

# MTXQCvX - Part1: pSIRM \*

**test**     *test*

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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

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## MTXQCvX part1

### *Summary*

**\*\* Summarise your major findings and important details. DO NOT skip this part.\*\***

### *General project settings*

```
##
## Attaching package: 'gplots'

## The following object is masked from 'package:stats':
##
##     lowess
```

### *Data import*

```
## MTXQCparams.csv imported!

## Metmax_params.csv imported.
```

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\*Kempa Lab - Template MTXQCvX part1 - processed 'September 27, 2018'

```

## Experimental setup does not include additional quantification standards!

## File imported! annotation.csv

## File imported! Sample_extracts.csv

## WARNING: No file detected: InternalStandard.csv

## File imported! Alkane_intensities.csv

## No file with m/z 73 values defined for this input format!

## No file defined for this input format!

## File imported! quantMassAreasMatrix.csv

## It's not a pSIRM experiment!

## Correct column names in file sample_extracts.csv

## Correct column names in sample annotation

## Input files checked!

## Annotation and Sample_extract.csv correctly imported!

```

## MTXQC - GC-MS perfomance

### *Alkane standards*

```
## QC-metric succesfully exported: alkanes
```

### *Data normalization*

#### *Internal standard cinnamic acid*

```
## Empty data frame OR no peak areas for internal standard detectable!
```

#### *Sum of Area of annotated metabolites per file*

```
## No SumOfArea file generated in Metmax parser!
```

### *Derivatization check*

```
## No input files detected. Either MassSum-73.csv or PeakDensities-Chroma.csv
```

### *HeatMap - GC-MS performance*

Table 1: Summary of parameter evaluating GC-Performance

Batch_Id	qc_metric	title
e18627jg	0.9663448	alkanes

```
## Export of GC-Performance values done!
```

