

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

MTXQCvX part1

Summary

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

General project settings

##

Attaching package: 'gplots'

*Kempa Lab - Template MTXQCvX part1 - processed 'September 25, 2018'

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

Data import

```
## MTXQCparams.csv imported!  
## Maui_params.csv imported.  
## Required table containing additional Quant1-values detected!  
## File imported! Annotation_allbatches.csv  
## File imported! Sample_extract_allbatches.csv  
## File imported! InternalStandard.csv  
## File imported! Alkane_intensities.csv  
## File imported! MassSum-73.csv  
## File imported! PeakDensities-Chroma.csv  
## File imported! quantMassAreasMatrix_manVal.csv  
## File imported! pSIRM_SpectraData.csv  
## File imported! DataMatrix.csv  
## 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

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

Sum of Area of annotated metabolites per file

```
## Files with less than 50% of max(N) should be excluded from SumofArea normalisation.  
## QC-metric succesfully exported: sumofarea
```

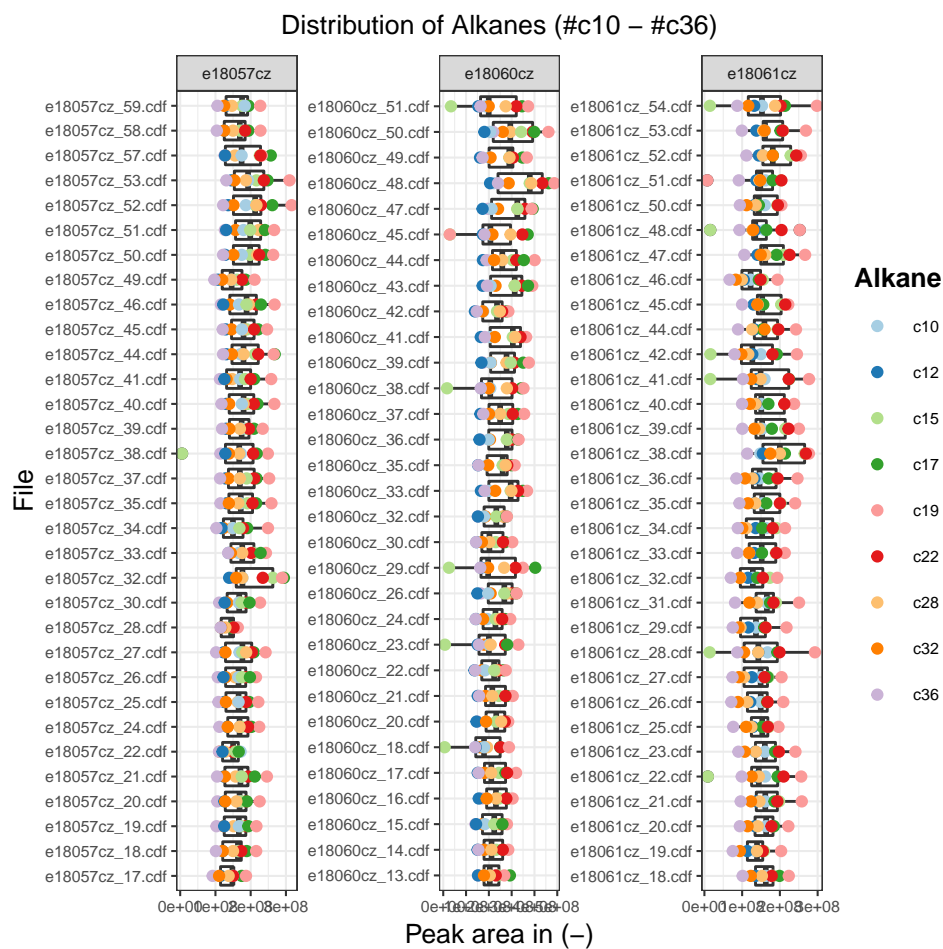


