

Supplementary Materials

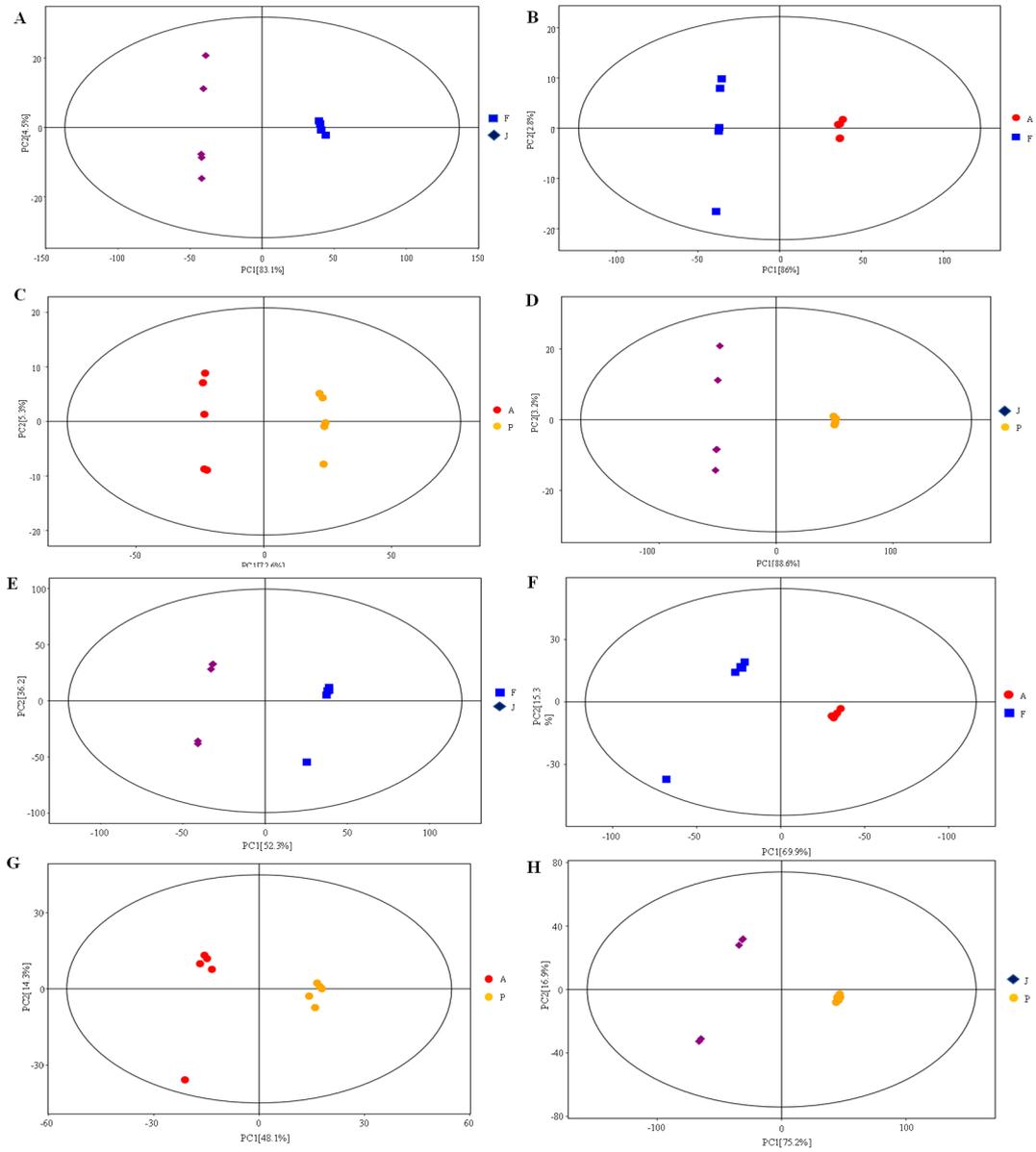


Figure S1. Plot of PCA scores between different stages in ESI^+ (A–D) and ESI^- (E–H). (Purple: J stage; Blue: F stage; Red: A stage; Orang: P stage)

