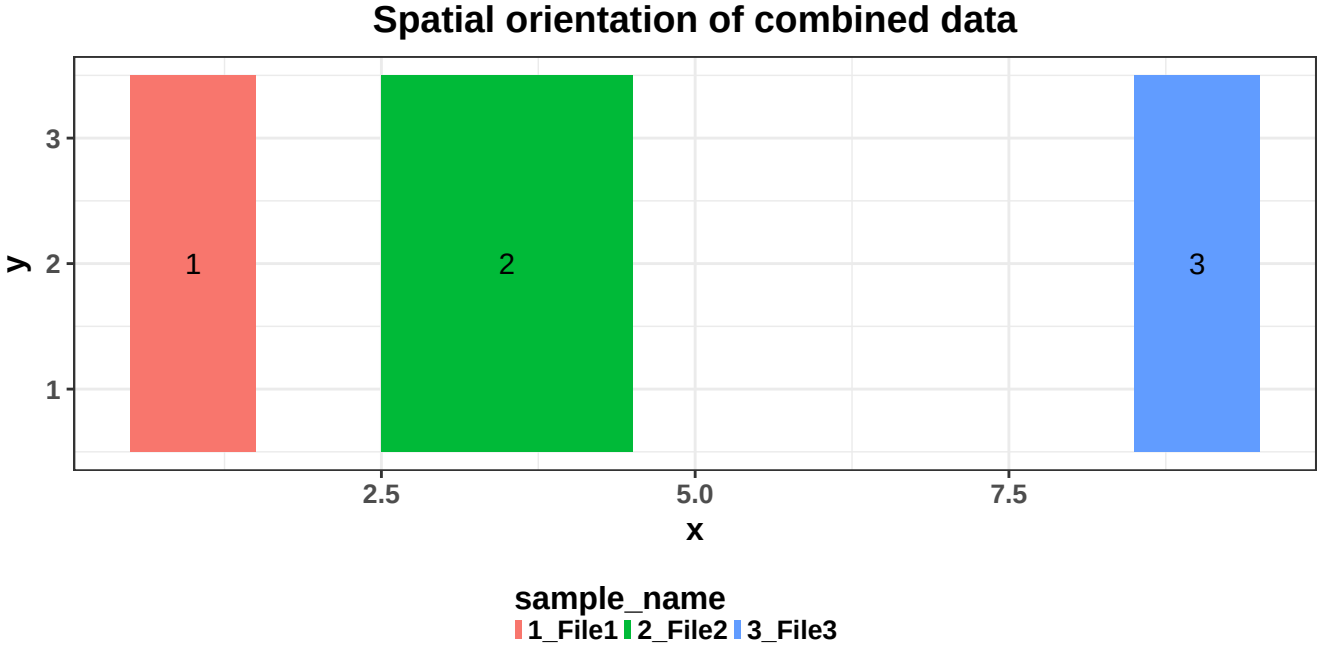
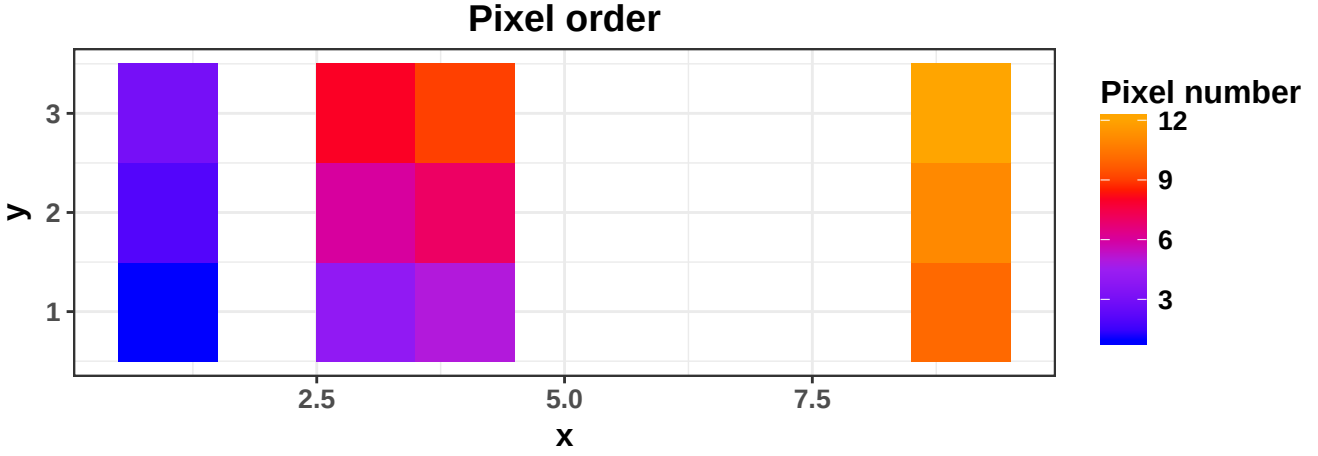
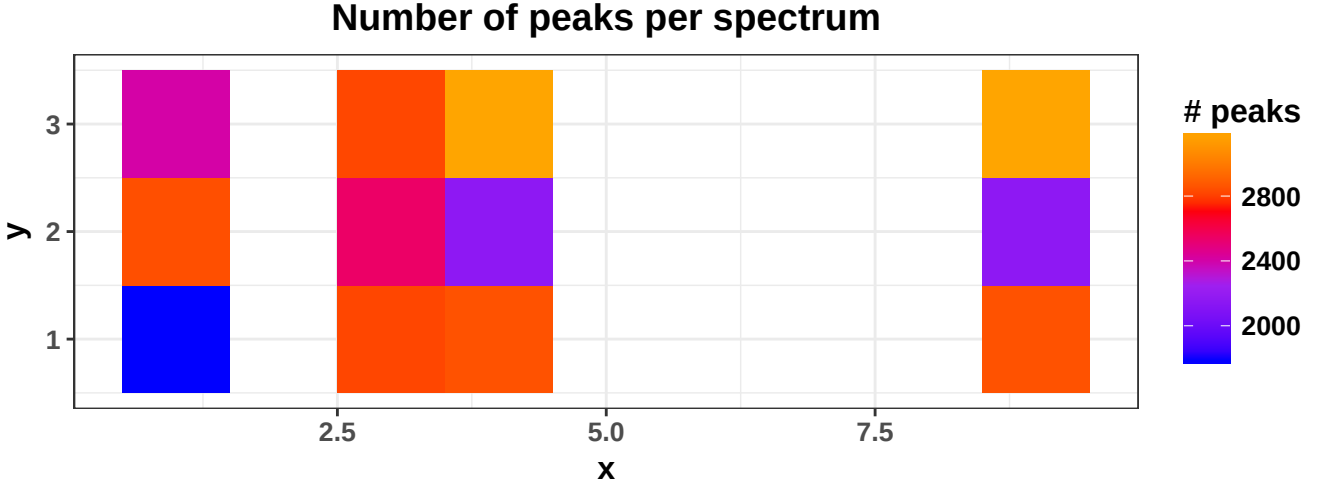
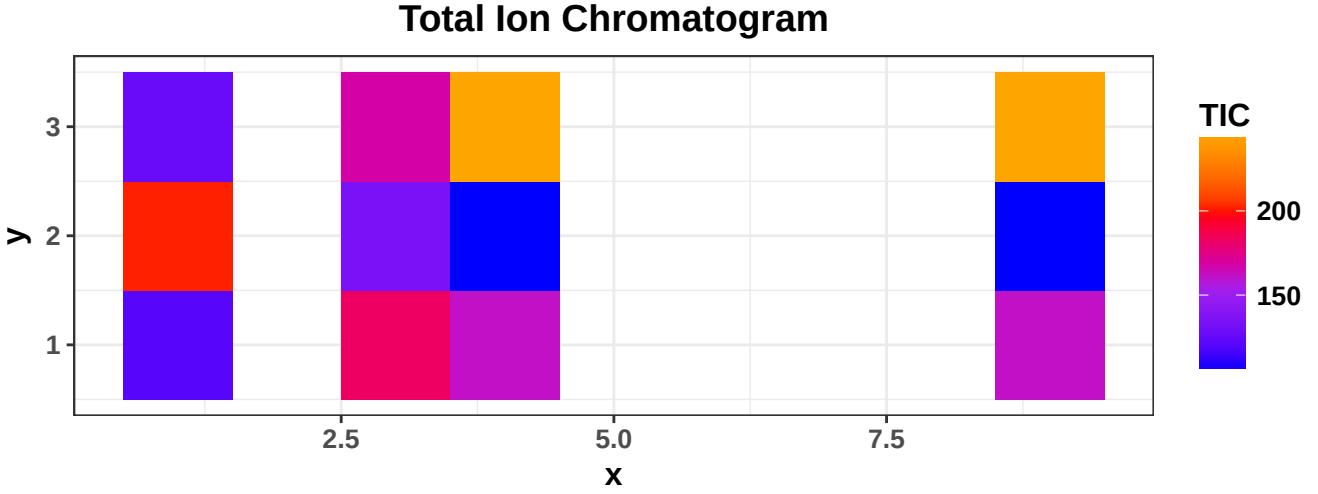
Testfile_rdata

