

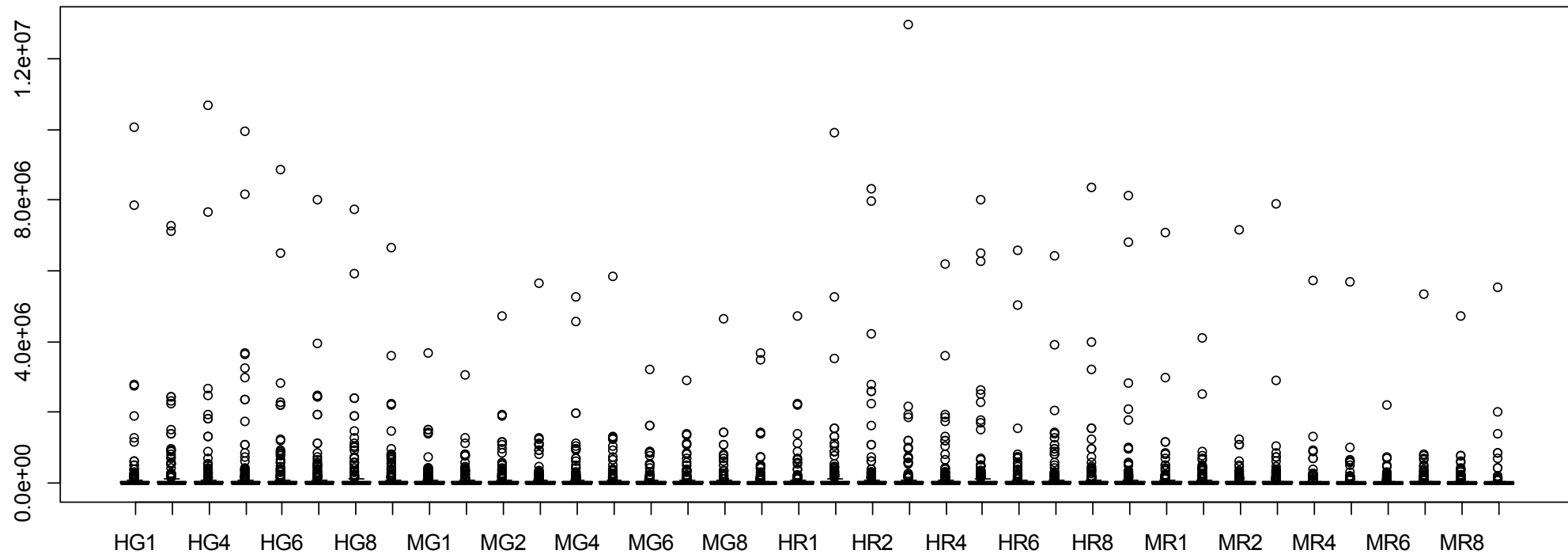
Processing and Visualization of Metabolomics Data Using R

