

# ● Analysis Report

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

Sample ID: ALZ\_Urine\_Rack01\_RCM\_221214\_expno260.100000.10r

Measuring Date: 23-Dec-2014 19:51:01

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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	3.2	0.3	3.167	100 ●	0.049	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	0.14	45	31	0.142	100 ●	0.002	$\leq 54$ 
Trimethylamine	< 0.01	< 2	2	0.002	80 ○	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	< 0.05	< 15	15	0.000	0 ○	0.162	$\leq 15$ 
2-Furoylglycine	< 0.12	< 39	39	0.000	0 ○	0.021	$\leq 40$ 
4-Aminobutyric acid	< 0.06	< 20	20	0.046	55 ○	0.065	$\leq 20$ 
Alanine	0.11	36	10	0.115	100 ●	0.005	11 - 72 
Arginine	< 2.4	< 750	750	0.206	19 ○	2.902	$\leq 750$ 
Betaine	0.06	18	7	0.058	100 ●	0.019	9 - 78 
Creatine	< 0.16	< 50	50	0.080	100 ●	0.049	$\leq 280$ 
Glycine	0.23	72	34	0.227	100 ●	0.007	38 - 440 
Guanidinoacetic acid	< 0.33	< 100	100	0.248	96 ●	0.083	$\leq 140$ 
Methionine	< 0.06	< 18	18	0.000	0 ○	0.139	$\leq 18$ 
N,N-Dimethylglycine	0.02	7	5	0.023	98 ●	0.005	$\leq 15$ 
Sarcosine	< 0.01	< 2	2	0.005	33 ○	0.004	$\leq 7$ 
Taurine	0.52	160	140	0.516	97 ●	0.125	$\leq 170$ 
Valine	0.02	6	2	0.018	93 ●	0.004	$\leq 7$ 











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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	< 0.03	< 10	10	0.000	0○	0.024	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0○	0.040	2 - 17 
Hippuric acid	< 0.54	< 170	170	0.416	99●	0.048	≤ 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	11	5	0.035	91●	0.010	≤ 51 
Citric acid	1.1	360	40	1.139	100●	0.096	≤ 700 
Formic acid	0.03	10	10	0.031	100●	0.001	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.002	87●	0.001	≤ 3 
Imidazole	< 0.15	< 48	48	0.000	0○	0.080	≤ 48 
Lactic acid	< 0.15	< 49	49	0.074	96●	0.024	≤ 110 
Proline betaine	0.11	36	25	0.114	99●	0.012	≤ 280 
Succinic acid	< 0.01	< 5	5	0.015	56○	0.009	≤ 39 
Tartaric acid	0.02	7	5	0.023	98●	0.004	≤ 110 
Trigonelline	< 0.11	< 35	35	0.065	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	< 0.15	< 48	48	0.000	0○	0.150	≤ 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	< 0.29	< 92	92	0.028	58 ○	0.119	≤ 92 
3-Hydroxybutyric acid	< 0.33	< 100	100	0.000	0 ○	0.363	≤ 100 
Acetoacetic acid	< 0.04	< 14	14	0.042	83 ○	0.032	≤ 30 
Acetone	0.01	4	2	0.012	99 ●	0.002	≤ 7 
Oxaloacetic acid	0.09	28	17	0.089	87 ●	0.063	≤ 66 
Pyruvic acid	< 0.03	< 9	9	0.017	100 ●	0.001	≤ 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	< 0.02	< 5	5	0.000	0 ○	0.090	≤ 5 
1-Methylnicotinamide	< 0.10	< 32	32	0.034	94 ●	0.009	≤ 32 
Adenosine	< 1.2	< 390	390	0.000	0 ○	0.696	≤ 390 
Allantoin	< 0.05	< 17	17	0.043	99 ●	0.005	≤ 47 
Allopurinol	< 0.03	< 10	10	0.022	87 ●	0.026	≤ 11 
Caffeine	< 0.14	< 45	45	0.098	74 ○	0.086	≤ 61 
Inosine	< 0.06	< 19	19	0.028	73 ○	0.028	≤ 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	< 0.14	< 43	43	0.000	0 ○	0.015	≤ 44 
D-Glucose	< 0.11	< 34	34	0.101	82 ○	0.039	≤ 140 
D-Lactose	< 0.30	< 96	96	0.021	87 ●	0.021	≤ 96 
D-Mannitol	< 0.58	< 180	180	0.000	0 ○	1.265	≤ 180 
D-Mannose	< 0.02	< 6	6	0.000	0 ○	0.040	≤ 8 
Myo-Inositol	< 14	< 4400	4400	0.000	0 ○	5.443	≤ 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

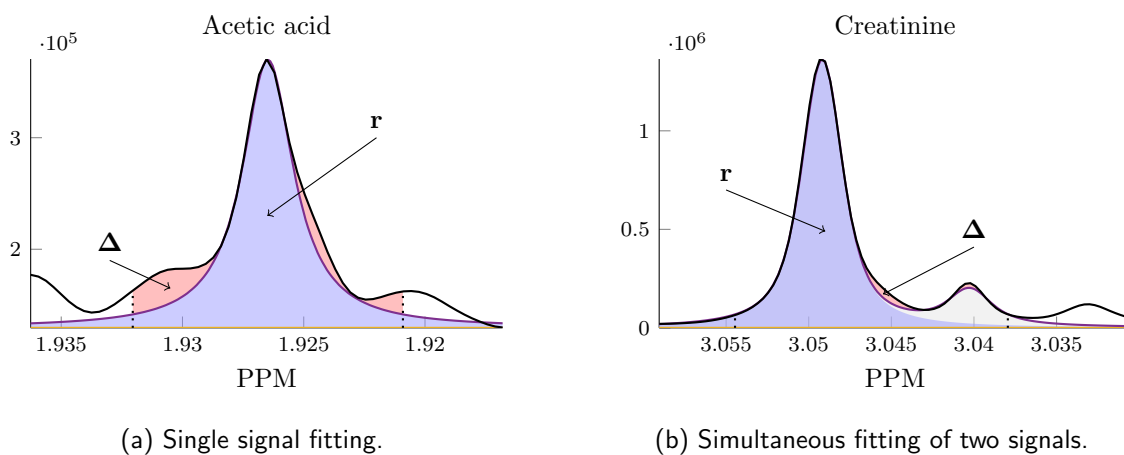


Figure 1: Examples of fitting.

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.

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