

# ● Analysis Report

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

Sample ID: ALZ\_Urine\_Rack01\_RCM\_221214\_expno740.100000.10r

Measuring Date: 24-Dec-2014 07:16:04

Reporting Date: 12-Dec-2020 15:51:52, 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

The following metabolites were found with concentrations outside the 95% range of Bruker Quant-UR B.1.1.0 urine metabolite concentration database:


Amino acids and derivatives: Betaine ( $< 7 \text{ mmol/mol Crea}$ ).

Further detailed information is provided on the following pages.

## 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	5.5	0.3	5.547	100 ●	0.096	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	< 0.17	< 31	31	0.167	100 ●	0.005	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.006	100 ●	0.000	≤ 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	< 0.08	< 15	15	0.023	72 ○	0.012	≤ 15 
2-Furoylglycine	< 0.21	< 39	39	0.117	99 ●	0.018	≤ 40 
4-Aminobutyric acid	< 0.11	< 20	20	0.065	57 ○	0.058	≤ 20 
Alanine	0.16	28	10	0.158	100 ●	0.006	11 - 72 
Arginine	< 4.1	< 750	750	0.000	0 ○	3.587	≤ 750 
Betaine	< 0.04	< 7	7	0.000	99 ●	0.052	9 - 78 
Creatine	< 0.28	< 50	50	0.165	100 ●	0.096	≤ 280 
Glycine	0.70	130	34	0.697	100 ●	0.032	38 - 440 
Guanidinoacetic acid	< 0.57	< 100	100	0.351	88 ●	0.144	≤ 140 
Methionine	< 0.10	< 18	18	0.000	0 ○	0.430	≤ 18 
N,N-Dimethylglycine	0.04	6	5	0.035	75 ○	0.015	≤ 15 
Sarcosine	< 0.01	< 2	2	0.000	0 ○	0.004	≤ 7 
Taurine	< 0.79	< 140	140	0.419	94 ●	0.143	≤ 170 
Valine	0.02	4	2	0.022	75 ○	0.013	≤ 7 











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## 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 ○	0.025	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.004	16 ○	0.004	2 - 17 
Hippuric acid	1.1	210	170	1.142	99 ●	0.105	≤ 660 


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## 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	0.08	15	5	0.082	99 ●	0.009	≤ 51 
Citric acid	1.7	310	40	1.718	100 ●	0.150	≤ 700 
Formic acid	0.12	21	10	0.117	100 ●	0.002	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.004	77 ○	0.002	≤ 3 
Imidazole	< 0.27	< 48	48	0.029	35 ○	0.034	≤ 48 
Lactic acid	< 0.27	< 49	49	0.030	0 ○	0.160	≤ 110 
Proline betaine	0.29	52	25	0.286	98 ●	0.032	≤ 280 
Succinic acid	0.13	23	5	0.129	98 ●	0.018	≤ 39 
Tartaric acid	0.06	11	5	0.061	99 ●	0.011	≤ 110 
Trigonelline	< 0.19	< 35	35	0.134	100 ●	0.003	≤ 67 







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## 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	< 0.26	< 48	48	0.000	0 ○	0.200	≤ 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	< 0.51	< 92	92	0.028	46 ○	0.128	≤ 92 
3-Hydroxybutyric acid	< 0.57	< 100	100	0.034	12 ○	0.185	≤ 100 
Acetoacetic acid	< 0.08	< 14	14	0.069	86 ●	0.031	≤ 30 
Acetone	0.02	4	2	0.021	99 ●	0.002	≤ 7 
Oxaloacetic acid	< 0.10	< 17	17	0.077	73 ○	0.081	≤ 66 
Pyruvic acid	< 0.05	< 9	9	0.032	94 ●	0.007	≤ 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 ○	0.118	≤ 5 
1-Methylnicotinamide	< 0.18	< 32	32	0.051	98 ●	0.009	≤ 32 
Adenosine	< 2.2	< 390	390	0.000	0 ○	0.970	≤ 390 
Allantoin	< 0.09	< 17	17	0.061	100 ●	0.003	≤ 47 
Allopurinol	< 0.06	< 10	10	0.029	64 ○	0.055	≤ 11 
Caffeine	< 0.25	< 45	45	0.107	86 ●	0.118	≤ 61 
Inosine	< 0.10	< 19	19	0.010	90 ●	0.045	≤ 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	< 0.24	< 43	43	0.000	0 ○	0.038	≤ 44 
D-Glucose	0.21	37	34	0.205	83 ○	0.080	≤ 140 
D-Lactose	< 0.53	< 96	96	0.185	89 ●	0.070	≤ 96 
D-Mannitol	< 1.00	< 180	180	0.000	0 ○	1.928	≤ 180 
D-Mannose	< 0.03	< 6	6	0.000	0 ○	0.063	≤ 8 
Myo-Inositol	< 25	< 4400	4400	0.000	0 ○	4.892	≤ 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.

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