

MTXQCvX - Part3: ManualValidation template *

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This document provides the manual validation of GC-MS derived data (MTXQC part 3). That 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 - either 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 performed for: PeakArea

Input files

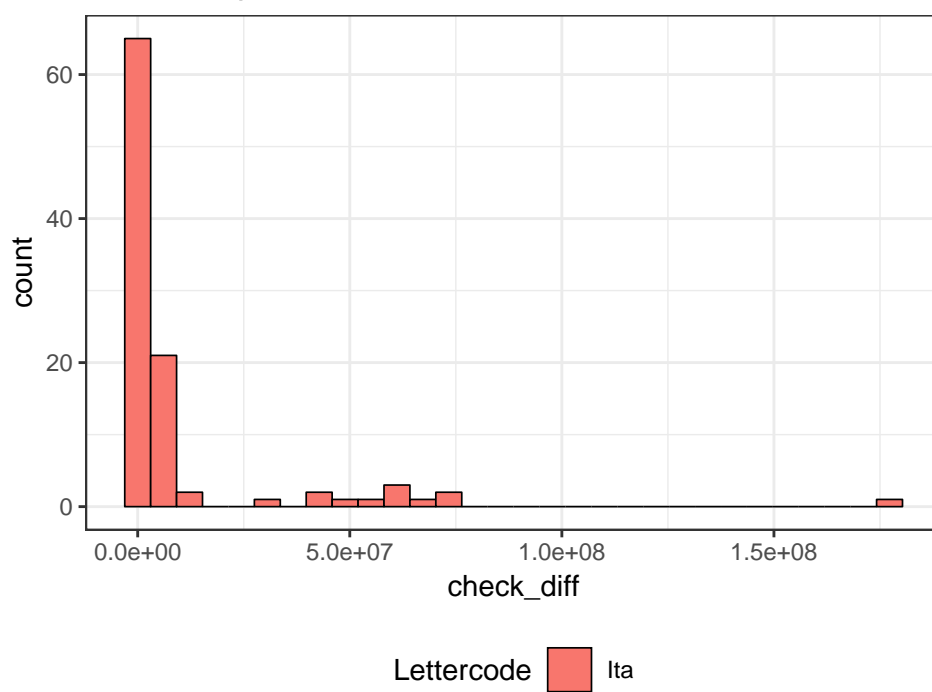
MTXQCparams.csv imported!

Maui_params.csv imported.

Number of modified peak areas: 100

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

Validated peak area: $\text{check_diff} = \text{ManVal} - \text{PeakArea}$



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

Validation of peak areas