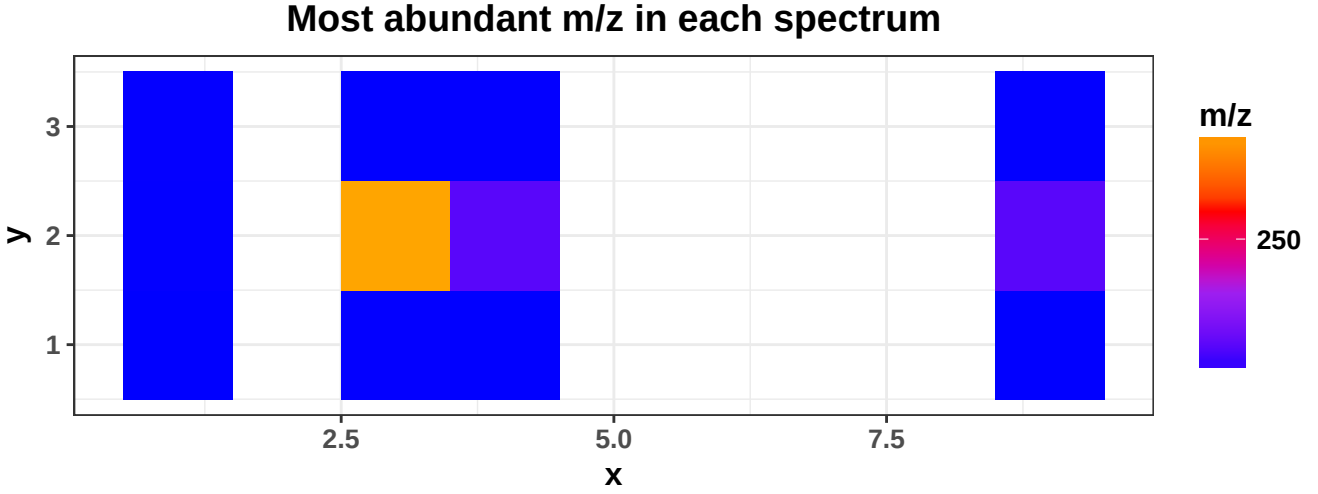
properties	values
Number of m/z features	8399
Range of m/z values	100.08 − 799.92
Number of pixels	12
Range of x coordinates	1 − 9
Range of y coordinates	1 − 3
Range of intensities	0 − 9.24
Median of intensities	0
Intensities > 0	31.29 %
Number of zero TICs	0
Median TIC	161.81
Median # peaks per spectrum	2811
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE
# peptides in None	0 / 0
# calibrants in None	0 / 0

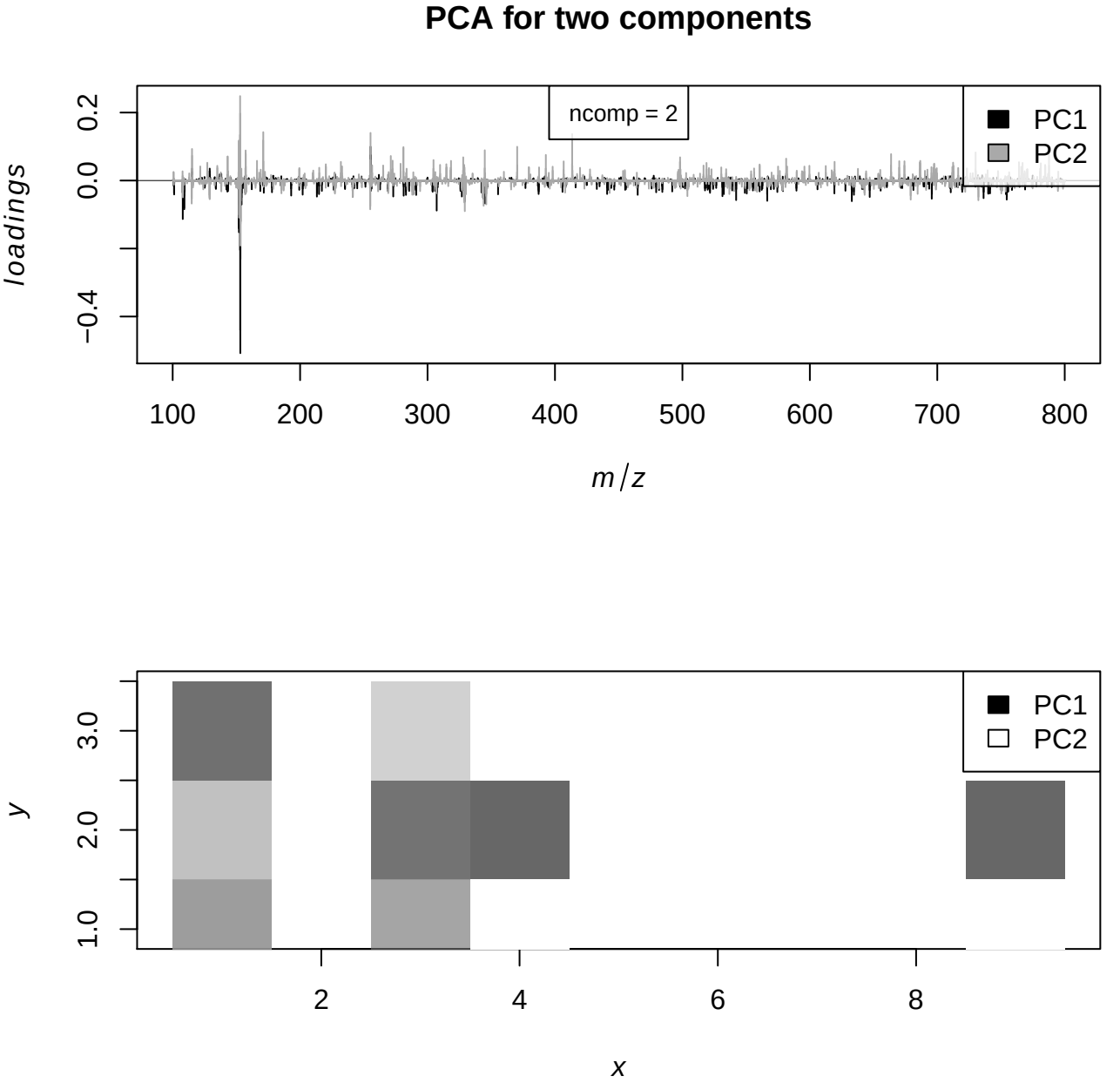

Spatial orientation of combined data
y
3
2
1
1
2
3
2.5
5.0
7.5
x
sample_name
1_File1
2_File2
3_File3

