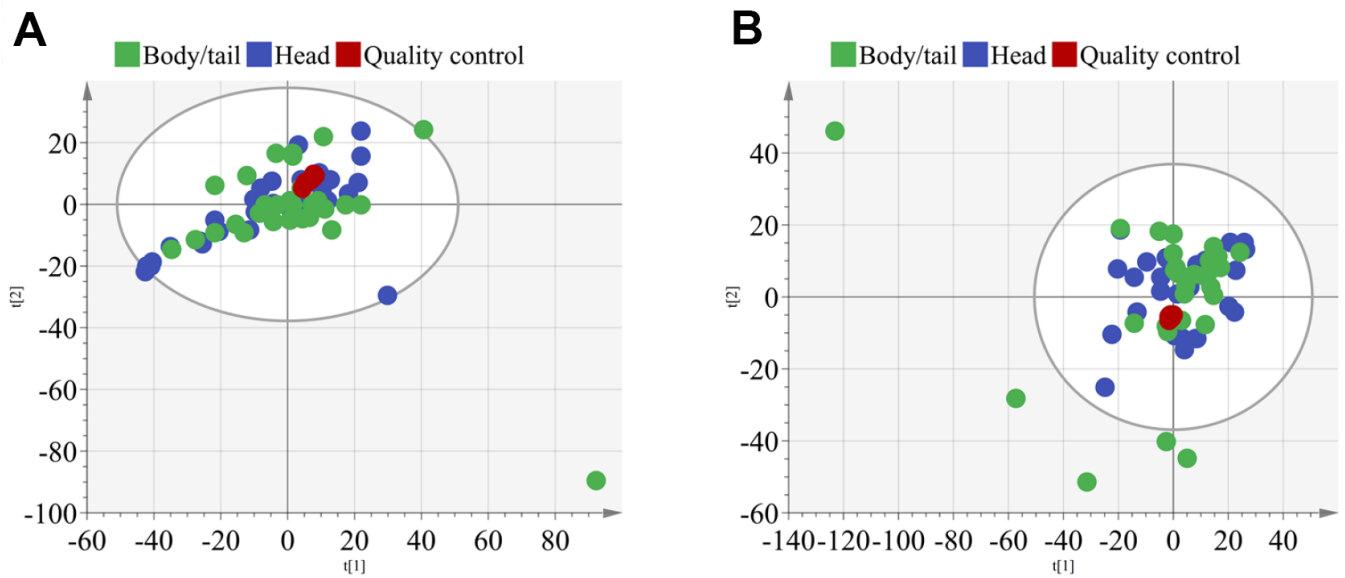
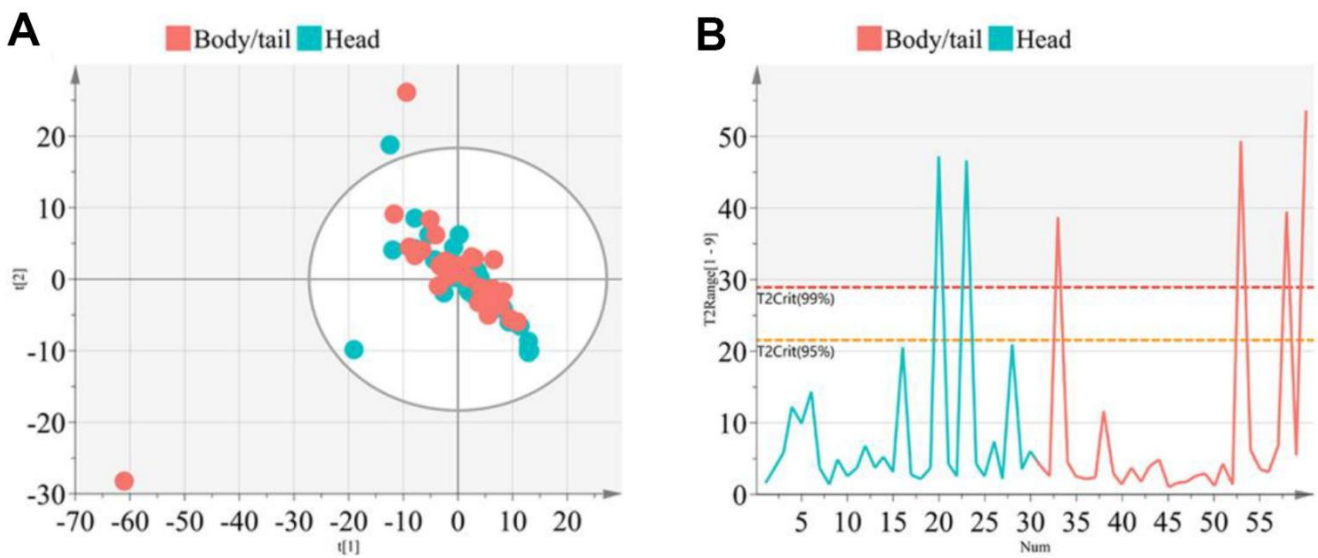


## SUPPLEMENTARY FIGURES

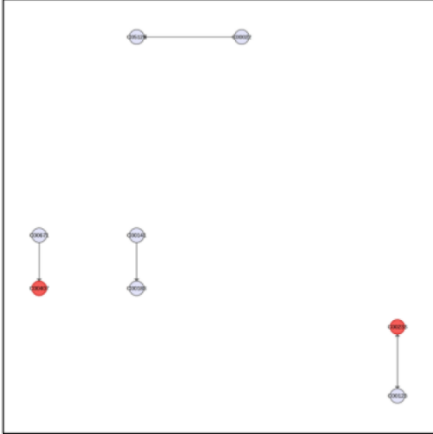


**Supplementary Figure 1. The quality control testing by including quality control samples into the PCA analysis. (A) the PCA plot in ESI<sup>+</sup> mode. (B) the PCA plot in ESI<sup>-</sup> mode.**

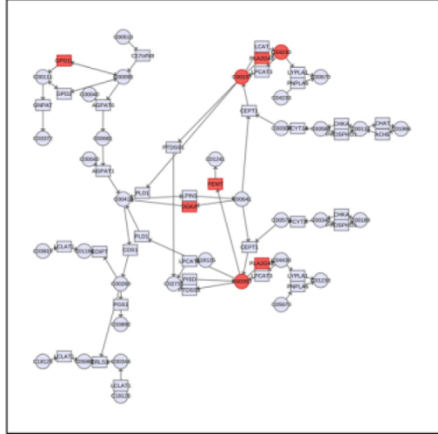


**Supplementary Figure 2. The total PCA analysis indicated the six outliers. (A) the PCA plot. (B) Hotelling's T2 plot shows six cases with values larger than the 99% confidence limit were considered as outlier.**

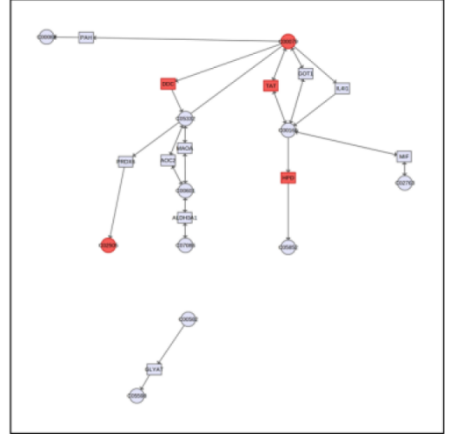
Valine, leucine and isoleucine biosynthesis



Glycerophospholipid metabolism



Phenylalanine metabolism



Supplementary Figure 3. The metabolism pathway of the top three enriched items, labeled with metabolites and enzyme-coded genes.