Figure 1: Alkane intensities summarised per each file. Drop of intensities shows questionable files.

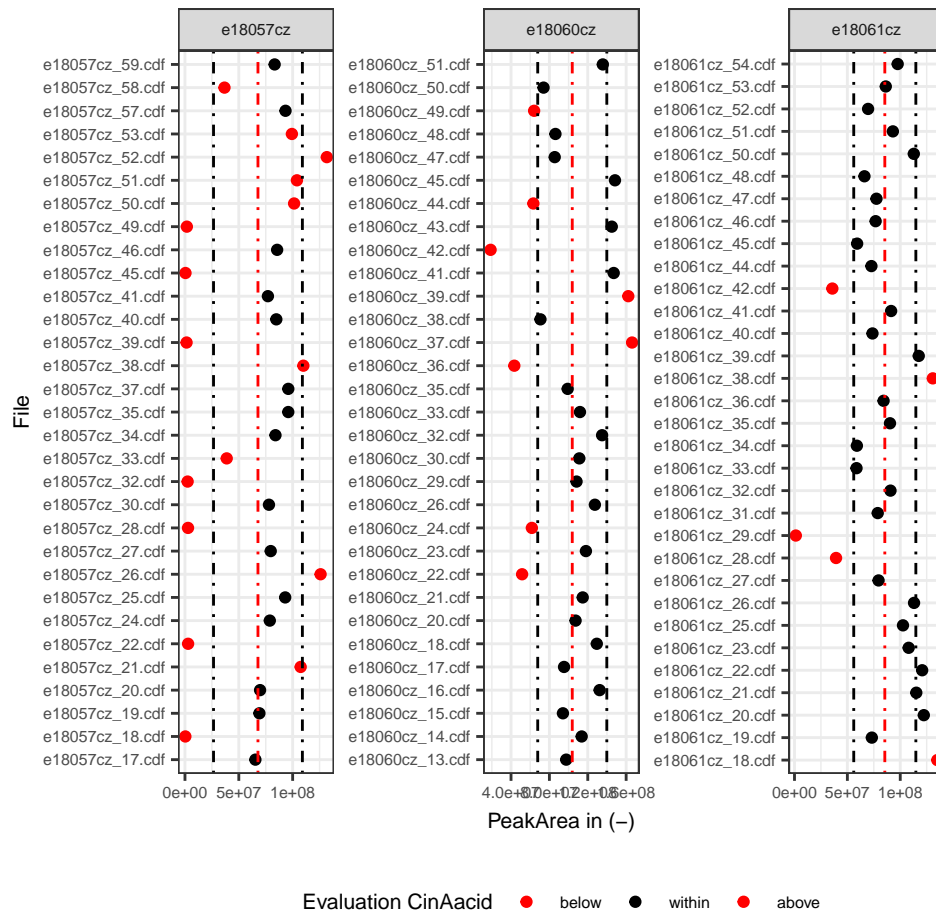


Figure 2: Quantification of internal extraction standard

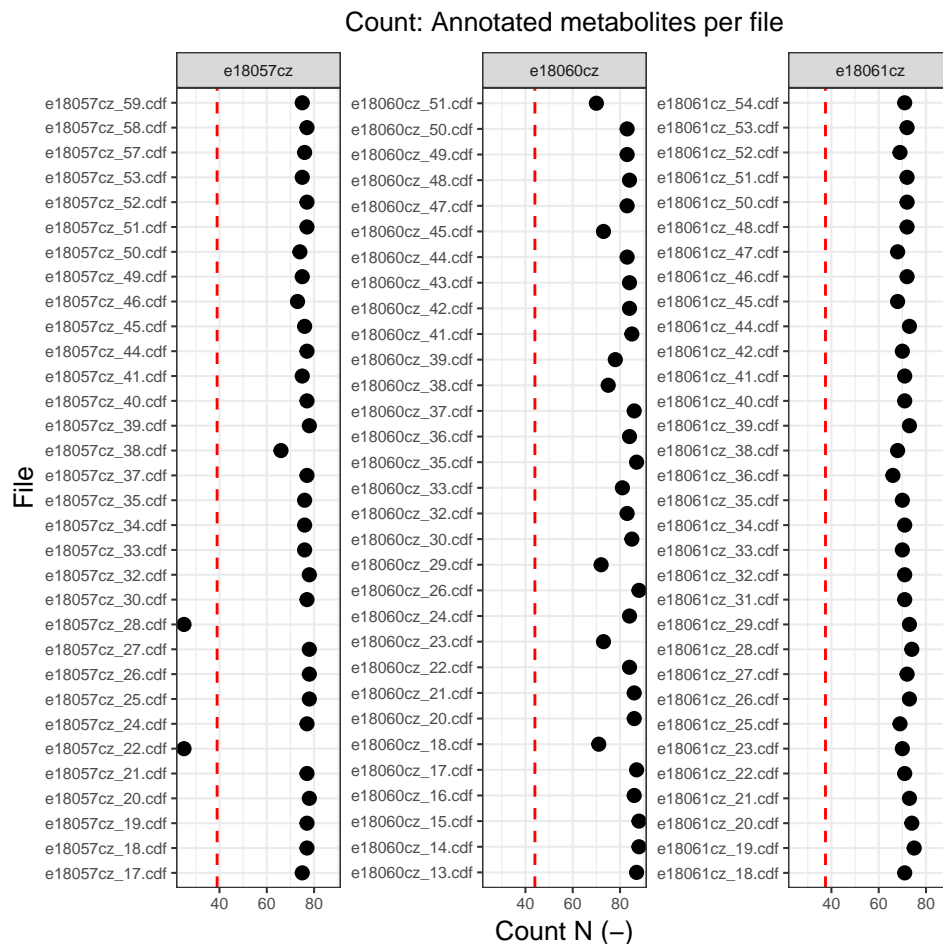


Figure 3: Count N: Annotated intermediates per file. Evaluate careful for SumOfArea normalisation.

Batch_Id	n_50
e18057cz	39.0
e18060cz	44.0
e18061cz	37.5

Derivatization check

QC-metric succesfully exported: mz73

HeatMap - GC-MS performance

Table 2: Summary of parameter evaluating GC-Performance

Batch_Id	qc_metric	title
e18057cz	0.9371664	alkanes
e18060cz	0.9104125	alkanes
e18061cz	0.9173959	alkanes

Batch_Id	qc_metric	title
e18057cz	0.3914688	cinacid
e18060cz	0.6531375	cinacid
e18061cz	0.6563009	cinacid
e18057cz	0.6818946	mz73
e18060cz	0.8585613	mz73
e18061cz	0.7720460	mz73
e18057cz	0.6512975	sumofarea
e18060cz	0.7576846	sumofarea
e18061cz	0.6644690	sumofarea

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

MTXQC - Quantitative metabolomics

Generation of ManualQuantTable: Quant-Standards (Qstd)

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

```
## Correct matching of ManualQuantTable files and annotation file content!
```

```
## ManualQuantTable for standard calibration curves has been generated. Quant1_v3
```

