

Figure S1. The glucosinolates content of parents and their F₂ population.

(A) Comparison of glucosinolates content between B0401 and MS84003 at commercial stage. RAA, (*R_S*)-4-(methylsulfinyl)butyl GSL (Glucoraphanin), GBC, Indol-3-methyl GSL (Glucobrassicin), ERU, 4-(Methylsulfonyl)butyl GSL (Glucoerucin), ALY, (*R_S*)-5-(Methylsulfinyl)pentyl GSL (Glucoalyssin), 4ME, 4-Methoxyindol-3-ylmethyl GSL (4-methoxyglucobrassicin), NEO, 1-Methoxyindol-3-ylmethyl GSL (Neoglucobrassicin). *** $P < 0.01$. Frequency histogram of RAA in leaf (B), stalk (C) at vegetative growth stage and floret (D) at commercial stage in F₂ plants. FW, fresh weight; DW, dry weight.

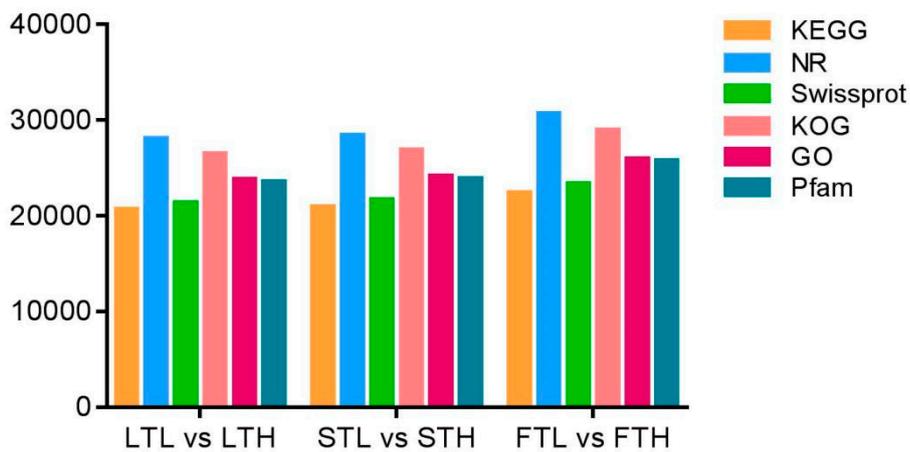


Figure S2. The number of transcripts annotated by KEGG, nonredundant (NR), Swiss-Prot, EuKaryotic Orthologous Groups (KOG), GO and Pfam databases.

LTL, STL and FTL represent low RAA content pools in leaf, stalk and floret, respectively. LTH, STH and FTH represent high RAA content pools in leaf, stalk and floret, respectively.

