

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 21, 2018'

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

Data import

```
## MTXQCparams.csv imported!  
## Metmax_params.csv imported.  
## Experimental setup does not include additional quantification standards!  
## File imported! annotation.csv  
## File imported! Sample_extracts.csv  
## File imported! InternalStandard.csv  
## File imported! Alkane_intensities.csv  
## File imported! MassSum-73.csv  
## File imported! PeakDensities-Chroma.csv  
## File imported! quantMassAreasMatrix.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
```

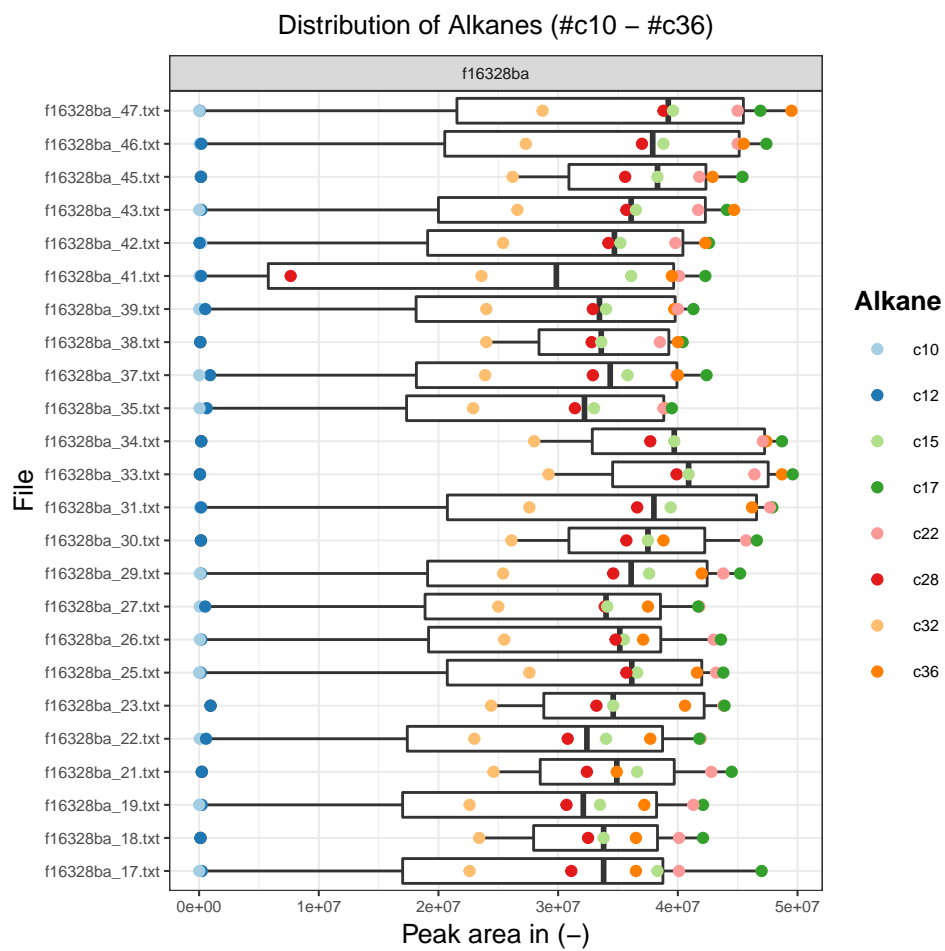


Figure 1: Alkane intensities summarised per each file. Drop of intensities shows questionable files.