```
## ManualQuantTable generated and exported!
```

Generation of ManualQuantTable: Additional calibration curves (Qadd)

```
## Additional quant1-values imported for metabolites: 3
```

```
## Additional calibration curves have been defined for all included batches!
```

```
## Additional calibration curves have been duplicated and added for all batches!
```

```
## ManualQuantTable for additional calibration curves has been generated. Quant1-values: Quant_ext
```

```
## Additional Quant-Standards have been added to MQT_integrated.csv
```

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")
}
```

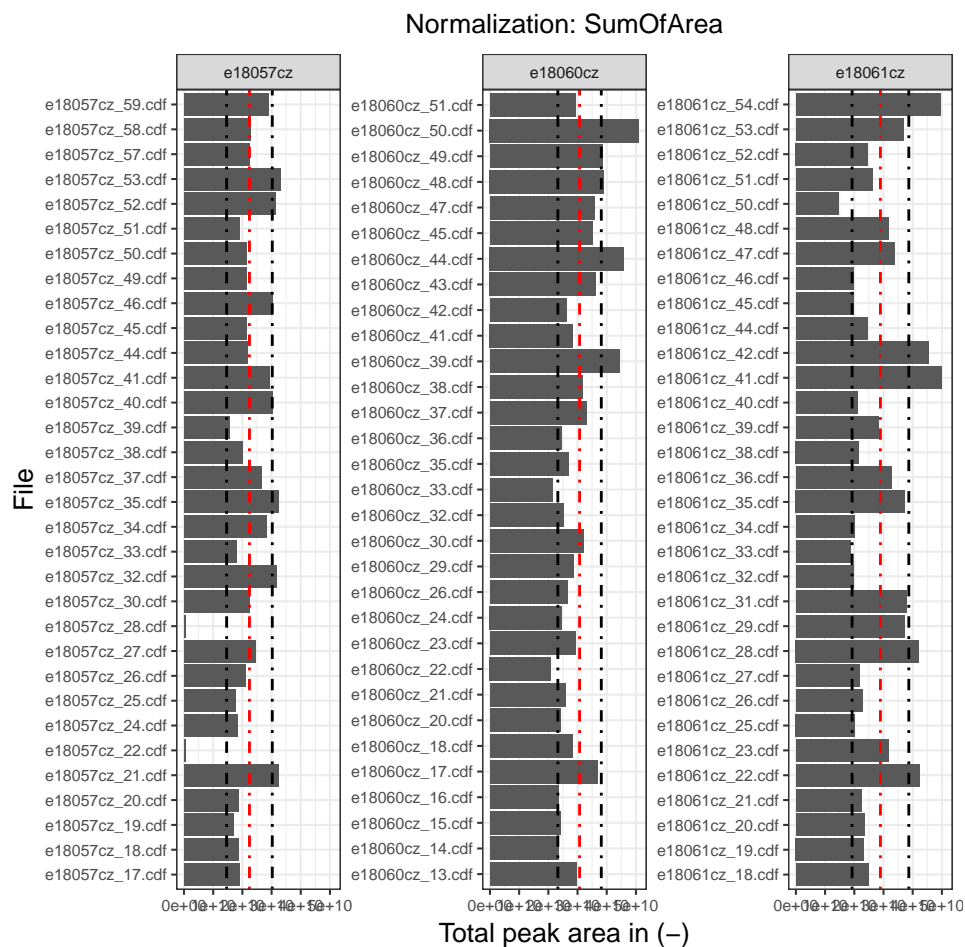


Figure 4: Total peak area of all annotated metabolite per file.

