

● Analysis Report

Bruker IVDr Quantification in URine B.I.Quant-UR bTM

Sample ID: ALZ_Urine_Rack03_RCM_06012015_expno320.100000.10

Measuring Date: 14-Jan-2015 17:43:58

Reporting Date: 14-Dec-2020 15:11:38, 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.

Contents



1	Creatinine	3
2	Amines and derivatives	3
3	Amino acids and derivatives	3
4	Benzene and substituted derivatives	4
5	Carboxylic acids	4
6	Fatty acids and derivatives	4
7	Keto acids and derivatives	5
8	Purine, Pyridine and Pyrimidine derivatives	5
9	Sugars and derivatives	5
10	Explanations	6

1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	ρ %	Δ mmol/L	95% Range ^(*) mmol/L
Creatinine	8.6	0.3	8.594	100 ●	0.258	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	0.31	37	31	0.315	100 ●	0.006	≤ 54 
Trimethylamine	< 0.02	< 2	2	0.010	5 ○	0.018	≤ 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	0.078	31 ○	0.213	≤ 15 
2-Furoylglycine	< 0.33	< 39	39	0.107	47 ○	0.039	≤ 40 
4-Aminobutyric acid	< 0.17	< 20	20	0.000	0 ○	0.456	≤ 20 
Alanine	0.28	33	10	0.280	100 ●	0.019	11 - 72 
Arginine	< 6.4	< 750	750	0.703	0 ○	2.680	≤ 750 
Betaine	0.20	23	7	0.197	100 ●	0.024	9 - 78 
Creatine	0.50	58	50	0.496	100 ●	0.258	≤ 280 
Glycine	1.00	120	34	1.033	100 ●	0.035	38 - 440 
Guanidinoacetic acid	< 0.89	< 100	100	0.419	61 ○	0.219	≤ 140 
Methionine	< 0.15	< 18	18	0.000	0 ○	0.430	≤ 18 
N,N-Dimethylglycine	0.05	5	5	0.046	88 ●	0.014	≤ 15 
Sarcosine	< 0.02	< 2	2	0.000	0 ○	0.006	≤ 7 
Taurine	< 1.2	< 140	140	0.763	88 ●	0.267	≤ 170 
Valine	0.04	4	2	0.035	87 ●	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	0.088	100 ●	0.005	≤ 10 
D-Mandelic acid	< 0.02	< 2	2	0.000	0 ○	0.126	2 - 17 
Hippuric acid	3.6	420	170	3.649	99 ●	0.290	≤ 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	0.25	29	5	0.251	100 ●	0.020	≤ 51 
Citric acid	2.4	280	40	2.421	100 ●	0.247	≤ 700 
Formic acid	0.34	39	10	0.337	100 ●	0.013	≤ 43 
Fumaric acid	< 0.02	< 2	2	0.007	99 ●	0.001	≤ 3 
Imidazole	< 0.41	< 48	48	0.000	0 ○	0.174	≤ 48 
Lactic acid	< 0.42	< 49	49	0.198	97 ●	0.065	≤ 110 
Proline betaine	0.32	38	25	0.325	99 ●	0.040	≤ 280 
Succinic acid	0.16	18	5	0.159	99 ●	0.017	≤ 39 
Tartaric acid	0.13	15	5	0.128	99 ●	0.015	≤ 110 
Trigonelline	0.35	41	35	0.352	100 ●	0.006	≤ 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	0.047	5 ○	0.129	≤ 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	< 0.79	< 92	92	0.015	0 ○	0.169	≤ 92 
3-Hydroxybutyric acid	< 0.89	< 100	100	0.091	24 ○	0.369	≤ 100 
Acetoacetic acid	< 0.12	< 14	14	0.111	94 ●	0.053	≤ 30 
Acetone	0.03	3	2	0.027	99 ●	0.004	≤ 7 
Oxaloacetic acid	0.24	28	17	0.242	90 ●	0.127	≤ 66 
Pyruvic acid	< 0.08	< 9	9	0.036	95 ●	0.008	≤ 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 ○	0.146	≤ 5 
1-Methylnicotinamide	< 0.27	< 32	32	0.065	98 ●	0.008	≤ 32 
Adenosine	< 3.3	< 390	390	0.000	0 ○	1.744	≤ 390 
Allantoin	< 0.14	< 17	17	0.130	97 ●	0.017	≤ 47 
Allopurinol	< 0.09	< 10	10	0.049	74 ○	0.048	≤ 11 
Caffeine	< 0.39	< 45	45	0.194	91 ●	0.224	≤ 61 
Inosine	< 0.16	< 19	19	0.035	78 ○	0.054	≤ 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	< 0.37	< 43	43	0.026	95 ●	0.004	≤ 44 
D-Glucose	0.85	99	34	0.852	93 ●	0.148	≤ 140 
D-Lactose	< 0.82	< 96	96	0.038	75 ○	0.061	≤ 96 
D-Mannitol	< 1.6	< 180	180	0.000	0 ○	4.062	≤ 180 
D-Mannose	< 0.05	< 6	6	0.039	2 ○	0.041	≤ 8 
Myo-Inositol	< 38	< 4400	4400	0.000	0 ○	10.64	≤ 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 r , ρ and Δ .

10.1 How to read the result



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 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

- Conc.** is the final result concentration of the metabolite,
- LOD** is the *limit of detection* of the given metabolite,
- 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),
- 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) r (*raw concentration*) is defined as

$$r = \frac{1}{P_N} \int_{\mathbb{R}} f(\xi) d\xi.$$

β) ρ is the *correlation* of the functions s and $f + b$, i.e.

$$\rho = \max(0, \text{corr}(\bar{s}, \overline{f+b})),$$

where \bar{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.

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