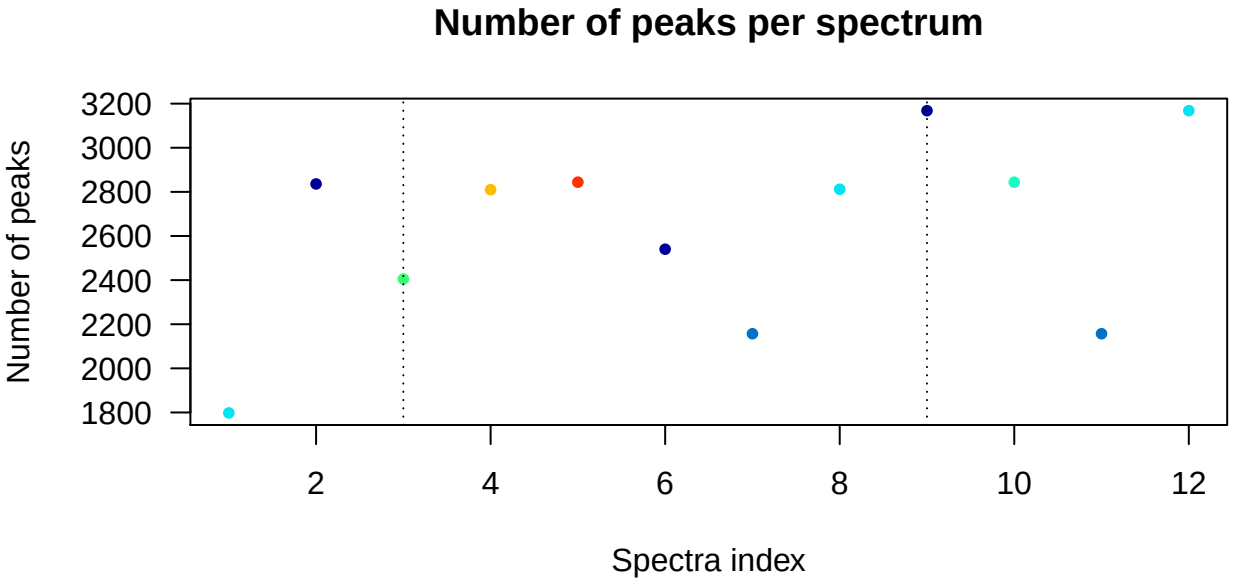

Pixel order
y
3
2
1
2.5
5.0
7.5
x
Pixel number
12
9
6
3

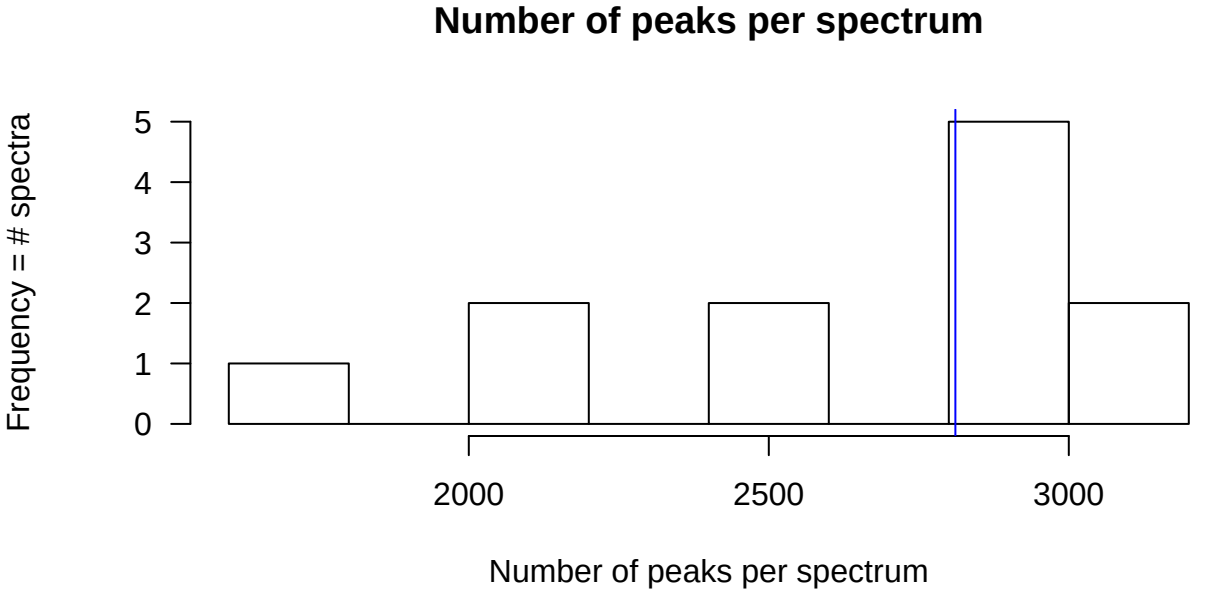

Number of peaks per spectrum
y
3
2
1
2.5
5.0
7.5
x
peaks
2800
2400
2000

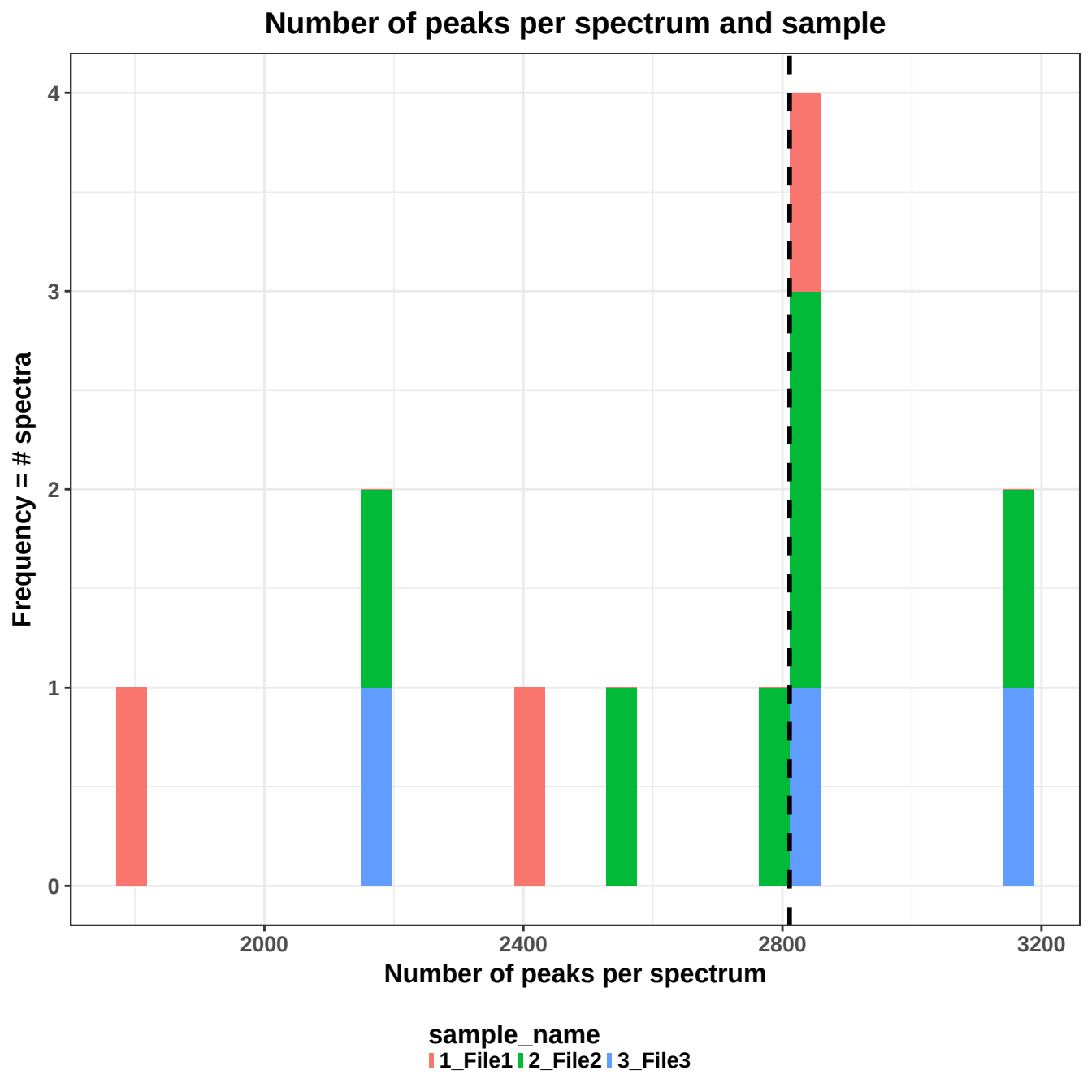

Total Ion Chromatogram
y
3
2
1
2.5
5.0
7.5