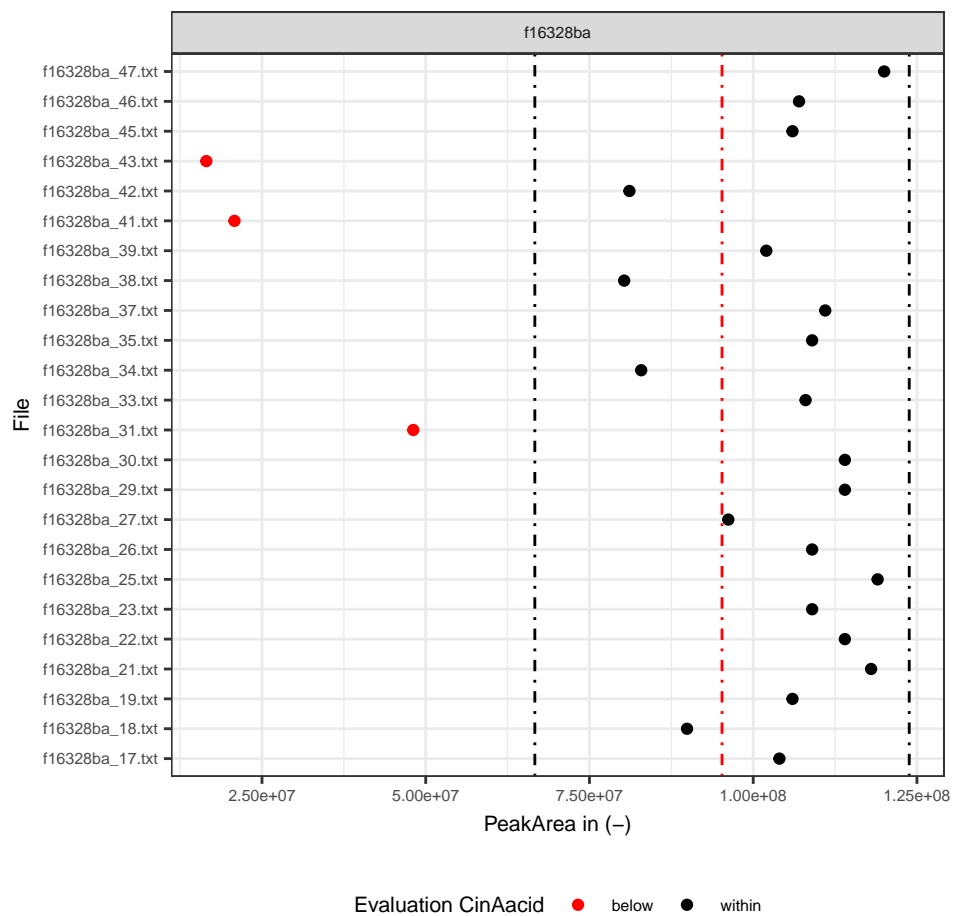


Figure 2: Quantification of internal extraction standard

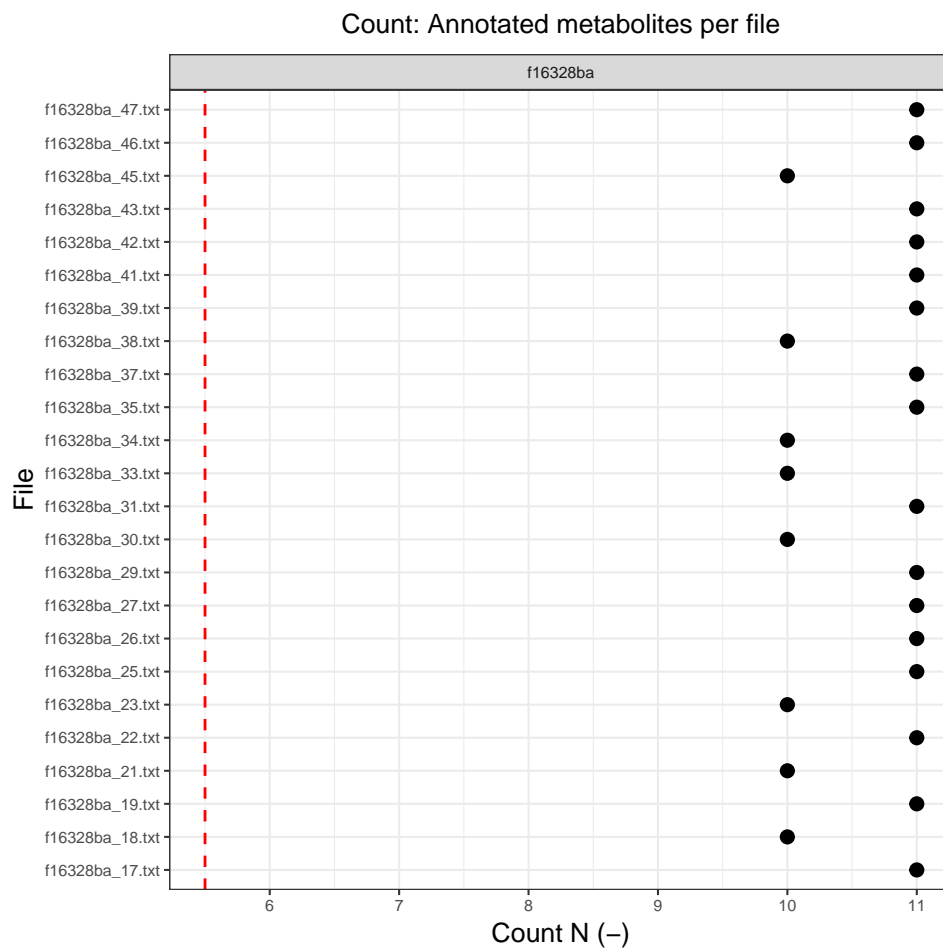


Figure 3: Count N: Annotated intermediates per file. Evaluate careful for SumOfArea normalisation.