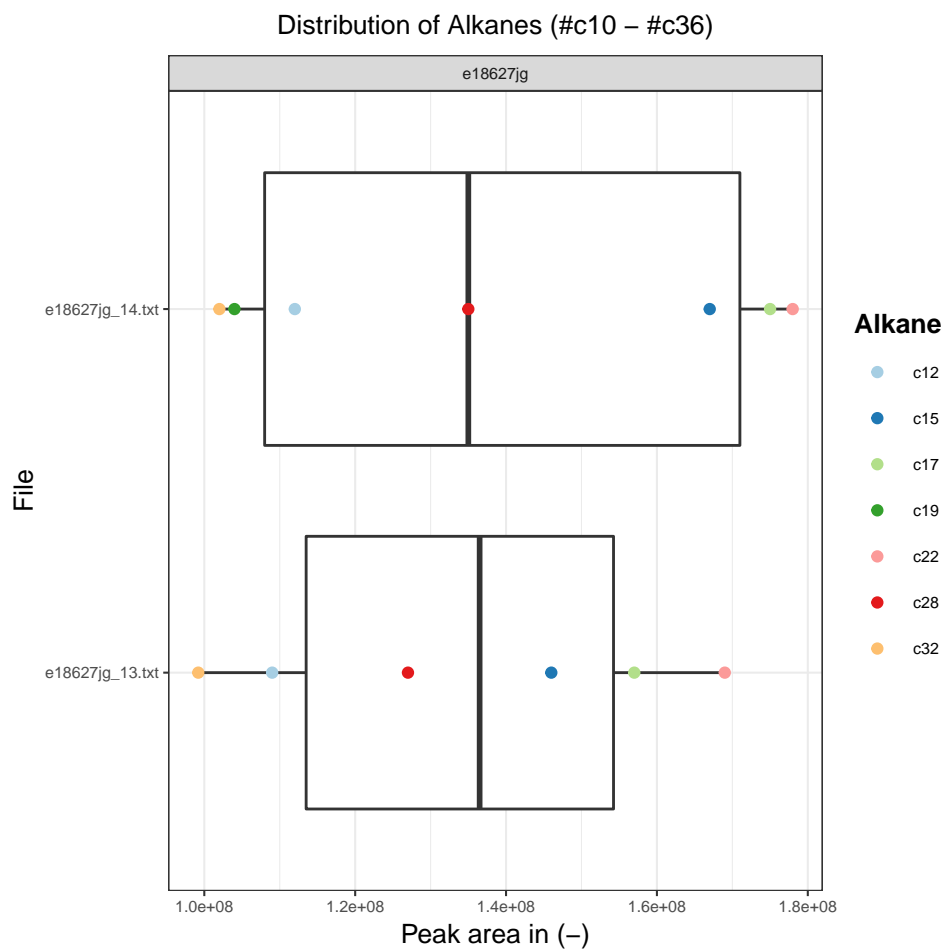


Figure 1: Alkane intensities summarised per each file. Drop of intensities shows questionable files.

## MTXQC - Quantitative metabolomics

*Generation of ManualQuantTable: Quant-Standards (Qstd)*

```
## File imported! quant1_values.csv
```

```
## ManualQuantTable imported!
```

*Generation of ManualQuantTable: Additional calibration curves (Qadd)*

*Determination of calibration curves*

```
## top5_QMQcurveInfo.csv generated!
```

```
if (nrow(qc_calcurve != 0)) {  
  ggplot(qc_calcurve, aes(Lettercode, Par_value, color = Parameter)) +  
    geom_point(aes(shape = Parameter), size = 3) +  
    coord_flip() +  
    ggtitle('Calibration curve: adj. R square and nb of data points') +  
    ylim(0,1) +  
    geom_hline(aes(yintercept = 0.75), linetype = 'dashed', color = 'grey30') +  
    scale_color_manual(values = c('tomato3', 'black')) +  
    scale_shape_manual(values = c(17, 20)) +  
    facet_grid(Origin ~ Batch_Id, scales = "free_y") +  
    xlab('Derivate') +  
    ylab('Parameter value in (-)') +  
    theme(legend.position = "bottom")  
}
```

*Evaluation of experimental data*

*Determination extraction factor*

```
## The quantification factor for that experimental setup: 0.333333333333333
```

```
## The sample factor for that experimental setup: 1
```

```
## The extraction factor for that experimental setup: 0.333333333333333
```

*Quantification range and limits*

```
## Position of data points regarding calibration curves evaluated.
```