x
TIC
200
150

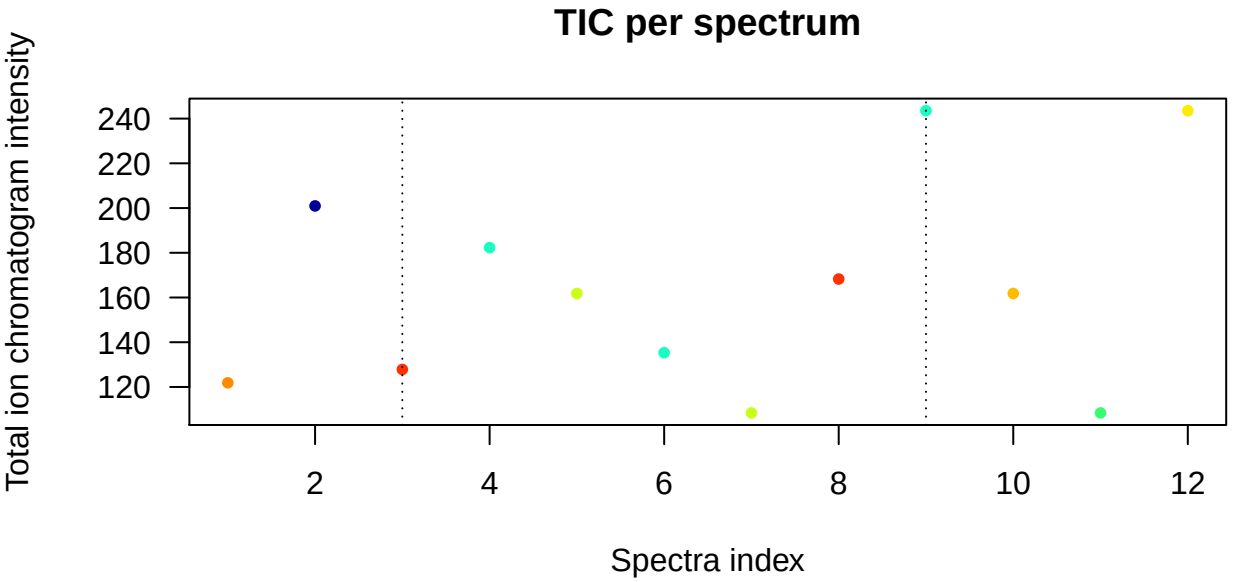

Most abundant m/z in each spectrum
y
3
2
1
2.5
5.0
7.5
x
m/z
250

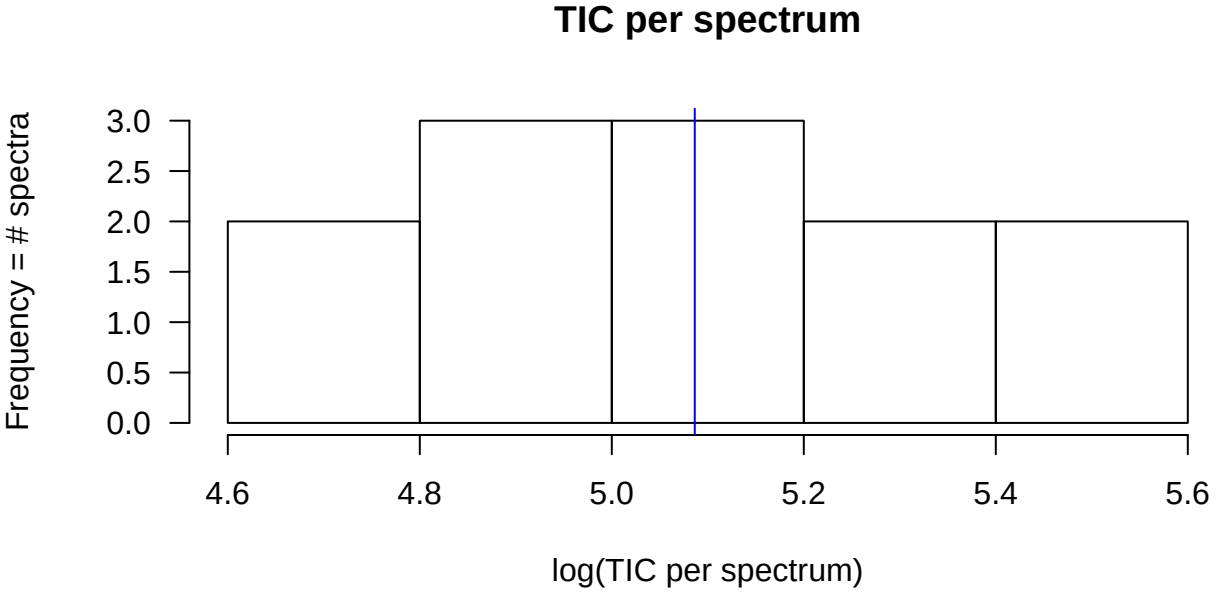

PCA for two components
ncomp = 2
PC1
PC2
loadings
0.2
0.0
−0.4
100
200
300
400
500
600
700
800
m/z
PC1
PC2
y
3.0
2.0
1.0
2
4
6
8
x