Batch_Id	n_50
f16328ba	5.5

Derivatization check

QC-metric succesfully exported: mz73

HeatMap - GC-MS performance

Table 2: Summary of parameter evaluating GC-Performance

Batch_Id	qc_metric	title
f16328ba	0.9449839	alkanes
f16328ba	0.6998855	cinacid
f16328ba	0.9533990	mz73
f16328ba	0.8627827	sumofarea

Export of GC-Performance values done!

MTXQC - Quantitative metabolomics

5

Generation of ManualQuantTable: Quant-Standards (Qstd)

File imported! quant1 values.csv

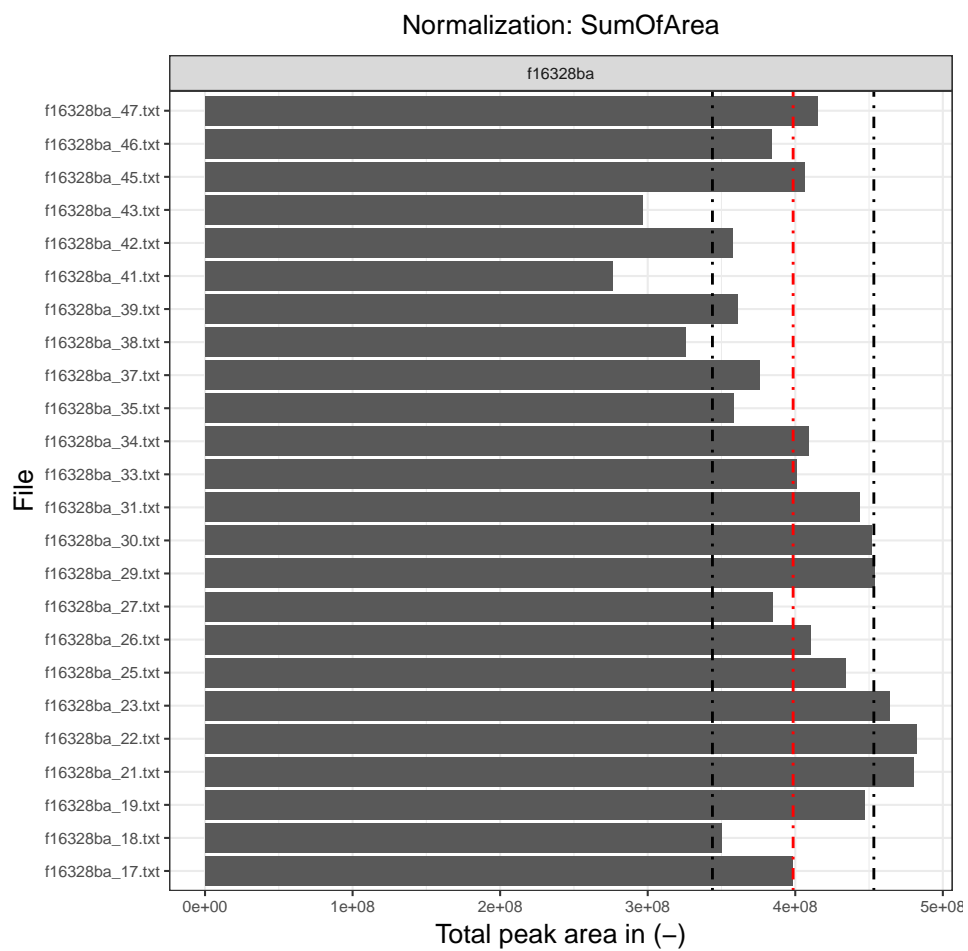


Figure 4: Total peak area of all annotated metabolite per file.

