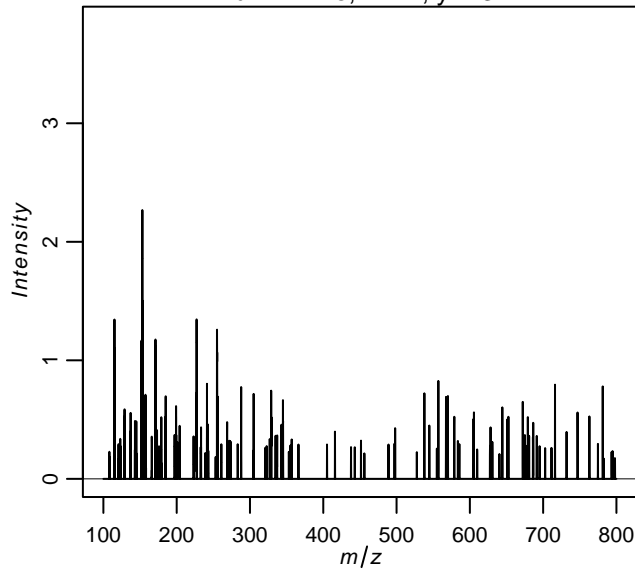


Quality control during preprocessing

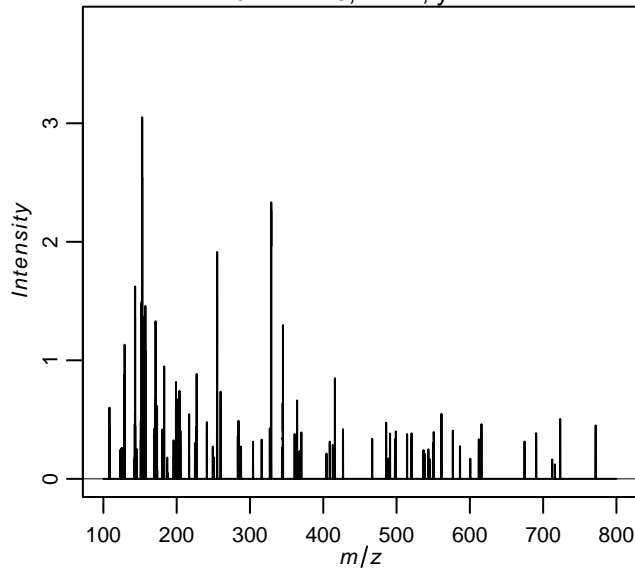
Filename: Composite Dataset

Input spectra

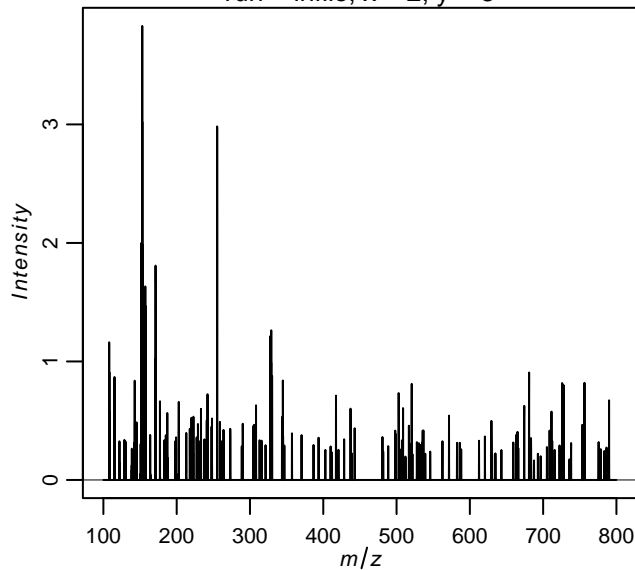
run = infile, x = 1, y = 3



