Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno460.100000.10r

Measuring Date: 24-Dec-2014 00:47:44
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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

The following metabolites were found with concentrations outside the 95% range of Bruker Quant-UR B.1.1.0 urine metabolite concentration database:

Sugars and derivatives: D-Glucose (240 mmol/mol Crea).

Further detailed information is provided on the following pages.

Contents

1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	ρ %	Δ mmol/L	95% Range(*) mmol/L
Creatinine	11	0.3	10.89	100 ●	0.161	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	< 0.33	< 31	31	0.292	100 ●	0.014	≤ 54
Trimethylamine	< 0.02	< 2	2	0.001	0 ○	0.008	≤ 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	< 0.16	< 15	15	0.064	74 ○	0.050	≤ 15
2-Furoylglycine	< 0.42	< 39	39	0.000	0 ○	0.051	≤ 40
4-Aminobutyric acid	< 0.22	< 20	20	0.045	6 ○	0.152	≤ 20
Alanine	0.44	40	10	0.439	100 ●	0.038	11 - 72
Arginine	< 8.1	< 750	750	1.414	23 ○	4.190	≤ 750
Betaine	0.78	71	7	0.778	100 ●	0.121	9 - 78
Creatine	< 0.54	< 50	50	0.139	100 ●	0.161	≤ 280
Glycine	0.99	91	34	0.994	100 ●	0.043	38 - 440
Guanidinoacetic acid	< 1.1	< 100	100	0.526	90 ●	0.270	≤ 140
Methionine	< 0.19	< 18	18	0.000	0 ○	0.398	≤ 18
N,N-Dimethylglycine	0.08	7	5	0.076	86 ●	0.026	≤ 15
Sarcosine	< 0.02	< 2	2	0.011	0 ○	0.024	≤ 7
Taurine	< 1.6	< 140	140	1.459	69 ○	0.945	≤ 170
Valine	0.04	4	2	0.042	89 ●	0.012	≤ 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	< 0.10	< 10	10	0.000	0 ○	0.033	≤ 10
D-Mandelic acid	< 0.02	< 2	2	0.000	0 ○	0.008	2 - 17
Hippuric acid	3.0	270	170	2.985	99 ●	0.294	≤ 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	0.06	5	5	0.056	91 ●	0.027	≤ 51
Citric acid	3.1	280	40	3.078	100 ●	0.294	≤ 700
Formic acid	0.18	16	10	0.177	100 ●	0.009	≤ 43
Fumaric acid	< 0.02	< 2	2	0.015	93 ●	0.003	≤ 3
Imidazole	< 0.52	< 48	48	0.165	100 ●	0.300	≤ 48
Lactic acid	< 0.53	< 49	49	0.200	98 ●	0.195	≤ 110
Proline betaine	< 0.27	< 25	25	0.132	98 ●	0.059	≤ 280
Succinic acid	< 0.05	< 5	5	0.034	70 ○	0.013	≤ 39
Tartaric acid	< 0.05	< 5	5	0.016	81 ○	0.006	≤ 110
Trigonelline	< 0.38	< 35	35	0.248	100 ●	0.005	≤ 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	< 0.52	< 48	48	0.000	0 ○	0.436	≤ 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	< 1.00	< 92	92	0.188	77 ○	0.363	≤ 92
3-Hydroxybutyric acid	< 1.1	< 100	100	0.000	0 ○	0.777	≤ 100
Acetoacetic acid	< 0.16	< 14	14	0.033	92 ●	0.059	≤ 30
Acetone	< 0.02	< 2	2	0.020	87 ●	0.010	≤ 7
Oxaloacetic acid	< 0.19	< 17	17	0.091	61 ○	0.112	≤ 66
Pyruvic acid	< 0.10	< 9	9	0.036	97 ●	0.009	≤ 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 ○	0.128	≤ 5
1-Methylnicotinamide	< 0.34	< 32	32	0.067	99 ●	0.005	≤ 32
Adenosine	< 4.2	< 390	390	0.000	0 ○	1.870	≤ 390
Allantoin	< 0.18	< 17	17	0.141	93 ●	0.029	≤ 47
Allopurinol	< 0.11	< 10	10	0.034	92 ●	0.066	≤ 11
Caffeine	< 0.49	< 45	45	0.376	86 ●	0.224	≤ 61
Inosine	< 0.21	< 19	19	0.028	95 ●	0.060	≤ 19

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

9 Sugars and derivatives

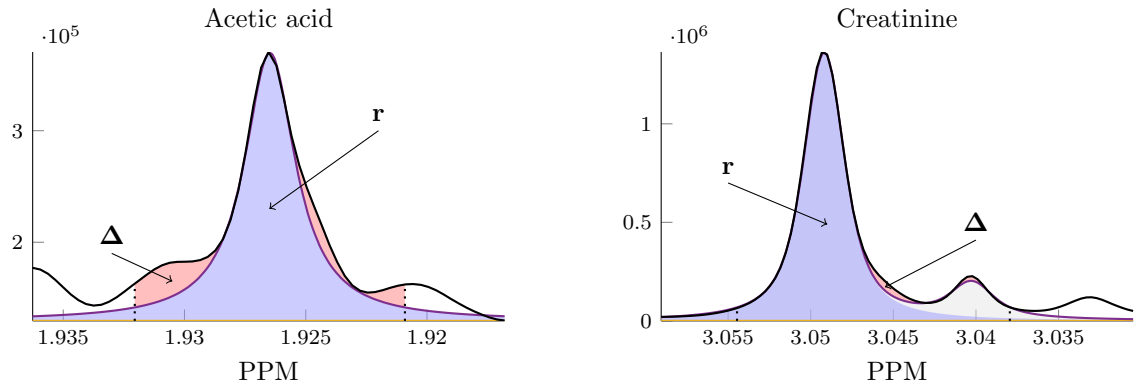
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.47	< 43	43	0.000	0 ○	0.040	≤ 44
D-Glucose	2.6	240	34	2.595	100 ●	0.110	≤ 140
D-Lactose	< 1.00	< 96	96	0.179	88 ●	0.113	≤ 96
D-Mannitol	< 2.0	< 180	180	0.000	0 ○	3.121	≤ 180
D-Mannose	< 0.07	< 6	6	0.025	98 ●	0.002	≤ 8
Myo-Inositol	< 48	< 4400	4400	0.000	0 ○	16.21	≤ 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.

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