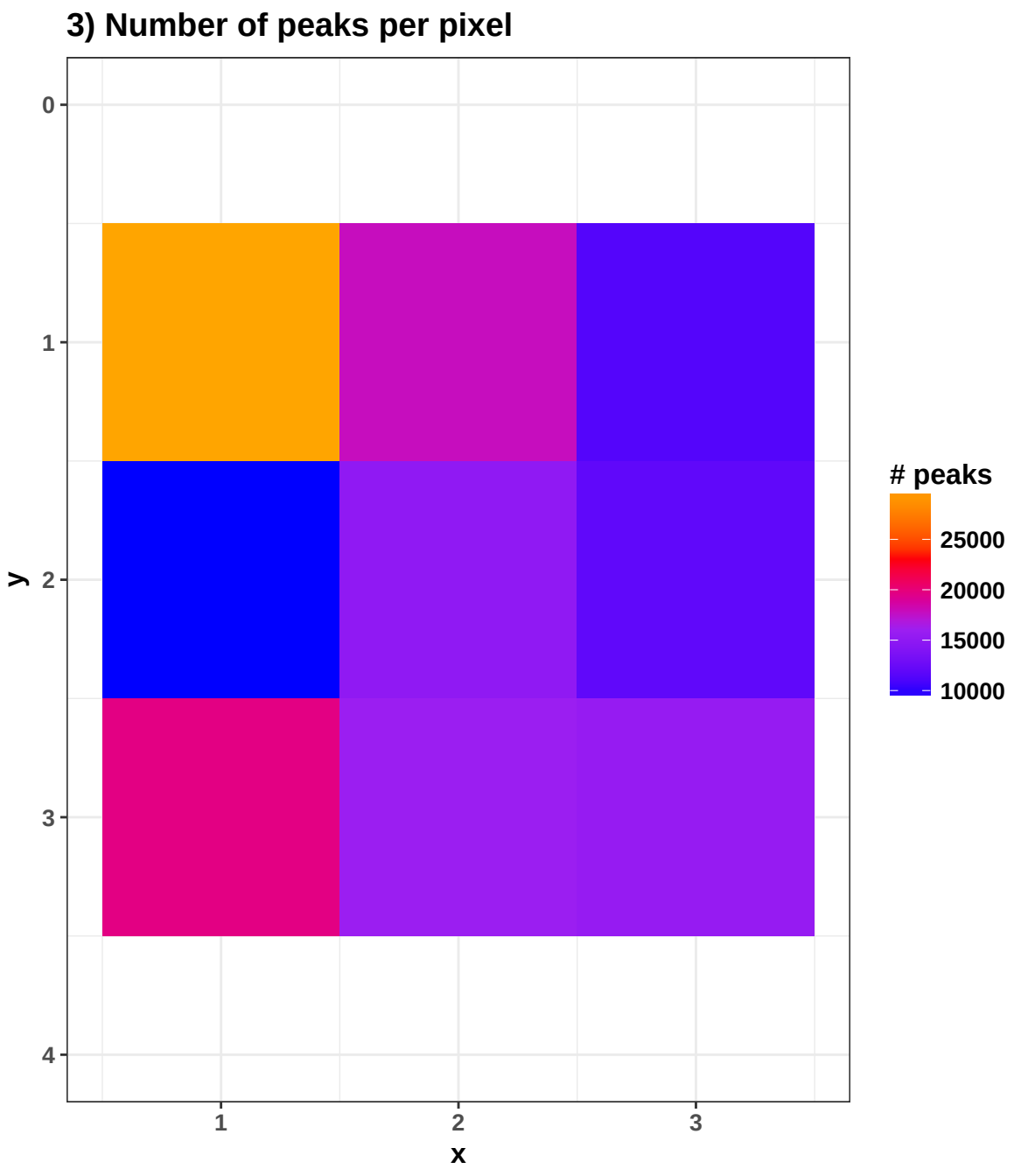
properties	values
Number of mz features	58031
Range of mz values [Da]	699.75 − 1916.29
Number of pixels	9
Range of x coordinates	1 − 3
Range of y coordinates	1 − 3
Range of intensities	0 − 146
Median of intensities	0
Intensities > 0	28.02 %
Number of zero TICs	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# valid peptidemasses	2