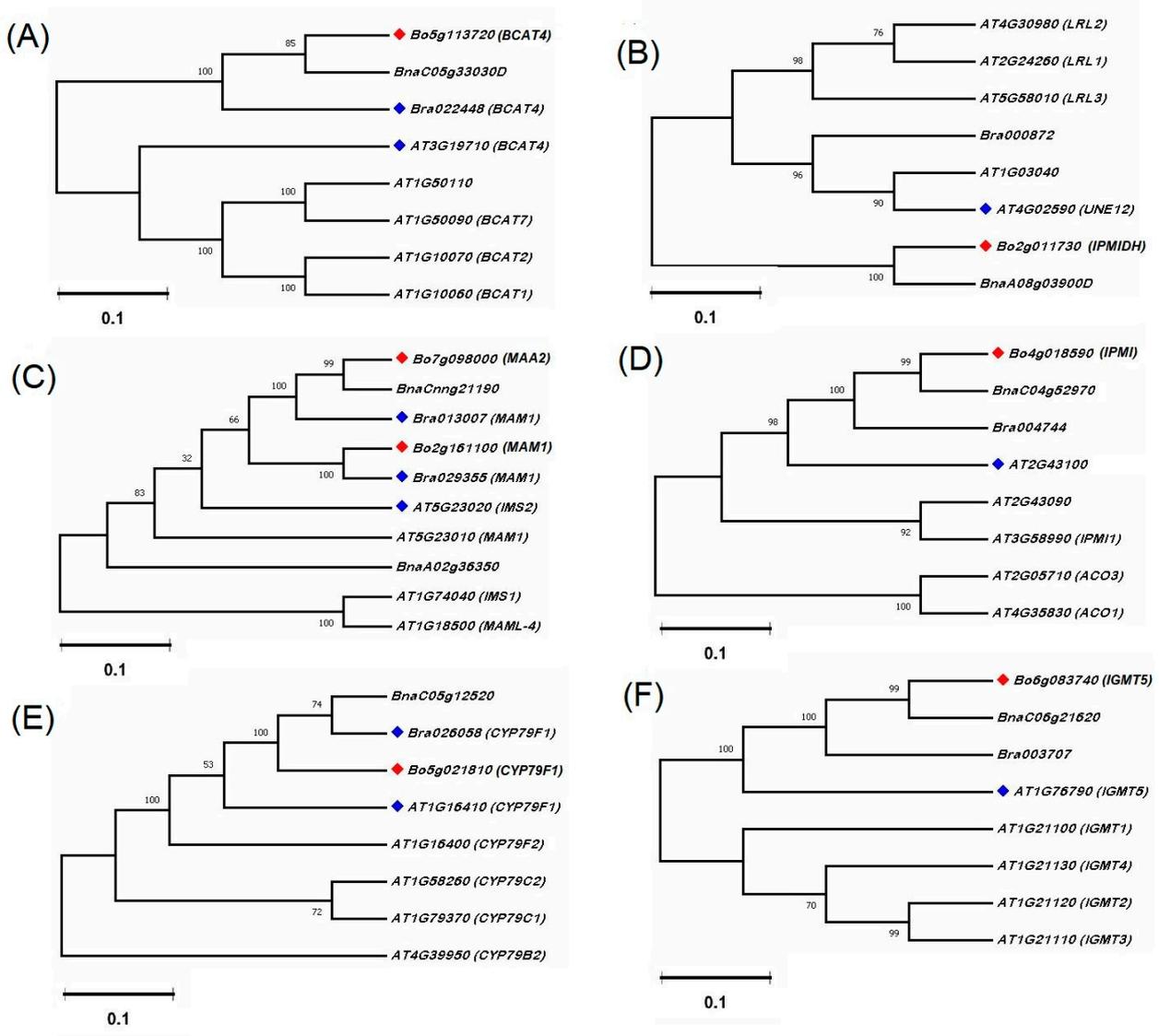


Figure S4. Phylogenetic analysis of DEGs involved in glucosinolate biosynthesis.

Phylogenetic tree of *Bo5g113720* (A), *Bo2g011730* (B), *Bo2g161100* and *Bo7g098000* (C), *Bo4g018590* (D), *Bo5g021810* (E) and *Bo6g083740* (F). Mega 7.0 was used to build the phylogenetic tree by the neighbor-joining method (<https://www.megasoftware.net/>). The scale bar indicates a branch length of 0.1. Red and blue boxes represent the gene itself and genes with functional annotations in *Brassica rapa* and *Arabidopsis thaliana*.

