

● Analysis Report

Bruker IVDr Quantification in URine B.I.Quant-UR bTM

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno340.100000.10r

Measuring Date: 23-Dec-2014 21:50:43

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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

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: Guanidinoacetic acid (260 mmol/mol Crea),

Carboxylic acids: Formic acid (73 mmol/mol Crea), Trigonelline (100 mmol/mol Crea),

Keto acids and derivatives: Oxaloacetic acid (210 mmol/mol Crea),


Sugars and derivatives: D-Mannitol (1100 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	ρ %	Δ mmol/L	95% Range ^(*) mmol/L
Creatinine	3.1	0.3	3.069	100 ●	0.044	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	ρ %	Δ mmol/L	95% Range ^(*) $\frac{\text{mmol}}{\text{mol Crea}}$
Dimethylamine	< 0.09	< 31	31	0.092	100 ●	0.002	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.002	99 ●	0.000	≤ 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	ρ %	Δ mmol/L	95% Range ^(*) $\frac{\text{mmol}}{\text{mol Crea}}$
1-Methylhistidine	< 0.05	< 15	15	0.000	0 ○	0.040	≤ 15 
2-Furoylglycine	< 0.12	< 39	39	0.000	0 ○	0.036	≤ 40 
4-Aminobutyric acid	< 0.06	< 20	20	0.000	0 ○	0.135	≤ 20 
Alanine	0.10	32	10	0.099	100 ●	0.004	11 - 72 
Arginine	< 2.3	< 750	750	0.382	27 ○	1.127	≤ 750 
Betaine	0.03	11	7	0.034	100 ●	0.010	9 - 78 
Creatine	< 0.15	< 50	50	0.044	100 ●	0.044	≤ 280 
Glycine	0.26	86	34	0.264	100 ●	0.006	38 - 440 
Guanidinoacetic acid	0.79	260	100	0.794	53 ○	0.556	≤ 140 
Methionine	< 0.06	< 18	18	0.000	0 ○	0.137	≤ 18 
N,N-Dimethylglycine	< 0.02	< 5	5	0.007	93 ●	0.010	≤ 15 
Sarcosine	< 0.01	< 2	2	0.005	0 ○	0.011	≤ 7 
Taurine	< 0.44	< 140	140	0.330	97 ●	0.097	≤ 170 
Valine	0.01	5	2	0.015	91 ●	0.005	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
Benzoic acid	< 0.03	< 10	10	0.000	0○	0.014	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0○	0.136	2 - 17 
Hippuric acid	1.1	360	170	1.113	99●	0.107	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
Acetic acid	0.06	18	5	0.055	98●	0.009	≤ 51 
Citric acid	0.49	160	40	0.491	100●	0.062	≤ 700 
Formic acid	0.23	73	10	0.225	100●	0.006	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.002	0○	0.003	≤ 3 
Imidazole	< 0.15	< 48	48	0.000	0○	0.069	≤ 48 
Lactic acid	< 0.15	< 49	49	0.087	96●	0.021	≤ 110 
Proline betaine	< 0.08	< 25	25	0.054	0○	0.081	≤ 280 
Succinic acid	0.02	7	5	0.020	79○	0.008	≤ 39 
Tartaric acid	< 0.01	< 5	5	0.006	94●	0.002	≤ 110 
Trigonelline	0.31	100	35	0.312	100●	0.007	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
2-Methylsuccinic acid	< 0.15	< 48	48	0.000	0○	0.110	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
2-Oxoglutaric acid	< 0.28	< 92	92	0.037	54 ○	0.098	≤ 92 
3-Hydroxybutyric acid	< 0.32	< 100	100	0.000	0 ○	0.306	≤ 100 
Acetoacetic acid	0.05	16	14	0.048	79 ○	0.024	≤ 30 
Acetone	0.01	4	2	0.011	99 ●	0.001	≤ 7 
Oxaloacetic acid	0.66	210	17	0.659	99 ●	0.115	≤ 66 
Pyruvic acid	< 0.03	< 9	9	0.017	88 ●	0.006	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
1-Methyladenosine	< 0.01	< 5	5	0.000	0 ○	0.074	≤ 5 
1-Methylnicotinamide	< 0.10	< 32	32	0.027	93 ●	0.010	≤ 32 
Adenosine	< 1.2	< 390	390	0.000	0 ○	0.609	≤ 390 
Allantoin	0.08	25	17	0.076	99 ●	0.005	≤ 47 
Allopurinol	< 0.03	< 10	10	0.018	81 ○	0.017	≤ 11 
Caffeine	< 0.14	< 45	45	0.054	92 ●	0.050	≤ 61 
Inosine	< 0.06	< 19	19	0.011	97 ●	0.015	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.13	< 43	43	0.063	99 ●	0.002	≤ 44 
D-Glucose	< 0.10	< 34	34	0.099	74 ○	0.037	≤ 140 
D-Lactose	< 0.29	< 96	96	0.040	83 ○	0.036	≤ 96 
D-Mannitol	3.5	1100	180	3.471	99 ●	0.444	≤ 180 
D-Mannose	< 0.02	< 6	6	0.000	0 ○	0.030	≤ 8 
Myo-Inositol	< 14	< 4400	4400	0.000	0 ○	2.539	≤ 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 , ρ and Δ .

10.1 How to read the result

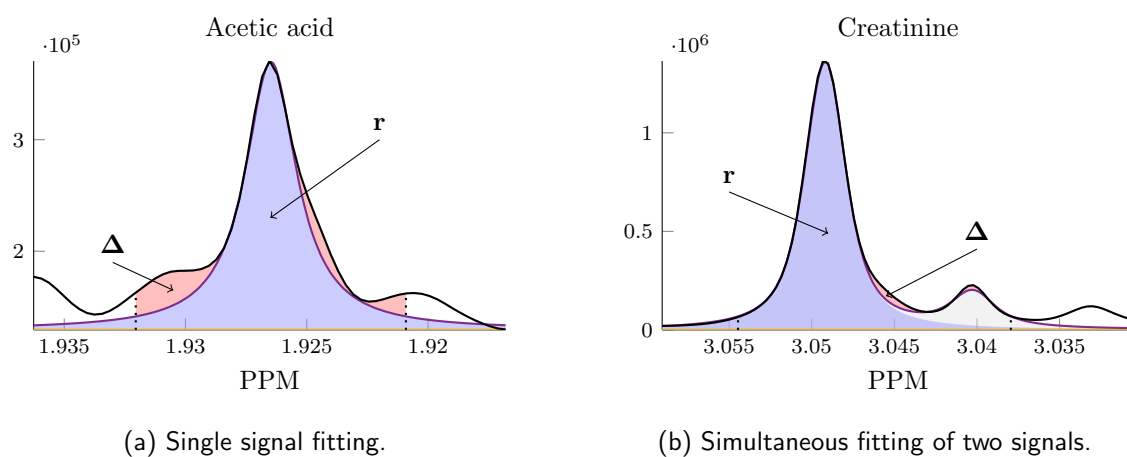


Figure 1: Examples of fitting.

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 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. α),
- ρ is the correlation of lineshape metabolite signal with calculated fit characterizing the match between metabolite signal and fit (cf. β). Depending on the value of ρ , 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) Δ is the concentration equivalent of the difference between metabolite signal and calculated fit (residue corresponding to the **the red area**, cf. γ)).

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.

α) r (*raw concentration*) is defined as

$$r = \frac{1}{P_N} \int_{\mathbb{R}} f(\xi) d\xi.$$

β) ρ 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 .

γ) Δ 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.

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