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1  |--BASELINE CORRECTION FOR MULTIPLE SPECTRA--
2
3  # Load necessary libraries
4  library(readxl)
5  library(baseline)
6  library(writexl)
7  library(tidyr)
8  library(reshape2)
9  library(dplyr)
10
11 # Read data from excel file into a data frame
12 input_data <- read_excel("C:\\Users\\barbi\\Desktop\\input_data.xlsx")
13
14 # Changes the data from a data frame to a matrix
15 input_matrix <- as.matrix(input_data)
16
17 sum(is.na(input_matrix))
18 sum(is.infinite(input_matrix))
19
20 # Perform baseline correction on the current spectrum
21 corrected_spectrum <- baseline(as.matrix(input_data), method = "fillPeaks", lambda = 0.1875, hwi=400, it=5, int=12.5)
22
23 # Changes the format from a long table to a wide table
24 corrected_df <- data.frame(wave_number = seq_len(nrow(input_data)), as.data.frame(corrected_spectrum@corrected))
25 corrected_df <- data.frame(corrected_df)
26 corrected_df <- corrected_df[,-1] #eliminates first column
27
28 # Eliminate the first column in corrected_df
29 corrected_df <- corrected_df %>% select(-1)
30
31 # Add the first column in input_data as the new first column in corrected_df
32 corrected_df <- cbind(input_data[,1], corrected_df)
33
34 # Change the name of the first column to "wave_number"
35 names(corrected_df)[1] <- "wave_number"
36
37 # Converting "corrected_df" to a data frame again
38 corrected_df <- data.frame(corrected_df)
39
40 # Exports the data frame in a new .xlsx file
41 write_xlsx(corrected_df, "C:\\Users\\barbi\\Desktop\\baseline_corrected.xlsx")

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