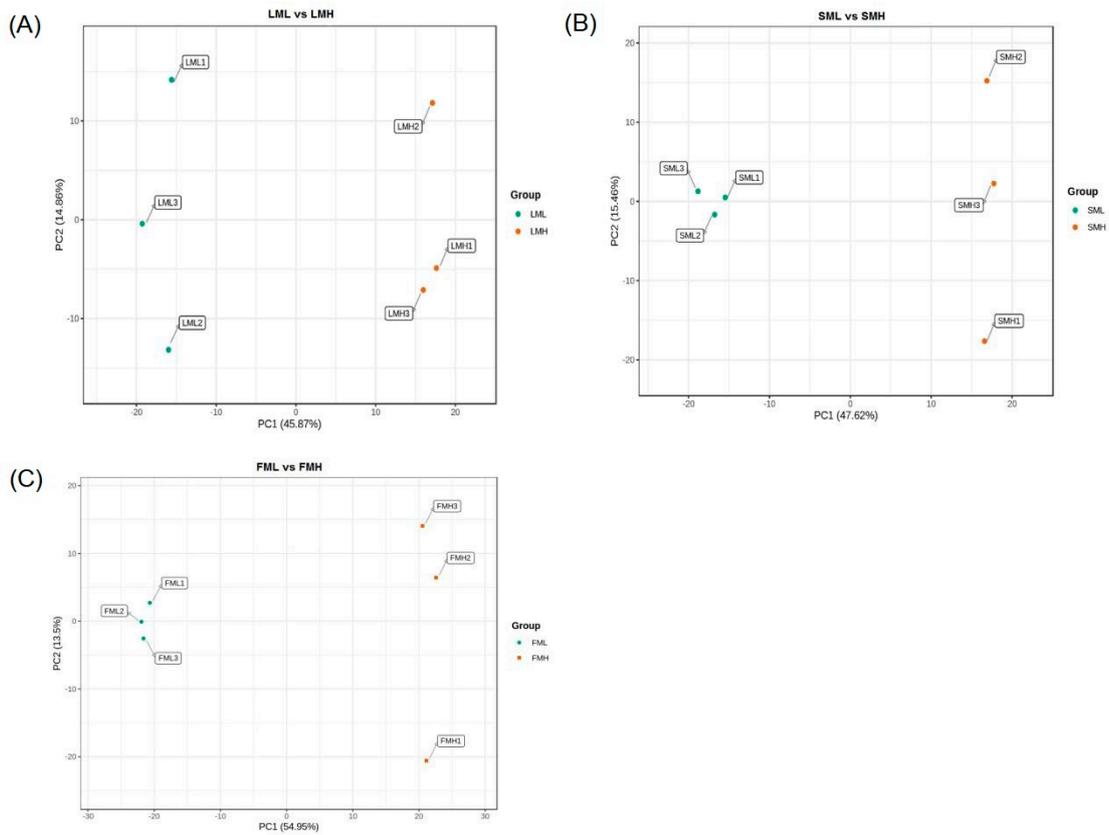


Figure S5. PCA of differentially accumulated metabolites in LML vs LMH (A), SML vs SMH (B), and FML vs FMH (C).

LML, SML and FML represent low RAA content pools in leaf, stalk and floret, respectively. LMH, SMH and FMH represent high RAA content pools in leaf, stalk and floret, respectively.

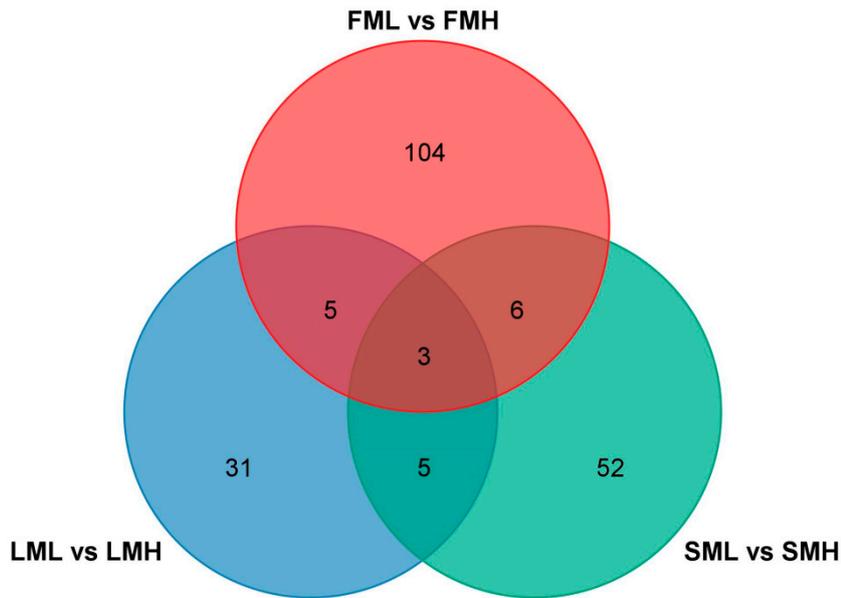


Figure S6. Coregulation among DAMs in all comparison groups.

LML, SML and FML represent low RAA content pools in leaf, stalk and floret, respectively. LMH, SMH and FMH represent high RAA content pools in leaf, stalk and floret, respectively.

