Using PTRMSR for automatizing pre-processing

Contents

This vignette shows how to use PTRMSR package to read .txt files, calculate AUC and return statistical analyses.

General principle

In this package, the functions beginning by ptrv use a single dataset as input. The functions beginning by ptrvList use names of several files to be used and a metaData file containing information about the different files. The objective of this paper is to use files produced by ptrViewer (or any other preprocessing of PTR-MS device returning files with ion, intensity and time as columns) then return curves and relevant statistics on the evaluations. Several biases can be corrected: (i) the breathing of the subject by calculating statistics by breathing cycle (use the parameter correction="cycle"), (ii) blank period during the evaluation that can be removed from the intensities (use blankCorrection = TRUE and noisePeriod=...). Some statistics are returned.

Loading the library

```
library(PTRMSR)
```

Loading metadata and list of files to be processed

All the data files (.txt from ptrViewer) and the metadata file (.csv) should be in a single repository

```
repo="./../inst/extdata"
listFiles=list.files(repo,pattern="*.txt")
metaData=read.table(paste0(repo,"/metaData.csv"),sep=";",header=T)
head(metaData)
```

```
##        file rep breathing     into start nothing     stop product subject
## 1 file1.txt   1  m69.0690 36.93347     0      NA 129.8109       B    S002
## 2 file2.txt   1  m69.0690 39.02045     0      NA 140.6618       A    S002
```

AUC calculations of several PTR-Viewer files with noise and breathing correction

This function allows statistics to be calculated for each file after breathing correction

The results can be saved into csv files

```
write.table(file="auc.csv",sep=";",res_auc$listRes,row.names=F)
```

The stat option can be used to select the statistic.

```
res_tmax=ptrvListIntensityByTime(listFiles=listFiles,metaData=metaData,ions=c("m31.0183", "m31.0259",
                                                                              "m33.0324"),stat="tmax")
```

The breathing cycles can be observed with this command.

```
grid.arrange(grobs=res_tmax$cycleLimits[1:4])
```

Documentations on the functions are available in the R documentation

```
?detectCycle
?ptrvIntensityByTime # for only one dataset,
?ptrvIntensity # for summarizing the time of one dataset
?ptrvListIntensityByTime # for only one dataset,
?ptrvListIntensity # for summarizing several datasets
```