MTXQCvX - Part1: pSIRM *

test *test*

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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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 19, 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! Alcane_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
```

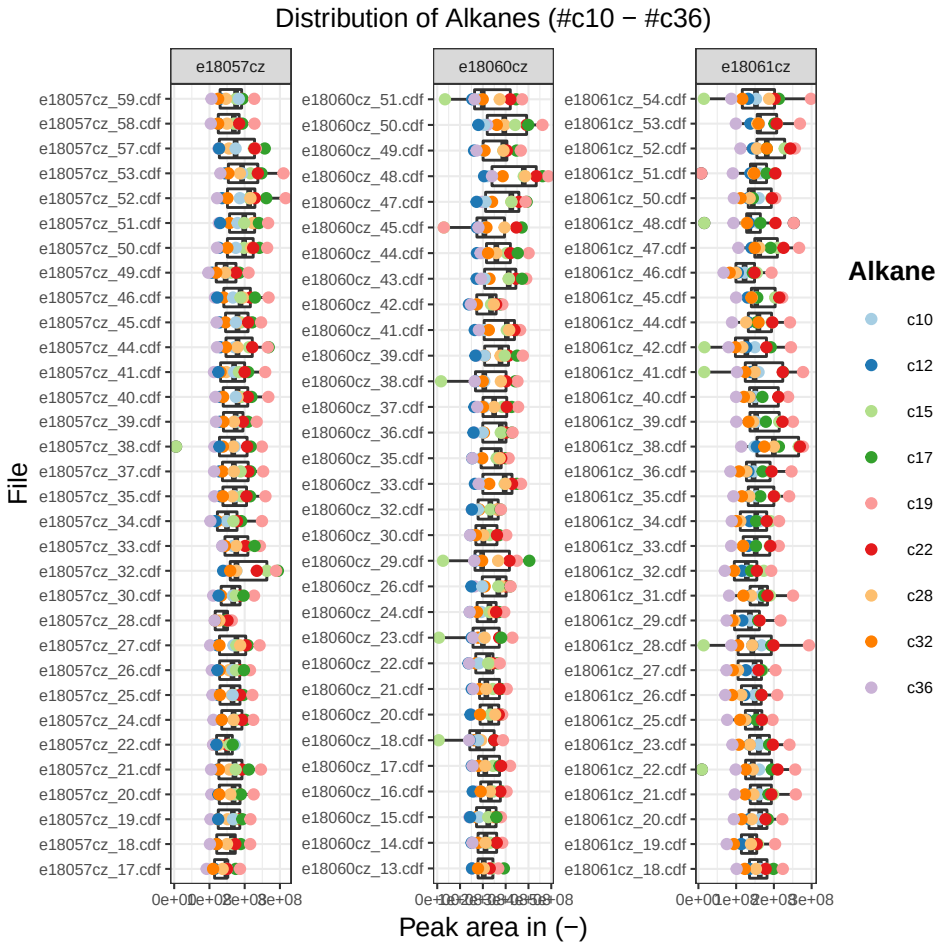


Figure 1: Alkane intensities summarised per each file. Drop of intensities shows questionable files.

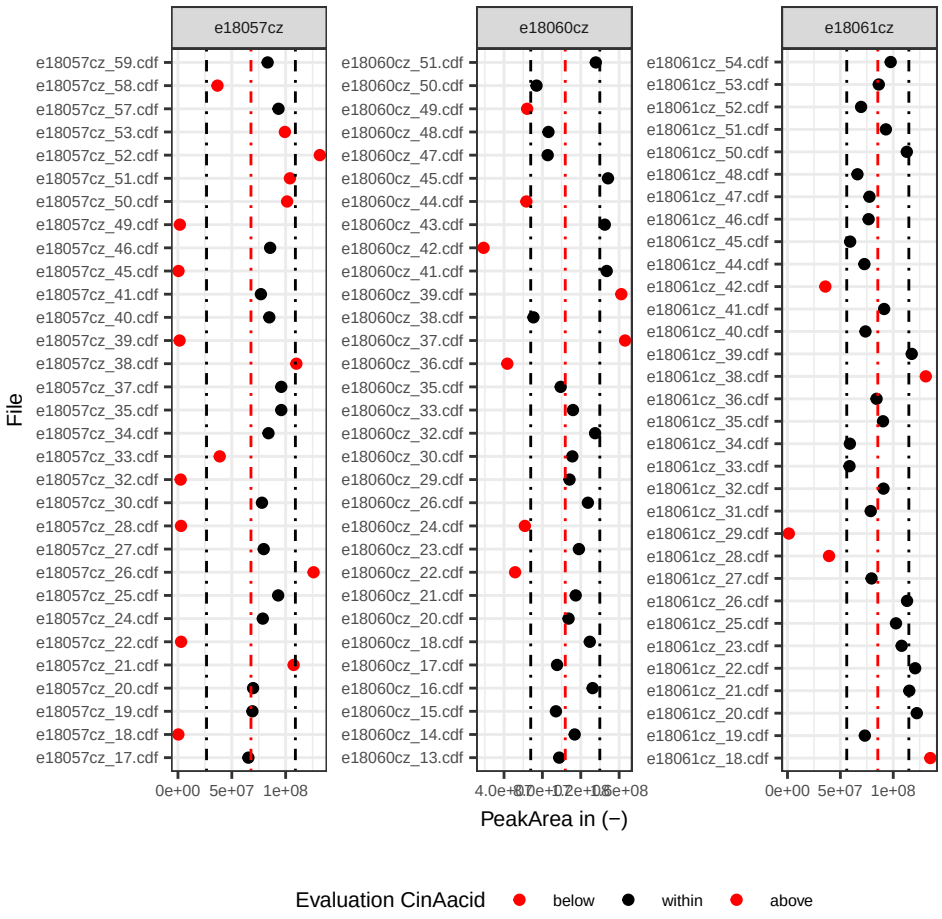


Figure 2: Quantification of internal extraction standard

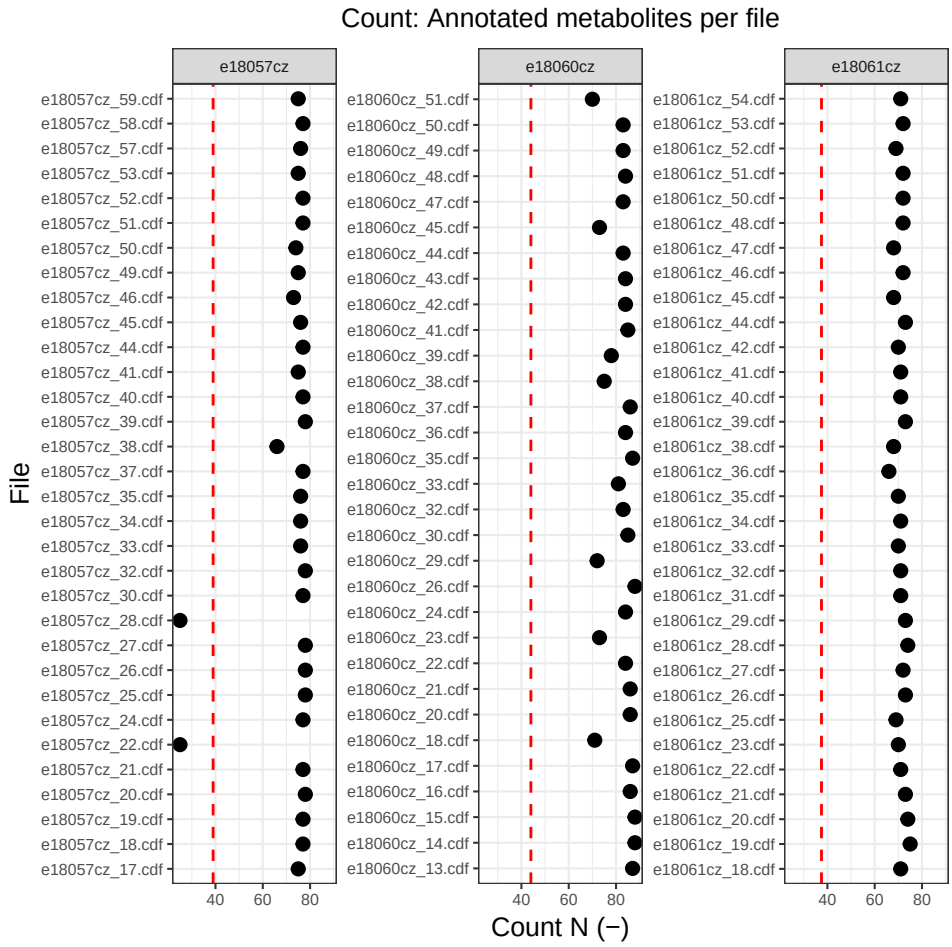


Figure 3: Count N: Annotated intermediates per file. Evaluate careful for SumOfArea normalisation.

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 not defined for all batches included in the annotation file!
```

```
## Batch Id containing additional calibration curves: e18060cz
```

```
## 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")
}
```

