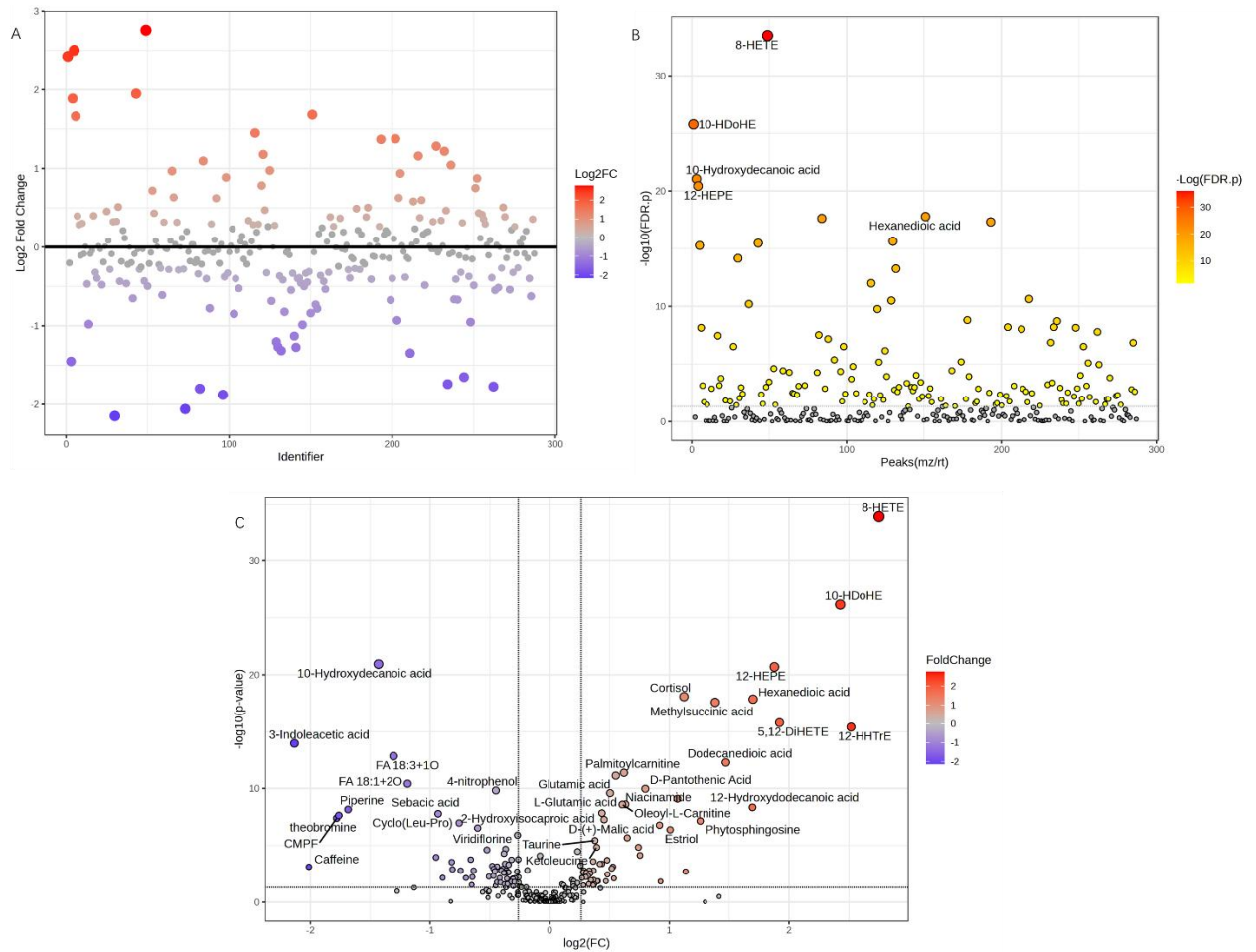
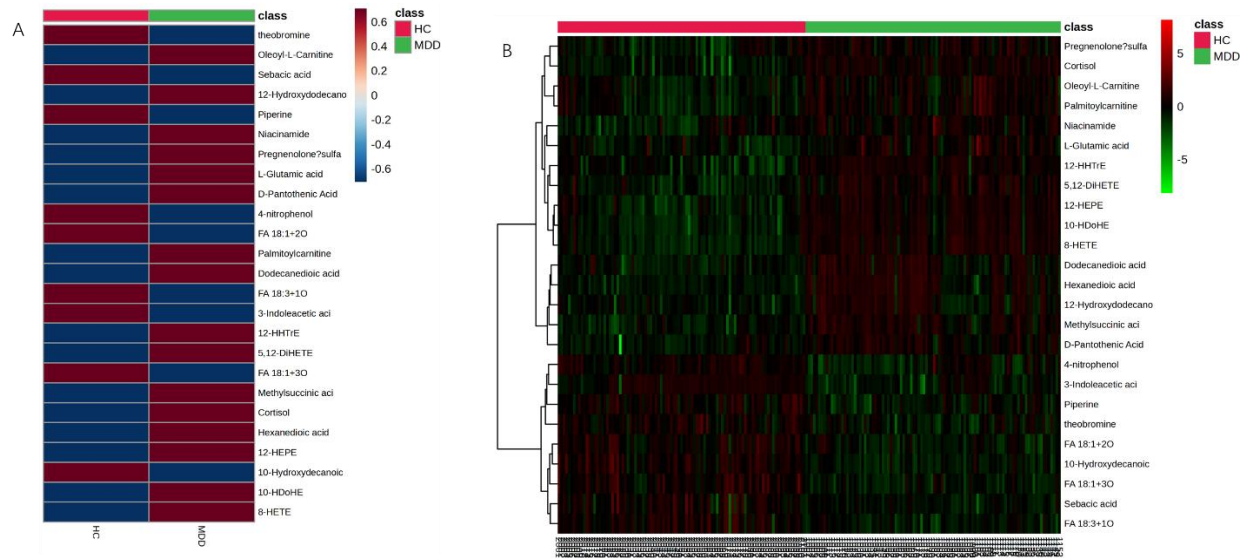