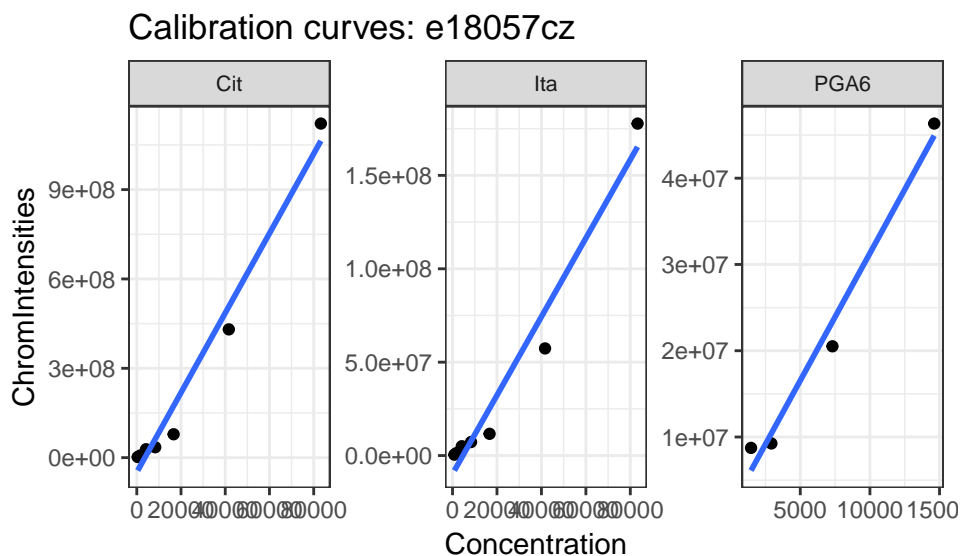


Figure 5: Additional Calibration curves

Calibration curves: e18060cz

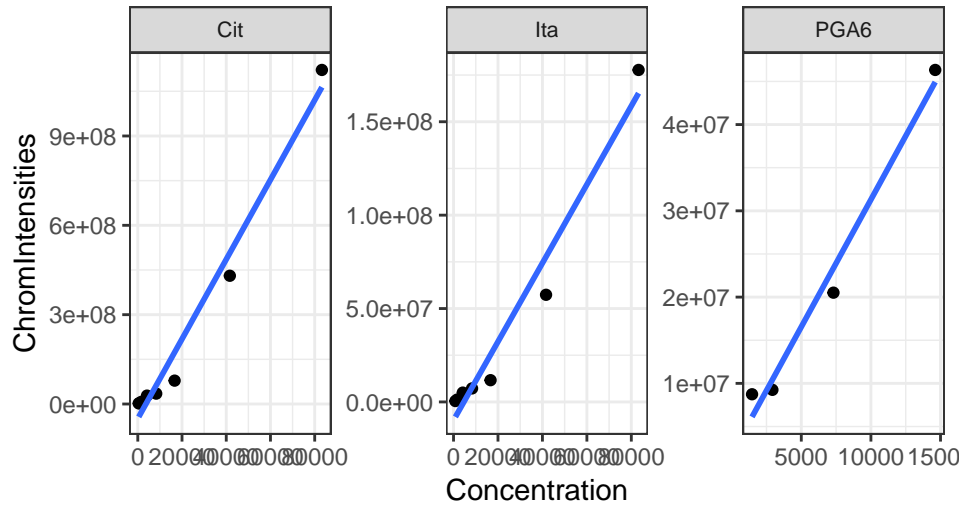


Figure 6: Additional Calibration curves

Calibration curves: e18061cz

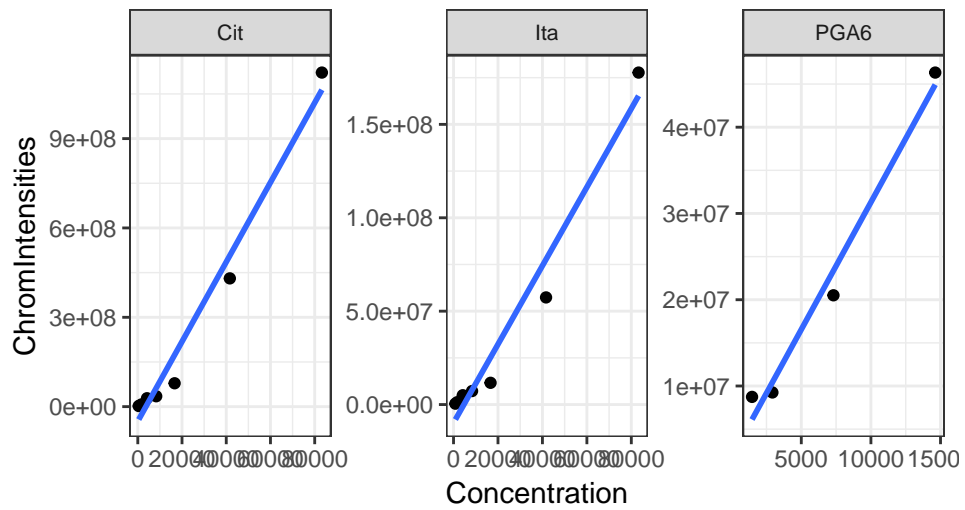


Figure 7: Additional Calibration curves

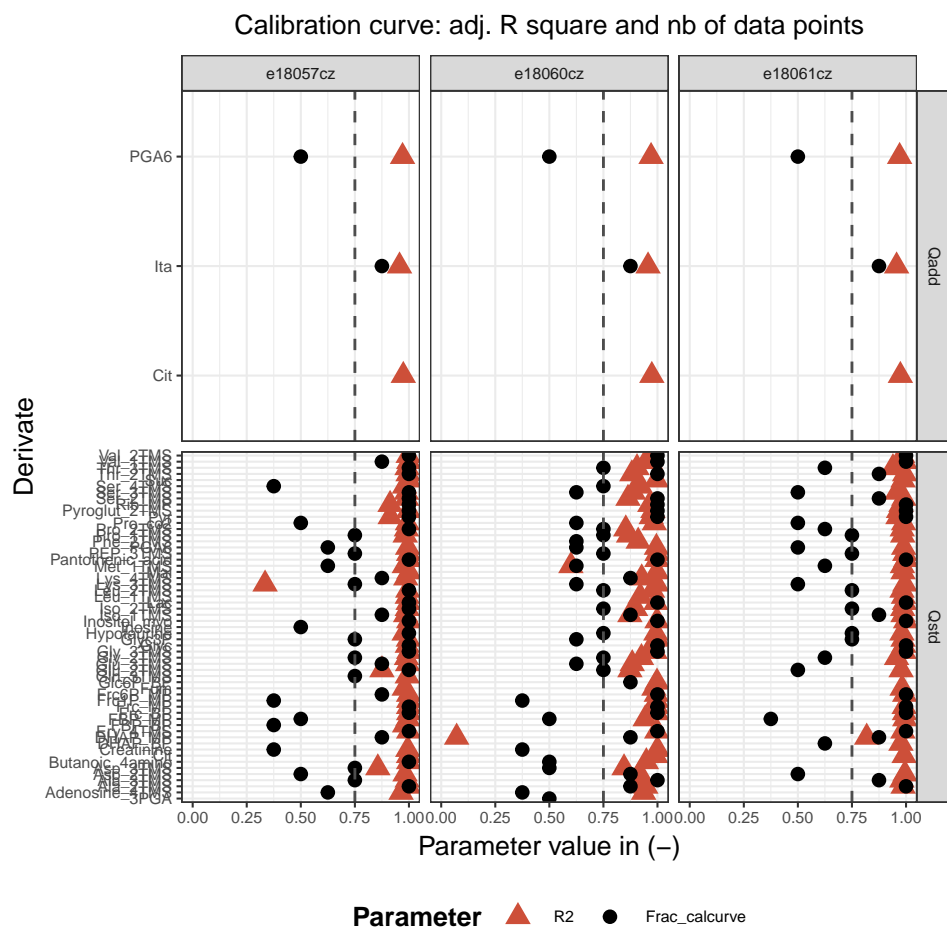


Figure 8: Calibration curves: Nb. of data points.

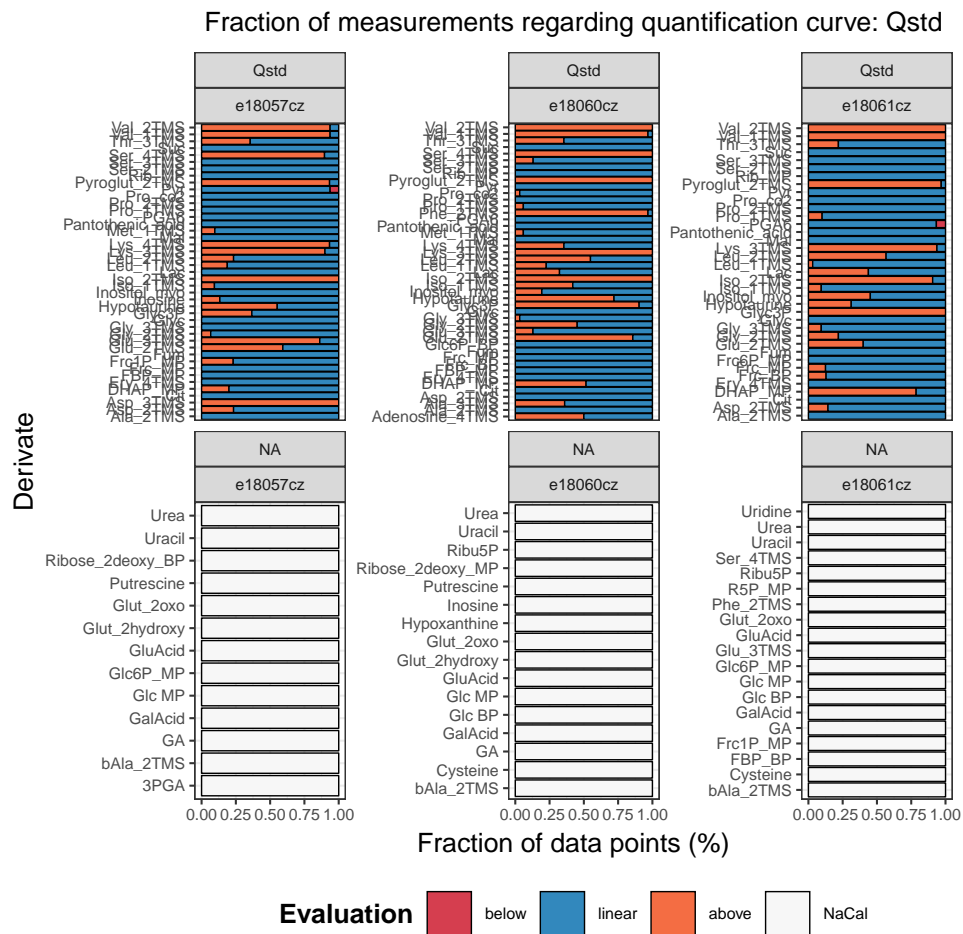


Figure 10: Distribution of data points regarding linear range of the calibration curve

Evaluation of experimental data

Determination extraction factor

The quantification factor for that experimental setup: 0.3333333333333333

The sample factor for that experimental setup: 1

The extraction factor for that experimental setup: 0.3333333333333333

Quantification range and limits

Position of data points regarding calibration curves evaluated.

