Electronic Supplementary Material (ESI) for Molecular BioSystems.

Electronic supplementary information (ESI)

Fig. S1 PCA score plot for methods A-F (R^2X (cum) = 0.903, Q^2 (cum) = 0.635)

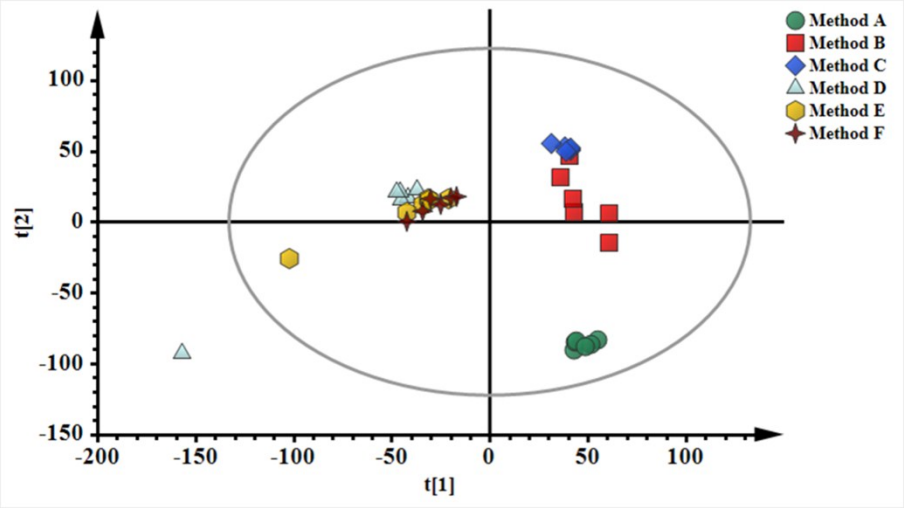


Fig. S2 Representative base peak intensity (BPI) chromatograms of (+) ESI-MS (A) and (-) ESI-MS (B) from serum samples of Con A-treated mice (upper) and control mice (lower), respectively.

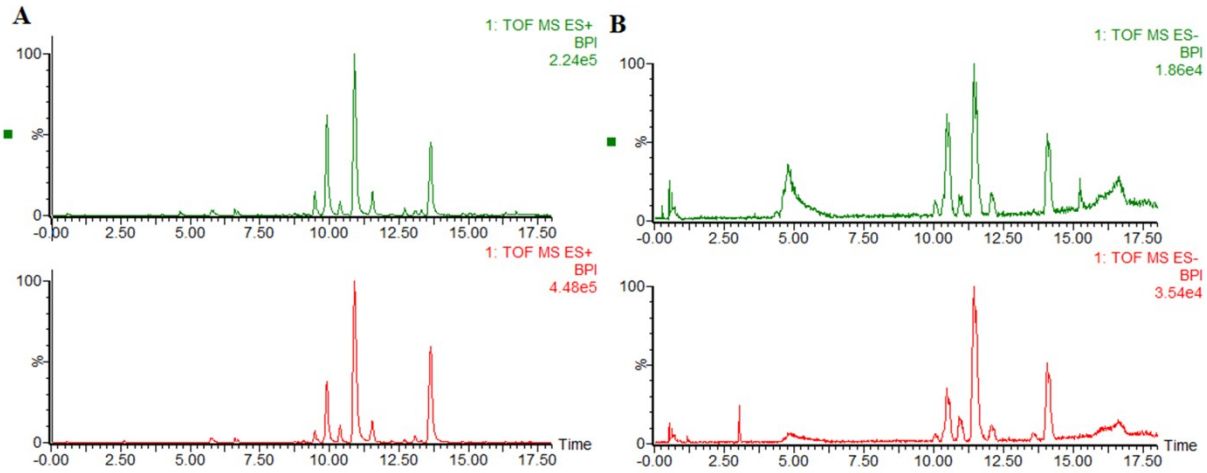
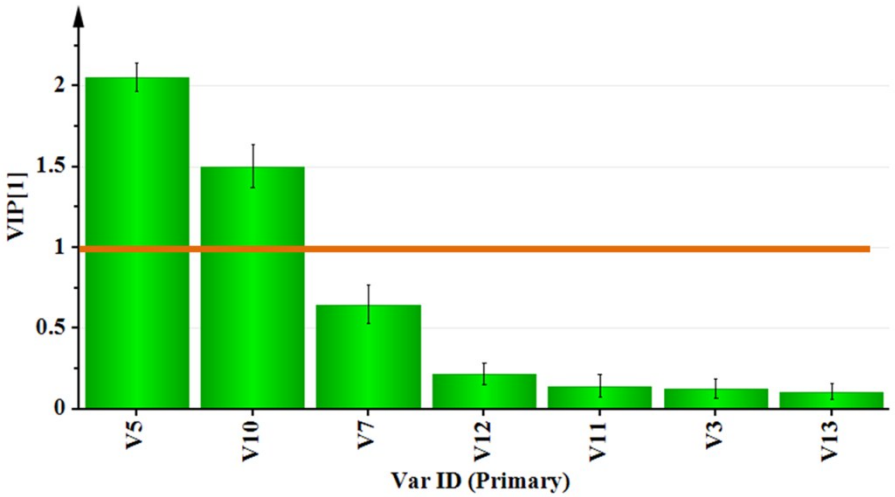


