

● Analysis Report

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

Sample ID: Demo-2

Measuring Date: 26-Apr-2017 17:02:01

Reporting Date: 26-Jul-2017 19:00:04, 9 page(s), Version 1.0.0

Quantification Method Version: Quant-UR NE.1.0.0

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.

Contents

1 Targeted Analysis	2
1.1 Creatinine	2
1.2 Alcohols and derivatives	2
1.3 Amines and derivatives	2
1.4 Amino acids and derivatives	3
1.5 Benzene and substituted derivatives	4
1.6 Carboxylic acids	4
1.7 Cosmetics, vitamins, drugs and drug metabolites	5
1.8 Fatty acids and derivatives	5
1.9 Hydroxy acids and derivatives	6
1.10 Keto acids and derivatives	6
1.11 Purine,Pyridine and Pyrimidine derivatives	7
1.12 Sugars and derivatives	7
2 Non-Targeted Analysis	8
2.1 Univariate analysis	8
2.2 Multivariate analysis	8
2.3 Spectroscopical overview	9





1 Targeted Analysis

1.1 Creatinine

Compound	Conc. mmol/L	LOD mmol/L	95% Range mmol/L	Graphics (*)
Creatinine	0.60	0.3	0 - 12	





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

1.2 Alcohols and derivatives

Compound	Conc. mmol/L	Conc. mmol/mol Crea	LOD mmol/mol Crea	95% Range mmol/mol Crea	Graphics (*)
Ethanol	< 0.50	< 840	840	≤ 840	
Isopropanol	< 0.01	< 9	9	≤ 9	
Methanol	0.07	120	91	≤ 400	
Propylene glycol	0.52	870	45	≤ 1200	

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

1.3 Amines and derivatives

Compound	Conc. mmol/L	Conc. mmol/mol Crea	LOD mmol/mol Crea	95% Range mmol/mol Crea	Graphics (*)
1-Methylguanidine	0.08	140	98	≤ 160	
Dimethylamine	0.07	110	8	38 - 160	
Trimethylamine	0.01	10	2	≤ 6	
Tyramine	< 0.05	< 86	86	≤ 86	

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

1.4 Amino acids and derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
1-Methylhistidine	< 0.23	< 380	380	≤ 380	
2-Furoylglycine	< 0.02	< 39	39	≤ 39	
3-Aminoisobutyric acid	< 0.18	< 300	300	≤ 390	
3-Methylcrotonylglycine	< 0.04	< 60	60	≤ 60	
4-Aminobutyric acid	< 0.01	< 17	17	≤ 20	
5-Aminopentanoic acid	< 0.10	< 170	170	≤ 170	
Alanine	0.32	540	14	27 - 350	
Arginine	< 2.8	< 4800	4800	≤ 4800	
Argininosuccinic acid	< 0.06	< 99	99	≤ 99	
Betaine	0.57	960	44	≤ 1200	
Citrulline	12	20000	780	≤ 780	
Creatine	0.12	210	50	≤ 680	
Cystine	< 0.04	< 75	75	≤ 75	
DL-Alloisoleucine	< 0.03	< 47	47	≤ 47	
DL-Tyrosine	< 0.03	< 43	43	≤ 43	
Glutamic acid	< 0.19	< 330	330	≤ 330	
Glutamine	< 0.50	< 830	830	≤ 830	
Glycine	0.85	1400	30	87 - 1900	
Guanidinoacetic acid	0.13	210	93	≤ 190	
Isobutyrylglycine	< 0.02	< 29	29	≤ 29	
L-Homocystine	< 0.10	< 170	170	≤ 170	
L-Isoleucine	< 0.03	< 47	47	≤ 47	
L-Pyroglutamic acid	0.14	230	5	≤ 44	
L-Tryptophan	0.03	50	49	≤ 49	
Leucine	0.04	63	13	≤ 40	
Methionine	< 0.01	< 13	13	≤ 22	
N,N-Dimethylglycine	0.03	54	15	≤ 220	
N-Acetylaspartic acid	< 0.03	< 48	48	≤ 48	
N-Acetylglutamate	< 0.03	< 42	42	≤ 42	
N-Acetylphenylalanine	< 0.05	< 87	87	≤ 87	
N-Acetyltyrosine	< 0.65	< 1100	1100	≤ 1100	
N-Isovaleroylglycine	0.00	4	2	≤ 5	
Phenylalanine	< 0.07	< 120	120	≤ 120	
Proline betaine	0.09	150	24	≤ 120	
Propionylglycine	< 0.01	< 2	2	≤ 2	
Sarcosine	0.01	13	5	≤ 25	
Taurine	0.50	830	250	≤ 910	
Tiglylglycine	< 0.04	< 74	74	≤ 74	
Valine	0.02	31	5	≤ 24	