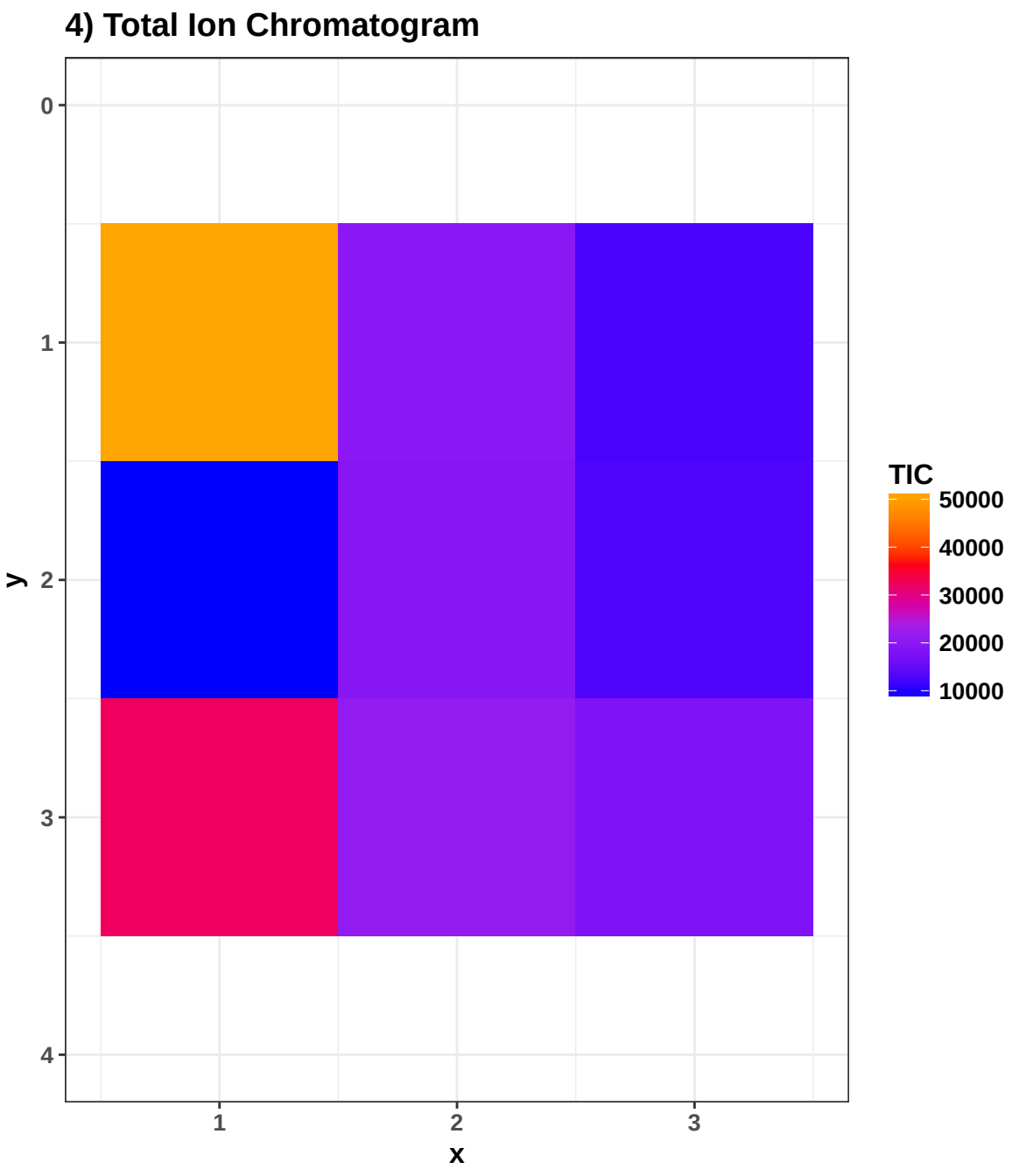
1) Order of Acquisition

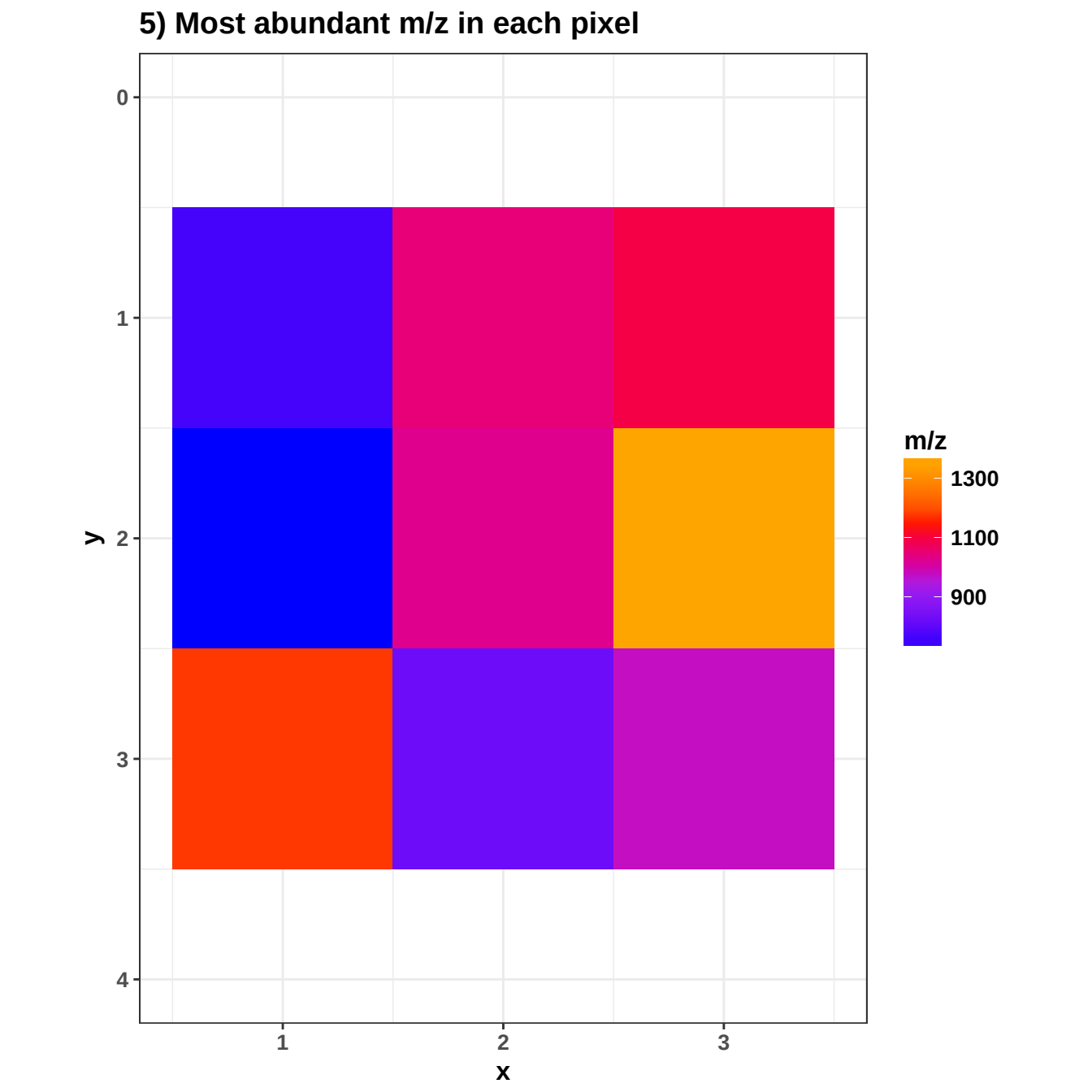



2A) mass1 (854.5 Da)
m/z = 854.5
1.12
0.01
0.5
1.0
1.5
2.0
2.5
3.0
3.5
y
x

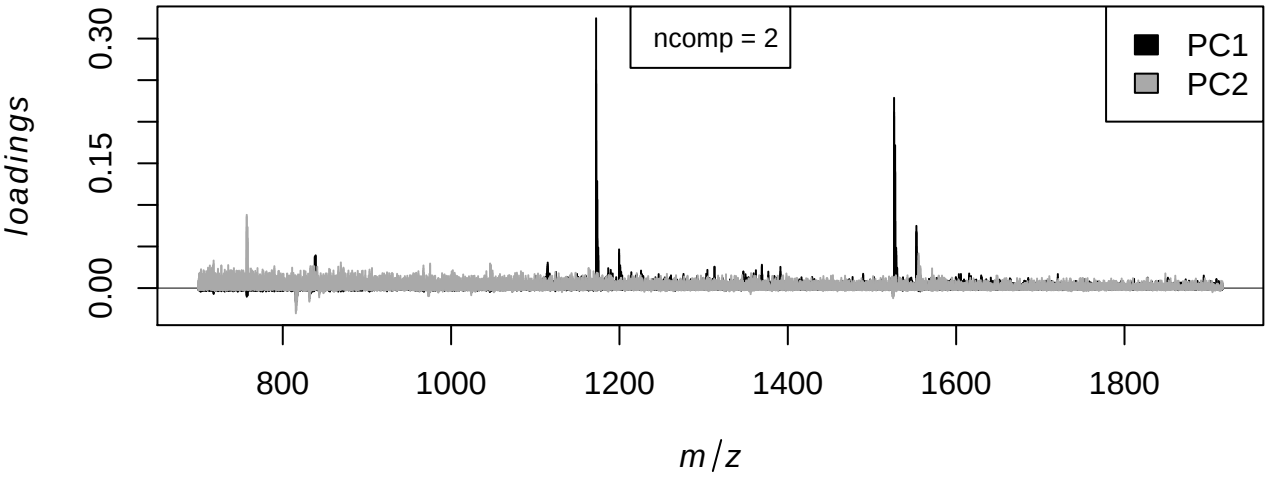

2B) mass2 (1296.7 Da)
m/z = 1296.71
0.67
0.01
y
x
0.5
1.0
1.5