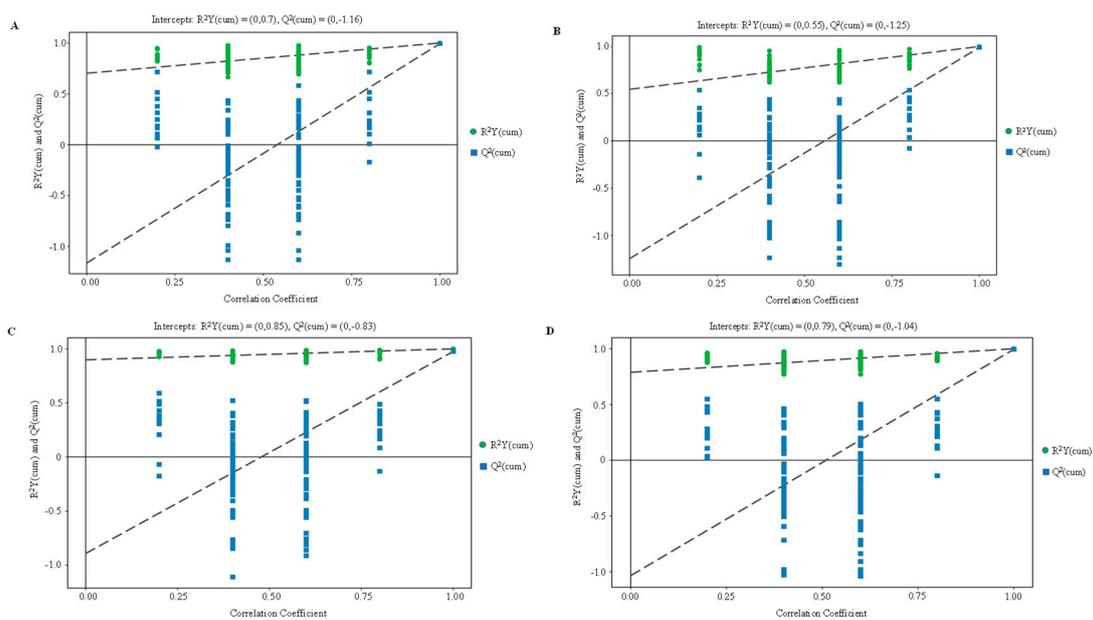


Figure S2. Cross-Validation and Alternate Testing of OPLS-DA Models (ESI^+). ((A): J vs F; (B): F vs A; (C): A vs P; (D): J vs P).

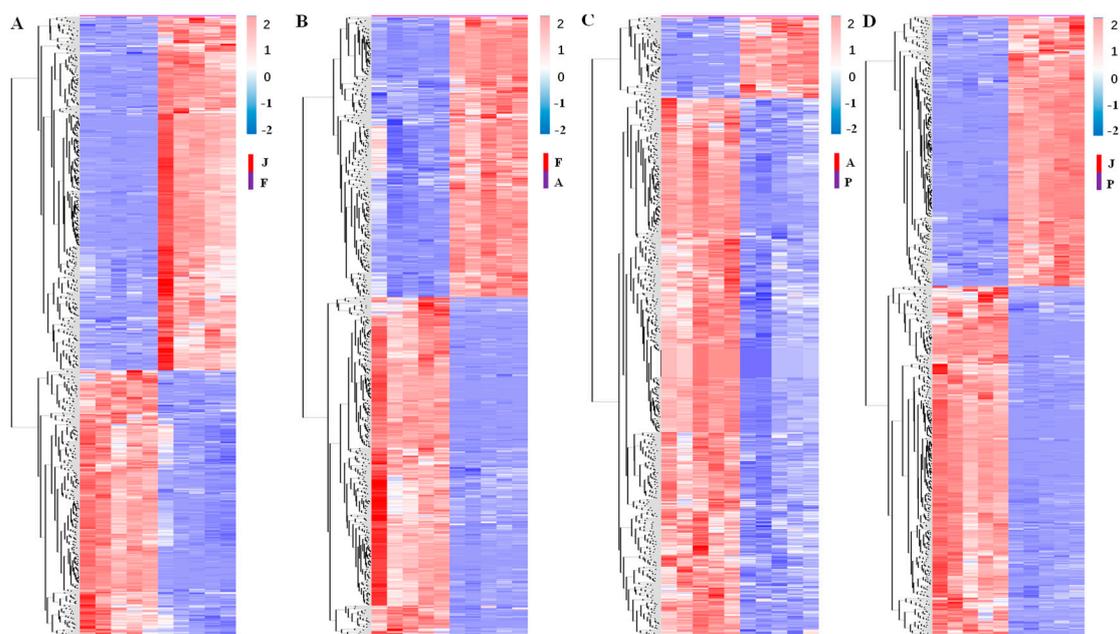


Figure S3. Hierarchical cluster analysis heat map of different brewing stages of mulberry wine. The sample names are displayed in the abscissa, and the differential metabolites are displayed in the ordinate. The color transformation from blue to red represents the relative abundance of metabolite expression from low to high. ((**A**): J vs F; (**B**): F vs A; (**C**): A vs F; (**D**): J vs P).