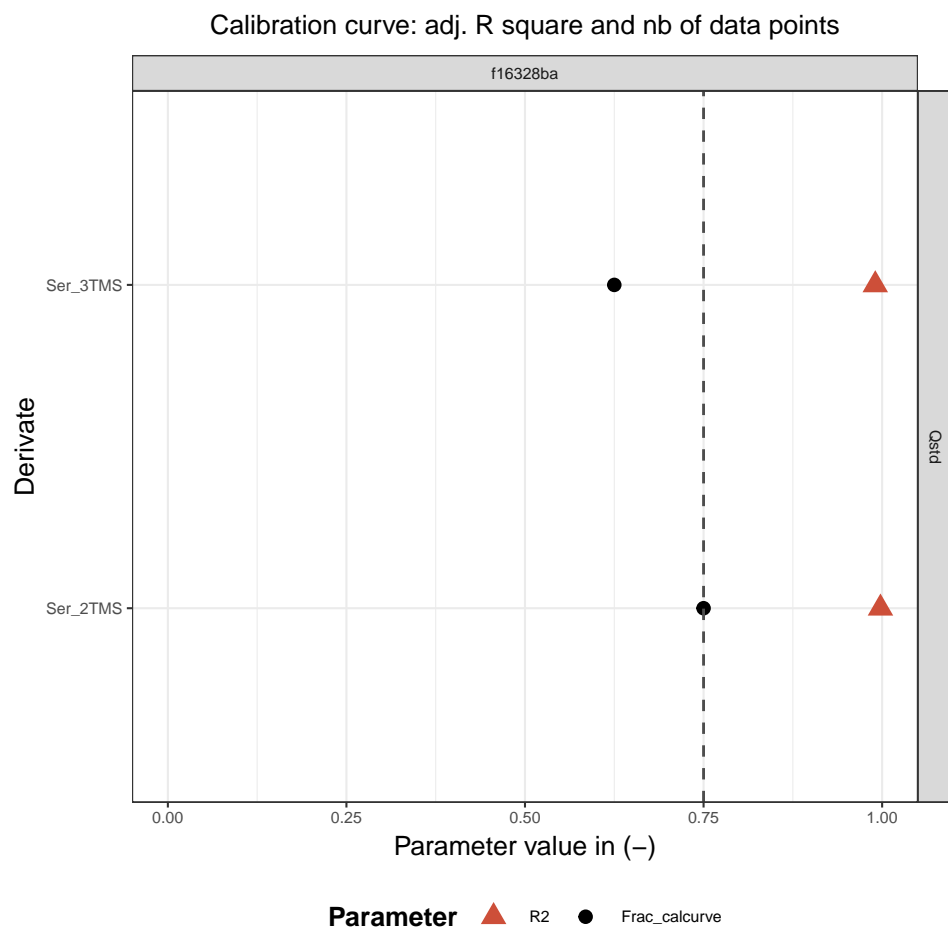


Figure 5: Calibration curves: Nb. of data points.

