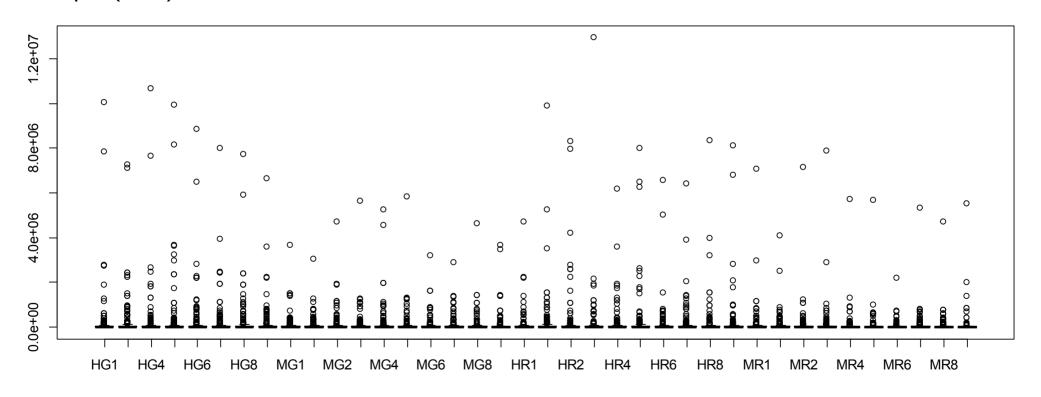
Processing and Visualization of Metabolomics Data Using R

Log transformation

Normalization and scaling

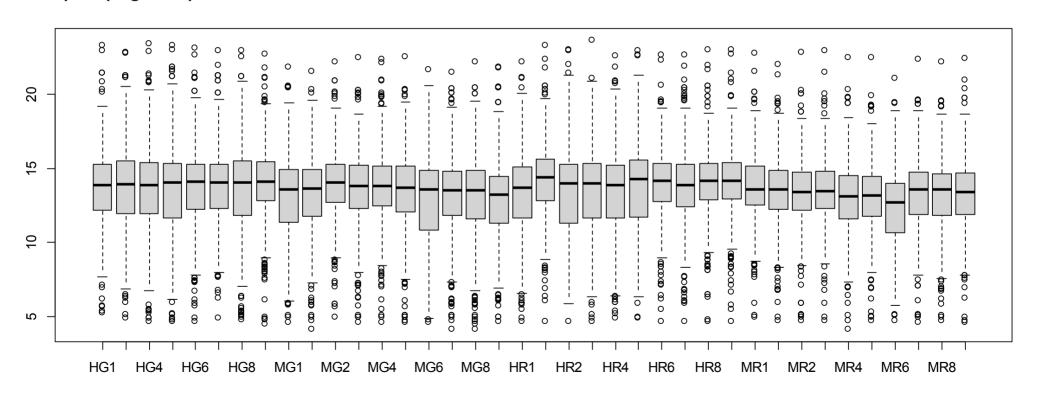
Raw Data

dat1 <- read.csv("xcmsresults.csv", header=T, row.names=1)
boxplot(dat1)</pre>



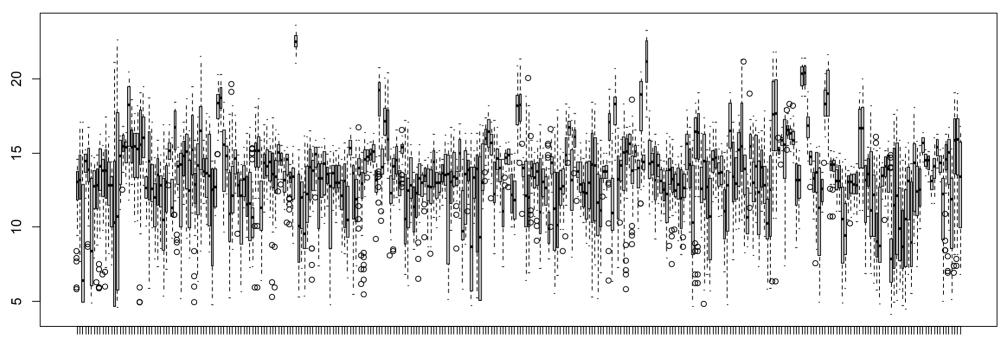
Nach log (spaltenweise = einzelne Pflanzen)

dat2 <- as.data.frame(t(apply(dat1, 1, replacezero)))
logdata <- log(dat2, 2)
boxplot(logdata)</pre>