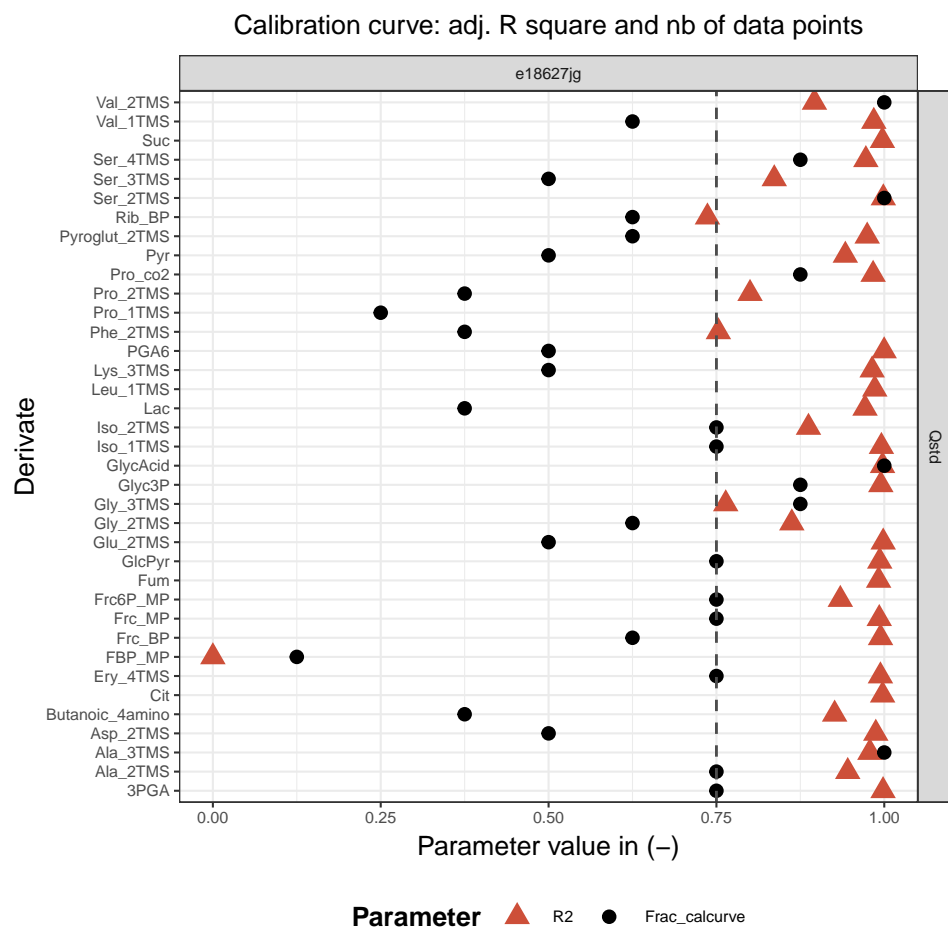


Figure 2: Calibration curves: Nb. of data points.