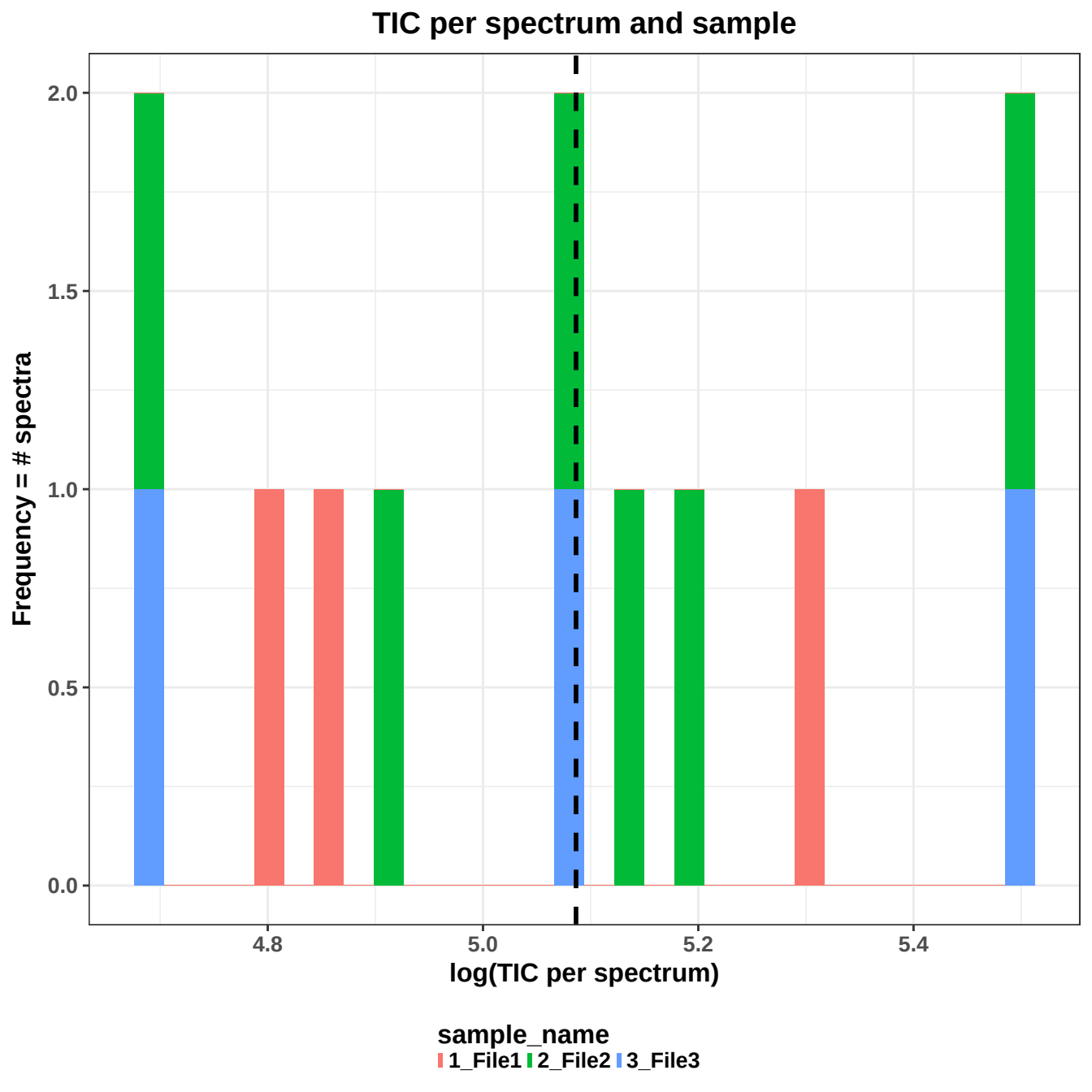

Number of peaks per spectrum
Number of peaks
3200
3000
2800
2600
2400
2200
2000
1800
2
4
6
8
10
12
Spectra index

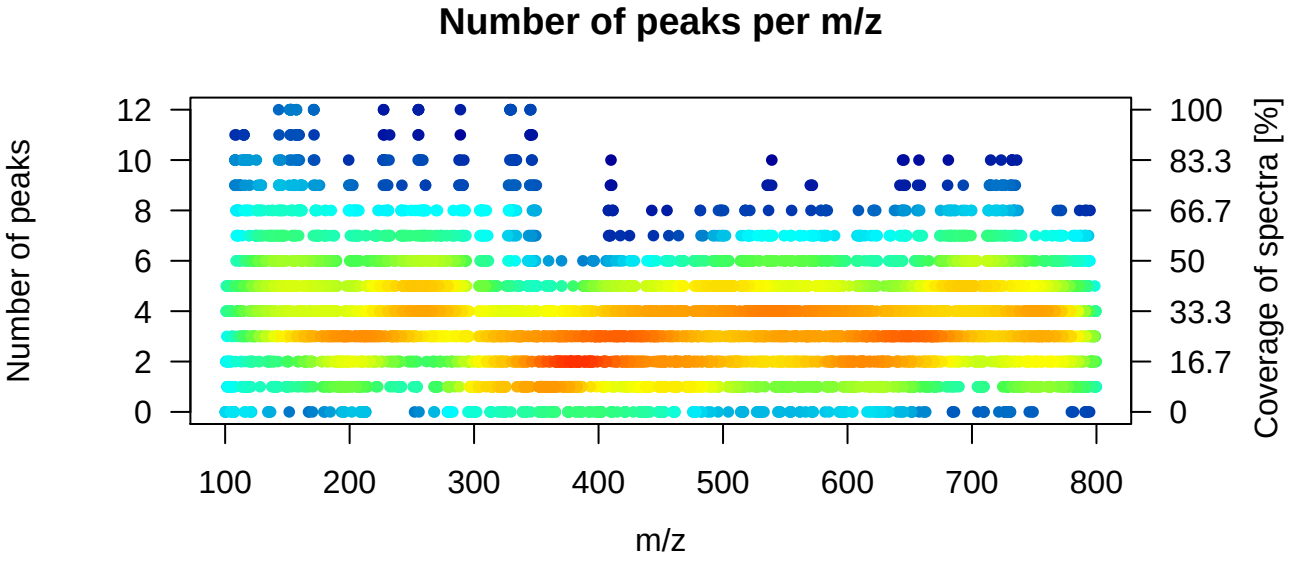

Number of peaks per spectrum
Frequency = # spectra
5
4
3
2
1
0
2000
2500
3000
Number of peaks per spectrum

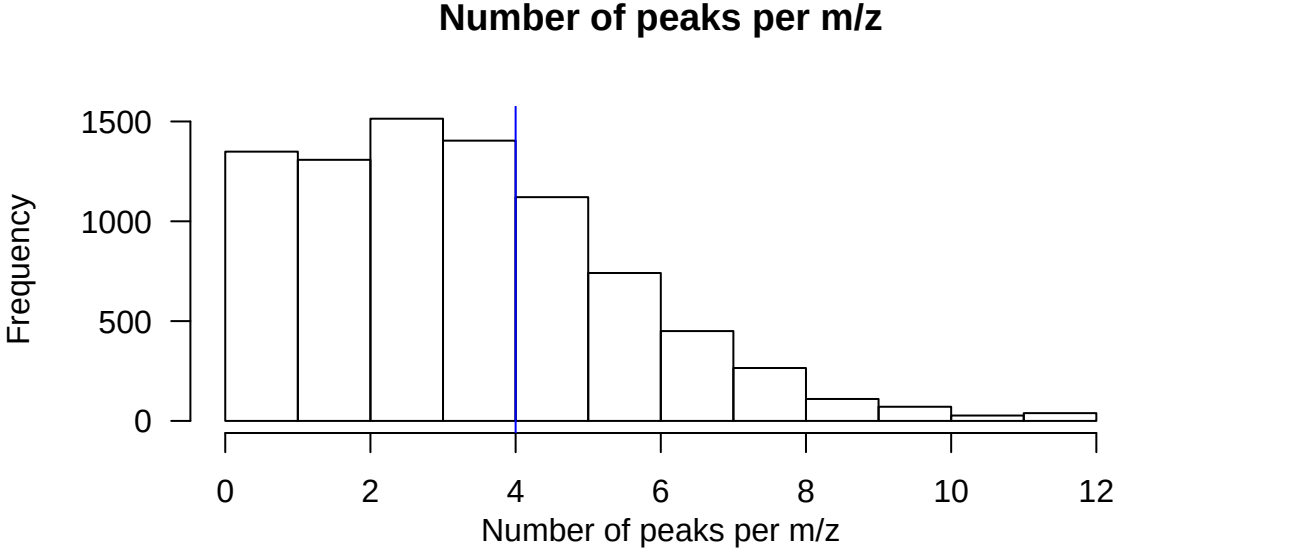

Number of peaks per spectrum and sample
Frequency = # spectra
4
3
2
1
0
2000
2400
2800
3200
Number of peaks per spectrum
sample_name
1_File1
2_File2
3_File3