2.0
2.5
3.0
3.5

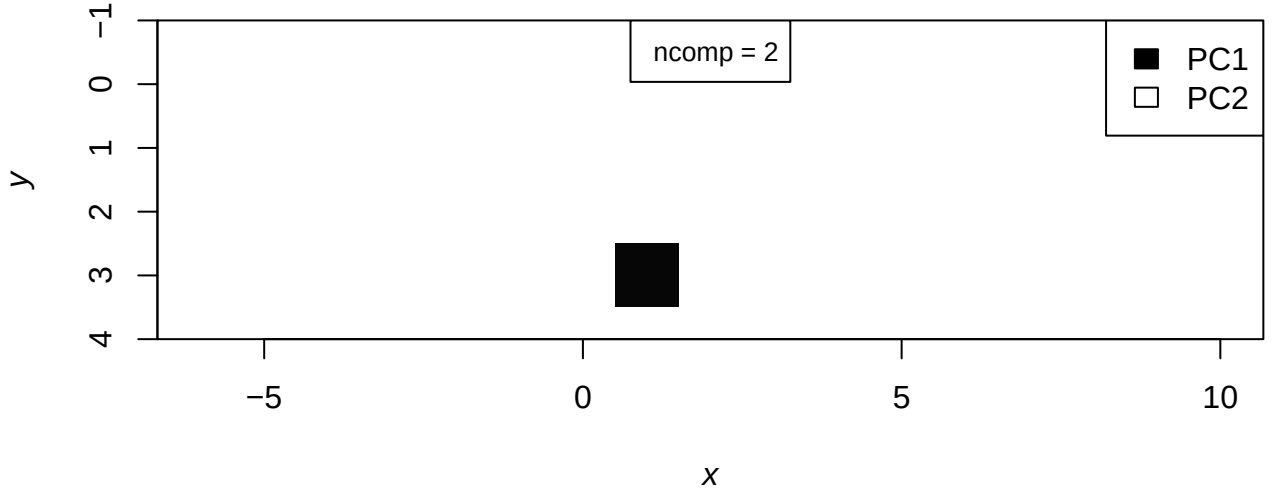

3) Number of peaks per pixel
0
1
2
3
4
y
1
2
3
x
peaks
25000
20000
15000
10000

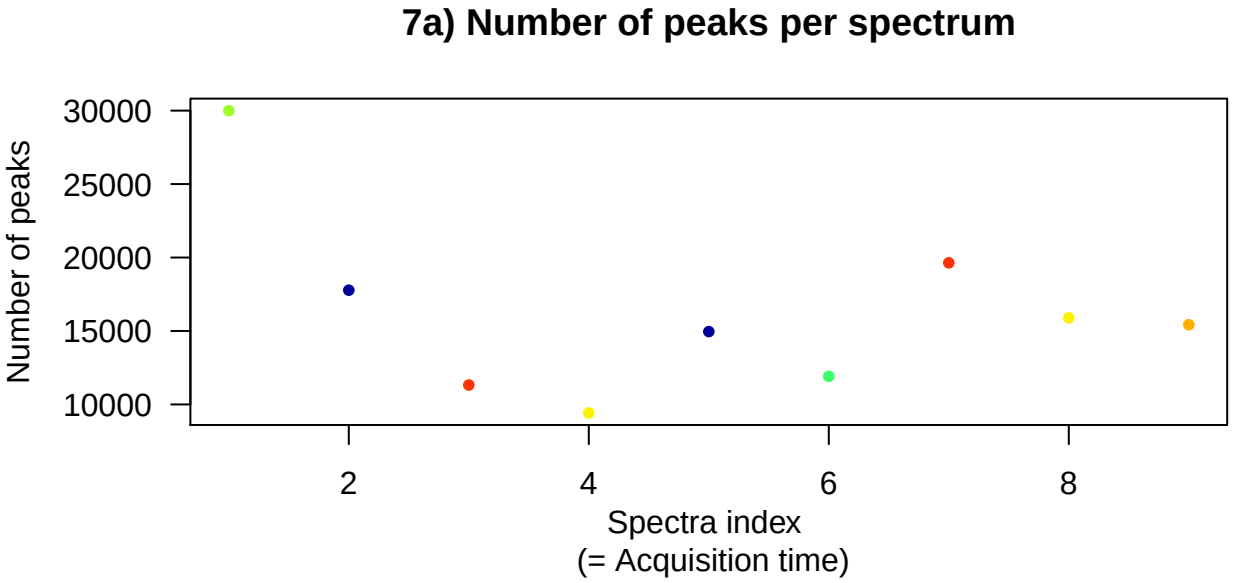

4) Total Ion Chromatogram
0
1
2
3
4
y
1
2
3
x
TIC
50000
40000
30000
20000
10000

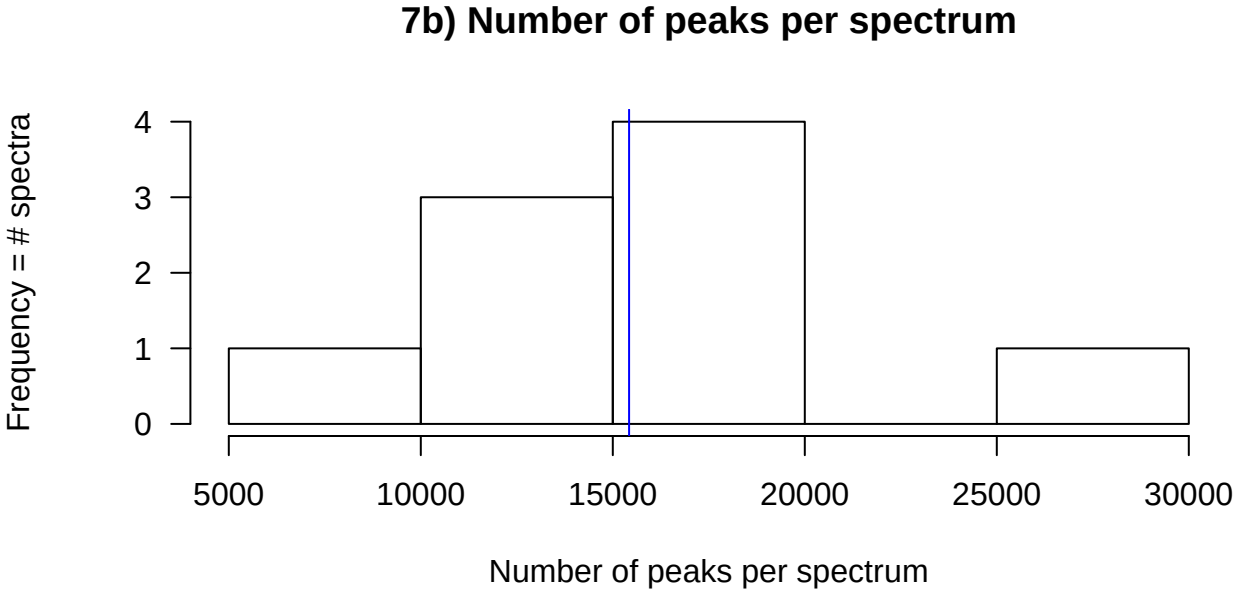