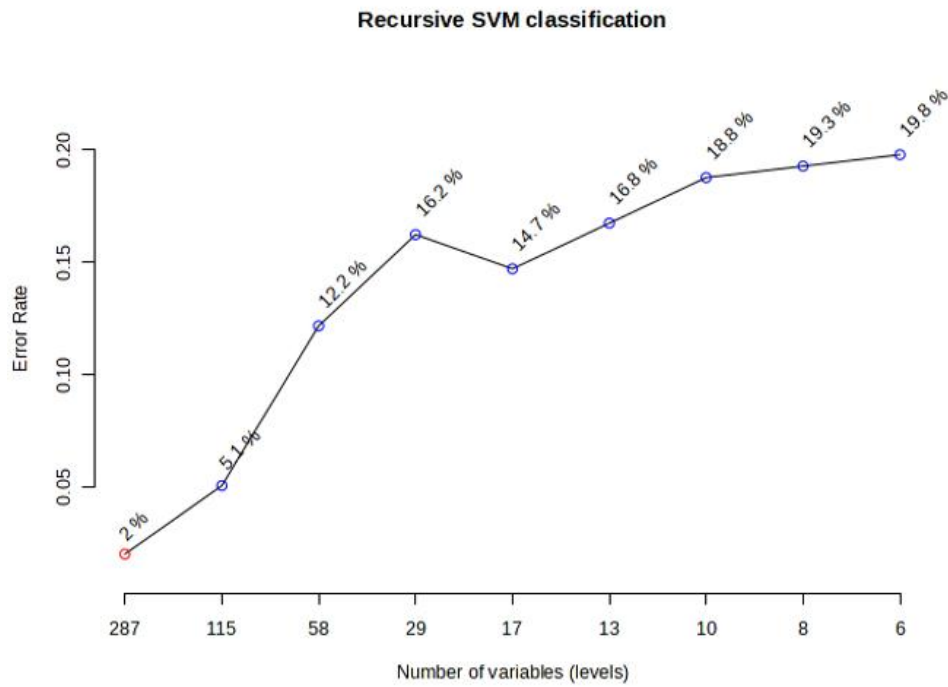
**Supplemental Figure 1 Overview of principal component analysis results for major depressive disorder and healthy control.** A: Top 2 components of principal component analysis for untargeted metabolomic profiling of serum samples in major depressive disorder, and healthy control samples; B: Screen plot of top 5 components. HC: Healthy control; MDD: Major depressive disorder.



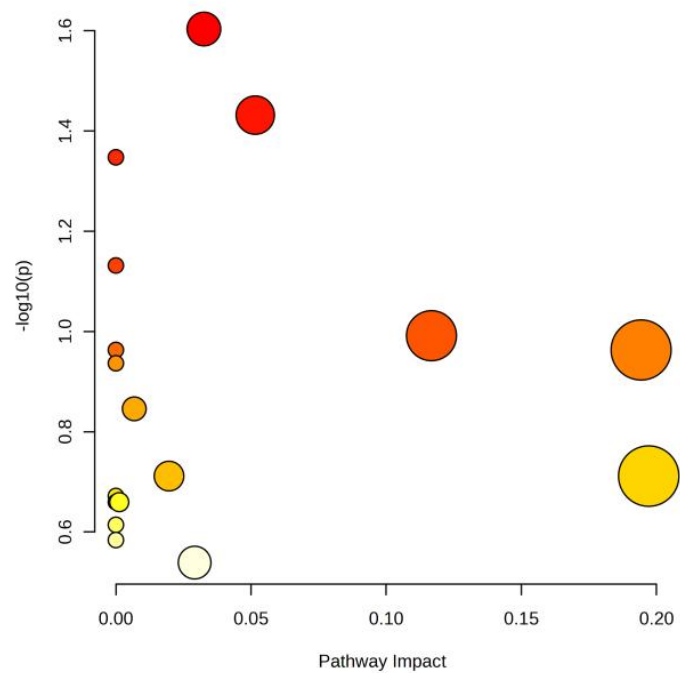
**Supplemental Figure 2 Metabolite differential analysis.** A: The fold change analysis is to compare the absolute values of change between two group means; B and C: Two-sample *t*-tests (B) Volcano plot (C). Red indicates the metabolites with significant up-regulation, blue represents the metabolites with significant down-regulation, and black denotes the metabolites with no significant difference.



**Supplemental Figure 3 Heatmap of top 25 features of t test.** A and B: Red indicates that the value in the major depressive disorder group is significantly greater than that in the healthy control (HC) group, and blue indicates that it is significantly less than that in the HC group. HC: Healthy control; MDD: Major depressive disorder.



**Supplemental Figure 4 R-SVM uses SVM (with linear kernel) to perform classification recursively using different feature subsets. The features used by the best model are plotted.**



**Supplemental Figure 5** Pathway analysis of potential metabolic mechanism of candidate metabolic biomarkers for major depressive disorder.