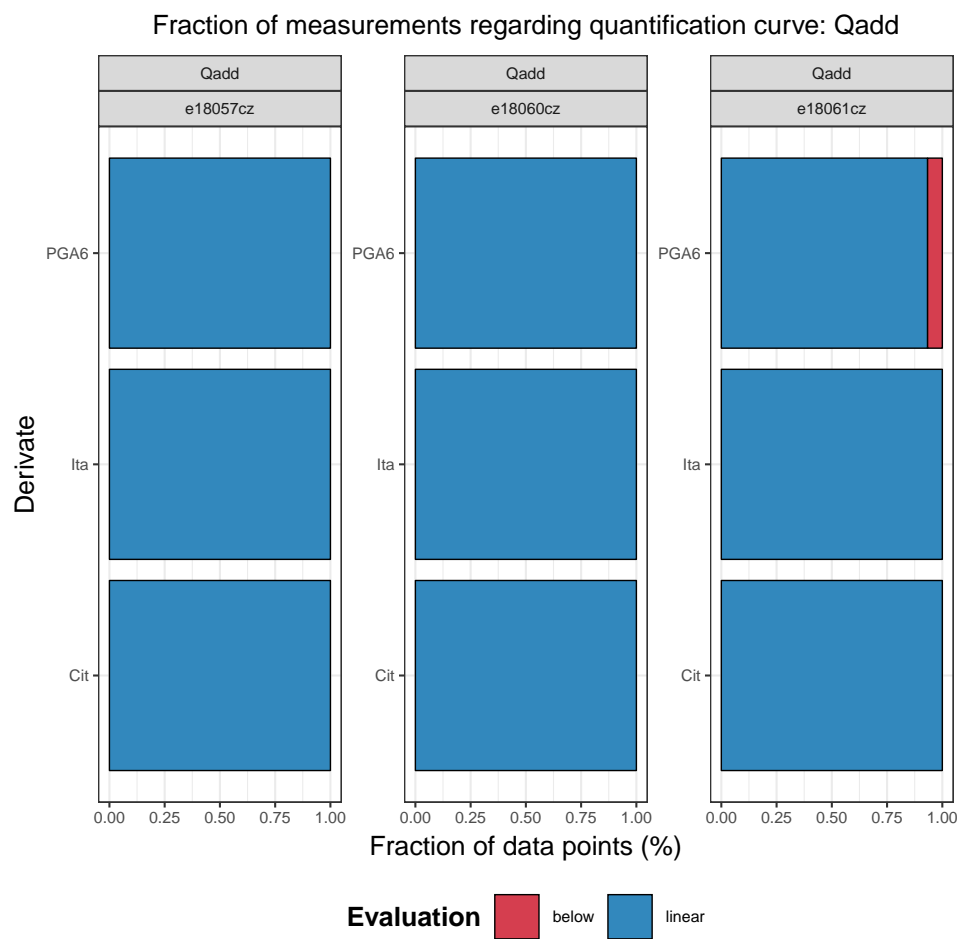
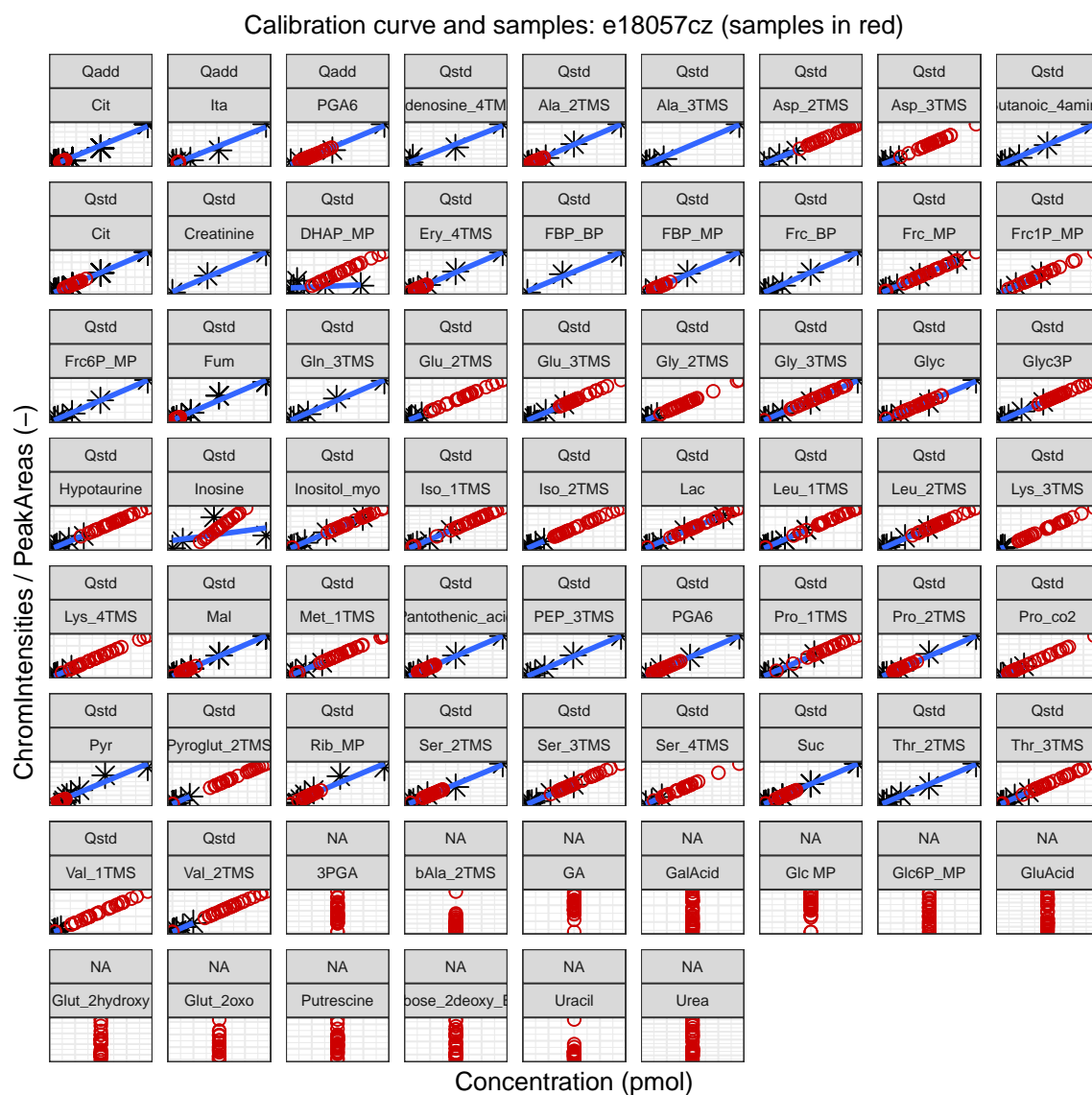


