

# ● Analysis Report

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

Sample ID: ALZ\_Urine\_Rack01\_RCM\_221214\_expno580.100000.10r

Measuring Date: 24-Dec-2014 03:43:44

Reporting Date: 12-Dec-2020 02:24:39, 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 (8 mmol/mol Crea),


Carboxylic acids: Trigonelline (89 mmol/mol Crea).

Further detailed information is provided on the following pages.

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## 1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	$\rho$ %	$\Delta$ mmol/L	95% Range <sup>(*)</sup> mmol/L
Creatinine	5.8	0.3	5.802	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	< 0.18	< 31	31	0.172	100 ●	0.002	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.005	98 ●	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	< 0.09	< 15	15	0.027	0 ○	0.058	≤ 15 
2-Furoylglycine	< 0.22	< 39	39	0.056	90 ●	0.016	≤ 40 
4-Aminobutyric acid	< 0.11	< 20	20	0.012	0 ○	0.397	≤ 20 
Alanine	0.16	27	10	0.159	100 ●	0.006	11 - 72 
Arginine	< 4.3	< 750	750	0.350	0 ○	1.784	≤ 750 
Betaine	0.05	8	7	0.046	100 ●	0.006	9 - 78 
Creatine	1.2	200	50	1.169	100 ●	0.096	≤ 280 
Glycine	0.68	120	34	0.682	100 ●	0.018	38 - 440 
Guanidinoacetic acid	< 0.60	< 100	100	0.487	94 ●	0.089	≤ 140 
Methionine	< 0.10	< 18	18	0.000	0 ○	0.264	≤ 18 
N,N-Dimethylglycine	0.05	8	5	0.046	83 ○	0.016	≤ 15 
Sarcosine	< 0.01	< 2	2	0.006	0 ○	0.009	≤ 7 
Taurine	< 0.83	< 140	140	0.148	39 ○	0.205	≤ 170 
Valine	0.03	5	2	0.028	74 ○	0.012	≤ 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	< 0.06	< 10	10	0.000	0○	0.033	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0○	0.002	2 - 17 
Hippuric acid	3.3	560	170	3.257	99●	0.344	≤ 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	0.12	20	5	0.116	99●	0.014	≤ 51 
Citric acid	1.5	260	40	1.532	100●	0.128	≤ 700 
Formic acid	0.17	29	10	0.170	100●	0.003	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.005	65○	0.004	≤ 3 
Imidazole	< 0.28	< 48	48	0.000	0○	0.097	≤ 48 
Lactic acid	< 0.28	< 49	49	0.138	97●	0.028	≤ 110 
Proline betaine	0.25	42	25	0.246	99●	0.024	≤ 280 
Succinic acid	0.04	7	5	0.038	89●	0.010	≤ 39 
Tartaric acid	0.03	5	5	0.031	93●	0.012	≤ 110 
Trigonelline	0.51	89	35	0.515	100●	0.015	≤ 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	< 0.28	< 48	48	0.000	0○	0.199	≤ 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	< 0.54	< 92	92	0.111	75 ○	0.159	≤ 92 
3-Hydroxybutyric acid	< 0.60	< 100	100	0.029	0 ○	0.810	≤ 100 
Acetoacetic acid	< 0.08	< 14	14	0.077	90 ●	0.044	≤ 30 
Acetone	0.03	4	2	0.025	91 ●	0.006	≤ 7 
Oxaloacetic acid	0.22	38	17	0.222	93 ●	0.088	≤ 66 
Pyruvic acid	< 0.05	< 9	9	0.022	87 ●	0.008	≤ 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 ○	0.122	≤ 5 
1-Methylnicotinamide	< 0.18	< 32	32	0.050	98 ●	0.007	≤ 32 
Adenosine	< 2.3	< 390	390	0.000	0 ○	1.163	≤ 390 
Allantoin	0.14	24	17	0.141	100 ●	0.005	≤ 47 
Allopurinol	< 0.06	< 10	10	0.022	97 ●	0.024	≤ 11 
Caffeine	< 0.26	< 45	45	0.129	69 ○	0.146	≤ 61 
Inosine	< 0.11	< 19	19	0.017	98 ●	0.025	≤ 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	< 0.25	< 43	43	0.000	0 ○	0.022	≤ 44 
D-Glucose	0.23	40	34	0.229	82 ○	0.067	≤ 140 
D-Lactose	< 0.56	< 96	96	0.143	92 ●	0.065	≤ 96 
D-Mannitol	< 1.1	< 180	180	0.683	58 ○	0.736	≤ 180 
D-Mannose	< 0.03	< 6	6	0.000	0 ○	0.053	≤ 8 
Myo-Inositol	< 26	< 4400	4400	0.000	0 ○	4.668	≤ 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.

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