

# MTXQCvX Part4: PROJECT NAME \*

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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 <sup>13</sup>C-isotope incorporation.

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

## 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

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

```

## File imported! file annotation

## File imported! sample_extracts

## PeakArea matrix imported!

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

## No file for mass isotopomer distributions (MIDs) defined!

## Internal Standard definition detected in conversion_metabolite.csv.

## Alkane standard annotation detected in conversion_metabolite.csv.

GC-Performance

Internal extraction standard

## Data file for internal standard generated and exported to: input/gc/InternalStandard.csv

## Defined internal standard: CinAcid

Alkane intensity distribution

## Alkane intensities have been exported to input/gc/Alcane_Intensities.csv

PeakDensities

Derivatisation efficiency

## No input file generated. Check your parameter selection.

Absolute Quantification

Generation of ManualQuantTable and PeakArea-matrix

## ManualQuantTable for standard calibration curves has been generated. Quant1_v3

## quantMassAreaMatrix.csv has been generated and saved in input/quant/.

Stable isotope incorporation

Calculation of stable isotope incorporation

## No application of stable isotopes defined in the ExperimentalSetup.

```

*General report parameter*

## Metmax\_params.csv exported.

Parameter	Value
spath	test2/
matrix	metmax_area_ser.csv
mz	
mid	
inc_data	DataMatrix.csv
inputformat	metmax
intstd	TRUE
alkanes	TRUE
peakchroma	FALSE
mqt	TRUE
inc	FALSE