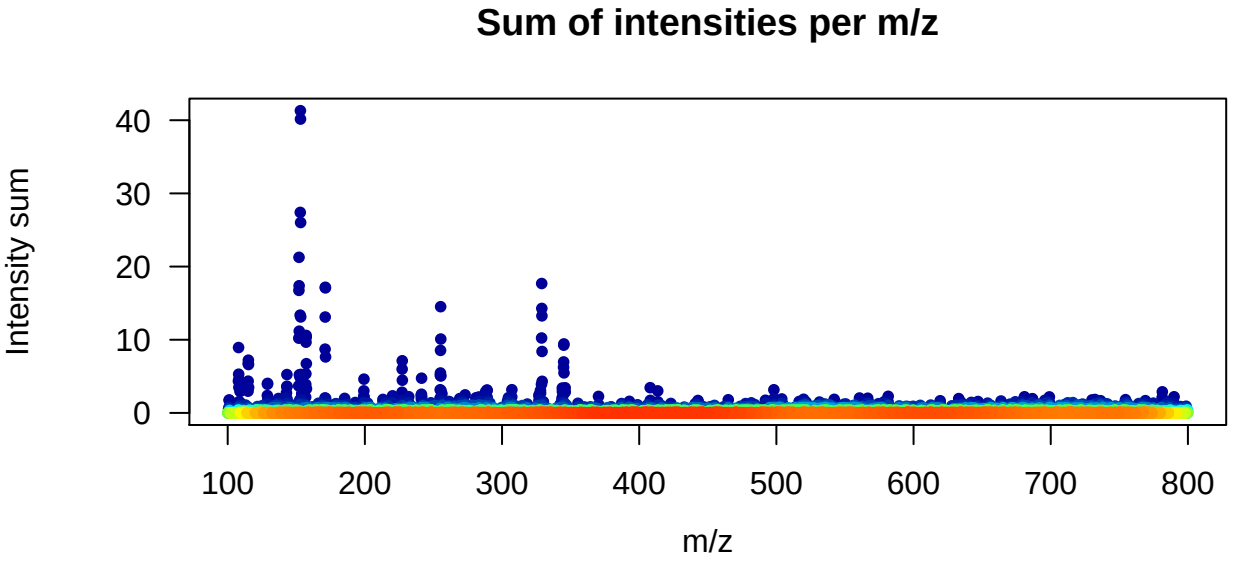

TIC per spectrum
Total ion chromatogram intensity
240
220
200
180
160
140
120
2
4
6
8
10
12
Spectra index

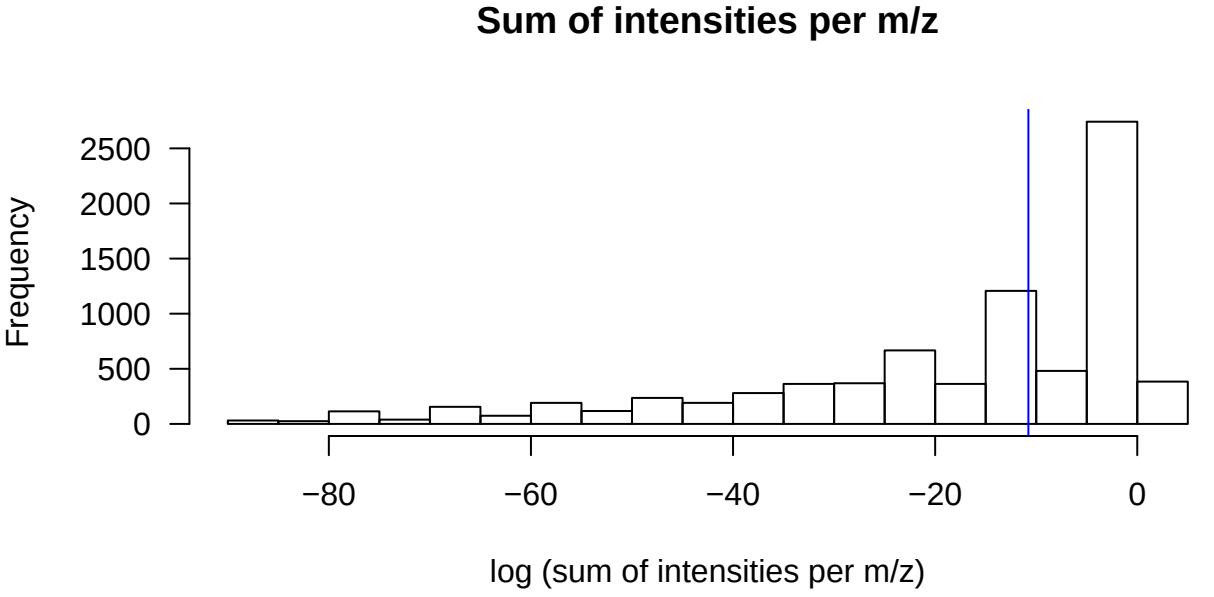

TIC per spectrum
Frequency = # spectra
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.6
4.8
5.0
5.2
5.4
5.6
log(TIC per spectrum)

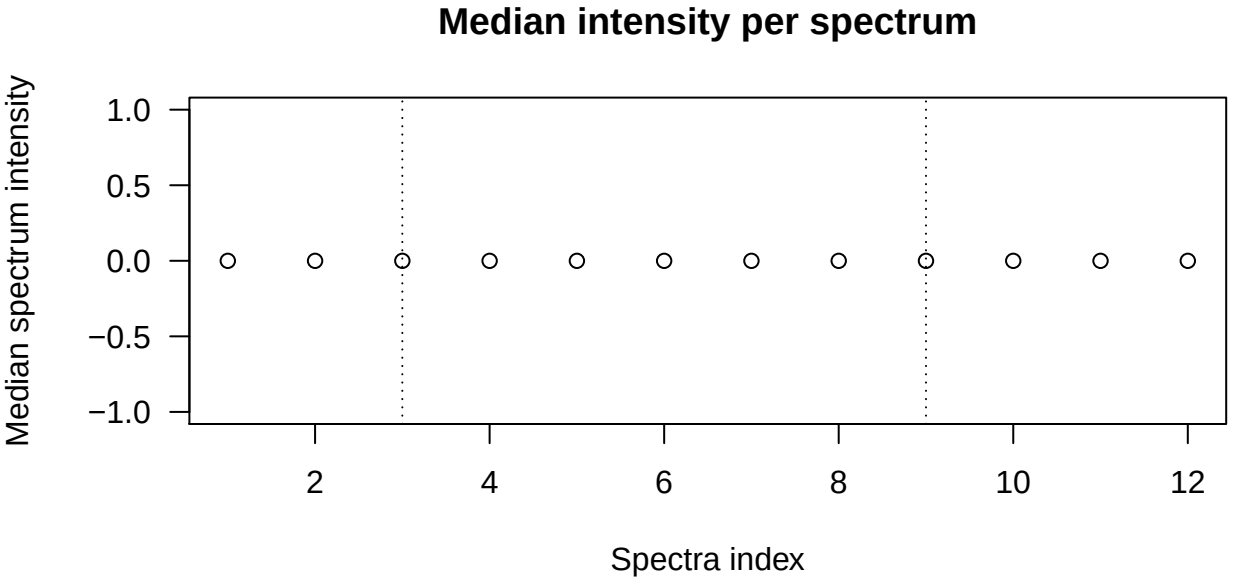

TIC per spectrum and sample
Frequency = # spectra
2.0
1.5
1.0
0.5
0.0
4.8
5.0
5.2
5.4
log(TIC per spectrum)
sample_name
1_File1
2_File2
3_File3

