MTXQCvX - Part3: ManualValidation template *

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Contents

This document provides the manual validation of GC-MS derived data (MTXQC part 3). Thats has been processed through MTXQCvX part1 before. It transforms your MAUI exports into easily modifiable tables (PrepData) and re-transform them after manual validation into csv-files usable for another round of MTXQC (EvalQuant; EvalInc). In case of Metmax input files run MTXQC part 4 first.

Keywords: MTXQCvX, manual validation

Data transformation for convenient manual validation

```
#if (params$inputformat != "maui") {
 # message("This input format is currently not integrated in this module! Sorry!")
#  knitr::knit_exit()
#}

if ((params$prep != "none") & (params$eval != "none")) {
  message("Please select only one action at a time - eiter data transformation or data integration!")
  knitr::knit_exit()
}
```

```
#MOD!
set_input = "input/"
set_output = "output/"

## subfolder for postprocessing
set_val = paste0(params$folder, "/")

if (set_val == "") {
  message("Please define a folder!")
  knitr::knit_exit()
}

#directory definition and figure_name definition
if (params$spath == "") {
  path_setup = ""
  set_fig = paste0(path_setup, 'figure/MTXQCp3-')
```

*Template MTXQCvX part3 written by Christin Zasada, Kempa Lab

```
} else {
  path_setup = paste0(params$spath, "/")
  set_fig = paste0(path_setup, 'figure/MTXQCp3-')
}

knitr::opts_chunk$set(fig.width = 5, fig.align = 'center', fig.height = 4,
                      fig.path = set_fig,
                      echo = FALSE,  #TRUE - show R code
                      warning = FALSE, #show warnings
                      message = TRUE) #show messages

#Create a folder and stop processing if it is already present performing PrepData
if (params$prep != "none") {
  if (!dir.exists(file.path(paste0(path_setup, set_output, set_val)))) {
      dir.create(paste0(path_setup, set_output, set_val))
  } else {
     message("Folder already exists! Please define a new folder where to save transformed data.")
  }
}
```

Choose the mode of the document!

```
## Data transformation performed for: none
```

```
## Data integration perfomed for: PeakArea
```

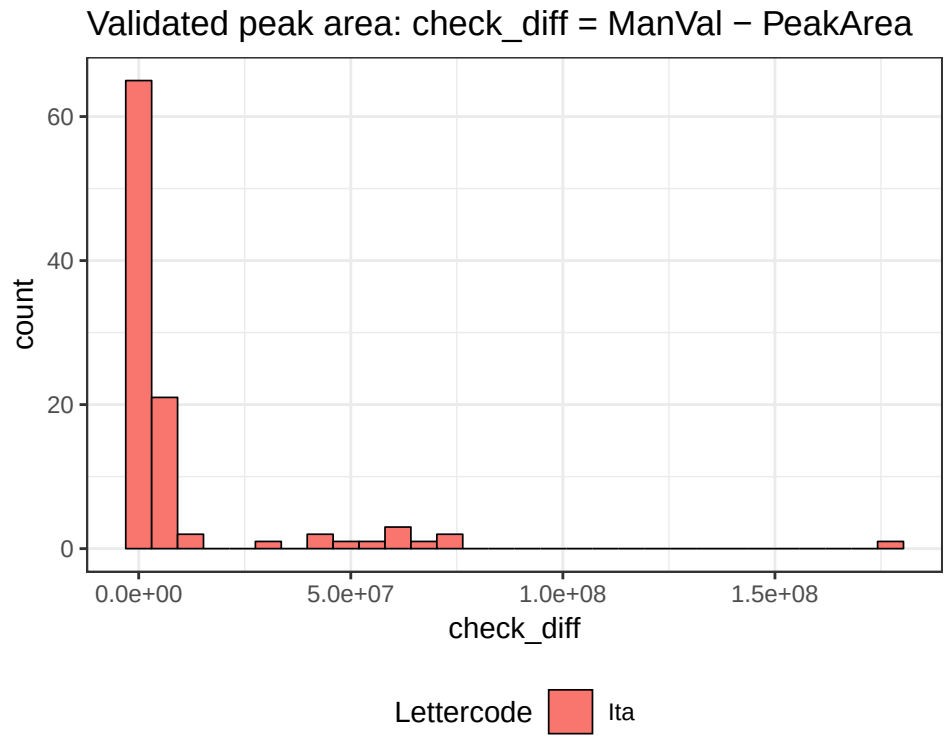
Input files

```
## MTXQCparams.csv imported!
```

```
## Maui_params.csv imported.
```

```
## Number of modified peak areas: 100
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```




```
## Manual validated peak areas have been merged original data and saved in: input/quant/MassAreasMatrix
```