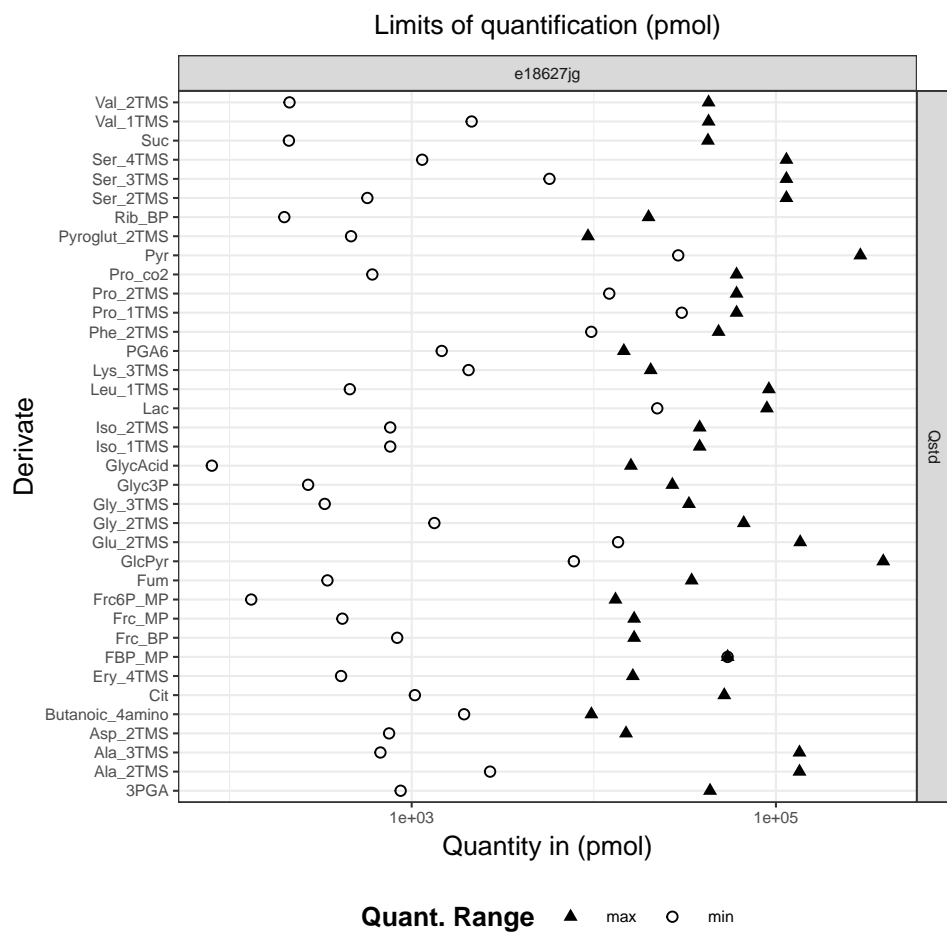


Figure 3: Limits of quantifiable range per metabolite

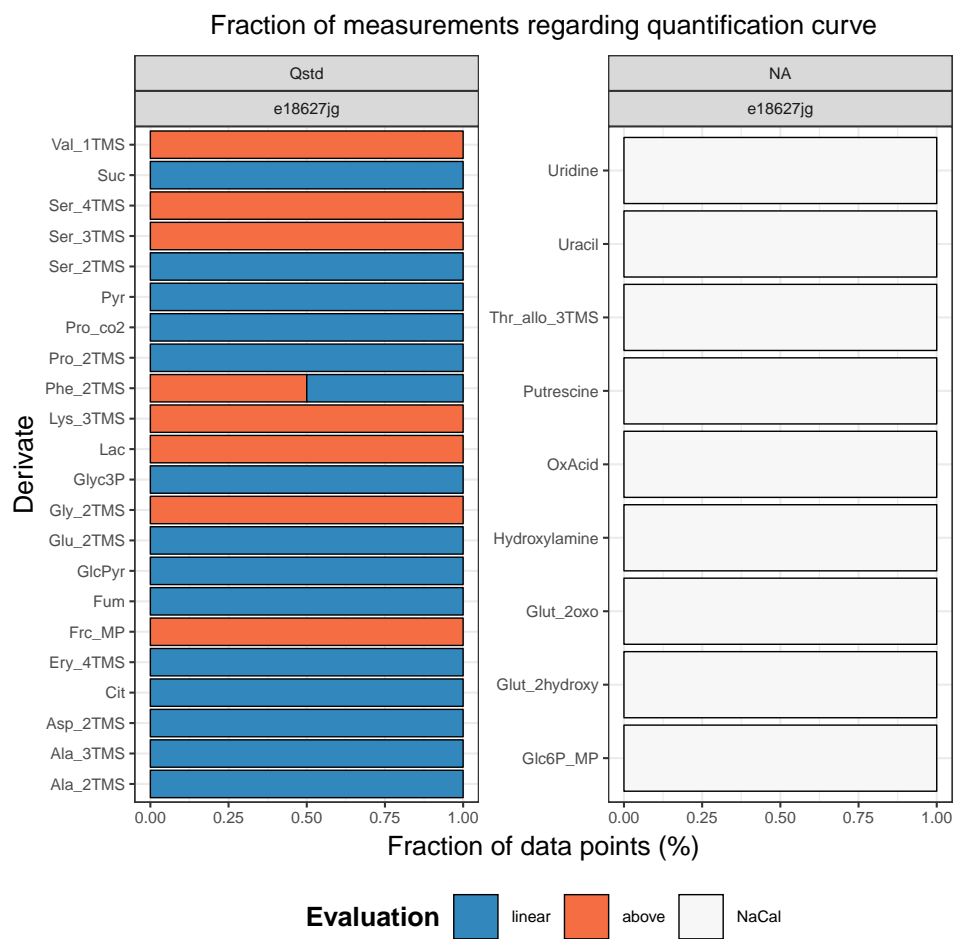