5) Most abundant m/z in each pixel
0
1
2
3
4
y
1
2
3
x
m/z
1300
1100
900

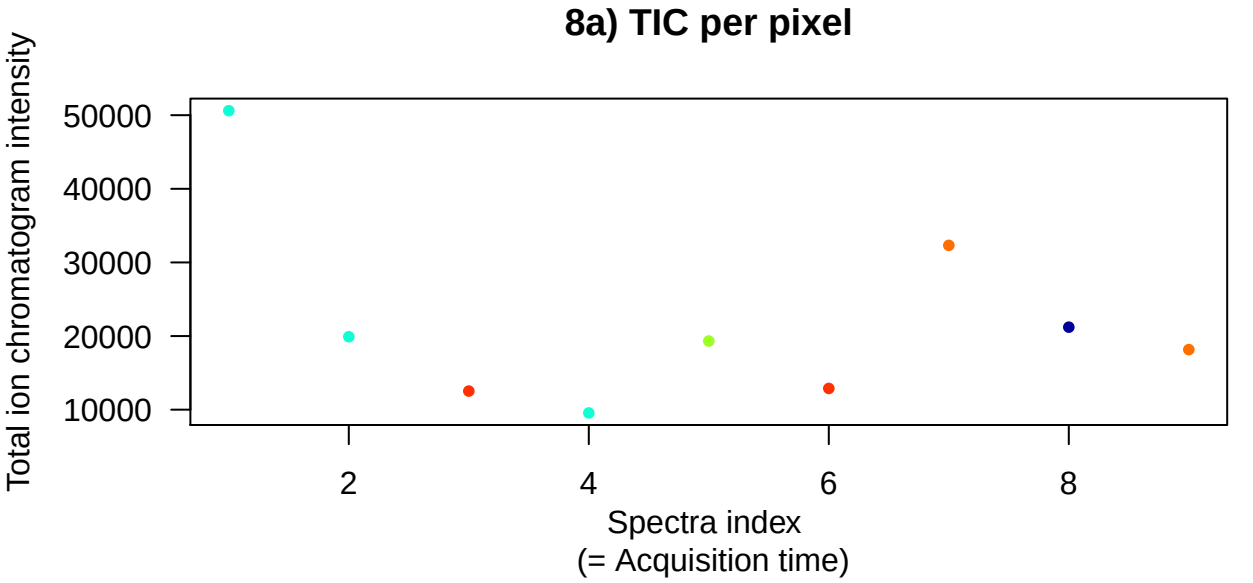
6) PCA for two components

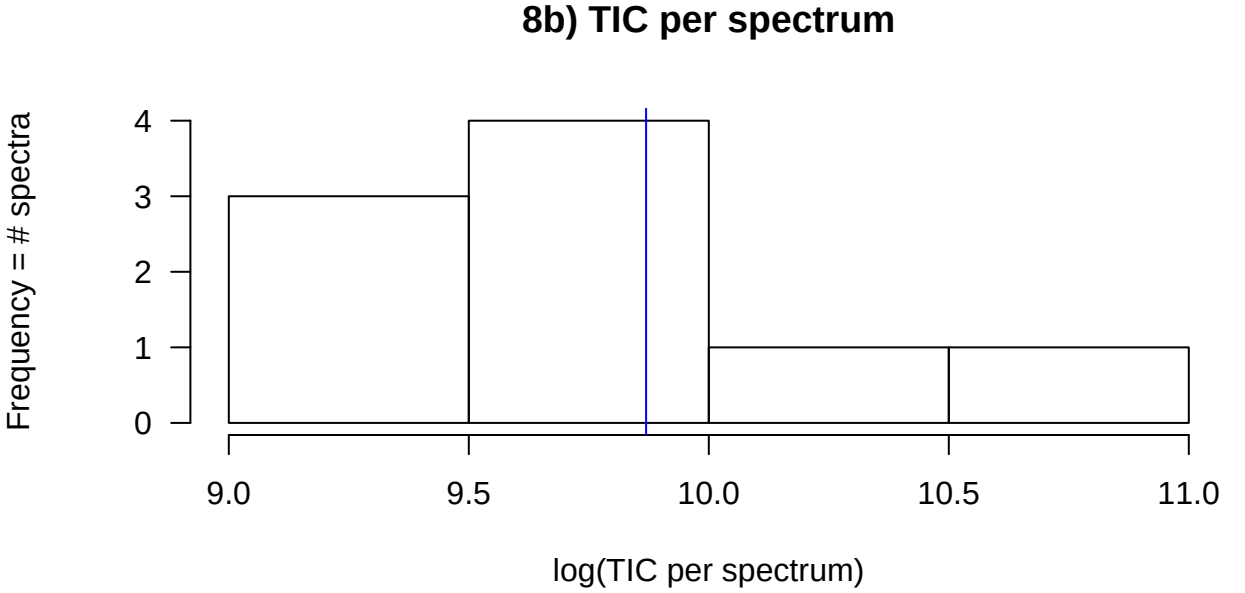


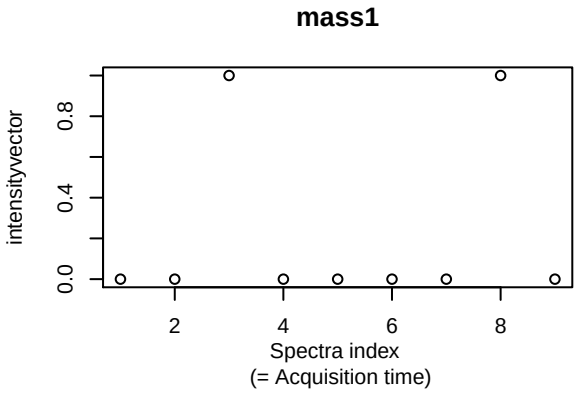


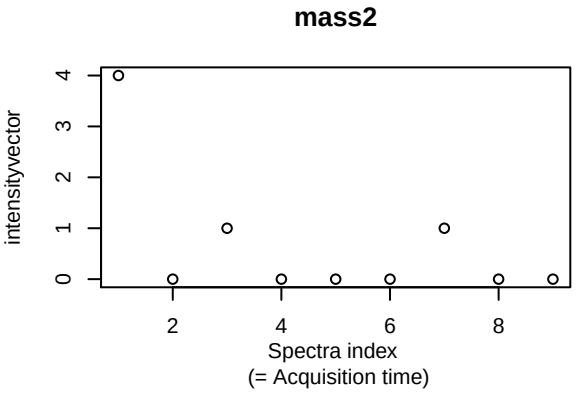