Fig. S3 VIP values of lysoPCs in PLS-RA model



Metabolites identification

Procedures of the metabolites identification are as follows: first, the quasimolecular ions were confirmed; secondly, the exact masses of the monoisotopic molecular weights were used to search the online databases, such as the Human Metabolome Database (http://www.hmdb.ca/), Metlin (http://metlin.scripps.edu/) and Mass Bank (http://www.massbank.jp/); then, the MS/MS spectra were also analyzed to verify the structure of the identified metabolites, and some of them were further confirmed using reference substances. The glycerophospholipids generally contain a quaternary ammonium salt group and a phosphate ester group. Hence, the fragment ions at *m/z* 184 ($[C_5H_{15}NO_4P]^+$) and 104 ($[C_5H_{14}NO]^+$) are characteristic ions of glycerophospholipids. And the length of the aliphatic chain is deduced from the accurate mass obtained via high-resulution mass spectrometry. Take lysoPC(18:0) (**V10**) as an example, it showed an accurate mass of $[M+H]^+$ and $[M+Na]^+$ at *m/z* 524.3718 and 546.3541, corresponding to the molecular formula $C_{26}H_{54}NO_7P$. Characteristic ions at *m/z* 184.0743 and 104.1074 were observed, and ion at 506.3609 were originated by the loss of H_2O (18 Da). By searching from the data base (HMDB), it was tentatively identified as lysoPC(18:0) (**V10**). The mass spectrum of lysoPC(18:0) (**V10**) is presented as **Fig. S4**. Carnitines have the similar skeletons as glycerophospholipids, but ions at *m/z* ~184 cannot be found in carnitines due to the lack of phosphate ester group. Therefore, by using this procedure, the structures of three long-chain acylcarnitines and seven glycerophospholipids were determined. Bile acids and bilirubin were validated by reference substance as shown in **Fig. S5-7**.

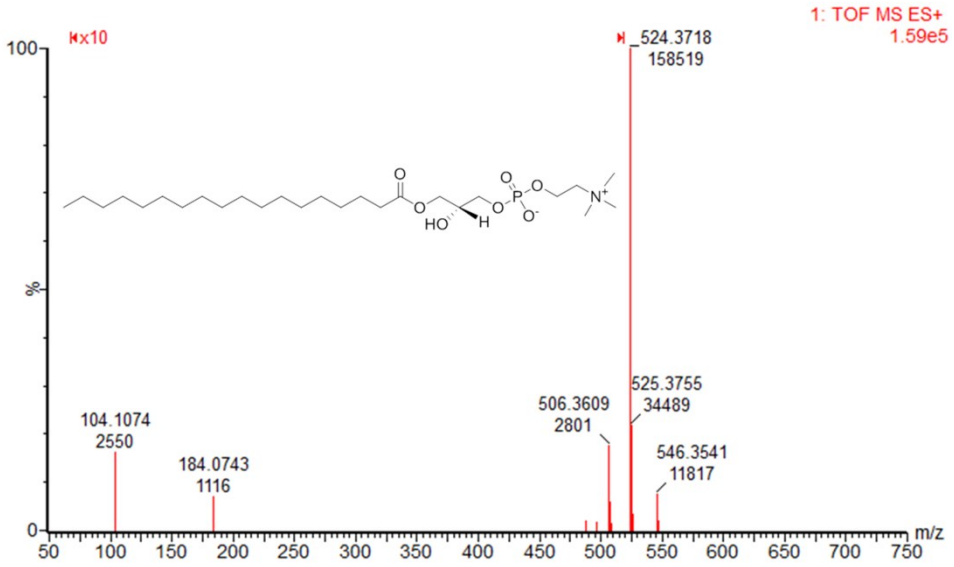


Fig. S4 Mass spectrum of lysoPC(18:0) (**V10**)

Fig. S5. (A) The UPLC-Q-TOF/MS base peak intensity (BPI) of taurocholic acid (**V1**). (B) The extracted ion chromatogram of ion at *m/z* 514 in a representative sample.