Nach log (zeilenweise = einzelne Metabolite)

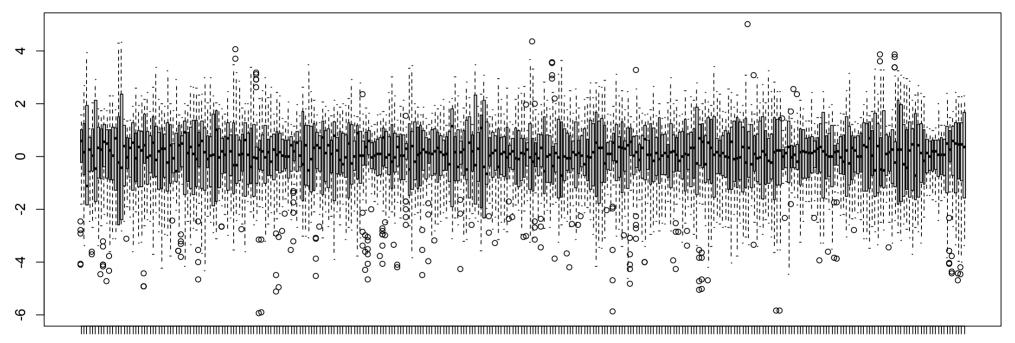
boxplot(t(logdata))



163.3/1327 294.3/286 367.6/1473 399.4/329 443.7/1246 495.2/296 532.6/267 595/1326 649.1/313 699.1/1934 762/1628 939.4/2089

Nach Pareto-Scaling (zeilenweise)

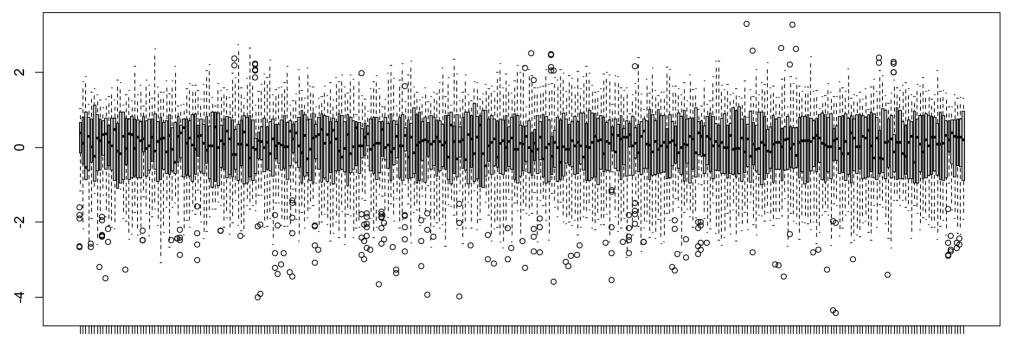
logdata.pareto <- paretoscale(logdata)
boxplot(t(logdata.pareto))</pre>



163.3/1327 294.3/286 367.6/1473 399.4/329 443.7/1246 495.2/296 532.6/267 595/1326 649.1/313 699.1/1934 762/1628 939.4/2089

Nach Z-Score-Scaling (zeilenweise)

boxplot(scale(t(logdata)))



163.3/1327 294.3/286 367.6/1473 399.4/329 443.7/1246 495.2/296 532.6/267 595/1326 649.1/313 699.1/1934 762/1628 939.4/2089