

Figure S1 The stacking diagram of the total ion chromatogram (TIC) in quality control samples.

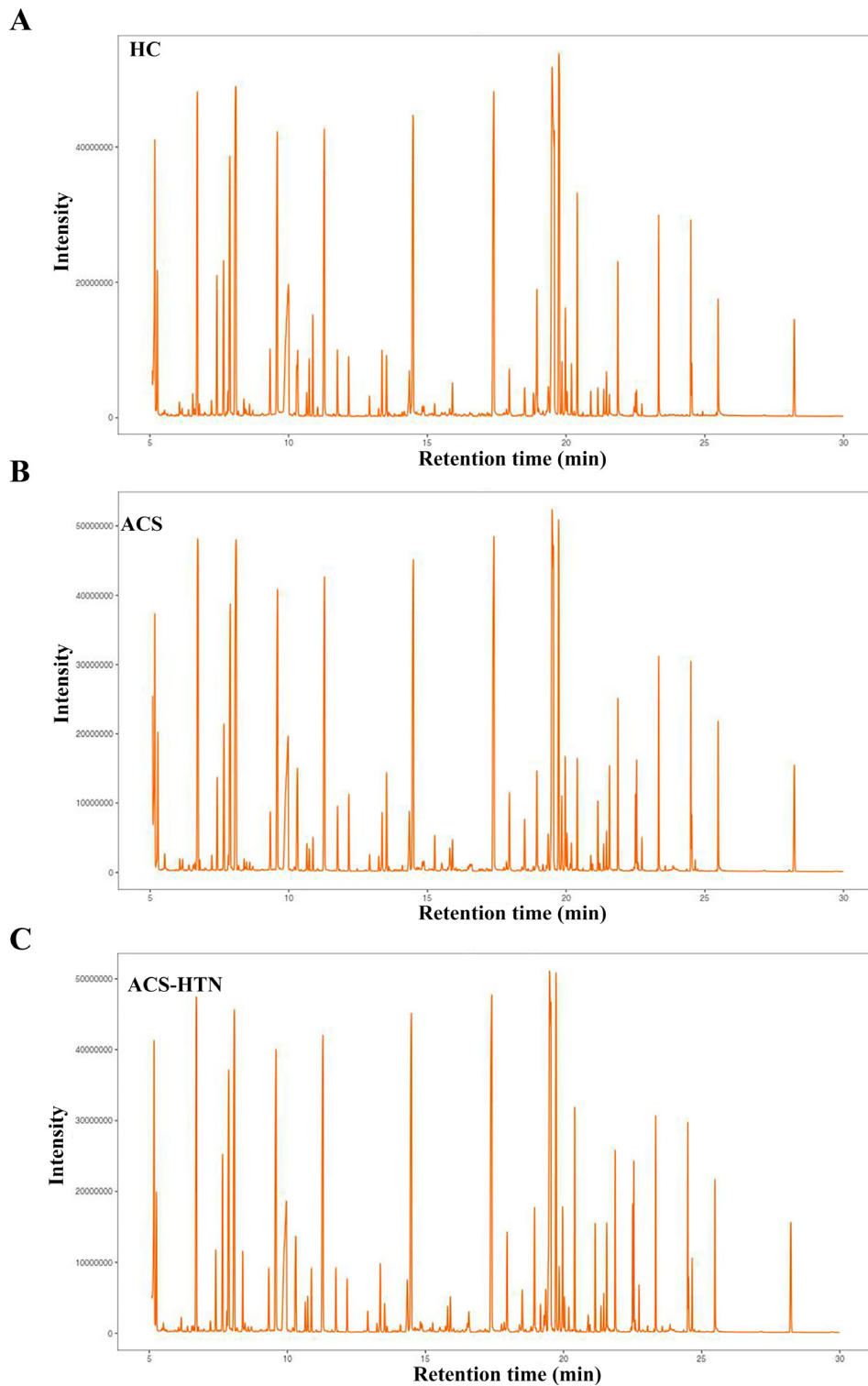


Figure S2 Mass spectrograms between the HC, ACS, and ACS-HTN groups. HC, healthy control; ACS, acute coronary syndrome; HTN, hypertension.

