

# ● Analysis Report

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

Sample ID: ALZ\_Urine\_Rack01\_RCM\_221214\_expno610.100000.10r

Measuring Date: 24-Dec-2014 04:27:57

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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.

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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	5.9	0.3	5.930	100 ●	0.111	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	0.28	47	31	0.279	100 ●	0.012	$\leq 54$ 
Trimethylamine	< 0.01	< 2	2	0.004	98 ●	0.001	$\leq 3$ 




(\*) 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	0.000	0 ○	0.049	$\leq 15$ 
2-Furoylglycine	< 0.23	< 39	39	0.044	88 ●	0.017	$\leq 40$ 
4-Aminobutyric acid	< 0.12	< 20	20	0.088	81 ○	0.075	$\leq 20$ 
Alanine	0.17	29	10	0.174	100 ●	0.016	11 - 72 
Arginine	< 4.4	< 750	750	0.408	0 ○	1.722	$\leq 750$ 
Betaine	0.17	28	7	0.168	100 ●	0.016	9 - 78 
Creatine	< 0.30	< 50	50	0.103	100 ●	0.111	$\leq 280$ 
Glycine	0.47	79	34	0.468	100 ●	0.025	38 - 440 
Guanidinoacetic acid	< 0.61	< 100	100	0.395	77 ○	0.210	$\leq 140$ 
Methionine	< 0.11	< 18	18	0.000	0 ○	0.187	$\leq 18$ 
N,N-Dimethylglycine	0.06	11	5	0.064	90 ●	0.019	$\leq 15$ 
Sarcosine	< 0.01	< 2	2	0.006	0 ○	0.011	$\leq 7$ 
Taurine	< 0.84	< 140	140	0.306	76 ○	0.149	$\leq 170$ 
Valine	0.02	4	2	0.023	80 ○	0.009	$\leq 7$ 











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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○	0.019	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0○	0.102	2 - 17 
Hippuric acid	< 1.00	< 170	170	0.978	91●	0.262	≤ 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	0.03	5	5	0.029	89●	0.009	≤ 51 
Citric acid	3.0	510	40	3.011	100●	0.259	≤ 700 
Formic acid	0.11	19	10	0.111	100●	0.006	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.002	94●	0.001	≤ 3 
Imidazole	< 0.28	< 48	48	0.036	16○	0.042	≤ 48 
Lactic acid	< 0.29	< 49	49	0.093	85●	0.052	≤ 110 
Proline betaine	0.36	61	25	0.361	100●	0.016	≤ 280 
Succinic acid	0.04	7	5	0.041	83○	0.015	≤ 39 
Tartaric acid	< 0.03	< 5	5	0.020	99●	0.002	≤ 110 
Trigonelline	< 0.21	< 35	35	0.127	99●	0.008	≤ 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	0.047	0○	0.094	≤ 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	< 0.55	< 92	92	0.106	54 ○	0.164	≤ 92 
3-Hydroxybutyric acid	< 0.61	< 100	100	0.000	0 ○	0.793	≤ 100 
Acetoacetic acid	< 0.09	< 14	14	0.063	94 ●	0.037	≤ 30 
Acetone	0.01	2	2	0.013	97 ●	0.002	≤ 7 
Oxaloacetic acid	0.25	43	17	0.254	95 ●	0.078	≤ 66 
Pyruvic acid	< 0.05	< 9	9	0.022	79 ○	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 ○	0.093	≤ 5 
1-Methylnicotinamide	< 0.19	< 32	32	0.025	78 ○	0.012	≤ 32 
Adenosine	< 2.3	< 390	390	0.000	0 ○	1.398	≤ 390 
Allantoin	0.11	19	17	0.113	89 ●	0.024	≤ 47 
Allopurinol	< 0.06	< 10	10	0.015	94 ●	0.033	≤ 11 
Caffeine	< 0.27	< 45	45	0.178	66 ○	0.207	≤ 61 
Inosine	< 0.11	< 19	19	0.015	97 ●	0.031	≤ 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	< 0.26	< 43	43	0.043	91 ●	0.005	≤ 44 
D-Glucose	0.26	43	34	0.257	81 ○	0.092	≤ 140 
D-Lactose	< 0.57	< 96	96	0.206	93 ●	0.070	≤ 96 
D-Mannitol	< 1.1	< 180	180	0.000	0 ○	3.155	≤ 180 
D-Mannose	< 0.04	< 6	6	0.000	0 ○	0.236	≤ 8 
Myo-Inositol	< 26	< 4400	4400	0.000	0 ○	4.855	≤ 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.

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