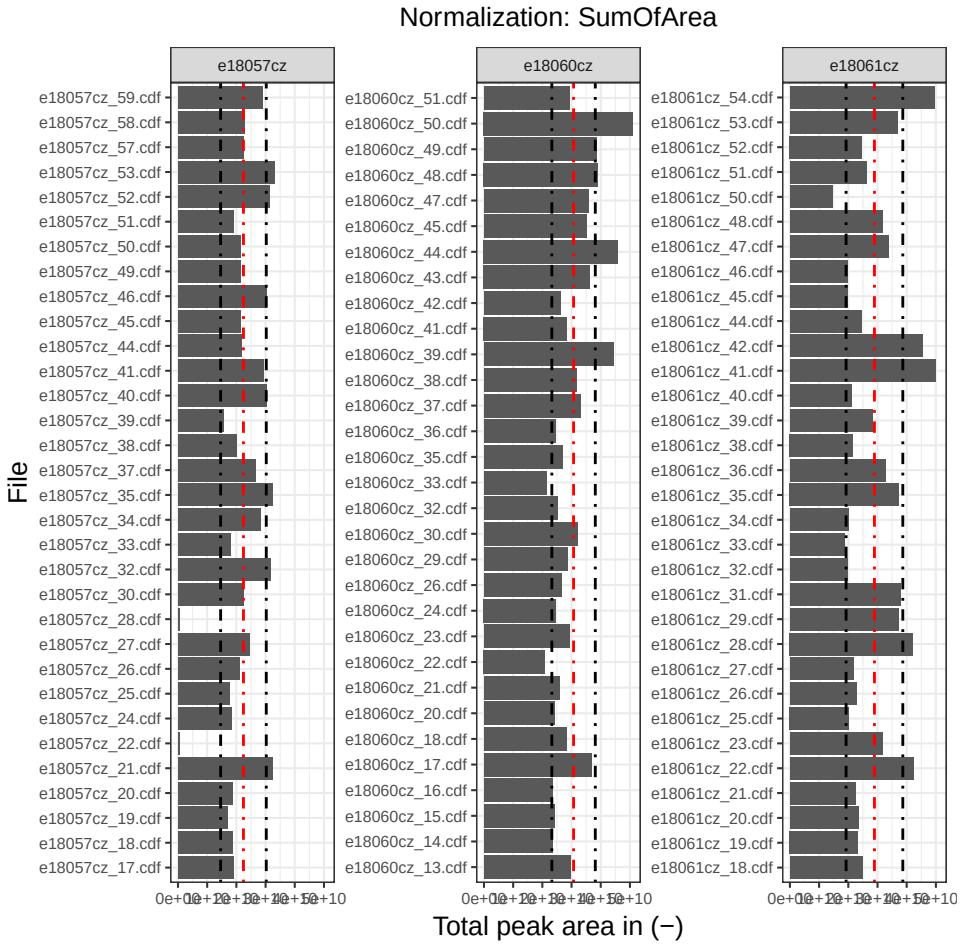


Figure 4: Total peak area of all annotated metabolite per file.

