

Experimental conditions are given in the paper:

Fadil, F.; Samol, C.; Berger, R.S.; Kellermeier, F.; Gronwald, W.; Oefner, P.J.; Dettmer, K. Isotope ratio analysis for urinary LC–TOFMS based metabolomics. *Metabolites* 2022, 12(8), 741.

Uploaded datasets comprise raw .mzML files from:

- The original experiment,
- the subsets used to test for batch effects,
- the calibration experiment,
- the data from the creatinine concentration test.

Note that:

- In MZmine, only retention times up to 15 minutes were considered for the analysis, as flushing and conditioning of the column took place afterwards.
- Sample numbering in the folders "Batch effects" and "Crea Concentration Test" correspond to the sample numbering in the folder "Original experiment".
- Samples in the Original experiments with "repeat" in their names, are technical replicates.
- The given dilution factors are the final dilutions, after the addition of the IS.
- Regarding the Quant concentrations, since only one value of tryptophan and only one value of methionine were below the lower limit of quantification (below LLOQ), these were assigned the lowest ranks when calculating spearman correlation coefficients.