```
##############################
####Quantification of SPE extracts
##############################


#packages
library(openxlsx)
library(effects)
library(investr)


###import data
setwd("C:\\Users\\charles.chappuis\\OneDrive - HESSO\\Documents\\Ra&D\\Lefort\\conf_publi")


ana <- read.xlsx("data_chappuis_2023.xlsx",sheet=3)
colnames(ana) <- c("name","rep","type","levels","istd","verb","meth","phero","panis")
str(ana)


###quantification
#values of blanks are neglected as they are very low. Headspace cells and cartridges were clean.


i=3
k=1


for(i in c(1:4)){
        prodi <- ana[,c(1,2,3,4,5,i+5)]
        nam <- names(prodi)[6]
                if(nam=="verb"){
                cali <- prodi[prodi$type=="Cal",]
                cali$levels <- cali$levels*0.992*0.94 #mass and purity taken into account
                cali$rel <- cali$verb/cali$istd
                mod <- lm(rel~levels,weight=1/levels,data=cali)
                summary(mod)
```

```r
}else{}


if(nam=="meth"){
cali <- prodi[prodi$type=="Cal",]
cali$levels <- cali$levels*1.187*0.98
cali$rel <- cali$meth/cali$istd
mod <- lm(rel~levels,weight=1/levels,data=cali)
summary(mod)
}else{}


if(nam=="phero"){
cali <- prodi[prodi$type=="Cal",]
cali$levels <- cali$levels*1.623*0.983
cali$rel <- cali$phero/cali$istd
calii <- cali[c(1:7),] #limit the calibration span, values above are useless
mod <- lm(rel~levels+I(levels^2),weight=1/levels^2,data=calii)#
summary(mod)
}else{}


if(nam=="panis"){
cali <- prodi[prodi$type=="Cal",]
cali$levels <- cali$levels*1.148*0.98
cali$rel <- cali$panis/cali$istd
mod <- lm(rel~levels,weight=1/levels,data=cali)
summary(mod)
}else{}
conc <- c()
for(k in c(1:nrow(prodi))){
prodi$rel <- prodi[,6]/prodi[,5]
xx <- prodi$rel[k]
pred <- invest(mod,xx,interval="none",extendInt="yes")
```

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            conci <- as.numeric(pred)

            conc <- c(conc,conci)

            }


      ana$pred <- conc

      colnames(ana)[9+i] <- paste(nam,"C",sep="")

}


ana

#write.table(ana,"quant_extracts_chappuis_2023.txt",sep="\t",col.names=T)


ana$verbCC <- 100*ana$verbC/(ana$levels*0.992*0.94)

ana$pheroCC <- 100*ana$pheroC/(ana$levels*1.623*0.983)

ana$methCC <- 100*ana$methC/(ana$levels*1.187*0.98)

ana$panisCC <- 100*ana$panisC/(ana$levels*1.148*0.98)


test <- ana$phero/ana$istd

(test+2.411e-04)/4.301e-05
```