

Table S1. Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway analysis with MetPA.

No	Pathway Name	Total	Expected	Hits	Raw p	Impact
1	Phenylalanine, tyrosine and tryptophan biosynthesis	4	0.0285	1	0.0283	0.5000
2	Valine, leucine and isoleucine biosynthesis	11	0.0785	1	0.0760	0.3333
3	Glycine, serine and threonine metabolism	32	0.2283	1	0.2068	0.2920
4	Tyrosine metabolism	42	0.2996	2	0.0339	0.1416
5	Primary bile acid biosynthesis	46	0.3281	1	0.2845	0.0298
6	Tryptophan metabolism	41	0.2924	3	0.0024	0.0166
7	Glutathione metabolism	26	0.1855	1	0.1712	0.0057
8	Aminoacyl-tRNA biosynthesis	67	0.4779	3	0.0098	0
9	Ubiquinone and other terpenoid-quinone biosynthesis	3	0.0214	1	0.0213	0
10	Cyanoamino acid metabolism	6	0.0428	1	0.0421	0
11	Phenylalanine metabolism	9	0.0642	1	0.0626	0
12	Methane metabolism	9	0.0642	1	0.0626	0
13	Nitrogen metabolism	9	0.0642	1	0.0626	0
14	Porphyrin and chlorophyll metabolism	27	0.1926	1	0.1772	0
15	Amino sugar and nucleotide sugar metabolism	37	0.2639	1	0.2353	0
16	Valine, leucine and isoleucine degradation	38	0.2710	1	0.2409	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 Impact is the pathway impact value calculated from pathway topology analysis.

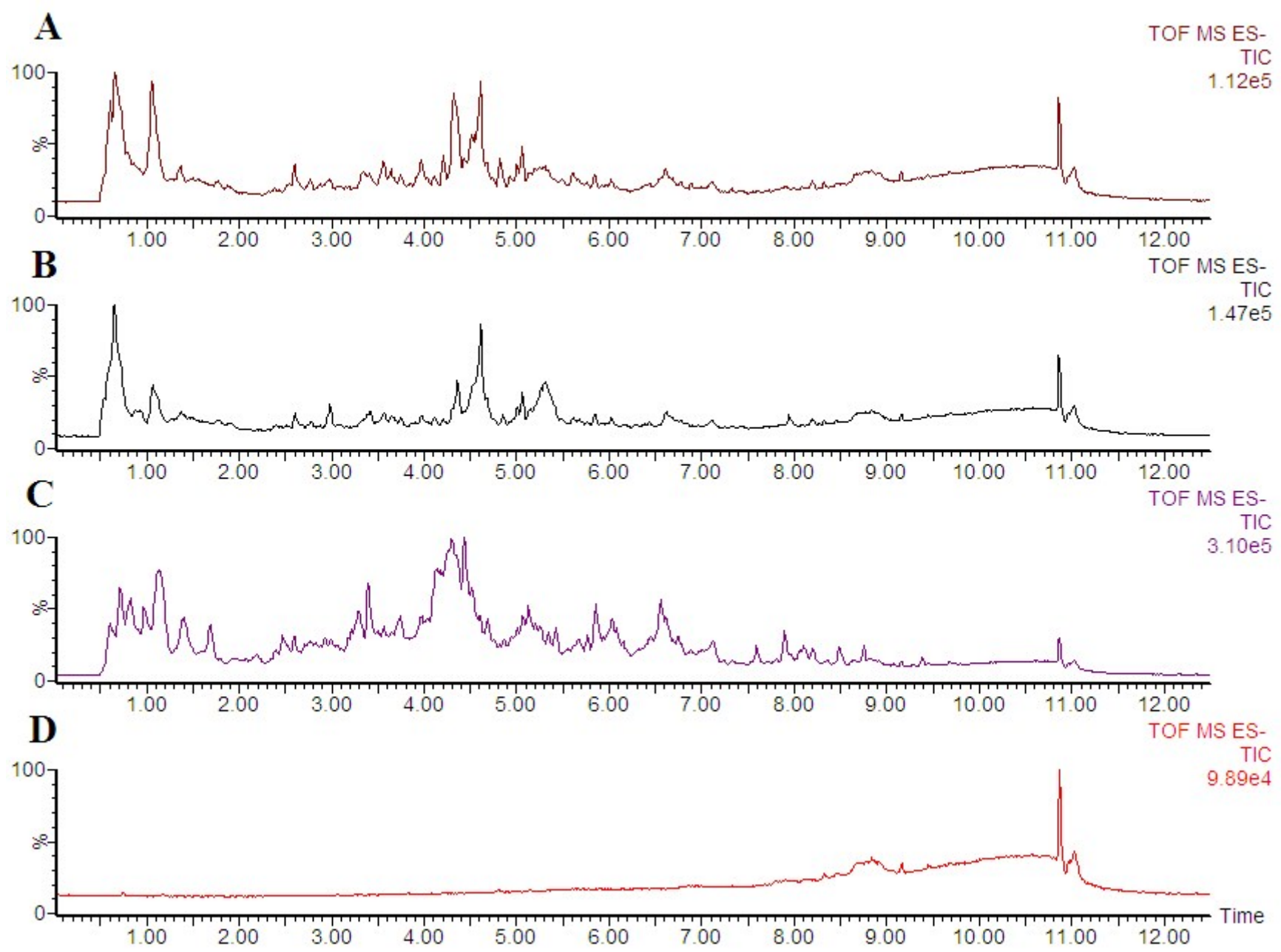


Fig. S1. Representative UPLC/MS spectra of urine samples.

Note: A, control group; B, model group; C, HXC group (ESI mode), D, black samples.