Analysis Report

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

Sample ID:	U8_A_expno10.100000.11r
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Quantification Method Version:	Quant-UR E.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 E 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 E.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 Alcohols and derivatives

Compound	Conc. mmol/L	Conc. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
Ethanol	< 0.85	< 70	70	0.000	0 ○	0.802	≤ 98
Isopropanol	< 0.04	< 3	3	0.000	0 ○	0.117	≤ 3
Methanol	< 0.58	< 48	48	0.468	99 ●	0.038	≤ 230
Propylene glycol	< 0.47	< 39	39	0.015	61 ○	0.020	≤ 50

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

3 Amines and derivatives

Compound	Conc. mmol/L	Conc. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
1-Methylguanidine	< 0.78	< 64	64	0.267	83 ○	0.227	≤ 72
Dimethylamine	< 0.37	< 31	31	0.242	100 ●	0.008	≤ 54
Trimethylamine	< 0.02	< 2	2	0.001	0 ○	0.003	≤ 3
Tyramine	< 0.96	< 80	80	0.000	0 ○	0.669	≤ 80

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

4 Amino acids and derivatives

Compound	Conc. mmol/L	Conc. mmol / mol Crea	LOD mmol / mol Crea	r mmol/L	ρ %	Δ mmol/L	95% Range(*) mmol / 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
3-Aminoisobutyric acid	< 1.00	< 85	85	0.000	0 ○	1.035	≤ 85
3-Methylcrotonylglycine	< 0.10	< 8	8	0.000	0 ○	0.010	≤ 8
4-Aminobutyric acid	< 0.24	< 20	20	0.000	0 ○	0.614	≤ 20
5-Aminopentanoic acid	< 1.1	< 94	94	0.000	0 ○	1.200	≤ 94
Alanine	0.14	12	10	0.141	99 ●	0.015	11 - 72
Arginine	< 9.0	< 750	750	0.559	0 ○	2.035	≤ 750
Argininosuccinic acid	< 0.34	< 29	29	0.000	0 ○	0.472	≤ 29
Betaine	0.14	12	7	0.139	100 ●	0.026	9 - 78
Citrulline	< 8.3	< 690	690	0.140	5 ○	0.969	≤ 690
Creatine	< 0.60	< 50	50	0.120	100 ●	0.334	≤ 280
Cystine	< 5.9	< 490	490	0.000	0 ○	5.784	≤ 490
DL-Alloisoleucine	< 0.58	< 48	48	0.000	0 ○	0.216	≤ 48
DL-Tyrosine	< 0.53	< 44	44	0.000	0 ○	0.187	≤ 44
Glutamic acid	< 5.5	< 460	460	0.000	0 ○	2.567	≤ 460
Glutamine	< 5.3	< 440	440	0.000	0 ○	7.771	≤ 440
Glycine	0.55	45	34	0.549	100 ●	0.032	38 - 440
Guanidinoacetic acid	< 1.2	< 100	100	0.281	96 ●	0.064	≤ 140
Isobutyrylglycine	< 0.08	< 7	7	0.000	0 ○	0.130	≤ 7
L-Carnosine	< 1.6	< 130	130	0.000	0 ○	0.285	≤ 130
L-Homocystine	< 11	< 910	910	0.000	0 ○	0.218	≤ 910
L-Isoleucine	< 0.19	< 16	16	0.000	0 ○	0.063	≤ 16
L-Pyroglutamic acid	< 0.39	< 32	32	0.000	0 ○	1.553	≤ 67
L-Tryptophan	< 1.2	< 97	97	0.046	17 ○	0.041	≤ 97
Leucine	< 0.26	< 22	22	0.052	64 ○	0.027	≤ 22
Methionine	< 0.22	< 18	18	0.000	0 ○	0.367	≤ 18
N,N-Dimethylglycine	< 0.06	< 5	5	0.059	88 ●	0.027	≤ 15
N-Acetylaspartic acid	< 1.2	< 99	99	0.064	38 ○	0.168	≤ 99
N-Acetylglutamate	< 0.51	< 42	42	0.000	0 ○	0.305	≤ 42
N-Acetylphenylalanine	< 1.6	< 130	130	0.000	0 ○	0.615	≤ 130
N-Acetyltyrosine	< 4.6	< 380	380	0.000	0 ○	1.227	≤ 380
N-Isovaleroylglycine	< 0.02	< 2	2	0.000	0 ○	0.072	≤ 5
Phenylalanine	< 2.4	< 200	200	0.091	0 ○	0.474	≤ 200
Proline betaine	0.57	47	25	0.573	100 ●	0.057	≤ 280
Propionylglycine	< 0.15	< 12	12	0.000	0 ○	0.303	≤ 12
Sarcosine	< 0.02	< 2	2	0.007	0 ○	0.010	≤ 7
Taurine	< 1.7	< 140	140	0.840	95 ●	0.284	≤ 170
Tiglylglycine	< 0.23	< 19	19	0.000	0 ○	0.077	≤ 19
Valine	0.04	3	2	0.042	65 ○	0.031	≤ 7

