

● Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno250.100000.10r

Measuring Date: 23-Dec-2014 19:36:24

Reporting Date: 12-Dec-2020 15:21:46, 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

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 (75 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	9.4	0.3	9.397	100 ●	0.204	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	< 0.29	< 31	31	0.252	100 ●	0.008	≤ 54 
Trimethylamine	< 0.02	< 2	2	0.002	0 ○	0.003	≤ 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	< 0.14	< 15	15	0.000	0 ○	0.078	≤ 15 
2-Furoylglycine	< 0.36	< 39	39	0.000	0 ○	0.042	≤ 40 
4-Aminobutyric acid	< 0.19	< 20	20	0.000	0 ○	0.725	≤ 20 
Alanine	0.12	13	10	0.123	99 ●	0.014	11 - 72 
Arginine	< 7.0	< 750	750	0.548	16 ○	2.007	≤ 750 
Betaine	0.27	29	7	0.269	100 ●	0.035	9 - 78 
Creatine	< 0.47	< 50	50	0.077	100 ●	0.204	≤ 280 
Glycine	1.1	110	34	1.070	100 ●	0.039	38 - 440 
Guanidinoacetic acid	< 0.97	< 100	100	0.328	83 ○	0.135	≤ 140 
Methionine	< 0.17	< 18	18	0.000	0 ○	0.452	≤ 18 
N,N-Dimethylglycine	0.08	9	5	0.080	91 ●	0.018	≤ 15 
Sarcosine	< 0.02	< 2	2	0.000	0 ○	0.004	≤ 7 
Taurine	< 1.3	< 140	140	0.338	25 ○	0.276	≤ 170 
Valine	0.03	3	2	0.026	87 ●	0.023	≤ 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	< 0.09	< 10	10	0.000	0 ○	0.036	≤ 10 
D-Mandelic acid	< 0.02	< 2	2	0.000	0 ○	0.128	2 - 17 
Hippuric acid	3.6	380	170	3.588	99 ●	0.425	≤ 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	0.08	8	5	0.079	99 ●	0.013	≤ 51 
Citric acid	5.1	540	40	5.108	100 ●	0.377	≤ 700 
Formic acid	0.19	21	10	0.193	99 ●	0.014	≤ 43 
Fumaric acid	< 0.02	< 2	2	0.008	94 ●	0.002	≤ 3 
Imidazole	< 0.45	< 48	48	0.000	0 ○	0.155	≤ 48 
Lactic acid	< 0.46	< 49	49	0.165	98 ●	0.036	≤ 110 
Proline betaine	1.3	130	25	1.261	100 ●	0.047	≤ 280 
Succinic acid	0.07	7	5	0.070	97 ●	0.010	≤ 39 
Tartaric acid	0.22	23	5	0.217	100 ●	0.006	≤ 110 
Trigonelline	0.71	75	35	0.709	100 ●	0.030	≤ 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	< 0.45	< 48	48	0.000	0 ○	0.309	≤ 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	< 0.87	< 92	92	0.000	40 ○	0.597	≤ 92 
3-Hydroxybutyric acid	< 0.97	< 100	100	0.102	4 ○	0.560	≤ 100 
Acetoacetic acid	0.20	21	14	0.198	99 ●	0.042	≤ 30 
Acetone	0.03	3	2	0.027	98 ●	0.005	≤ 7 
Oxaloacetic acid	0.17	18	17	0.166	89 ●	0.093	≤ 66 
Pyruvic acid	< 0.08	< 9	9	0.038	99 ●	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	< 0.05	< 5	5	0.000	0 ○	0.138	≤ 5 
1-Methylnicotinamide	< 0.30	< 32	32	0.054	97 ●	0.008	≤ 32 
Adenosine	< 3.6	< 390	390	0.000	0 ○	1.636	≤ 390 
Allantoin	0.18	19	17	0.180	100 ●	0.016	≤ 47 
Allopurinol	< 0.09	< 10	10	0.040	95 ●	0.039	≤ 11 
Caffeine	< 0.43	< 45	45	0.277	82 ○	0.220	≤ 61 
Inosine	< 0.18	< 19	19	0.023	95 ●	0.042	≤ 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	< 0.41	< 43	43	0.000	0 ○	0.037	≤ 44 
D-Glucose	< 0.32	< 34	34	0.307	95 ●	0.060	≤ 140 
D-Lactose	< 0.90	< 96	96	0.136	84 ○	0.085	≤ 96 
D-Mannitol	< 1.7	< 180	180	0.000	0 ○	2.557	≤ 180 
D-Mannose	< 0.06	< 6	6	0.000	0 ○	0.091	≤ 8 
Myo-Inositol	< 42	< 4400	4400	0.000	0 ○	10.18	≤ 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.

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