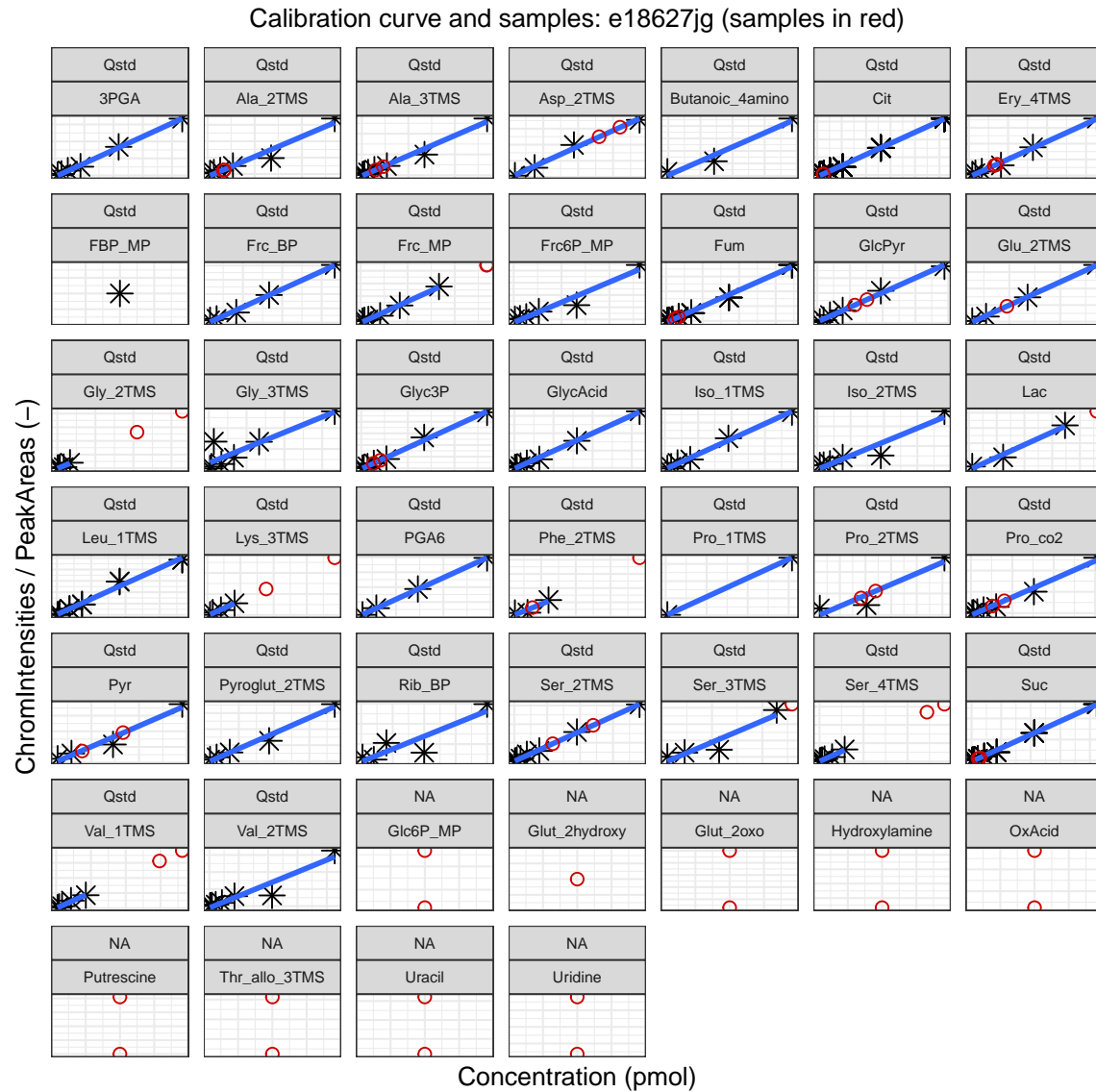


Figure 4: Distribution of data points regarding linear range of the calibration curve

