Analysis Report

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

Sample ID: ALZ_Urine_Rack01_RCM_221214_expno730.100000.10r

Measuring Date: 24-Dec-2014 07:01:27
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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	8.7	0.3	8.692	100	0.161	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	0.30	34	31	0.297	100	0.005	$\leq$ 54
Trimethylamine	$<$ 0.02	$<$ 2	2	0.005	96	0.001	$\leq$ 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	$<$ 0.13	$<$ 15	15	0.000	0	0.176	$\leq$ 15
2-Furoylglycine	$<$ 0.33	$<$ 39	39	0.112	54	0.037	$\leq$ 40
4-Aminobutyric acid	$<$ 0.17	$<$ 20	20	0.095	18	0.197	$\leq$ 20
Alanine	0.27	31	10	0.272	100	0.020	11 - 72
Arginine	$<$ 6.5	$<$ 750	750	0.713	0	3.226	$\leq$ 750
Betaine	0.20	24	7	0.205	100	0.033	9 - 78
Creatine	$<$ 0.43	$<$ 50	50	0.214	100	0.161	$\leq$ 280
Glycine	0.95	110	34	0.953	100	0.028	38 - 440
Guanidinoacetic acid	$<$ 0.90	$<$ 100	100	0.394	75	0.155	$\leq$ 140
Methionine	$<$ 0.16	$<$ 18	18	0.000	0	0.433	$\leq$ 18
N,N-Dimethylglycine	$<$ 0.04	$<$ 5	5	0.043	97	0.005	$\leq$ 15
Sarcosine	$<$ 0.02	$<$ 2	2	0.000	0	0.004	$\leq$ 7
Taurine	$<$ 1.2	$<$ 140	140	0.738	90	0.262	$\leq$ 170
Valine	0.03	3	2	0.028	95	0.009	$\leq$ 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	< 0.08	< 10	10	0.034	88 ●	0.014	≤ 10
D-Mandelic acid	< 0.02	< 2	2	0.000	0 ○	0.129	2 - 17
Hippuric acid	3.5	400	170	3.465	99 ●	0.334	≤ 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	0.21	24	5	0.209	99 ●	0.016	≤ 51
Citric acid	2.4	270	40	2.368	100 ●	0.224	≤ 700
Formic acid	0.29	34	10	0.294	100 ●	0.004	≤ 43
Fumaric acid	< 0.02	< 2	2	0.008	98 ●	0.001	≤ 3
Imidazole	< 0.42	< 48	48	0.000	0 ○	0.206	≤ 48
Lactic acid	< 0.42	< 49	49	0.200	99 ●	0.048	≤ 110
Proline betaine	0.28	32	25	0.280	98 ●	0.067	≤ 280
Succinic acid	0.12	14	5	0.124	99 ●	0.013	≤ 39
Tartaric acid	0.12	14	5	0.118	100 ●	0.012	≤ 110
Trigonelline	0.34	39	35	0.335	100 ●	0.008	≤ 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	< 0.41	< 48	48	0.042	50 ○	0.127	≤ 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	< 0.80	< 92	92	0.000	0 ○	0.585	≤ 92
3-Hydroxybutyric acid	< 0.90	< 100	100	0.086	24 ○	0.358	≤ 100
Acetoacetic acid	< 0.12	< 14	14	0.116	94 ●	0.060	≤ 30
Acetone	0.03	3	2	0.026	100 ●	0.004	≤ 7
Oxaloacetic acid	0.22	25	17	0.218	90 ●	0.120	≤ 66
Pyruvic acid	< 0.08	< 9	9	0.035	96 ●	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	< 0.04	< 5	5	0.000	0 ○	0.152	≤ 5
1-Methylnicotinamide	< 0.27	< 32	32	0.061	98 ●	0.009	≤ 32
Adenosine	< 3.4	< 390	390	0.000	0 ○	1.695	≤ 390
Allantoin	< 0.14	< 17	17	0.103	97 ●	0.013	≤ 47
Allopurinol	< 0.09	< 10	10	0.051	82 ○	0.048	≤ 11
Caffeine	< 0.39	< 45	45	0.186	93 ●	0.201	≤ 61
Inosine	< 0.16	< 19	19	0.031	97 ●	0.047	≤ 19

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

9 Sugars and derivatives

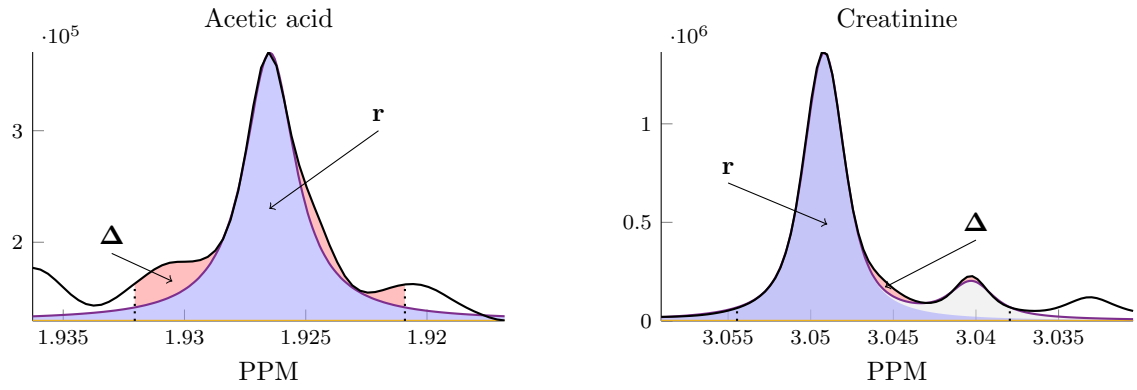
Compound	Conc. mmol/L	Conc. $\frac{\text{mmol}}{\text{mol Crea}}$	LOD $\frac{\text{mmol}}{\text{mol Crea}}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{\text{mmol}}{\text{mol Crea}}$
D-Galactose	< 0.38	< 43	43	0.024	95 ●	0.002	≤ 44
D-Glucose	0.77	89	34	0.771	94 ●	0.128	≤ 140
D-Lactose	< 0.83	< 96	96	0.199	84 ○	0.095	≤ 96
D-Mannitol	< 1.6	< 180	180	0.000	0 ○	3.923	≤ 180
D-Mannose	< 0.05	< 6	6	0.040	1 ○	0.038	≤ 8
Myo-Inositol	< 39	< 4400	4400	0.000	0 ○	10.20	≤ 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.

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