Figure 11: Distribution of data points regarding linear range of the calibration curve

Absolute quantification samples



Calibration curve and samples: e18060cz (samples in red)



Calibration curve and samples: e18061cz (samples in red)



Normalisation of absolute quantities

Absolute quantification and normalisation have been performed: CalculationFileData.csv

HeatMap - Quantification

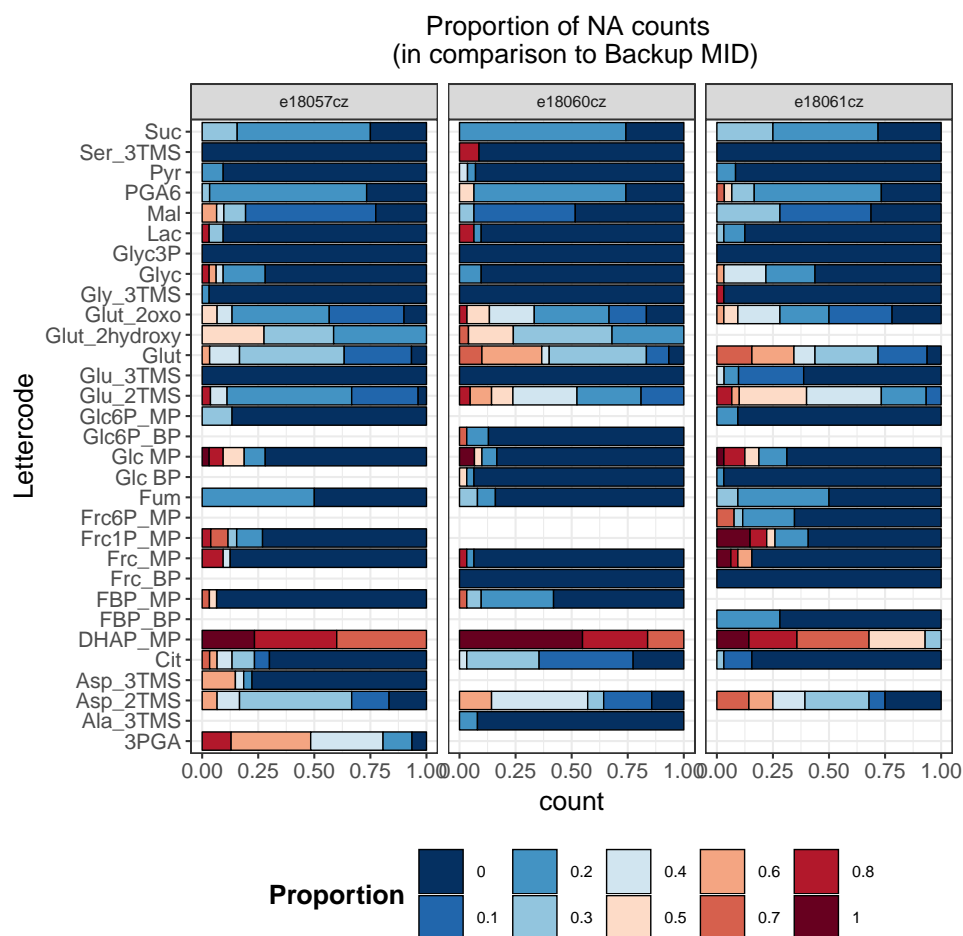


Figure 12: Missing values in mass isotopomer distributions (MID).

MTXQC - Stable isotope incorporation

NA count

3-Lowest of MID

3-Lowest of MID

¹³C-Isotope incorporation

No data for t=0 in the experimental setup defined!