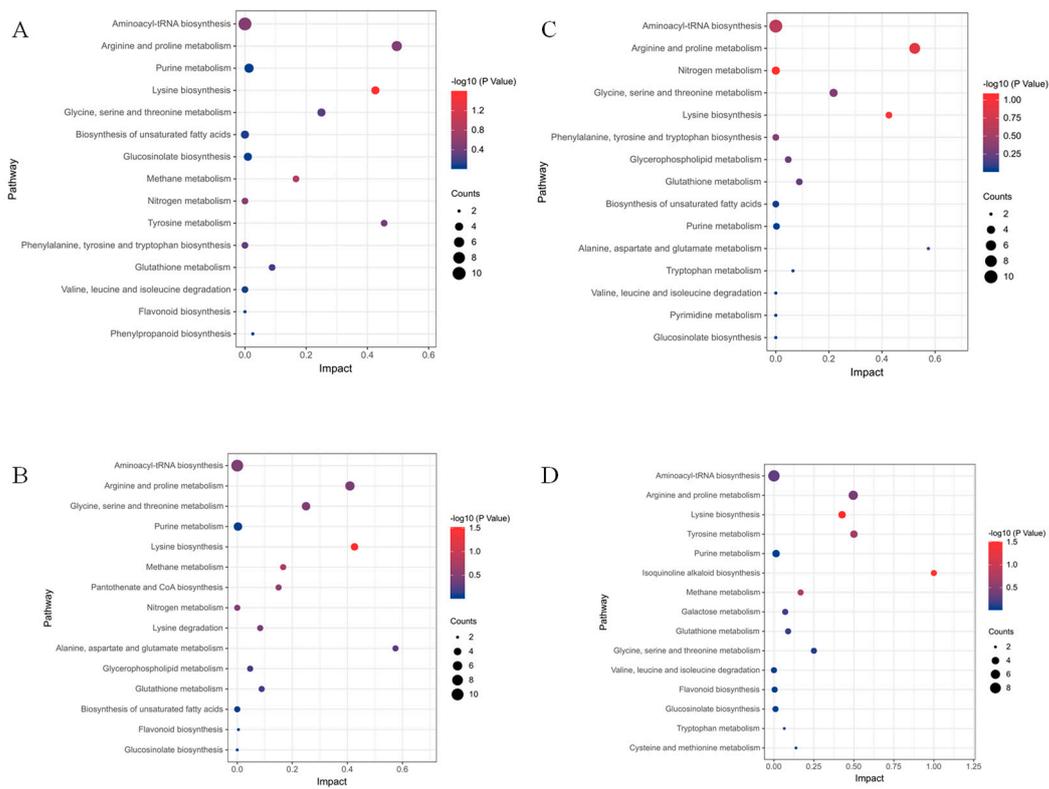


Figure S4. Enrichment analysis of differential metabolite pathways ((A): J vs F; (B): F vs A; (C): A vs P; (D): J vs P). The color represents the p-value and the bubble represents the number of enrichments of differential metabolites.

Supplementary Table S2. Mantel test result of the comparisons between major metabolites and physicochemical factors in mulberry wine brewing process.

Differential Metabolites	Physicochemical Factors	Mantel's r
Amino acids	pH	0.72
	TS	0.76
	TSS	0.21
	TA	0.29
	Alcohol	0.86
Aromatic compounds	pH	0.82
	TS	0.87
	TSS	0.18
	TA	0.50
	Alcohol	0.92
Fatty acids	pH	0.43
	TS	0.51
	TSS	0.52
	TA	0.22
	Alcohol	0.63
Organic acids	pH	0.59
	TS	0.69
	TSS	0.41
	TA	0.21
	Alcohol	0.77
Polyphenols	pH	0.49
	TS	0.58
	TSS	0.45
	TA	0.17
	Alcohol	0.68
Carbohydrates	pH	0.11
	TS	0.20
	TSS	0.73
	TA	0.12
	Alcohol	0.33