

● Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno490.100000.10r

Measuring Date: 24-Dec-2014 01:31:28

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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:


Carboxylic acids: *Trigonelline (160 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	6.4	0.3	6.381	100 ●	0.126	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	0.21	34	31	0.215	100 ●	0.006	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.003	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	< 0.10	< 15	15	0.000	0 ○	0.326	≤ 15 
2-Furoylglycine	< 0.25	< 39	39	0.171	99 ●	0.013	≤ 40 
4-Aminobutyric acid	< 0.13	< 20	20	0.017	42 ○	0.064	≤ 20 
Alanine	0.07	11	10	0.072	99 ●	0.009	11 - 72 
Arginine	< 4.8	< 750	750	0.452	7 ○	1.065	≤ 750 
Betaine	0.09	14	7	0.088	100 ●	0.026	9 - 78 
Creatine	< 0.32	< 50	50	0.180	100 ●	0.126	≤ 280 
Glycine	0.48	75	34	0.481	100 ●	0.024	38 - 440 
Guanidinoacetic acid	< 0.66	< 100	100	0.358	96 ●	0.084	≤ 140 
Methionine	< 0.11	< 18	18	0.000	0 ○	0.212	≤ 18 
N,N-Dimethylglycine	0.07	11	5	0.072	94 ●	0.016	≤ 15 
Sarcosine	< 0.01	< 2	2	0.003	0 ○	0.011	≤ 7 
Taurine	< 0.91	< 140	140	0.468	77 ○	0.265	≤ 170 
Valine	0.02	4	2	0.024	43 ○	0.024	≤ 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	< 0.06	< 10	10	0.000	0 ○	0.036	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.188	2 - 17 
Hippuric acid	< 1.1	< 170	170	0.990	99 ●	0.098	≤ 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	0.07	11	5	0.071	99 ●	0.007	≤ 51 
Citric acid	1.6	250	40	1.603	99 ●	0.249	≤ 700 
Formic acid	0.10	16	10	0.101	100 ●	0.004	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.009	91 ●	0.003	≤ 3 
Imidazole	< 0.31	< 48	48	0.086	51 ○	0.060	≤ 48 
Lactic acid	< 0.31	< 49	49	0.111	98 ●	0.025	≤ 110 
Proline betaine	< 0.16	< 25	25	0.137	95 ●	0.082	≤ 280 
Succinic acid	0.07	11	5	0.068	99 ●	0.008	≤ 39 
Tartaric acid	< 0.03	< 5	5	0.019	98 ●	0.009	≤ 110 
Trigonelline	1.00	160	35	1.047	100 ●	0.038	≤ 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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
2-Methylsuccinic acid	< 0.30	< 48	48	0.066	54 ○	0.102	≤ 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	< 0.59	< 92	92	0.084	51 ○	0.211	≤ 92 
3-Hydroxybutyric acid	< 0.66	< 100	100	0.207	72 ○	0.177	≤ 100 
Acetoacetic acid	0.19	30	14	0.195	100 ●	0.009	≤ 30 
Acetone	0.03	5	2	0.032	99 ●	0.006	≤ 7 
Oxaloacetic acid	< 0.11	< 17	17	0.058	61 ○	0.053	≤ 66 
Pyruvic acid	< 0.06	< 9	9	0.049	88 ●	0.021	≤ 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	< 0.03	< 5	5	0.000	0 ○	0.116	≤ 5 
1-Methylnicotinamide	< 0.20	< 32	32	0.067	98 ●	0.008	≤ 32 
Adenosine	< 2.5	< 390	390	0.000	0 ○	1.448	≤ 390 
Allantoin	0.12	19	17	0.122	90 ●	0.027	≤ 47 
Allopurinol	0.07	11	10	0.070	61 ○	0.070	≤ 11 
Caffeine	< 0.29	< 45	45	0.142	94 ●	0.129	≤ 61 
Inosine	< 0.12	< 19	19	0.036	67 ○	0.084	≤ 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	< 0.28	< 43	43	0.000	0 ○	0.027	≤ 44 
D-Glucose	0.32	50	34	0.319	90 ●	0.078	≤ 140 
D-Lactose	< 0.61	< 96	96	0.190	73 ○	3.509	≤ 96 
D-Mannitol	< 1.2	< 180	180	0.000	0 ○	1.803	≤ 180 
D-Mannose	< 0.04	< 6	6	0.000	0 ○	0.101	≤ 8 
Myo-Inositol	< 28	< 4400	4400	0.000	0 ○	5.171	≤ 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.

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