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

5 Benzene and substituted derivatives

Compound	Conc. mmol/L	Conc. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
2-Hydroxyphenylacetic acid	< 0.12	< 10	10	0.000	0 ○	0.296	≤ 10
3-Phenyllactic acid	< 1.1	< 89	89	0.070	16 ○	0.493	≤ 89
4-Aminohippuric acid	< 3.3	< 270	270	0.000	0 ○	0.271	≤ 270
4-Ethylphenol	< 0.15	< 13	13	0.000	0 ○	0.283	≤ 13
4-Hydroxyhippuric acid	< 0.32	< 26	26	0.000	0 ○	0.282	≤ 30
4-Hydroxyphenylacetic acid	< 0.22	< 18	18	0.051	96 ●	0.030	≤ 28
4-Hydroxyphenyllactic acid	< 0.52	< 43	43	0.000	0 ○	0.968	≤ 43
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
Phenylacetic acid	< 0.87	< 72	72	0.100	91 ●	0.096	≤ 72
Phenylpyruvic acid	< 1.2	< 98	98	0.042	0 ○	0.109	≤ 98
Pyrocatechol	< 2.1	< 170	170	0.000	0 ○	0.300	≤ 170
Syringic acid	< 0.46	< 38	38	0.097	98 ●	0.069	≤ 38

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

6 Carboxylic acids

Compound	Conc. mmol/L	Conc. $\frac{mmol}{mol\ Crea}$	LOD $\frac{mmol}{mol\ Crea}$	r mmol/L	ρ %	Δ mmol/L	95% Range(*) $\frac{mmol}{mol\ Crea}$
5-Aminolevulinic acid	< 0.02	< 2	2	0.000	0 ○	0.112	≤ 2
Acetic acid	< 0.06	< 5	5	0.042	65 ○	0.026	≤ 51
Citric acid	2.4	200	40	2.414	100 ●	0.248	≤ 700
E-Glutaconic acid	< 0.46	< 38	38	0.000	0 ○	0.062	≤ 38
Ethylmalonic acid	< 0.42	< 35	35	0.033	2 ○	0.080	≤ 35
Formic acid	< 0.11	< 10	10	0.104	99 ●	0.011	≤ 43
Fumaric acid	< 0.02	< 2	2	0.003	82 ○	0.001	≤ 3
Glutaric acid	< 2.1	< 170	170	0.022	0 ○	0.183	≤ 170
Imidazole	< 0.58	< 48	48	0.000	0 ○	0.201	≤ 48
Lactic acid	< 0.59	< 49	49	0.093	76 ○	0.097	≤ 110
Maleic acid	< 0.05	< 4	4	0.004	72 ○	0.003	≤ 8
Methylmalonic acid	< 0.20	< 17	17	0.000	0 ○	0.169	≤ 31
Propionic acid	< 0.62	< 51	51	0.069	58 ○	0.091	≤ 51
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
Xanthurenic acid	< 0.22	< 18	18	0.037	63 ○	0.021	≤ 18

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

7 Cosmetics, vitamines, drugs and drug metabolites

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(*) $\frac{\text{mmol}}{\text{mol Crea}}$
Choline	< 0.55	< 46	46	0.000	0 ○	0.231	≤ 46
D-Panthenol	< 0.20	< 17	17	0.000	0 ○	0.396	≤ 17
L-Ascorbic acid	< 1.9	< 160	160	0.000	0 ○	0.335	≤ 160
Pantothenic acid	< 0.19	< 16	16	0.056	72 ○	0.103	≤ 19
Paracetamol	< 0.60	< 50	50	0.000	0 ○	0.187	≤ 50
Paracetamol-glucuronide	< 0.28	< 24	24	0.000	0 ○	0.639	≤ 53