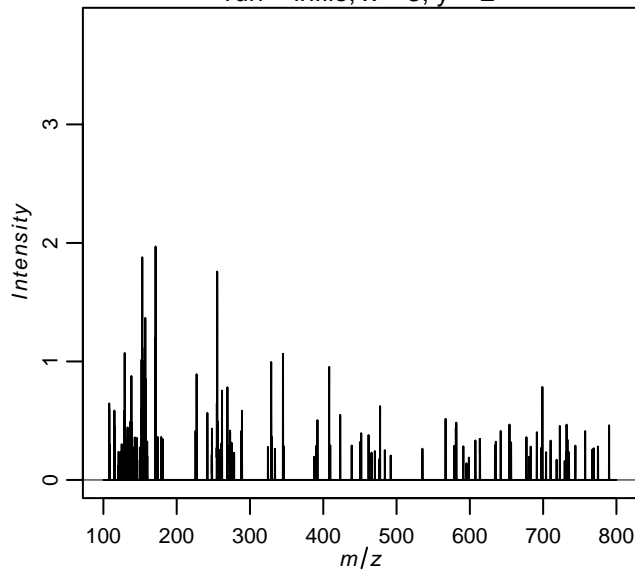
run = infile, x = 1, y = 1



run = infile, x = 2, y = 3

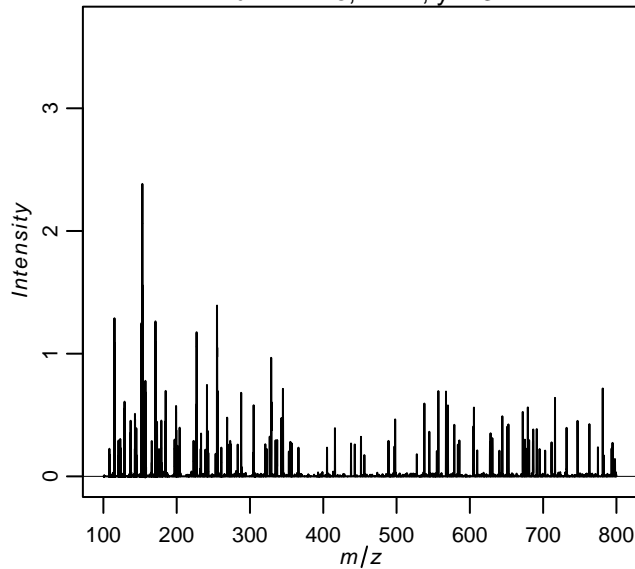


run = infile, x = 3, y = 2

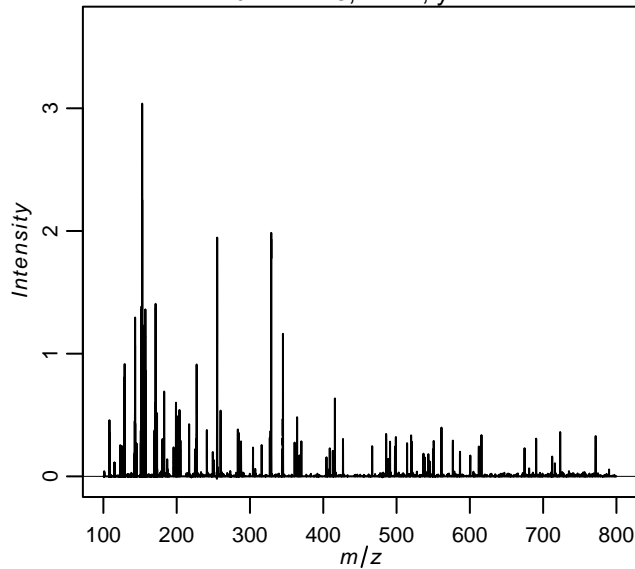


Spectra after ComBat batch correction

