

● Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno420.100000.10r

Measuring Date: 23-Dec-2014 23:49:00

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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	ρ %	Δ mmol/L	95% Range ^(*) mmol/L
Creatinine	3.5	0.3	3.523	100 ●	0.053	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	0.12	34	31	0.119	100 ●	0.004	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.001	89 ●	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 ○	0.076	≤ 15 
2-Furoylglycine	< 0.14	< 39	39	0.000	0 ○	0.033	≤ 40 
4-Aminobutyric acid	< 0.07	< 20	20	0.000	0 ○	0.245	≤ 20 
Alanine	0.05	15	10	0.053	99 ●	0.006	11 - 72 
Arginine	< 2.6	< 750	750	0.206	0 ○	1.455	≤ 750 
Betaine	0.04	10	7	0.035	100 ●	0.010	9 - 78 
Creatine	< 0.18	< 50	50	0.047	100 ●	0.053	≤ 280 
Glycine	0.15	42	34	0.149	100 ●	0.007	38 - 440 
Guanidinoacetic acid	< 0.36	< 100	100	0.185	80 ○	0.092	≤ 140 
Methionine	< 0.06	< 18	18	0.000	0 ○	0.078	≤ 18 
N,N-Dimethylglycine	0.02	7	5	0.023	89 ●	0.007	≤ 15 
Sarcosine	< 0.01	< 2	2	0.002	0 ○	0.004	≤ 7 
Taurine	< 0.50	< 140	140	0.172	96 ●	0.049	≤ 170 
Valine	0.01	2	2	0.009	58 ○	0.007	≤ 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 ○	0.042	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.070	2 - 17 
Hippuric acid	1.00	300	170	1.041	99 ●	0.093	≤ 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	0.03	10	5	0.034	78 ○	0.015	≤ 51 
Citric acid	0.61	170	40	0.610	100 ●	0.071	≤ 700 
Formic acid	< 0.03	< 10	10	0.028	100 ●	0.002	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.002	80 ○	0.001	≤ 3 
Imidazole	< 0.17	< 48	48	0.031	50 ○	0.022	≤ 48 
Lactic acid	< 0.17	< 49	49	0.047	85 ●	0.024	≤ 110 
Proline betaine	< 0.09	< 25	25	0.084	98 ●	0.012	≤ 280 
Succinic acid	0.03	9	5	0.031	86 ●	0.010	≤ 39 
Tartaric acid	< 0.02	< 5	5	0.005	94 ●	0.002	≤ 110 
Trigonelline	< 0.12	< 35	35	0.107	100 ●	0.003	≤ 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	< 0.17	< 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	< 0.33	< 92	92	0.061	51 ○	0.086	≤ 92 
3-Hydroxybutyric acid	< 0.36	< 100	100	0.058	18 ○	0.225	≤ 100 
Acetoacetic acid	0.07	21	14	0.073	81 ○	0.037	≤ 30 
Acetone	0.01	3	2	0.011	98 ●	0.002	≤ 7 
Oxaloacetic acid	0.21	59	17	0.210	96 ●	0.056	≤ 66 
Pyruvic acid	< 0.03	< 9	9	0.009	98 ●	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	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
1-Methyladenosine	< 0.02	< 5	5	0.000	0 ○	0.059	≤ 5 
1-Methylnicotinamide	< 0.11	< 32	32	0.024	87 ●	0.008	≤ 32 
Adenosine	< 1.4	< 390	390	0.000	0 ○	0.611	≤ 390 
Allantoin	0.07	19	17	0.068	99 ●	0.005	≤ 47 
Allopurinol	< 0.04	< 10	10	0.012	92 ●	0.018	≤ 11 
Caffeine	< 0.16	< 45	45	0.059	97 ●	0.055	≤ 61 
Inosine	< 0.07	< 19	19	0.013	81 ○	0.022	≤ 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	< 0.15	< 43	43	0.000	0 ○	0.029	≤ 44 
D-Glucose	0.13	36	34	0.125	61 ○	0.072	≤ 140 
D-Lactose	< 0.34	< 96	96	0.044	88 ●	0.028	≤ 96 
D-Mannitol	< 0.65	< 180	180	0.000	0 ○	1.315	≤ 180 
D-Mannose	< 0.02	< 6	6	0.000	0 ○	0.041	≤ 8 
Myo-Inositol	< 16	< 4400	4400	0.000	0 ○	3.090	≤ 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.

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