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

8 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-Hydroxy-4-methylvaleric acid	< 0.09	< 7	7	0.000	0 ○	0.055	≤ 7
2-Hydroxyisovaleric acid	< 0.05	< 4	4	0.011	49 ○	0.011	≤ 4
2-Methylsuccinic acid	< 0.58	< 48	48	0.000	0 ○	0.288	≤ 48
3-Hydroxy-3-methylglutaric acid	< 0.23	< 19	19	0.000	0 ○	1.186	≤ 19
3-Hydroxyisovaleric acid	< 0.43	< 36	36	0.081	100 ●	0.006	≤ 36
3-Hydroxyvaleric acid	< 0.03	< 2	2	0.000	0 ○	0.200	≤ 2
3-Methylglutaconic acid	< 0.19	< 16	16	0.041	89 ●	0.028	≤ 16
Butyric acid	< 0.19	< 15	15	0.071	16 ○	0.251	≤ 15
Citraconic acid	< 0.44	< 37	37	0.000	0 ○	0.479	≤ 37
L-Citramalic acid	< 1.2	< 100	100	0.109	68 ○	1.220	≤ 100
Pimelic acid	< 0.38	< 31	31	0.000	0 ○	0.432	≤ 31
Thymol	< 0.53	< 44	44	0.094	86 ●	0.196	≤ 44

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

9 Hydroxy 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(*) $\frac{\text{mmol}}{\text{mol Crea}}$
3-Hydroxyglutaric acid	< 0.59	< 49	49	0.026	0 ○	0.524	≤ 49
3-Hydroxypropionic acid	< 0.42	< 35	35	0.165	80 ○	0.323	≤ 35
D-Galactonic acid	< 0.69	< 57	57	0.000	0 ○	0.259	≤ 57
D-Gluconic acid	< 1.2	< 99	99	0.000	0 ○	1.076	≤ 99
Glycolic acid	< 2.2	< 180	180	0.425	100 ●	0.053	≤ 180
Malic acid	< 1.2	< 97	97	0.000	0 ○	4.359	≤ 97

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

10 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-Ketobutyric acid	< 0.82	< 68	68	0.000	0 ○	0.390	≤ 68
2-Oxoglutaric acid	< 1.1	< 92	92	0.000	41 ○	0.555	≤ 92
2-Oxoisocaproic acid	< 0.06	< 5	5	0.017	45 ○	0.022	≤ 5
2-Oxoisovaleric acid	< 0.11	< 9	9	0.000	0 ○	0.063	≤ 9
3-Hydroxybutyric acid	< 1.2	< 100	100	0.063	1 ○	0.544	≤ 100
3-Methyl-2-oxovaleric acid	< 0.36	< 29	29	0.028	0 ○	0.135	≤ 29
4-Hydroxyphenylpyruvic acid	< 0.60	< 50	50	0.000	0 ○	0.211	≤ 50
Acetoacetic acid	< 0.17	< 14	14	0.117	92 ●	0.055	≤ 30
Acetoine	< 0.17	< 14	14	0.000	0 ○	0.182	≤ 14
Acetone	< 0.02	< 2	2	0.019	99 ●	0.003	≤ 7
DL-Kynurenin	< 9.5	< 790	790	0.000	0 ○	0.532	≤ 790
Oxaloacetic acid	0.27	22	17	0.266	96 ●	0.091	≤ 66
Pyruvic acid	< 0.11	< 9	9	0.060	100 ●	0.004	≤ 13
Succinylacetone	< 1.6	< 130	130	0.000	0 ○	0.577	≤ 130

