Analysis Report

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

Sample ID:	U8_A_expno10.100000.10r
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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	12	0.3	12.08	100 ●	0.334	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	< 0.37	< 31	31	0.242	100 ●	0.008	≤ 54
Trimethylamine	< 0.02	< 2	2	0.001	0 ○	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	< 0.18	< 15	15	0.000	0 ○	0.237	≤ 15
2-Furoylglycine	< 0.47	< 39	39	0.000	0 ○	0.039	≤ 40
4-Aminobutyric acid	< 0.24	< 20	20	0.000	0 ○	0.614	≤ 20
Alanine	0.14	12	10	0.141	99 ●	0.015	11 - 72
Arginine	< 9.0	< 750	750	0.559	0 ○	2.035	≤ 750
Betaine	0.14	12	7	0.139	100 ●	0.026	9 - 78
Creatine	< 0.60	< 50	50	0.120	100 ●	0.334	≤ 280
Glycine	0.55	45	34	0.549	100 ●	0.032	38 - 440
Guanidinoacetic acid	< 1.2	< 100	100	0.281	96 ●	0.064	≤ 140
Methionine	< 0.22	< 18	18	0.000	0 ○	0.367	≤ 18
N,N-Dimethylglycine	< 0.06	< 5	5	0.059	88 ●	0.027	≤ 15
Sarcosine	< 0.02	< 2	2	0.007	0 ○	0.010	≤ 7
Taurine	< 1.7	< 140	140	0.840	95 ●	0.284	≤ 170
Valine	0.04	3	2	0.042	65 ○	0.031	≤ 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	< 0.12	< 10	10	0.000	0 ○	0.042	≤ 10
D-Mandelic acid	< 0.03	< 2	2	0.000	0 ○	0.003	2 - 17
Hippuric acid	< 2.1	< 170	170	1.596	100 ●	0.121	≤ 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	0.042	65 ○	0.026	≤ 51
Citric acid	2.4	200	40	2.414	100 ●	0.248	≤ 700
Formic acid	< 0.11	< 10	10	0.104	99 ●	0.011	≤ 43
Fumaric acid	< 0.02	< 2	2	0.003	82 ○	0.001	≤ 3
Imidazole	< 0.58	< 48	48	0.000	0 ○	0.201	≤ 48
Lactic acid	< 0.59	< 49	49	0.093	76 ○	0.097	≤ 110
Proline betaine	0.57	47	25	0.573	100 ●	0.057	≤ 280
Succinic acid	< 0.06	< 5	5	0.045	93 ●	0.011	≤ 39
Tartaric acid	< 0.06	< 5	5	0.055	98 ●	0.008	≤ 110
Trigonelline	< 0.42	< 35	35	0.042	99 ●	0.003	≤ 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	< 0.58	< 48	48	0.000	0 ○	0.288	≤ 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	< 1.1	< 92	92	0.000	41 ○	0.555	≤ 92
3-Hydroxybutyric acid	< 1.2	< 100	100	0.063	1 ○	0.544	≤ 100
Acetoacetic acid	< 0.17	< 14	14	0.117	92 ●	0.055	≤ 30
Acetone	< 0.02	< 2	2	0.019	99 ●	0.003	≤ 7
Oxaloacetic acid	0.27	22	17	0.266	96 ●	0.091	≤ 66
Pyruvic acid	< 0.11	< 9	9	0.060	100 ●	0.004	≤ 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	< 0.06	< 5	5	0.000	0 ○	0.107	≤ 5
1-Methylnicotinamide	< 0.38	< 32	32	0.107	100 ●	0.005	≤ 32
Adenosine	< 4.7	< 390	390	0.000	0 ○	1.554	≤ 390
Allantoin	< 0.20	< 17	17	0.019	72 ○	0.010	≤ 47
Allopurinol	< 0.12	< 10	10	0.082	69 ○	0.071	≤ 11
Caffeine	< 0.55	< 45	45	0.169	98 ●	0.127	≤ 61
Inosine	< 0.23	< 19	19	0.013	94 ●	0.073	≤ 19

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

9 Sugars and derivatives

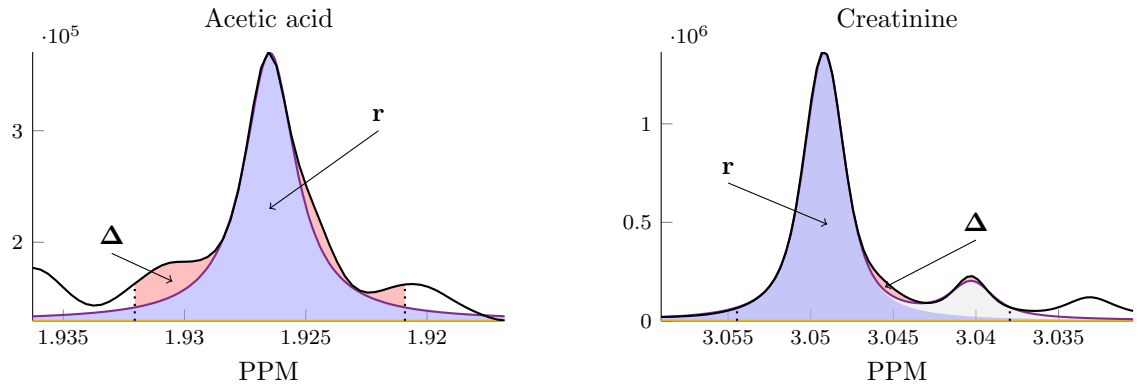
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.52	< 43	43	0.000	0 ○	0.019	≤ 44
D-Glucose	< 0.41	< 34	34	0.236	89 ●	0.067	≤ 140
D-Lactose	< 1.2	< 96	96	0.025	51 ○	0.042	≤ 96
D-Mannitol	< 2.2	< 180	180	0.000	0 ○	2.431	≤ 180
D-Mannose	< 0.07	< 6	6	0.000	0 ○	0.047	≤ 8
Myo-Inositol	< 54	< 4400	4400	0.000	0 ○	7.938	≤ 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.

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