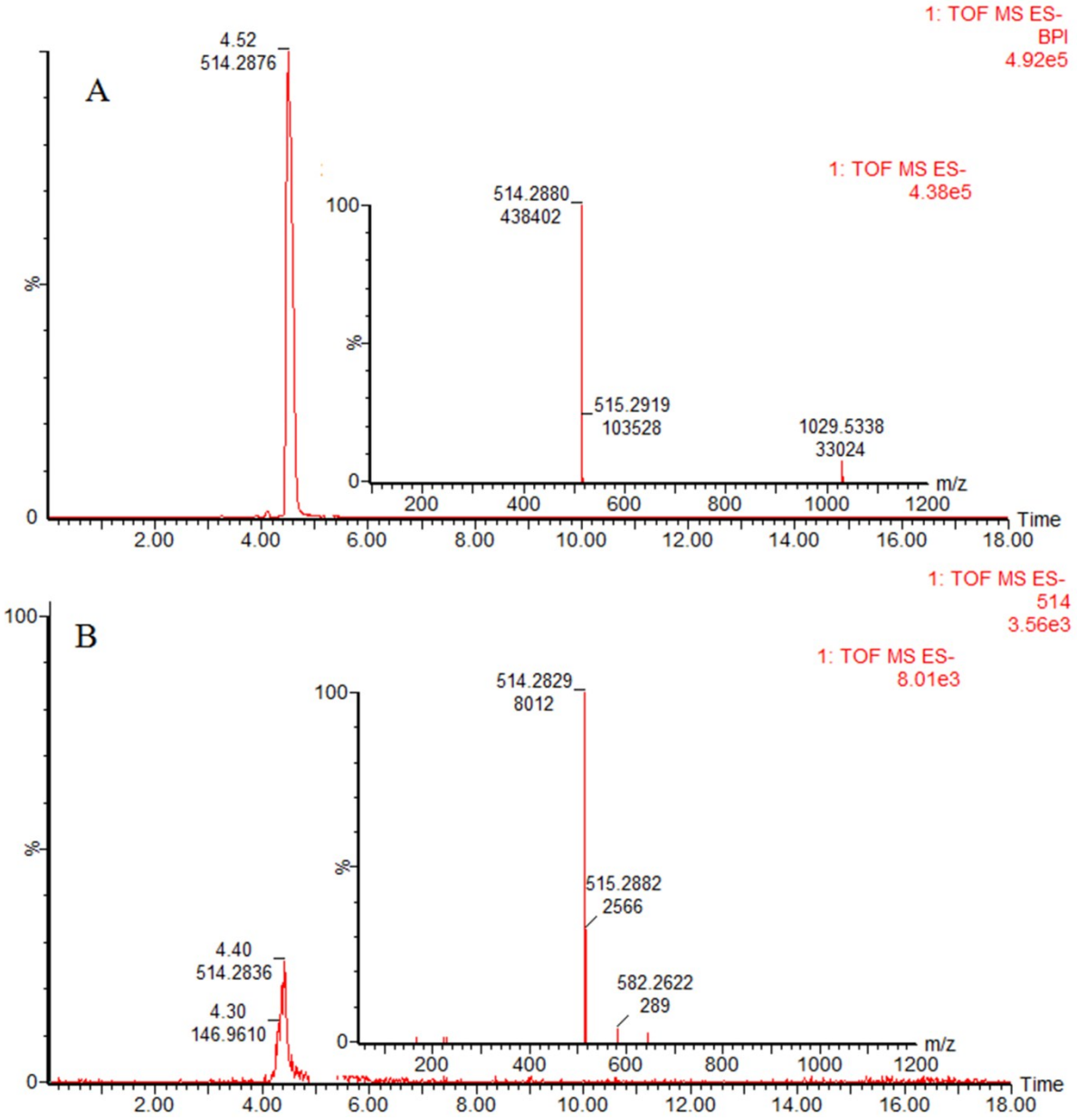


Fig. S6. (A) The UPLC-Q-TOF/MS base peak intensity (BPI) of taurochenodeoxycholic acid (**V2**). (B) The extracted ion chromatogram of ion at *m/z* 498 in a representative sample.