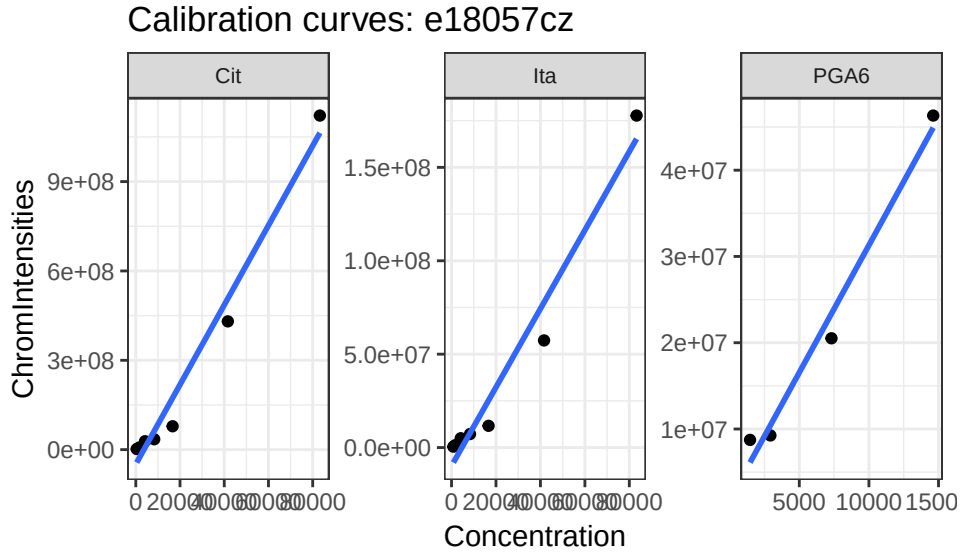


Figure 5: Additional Calibration curves

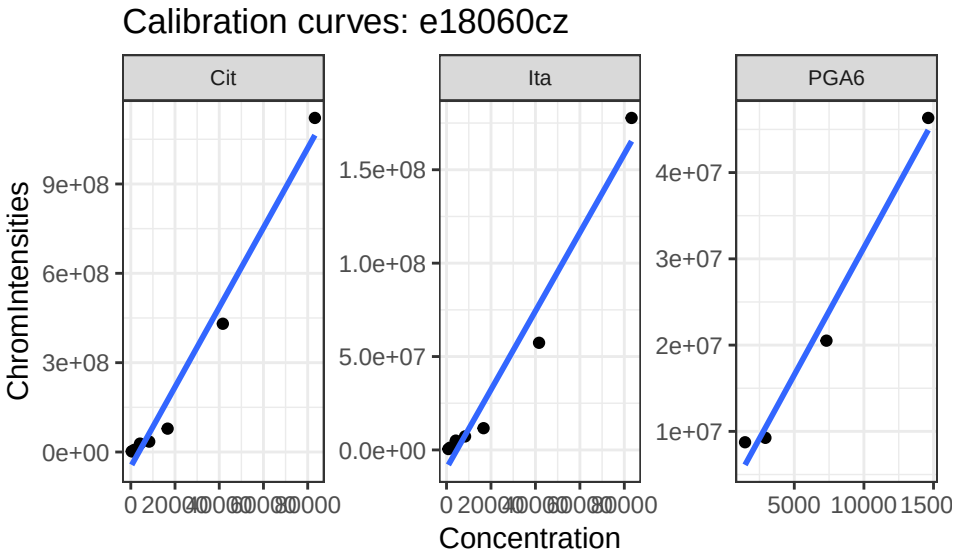


Figure 6: Additional Calibration curves

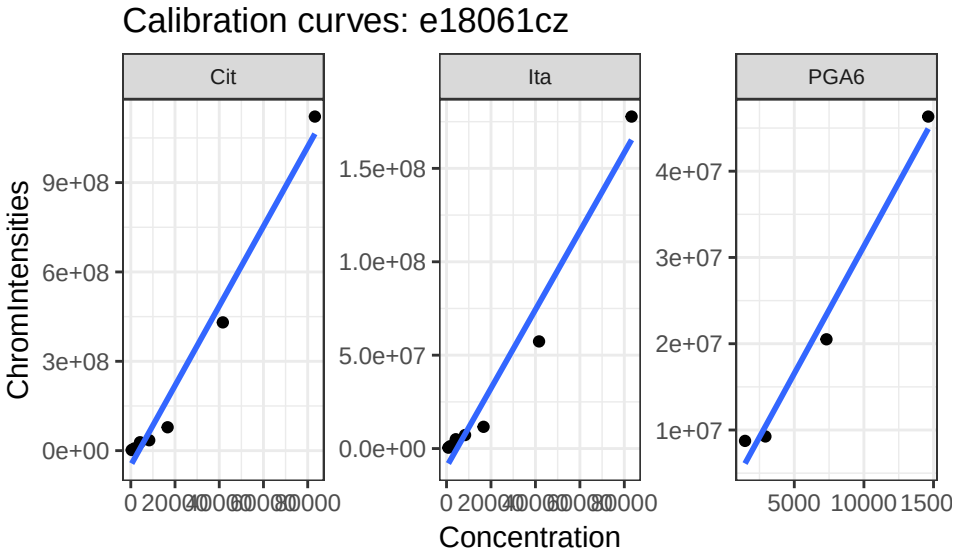


Figure 7: Additional Calibration curves

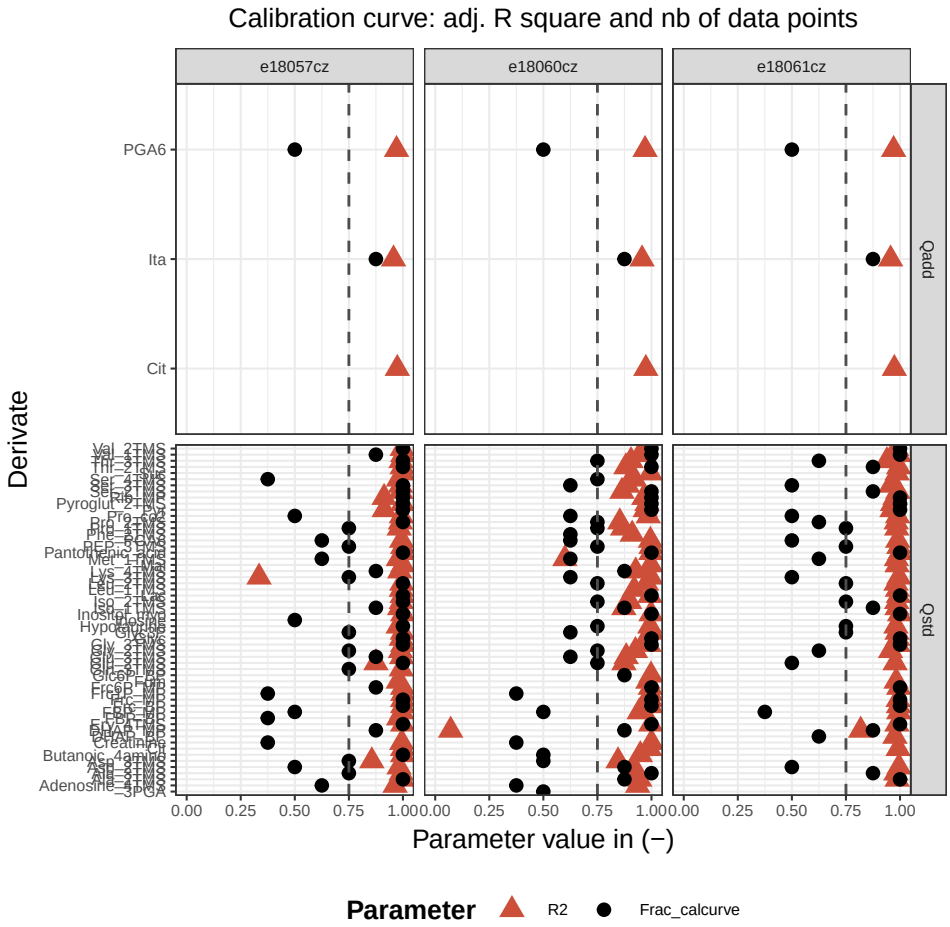


Figure 8: Calibration curves: Nb. of data points.

