

# ● Analysis Report

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

Sample ID: ALZ\_Urine\_Rack01\_RCM\_221214\_expno240.100000.10r

Measuring Date: 23-Dec-2014 19:21:48

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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	4.7	0.3	4.747	100 ●	0.090	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	0.16	33	31	0.158	100 ●	0.005	$\leq 54$ 
Trimethylamine	< 0.01	< 2	2	0.001	0 ○	0.004	$\leq 3$ 




(\*) 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	< 0.07	< 15	15	0.000	0 ○	0.062	$\leq 15$ 
2-Furoylglycine	< 0.18	< 39	39	0.165	100 ●	0.008	$\leq 40$ 
4-Aminobutyric acid	< 0.09	< 20	20	0.000	0 ○	0.226	$\leq 20$ 
Alanine	0.12	24	10	0.116	100 ●	0.008	11 - 72 
Arginine	< 3.5	< 750	750	0.402	3 ○	0.878	$\leq 750$ 
Betaine	0.07	15	7	0.071	99 ●	0.020	9 - 78 
Creatine	< 0.24	< 50	50	0.023	100 ●	0.090	$\leq 280$ 
Glycine	0.43	91	34	0.434	98 ●	0.047	38 - 440 
Guanidinoacetic acid	< 0.49	< 100	100	0.053	87 ●	0.023	$\leq 140$ 
Methionine	< 0.09	< 18	18	0.000	0 ○	0.226	$\leq 18$ 
N,N-Dimethylglycine	0.04	8	5	0.040	95 ●	0.008	$\leq 15$ 
Sarcosine	< 0.01	< 2	2	0.002	0 ○	0.007	$\leq 7$ 
Taurine	< 0.68	< 140	140	0.175	4 ○	0.263	$\leq 170$ 
Valine	0.02	3	2	0.016	89 ●	0.005	$\leq 7$ 











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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	< 0.05	< 10	10	0.000	0 ○	0.019	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.071	2 - 17 
Hippuric acid	< 0.81	< 170	170	0.309	99 ●	0.034	≤ 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	7	5	0.033	99 ●	0.004	≤ 51 
Citric acid	0.84	180	40	0.844	99 ●	0.160	≤ 700 
Formic acid	0.13	27	10	0.129	100 ●	0.005	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.003	93 ●	0.001	≤ 3 
Imidazole	< 0.23	< 48	48	0.050	69 ○	0.037	≤ 48 
Lactic acid	< 0.23	< 49	49	0.064	75 ○	0.044	≤ 110 
Proline betaine	0.55	120	25	0.546	100 ●	0.016	≤ 280 
Succinic acid	0.04	7	5	0.035	85 ●	0.012	≤ 39 
Tartaric acid	0.04	9	5	0.041	94 ●	0.010	≤ 110 
Trigonelline	0.21	44	35	0.211	100 ●	0.004	≤ 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	< 0.23	< 48	48	0.000	0 ○	0.140	≤ 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	< 0.44	< 92	92	0.028	15 ○	0.144	≤ 92 
3-Hydroxybutyric acid	< 0.49	< 100	100	0.000	0 ○	0.759	≤ 100 
Acetoacetic acid	< 0.07	< 14	14	0.031	55 ○	0.027	≤ 30 
Acetone	< 0.01	< 2	2	0.008	93 ●	0.002	≤ 7 
Oxaloacetic acid	< 0.08	< 17	17	0.065	87 ●	0.043	≤ 66 
Pyruvic acid	< 0.04	< 9	9	0.018	61 ○	0.014	≤ 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 ○	0.084	≤ 5 
1-Methylnicotinamide	< 0.15	< 32	32	0.027	94 ●	0.009	≤ 32 
Adenosine	< 1.8	< 390	390	0.000	0 ○	1.107	≤ 390 
Allantoin	0.08	17	17	0.083	95 ●	0.014	≤ 47 
Allopurinol	< 0.05	< 10	10	0.018	96 ●	0.027	≤ 11 
Caffeine	< 0.22	< 45	45	0.202	94 ●	0.149	≤ 61 
Inosine	< 0.09	< 19	19	0.012	97 ●	0.024	≤ 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	< 0.21	< 43	43	0.055	87 ●	0.005	≤ 44 
D-Glucose	0.26	56	34	0.264	74 ○	0.253	≤ 140 
D-Lactose	< 0.45	< 96	96	0.250	99 ●	0.030	≤ 96 
D-Mannitol	< 0.87	< 180	180	0.000	0 ○	2.598	≤ 180 
D-Mannose	< 0.03	< 6	6	0.000	0 ○	0.073	≤ 8 
Myo-Inositol	< 21	< 4400	4400	0.000	0 ○	4.105	≤ 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

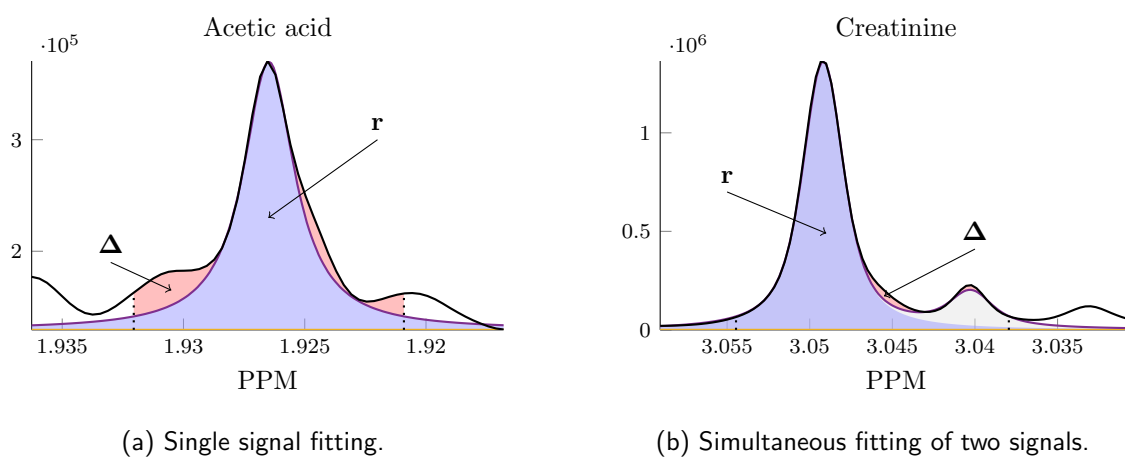


Figure 1: Examples of fitting.

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.

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