Log transformation

Normalization and scaling

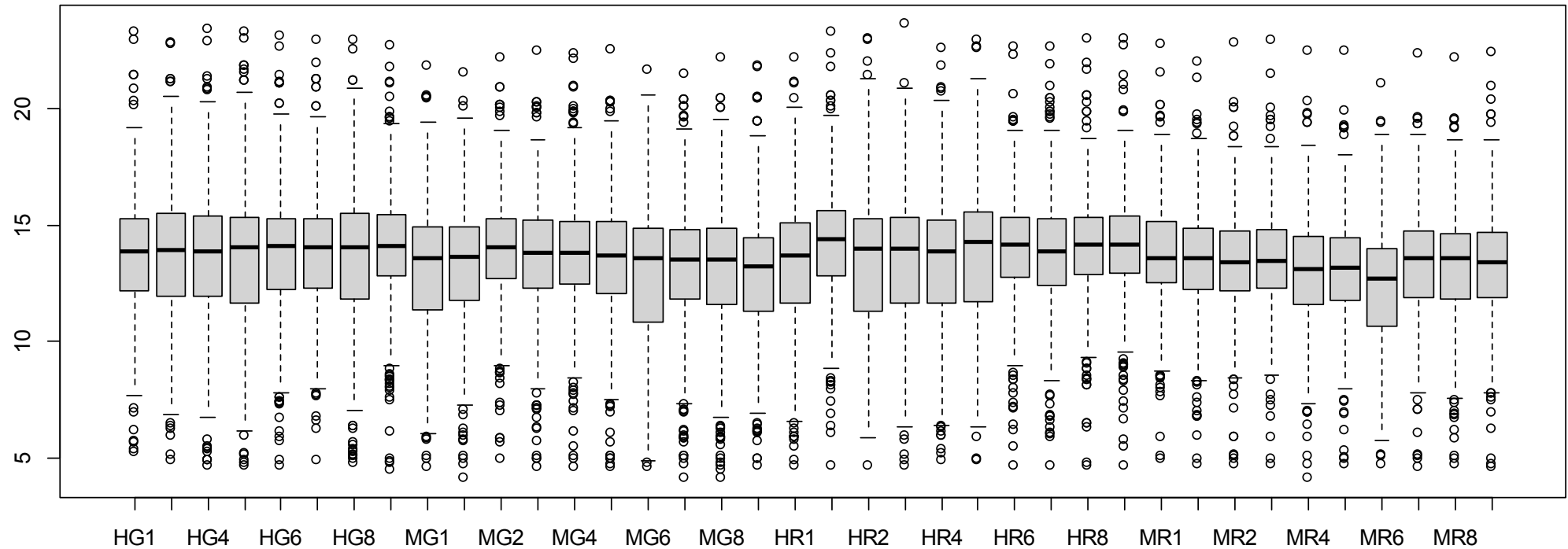
Raw Data

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



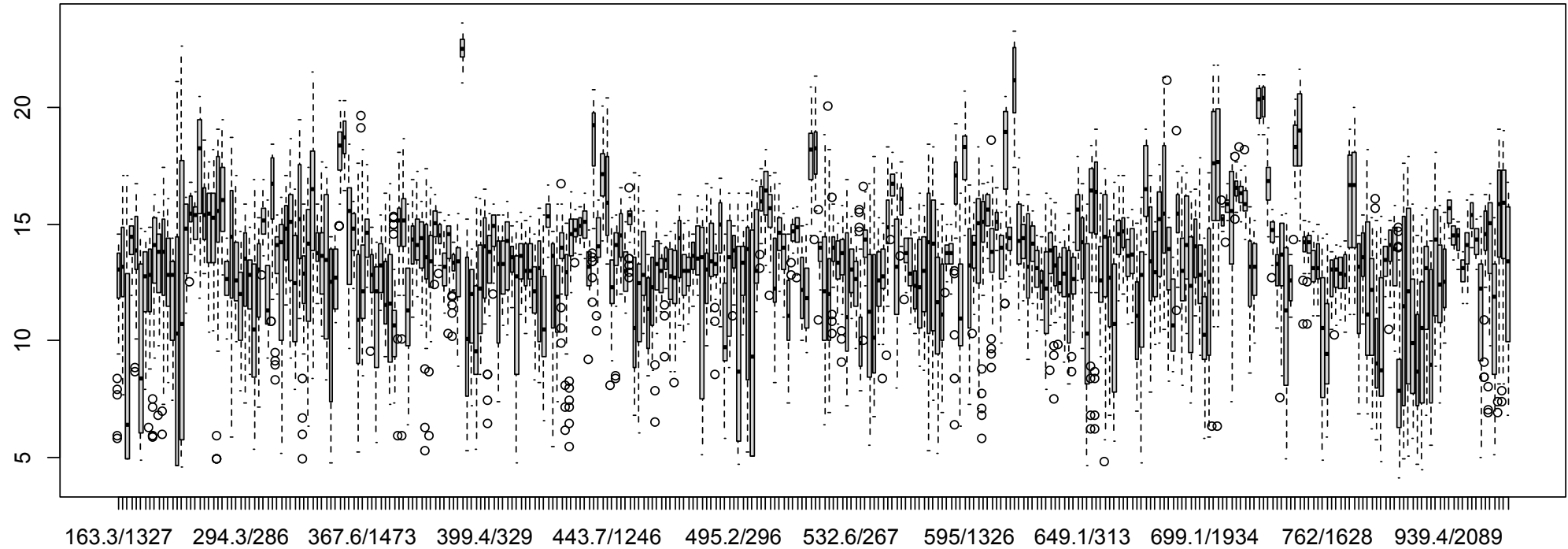
Nach log (spaltenweise = einzelne Pflanzen)