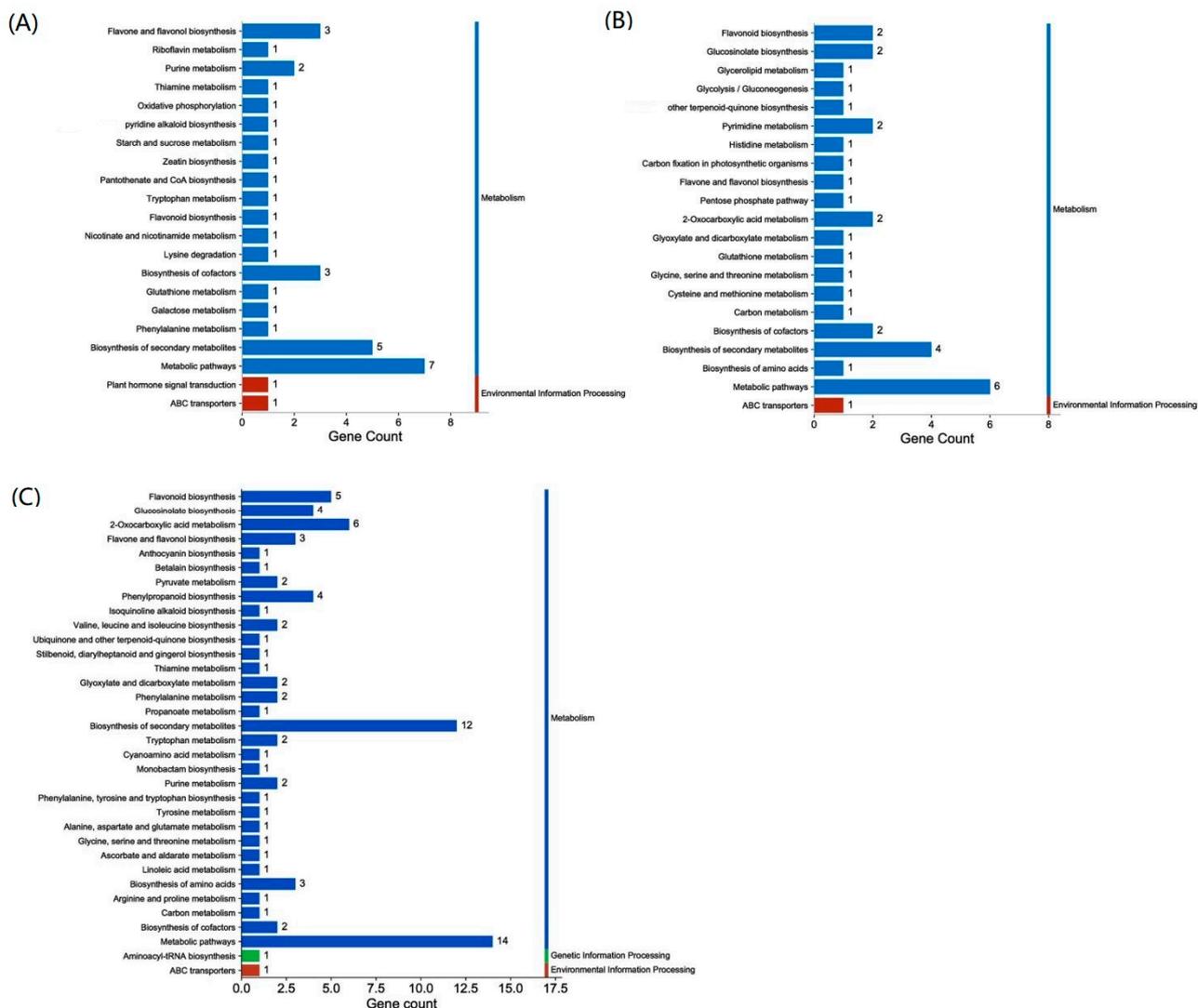


Figure S7. Kyoto Encyclopedia of Genes and Genomes (KEGG) functional classification of differential accumulated metabolites (DAMs) in LML vs LMH (A), SML vs SMH (B), and FML vs FMH (C) pools.

The X axis is the number of annotated genes to different categories of KEGG. The Y axis represents different categories of KEGG. Blue column, Metabolism systems; Brown column, Environmental information processing. LML, SML and FML represent low RAA content pools in leaf, stalk and floret, respectively. LMH, SMH and FMH represent high RAA content pools in leaf, stalk and floret, respectively.

