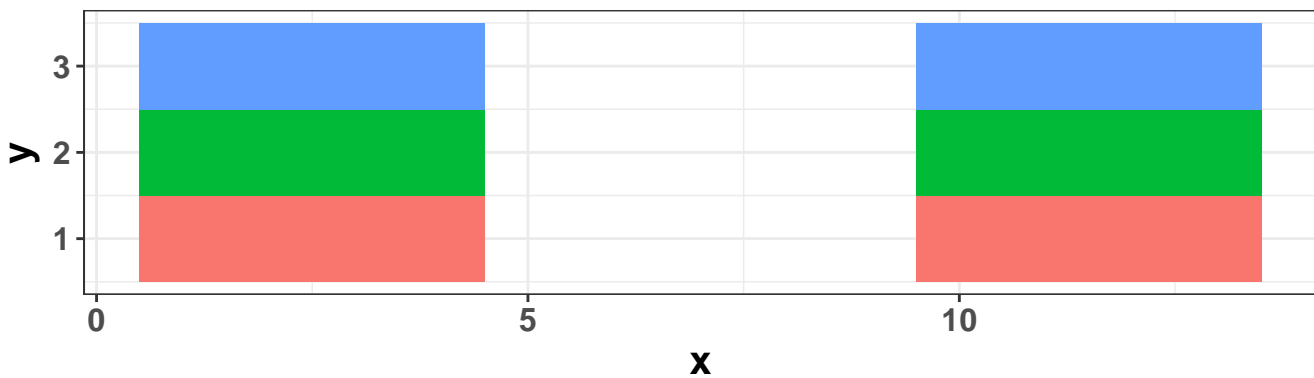


PLS for file:

testfile_squares.rdata

properties	values
Number of mz features	2718
Range of mz values	900 – 999.98
Number of pixels	24
Range of x coordinates	1 – 13
Range of y coordinates	1 – 3
Range of intensities	0 – 168
Median of intensities	3
Intensities > 0	98.75 %
Number of empty spectra	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE

Distribution of the response variable y



y_vector



A

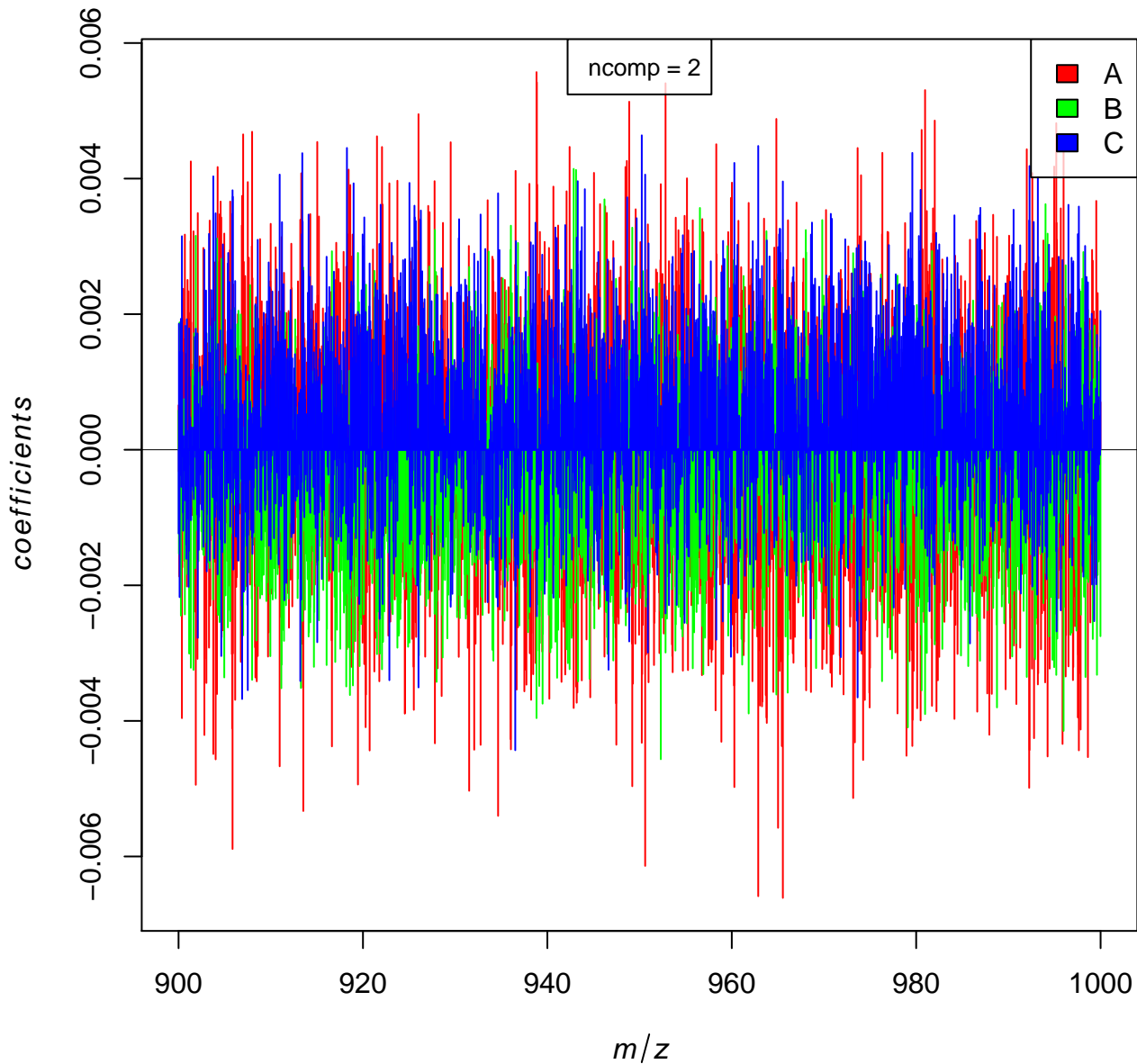


B



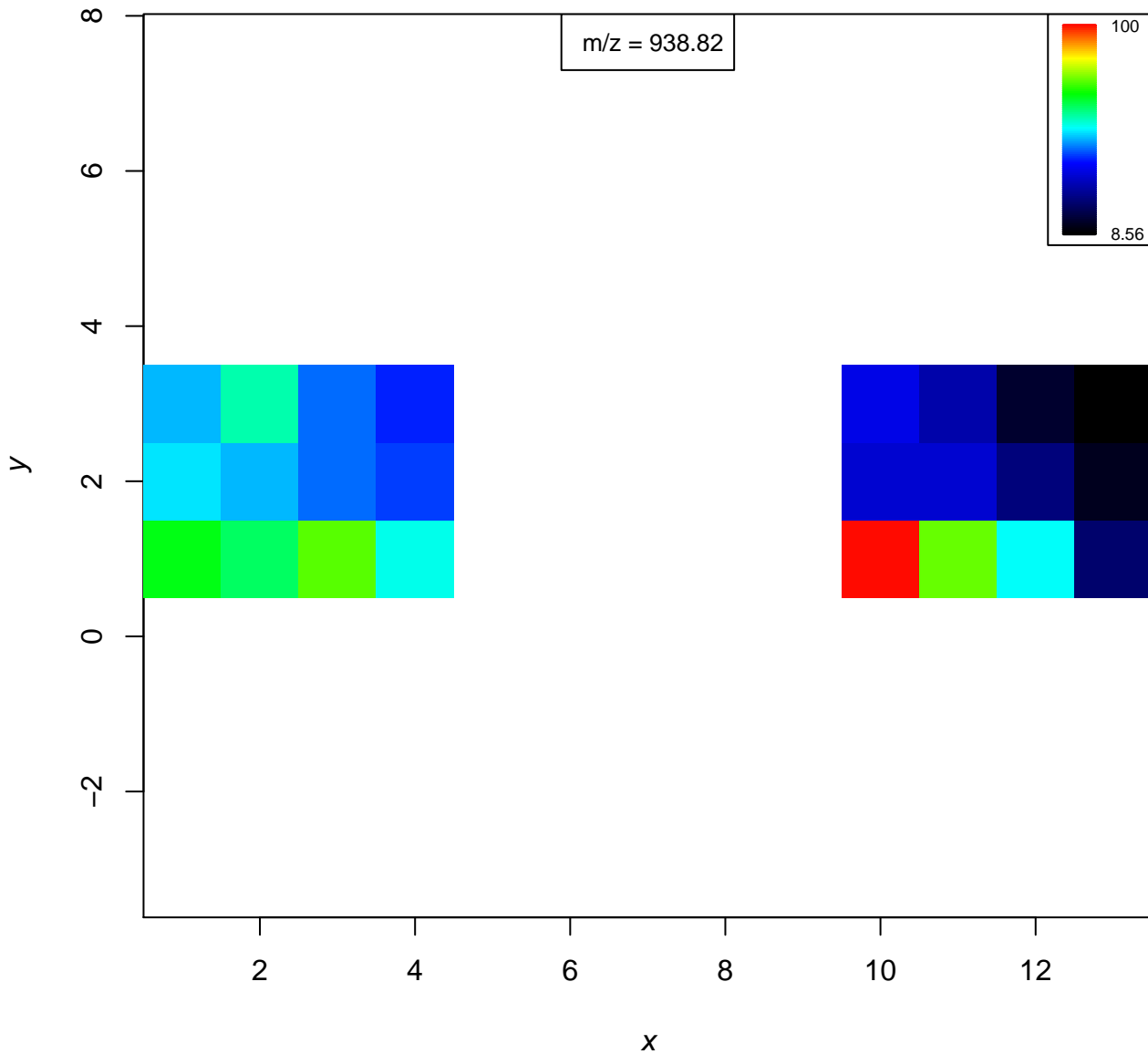
C

PLS coefficients per m/z

