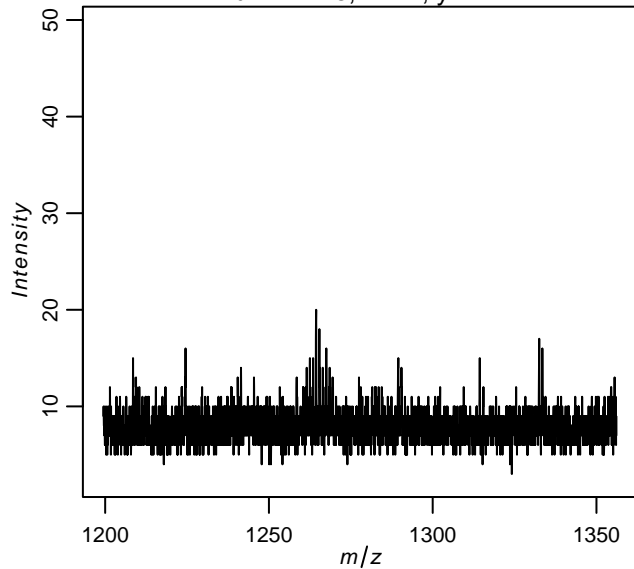


**Quality control during preprocessing**

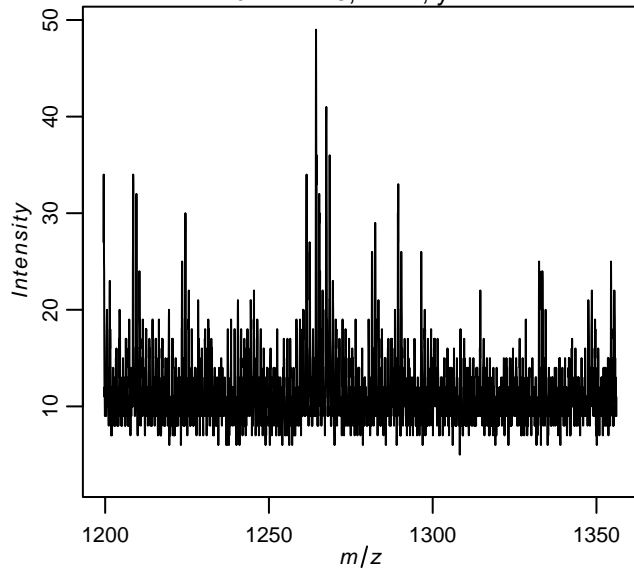
**Filename: Composite Dataset**

# Input spectra

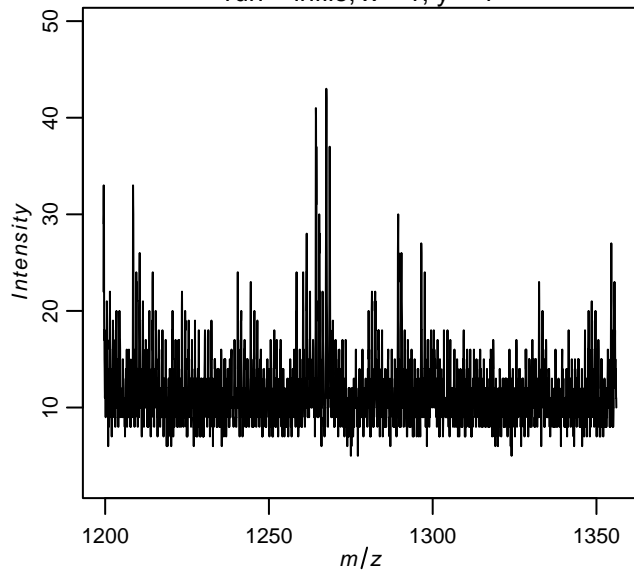
run = infile, x = 2, y = 1



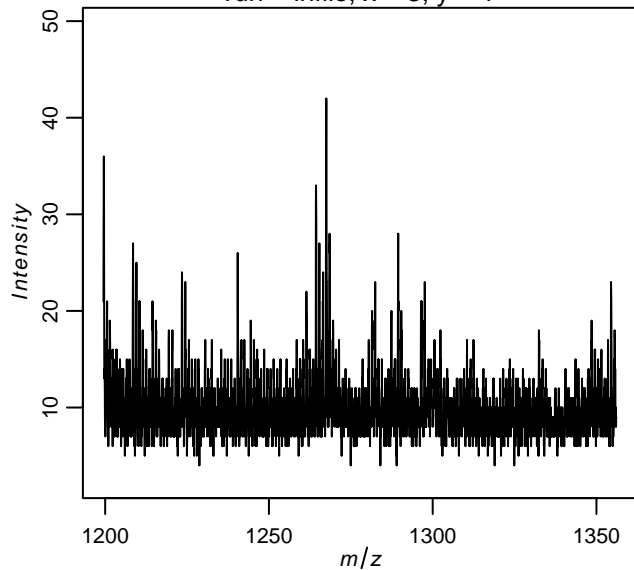
run = infile, x = 1, y = 2



