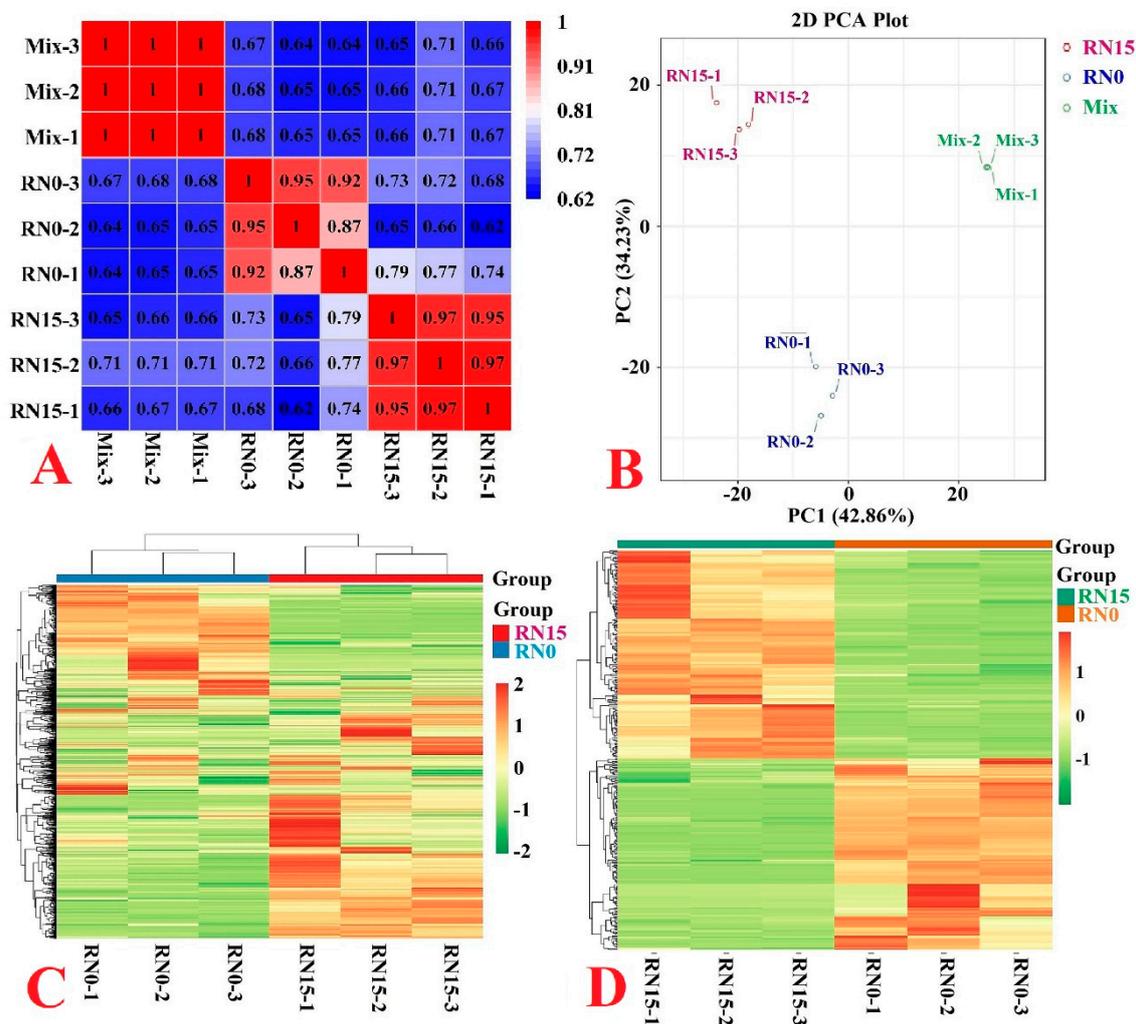
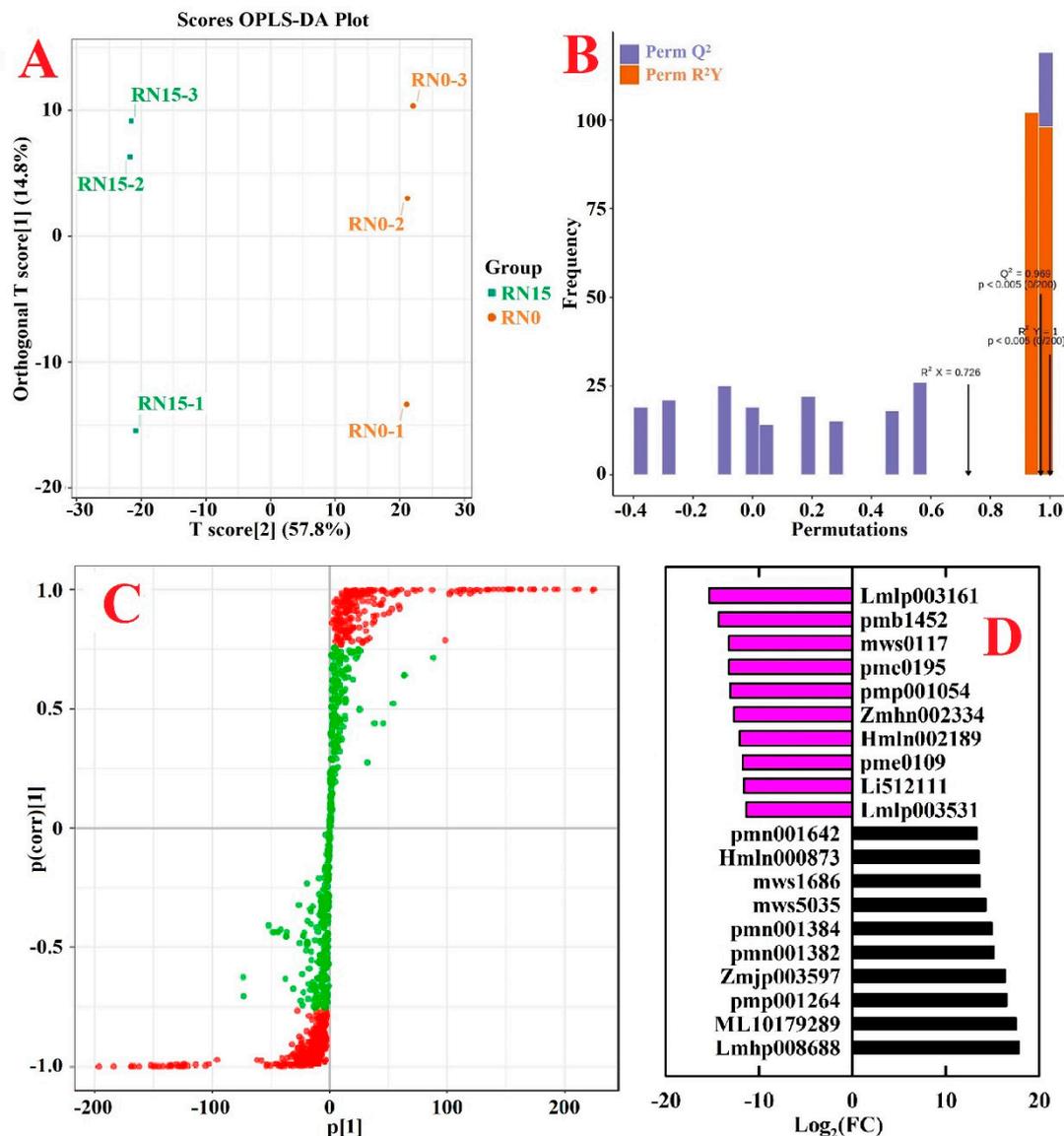


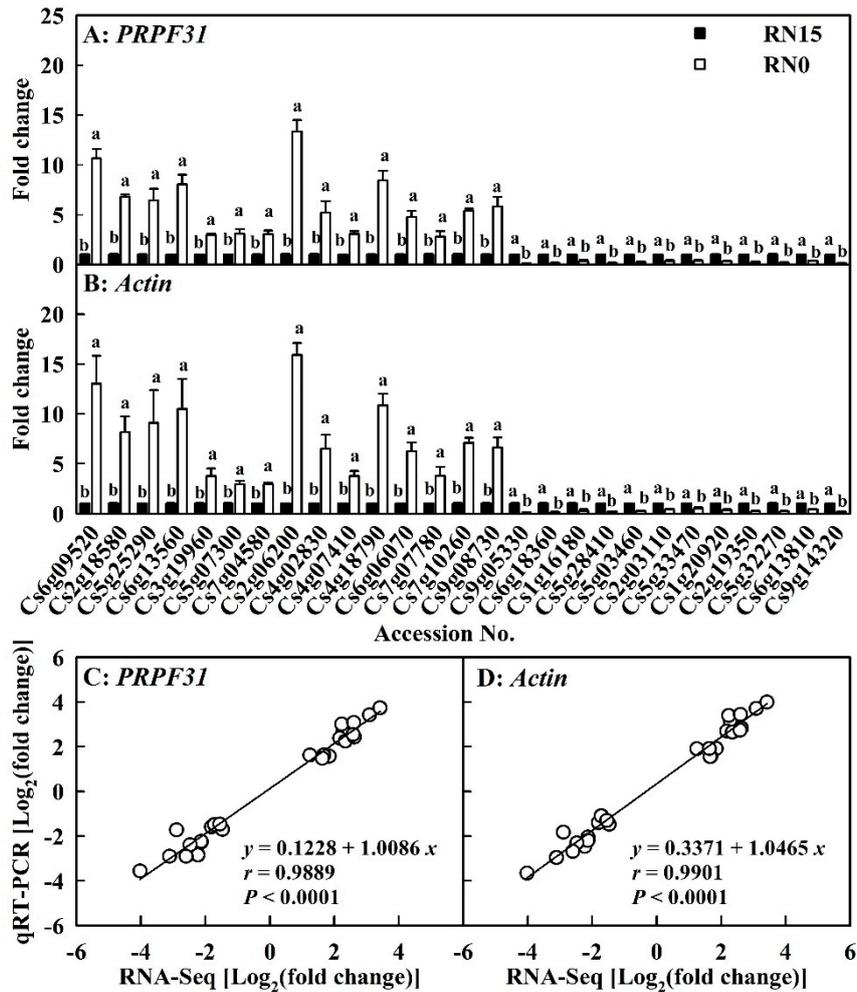
## Figures S1-S5



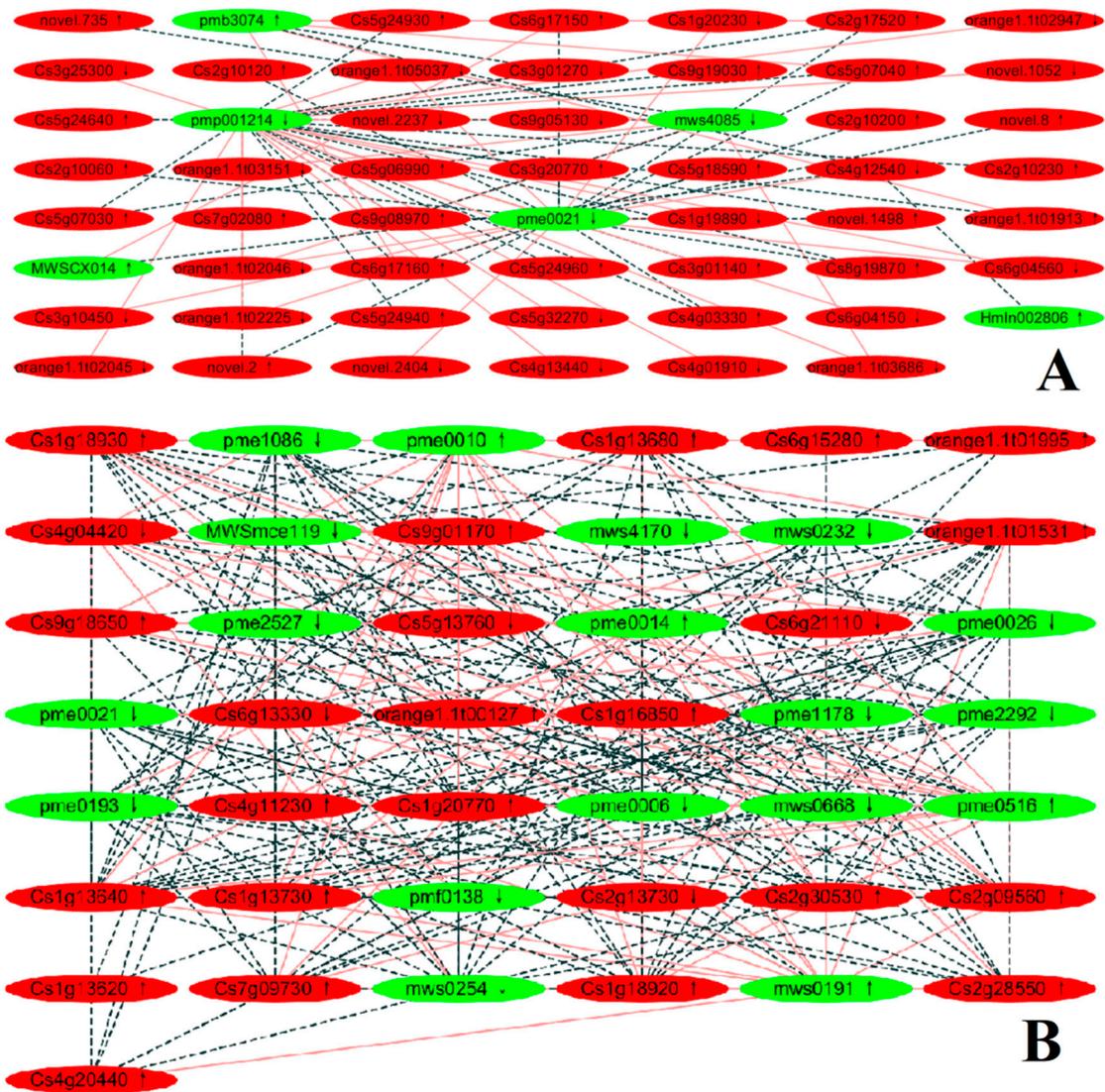
**Figure S1.** Pearson correlation coefficient ( $R^2$ ) matrix among RN15, RN0, and quality control samples (Mix; **A**), 2D PCA plot (**B**) and HCA (**C**) of total metabolites identified in RN15 and/or RN0, and HCA of differentially abundant metabolites (DAMs, **D**)



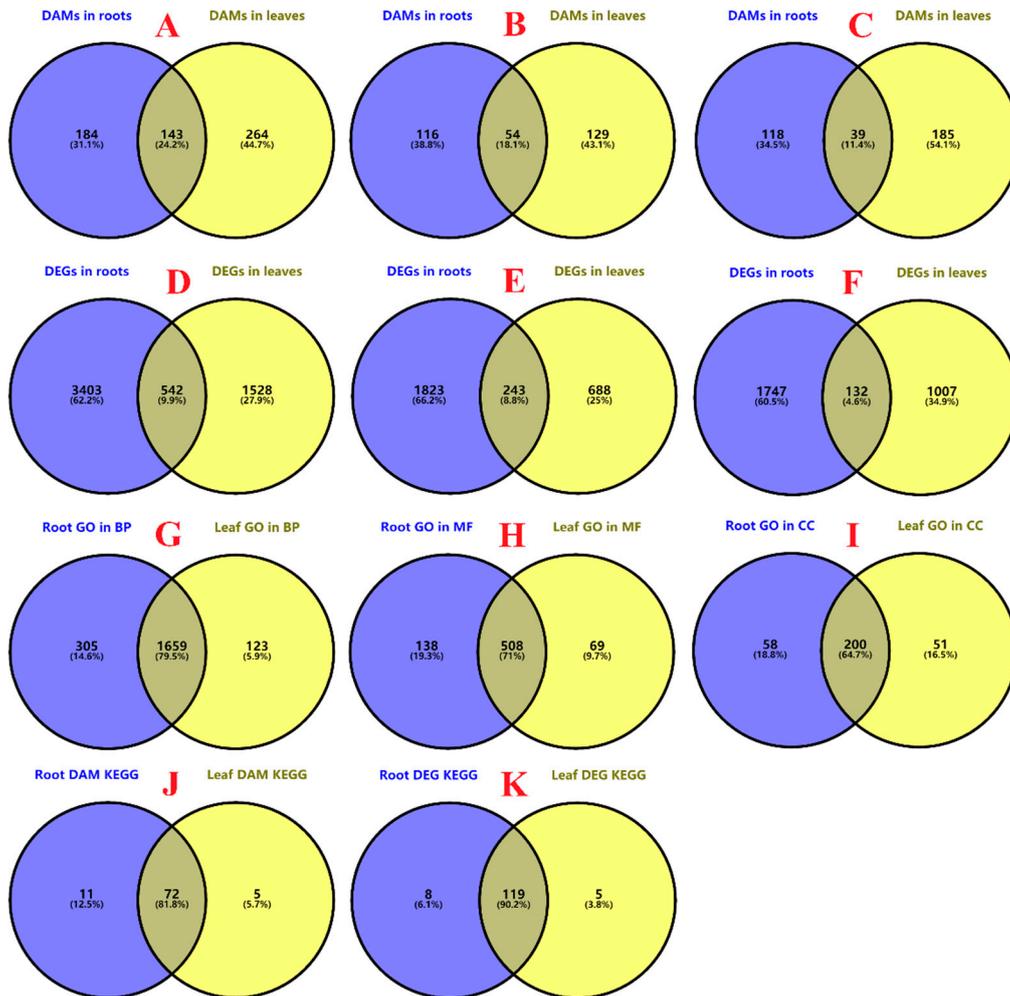