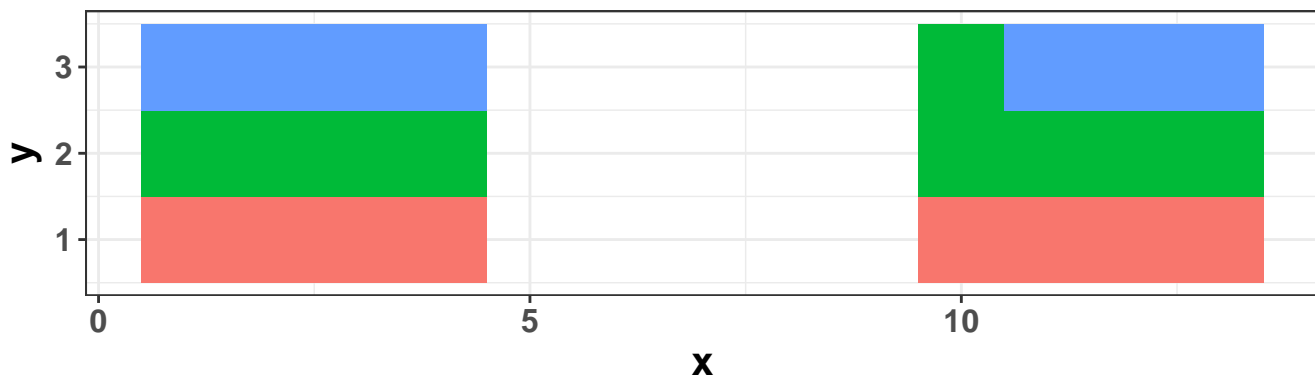


ncomp = 2	Accuracy	Sensitivity	Specificity	FDR
A	1	1	1	0
B	0.96	1	0.94	0.11
C	0.96	0.88	1	0

best m/z heatmap



Predicted condition for each pixel



predicted_classes

