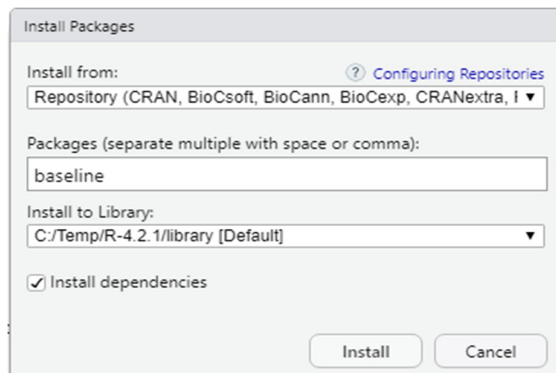**SUPPLEMENTARY MATERIAL**

Table S1. Steps for utilization of RStudio software for baseline correction

Step 1: Installation of packages > setRepositories() >1 2 3 4 5 6 7 >install("baseline") >install("gWidgets2") >install("gWidgets2tcltk") Another way to install the three packages is to go to Packages pane, select Install, write baseline to the packages and press Install.   The same procedure will be followed for the installation of gWidgets2 and gWidgets2tcltk.
Before any baseline correction the packages have to be always installed and selected via choosing them from Package pane or with the following commands: > library(baseline) > library(gWidgets2) > library(gWidgets2tcltk) > setwd("C:/Temp/CSVfiles") The command > setwd("C:/Temp/CSVfiles") sets the selected file as working directory, Temp in our case, which can also be done manually from Files pane.
Step 2: Baseline correction Import the table in .csv form of your interest. Go to Environment pane, press Import "From Text(reader) and browse to select your intended table (e.g., linearity3a.csv). Before pressing Import, you have to choose "Semicolon" as Delimiter.

```
> linearity3a <- as.matrix(linearity3a)
> baselineGUI(linearity3a)  or > baselineGUI (linearity3a, method= "als")
```


A new window appears where the appropriate algorithm and parameters can be selected. By pressings the buttons "Update plot" and "Apply to all", the baseline corrected chromatograms can be exported by pressing "Apply and export" in the following window:

Data can be exported as .CSV files:
> tran <- t(corrected.linearity3a@corrected)
> write.csv(tran, file="corrected.linearity3a.csv")

The new csv file is saved at the file we determined as working directory and can be uploaded to Fityk software for further process.