Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno470.100000.10r

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Quantification Method Version:	Quant-UR B.1.1.0

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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.

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1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	ρ %	Δ mmol/L	95% Range(*) mmol/L
Creatinine	1.1	0.3	1.081	100 ●	0.029	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	0.04	34	31	0.037	100 ●	0.001	≤ 54
Trimethylamine	< 0.01	< 2	2	0.001	15 ○	0.001	≤ 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	< 0.02	< 15	15	0.000	0 ○	0.017	≤ 15
2-Furoylglycine	< 0.04	< 39	39	0.000	0 ○	0.025	≤ 40
4-Aminobutyric acid	< 0.02	< 20	20	0.000	0 ○	0.052	≤ 20
Alanine	0.03	25	10	0.027	99 ●	0.003	11 - 72
Arginine	< 0.81	< 750	750	0.122	12 ○	0.419	≤ 750
Betaine	0.04	41	7	0.045	100 ●	0.002	9 - 78
Creatine	< 0.05	< 50	50	0.004	100 ●	0.029	≤ 280
Glycine	0.14	130	34	0.138	100 ●	0.006	38 - 440
Guanidinoacetic acid	< 0.11	< 100	100	0.078	80 ○	0.039	≤ 140
Methionine	< 0.02	< 18	18	0.000	0 ○	0.050	≤ 18
N,N-Dimethylglycine	0.01	9	5	0.010	96 ●	0.002	≤ 15
Sarcosine	0.00	2	2	0.002	0 ○	0.004	≤ 7
Taurine	< 0.15	< 140	140	0.108	97 ●	0.023	≤ 170
Valine	0.01	5	2	0.005	89 ●	0.003	≤ 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	< 0.01	< 10	10	0.000	0 ○	0.053	≤ 10
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.024	2 - 17
Hippuric acid	0.44	400	170	0.437	99 ●	0.038	≤ 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	0.02	15	5	0.016	97 ●	0.003	≤ 51
Citric acid	0.46	420	40	0.459	100 ●	0.024	≤ 700
Formic acid	0.04	36	10	0.038	100 ●	0.001	≤ 43
Fumaric acid	< 0.01	< 2	2	0.001	49 ○	0.001	≤ 3
Imidazole	< 0.05	< 48	48	0.000	0 ○	0.025	≤ 48
Lactic acid	< 0.05	< 49	49	0.013	97 ●	0.022	≤ 110
Proline betaine	0.04	35	25	0.037	92 ●	0.021	≤ 280
Succinic acid	0.01	9	5	0.010	95 ●	0.002	≤ 39
Tartaric acid	< 0.01	< 5	5	0.004	99 ●	0.001	≤ 110
Trigonelline	0.04	41	35	0.044	100 ●	0.002	≤ 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	< 0.05	< 48	48	0.000	0 ○	0.041	≤ 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	< 0.10	< 92	92	0.000	0 ○	0.106	≤ 92
3-Hydroxybutyric acid	< 0.11	< 100	100	0.000	0 ○	0.139	≤ 100
Acetoacetic acid	< 0.01	< 14	14	0.010	75 ○	0.006	≤ 30
Acetone	0.01	6	2	0.007	99 ●	0.001	≤ 7
Oxaloacetic acid	0.02	18	17	0.019	84 ○	0.015	≤ 66
Pyruvic acid	< 0.01	< 9	9	0.003	95 ●	0.001	≤ 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	< 0.01	< 5	5	0.000	0 ○	0.033	≤ 5
1-Methylnicotinamide	< 0.03	< 32	32	0.013	82 ○	0.006	≤ 32
Adenosine	< 0.42	< 390	390	0.000	0 ○	0.215	≤ 390
Allantoin	< 0.02	< 17	17	0.013	98 ●	0.002	≤ 47
Allopurinol	< 0.01	< 10	10	0.004	93 ●	0.008	≤ 11
Caffeine	< 0.05	< 45	45	0.027	93 ●	0.021	≤ 61
Inosine	< 0.02	< 19	19	0.004	95 ●	0.009	≤ 19

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

9 Sugars and derivatives

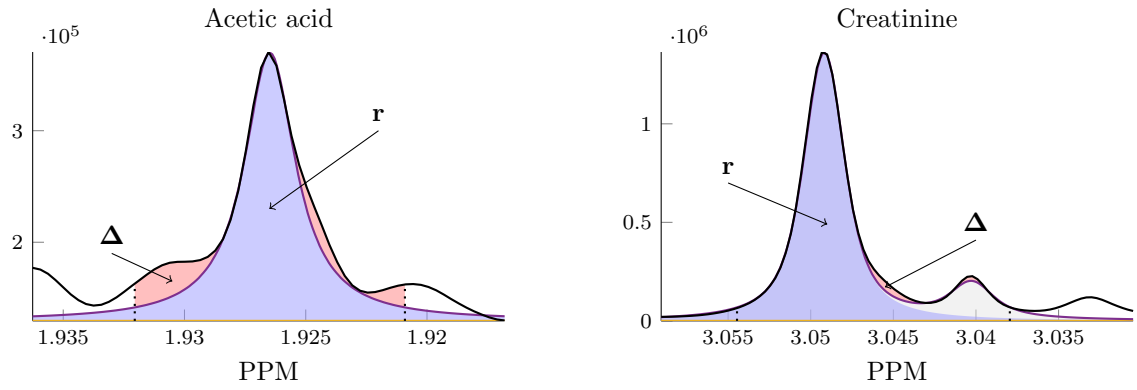
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.05	< 43	43	0.000	0 ○	0.021	≤ 44
D-Glucose	< 0.04	< 34	34	0.026	50 ○	0.030	≤ 140
D-Lactose	< 0.10	< 96	96	0.008	0 ○	0.051	≤ 96
D-Mannitol	< 0.20	< 180	180	0.000	0 ○	0.574	≤ 180
D-Mannose	< 0.01	< 6	6	0.000	0 ○	0.017	≤ 8
Myo-Inositol	< 4.8	< 4400	4400	0.000	0 ○	0.591	≤ 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.

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