run = infile, x = 1, y = 1

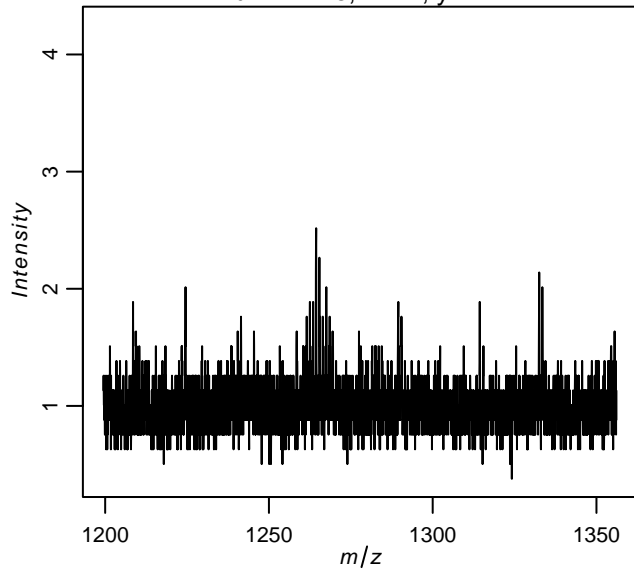


run = infile, x = 3, y = 1

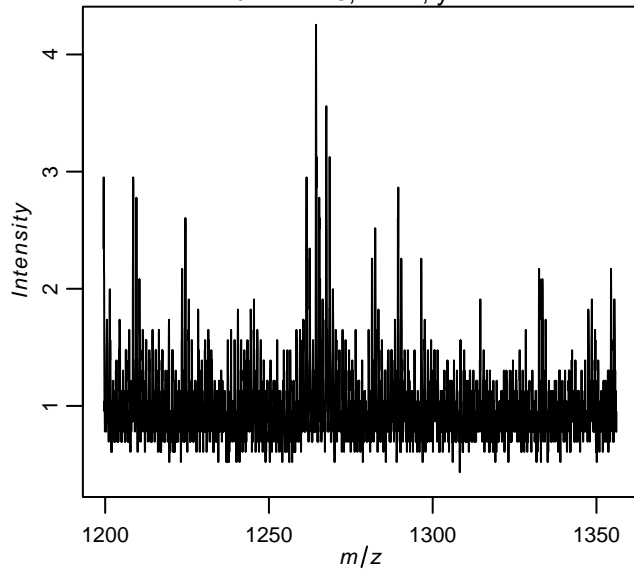


# Spectra after normalization

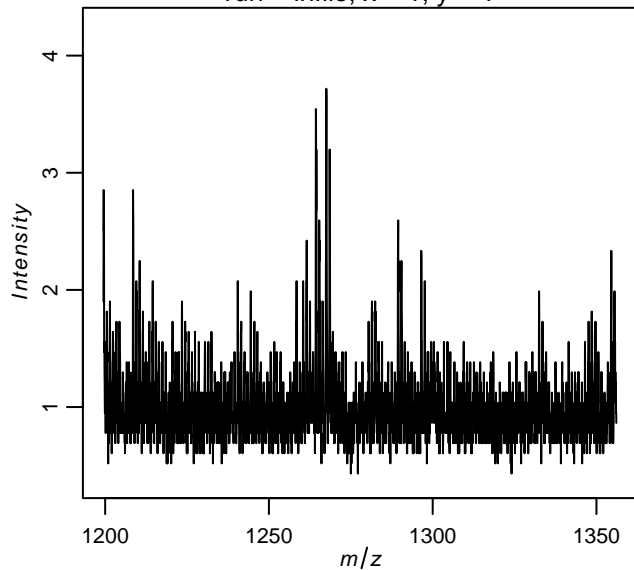
run = infile, x = 2, y = 1



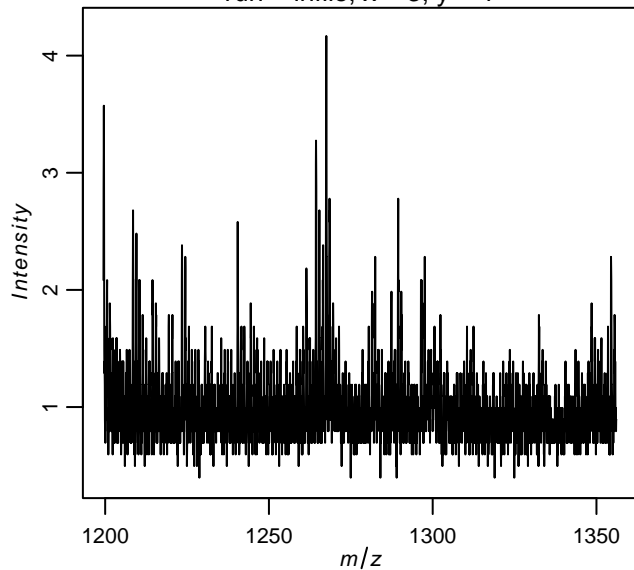
run = infile, x = 1, y = 2