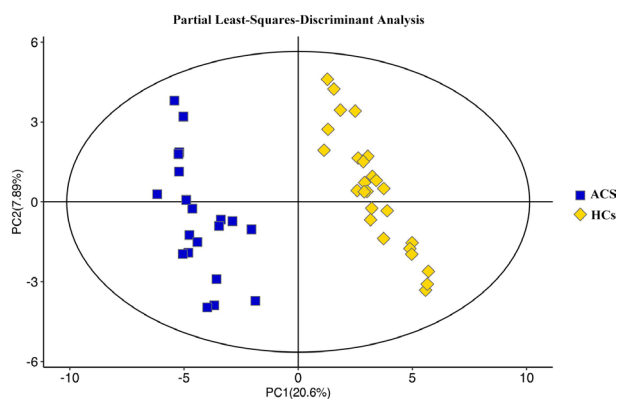


Figure S3 The partial least-squares-discriminant analysis comparing patients with ACS to HCs. HC, healthy control; ACS, acute coronary syndrome.

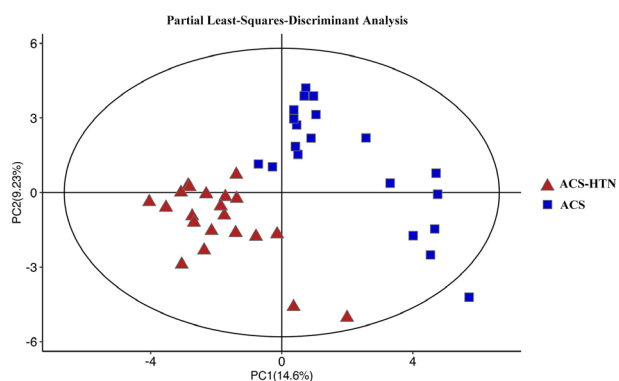


Figure S4 The partial least-squares-discriminant analysis comparing the ACS-HTN and ACS groups. ACS, acute coronary syndrome; HTN, hypertension.

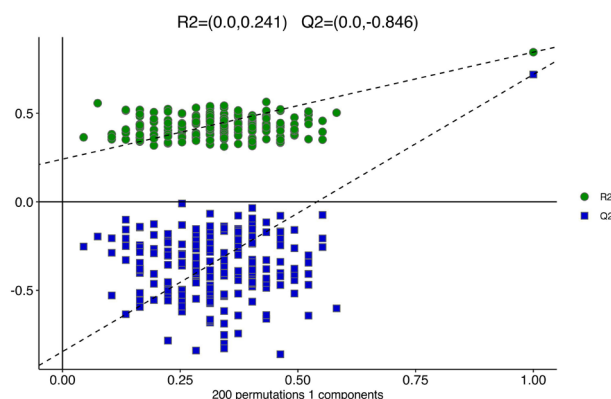


Figure S5 Response permutation testing between the HC, ACS, and ACS-HTN groups. The degree of fitting at OPLS-DA model was evaluated using 7-fold cross-validation and 200 RPT. Linear regression was conducted with R2Y and Q2Y of the original model, and the obtained intercept values between the regression line and Y-axis were R2 and Q2, respectively, evaluating whether the OPLS-DA model was overfitting. Generally, the closer the slope of R2Y and Q2Y lines was to the horizontal line, the more likely the model was to overfit. When using RPT tests, Q2 in this case was generally required to be less than zero. HC, healthy control; ACS, acute coronary syndrome; HTN, hypertension; RPT, response permutation testing.

