

Table S1. Identification of urinary biomarkers in model cases by TransOmics

No	Rt(min)	m/z	Compound ID	Adducts	Formula	Mass Error (ppm)	Description	Fold Change	Anova (p)
1	0.63	203.94	HMDB04143	M+Na	HTa	4.76	Tantalum	3.51	0.0021
2	2.48	175.11	HMDB03357	M+H	C7H14N2O3	-4.66	N-Acetylornithine	1.48	0.0051
3	2.73	244.11	HMDB01458	M+H	C10H17N3O2S	-3.63	Biotin amide	2.40	0.0056
4	2.77	241.13	HMDB00745	M+H	C10H16N4O3	-1.54	Homocarnosine	3.31	0.0052
5	2.82	154.00	HMDB03585	M+H	C3H7NO2S2	-1.09	Thiocysteine	6.98	0.0006
6	2.98	295.10	HMDB04810	M+Na	C16H16O4	3.58	5C-aglycone	2.02	0.0063
7	3.12	148.06	HMDB00148	M+H	C5H9NO4	3.61	L-Glutamic acid	1.59	0.0018
8	3.37	315.06	HMDB01308	M+H	C8H15N2O9P	-0.53	5'-Phosphoribosyl-N-formylglycinamide	15.12	0.0074
9	3.42	178.05	HMDB01015	M+H	C6H11NO3S	0.87	N-Formyl-L-methionine	1.99	0.0017
10	3.55	156.99	HMDB00816	M+H	C2H5O6P	2.77	Phosphoglycolic acid	2.21	0.0004
11	4.60	315.06	HMDB01308	M+H	C8H15N2O9P	0.92	5'-Phosphoribosyl-N-formylglycinamide	3.31	0.0008
12	4.78	220.01	HMDB03705	M+Na	C3H8N3O5P	3.52	Phosphoguanidinoacetate	6.42	0.0001
13	5.18	268.07	HMDB01410	M+H	C9H9N5O5	4.57	2-Amino-4-oxo-6-(1',2'-dioxopropyl)- 7,8-dihydroxypteridine	3.18	0.0006
14	5.78	291.13	HMDB00052	M+H	C10H18N4O6	0.50	Argininosuccinic acid	1.44	0.0022
15	5.86	371.19	HMDB06278	M+H	C19H30O5S	-3.89	5alpha-Dihydrotestosterone sulfate	6.81	0.0356
16	6.01	283.02	HMDB00645	M+Na	C6H13O9P	2.26	Galactose 1-phosphate	1.49	0.0042
17	7.21	337.08	HMDB04645	M+H	C10H16N4O7S	-2.05	S-Nitrosoglutathione	10.34	0.0077

Table S2. Result from ingenuity pathway analysis with MetPA.

Metabolic pathway	Total	Expected	Hits	Raw p	Impact
Arginine and proline metabolism	44	0.3766	3	0.0052089	0.11711
Alanine, aspartate and glutamate metabolism	24	0.20542	2	0.0167	0.28164
D-Glutamine and D-glutamate metabolism	5	0.042796	1	0.042129	1
Nitrogen metabolism	9	0.077033	1	0.074653	0
Histidine metabolism	15	0.12839	1	0.12155	0
Glyoxylate and dicarboxylate metabolism	16	0.13695	1	0.12915	0
Butanoate metabolism	20	0.17118	1	0.15895	0
Glutathione metabolism	26	0.22254	1	0.2019	0.05534
Galactose metabolism	26	0.22254	1	0.2019	0.13475
Porphyrin and chlorophyll metabolism	27	0.2311	1	0.20886	0
Cysteine and methionine metabolism	28	0.23966	1	0.21577	0
Amino sugar and nucleotide sugar metabolism	37	0.31669	1	0.27547	0.03099
Aminoacyl-tRNA biosynthesis	67	0.57347	1	0.44567	0
Purine metabolism	68	0.58203	1	0.45065	0.03915

Note: Total is the total number of compounds in the pathway; the Hits is the actually matched number from the user uploaded data; the Impact is the pathway impact value calculated from pathway topology analysis.