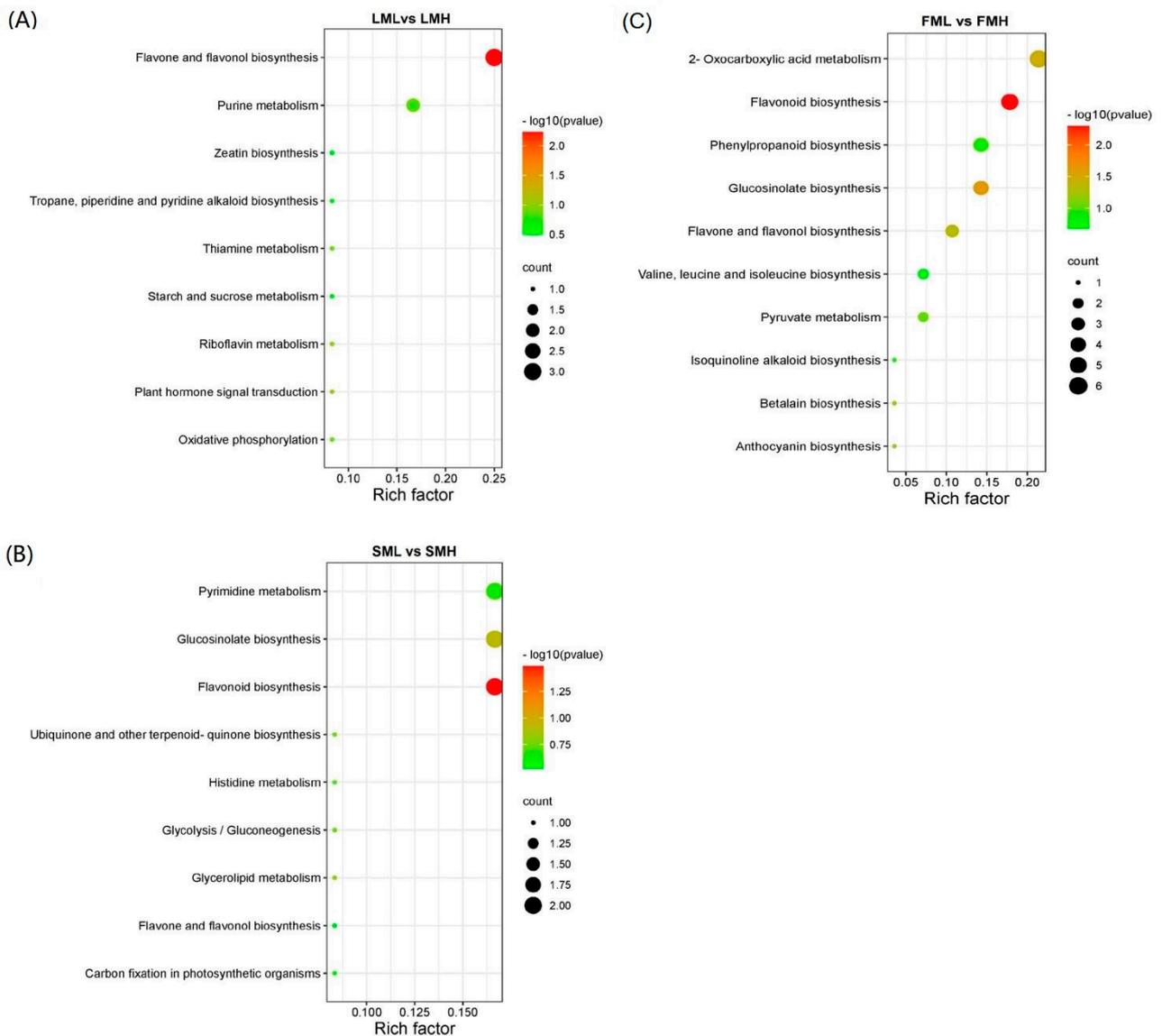


Figure S8. KEGG pathway of DAMs in LML vs LMH (A), SML vs SMH (B), and FML vs FMH (C) pools.

The X-axis is the rich factor; the Y-axis represents the name of the pathway. The bubbles size represents the number of DAMs involved. The bubbles color indicates the enrichment degree of pathway and the size represents the number of DAMs enrichment in the pathway. LML, SML and FML represent low RAA content pools in leaf, stalk and floret, respectively. LMH, SMH and FMH represent high RAA content pools in leaf, stalk and floret, respectively.

