

Table S1. Result from ingenuity pathway analysis with MetPA.

No	Pathway Name	Total	Hits	p	-log(p)	Impact
1a	Taurine and hypotaurine metabolism	8	1	0.082653	2.4931	0.42857
2b	Glyoxylate and dicarboxylate metabolism	16	1	0.1589	1.8395	0.2963
3c	Glycine, serine and threonine metabolism	32	2	0.044048	3.1225	0.29197
4d	Citrate cycle (TCA cycle)	20	2	0.01817	4.008	0.08044
5e	Glycerophospholipid metabolism	30	2	0.039109	3.2414	0.06759
6f	Primary bile acid biosynthesis	46	2	0.084338	2.4729	0.05952
7	Glutathione metabolism	26	1	0.24589	1.4029	0.00573
8	Alanine, aspartate and glutamate metabolism	24	1	0.22919	1.4732	0.00316
9	Purine metabolism	68	1	0.52745	0.6397	0.00275
10	Cyanoamino acid metabolism	6	1	0.06261	2.7708	0.0
11	Ascorbate and aldarate metabolism	9	1	0.092524	2.3803	0.0
12	Methane metabolism	9	1	0.092524	2.3803	0.0
13	Nitrogen metabolism	9	1	0.092524	2.3803	0.0
14	Caffeine metabolism	12	1	0.12155	2.1075	0.0
15	Porphyrin and chlorophyll metabolism	27	1	0.25411	1.37	0.0
16	Drug metabolism - other enzymes	30	1	0.27827	1.2792	0.0
17	Tyrosine metabolism	42	1	0.3678	1.0002	0.0
18	Arginine and proline metabolism	44	1	0.38168	0.96318	0.0
19	Aminoacyl-tRNA biosynthesis	67	1	0.52208	0.64993	0.0

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