1.5 Metabolic Profiling (GC-MS and LC-MS)

Method : GC-MS
Status : partially validated
Matrices : human and rat plasma and tissues
Reference : N/A : N/A

Analytes:

3OH-butyrate
Acetic acid
Alanine
Aminomalonate
Creatinine
Galactonic acid
Glucitol
Glucoronic acid
Glutamine
Glycine
Hippurate
Histidine
Indolacetate
Isocitrate
Isovalerate
Lactic acid
Oxalate
Proline
Pseudouridine
Pyruvic acid
Ribose
Serine
Succinate
Threonine
Tyrosine
Uric acid
Valine
Xylitol

Please note that only the major metabolites are listed. Typically, more than 100 metabolites can be detected within one GC-MS run, allowing either for quantitation or semi-quantitative comparison.

In addition, LC-TOF and LC-MS-TOF assays are set up and available. Metabolites can be identified using the METLIN / HMBD databases. However, it must be noted that due to the inherent problem of ion suppression in the electrospray source use of this data for semi-quantitative comparison may be limited.

1.6 Metabolic Profiling (^{1}H NMR)

Method : proton nuclear magnetic resonance spectroscopy (500, 600 and 900 MHz)
Status : partially validated
Matrices : human and rat plasma, urine and tissues
Reference : N/A

Analytes:

No.	Metabolite	1H [ppm]	13C [ppm]	blood	urine
1	Leucine	0.94	22	●	●
2	Leucine	0.96	23	●	●
3	Valine	0.97	18	●	
4	Isoleucine	1.00	16	●	●
5	Valine	1.03	19	●	
6	(isobutyrate / 3oxo-isovalerate)	1.13	23.1		●
7	3-hydroxybutyrate	1.19	23	●	
8	Threonine	1.29	20.5	●	
9	Lactate	1.32	21.3	●	●
10	Lysine	1.43 + 1.47	22.8	●	
11	Alanine	1.46	17.5	●	●
12	Arginine	1.67	25.3	●	
13	Leucine	1.68	25.0	●	●
14	Leucine	1.69	41.0	●	
15	Leucine	1.69	40.2	●	
16	Lysine	1.70	27.6	●	
17	2-hydroxyglutarate	1.83	31.9		●

No.	Metabolite	1H [ppm]	13C [ppm]	blood	urine
18	Lysine	1.87	31.5	●	
19	Arginine	1.87	29.3	●	
20	2-Hydroxyglutarate	1.98	31.5		
21	Acetate	2.02	23.4	●	●
22	Glutamate	2.08	28.3	●	
23	Glutamine	2.12	28	●	
24	Hydroxyglutarate	2.26	34.3		●
25	Glutamate	2.32	34.7	●	
26	Succinate	2.43	34		●
27	Glutamine	2.44	32.1	●	
28	2-Oxoglutarate	2.45	31.5		●
29	Glutathione (Glu) both froms	2.49	32.7	●	
30	Citrate	2.56	46.2		●
31	Dimethylamine	2.70	35.7		●
32	Citrate	2.71	46.2		●
33	Trimethylamine	2.87	45.7		●
34	GSSG (Cys) oxidized	2.95	39.9	●	
35	2-Oxoglutarate	2.97	36.8		●
36	Lysine	3.01	40.3	●	
37	Creatine	3.02	38.3	●	●
38	Creatinine	3.04	31.4	●	●
39	R-N+-$(CH_3)_3$ several signals	3.18 -3.27	53.1-55.5	●	●
40	Taurine	3.20	49.9	●	●
41	β-Glucose C2	3.23	75.3	●	●

No.	Metabolite	1H [ppm]	13C [ppm]	blood	urine
42	Arginine	3.23	41.7	●	
43	Trimethylamine N-oxide	3.25	60.8	●	● 3.3 ppm
44	Phenylalanine	3.28	36.9		●
45	GSSG (Cys) oxidized	3.30	39.8	●	
46	Taurine	3.32	36.8	●	●
47	α, β-Glucose C4	3.40	70.8	●	●
48	β-Glucose C3/C5	3.48	77.1	●	●
49	α-Glucose C2	3.52	72.6	●	●
50	Glycine	3.54	42.8	●	●
51	Glutathione+Gln+Glu	3.69	55.7	●	
52	α-Glucose C3	3.69	73.9	●	●
53	α, β-Gglucose C6	3.72	61.9	●	●
54	Glutathione (Gly) both forms	3.75	44.7	●	
55	Alanine	3.75	51.7	●	●
56	α-Glucose C5	3.82	72.6	●	●
57	α, β-Glucose C6	3.87	61.9	●	●
58	Creatine	3.91	55.0	●	●
59	Hippurate	3.94	45.1		●
60	Creatinine	4.09	56.9		●
61	Lactate	4.09	69.7	●	●
62	β-Glucose C1	4.64	97.1	●	●
63	α-Glucose C1	5.21	93.3	●	●
64	Urea	5.80	------		●
65	Phenylalanine	7.31	130.5		●

1.6 Metabolic Profiling (^{1}H NMR)

No.	Metabolite	1H [ppm]	13C [ppm]	blood	urine
66	Phenylalanine	7.34	128.0		●
67	Phenylalanine	7.41	129.9		●
68	Hippurate	7.50	129.9		●
69	Hippurate	7.59	133.2		●
70	Hippurate	7.79	128.2		●
71	Fumarate	8.46	147.9		