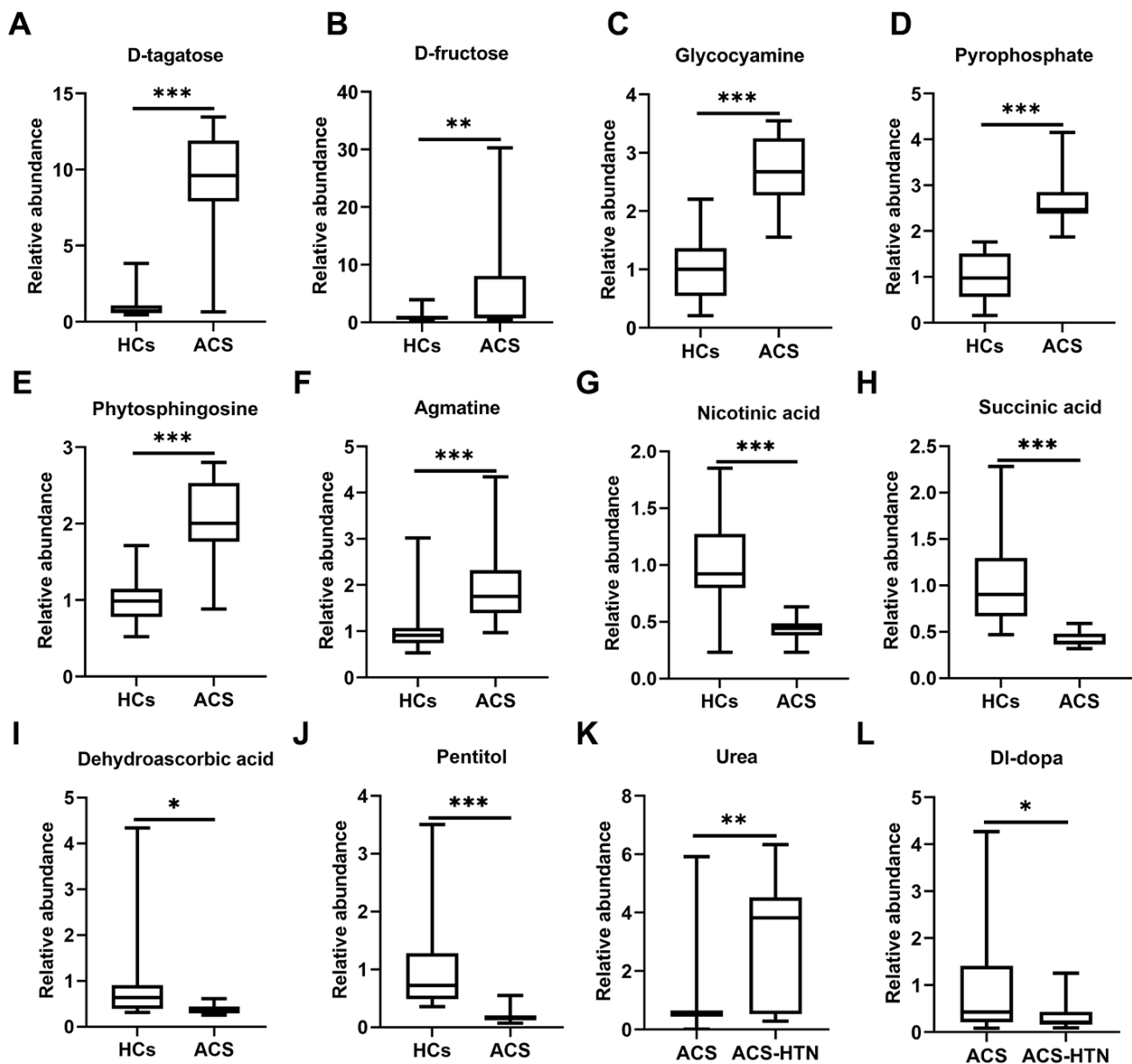


Figure S6 The significant metabolites identified for the different groups. In order to improve the accuracy of metabolites screening, the condition of $FC \geq 2$ or ≤ 0.5 was added, as the VIP values were greater than 1.0 and the P values were less than 0.05. (A-J) Compared to the HC group, the ACS group had 6 obviously upregulated metabolites and 4 significantly downregulated metabolites. (K-L) Compared to the ACS group, the ACS-HTN group had obviously upregulated urea levels and significantly downregulated DI-dopa levels. *, $P < 0.05$; **, $P < 0.01$; ***, $P < 0.001$. FC, fold change; VIP, variable importance in the project obtained from the two different groups; HC, healthy control; ACS, acute coronary syndrome; HTN, hypertension.