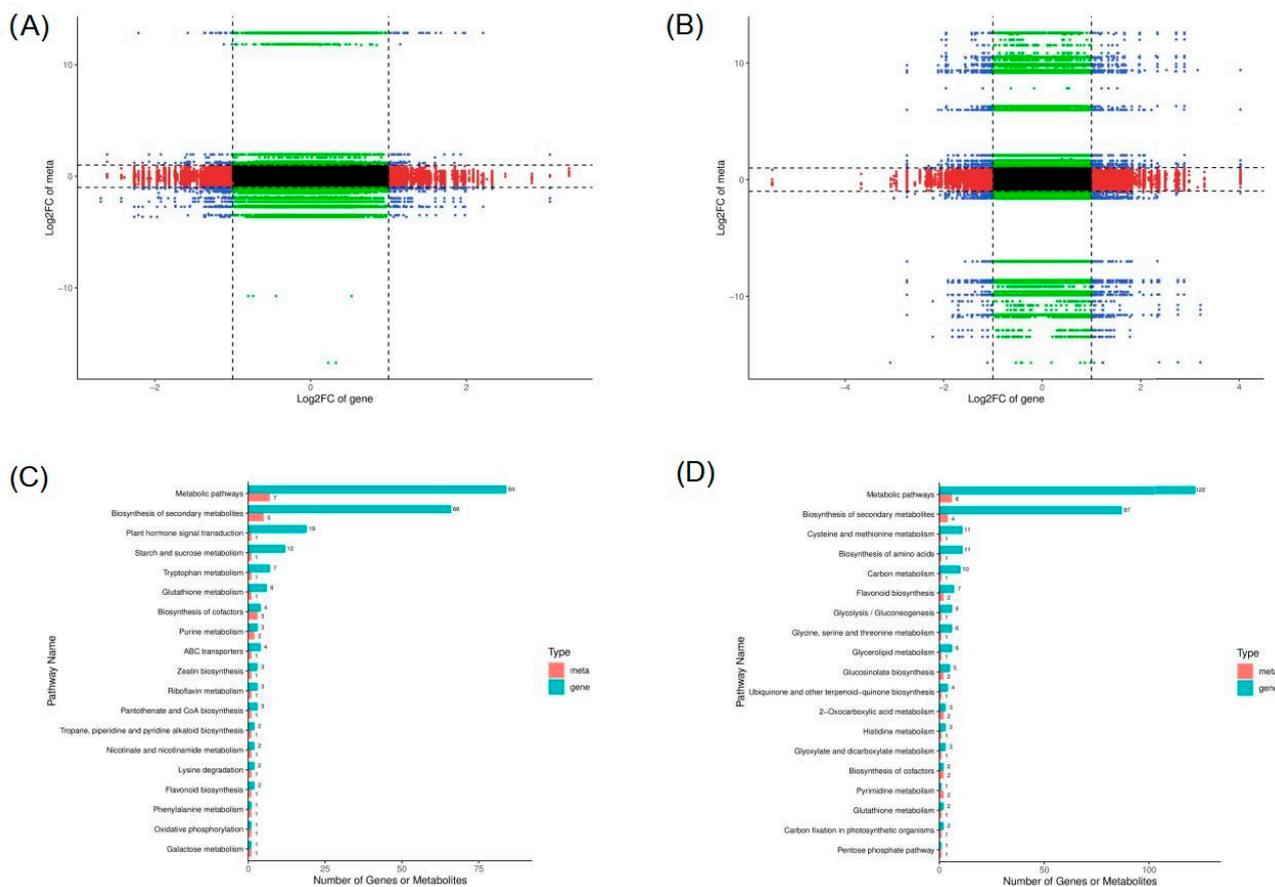


Figure S9. Correlation analysis between transcriptome and metabolome in LML vs LMH and SML vs SMH.

The nine-quadrant diagram shows the correlation of genes and compounds between LML and LMH (A), SML and SMH (B). KEGG enrichment analysis of DEGs (red column) and DAMs (blue column) enriched in the same pathway in LML vs LMH (C), SML vs SMH (D). LML and SML represent low RAA content pools in leaf and stalk, respectively. LMH and SMH represent high RAA content pools in leaf and stalk, respectively.