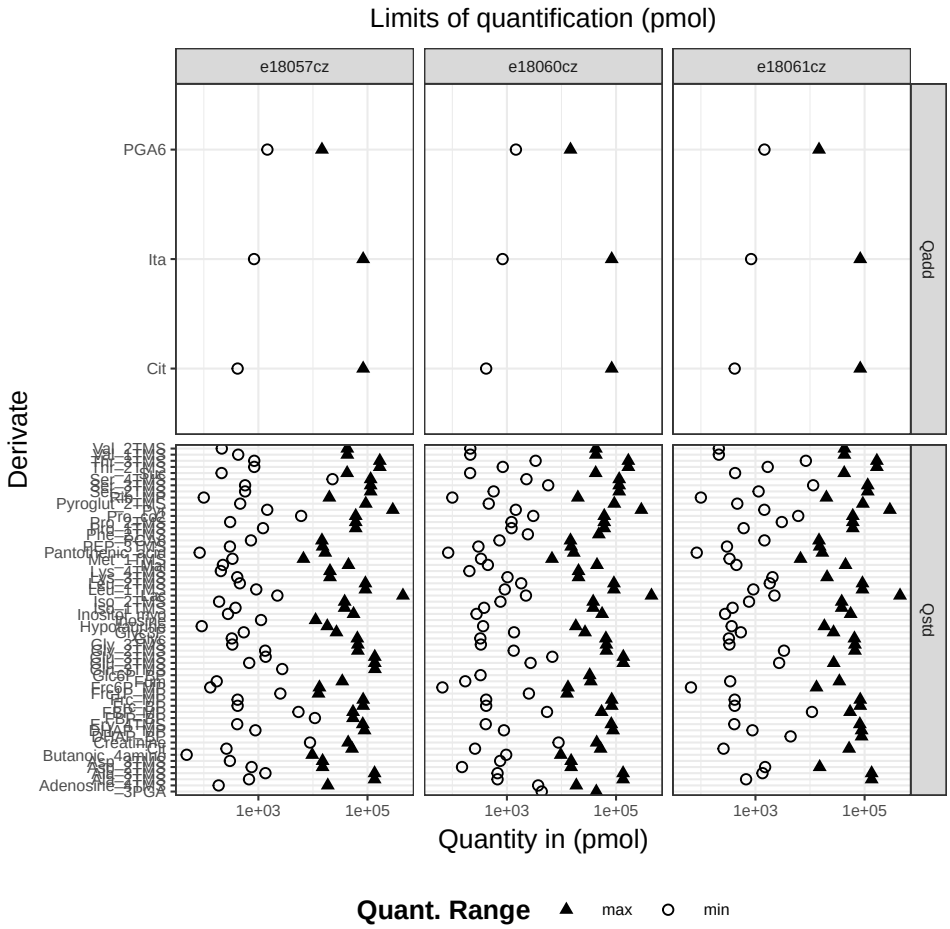


Figure 9: Limits of quantifiable range per metabolite

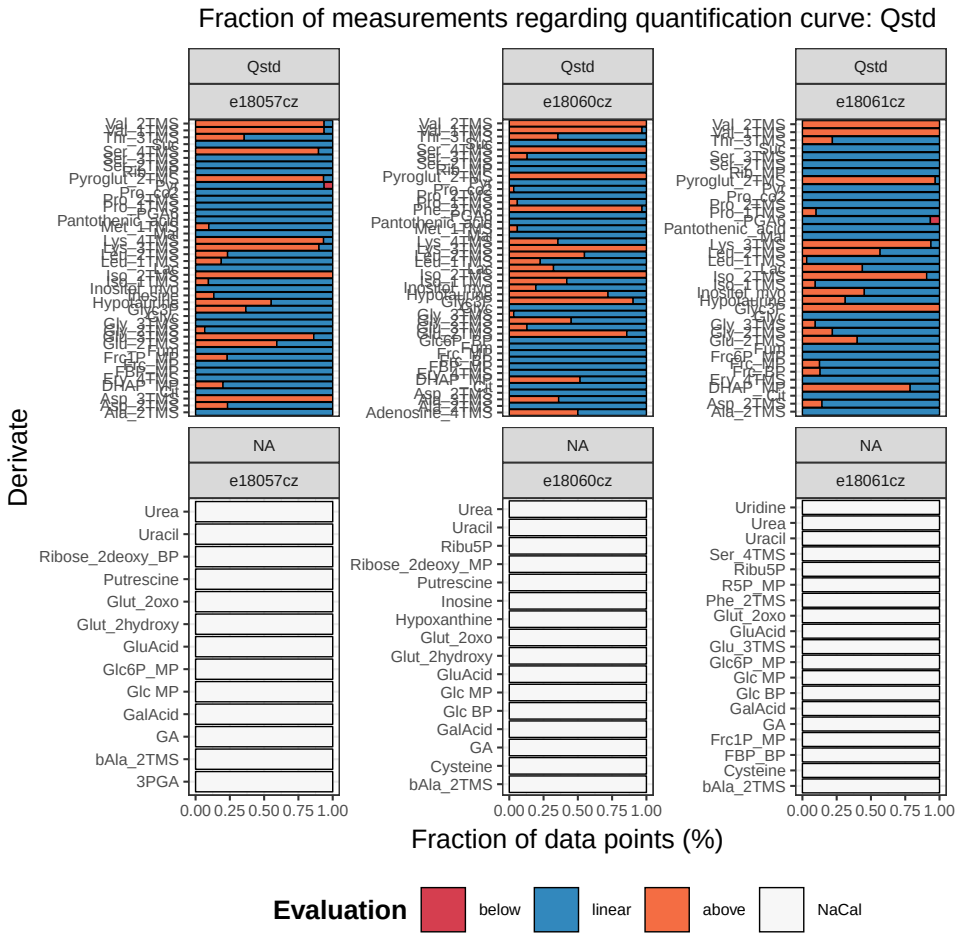


Figure 10: Distribution of data points regarding linear range of the calibration curve