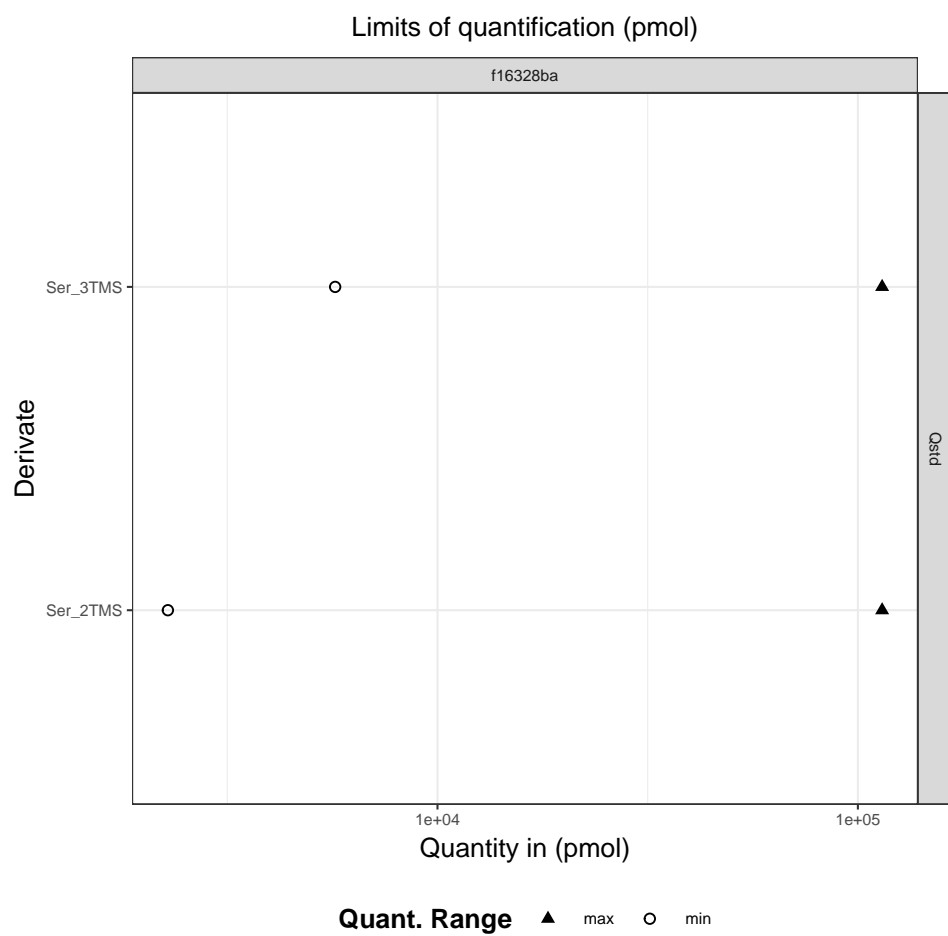


Figure 6: Limits of quantifiable range per metabolite

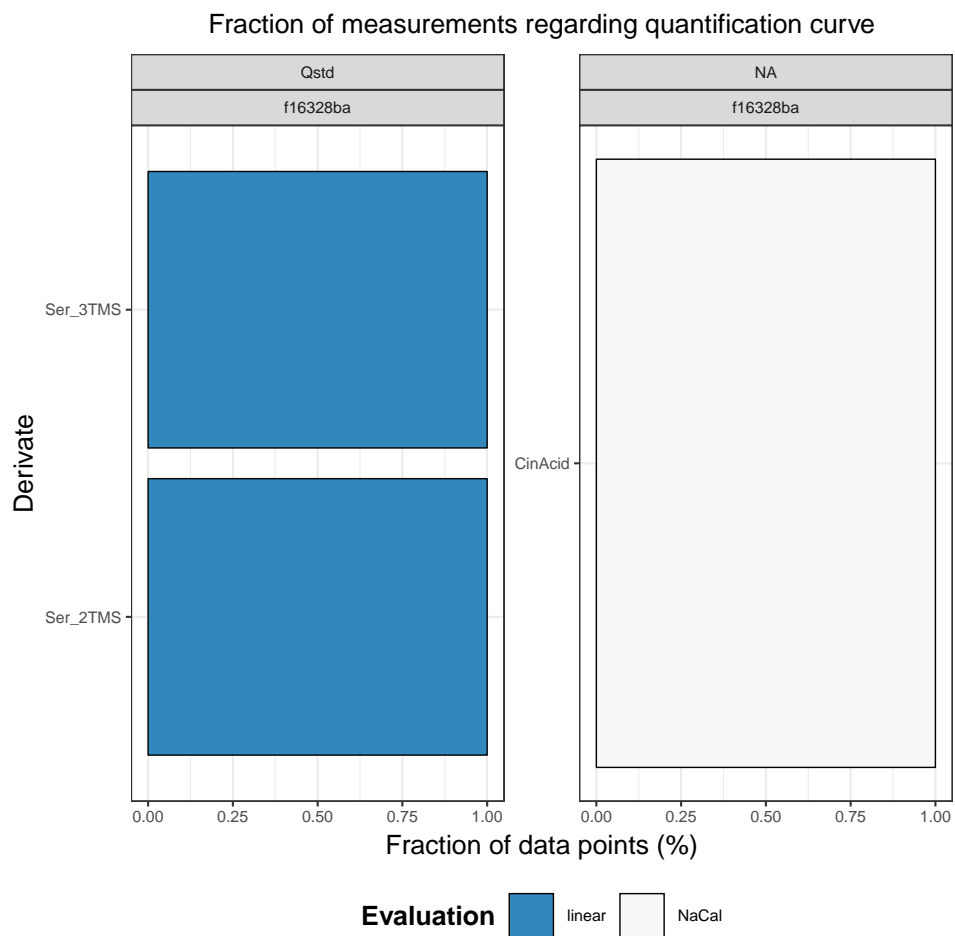


Figure 7: Distribution of data points regarding linear range of the calibration curve

