MTXQCvX Part4: PROJECT NAME *

Secret   *Secret*
Christin   *Kempa Lab*

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

Metmax-parser for MTXQC

Project settings

```r
#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 defintion detected in conversion_metabolite.csv.

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

GC-Performance

Internal extraction standard

```
## Defined internal standard: CinAcid

## WARNING: No peak areas detected for internal standard in peak area matrix.
```

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	test/
matrix	metmax_area.csv
mz	
mid	
inc_data	DataMatrix.csv
inputformat	metmax
intstd	TRUE
alkanes	TRUE
peakchroma	FALSE
mqt	TRUE
inc	FALSE