7a) Number of peaks per spectrum
Number of peaks
30000
25000
20000
15000
10000
2
4
6
8
Spectra index
(= Acquisition time)

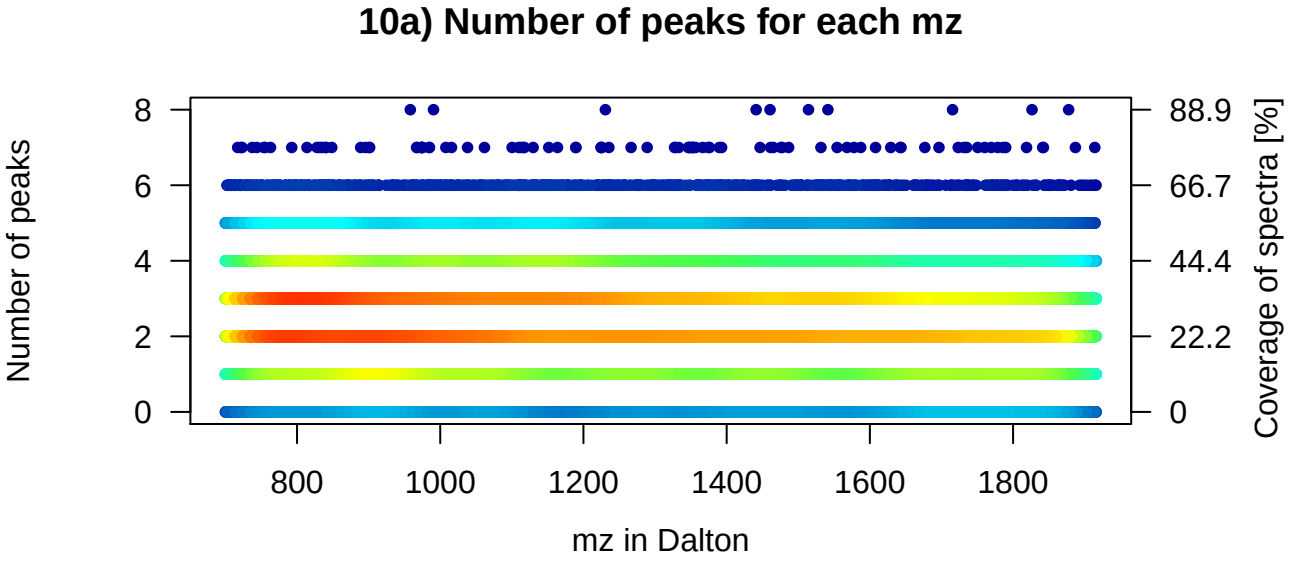

7b) Number of peaks per spectrum
Frequency = # spectra
4
3
2
1
0
5000
10000
15000
20000
25000
30000
Number of peaks per spectrum