run = infile, x = 1, y = 1

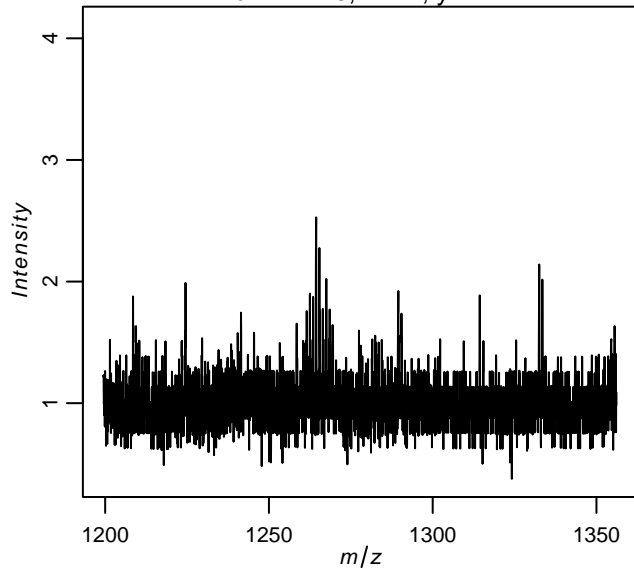


run = infile, x = 3, y = 1

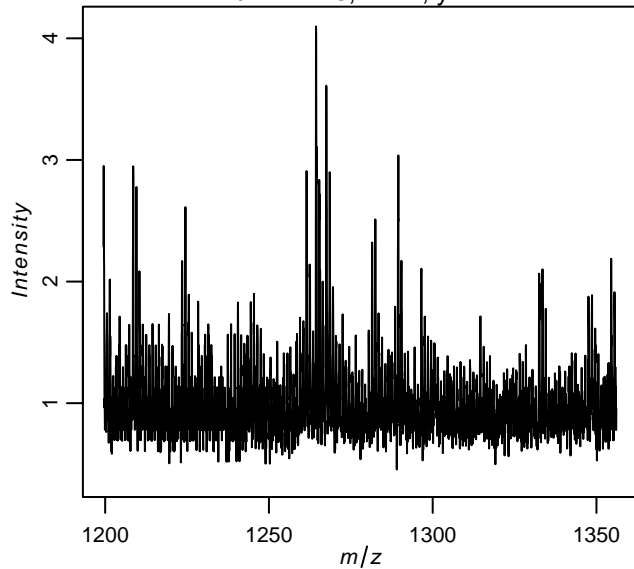


# Spectra after $m/z$ alignment

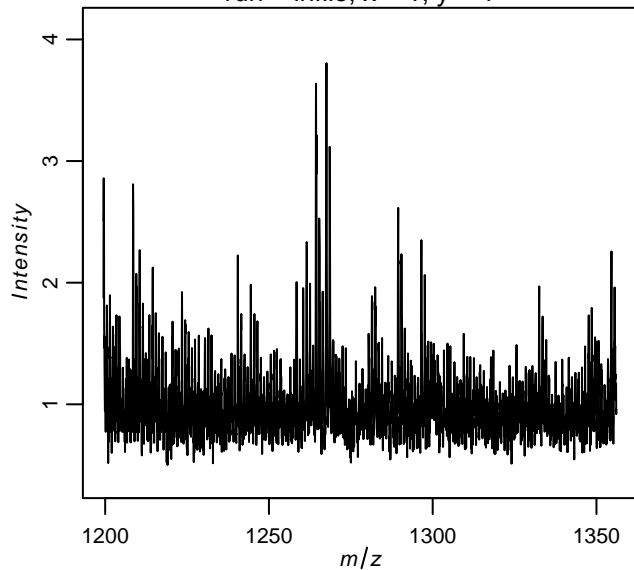
run = infile, x = 2, y = 1



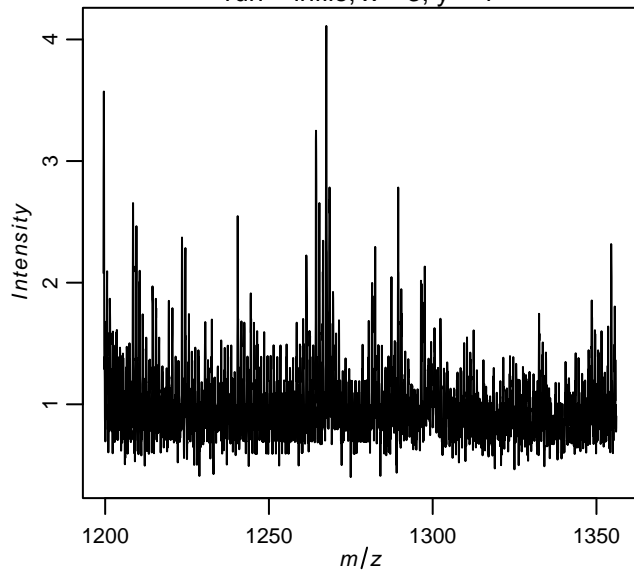
run = infile, x = 1, y = 2



