

# ● Analysis Report

## Bruker IVDr Quantification in URine B.I.Quant-UR b<sup>TM</sup>

Sample ID: ALZ\_Urine\_Rack05\_RCM\_161214\_expno310.100000.10r

Measuring Date: 16-Dec-2014 22:25:16

Reporting Date: 14-Dec-2020 20:43:52, 7 page(s), Version 1.1.0

Quantification Method Version: Quant-UR B.1.1.0

### Disclaimer

RESEARCH USE ONLY: This is no clinical diagnostic analysis report. Must not be used for clinical (medical or IVD) diagnosis or for patient management! Additional concentration range information (95% range) provided numerically or graphically in this report must not be used for clinical diagnostic interpretation.

Application of B.I.Quant-UR B 1.1.0 requires use of Bruker's B.I.Methods SOP for urine.


### Summary

All metabolites were found with concentrations inside the 95% range of Bruker Quant-UR B.1.1.0 urine metabolite concentration database.

## Contents



1	Creatinine	3
2	Amines and derivatives	3
3	Amino acids and derivatives	3
4	Benzene and substituted derivatives	4
5	Carboxylic acids	4
6	Fatty acids and derivatives	4
7	Keto acids and derivatives	5
8	Purine, Pyridine and Pyrimidine derivatives	5
9	Sugars and derivatives	5
10	Explanations	6

## 1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range <sup>(*)</sup> mmol/L
Creatinine	5.0	0.3	5.029	100 ●	0.100	1 - 19 















(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 2 Amines and derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range <sup>(*)</sup> $\frac{\text{mmol}}{\text{mol Crea}}$
Dimethylamine	< 0.15	< 31	31	0.151	100 ●	0.004	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.003	89 ●	0.001	≤ 3 




(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 3 Amino acids and derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range <sup>(*)</sup> $\frac{\text{mmol}}{\text{mol Crea}}$
1-Methylhistidine	< 0.07	< 15	15	0.000	0 ○	0.111	≤ 15 
2-Furoylglycine	< 0.19	< 39	39	0.106	99 ●	0.007	≤ 40 
4-Aminobutyric acid	< 0.10	< 20	20	0.000	0 ○	0.217	≤ 20 
Alanine	0.15	29	10	0.148	100 ●	0.007	11 - 72 
Arginine	< 3.8	< 750	750	0.342	0 ○	2.384	≤ 750 
Betaine	0.06	12	7	0.060	100 ●	0.008	9 - 78 
Creatine	< 0.25	< 50	50	0.120	100 ●	0.100	≤ 280 
Glycine	0.63	130	34	0.633	100 ●	0.022	38 - 440 
Guanidinoacetic acid	< 0.52	< 100	100	0.309	90 ●	0.113	≤ 140 
Methionine	< 0.09	< 18	18	0.000	0 ○	0.238	≤ 18 
N,N-Dimethylglycine	0.04	8	5	0.040	93 ●	0.010	≤ 15 
Sarcosine	< 0.01	< 2	2	0.003	0 ○	0.008	≤ 7 
Taurine	< 0.72	< 140	140	0.372	96 ●	0.141	≤ 170 
Valine	0.02	4	2	0.018	68 ○	0.010	≤ 7 











(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 4 Benzene and substituted derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
Benzoic acid	< 0.05	< 10	10	0.000	0 ○	0.027	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.049	2 - 17 
Hippuric acid	1.1	210	170	1.060	99 ●	0.073	≤ 660 


(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 5 Carboxylic acids

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
Acetic acid	0.05	10	5	0.051	96 ●	0.013	≤ 51 
Citric acid	1.6	320	40	1.606	100 ●	0.109	≤ 700 
Formic acid	0.10	19	10	0.096	98 ●	0.014	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.003	86 ●	0.001	≤ 3 
Imidazole	< 0.24	< 48	48	0.028	5 ○	0.036	≤ 48 
Lactic acid	< 0.24	< 49	49	0.060	92 ●	0.096	≤ 110 
Proline betaine	0.25	50	25	0.254	95 ●	0.040	≤ 280 
Succinic acid	0.05	10	5	0.052	89 ●	0.016	≤ 39 
Tartaric acid	0.05	11	5	0.054	98 ●	0.008	≤ 110 
Trigonelline	< 0.17	< 35	35	0.133	100 ●	0.004	≤ 67 







(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 6 Fatty acids and derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
2-Methylsuccinic acid	< 0.24	< 48	48	0.000	0 ○	0.183	≤ 48 








