Analysis Report

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

Sample ID: ALZ_Urine_Rack04_RCM_191214_expno310.100000.10r

Measuring Date: 19-Dec-2014 23:30:56
Reporting Date: 14-Dec-2020 16:59:29, 7 page(s), Version 1.1.0
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.

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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	5.9	0.3	5.866	100 ●	0.062	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	< 0.18	< 31	31	0.176	100 ●	0.003	≤ 54
Trimethylamine	< 0.01	< 2	2	0.003	23 ○	0.002	≤ 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	< 0.09	< 15	15	0.000	0 ○	0.044	≤ 15
2-Furoylglycine	< 0.23	< 39	39	0.134	99 ●	0.009	≤ 40
4-Aminobutyric acid	< 0.12	< 20	20	0.000	0 ○	0.238	≤ 20
Alanine	0.16	27	10	0.160	100 ●	0.011	11 - 72
Arginine	< 4.4	< 750	750	0.463	2 ○	0.750	≤ 750
Betaine	0.11	19	7	0.110	100 ●	0.023	9 - 78
Creatine	< 0.29	< 50	50	0.142	100 ●	0.062	≤ 280
Glycine	0.74	130	34	0.741	100 ●	0.019	38 - 440
Guanidinoacetic acid	< 0.61	< 100	100	0.345	88 ●	0.137	≤ 140
Methionine	< 0.11	< 18	18	0.000	0 ○	0.463	≤ 18
N,N-Dimethylglycine	0.04	6	5	0.036	75 ○	0.017	≤ 15
Sarcosine	< 0.01	< 2	2	0.000	0 ○	0.004	≤ 7
Taurine	< 0.84	< 140	140	0.406	95 ●	0.156	≤ 170
Valine	0.02	4	2	0.024	69 ○	0.013	≤ 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	< 0.06	< 10	10	0.000	0 ○	0.031	≤ 10
D-Mandelic acid	< 0.01	< 2	2	0.000	0 ○	0.080	2 - 17
Hippuric acid	1.2	200	170	1.186	99 ●	0.124	≤ 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	13	5	0.076	98 ●	0.010	≤ 51
Citric acid	1.9	320	40	1.850	100 ●	0.118	≤ 700
Formic acid	0.11	19	10	0.113	100 ●	0.005	≤ 43
Fumaric acid	< 0.01	< 2	2	0.003	73 ○	0.001	≤ 3
Imidazole	< 0.28	< 48	48	0.030	43 ○	0.035	≤ 48
Lactic acid	< 0.28	< 49	49	0.135	99 ●	0.052	≤ 110
Proline betaine	0.28	47	25	0.277	99 ●	0.024	≤ 280
Succinic acid	0.11	19	5	0.111	96 ●	0.019	≤ 39
Tartaric acid	0.06	10	5	0.060	98 ●	0.012	≤ 110
Trigonelline	< 0.20	< 35	35	0.137	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	< 0.28	< 48	48	0.000	0 ○	0.208	≤ 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	< 0.54	< 92	92	0.081	64 ○	0.172	≤ 92
3-Hydroxybutyric acid	< 0.60	< 100	100	0.000	0 ○	0.555	≤ 100
Acetoacetic acid	< 0.08	< 14	14	0.074	87 ●	0.038	≤ 30
Acetone	0.02	4	2	0.022	100 ●	0.002	≤ 7
Oxaloacetic acid	< 0.10	< 17	17	0.084	73 ○	0.088	≤ 66
Pyruvic acid	< 0.05	< 9	9	0.035	95 ●	0.007	≤ 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	< 0.03	< 5	5	0.000	0 ○	0.122	≤ 5
1-Methylnicotinamide	< 0.19	< 32	32	0.057	98 ●	0.012	≤ 32
Adenosine	< 2.3	< 390	390	0.000	0 ○	1.016	≤ 390
Allantoin	< 0.10	< 17	17	0.066	100 ●	0.003	≤ 47
Allopurinol	< 0.06	< 10	10	0.035	97 ●	0.050	≤ 11
Caffeine	< 0.27	< 45	45	0.117	90 ●	0.120	≤ 61
Inosine	< 0.11	< 19	19	0.012	95 ●	0.053	≤ 19

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

9 Sugars and derivatives

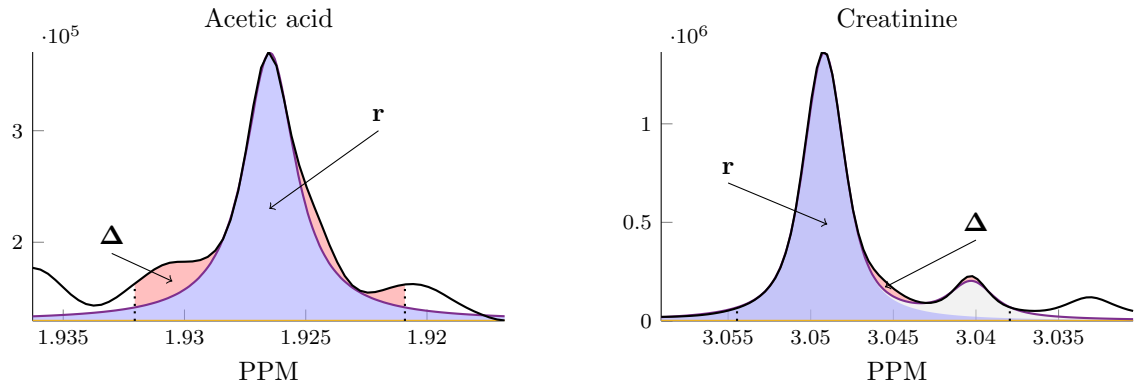
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.25	< 43	43	0.040	96 ●	0.002	≤ 44
D-Glucose	0.21	36	34	0.211	88 ●	0.048	≤ 140
D-Lactose	< 0.56	< 96	96	0.166	88 ●	0.074	≤ 96
D-Mannitol	< 1.1	< 180	180	0.000	0 ○	2.040	≤ 180
D-Mannose	< 0.04	< 6	6	0.000	0 ○	0.060	≤ 8
Myo-Inositol	< 26	< 4400	4400	0.000	0 ○	5.508	≤ 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.

$$\rho = \max\bigl(0, \operatorname{corr}\bigl(\overline{s}, \overline{f+b}\bigr)\bigr)\,,$$

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.

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