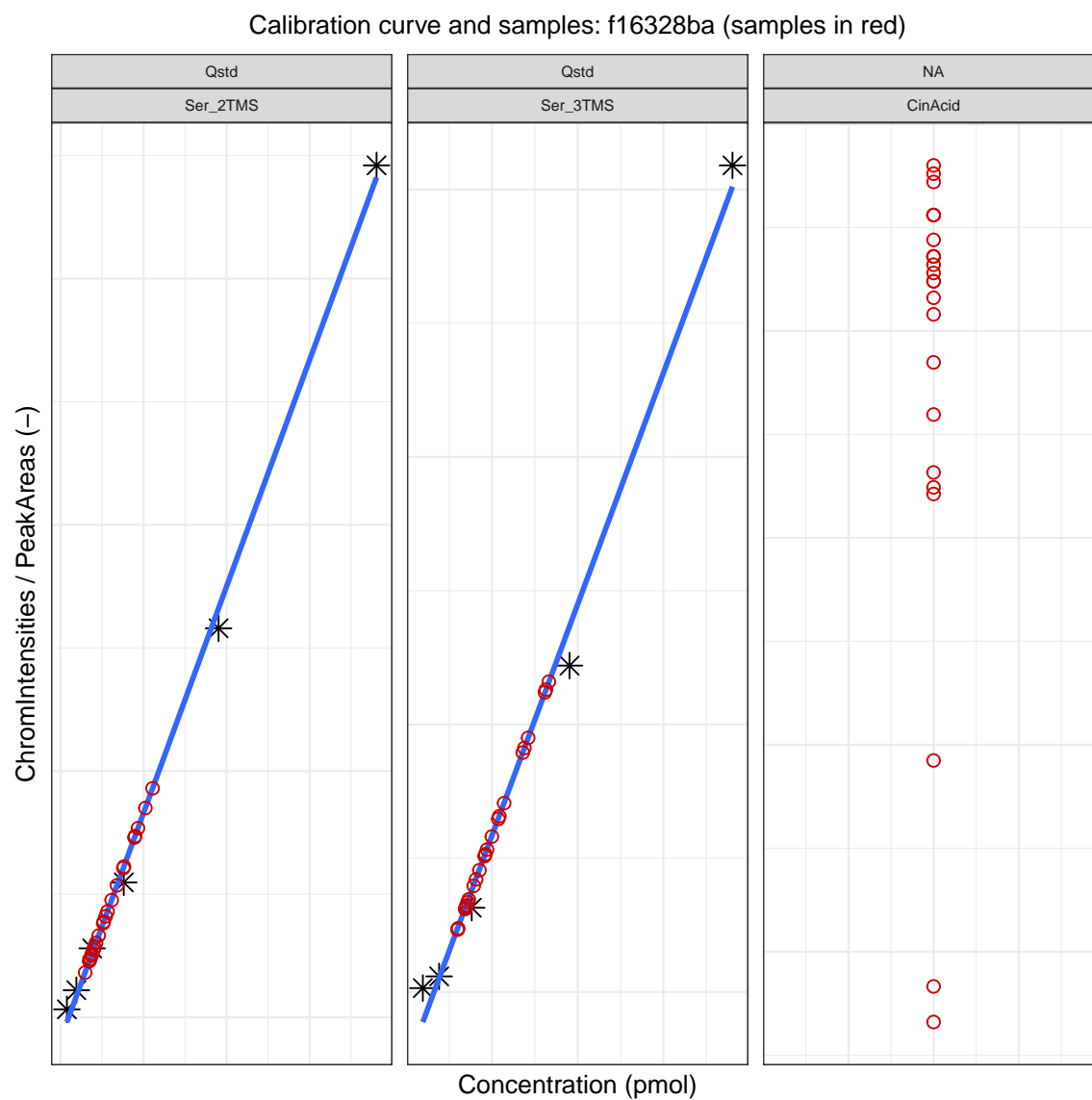
The sample factor for that experimental setup: 1

The extraction factor for that experimental setup: 0.3333333333333333

Quantification range and limits

Position of data points regarding calibration curves evaluated.

Absolute quantification samples



Normalisation of absolute quantities

Absolute quantification and normalisation have been performed: CalculationFileData.csv