**Figure S2.** Score scatter plots of OPLS-DA model (A), permutation test of OPLS-DA model (B), and S-plot of OPLS-DA (C) for RN0 vs. RN15, and top abundant 10 upregulated and 10 downregulated metabolites detected in RN0 (D). For (A), the abscissa represents the predicted scores of PC1, and the ordinate represents the scores of the orthogonal principal components. For (B),  $R^2Y$  and  $R^2X$  are the explanatory rate of the model to  $y$  and  $x$  matrix, respectively, and  $Q^2$  is the predicative ability of the model. For (C), red dot and green dots represent  $VIP \geq 1$  and  $< 1$ , respectively; the abscissa represents the covariance of the principal components and metabolites, and the ordinate represents the correlation coefficient between the principal component and the metabolites.



**Figure S3.** qRT-PCR validation of 27 DEGs detected in RN0 using *PRPF31* (A) and *Actin* (B) as internal standards, and the correlation analysis of RNA-Seq data and qRT-PCR results using *PRPF31* (C) and *actin* (D) as internal standards. Bars represent means  $\pm$  SE of two technique and three biological replicates. For the same genes, different letters above the bars indicate a significant difference at  $P < 0.05$ .



**Figure S4.** DAM-DEG Pearson correlation networks involved in phenylpropanoid biosynthesis (ko00940; **A**) and ABC transporters (ko02010; **B**) in RN0. Metabolite-gene pairs were connected by edges; red solid and black dashed lines represent positive and negative correlation, respectively; green and red nodes represent DAMs and DEGs, respectively. ↓, downregulation; ↑, upregulation.



**Figure S5.** Venn analysis of total (A), downregulated (B), and upregulated (C) DAMs detected in RN0 and LN0, total (D), downregulated (E), and upregulated (F) DEGs isolated in RN0 and LN0, enriched GO terms for DEGs isolated in RN0 and LN0 in BP (G), MF (H), and CC (I), and enriched KEGG pathways for DAMs (J) and DEGs (K) isolated in RN0 and LN0.