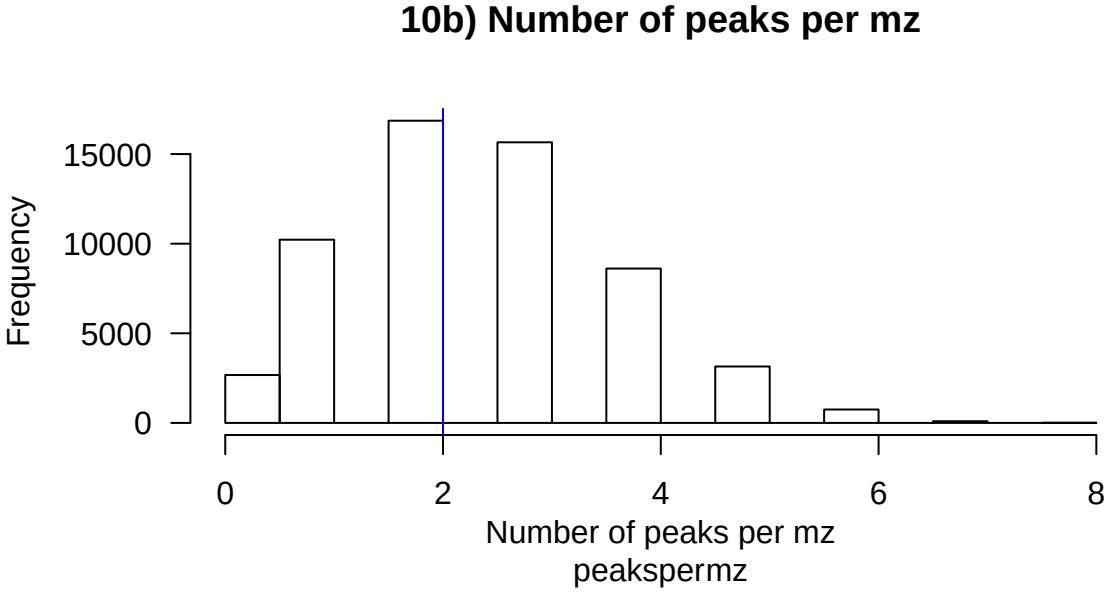

8a) TIC per pixel
Total ion chromatogram intensity
50000
40000
30000
20000
10000
2
4
6
8
Spectra index
(= Acquisition time)

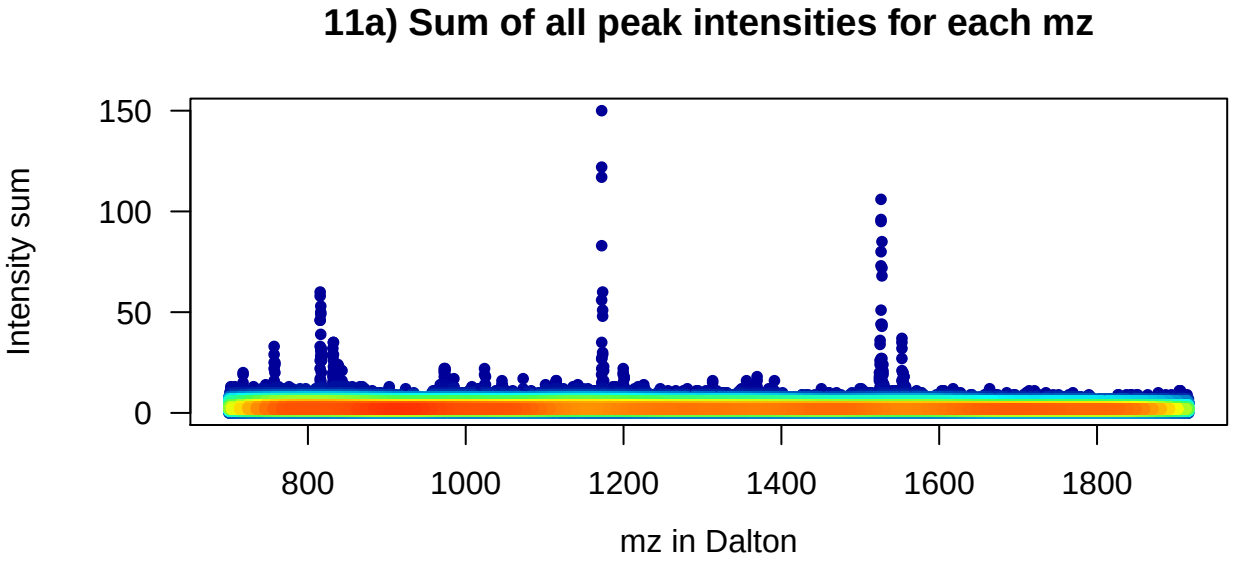

8b) TIC per spectrum
Frequency = # spectra
4
3
2
1
0
9.0
9.5
10.0
10.5
11.0
log(TIC per spectrum)