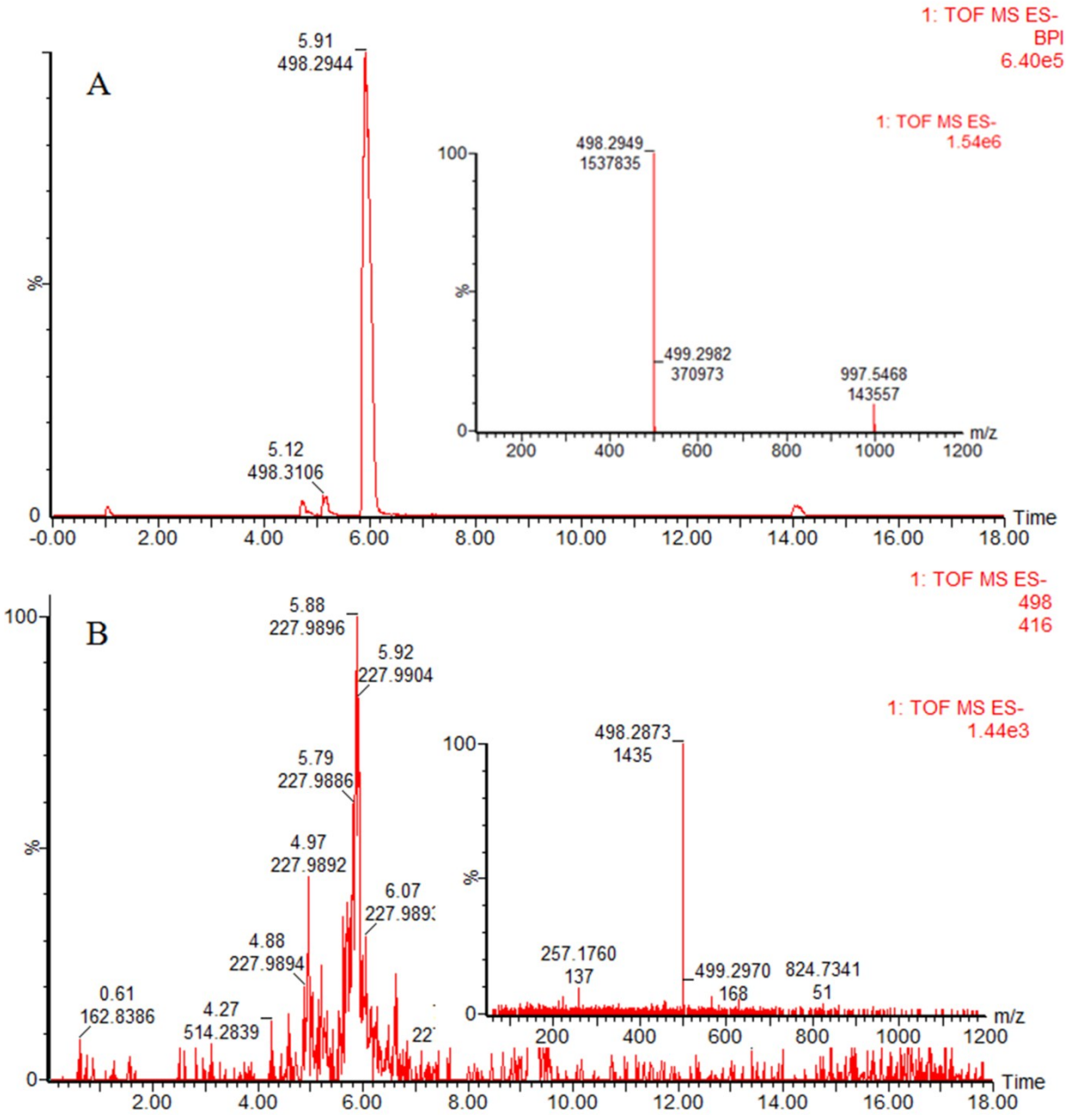


Fig. S7. (A) The UPLC-Q-TOF/MS base peak intensity (BPI) of bilirubin (**V14**). (B) The extracted ion chromatogram of ion at *m/z* 607 in a representative sample.