MTXQCvX Part4: PROJECT NAME *

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Contents

MTXQC part 4 provides the transformation of Metmax-derived files for the usage as input files for MTXQC part 1. This report provides three modes - (1) basic - creates tables required for GC-MS performance, (2) Quant - Generation of ManualQuantTable (3) Inc - Calculation of 13C-isotope incorporation.

Keywords: MTXQCvX, pSIRM time course, cell extracts, manual validation, quantities, stable isotope incorporation

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Metmax-parser for MTXQC

Project settings

```
#set path for figure export and size

set_input = "input/"
set_output = "output/"
## subfolder for postprocessing

#directory definition and figure_name definition
if (params$spath == "") {
  path_setup = ""
  set_fig = paste0(path_setup, 'figure/MTXQCp4-')
} else {
  path_setup = paste0(params$spath, "/")
  set_fig = paste0(path_setup, 'figure/MTXQCp4-')
}

knitr::opts_chunk$set(fig.width = 8, fig.align = 'center', fig.height = 7,
                      fig.path = set_fig,
                      echo = FALSE,  #TRUE - show R code
                      warning = FALSE, #show warnings
                      message = TRUE,
                      eval = TRUE
                      ) #show messages
```

```
## Correct input format of files defined! metmax

## File imported! file annotation

## File imported! sample_extracts
```

*Template MTXQCvX part 4 written by Christin Zasada, Kempa Lab

```
## PeakArea matrix imported!

## No file for m/z 73 values defined!

## No file with MIDs defined!

## Please define your internal standard in the conversion_metabolite.csv file!

## Alkane standard annotation detected in conversion_metabolite.csv.
```