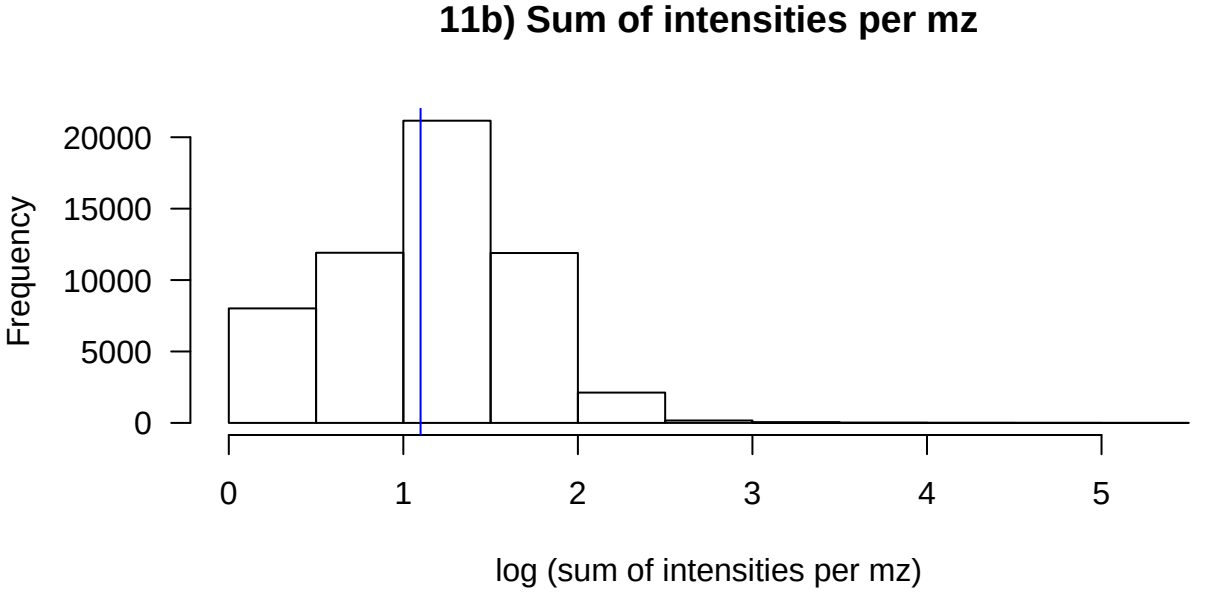

mass1
intensityvector
0.0
0.4
0.8
2
4
6
8
Spectra index
(= Acquisition time)


mass2
intensityvector
0
1
2
3
4
2
4
6
8
Spectra index
(= Acquisition time)

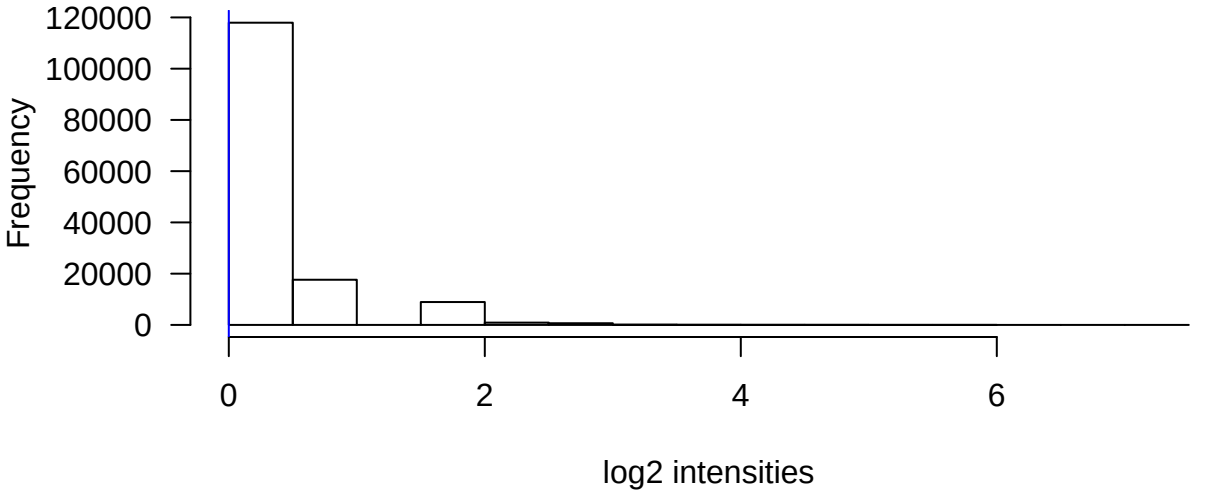

10a) Number of peaks for each mz
Number of peaks
0
2
4
6
8
Coverage of spectra [%]
0
22.2
44.4
66.7
88.9
800
1000
1200
1400
1600
1800
mz in Dalton


10b) Number of peaks per mz
Frequency
0
5000
10000
15000
0
2
4
6
8
Number of peaks per mz
peakspermz

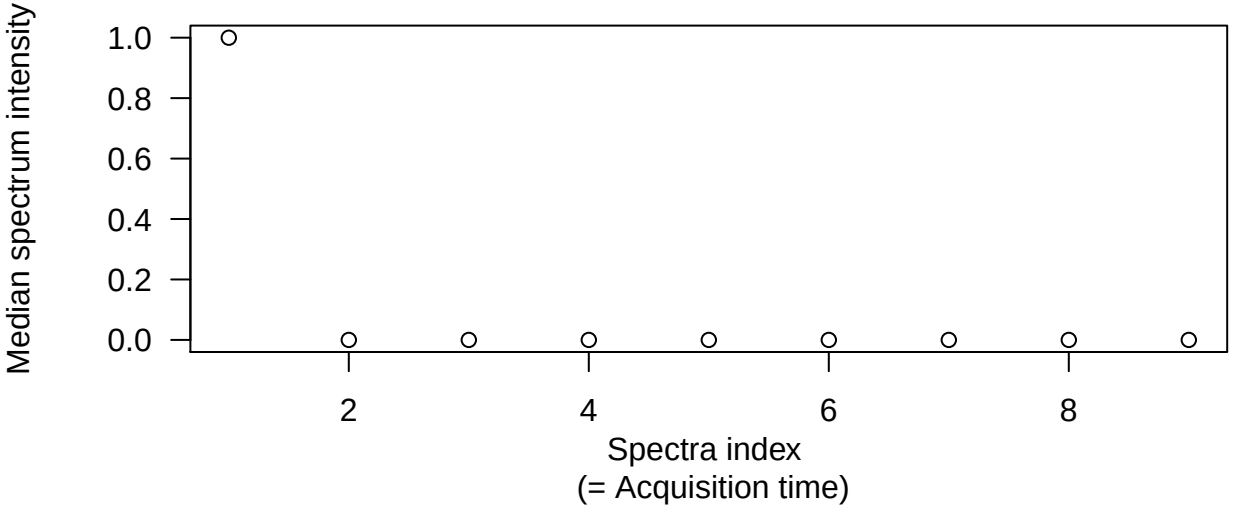

11a) Sum of all peak intensities for each mz
Intensity sum
150
100
50
0
800
1000
1200
1400
1600
1800
mz in Dalton