Evaluation of experimental data

Determination extraction factor

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

## 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.
```

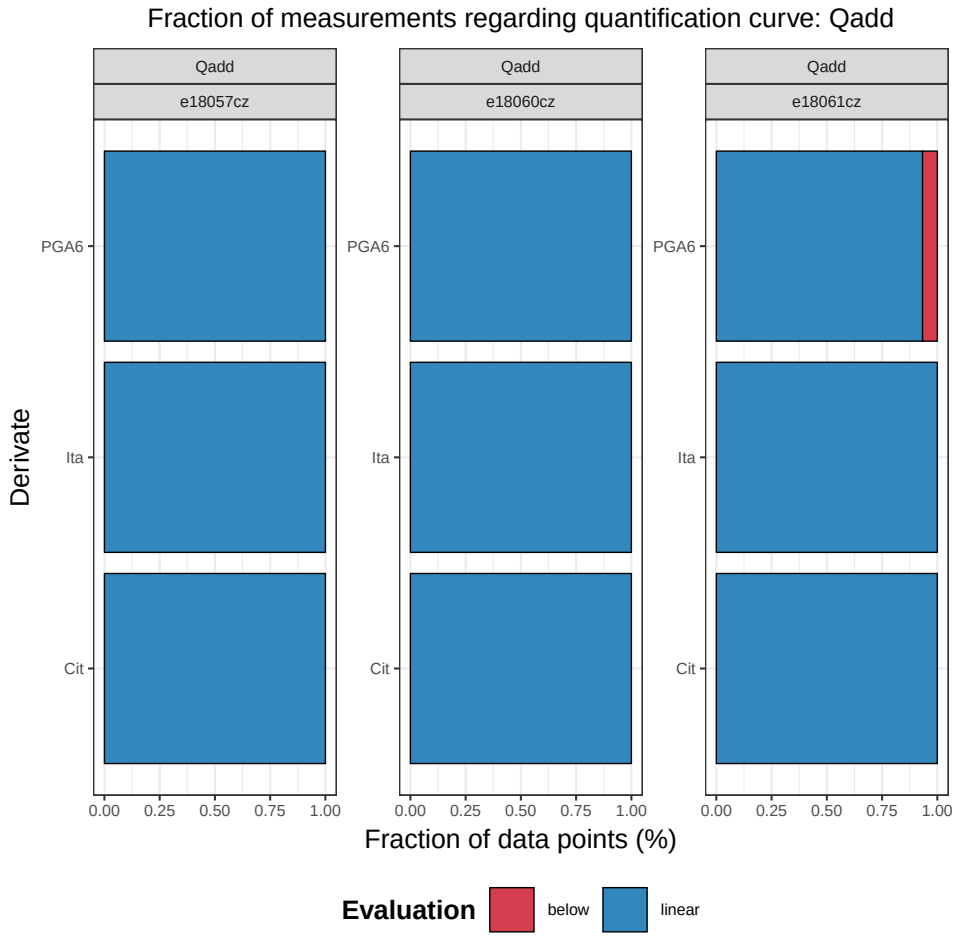
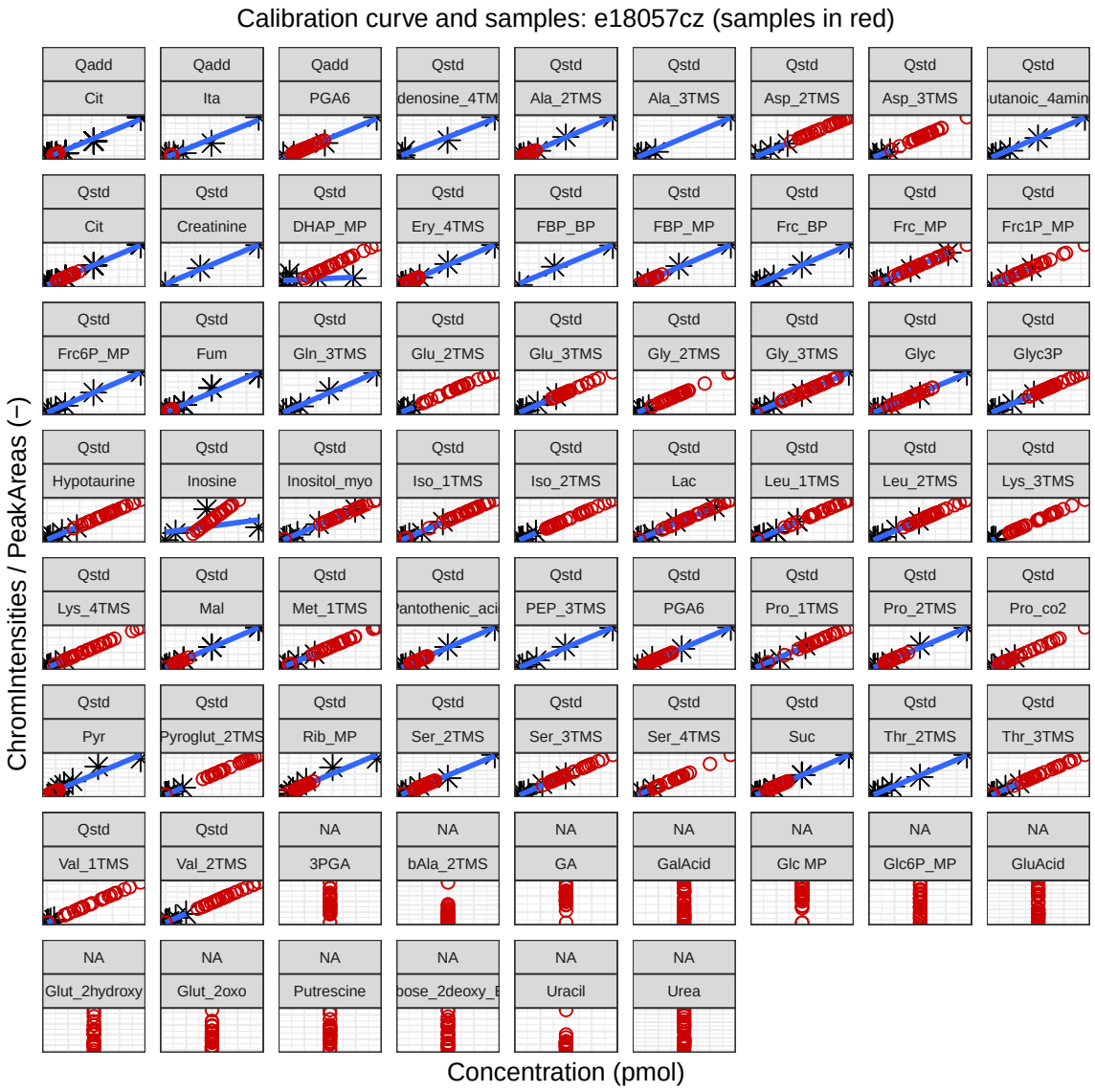
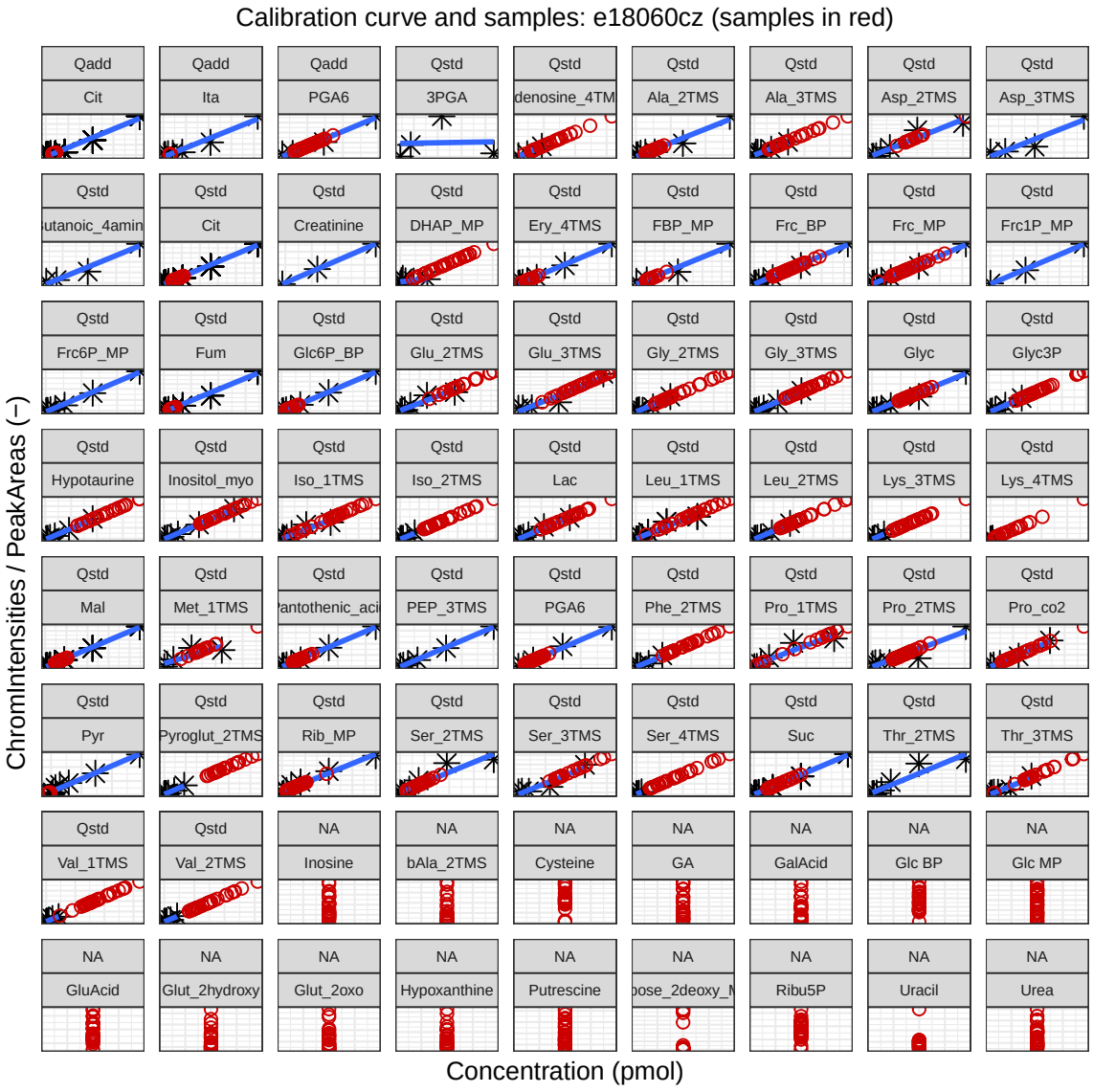
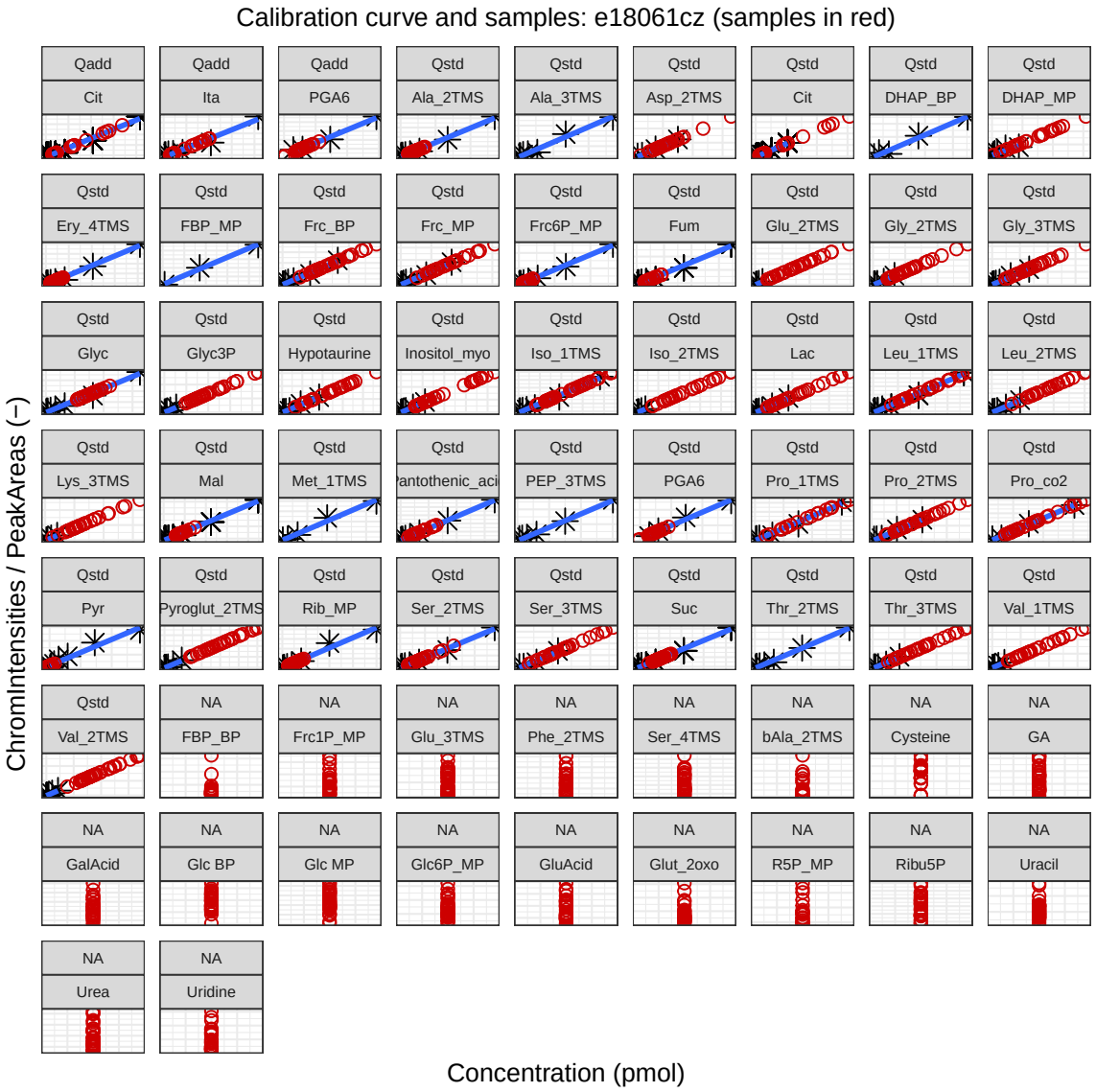


Figure 11: Distribution of data points regarding linear range of the calibration curve

Absolute quantification samples




Calibration curve and samples: e18060cz (samples in red)
ChromIntensities / PeakAreas (−)
