

MTXQCvX - Experimental Setup - PROJECT TITLE *

NAME ONE *LAB, LAB LOCATION*
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This document provides an evaluation of GC-MS derived metabolomics data. It assesses GC-MS performance, the absolute quantification and the stable isotope incorporation. ADD HERE FURTHER PROJECT RELEVANT FACTS.

Keywords: MTXQCvX, GC-MS, metabolomics, data analysis and processing

Project-related experimental setup

Sample extraction and derivatisation have been performed by Jenny. According to her notes documented in OneNote section: Collaborations/Landthaler/ODC1 experiment

Sample extraction

Extraction protocol:

1. 5 ml MeOH (50%)
2. 1 ml Chlorform
3. dried 3.5 ml of polar phase
4. 2nd extraction: yes (in two replicates)

Polar phases have been split into two equal fractions of 280 ul (added 600 ul 20% MeOH).

Quant-Mix extraction protocol

Quant-Mixes batch: *Quant_v4*

1. 1 ml MCW for extraction
2. 0.5 ml H2O for phase separation
3. dried 0.5 ml of polar phase (twice)

*Kempa Lab - MTXQCvX ExperimentalSetup, provided by Ch. Zasada, processed 'September 26, 2018'

Derivatisation protocol

Applied the following protocol for derivatisation protocol

1. MEOX/Pyridine (final conc: 40 mg MEOX/ 1 ml Pyridine)
 - Volume: 20 ul
 - Incubation time: 90 min
 - Temp: 30 C
2. Alkan-mix/MSTFA (10 ul mix/1 ml MSTFA)
 - Volume: 80 ul
 - Incubation time: 60 min
 - Temp: 37 C

Prepared aliquots: three-times 28 ul, big glas vials, crimped.

GC-MS measurement

Samples have been measured using the following methods

1. Injector-method: hamilton_1ul
2. GC-method: 5/7/12 1.2ml/min
3. Split: 1:5
4. MS-method: Lizzy-like

General MTXQC parameter

MTXQC_params.csv written.

Proceed with MTXQC_metmax in order to generate required input files.

Table 1: Experimental parameters of the project.

| Value | Parameter |
|---------------------|-------------|
| annotation.csv | ann |
| Sample_extracts.csv | sample_ext |
| qMTX | data |
| TRUE | instd |
| Quant1_v3 | quant |
| none | substr |
| 500 | quant_vol |
| no | addQ_Int |
| no | addQ |
| metmax | inputformat |
| 2 | backups |
| cell extracts | samples |
| test2 | subf |