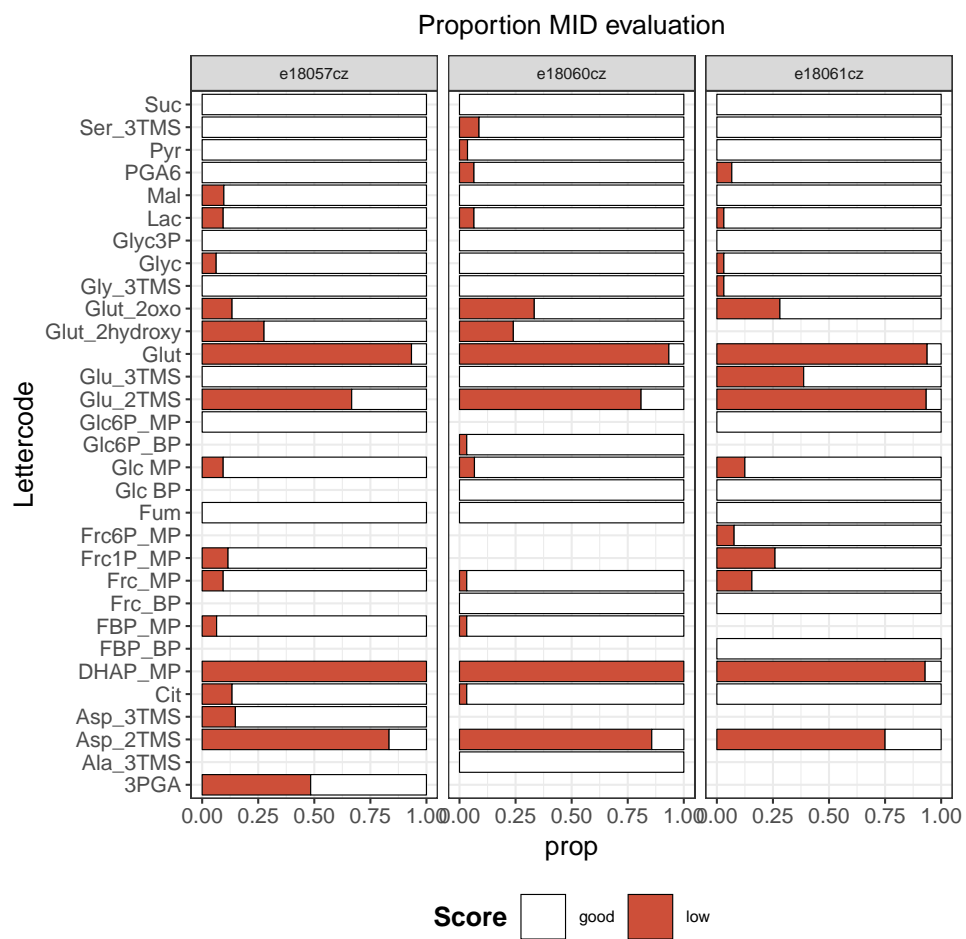


Figure 13: MID quality

Heatmap Isotope incorporation

MTXQC Heatmap compilation: Quantifitation and stable isotope incorporation

End of the document

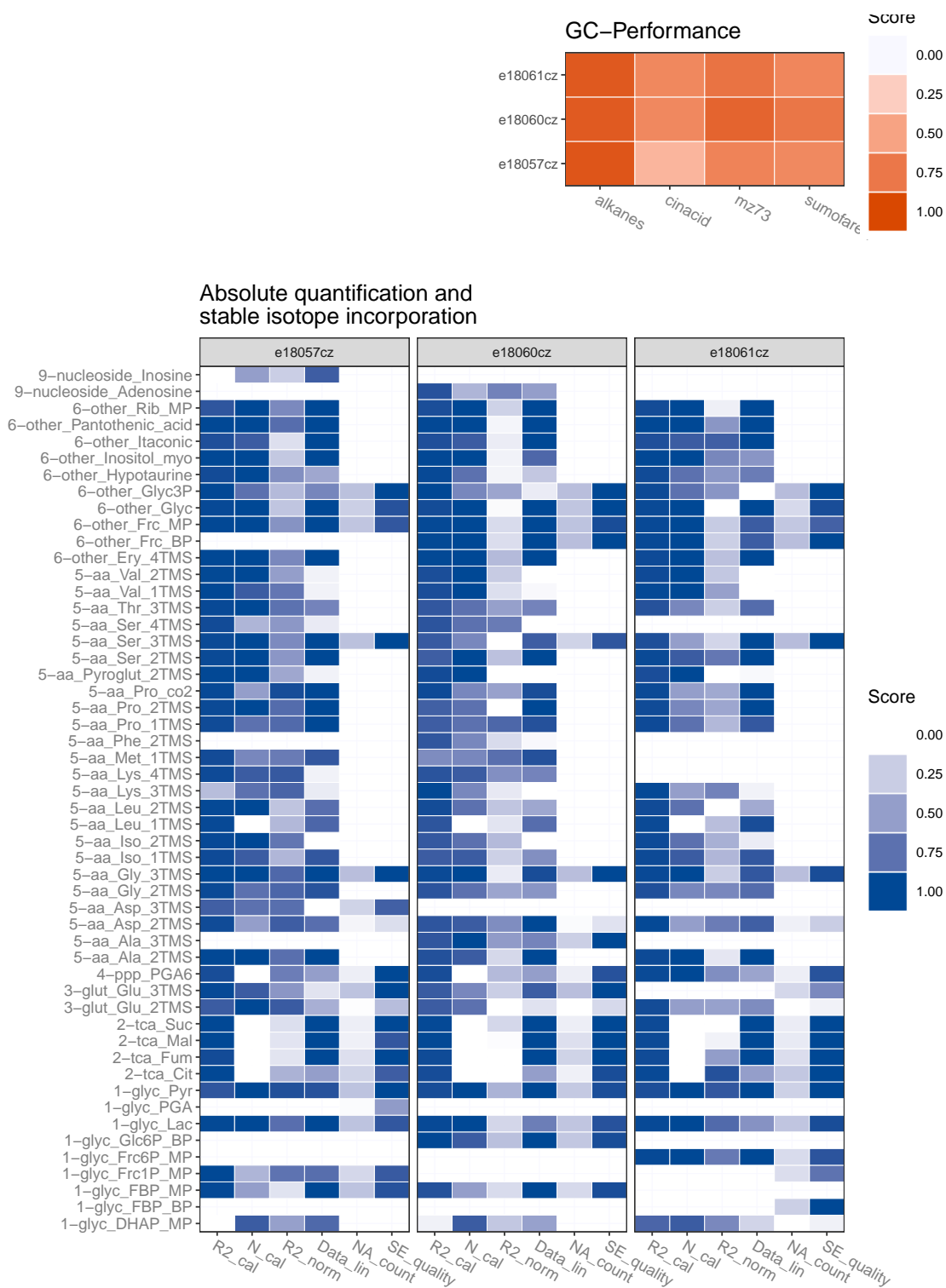


Figure 14: MTXQCvX - Heatmap overview