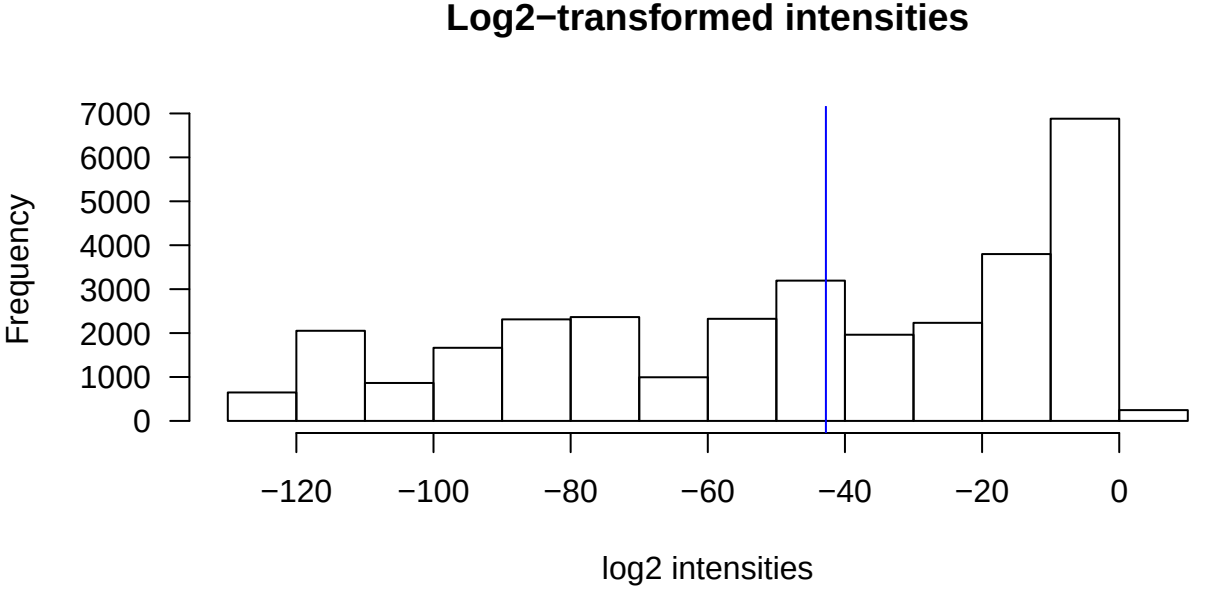

Number of peaks per m/z
Number of peaks
Coverage of spectra [%]
m/z
0
2
4
6
8
10
12
0
16.7
33.3
50
66.7
83.3
100
100
200
300
400
500
600
700
800

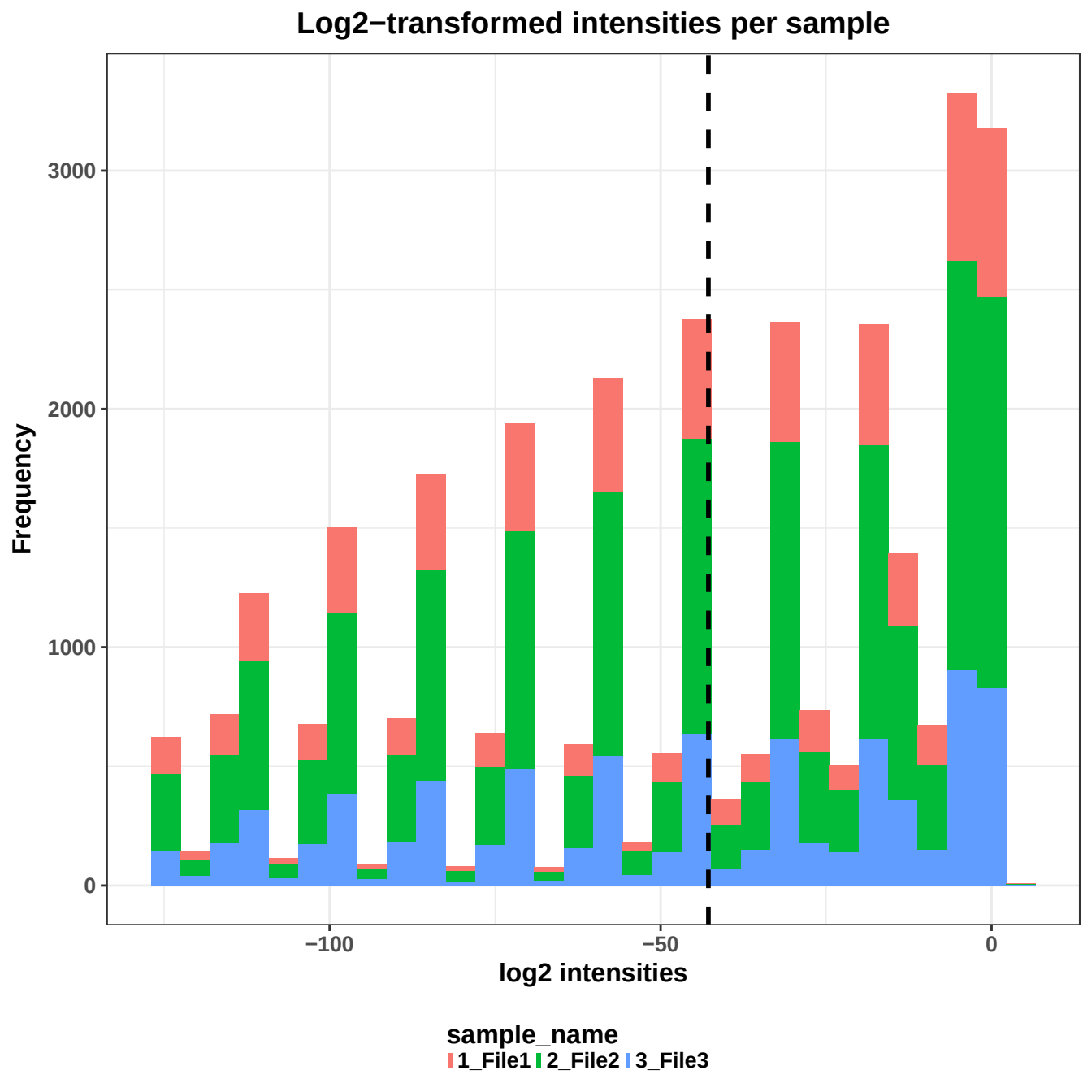

Number of peaks per m/z
Frequency
Number of peaks per m/z
0
500
1000
1500
0
2
4
6
8
10
12


Sum of intensities per m/z
Intensity sum
0
10
20
30
40
100
200
300
400
500
600
700
800
m/z

