Analysis Report

Bruker IVDr Quantification in URine B.I.Quant-UR b™

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno170.100000.10r

Measuring Date: 23-Dec-2014 17:37:49
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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.

Contents

1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	ρ %	Δ mmol/L	95% Range(*) mmol/L
Creatinine	7.0	0.3	7.048	100 ●	0.151	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	< 31	31	0.205	100 ●	0.007	≤ 54
Trimethylamine	< 0.01	< 2	2	0.006	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	< 0.11	< 15	15	0.000	0 ○	0.209	≤ 15
2-Furoylglycine	< 0.27	< 39	39	0.000	0 ○	0.049	≤ 40
4-Aminobutyric acid	< 0.14	< 20	20	0.000	0 ○	0.283	≤ 20
Alanine	0.45	63	10	0.445	100 ●	0.018	11 - 72
Arginine	< 5.3	< 750	750	0.476	0 ○	2.267	≤ 750
Betaine	0.14	20	7	0.139	100 ●	0.010	9 - 78
Creatine	< 0.35	< 50	50	0.053	100 ●	0.151	≤ 280
Glycine	1.1	160	34	1.098	100 ●	0.034	38 - 440
Guanidinoacetic acid	< 0.73	< 100	100	0.352	77 ○	0.188	≤ 140
Methionine	< 0.13	< 18	18	0.000	0 ○	0.355	≤ 18
N,N-Dimethylglycine	0.06	8	5	0.056	97 ●	0.011	≤ 15
Sarcosine	< 0.01	< 2	2	0.009	4 ○	0.010	≤ 7
Taurine	< 1.00	< 140	140	0.728	98 ●	0.140	≤ 170
Valine	0.05	7	2	0.046	96 ●	0.008	≤ 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	< 0.07	< 10	10	0.000	0 ○	0.028	≤ 10
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.004	2 - 17
Hippuric acid	< 1.2	< 170	170	1.018	99 ●	0.095	≤ 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	10	5	0.069	93 ●	0.018	≤ 51
Citric acid	2.8	400	40	2.826	100 ●	0.203	≤ 700
Formic acid	0.08	12	10	0.083	99 ●	0.007	≤ 43
Fumaric acid	< 0.01	< 2	2	0.006	100 ●	0.000	≤ 3
Imidazole	< 0.34	< 48	48	0.000	0 ○	0.157	≤ 48
Lactic acid	< 0.34	< 49	49	0.248	98 ●	0.129	≤ 110
Proline betaine	< 0.18	< 25	25	0.074	65 ○	0.073	≤ 280
Succinic acid	< 0.03	< 5	5	0.029	77 ○	0.012	≤ 39
Tartaric acid	0.05	7	5	0.048	98 ●	0.007	≤ 110
Trigonelline	< 0.24	< 35	35	0.073	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	< 0.34	< 48	48	0.059	0 ○	0.122	≤ 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	< 0.65	< 92	92	0.153	32 ○	0.248	≤ 92
3-Hydroxybutyric acid	< 0.73	< 100	100	0.000	0 ○	0.567	≤ 100
Acetoacetic acid	< 0.10	< 14	14	0.077	92 ●	0.043	≤ 30
Acetone	0.01	2	2	0.014	88 ●	0.004	≤ 7
Oxaloacetic acid	0.24	33	17	0.236	91 ●	0.114	≤ 66
Pyruvic acid	< 0.06	< 9	9	0.042	99 ●	0.004	≤ 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	< 0.04	< 5	5	0.000	0 ○	0.104	≤ 5
1-Methylnicotinamide	< 0.22	< 32	32	0.044	97 ●	0.007	≤ 32
Adenosine	< 2.7	< 390	390	0.000	0 ○	1.082	≤ 390
Allantoin	< 0.12	< 17	17	0.028	85 ●	0.011	≤ 47
Allopurinol	< 0.07	< 10	10	0.029	89 ●	0.029	≤ 11
Caffeine	< 0.32	< 45	45	0.090	80 ○	0.110	≤ 61
Inosine	< 0.13	< 19	19	0.017	96 ●	0.031	≤ 19

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

9 Sugars and derivatives

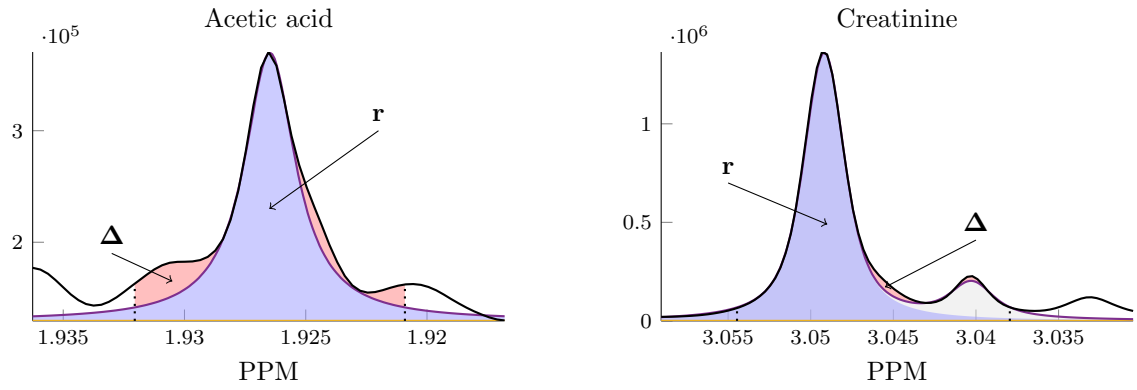
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.30	< 43	43	0.017	94 ●	0.001	≤ 44
D-Glucose	0.37	52	34	0.365	91 ●	0.077	≤ 140
D-Lactose	< 0.67	< 96	96	0.028	2 ○	0.047	≤ 96
D-Mannitol	< 1.3	< 180	180	0.373	32 ○	1.088	≤ 180
D-Mannose	< 0.04	< 6	6	0.000	0 ○	0.067	≤ 8
Myo-Inositol	< 31	< 4400	4400	0.000	0 ○	4.188	≤ 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 $\mathbf{r}$, ρ and $\mathbf{\Delta}$.

10.1 How to read the result



(a) Single signal fitting.

(b) Simultaneous fitting of two signals.

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 $\mathrm{CH_3}$ 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

a) **Conc.** is the final result concentration of the metabolite,

b) **LOD** is the *limit of detection* of the given metabolite,

c) $\mathbf{r}$ 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)),

d) 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) $\mathbf{r}$ (*raw concentration*) is defined as

$$\mathbf{r} = \frac{1}{P_N} \int_{\mathbb{R}} f(\xi)\, \mathrm{d}\xi.$$

β) ρ is the *correlation* of the functions s and $f + b$, i.e.

$$\rho = \max\left(0, \operatorname{corr}\left(\overline{s}, \overline{f + b}\right)\right),$$

where $\overline{s}$, $\overline{f + b}$ 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.

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