Correlation

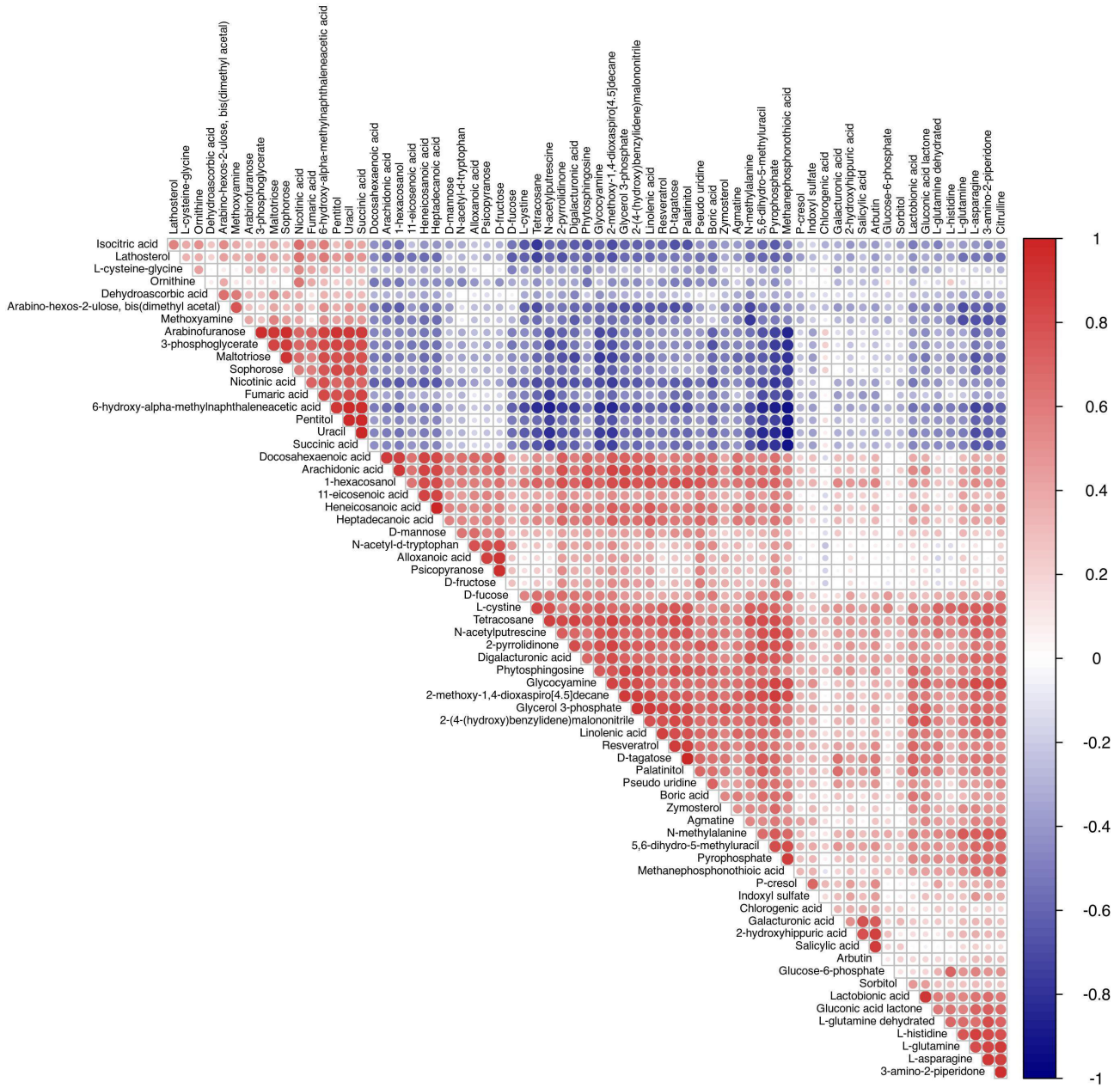


Figure S7 The correlation of metabolites between healthy controls and the patients with acute coronary syndrome. The color of the circle represents the size of correlation in the data with different levels of significance, with blue being the lowest value and red being the highest value.

