

● Analysis Report

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

Sample ID: ALZ_Urine_Rack04_RCM_191214_expno730.100000.10r

Measuring Date: 20-Dec-2014 09:15:23

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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	5.4	0.3	5.355	100 ●	0.111	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	< 0.16	< 31	31	0.155	100 ●	0.004	≤ 54 
Trimethylamine	< 0.01	< 2	2	0.003	94 ●	0.001	≤ 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	< 0.08	< 15	15	0.000	0 ○	0.043	≤ 15 
2-Furoylglycine	< 0.21	< 39	39	0.115	99 ●	0.008	≤ 40 
4-Aminobutyric acid	< 0.11	< 20	20	0.000	0 ○	0.218	≤ 20 
Alanine	0.14	27	10	0.142	100 ●	0.009	11 - 72 
Arginine	< 4.0	< 750	750	0.436	7 ○	0.653	≤ 750 
Betaine	0.06	11	7	0.058	100 ●	0.016	9 - 78 
Creatine	< 0.27	< 50	50	0.127	100 ●	0.111	≤ 280 
Glycine	0.65	120	34	0.654	100 ●	0.018	38 - 440 
Guanidinoacetic acid	< 0.55	< 100	100	0.313	88 ●	0.125	≤ 140 
Methionine	< 0.10	< 18	18	0.000	0 ○	0.425	≤ 18 
N,N-Dimethylglycine	0.03	6	5	0.032	75 ○	0.015	≤ 15 
Sarcosine	< 0.01	< 2	2	0.003	0 ○	0.006	≤ 7 
Taurine	< 0.76	< 140	140	0.360	95 ●	0.134	≤ 170 
Valine	0.02	4	2	0.021	71 ○	0.012	≤ 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	< 0.05	< 10	10	0.000	0 ○	0.027	≤ 10 
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.058	2 - 17 
Hippuric acid	1.1	200	170	1.087	100 ●	0.079	≤ 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	13	5	0.070	98 ●	0.009	≤ 51 
Citric acid	1.6	300	40	1.613	100 ●	0.137	≤ 700 
Formic acid	0.10	18	10	0.098	99 ●	0.009	≤ 43 
Fumaric acid	< 0.01	< 2	2	0.004	57 ○	0.002	≤ 3 
Imidazole	< 0.26	< 48	48	0.029	33 ○	0.031	≤ 48 
Lactic acid	< 0.26	< 49	49	0.124	99 ●	0.047	≤ 110 
Proline betaine	0.26	48	25	0.258	99 ●	0.021	≤ 280 
Succinic acid	0.10	19	5	0.104	97 ●	0.018	≤ 39 
Tartaric acid	0.05	10	5	0.054	98 ●	0.012	≤ 110 
Trigonelline	< 0.19	< 35	35	0.128	100 ●	0.002	≤ 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	< 0.26	< 48	48	0.000	0 ○	0.189	≤ 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	< 0.49	< 92	92	0.032	5 ○	0.146	≤ 92 
3-Hydroxybutyric acid	< 0.55	< 100	100	0.000	0 ○	0.503	≤ 100 
Acetoacetic acid	< 0.08	< 14	14	0.062	87 ●	0.029	≤ 30 
Acetone	0.02	4	2	0.022	100 ●	0.001	≤ 7 
Oxaloacetic acid	< 0.09	< 17	17	0.077	76 ○	0.077	≤ 66 
Pyruvic acid	< 0.05	< 9	9	0.029	96 ●	0.005	≤ 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 ○	0.105	≤ 5 
1-Methylnicotinamide	< 0.17	< 32	32	0.055	98 ●	0.012	≤ 32 
Adenosine	< 2.1	< 390	390	0.000	0 ○	0.925	≤ 390 
Allantoin	< 0.09	< 17	17	0.061	100 ●	0.004	≤ 47 
Allopurinol	< 0.05	< 10	10	0.030	97 ●	0.047	≤ 11 
Caffeine	< 0.24	< 45	45	0.105	91 ●	0.109	≤ 61 
Inosine	< 0.10	< 19	19	0.007	95 ●	0.050	≤ 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	< 0.23	< 43	43	0.030	87 ●	0.004	≤ 44 
D-Glucose	< 0.18	< 34	34	0.121	69 ○	0.075	≤ 140 
D-Lactose	< 0.51	< 96	96	0.148	86 ●	0.069	≤ 96 
D-Mannitol	< 0.98	< 180	180	0.000	0 ○	1.845	≤ 180 
D-Mannose	< 0.03	< 6	6	0.000	0 ○	0.057	≤ 8 
Myo-Inositol	< 24	< 4400	4400	0.000	0 ○	4.971	≤ 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.

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