Concentration (pmol)
Qadd Cit
Qadd Ita
Qadd PGA6
Qstd 3PGA
Qstd denosine_4TM
Qstd Ala_2TMS
Qstd Ala_3TMS
Qstd Asp_2TMS
Qstd Asp_3TMS
Qstd utanoic_4amin
Qstd Cit
Qstd Creatinine
Qstd DHAP_MP
Qstd Ery_4TMS
Qstd FBP_MP
Qstd Frc_BP
Qstd Frc_MP
Qstd Frc1P_MP
Qstd Frc6P_MP
Qstd Fum
Qstd Glc6P_BP
Qstd Glu_2TMS
Qstd Glu_3TMS
Qstd Gly_2TMS
Qstd Gly_3TMS
Qstd Glyc
Qstd Glyc3P
Qstd Hypotaurine
Qstd Inositol_myo
Qstd Iso_1TMS
Qstd Iso_2TMS
Qstd Lac
Qstd Leu_1TMS
Qstd Leu_2TMS
Qstd Lys_3TMS
Qstd Lys_4TMS
Qstd Mal
Qstd Met_1TMS
Qstd antothenic_aci
Qstd PEP_3TMS
Qstd PGA6
Qstd Phe_2TMS
Qstd Pro_1TMS
Qstd Pro_2TMS
Qstd Pro_co2
Qstd Pyr
Qstd Pyroglut_2TMS
Qstd Rib_MP
Qstd Ser_2TMS
Qstd Ser_3TMS
Qstd Ser_4TMS
Qstd Suc
Qstd Thr_2TMS
Qstd Thr_3TMS
Qstd Val_1TMS
Qstd Val_2TMS
NA Inosine
NA bAla_2TMS
NA Cysteine
NA GA
NA GalAcid
NA Glc BP
NA Glc MP
NA GluAcid
NA Glut_2hydroxy
NA Glut_2oxo
NA Hypoxanthine
NA Putrescine
NA ose_2deoxy_M
NA Ribu5P
NA Uracil
NA Urea



Normalisation of absolute quantities

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

HeatMap - Quantification

