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
```

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

```
## File imported! file annotation

## File imported! sample_extracts

## PeakArea matrix imported!

## Matrix with m/z 73-values imported

## MIDs-matrix imported!

## Internal Standard defintion 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

```
## Peak-Densities table has been exported. Check input/gc/PeakDensities-Chroma.csv
```

Derivatisation efficiency

```
## A modified table for the target mass m/z=73 has been generated and exported!
```

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

```
## The Metmax-exported MIDS have been converted.

## Determined 13C-incorporation has been saved: input/inc/DataMatrix.csv

## Metmax-derived MIDs have been transformed into classical MTXQC input format.

## File saved in input/inc/pSIRM_SpectraData.csv.
```

General report parameter

```
## Metmax_params.csv exported.
```

Parameter	Value
spath	test/
matrix	metmax_area.csv
mz	mz73_ser.csv
mid	mids_metmax.csv
inc_data	DataMatrix.csv
inputformat	metmax
intstd	TRUE
alkanes	TRUE
peakchroma	TRUE
mqt	TRUE
inc	TRUE