HeatMap - Quantification

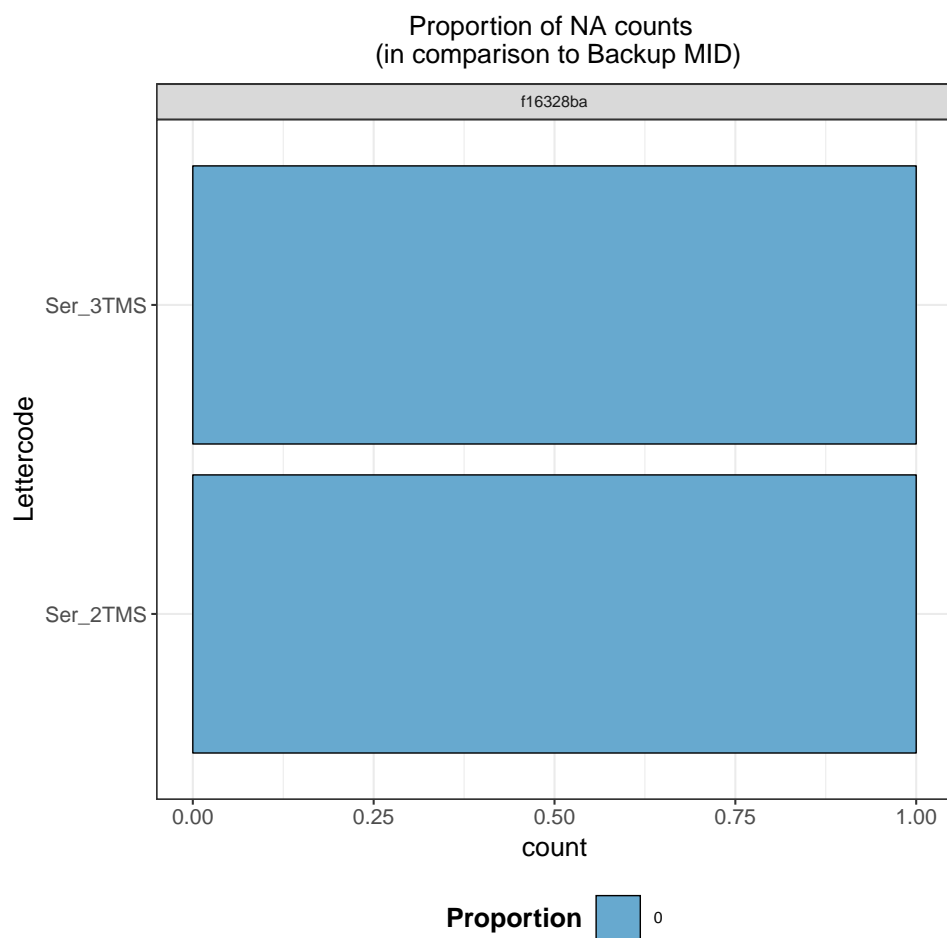


Figure 8: Missing values in mass isotopomer distributions (MID).

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!