(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 7 Keto acids and derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
2-Oxoglutaric acid	< 0.46	< 92	92	0.042	49 ○	0.170	≤ 92 
3-Hydroxybutyric acid	< 0.52	< 100	100	0.000	0 ○	0.499	≤ 100 
Acetoacetic acid	< 0.07	< 14	14	0.067	94 ●	0.036	≤ 30 
Acetone	0.02	4	2	0.018	100 ●	0.001	≤ 7 
Oxaloacetic acid	0.09	18	17	0.088	87 ●	0.062	≤ 66 
Pyruvic acid	< 0.04	< 9	9	0.034	85 ●	0.011	≤ 13 







(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 8 Purine, Pyridine and Pyrimidine derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
1-Methyladenosine	< 0.03	< 5	5	0.000	0 ○	0.080	≤ 5 
1-Methylnicotinamide	< 0.16	< 32	32	0.046	98 ●	0.007	≤ 32 
Adenosine	< 2.0	< 390	390	0.000	0 ○	0.875	≤ 390 
Allantoin	< 0.08	< 17	17	0.052	100 ●	0.003	≤ 47 
Allopurinol	< 0.05	< 10	10	0.040	64 ○	0.039	≤ 11 
Caffeine	< 0.23	< 45	45	0.099	93 ●	0.112	≤ 61 
Inosine	< 0.10	< 19	19	0.012	93 ●	0.033	≤ 19 

(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 9 Sugars and derivatives

Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.22	< 43	43	0.038	93 ●	0.003	≤ 44 
D-Glucose	0.20	40	34	0.204	90 ●	0.044	≤ 140 
D-Lactose	< 0.48	< 96	96	0.138	79 ○	0.428	≤ 96 
D-Mannitol	< 0.92	< 180	180	0.191	37 ○	0.380	≤ 180 
D-Mannose	< 0.03	< 6	6	0.000	0 ○	0.050	≤ 8 
Myo-Inositol	< 22	< 4400	4400	0.000	0 ○	5.467	≤ 4400 

(\*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

## 10 Explanations

This section contains the definition of the parameters used above. In the section 10.1 a short manual, how to interpret the results, is presented. The section 10.3 contains the exact definitions of the parameters  $r$ ,  $\rho$  and  $\Delta$ .

### 10.1 How to read the result



Figure 1: Examples of fitting.

In the figure 1(a), the black line, the blue line and the yellow line represent the original spectrum, the calculated signal fit and its baseline, respectively.

The blue area relates to the metabolite concentration to be determined and the red area represents a residue.

In case of the signal overlap a different approach is used: two or more overlapping signals are being fitted simultaneously. The most iconic example of such signals are the ones generated by  $\text{CH}_3$  groups of Creatinine and Creatine. In such a case, the blue line and the grey area relate the sum of all fitted signals. The blue area corresponds to the concentration of the metabolite of interest (cf. figure 1(b)).

### 10.2 Result parameters

- Conc.** is the final result concentration of the metabolite,
- LOD** is the *limit of detection* of the given metabolite,
- r** is the *raw concentration* i.e. the concentration equivalent of the resulting signal fit prior to comparing to **LOD** (relates to the blue area, cf.  $\alpha$ ),
- $\rho$  is the correlation of lineshape metabolite signal with calculated fit characterizing the match between metabolite signal and fit (cf.  $\beta$ ). Depending on the value of  $\rho$ , the following *flag* is displayed:

- ●, if the correlation is 95%,
  - ●, if the correlation is in between 85% and 95%,
  - ○, if the correlation is less than 85%,
- e)  $\Delta$  is the concentration equivalent of the difference between metabolite signal and calculated fit (residue corresponding to the **the red area**, cf.  $\gamma$ )).

### 10.3 Detailed definitions

Let  $s$ ,  $f$  and  $b$  denote the functions describing the *raw spectra*, *fitted curve* and *(fitted) baseline* respectively. These functions are chosen such that  $s \approx f + b$ . Moreover, let  $I$  be a relevant PPM interval and  $P_N$  be the proton number for given metabolite/signal.

$\alpha$ )  $r$  (*raw concentration*) is defined as

$$r = \frac{1}{P_N} \int_{\mathbb{R}} f(\xi) d\xi.$$

$\beta$ )  $\rho$  is the *correlation* of the functions  $s$  and  $f + b$ , i.e.

$$\rho = \max(0, \text{corr}(\bar{s}, \overline{f+b})),$$

where  $\bar{s}$ ,  $\overline{f+b}$  are numerical representations of the functions  $s$  and  $f + b$  on sufficiently fine mesh of the interval  $I$ .

$\gamma$ )  $\Delta$  is the the area between the raw signal  $s$  and the fitted data  $f + b$  on the interval  $I$  expressed in the terms of the concentration, i.e.

$$\Delta = \frac{1}{P_N} \int_I |s(\xi) - f(\xi) - b(\xi)| d\xi.$$