Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno380.100000.10r

Measuring Date: 23-Dec-2014 22:49:54
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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:

Keto acids and derivatives: Acetoacetic acid (38 mmol/mol Crea), Oxaloacetic acid (110 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	8.7	0.3	8.653	100 ●	0.169	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	0.30	34	31	0.297	100 ●	0.009	$\leq$ 54
Trimethylamine	$<$ 0.02	$<$ 2	2	0.001	0 ○	0.002	$\leq$ 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	$<$ 0.13	$<$ 15	15	0.000	0 ○	0.157	$\leq$ 15
2-Furoylglycine	$<$ 0.33	$<$ 39	39	0.000	0 ○	0.026	$\leq$ 40
4-Aminobutyric acid	$<$ 0.17	$<$ 20	20	0.000	0 ○	1.201	$\leq$ 20
Alanine	0.12	14	10	0.119	99 ●	0.013	11 - 72
Arginine	$<$ 6.5	$<$ 750	750	0.474	26 ○	0.905	$\leq$ 750
Betaine	0.07	9	7	0.075	100 ●	0.029	9 - 78
Creatine	$<$ 0.43	$<$ 50	50	0.028	100 ●	0.169	$\leq$ 280
Glycine	0.47	54	34	0.470	100 ●	0.039	38 - 440
Guanidinoacetic acid	$<$ 0.89	$<$ 100	100	0.270	8 ○	0.345	$\leq$ 140
Methionine	$<$ 0.15	$<$ 18	18	0.000	0 ○	0.416	$\leq$ 18
N,N-Dimethylglycine	$<$ 0.04	$<$ 5	5	0.020	98 ●	0.008	$\leq$ 15
Sarcosine	0.02	2	2	0.019	30 ○	0.016	$\leq$ 7
Taurine	$<$ 1.2	$<$ 140	140	0.344	97 ●	0.108	$\leq$ 170
Valine	0.03	3	2	0.028	64 ○	0.072	$\leq$ 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	< 0.08	< 10	10	0.000	0 ○	0.049	≤ 10
D-Mandelic acid	< 0.02	< 2	2	0.000	0 ○	0.090	2 - 17
Hippuric acid	1.9	210	170	1.859	99 ●	0.194	≤ 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	0.05	6	5	0.047	44 ○	0.039	≤ 51
Citric acid	2.2	260	40	2.210	100 ●	0.282	≤ 700
Formic acid	< 0.08	< 10	10	0.080	100 ●	0.005	≤ 43
Fumaric acid	< 0.02	< 2	2	0.011	80 ○	0.004	≤ 3
Imidazole	< 0.41	< 48	48	0.000	0 ○	0.121	≤ 48
Lactic acid	< 0.42	< 49	49	0.175	96 ●	0.164	≤ 110
Proline betaine	< 0.22	< 25	25	0.130	97 ●	0.025	≤ 280
Succinic acid	0.07	8	5	0.072	99 ●	0.006	≤ 39
Tartaric acid	< 0.04	< 5	5	0.009	27 ○	0.013	≤ 110
Trigonelline	< 0.30	< 35	35	0.140	100 ●	0.004	≤ 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	< 0.41	< 48	48	0.000	0 ○	0.286	≤ 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	< 0.80	< 92	92	0.148	17 ○	0.327	≤ 92
3-Hydroxybutyric acid	< 0.89	< 100	100	0.052	17 ○	0.682	≤ 100
Acetoacetic acid	0.33	38	14	0.325	96 ●	0.125	≤ 30
Acetone	0.03	3	2	0.027	98 ●	0.009	≤ 7
Oxaloacetic acid	0.91	110	17	0.914	97 ●	0.263	≤ 66
Pyruvic acid	< 0.08	< 9	9	0.030	99 ●	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	< 0.04	< 5	5	0.000	0 ○	0.155	≤ 5
1-Methylnicotinamide	< 0.27	< 32	32	0.047	98 ●	0.005	≤ 32
Adenosine	< 3.4	< 390	390	0.000	0 ○	1.550	≤ 390
Allantoin	< 0.14	< 17	17	0.066	98 ●	0.007	≤ 47
Allopurinol	< 0.09	< 10	10	0.033	71 ○	0.031	≤ 11
Caffeine	< 0.39	< 45	45	0.155	94 ●	0.183	≤ 61
Inosine	< 0.16	< 19	19	0.015	97 ●	0.028	≤ 19

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

9 Sugars and derivatives

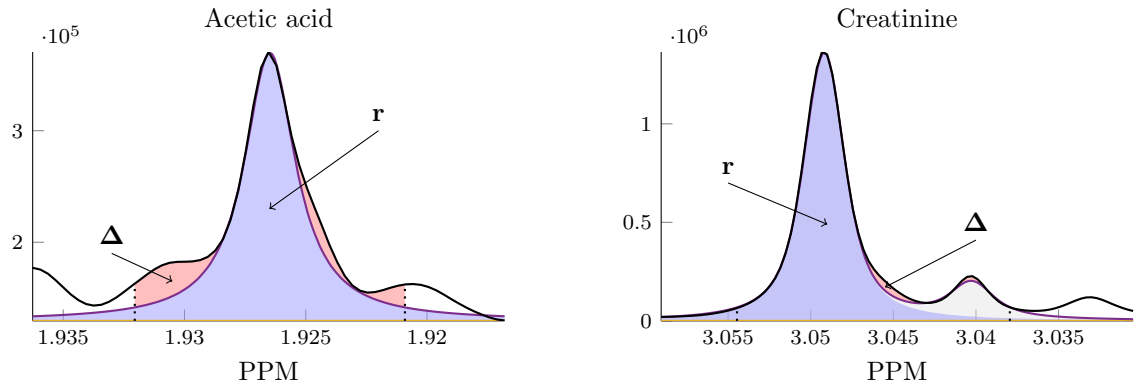
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.37	< 43	43	0.120	78 ○	0.022	≤ 44
D-Glucose	< 0.29	< 34	34	0.204	80 ○	0.129	≤ 140
D-Lactose	< 0.83	< 96	96	0.035	66 ○	0.036	≤ 96
D-Mannitol	< 1.6	< 180	180	0.609	32 ○	1.565	≤ 180
D-Mannose	< 0.05	< 6	6	0.000	0 ○	0.090	≤ 8
Myo-Inositol	< 38	< 4400	4400	0.000	0 ○	5.909	≤ 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 $\boldsymbol{\Delta}$.

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.

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