## Absolute quantification samples



## Normalisation of absolute quantities

## WARNING: Sum of area normalisation factor set to value = 1 due to missing input.

## WARNING: Internal Standard normalisation factor set to value = 1 due to missing input.

## Absolute quantification and normalisation have been performed: CalculationFileData.csv

## HeatMap - Quantification

## WARNING: Correlation between internal standard and sum of area normalisation not possible!

## No evaluation of isotope data included.



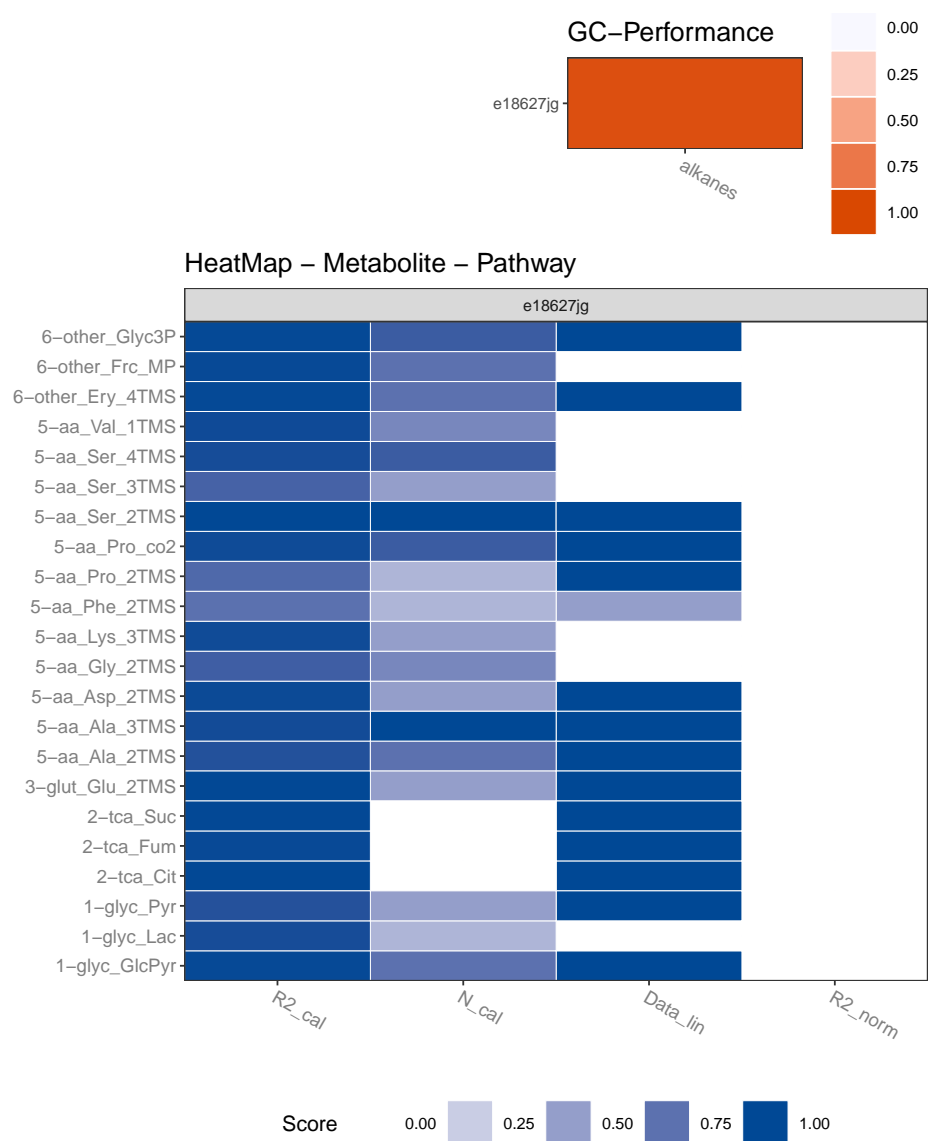


Figure 5: MTXQCvX - Heatmap overview