Electronic Supplementary Material (ESI) for Molecular BioSystems

Electronic Supplementary Information

For metabolomic analysis, the stability and reproducibility of the analytical method is very vital to obtain valid data. Therefore, we performed the PCA analysis of the QC samples to demonstrate the stability and reproducibility of the analytical method during the sequence. As shown in Fig. S1, the QC samples were clustered together in both positive and negative modes, indicating the excellent stability and reproducibility of our measurement during the whole sequence.

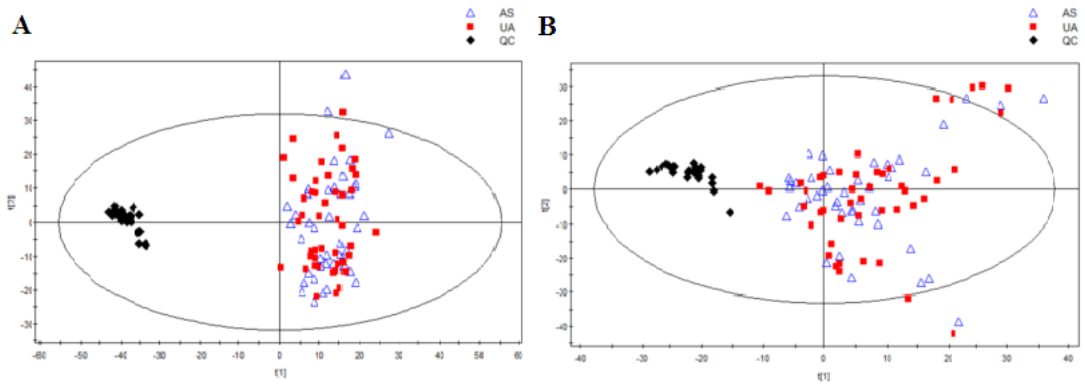

Fig. S1. PCA scores plots based on the data of the QC samples acquired in (A) positive mode and (B) negative mode.

The identification information of two typical metabolites from online database and our experimental data were demonstrated in Fig. S2-S3.

