MTXQCvX2 for Maui-projects

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Introduction

The following article describes briefly how to use MTXQCvX2 in case you used MAUI for the annotation of your metabolomics project. It does not matter if you have performed an experiment including stable isotopes or if you just aim for the quantification of few intermediates.

A **short** summary of the general workflow is shown below, followed by more detailed instructions explaining required input files. Check out the **sidenotes**[1] for some helpful hints and suggestions.

[1] exactly, this is one… :)

Quick view

1. Setup R-project and copy MTXQC-files[2]
2. Knit with parameter: MTXQC_init.Rmd
3. Copy input files
4. Create annotation.csv and sample_extracts.csv files[3]
5. Define the internal standard[4]
6. Knit with parameter: MTXQC_ExperimentalSetup.Rmd
7. Knit with parameter: MTXQC_part1.Rmd
8. Knit with parameter: MTXQC_part2.Rmd
9. If required - proceed with ManualValidation[5]

[2] Check for the latest release: github.com/ChrisZasa/fluffy-adventure

[3] Details further down this document

[4] see below InternalStandard

[5] see vignettes/MTXQCvX2_part3

Single MAUI-project

Input-Folder: gc

- Alcane_intensities.csv (Diagnostics/Export Alcane intensities)
- InternalStandard.csv [6]
- MassSum-73.csv (Diagnostics/QC Mass Sum Export for mass 73)
- PeakDensities-Chroma.csv (Diagnostics/ExportPeakDensities)

[6] see more details below

Input-Folder: quant

- ManualQuantTable.tsv - rename it - e.g., e18125cz.tsv [7] [8]
- quantMassAreasMatrix.csv (Quantification export of samplesPeakGroups)

[7] Location: Maui-project/export/QM-AbsoluteQuantification/…

[8] C://Users/Username/MauiProjects/…

Input-Folder: inc

- DataMatrix.csv (Export % Label of pSIRM-samplesPeakGroups)
- pSIRM_SpectraData.csv (pSIRM Spectra Export)[9]

[9] Requires the selection of Natural_MIDs.txt

Multiple MAUI-projects

Certain circumstances might require the combination of multiple MAUI-projects into one MTXQC-project. This might be the case when you run the same samples in split and splitless or your experimental setup has been measured in multiple batches in order to avoid derivatisation effects.

1. Create in the MTXQC-project folder a new folder, e.g., raw-data
2. Create subfolder for each MAUI-run
3. Copy the required files into each subfolder
4. Update the parameter of **combine-sets.R** file[10]
5. Execute the script
6. Merged files have been generated and copied into input-folder
7. Copy the renamed tsv-files separately into input/quant/…

[10] inst/template_files/…

Annotation-file

The annotation file relate file names with experimental conditions or specify quantification standards in your batch. Two columns - **File and Type** are obligatory and in the case of absence MTXQCvX_part1 stops and shows an error message.

1. Copy first row of quantMassAreaMatrix.csv file
2. Paste & transpose the content into a new Excel-File
3. Rename Metabolite into File
4. Remove QuantMasses (last entry of the column)
5. Add column **Type** and specify either as **sample** or **addQ1_dilution**[11]
6. Add further columns specifying your experimental conditions, e.g., Cellline, Treatment …[12]
7. Save as csv-file (folder: input/…)

[11] additional quantification standards included in your setup, see for further details vignettes/additionalQuant

[12] optimal 2-3 parameter, maximum 4 parameter. Think about possible combinations like: HCT116-control, HCT116-BPTES

Sample_extracts-file

The sample_extracts.csv file helps to determine correct absolute quantities in the manner of pmol/1e+6 cells or pmol/mg tissue. Two columns are obligatory and have to be included: **Extract_vol** and **Unit**[13]. Please specify for each experimental condition that differs in extracted quantities. Column names of the experimental conditions have to match with the annotation file. Otherwise MTXQCvX2_part1 stops processing and throws an error message in the report. An example file can be modified and reused[14]. Save the created file as csv-file into the input folder as well.

[13] Define: count, mg or ul

[14] inst/template_files/…

Internal Standard

15 16

[15] Either generated using Quantification Export of cinacid-peakcontainer or manually generated from quantMassAreasMatrix.csv. File has to be renamed accordingly.

[16] Internal standards have to be defined in config_mtx/conversion_metabolite.csv