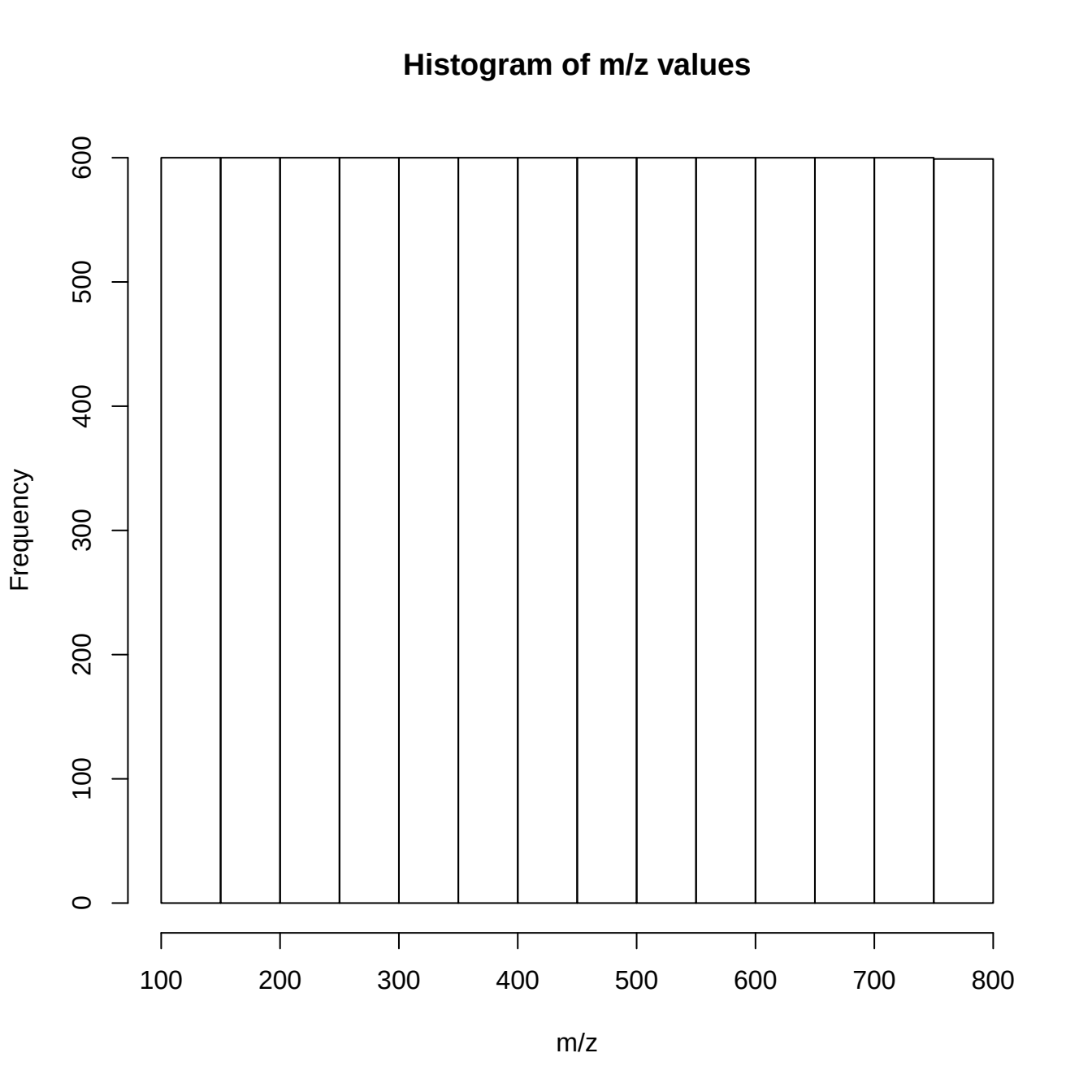

Sum of intensities per m/z
Frequency
0
500
1000
1500
2000
2500
−80
−60
−40
−20
0
log (sum of intensities per m/z)

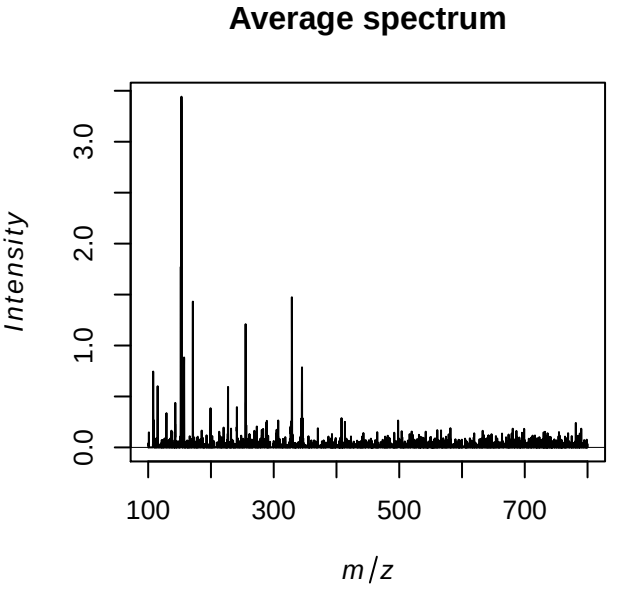

Median intensity per spectrum
Median spectrum intensity
1.0
0.5
0.0
−0.5
−1.0
2
4
6
8
10
12
Spectra index

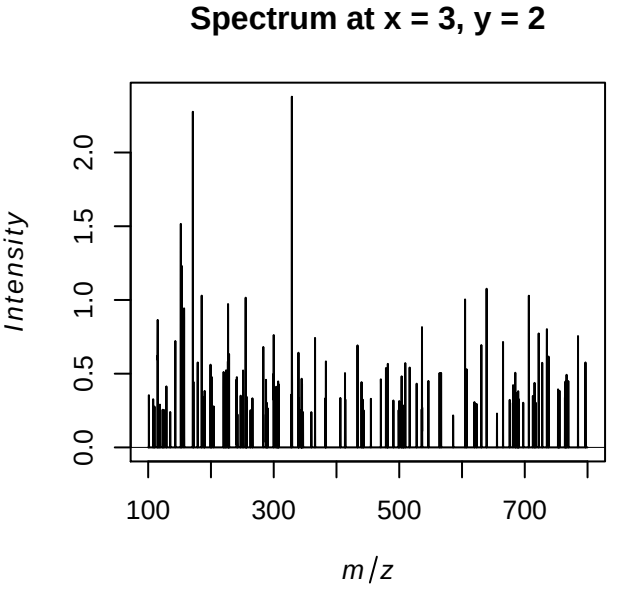

Log2−transformed intensities
Frequency
7000
6000
5000
4000
3000
2000
1000
0
−120
−100
−80
−60
−40
−20
0
log2 intensities

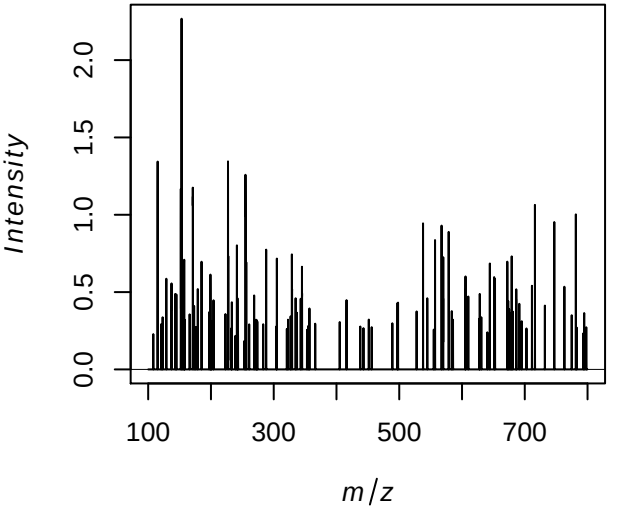

Log2−transformed intensities per sample
Frequency
3000
2000
1000
0
−100
−50
0
log2 intensities
sample_name
1_File1
2_File2
3_File3

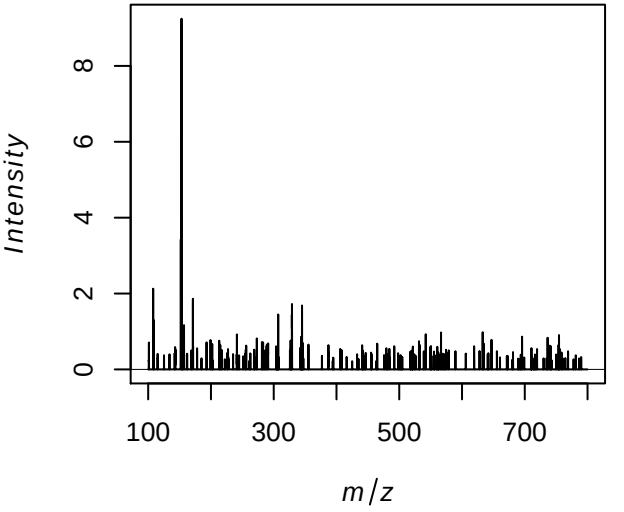
Mean intensities per m/z and sample
log2 mean intensity per m/z
0
−40
−80
−120
1_File1
2_File2
3_File3


Histogram of m/z values
Frequency
0
100
200
300
400
500
600
100
200
300
400
500
600
700
800
m/z


Average spectrum
Intensity
0.0
1.0
2.0
3.0
100
300
500
700
m/z


Spectrum at x = 3, y = 2
Intensity
0.0
0.5
1.0
1.5
2.0
100
300
500
700
m/z


Spectrum at x = 1, y = 3
Intensity
0.0
0.5
1.0
1.5
2.0
100
300
500
700
m/z


Spectrum at x = 4, y = 3
Intensity
0
2
4
6
8
100
300
500
700
m/z