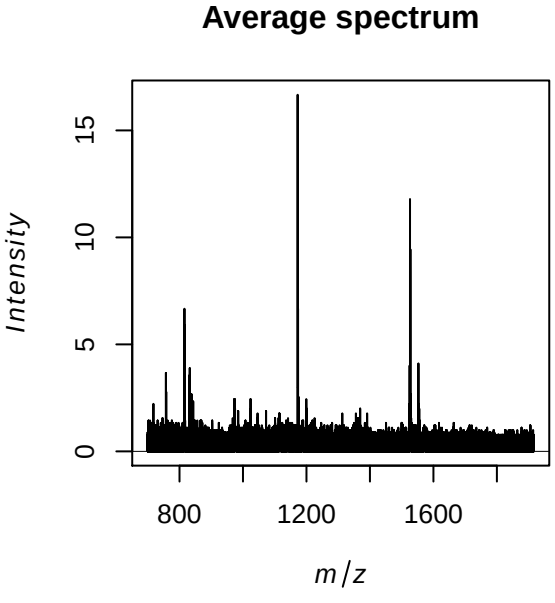

11b) Sum of intensities per mz
Frequency
20000
15000
10000
5000
0
0
1
2
3
4
5
log (sum of intensities per mz)

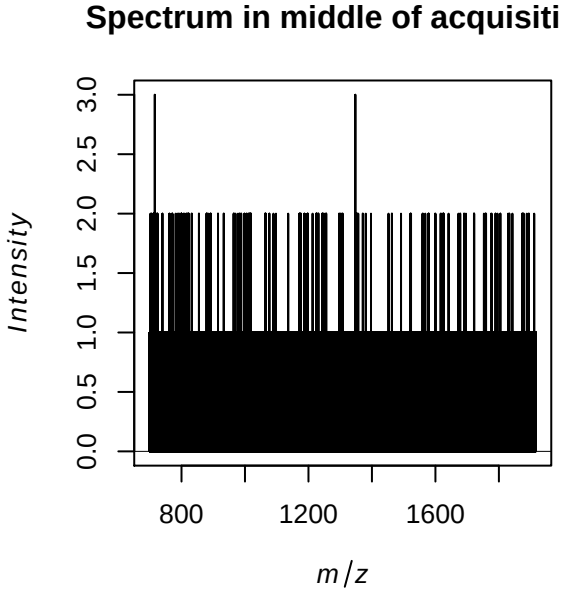
12a) Log2−transformed intensities

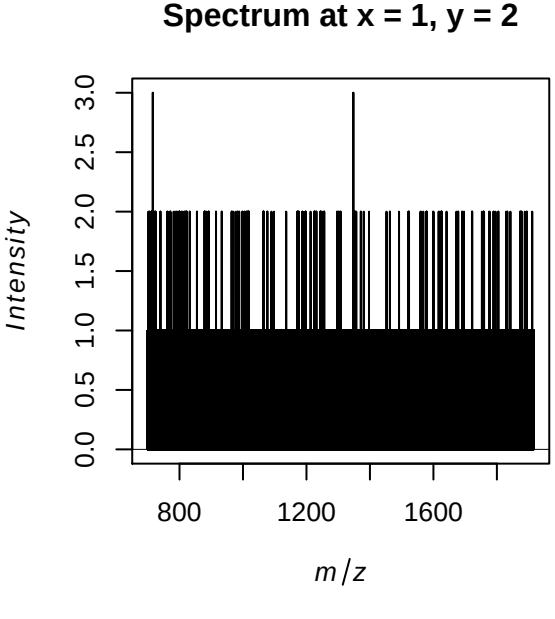


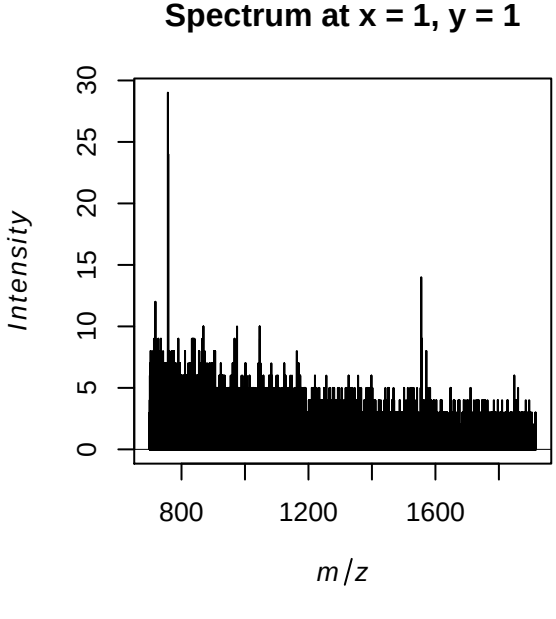
12b) Median intensity per spectrum




Average spectrum
Intensity
0
5
10
15
800
1200
1600
m/z


Spectrum in middle of acquisition
Intensity
0.0
0.5
1.0
1.5
2.0
2.5
3.0
800
1200
1600
m/z


Spectrum at x = 1, y = 2
Intensity
0.0
0.5
1.0
1.5
2.0
2.5
3.0
800
1200
1600
m/z


Spectrum at x = 1, y = 1
Intensity
0
5
10
15
20
25
30
800
1200
1600
m/z