Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno590.100000.10r

Measuring Date: 24-Dec-2014 03:58:18
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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	9.0	0.3	8.957	100 ●	0.080	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	< 0.27	< 31	31	0.257	100 ●	0.010	≤ 54
Trimethylamine	< 0.02	< 2	2	0.005	51 ○	0.003	≤ 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	0.065	0 ○	0.101	≤ 15
2-Furoylglycine	< 0.34	< 39	39	0.000	0 ○	0.066	≤ 40
4-Aminobutyric acid	< 0.18	< 20	20	0.000	0 ○	0.677	≤ 20
Alanine	0.15	16	10	0.146	100 ●	0.011	11 - 72
Arginine	< 6.7	< 750	750	0.516	0 ○	5.261	≤ 750
Betaine	0.21	23	7	0.209	100 ●	0.015	9 - 78
Creatine	< 0.45	< 50	50	0.001	100 ●	0.080	≤ 280
Glycine	0.48	54	34	0.479	100 ●	0.020	38 - 440
Guanidinoacetic acid	< 0.93	< 100	100	0.393	91 ●	0.135	≤ 140
Methionine	< 0.16	< 18	18	0.000	0 ○	0.266	≤ 18
N,N-Dimethylglycine	< 0.05	< 5	5	0.045	68 ○	0.018	≤ 15
Sarcosine	< 0.02	< 2	2	0.012	0 ○	0.020	≤ 7
Taurine	< 1.3	< 140	140	0.398	68 ○	0.279	≤ 170
Valine	0.04	4	2	0.036	84 ○	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	< 0.09	< 10	10	0.000	0 ○	0.031	≤ 10
D-Mandelic acid	< 0.02	< 2	2	0.000	0 ○	0.076	2 - 17
Hippuric acid	3.1	350	170	3.090	99 ●	0.299	≤ 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	8	5	0.074	71 ○	0.041	≤ 51
Citric acid	2.9	330	40	2.932	100 ●	0.311	≤ 700
Formic acid	< 0.09	< 10	10	0.084	99 ●	0.012	≤ 43
Fumaric acid	< 0.02	< 2	2	0.008	98 ●	0.001	≤ 3
Imidazole	< 0.43	< 48	48	0.000	0 ○	0.136	≤ 48
Lactic acid	< 0.43	< 49	49	0.177	71 ○	0.104	≤ 110
Proline betaine	0.38	43	25	0.384	99 ●	0.072	≤ 280
Succinic acid	< 0.04	< 5	5	0.041	80 ○	0.015	≤ 39
Tartaric acid	0.22	24	5	0.218	100 ●	0.012	≤ 110
Trigonelline	< 0.31	< 35	35	0.134	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	< 0.43	< 48	48	0.067	53 ○	0.158	≤ 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	< 0.83	< 92	92	0.000	0 ○	0.359	≤ 92
3-Hydroxybutyric acid	< 0.92	< 100	100	0.000	0 ○	1.312	≤ 100
Acetoacetic acid	0.23	26	14	0.232	87 ●	0.113	≤ 30
Acetone	0.02	2	2	0.019	96 ●	0.005	≤ 7
Oxaloacetic acid	0.46	51	17	0.460	93 ●	0.208	≤ 66
Pyruvic acid	< 0.08	< 9	9	0.040	98 ●	0.005	≤ 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 ○	0.149	≤ 5
1-Methylnicotinamide	< 0.28	< 32	32	0.044	98 ●	0.005	≤ 32
Adenosine	< 3.5	< 390	390	0.000	0 ○	1.585	≤ 390
Allantoin	< 0.15	< 17	17	0.141	99 ●	0.013	≤ 47
Allopurinol	< 0.09	< 10	10	0.043	97 ●	0.046	≤ 11
Caffeine	< 0.41	< 45	45	0.164	85 ●	0.208	≤ 61
Inosine	< 0.17	< 19	19	0.017	95 ●	0.053	≤ 19

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

9 Sugars and derivatives

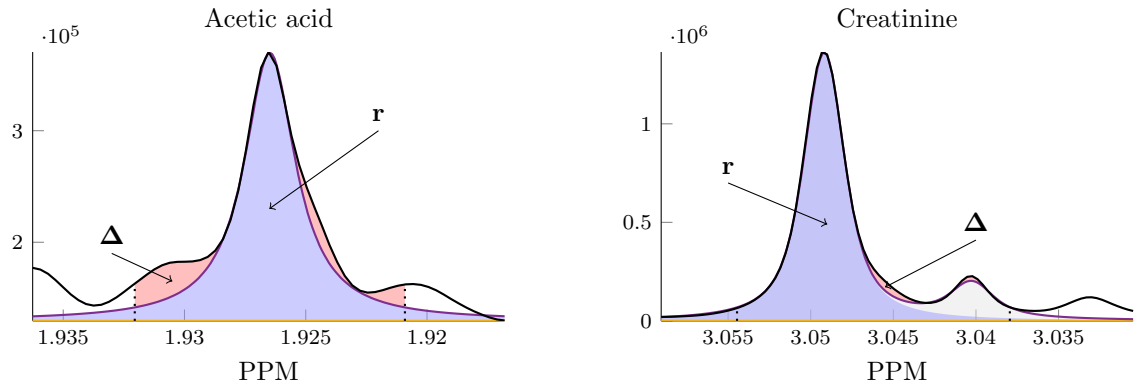
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.39	< 43	43	0.113	90 ●	0.008	≤ 44
D-Glucose	< 0.30	< 34	34	0.227	82 ○	0.079	≤ 140
D-Lactose	< 0.86	< 96	96	0.334	97 ●	0.063	≤ 96
D-Mannitol	< 1.6	< 180	180	0.000	0 ○	3.995	≤ 180
D-Mannose	< 0.05	< 6	6	0.000	0 ○	0.083	≤ 8
Myo-Inositol	< 40	< 4400	4400	0.000	0 ○	11.34	≤ 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.

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