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



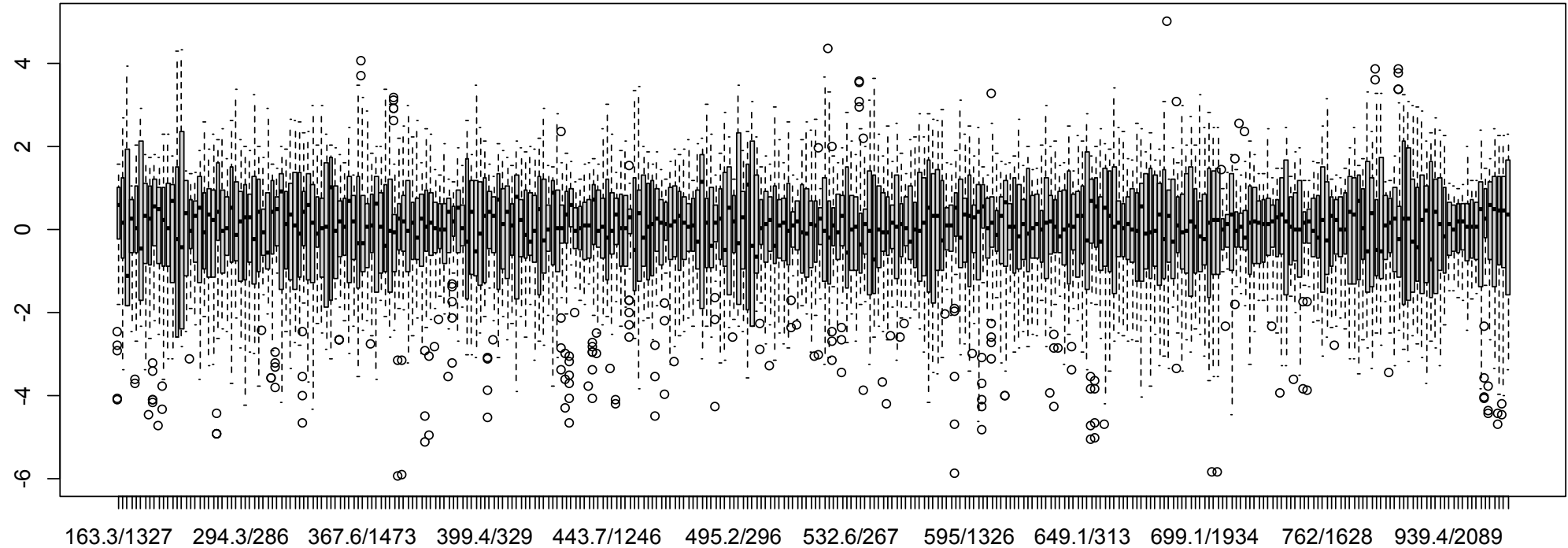
Nach log (zeilenweise = einzelne Metabolite)

boxplot(t(logdata))



Nach Pareto-Scaling (zeilenweise)

```
logdata.pareto <- paretoscale(logdata)  
boxplot(t(logdata.pareto))
```



Nach Z-Score-Scaling (zeilenweise)

```
boxplot(scale(t(logdata)))
```