run = infile, x = 1, y = 1

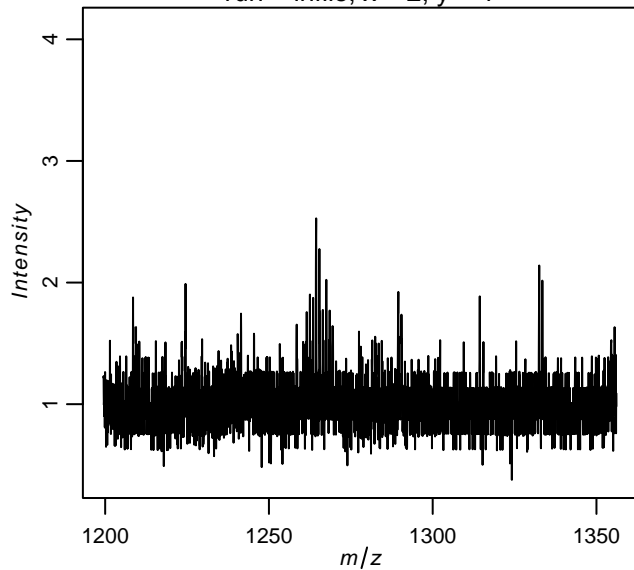


run = infile, x = 3, y = 1

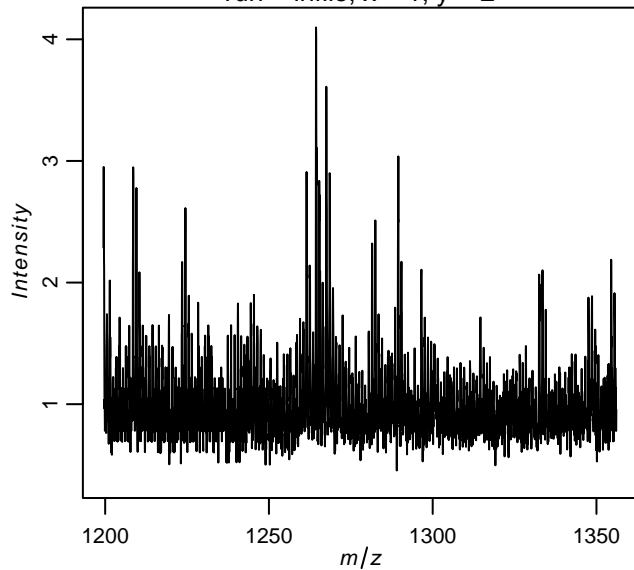


# Spectra after $m/z$ recalibration

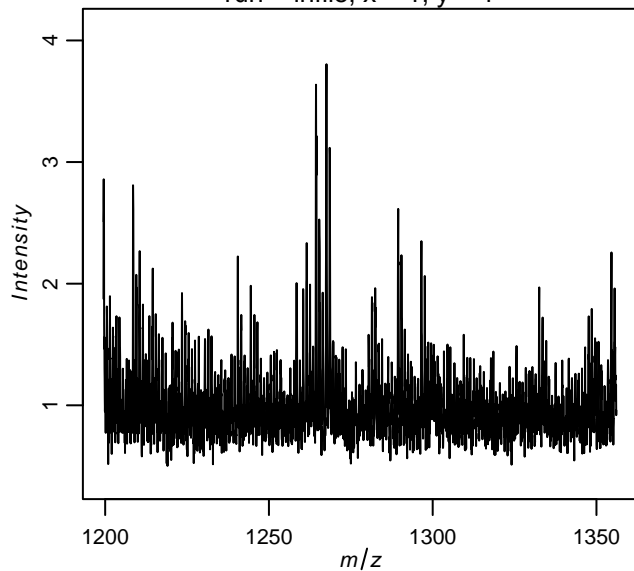
run = infile, x = 2, y = 1



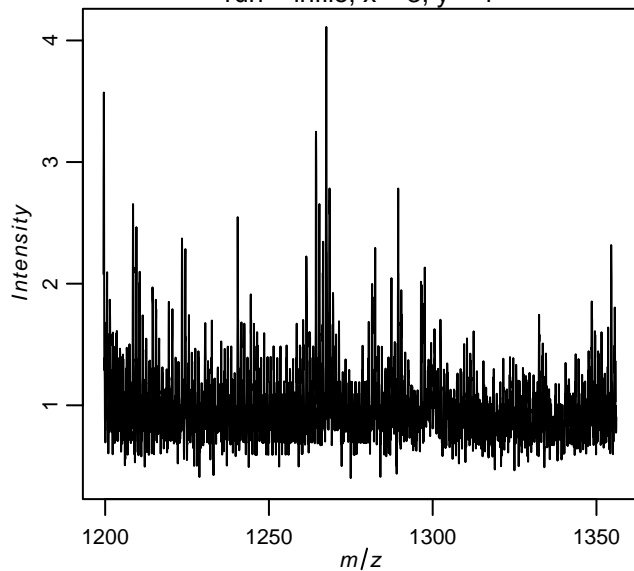
run = infile, x = 1, y = 2