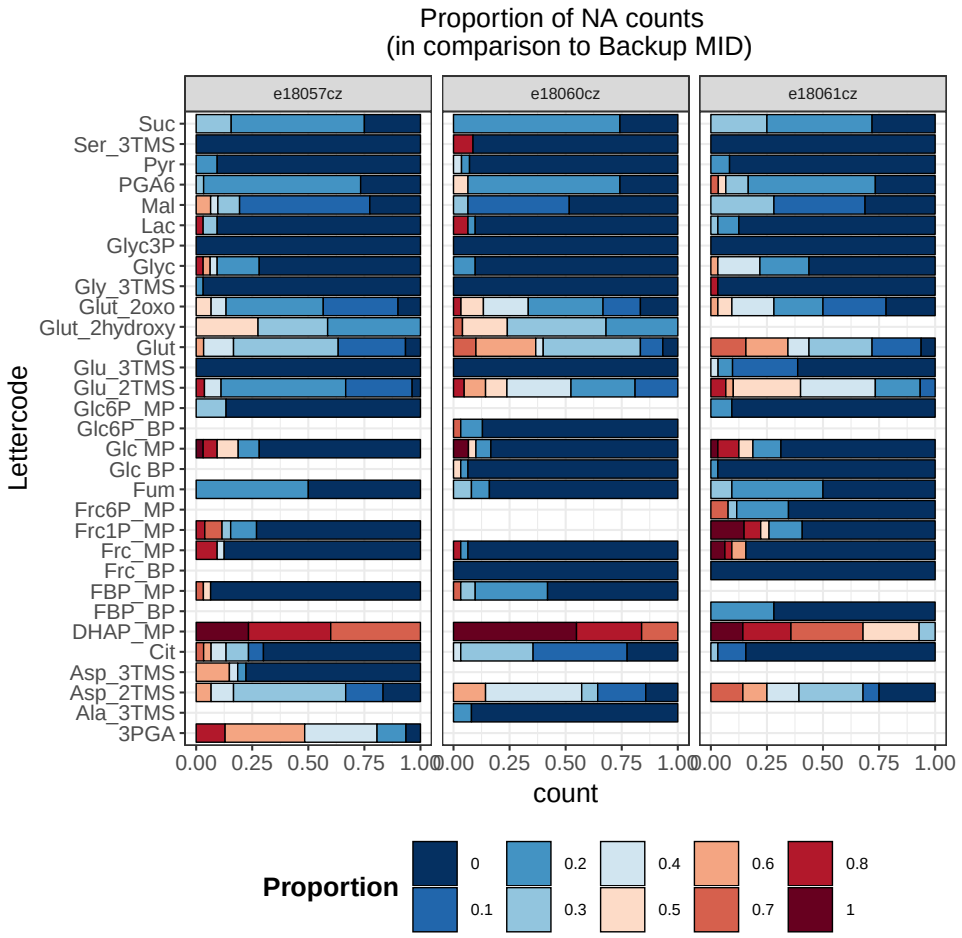


Figure 12: Missing values in mass isotopomer distributions (MID).

MTXQC - Stable isotope incorporation

NA count

3-Lowest of MID

3-Lowest of MID

^{13}*C-Isotope incorporation*

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

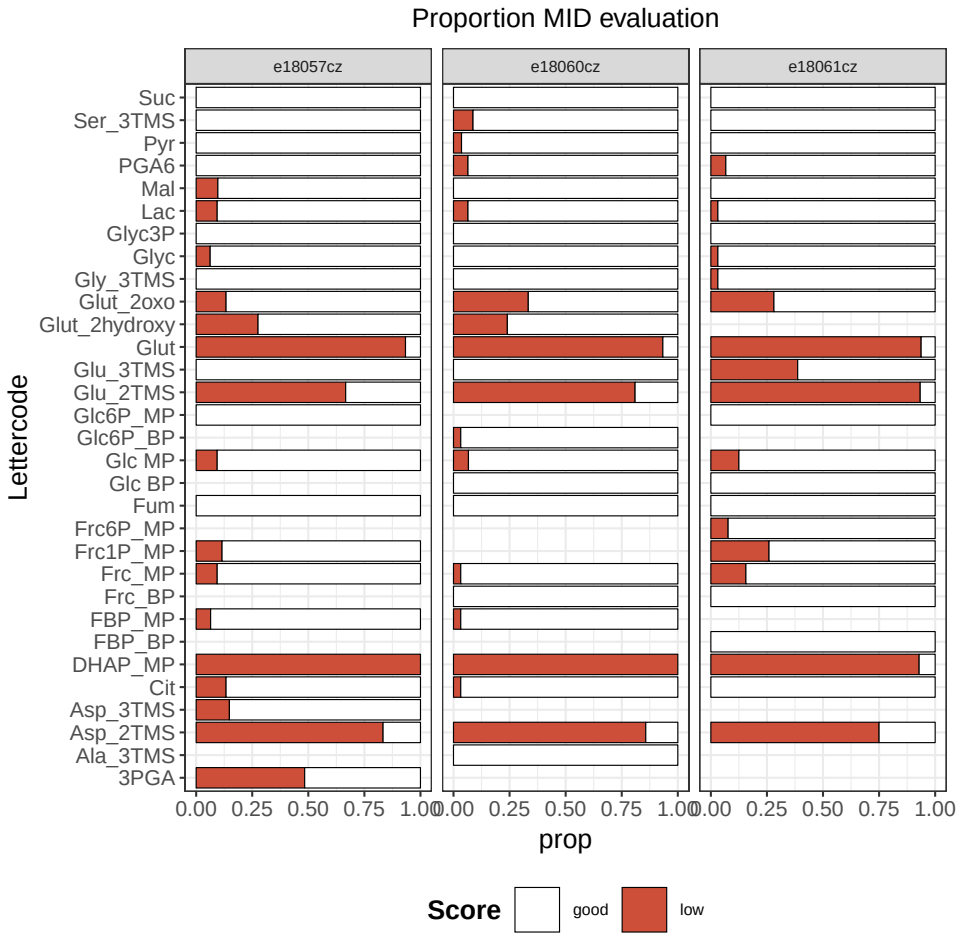


Figure 13: MID quality

Heatmap Isotope incorporation

MTXQC Heatmap compilation: Quantifitation and stable isotope incorporation

End of the document

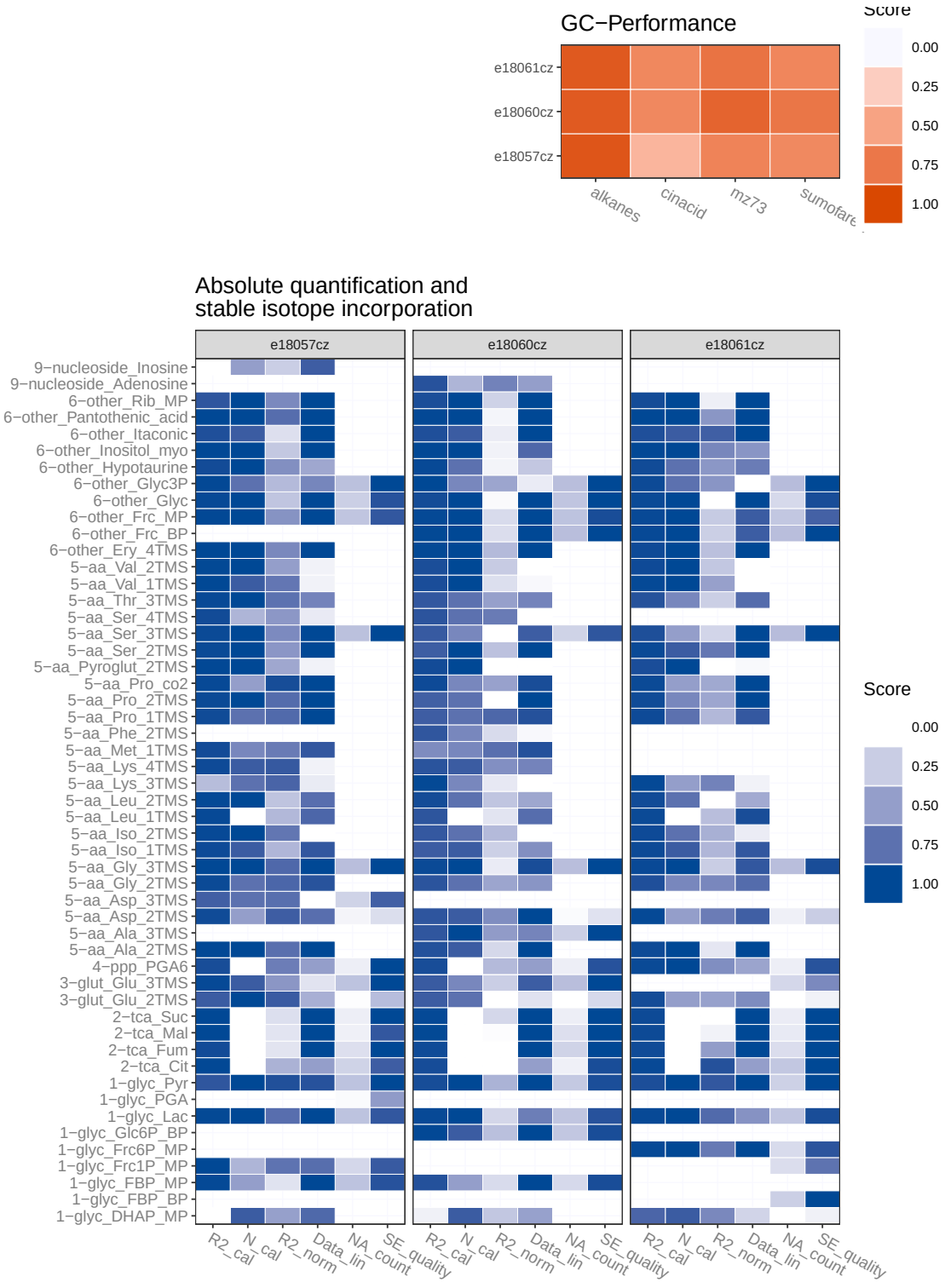


Figure 14: MTXQCvX - Heatmap overview