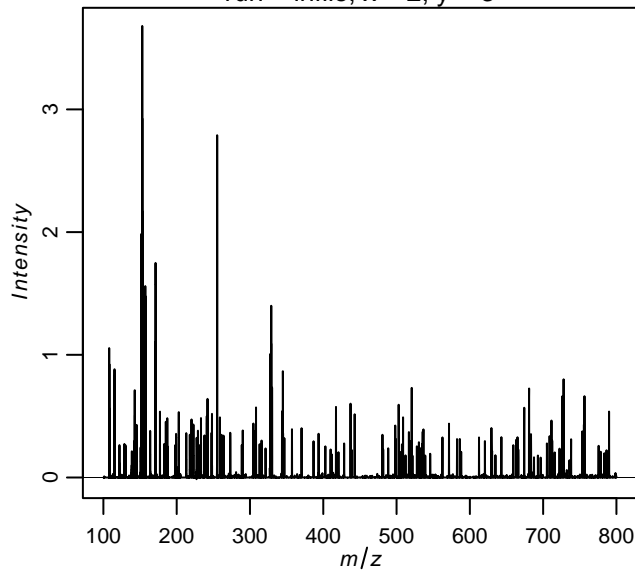
run = infile, x = 1, y = 3



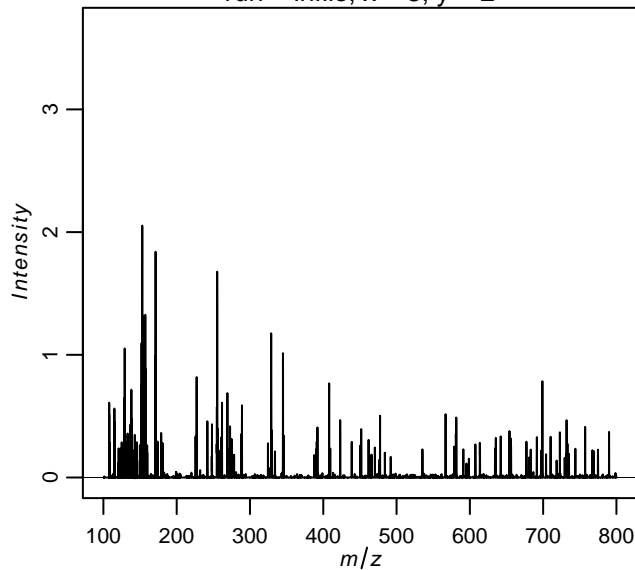
run = infile, x = 1, y = 1



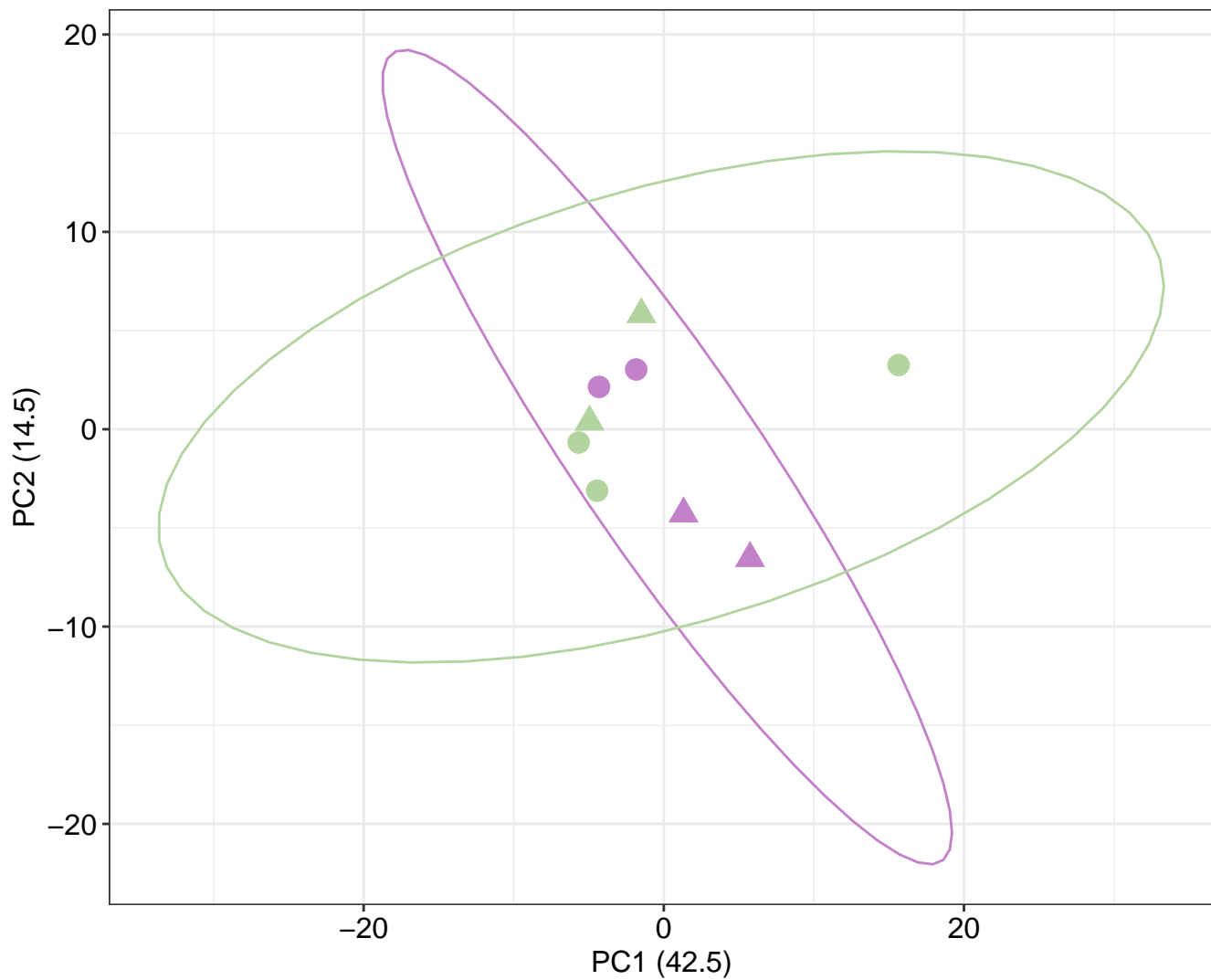
run = infile, x = 2, y = 3



run = infile, x = 3, y = 2



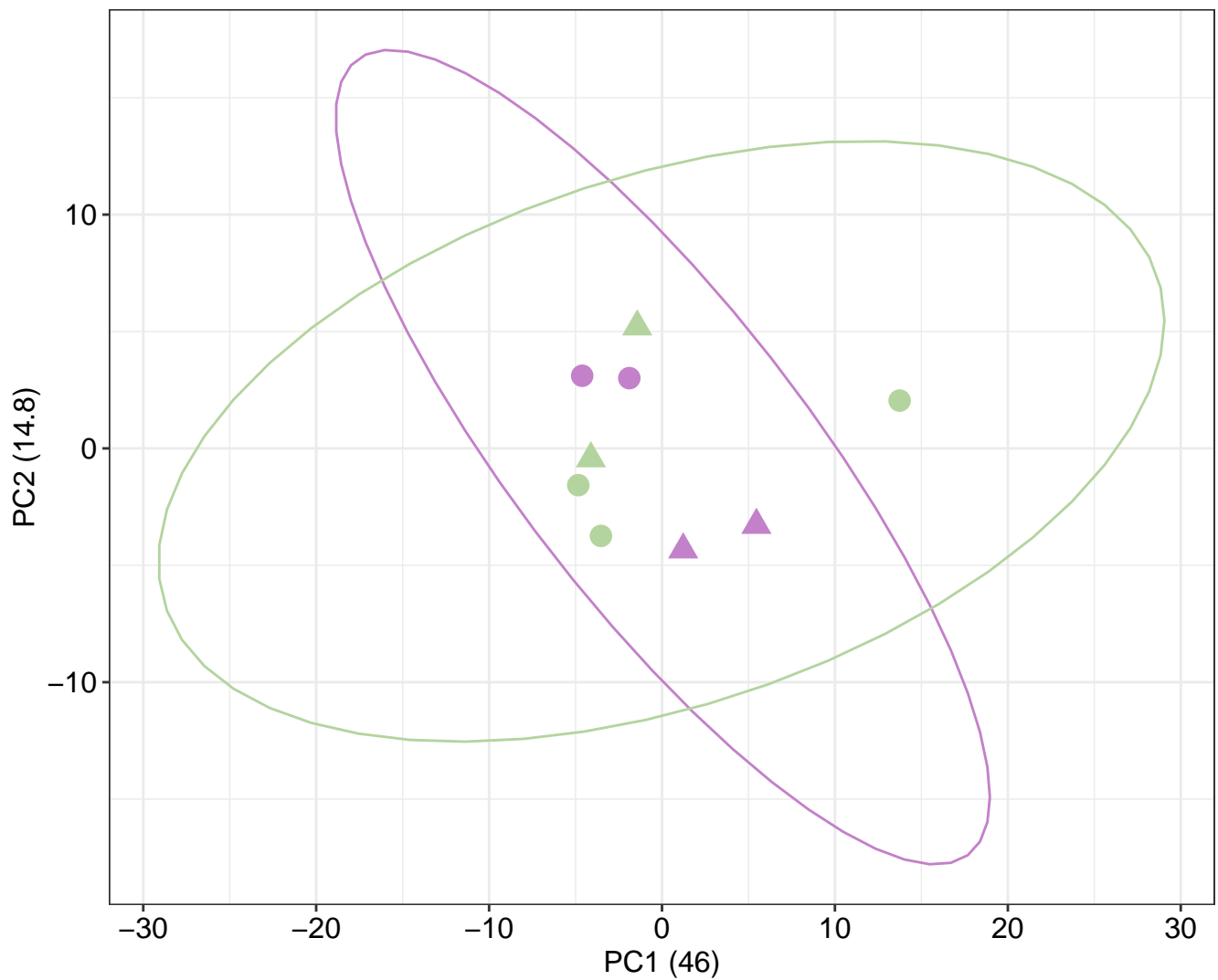
before batch correction



Batches ● B_1 ● B_2

Conditions ● A ▲ B

batch corrected



Batches ● B_1 ● B_2

Conditions ● A ▲ B

	min m/z	max mz	# features	# spectra
<i>inputdata</i>	100	799.97	10398	9
<i>batch_corrected</i>	100	799.97	10398	9