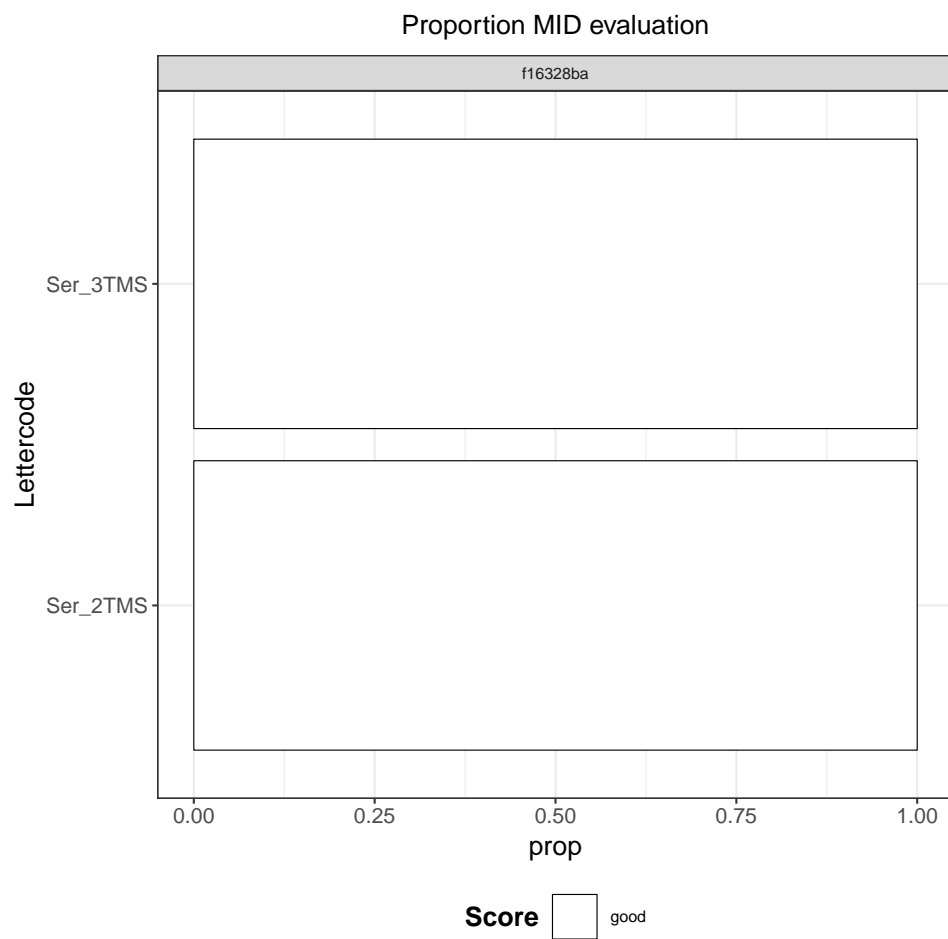


Figure 9: MID quality

Heatmap Isotope incorporation

MTXQC Heatmap compilation: Quantifitation and stable isotope incorporation

End of the document

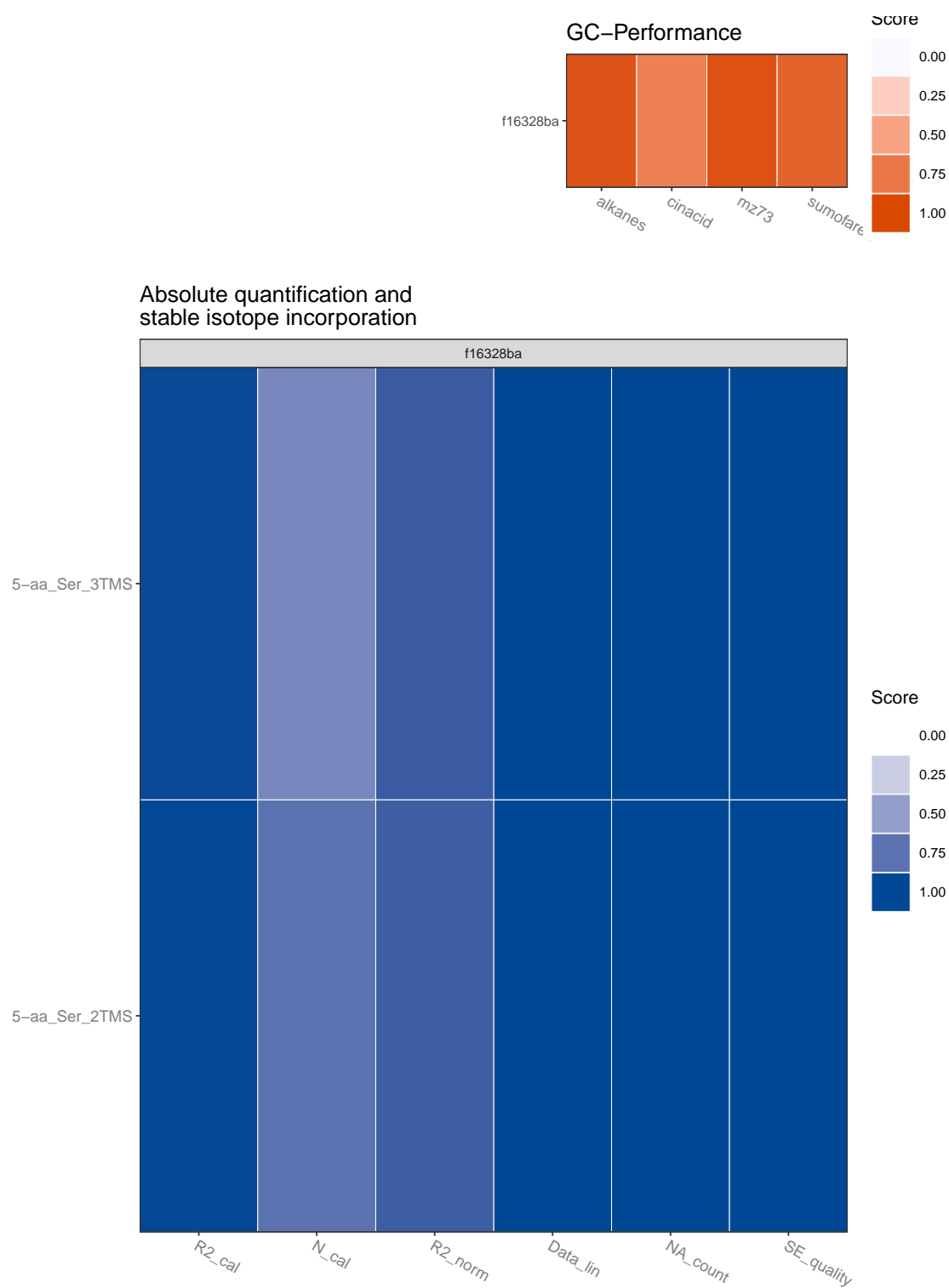


Figure 10: MTXQCvX - Heatmap overview