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

1.5 Benzene and substituted derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
2-Hydroxyphenylacetic acid	< 0.01	< 10	10	≤ 10	
3-Phenyllactic acid	< 0.05	< 85	85	≤ 85	
4-Aminohippuric acid	< 0.99	< 1700	1700	≤ 1700	
4-Ethylphenol	< 0.01	< 8	8	≤ 8	
4-Hydroxyhippuric acid	< 0.58	< 980	980	≤ 980	
4-Hydroxyphenylacetic acid	< 0.02	< 36	36	≤ 69	
4-Hydroxyphenyllactic acid	< 0.28	< 470	470	≤ 470	
Benzoic acid	< 0.01	< 12	12	≤ 12	
D-Mandelic acid	< 0.01	< 4	4	≤ 43	
Hippuric acid	0.04	74	49	≤ 510	
Phenylacetic acid	< 0.28	< 470	470	≤ 470	
Phenylpyruvic acid	< 0.05	< 85	85	≤ 85	
Pyrocatechol	< 0.10	< 170	170	≤ 170	
Syringic acid	0.01	14	10	≤ 23	







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

1.6 Carboxylic acids

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
5-Aminolevulinic acid	< 0.01	< 3	3	≤ 3	
Acetic acid	0.25	410	10	≤ 790	
Citric acid	0.26	440	46	≤ 1400	
E-Glutaconic acid	< 0.07	< 130	130	≤ 130	
Ethylmalonic acid	< 0.01	< 20	20	≤ 42	
Formic acid	0.08	130	92	≤ 660	
Fumaric acid	0.01	21	2	≤ 40	
Glutaric acid	< 0.04	< 67	67	≤ 67	
Imidazole	< 0.02	< 38	38	< 38	
Lactic acid	0.33	550	45	≤ 410	
Maleic acid	0.00	7	7	≤ 10	
Methylmalonic acid	0.03	45	10	≤ 20	
Propionic acid	< 0.05	< 76	76	≤ 76	
Succinic acid	0.16	260	8	9 - 360	
Tartaric acid	< 0.03	< 45	45	≤ 60	
Trigonelline	< 0.02	< 33	33	≤ 33	
Xanthurenic acid	< 0.01	< 18	18	< 18	







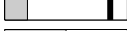




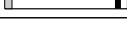
(*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

1.7 Cosmetics, vitamins, drugs and drug metabolites

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
Choline	< 0.06	< 94	94	≤ 94	
D-Panthenol	< 0.01	< 19	19	≤ 19	
L-Ascorbic acid	< 0.16	< 270	270	≤ 270	
Pantothenic acid	0.02	41	20	≤ 50	
Paracetamol	< 0.03	< 50	50	≤ 50	
Paracetamol-glucuronide	< 0.89	< 1500	1500	≤ 1500	







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

1.8 Fatty acids and derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
2-Hydroxy-4-methylvaleric acid	< 0.02	< 37	37	≤ 37	
2-Hydroxyisovaleric acid	0.01	10	4	≤ 4	
2-Methylsuccinic acid	0.13	210	34	≤ 34	
3-Hydroxy-3-methylglutaric acid	< 0.06	< 110	110	≤ 110	
3-Hydroxyisovaleric acid	< 0.01	< 18	18	≤ 33	
3-Hydroxyvaleric acid	< 0.01	< 6	6	≤ 8	
3-Methylglutaconic acid	0.07	120	17	≤ 26	
Butyric acid	< 0.02	< 26	26	≤ 34	
Citraconic acid	< 0.05	< 86	86	≤ 86	
L-Citramalic acid	< 0.34	< 560	560	≤ 560	
Pimelic acid	< 0.04	< 74	74	≤ 74	
Thymol	1.5	2600	170	≤ 170	














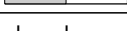
(*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

1.9 Hydroxy acids and derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
3-Hydroxyglutaric acid	< 0.02	< 41	41	≤ 44	
3-Hydroxypropionic acid	< 0.06	< 93	93	≤ 93	
D-Galactonic acid	< 0.08	< 130	130	≤ 130	
D-Gluconic acid	0.39	650	190	≤ 550	
Glycolic acid	0.28	470	190	≤ 480	
Malic acid	< 0.05	< 81	81	≤ 250	

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

1.10 Keto acids and derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
2-Ketobutyric acid	< 0.03	< 54	54	≤ 54	
2-Oxoglutaric acid	0.30	500	160	≤ 590	
2-Oxoisocaproic acid	0.01	10	5	≤ 10	
2-Oxoisovaleric acid	< 0.01	< 4	4	≤ 4	
3-Hydroxybutyric acid	< 0.06	< 97	97	≤ 100	
3-Methyl-2-oxovaleric acid	< 0.01	< 19	19	≤ 19	
4-Hydroxyphenylpyruvic acid	< 0.03	< 45	45	≤ 45	
Acetoacetic acid	0.02	33	5	≤ 28	
Acetoine	< 0.01	< 9	9	≤ 9	
Acetone	0.07	120	14	≤ 110	
DL-Kynurenin	< 0.47	< 790	790	≤ 790	
Oxaloacetic acid	0.06	100	44	≤ 210	
Pyruvic acid	0.03	57	13	≤ 41	
Succinylacetone	< 0.24	< 410	410	≤ 410	