run = infile, x = 1, y = 1

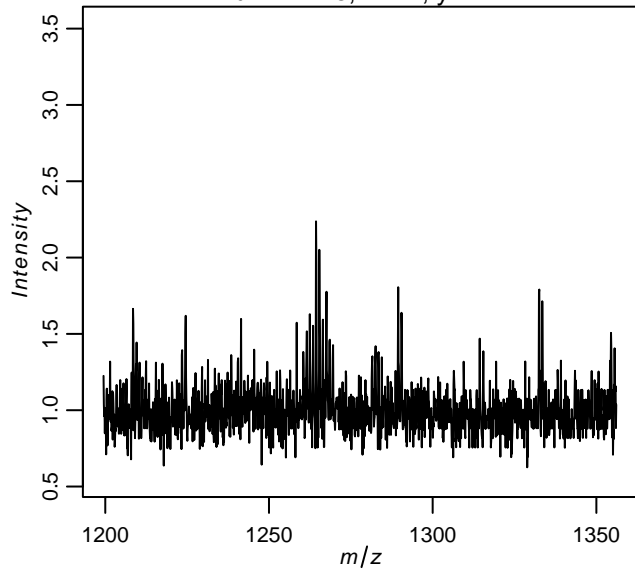


run = infile, x = 3, y = 1

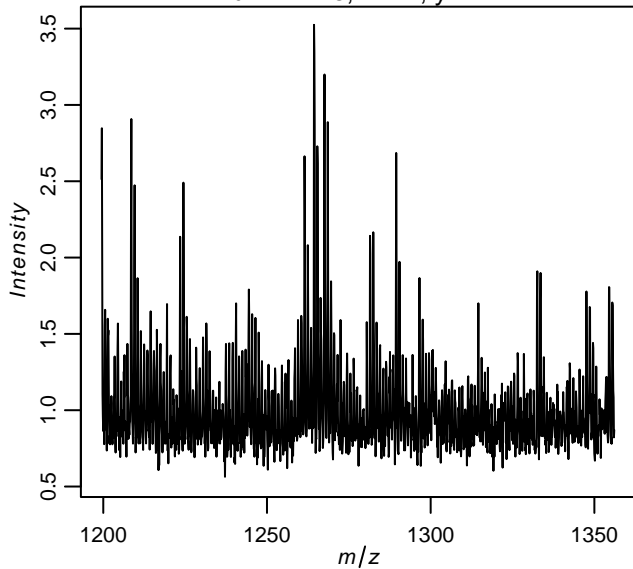


# Spectra after $m/z$ binning

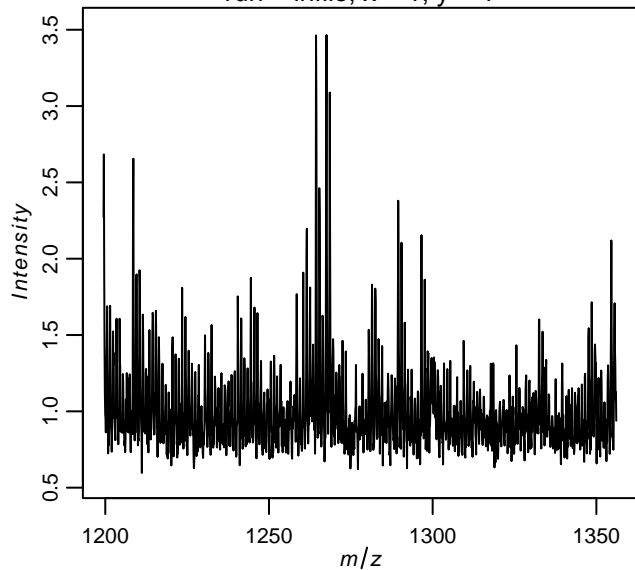
run = infile, x = 2, y = 1



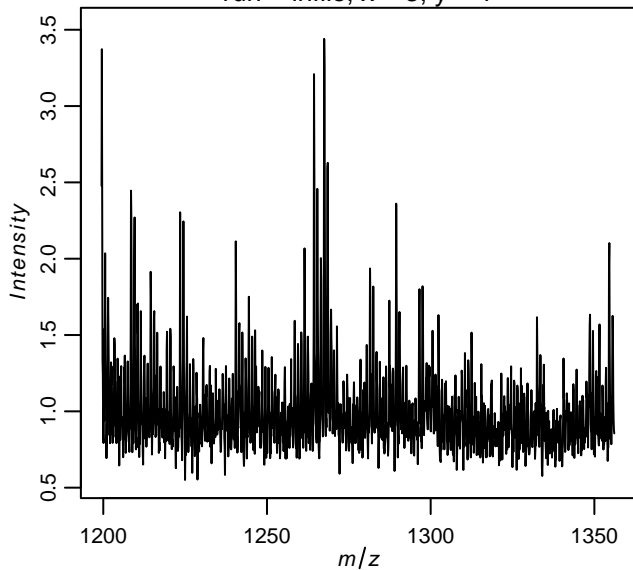
run = infile, x = 1, y = 2



run = infile, x = 1, y = 1



run = infile, x = 3, y = 1



	<b>min m/z</b>	<b>max mz</b>	<b># features</b>	<b># spectra</b>
<i>inputdata</i>	1199.47	1356.08	3672	9
<i>normalized</i>	1199.47	1356.08	3672	9
<i>mz_aligned</i>	1199.47	1356.08	3672	9
<i>mz_recal</i>	1199.47	1356.08	3672	9
<i>reduced</i>	1199.47	1356.07	1567	9