**Research Article**                                                                 **Open Access**

# Supplementary Information

## R Method

1. Copy and paste all mass-to-charge (m/z) values and the corresponding intensity values into an excel spreadsheet, organized by sample.

2. Save the spreadsheet as a comma separated values file (.csv), along with the "new_alignment.R" file. The code of this file is written below this procedure.

3. Open R and click "Misc" at the top of the screen. Click "Change Working Directory, and find the folder that contains the .csv file and the "new_alignment.R" file.

4. Click "Misc" at the top of the screen. Click "Get Working Directory, and find the folder that contains the .csv file and the "new_alignment.R" file. Click to open.

5. Open the "new_alignment.R" file, and change the name of the first "[DATA NAME HERE]" to the name of the .csv file. Change the name of "[OUTPUT NAME HERE]" to a new name for the output file.

6. Copy and paste the edited code into the R console, and press enter. The data will be output as a .csv file using the name given in step 5 in the same location as the input file.

## R Code

```r
alignment <- read.csv("[DATA NAME HERE].csv")
col_idx <- seq(1, ncol(alignment), by=2)
dat_pieces <- lapply(col_idx, function(i) {dat_piece <- alignment[, c(i, i+1)]
names(dat_piece)[1] <- "ID" return(dat_piece)
})
merged <- Reduce(
function(a, b) merge(a, b, by = 'ID', all.x =T, all.y=T), dat_pieces)
delete.na <- function(DF, n=0) { DF[rowSums(is.na(DF)) <= n,]
}
nc <- ncol(merged-1)
merged <- delete.na(merged,nc-1)
merged[is.na(merged)] <- 0
dx <- seq(2, ncol(merged), by=1)
data <- lapply(dx, function(i) {dx_piece <- merged[, c(1, i)]
names(dx_piece)[1] <- "ID" return(dx_piece)
})
new <- as.data.frame(do.call(cbind, data))
write.table(new, file = "[OUTPUT NAME HERE].csv", sep = ",", col.names = NA, qmethod = "double")
```

## Manual Alignment Method

1. Copy and paste all mass-to-charge ratio (m/z) values and intensity values of each sample into an Excel spreadsheet.

2. Create a new sheet, and label columns using the same sample names, ensuring that each sample has two columns, one for the m/z value, and the other for the corresponding intensity value. This is the alignment sheet.

3. Copy and paste the smallest m/z value along with its corresponding intensity value into the alignment sheet under its respective sample header.

4. If the m/z difference between two peaks is smaller than 0.5 Da (e.g., 834.1 and 834.4), place them in the same row.

5. Copy and paste the next m/z and intensity values in the dataset into the second row of alignment.

6. Repeat steps 4 and 5 until all data has been aligned.