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

1.11 Purine,Pyridine and Pyrimidine derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
1,3-Dimethyluric acid	0.05	88	13	20 - 150	
1-Methyladenosine	< 0.01	< 9	9	≤ 9	
1-Methylhydantoin	0.04	71	49	≤ 370	
1-Methylnicotinamide	< 0.03	< 46	46	≤ 120	
4-Pyridoxic acid	0.01	25	6	11 - 92	
Adenine	< 0.01	< 13	13	≤ 20	
Adenosine	< 0.57	< 950	950	≤ 950	
Allantoin	0.01	25	19	≤ 120	
Allopurinol	0.01	20	18	≤ 23	
Caffeine	< 0.01	< 8	8	21 - 450	
Cytosine	< 0.01	< 9	9	≤ 9	
Dihydrothymine	< 0.26	< 430	430	≤ 560	
Dihydrouracil	< 0.08	< 130	130	≤ 130	
Inosine	< 0.01	< 17	17	≤ 17	
Neopterin	< 0.01	< 17	17	≤ 17	
Orotic acid	0.04	65	5	≤ 6	
Oxypurinol	0.03	41	19	≤ 37	
Quinolinic acid	< 0.02	< 38	38	≤ 38	
Theobromine	0.07	110	81	≤ 150	
Thymine	< 0.01	< 4	4	≤ 4	
Uracil	< 0.01	< 8	8	≤ 110	
Uridine	< 0.01	< 15	15	≤ 15	

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

1.12 Sugars and derivatives

Compound	Conc.	Conc.	LOD	95% Range	Graphics (*)
	mmol/L	mmol/mol Crea	mmol/mol Crea	mmol/mol Crea	
D-Galactose	0.08	140	85	≤ 1400	
D-Glucose	1.8	3000	76	≤ 810	
D-Lactose	0.25	430	96	≤ 850	
D-Mannitol	< 0.25	< 430	430	≤ 430	
D-Mannose	0.03	52	20	≤ 310	
D-Xylose	< 0.50	< 840	840	≤ 840	
Galactitol	< 0.18	< 300	300	≤ 300	
Glycerol	< 0.47	< 790	790	≤ 790	
L-Fucose	< 0.18	< 300	300	≤ 460	
L-Threonic acid	< 0.11	< 180	180	≤ 180	
Myo-Inositol	< 1.5	< 2500	2500	≤ 2500	

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

2 Non-Targeted Analysis

2.1 Univariate analysis

Result: Univariate analysis detected significant deviations in the following chemical shifts (in ppm): 1.183, 1.191, 1.431, 1.498, 1.506, 1.513, 1.521, 1.528, 1.536, 1.543, 1.551, 1.558, 1.566, 1.573, 1.581, 1.588, 1.596, 1.603, 1.611, 1.618, 1.626, 1.633, 1.641, 1.648, 1.656, 1.663, 1.821, 1.829, 1.836, 1.844, 1.851, 1.859, 1.866, 1.874, 1.881, 1.889, 1.896, 1.904, 1.911, 2.009, 2.016, 2.024, 2.031, 2.039, 2.114, 2.151, 2.219, 2.226, 2.249, 2.256, 2.264, 2.422, 2.437, 2.444, 2.459, 2.474, 2.482, 2.497, 2.504, 2.512, 2.519, 2.639, 2.797, 2.804, 2.894, 3.105, 3.120, 3.127, 3.135, 3.142, 3.150, 3.157, 3.165, 3.172, 3.180, 3.187, 3.195, 3.225, 3.232, 3.240, 3.255, 3.405, 3.427, 3.442, 3.750, 3.758, 3.765, 3.773, 3.840, 3.915, 4.005, 4.013, 4.020, 4.238, 6.362, 6.370, 6.377, 6.385, 6.392, 6.400, 6.407, 6.415, 6.422, 6.430, 6.437, 6.445, 6.768, 6.775, 6.783, 6.820, 6.828, 6.835, 6.843, 6.850, 6.963, 7.038, 7.211, 7.218, 7.226, 7.233,

2.2 Multivariate analysis

Result: Multivariate analysis detected significant deviations in the following chemical shift regions (in ppm):

- 1.439 - 1.617
- 1.627 - 1.805
- 1.815 - 1.993
- 2.002 - 2.180
- 2.190 - 2.368
- 2.378 - 2.556
- 3.128 - 3.306
- 3.316 - 3.494
- 3.504 - 3.682
- 3.691 - 3.869
- 6.694 - 6.872
- 0.501 - 0.867
- 1.252 - 1.617
- 1.627 - 1.993
- 2.002 - 2.368
- 2.378 - 2.743
- 3.128 - 3.494
- 3.504 - 3.869
- 4.254 - 6.121
- 6.506 - 6.872
- 0.501 - 2.368
- 2.378 - 4.245
- 4.254 - 7.622
- 0.501 - 9.499

2.3 Spectroscopical overview

The following figure shows if any ppm region in the spectrum is affected by any significant deviations from the reference data. Each stripe represents an individual verification model. Chemical shifts or chemical shift regions with deviations from the reference are colored red. At the top, results of the univariate analysis are presented while the following stripes represent the multivariate analysis for different subdivisions of the entire spectrum.

