

Supplementary material

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#Trace Element Peak and Valley R Script

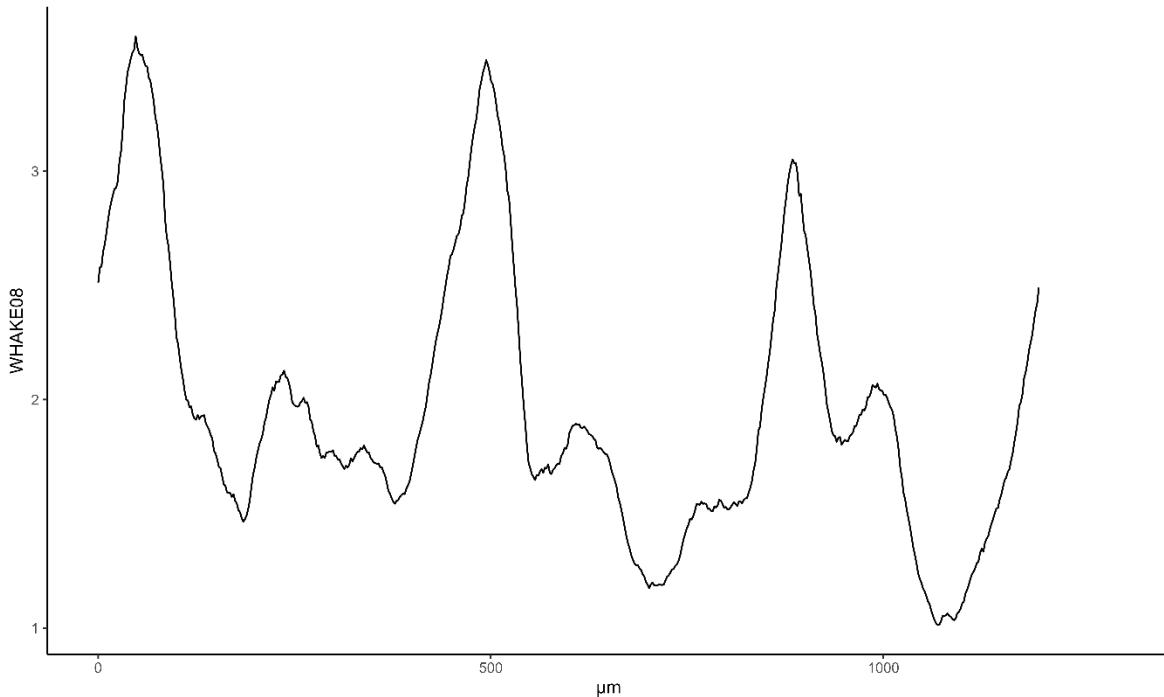
library(tidyverse)

## -- Attaching packages ----- tidyverse 1.3.2 --
## v ggplot2 3.3.6      v purrr   0.3.5
## v tibble  3.1.8      v dplyr   1.0.10
## v tidyrr  1.2.1      v stringr 1.4.1
## v readr   2.1.3      v forcats 0.5.2

mydata <- read.table("c:\\\\Users\\\\benla\\\\Desktop\\\\Mn55_Master25.csv",
header=TRUE, sep=",") #Input data set

library(ggplot2)

ggplot(data = mydata, aes(x = μm, y = WHAKE08)) +
  geom_line(color="black") + #Line plot of elemental concentration
  xlim(0,1300) + #Set the x-axis limit
  theme_classic() #Set theme to classic, white background
```



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library(caret)
library(lattice)
library(ggpmisc)
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library(ggpp)

mydata_ss <- preProcess(as.data.frame(mydata[,c(2:74)]), method=c("range"))
#Select data column range you wish to normalize

mydata_A <- predict(mydata_ss, as.data.frame(mydata[, c(2:74)]))
#Normalize data columns

mydata_A$Distance <- mydata$μm #Add Laser distance to new normalized data set

ggplot(data = mydata_A, aes(x = Distance, y = WHAKE08)) + #select normalized data set, x and y variables
  geom_line(color="black") + #Draw line plot of element concentrations
  ylim(0:1) + xlim(0,1300) + #Set x and y axes limits
  stat_peaks(colour = "green", size = 1.5, span = 101, ignore_threshold = 0.15, strict = TRUE, geom = "rug", sides = "b") + #peaks on rug
  stat_peaks(colour = "green", size = 1.5, span = 101, ignore_threshold = 0.15, strict = TRUE, geom = "point") + #peaks on line plot
  stat_valleys(colour = "red", size= 1.5, span = 151, ignore_threshold = 0.80, strict = TRUE, geom = "rug", sides = "b") + #valleys on rug
  stat_valleys(colour = "red", size = 1.5, span = 151, ignore_threshold = 0.80, strict = TRUE, geom = "point") + #valleys on line plot
  theme_classic() #set theme to classic

```

