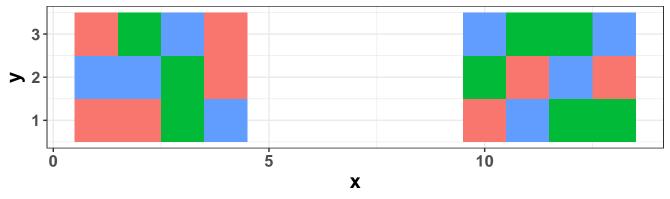
#### **OPLS** for file:

### testfile\_squares.rdata

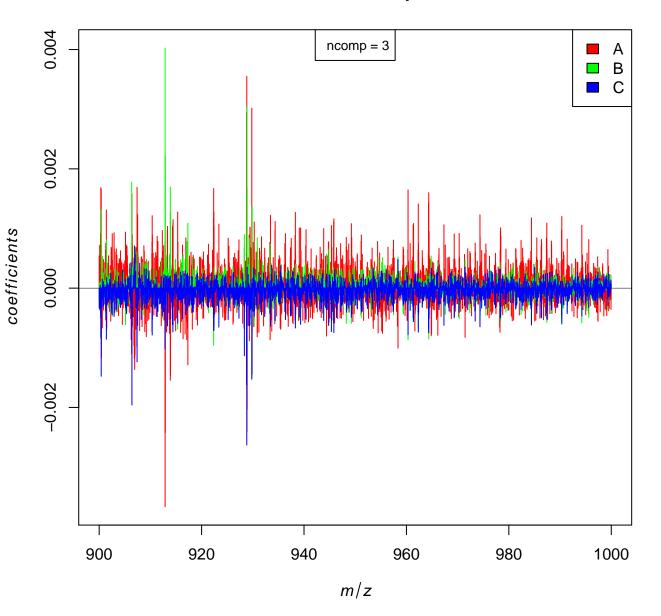
properties	values	
Number of mz features	2718	
Range of mz values	900 – 999.98	
Number of pixels	24	
Range of x coordinates	1 – 13	
Range of y coordinates	1 – 3	
Range of intensities	0 – 168	
Median of intensities	3	
Intensities > 0	98.75 %	
Number of empty spectra	0	
Preprocessing		
Normalization	FALSE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

# Distribution of the response variable y



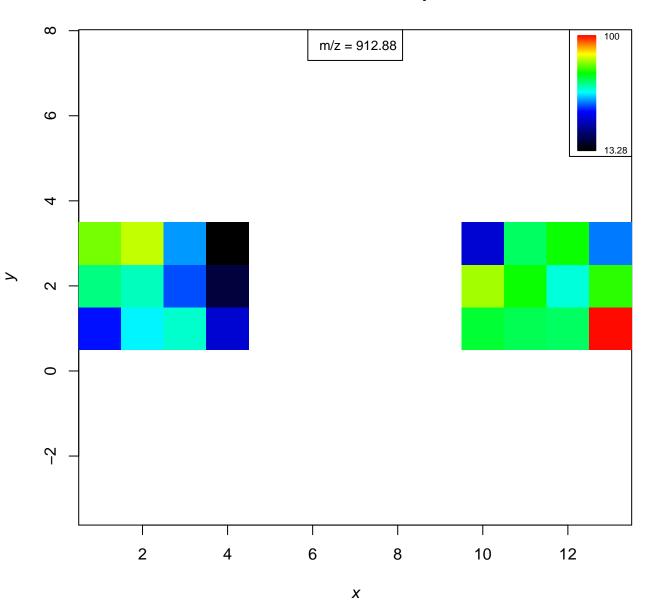


### OPLS coefficients per m/z



ncomp = 3	Accuracy	Sensitivity	Specificity	FDR
Α	0.96	0.88	1	0
В	0.96	0.88	1	0
С	0.92	1	0.88	0.2

### best m/z heatmap



## **Predicted condition for each pixel**

