Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno230.100000.10r

Measuring Date: 23-Dec-2014 19:06:53
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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:

Amino acids and derivatives: Sarcosine (10 mmol/mol Crea),
Carboxylic acids: Formic acid (45 mmol/mol Crea),
Sugars and derivatives: D-Mannose (74 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	3.5	0.3	3.536	91 ●	1.491	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	0.12	35	31	0.125	71 ○	0.059	$\leq$ 54
Trimethylamine	$<$ 0.01	$<$ 2	2	0.003	11 ○	0.004	$\leq$ 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	$<$ 0.05	$<$ 15	15	0.000	0 ○	0.097	$\leq$ 15
2-Furoylglycine	$<$ 0.14	$<$ 39	39	0.000	0 ○	0.066	$\leq$ 40
4-Aminobutyric acid	$<$ 0.07	$<$ 20	20	0.000	0 ○	0.248	$\leq$ 20
Alanine	0.06	17	10	0.059	84 ○	0.019	11 - 72
Arginine	$<$ 2.6	$<$ 750	750	0.341	0 ○	1.102	$\leq$ 750
Betaine	0.13	37	7	0.132	75 ○	0.063	9 - 78
Creatine	0.65	180	50	0.649	91 ●	1.491	$\leq$ 280
Glycine	0.25	70	34	0.248	64 ○	0.124	38 - 440
Guanidinoacetic acid	$<$ 0.37	$<$ 100	100	0.129	56 ○	0.085	$\leq$ 140
Methionine	$<$ 0.06	$<$ 18	18	0.038	85 ●	0.021	$\leq$ 18
N,N-Dimethylglycine	0.05	15	5	0.054	84 ○	0.022	$\leq$ 15
Sarcosine	0.04	10	2	0.035	0 ○	0.070	$\leq$ 7
Taurine	$<$ 0.50	$<$ 140	140	0.094	57 ○	0.136	$\leq$ 170
Valine	$<$ 0.01	$<$ 2	2	0.000	0 ○	0.131	$\leq$ 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	< 0.03	< 10	10	0.000	0 ○	0.065	≤ 10
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	2.593	2 - 17
Hippuric acid	1.00	290	170	1.038	87 ●	0.507	≤ 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	0.08	22	5	0.077	74 ○	0.045	≤ 51
Citric acid	1.6	440	40	1.556	85 ●	0.899	≤ 700
Formic acid	0.16	45	10	0.158	64 ○	0.081	≤ 43
Fumaric acid	0.01	2	2	0.007	40 ○	0.006	≤ 3
Imidazole	< 0.17	< 48	48	0.047	0 ○	0.045	≤ 48
Lactic acid	< 0.17	< 49	49	0.067	35 ○	0.097	≤ 110
Proline betaine	< 0.09	< 25	25	0.027	0 ○	0.056	≤ 280
Succinic acid	0.04	10	5	0.036	83 ○	0.011	≤ 39
Tartaric acid	< 0.02	< 5	5	0.011	67 ○	0.005	≤ 110
Trigonelline	0.17	47	35	0.168	99 ●	0.011	≤ 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	< 0.17	< 48	48	0.043	44 ○	0.046	≤ 48

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

7 Keto acids and derivatives

Compound	Conc. mmol/L	Conc. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
2-Oxoglutaric acid	< 0.33	< 92	92	0.053	15 ○	0.129	≤ 92
3-Hydroxybutyric acid	< 0.36	< 100	100	0.000	0 ○	0.671	≤ 100
Acetoacetic acid	0.05	15	14	0.054	91 ●	0.039	≤ 30
Acetone	0.02	4	2	0.016	71 ○	0.012	≤ 7
Oxaloacetic acid	0.17	49	17	0.175	80 ○	0.115	≤ 66
Pyruvic acid	< 0.03	< 9	9	0.012	35 ○	0.011	≤ 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. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
1-Methyladenosine	< 0.02	< 5	5	0.000	0 ○	0.183	≤ 5
1-Methylnicotinamide	< 0.11	< 32	32	0.055	21 ○	0.049	≤ 32
Adenosine	< 1.4	< 390	390	0.000	0 ○	1.323	≤ 390
Allantoin	< 0.06	< 17	17	0.041	42 ○	0.036	≤ 47
Allopurinol	< 0.04	< 10	10	0.019	28 ○	0.022	≤ 11
Caffeine	< 0.16	< 45	45	0.077	34 ○	0.111	≤ 61
Inosine	< 0.07	< 19	19	0.014	60 ○	0.026	≤ 19

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

9 Sugars and derivatives

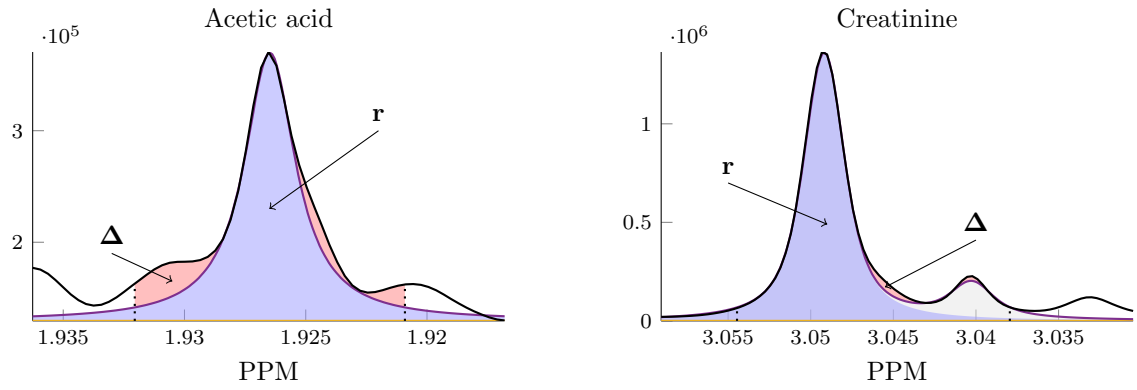
Compound	Conc. mmol/L	Conc. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
D-Galactose	< 0.15	< 43	43	0.000	0 ○	0.315	≤ 44
D-Glucose	< 0.12	< 34	34	0.109	80 ○	0.039	≤ 140
D-Lactose	< 0.34	< 96	96	0.079	62 ○	0.551	≤ 96
D-Mannitol	< 0.65	< 180	180	0.000	0 ○	2.783	≤ 180
D-Mannose	0.26	74	6	0.262	0 ○	0.239	≤ 8
Myo-Inositol	< 16	< 4400	4400	0.000	0 ○	2.512	≤ 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.

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