Supplementary



Figure S1 Quality control sample analysis. (A) TIC in the negative ion mode; (B) TIC in the positive ion mode; (C) PCA plot in the negative ion mode; (D) PCA plot in the positive ion mode. TIC, total ion chromatogram; PCA, principal component analysis.



Figure S2 Univariate statistical analysis between groups on day 7. (A) Metabolites with differential expression in the negative ion mode between the C7 group and T7 group; (B) metabolites with differential expression in the positive ion mode between the C7 group and T7 group; (C) metabolites with differential expression in the negative ion mode between the T7 group and TL7 group; (D) metabolites with differential expression in the positive ion mode between the T7 group and TL7 group; (E) metabolites with differential expression in the negative ion mode between the T7 group; (E) metabolites with differential expression in the negative ion mode between the T17 group; (E) metabolites with differential expression in the negative ion mode between the TL7 group and TL7 group; (F) metabolites with differential expression in the positive ion mode between the TL7 group and TH7 group.



Figure S3 Univariate statistical analysis between groups on day 28. (A) Metabolites with differential expression in the negative ion mode between the C28 group and T28 group; (B) metabolites with differential expression in the positive ion mode between the C28 group and T28 group; (C) metabolites with differential expression in the negative ion mode between the T28 group and TL28 group; (D) metabolites with differential expression in the positive ion mode between the T28 group; (E) metabolites with differential expression in the positive ion mode between the T28 group; (E) metabolites with differential expression in the negative ion mode between the T28 group; (E) metabolites with differential expression in the negative ion mode between the TL28 group and TL28 group; (F) metabolites with differential expression in the positive ion mode between the TL28 group and TH28 group; (F) metabolites with differential expression in the positive ion mode between the TL28 group and TH28 group.



Figure S4 Hierarchical clustering heatmap of significantly different metabolites. (A) Hierarchical clustering heatmap of differentially expressed metabolites between the C7 group and T7 group in the positive ion mode; (B) hierarchical clustering heatmap of differentially expressed metabolites between the TH7 group and TL7 group in the negative ion mode; (C) hierarchical clustering heatmap of differentially expressed metabolites between the TH7 group and TL7 group in the positive ion mode; (D) hierarchical clustering heatmap of differentially expressed metabolites between the TH7 group and TL28 group in the positive ion mode; (E) hierarchical clustering heatmap of differentially expressed metabolites between the TL28 group and TL28 group in the negative ion mode; (F) hierarchical clustering heatmap of differentially expressed metabolites between the TL28 group and TH28 group in the negative ion mode; (F) hierarchical clustering heatmap of differentially expressed metabolites between the TL28 group and TH28 group in the positive ion mode; (F) hierarchical clustering heatmap of differentially expressed metabolites between the TL28 group and TH28 group in the positive ion mode; (F) hierarchical clustering heatmap of differentially expressed metabolites between the TL28 group and TH28 group in the positive ion mode; (F) hierarchical clustering heatmap of differentially expressed metabolites between the TL28 group and TH28 group in the positive ion mode.



Figure S5 Metabolic pathways. TCA, tricarboxylic acid cycle; GPI, glucose-6-phosphate isomerase.