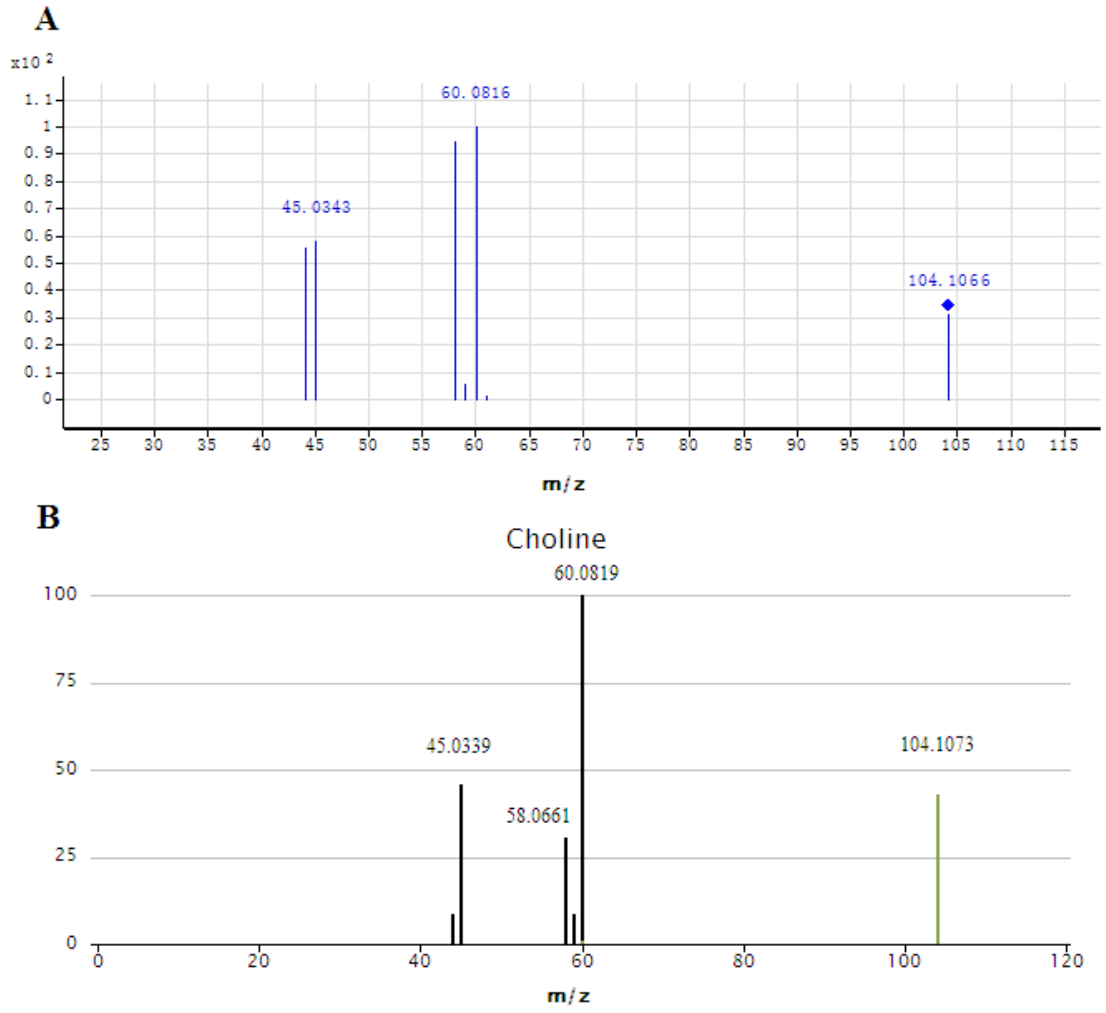

Fig.S2. The identification information of potential biomarker choline in positive mode. (A) The MS/MS spectrum of quasi-molecular ion ($[M+H]^+$) at m/z 104.1068 at 23.76 min in a plasma sample. (B) The corresponding MS/MS spectrum of biomarker choline in database of METLIN (20V).

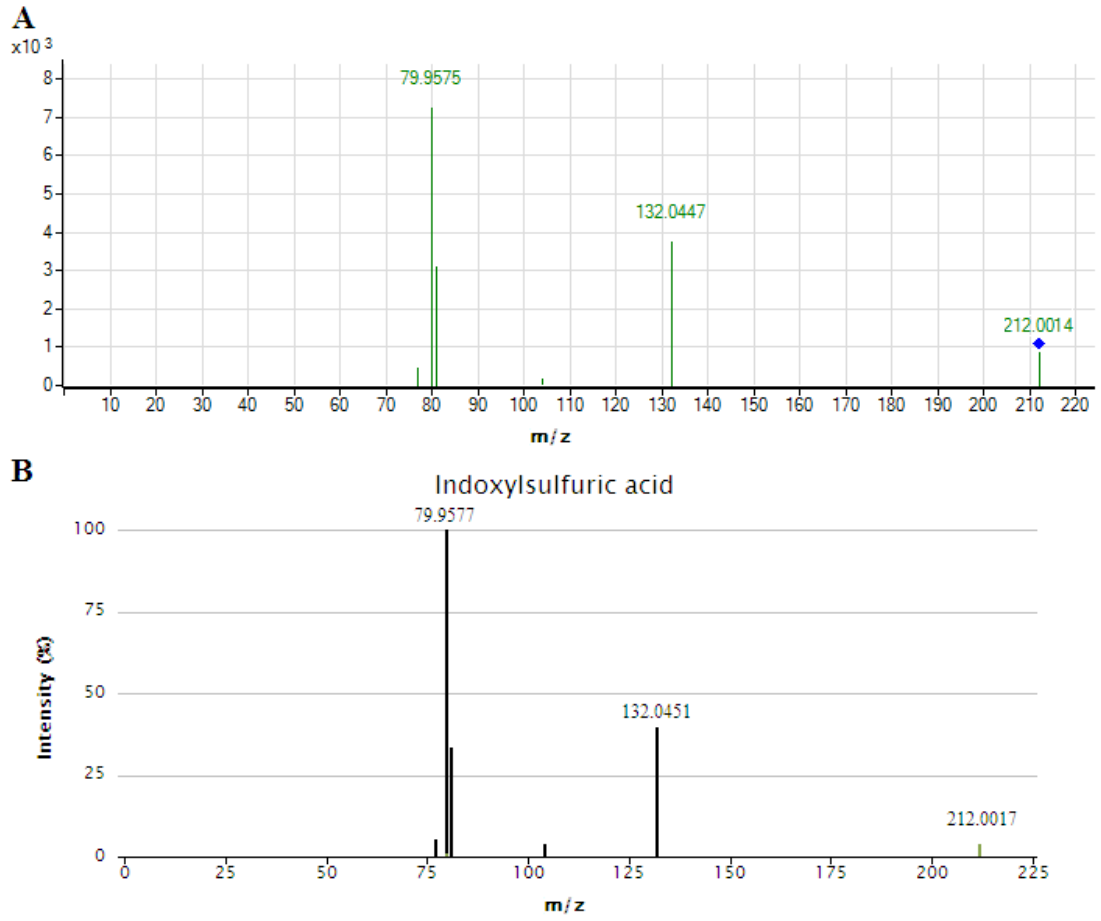

Fig.S3. The identification information of potential biomarker indoxylsulfuric acid in negative mode. (A) The MS/MS spectrum of quasi-molecular ion ($[M-H]^-$) at m/z 212.0014 at 6.59 min in a plasma sample. (B) The corresponding MS/MS spectrum of biomarker indoxylsulfuric acid in database of METLIN (20V).