Correlation

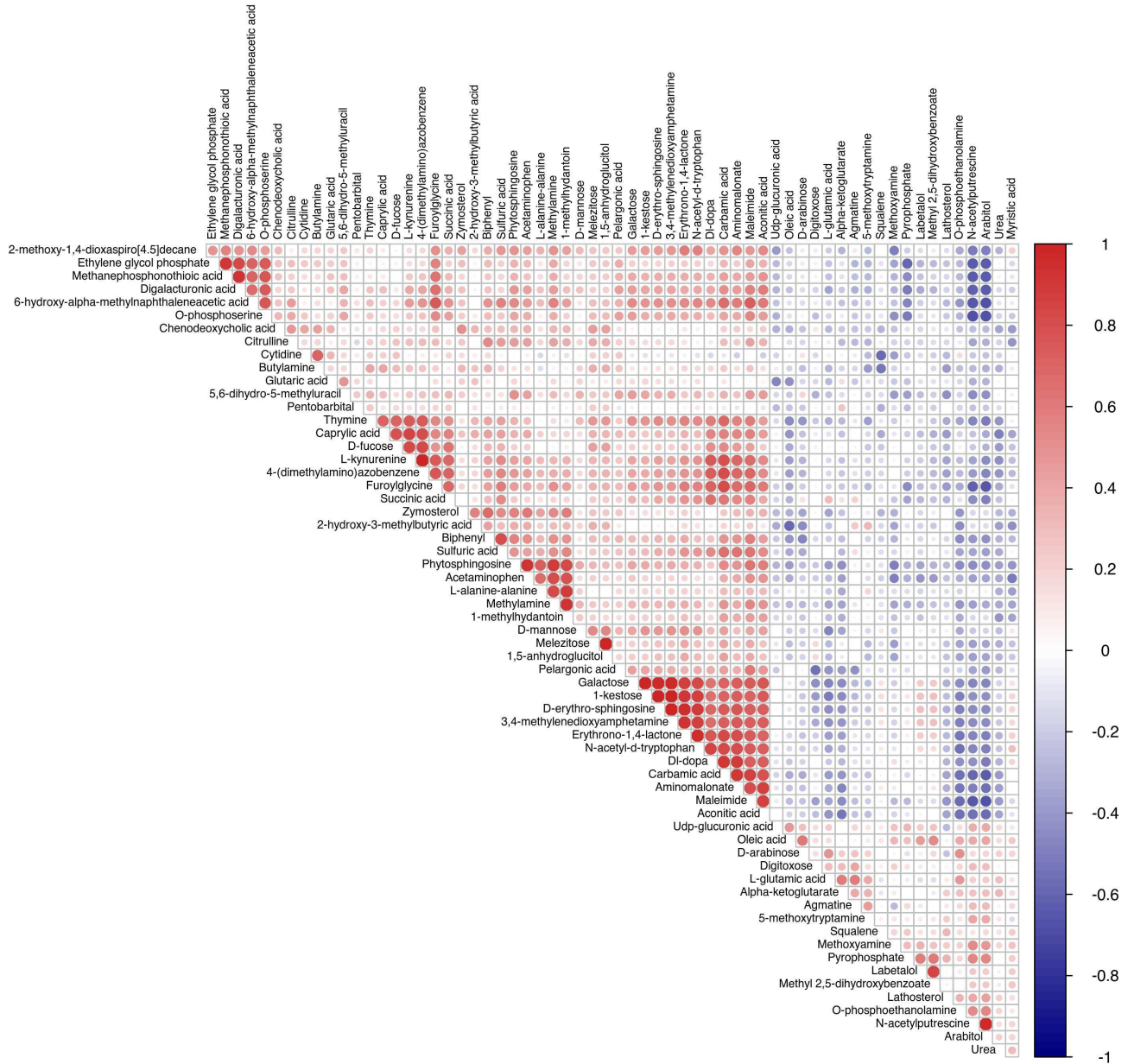


Figure S8 The correlation of metabolites between the ACS and ACS-HTN groups. The color of the circle represents the size of correlation in the data, with blue being the lowest value and red being the highest value. ACS, acute coronary syndrome; HTN, hypertension.