MTXQCvX - Experimental Setup - Macrophage differentiation - Glc labeling *

Sabrina Geisenberger *Mueller lab, MDC Berlin*
Christin Zasada *Kempa Lab, MDC*

Contents

This document provides an evaluation of GC-MS derived metabolomics data. It asseses 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

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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 18, 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
metmax	inputformat
annotation.csv	ann
Sample_extracts.csv	sample_ext
TRUE	instd
Quant1_v3	quant
glc	substr
pSIRM	data
500	quant_vol
no	addQ
test_ser	subf
1	backups
cell extracts	samples