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

11 Purine, Pyridine and Pyrimidine derivatives

Compound	Conc. mmol/L	Conc. mmol / mol Crea	LOD mmol / mol Crea	r mmol/L	ρ %	Δ mmol/L	95% Range(*) mmol / mol Crea
1,3-Dimethyluric acid	< 0.20	< 17	17	0.009	87	0.004	≤ 49
1-Methyladenosine	< 0.06	< 5	5	0.000	0	0.107	≤ 5
1-Methylhydantoin	< 0.51	< 42	42	0.074	96	0.017	≤ 47
1-Methylnicotinamide	< 0.38	< 32	32	0.107	100	0.005	≤ 32
4-Pyridoxic acid	< 0.13	< 11	11	0.020	38	0.024	≤ 30
Adenine	< 0.12	< 10	10	0.030	0	0.097	≤ 10
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
Cytosine	< 0.06	< 5	5	0.000	0	0.540	≤ 12
Dihydrothymine	< 1.1	< 94	94	0.337	90	0.190	≤ 110
Dihydrouracil	< 8.6	< 710	710	0.000	0	2.711	≤ 710
Inosine	< 0.23	< 19	19	0.013	94	0.073	≤ 19
Neopterin	< 0.28	< 23	23	0.005	67	0.005	≤ 30
Orotic acid	< 0.06	< 5	5	0.004	97	0.001	≤ 5
Oxypurinol	< 0.24	< 20	20	0.135	99	0.021	≤ 36
Quinolinic acid	< 0.82	< 68	68	0.000	0	0.898	≤ 68
Theobromine	< 1.4	< 120	120	0.071	100	0.028	≤ 120
Thymine	< 0.06	< 5	5	0.000	0	0.218	≤ 5
Uracil	0.64	53	50	0.641	67	0.859	≤ 230
Uridine	< 0.23	< 19	19	0.029	25	0.400	≤ 19

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

12 Sugars and derivatives

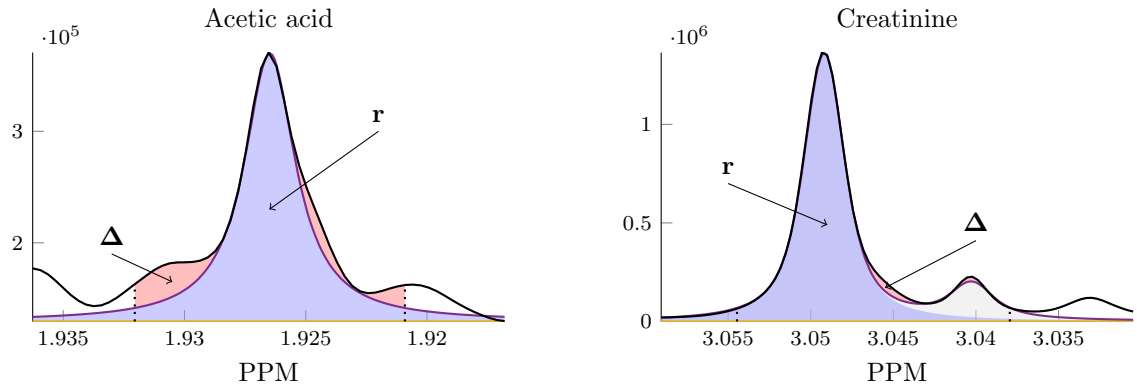
Compound	Conc. mmol/L	Conc. mmol / mol Crea	LOD mmol / mol Crea	r mmol/L	ρ %	Δ mmol/L	95% Range(*) mmol / mol Crea
D-Galactose	< 0.52	< 43	43	0.000	0	0.019	≤ 44
D-Glucose	< 0.41	< 34	34	0.236	89	0.067	≤ 140
D-Lactose	< 1.2	< 96	96	0.025	51	0.042	≤ 96
D-Mannitol	< 2.2	< 180	180	0.000	0	2.431	≤ 180
D-Mannose	< 0.07	< 6	6	0.000	0	0.047	≤ 8
Galactitol	< 4.5	< 370	370	0.000	0	1.657	≤ 370
Glycerol	< 2.3	< 190	190	0.000	0	4.383	≤ 190
L-Fucose	< 3.6	< 300	300	0.411	0	0.408	≤ 300
L-Threonic acid	< 3.9	< 320	320	0.000	0	2.689	≤ 320
Myo-Inositol	< 54	< 4400	4400	0.000	0	7.938	≤ 4400

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

13 Explanations

This section contains the definition of the parameters used above. In the section 13.1 a short manual, how to interpret the results, is presented. The section 13.3 contains the exact definitions of the parameters $\mathbf{r}$, ρ and $\boldsymbol{\Delta}$.

13.1 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 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)).

13.2 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)).

13.3 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.

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