

# ● Analysis Report

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

Sample ID: ALZ\_Urine\_Rack01\_RCM\_221214\_expno280.100000.10r

Measuring Date: 23-Dec-2014 20:20:32

Reporting Date: 12-Dec-2020 01:50:42, 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



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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	6.5	0.3	6.482	100 ●	0.107	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	< 0.20	< 31	31	0.174	100 ●	0.007	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.003	90 ●	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	< 0.10	< 15	15	0.015	64 ○	0.030	≤ 15 
2-Furoylglycine	< 0.25	< 39	39	0.000	0 ○	0.046	≤ 40 
4-Aminobutyric acid	< 0.13	< 20	20	0.000	0 ○	0.336	≤ 20 
Alanine	0.13	21	10	0.133	100 ●	0.008	11 - 72 
Arginine	< 4.8	< 750	750	0.210	0 ○	0.371	≤ 750 
Betaine	0.08	12	7	0.081	100 ●	0.029	9 - 78 
Creatine	< 0.32	< 50	50	0.048	100 ●	0.107	≤ 280 
Glycine	0.47	73	34	0.473	100 ●	0.020	38 - 440 
Guanidinoacetic acid	< 0.67	< 100	100	0.220	76 ○	0.121	≤ 140 
Methionine	< 0.12	< 18	18	0.000	0 ○	0.181	≤ 18 
N,N-Dimethylglycine	0.05	7	5	0.046	87 ●	0.014	≤ 15 
Sarcosine	< 0.01	< 2	2	0.000	0 ○	0.003	≤ 7 
Taurine	< 0.92	< 140	140	0.000	0 ○	0.424	≤ 170 
Valine	0.02	3	2	0.019	86 ●	0.007	≤ 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	0.018	74 ○	0.009	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.003	2 - 17 
Hippuric acid	1.7	270	170	1.741	99 ●	0.194	≤ 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	0.04	6	5	0.041	86 ●	0.016	≤ 51 
Citric acid	2.5	380	40	2.476	100 ●	0.173	≤ 700 
Formic acid	0.10	15	10	0.098	99 ●	0.011	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.001	97 ●	0.000	≤ 3 
Imidazole	< 0.31	< 48	48	0.029	72 ○	0.029	≤ 48 
Lactic acid	< 0.31	< 49	49	0.136	97 ●	0.035	≤ 110 
Proline betaine	0.33	51	25	0.332	100 ●	0.008	≤ 280 
Succinic acid	0.06	10	5	0.062	99 ●	0.006	≤ 39 
Tartaric acid	< 0.03	< 5	5	0.011	47 ○	0.017	≤ 110 
Trigonelline	< 0.22	< 35	35	0.055	100 ●	0.002	≤ 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	< 0.31	< 48	48	0.000	0 ○	0.178	≤ 48 








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## 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	< 0.60	< 92	92	0.000	0 ○	0.352	≤ 92 
3-Hydroxybutyric acid	< 0.67	< 100	100	0.000	0 ○	0.564	≤ 100 
Acetoacetic acid	0.10	15	14	0.098	89 ●	0.047	≤ 30 
Acetone	< 0.01	< 2	2	0.010	95 ●	0.002	≤ 7 
Oxaloacetic acid	0.24	37	17	0.243	91 ●	0.118	≤ 66 
Pyruvic acid	< 0.06	< 9	9	0.011	97 ●	0.003	≤ 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 ○	0.076	≤ 5 
1-Methylnicotinamide	< 0.20	< 32	32	0.057	97 ●	0.010	≤ 32 
Adenosine	< 2.5	< 390	390	0.000	0 ○	1.060	≤ 390 
Allantoin	< 0.11	< 17	17	0.035	90 ●	0.012	≤ 47 
Allopurinol	< 0.06	< 10	10	0.058	61 ○	0.077	≤ 11 
Caffeine	< 0.29	< 45	45	0.107	80 ○	0.112	≤ 61 
Inosine	< 0.12	< 19	19	0.012	93 ●	0.062	≤ 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	< 0.28	< 43	43	0.000	0 ○	0.056	≤ 44 
D-Glucose	0.24	37	34	0.241	88 ●	0.049	≤ 140 
D-Lactose	< 0.62	< 96	96	0.026	82 ○	0.029	≤ 96 
D-Mannitol	< 1.2	< 180	180	0.000	0 ○	2.325	≤ 180 
D-Mannose	< 0.04	< 6	6	0.019	79 ○	0.005	≤ 8 
Myo-Inositol	< 29	< 4400	4400	0.000	0 ○	4.677	≤ 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.

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