

● Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno110.100000.10r

Measuring Date: 23-Dec-2014 16:39:27

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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	13	0.3	12.97	98 ●	1.806	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	< 0.40	< 31	31	0.197	100 ●	0.004	≤ 54 
Trimethylamine	< 0.03	< 2	2	0.007	91 ●	0.002	≤ 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	< 0.19	< 15	15	0.000	0 ○	0.168	≤ 15 
2-Furoylglycine	< 0.50	< 39	39	0.045	97 ●	0.006	≤ 40 
4-Aminobutyric acid	< 0.26	< 20	20	0.000	0 ○	0.242	≤ 20 
Alanine	0.60	47	10	0.604	100 ●	0.019	11 - 72 
Arginine	< 9.7	< 750	750	0.604	0 ○	2.753	≤ 750 
Betaine	0.18	14	7	0.181	100 ●	0.013	9 - 78 
Creatine	< 0.65	< 50	50	0.009	98 ●	1.806	≤ 280 
Glycine	1.9	150	34	1.884	100 ●	0.040	38 - 440 
Guanidinoacetic acid	< 1.3	< 100	100	0.237	92 ●	0.082	≤ 140 
Methionine	< 0.23	< 18	18	0.000	0 ○	0.253	≤ 18 
N,N-Dimethylglycine	0.11	9	5	0.114	97 ●	0.020	≤ 15 
Sarcosine	< 0.03	< 2	2	0.009	27 ○	0.007	≤ 7 
Taurine	< 1.8	< 140	140	0.103	24 ○	0.217	≤ 170 
Valine	0.03	2	2	0.029	19 ○	0.033	≤ 7 











(*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

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	< 0.12	< 10	10	0.000	0 ○	0.032	≤ 10 
D-Mandelic acid	< 0.03	< 2	2	0.000	0 ○	0.184	2 - 17 
Hippuric acid	3.0	230	170	2.995	99 ●	0.315	≤ 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	6	5	0.073	94 ●	0.018	≤ 51 
Citric acid	4.1	310	40	4.065	100 ●	0.237	≤ 700 
Formic acid	< 0.12	< 10	10	0.095	100 ●	0.002	≤ 43 
Fumaric acid	< 0.03	< 2	2	0.015	100 ●	0.001	≤ 3 
Imidazole	< 0.62	< 48	48	0.000	0 ○	0.114	≤ 48 
Lactic acid	< 0.63	< 49	49	0.205	93 ●	0.138	≤ 110 
Proline betaine	< 0.33	< 25	25	0.048	23 ○	0.041	≤ 280 
Succinic acid	< 0.06	< 5	5	0.044	98 ●	0.006	≤ 39 
Tartaric acid	< 0.06	< 5	5	0.024	94 ●	0.007	≤ 110 
Trigonelline	0.61	47	35	0.606	100 ●	0.021	≤ 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	< 0.62	< 48	48	0.000	0 ○	0.224	≤ 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	< 1.2	< 92	92	0.134	31 ○	0.288	≤ 92 
3-Hydroxybutyric acid	< 1.3	< 100	100	0.000	0 ○	0.602	≤ 100 
Acetoacetic acid	< 0.19	< 14	14	0.078	86 ●	0.059	≤ 30 
Acetone	< 0.03	< 2	2	0.018	99 ●	0.003	≤ 7 
Oxaloacetic acid	< 0.22	< 17	17	0.198	90 ●	0.112	≤ 66 
Pyruvic acid	< 0.12	< 9	9	0.054	100 ●	0.003	≤ 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	< 0.06	< 5	5	0.000	0 ○	0.093	≤ 5 
1-Methylnicotinamide	< 0.41	< 32	32	0.019	79 ○	0.011	≤ 32 
Adenosine	< 5.0	< 390	390	0.000	0 ○	1.076	≤ 390 
Allantoin	< 0.22	< 17	17	0.082	99 ●	0.008	≤ 47 
Allopurinol	< 0.13	< 10	10	0.017	90 ●	0.017	≤ 11 
Caffeine	< 0.59	< 45	45	0.155	99 ●	0.083	≤ 61 
Inosine	< 0.25	< 19	19	0.017	92 ●	0.023	≤ 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	< 0.56	< 43	43	0.000	0 ○	0.018	≤ 44 
D-Glucose	< 0.44	< 34	34	0.369	89 ●	0.084	≤ 140 
D-Lactose	< 1.2	< 96	96	0.054	63 ○	0.029	≤ 96 
D-Mannitol	< 2.4	< 180	180	0.000	0 ○	2.176	≤ 180 
D-Mannose	< 0.08	< 6	6	0.000	0 ○	0.060	≤ 8 
Myo-Inositol	< 58	< 4400	4400	0.000	0 ○	5.900	≤ 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.

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