

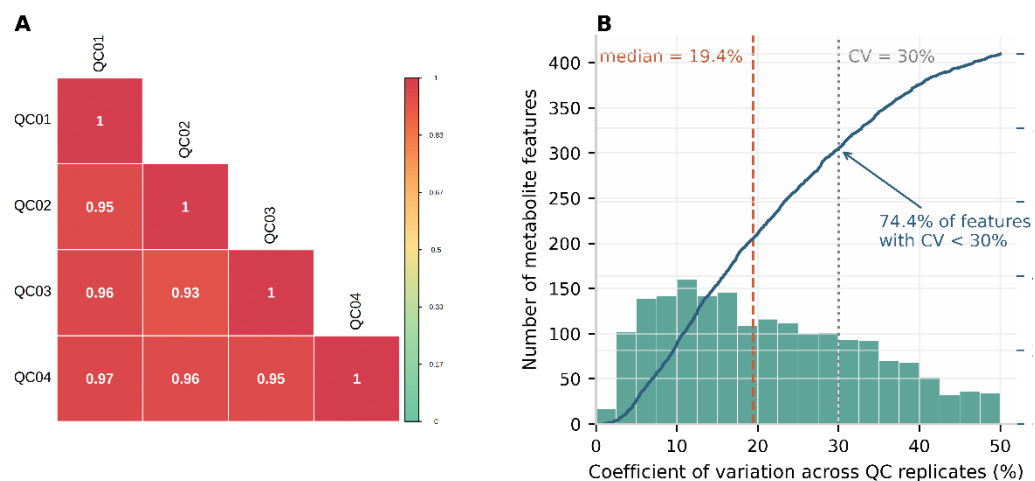


Figure S1: Pearson correlations among the four QC injections and the distribution of peak-area coefficients of variation. **(A)** Pearson correlations among the four quality-control (QC) injections ($r = 0.93\text{--}0.97$). **(B)** Distribution of peak-area coefficients of variation (CV) across QC replicates for all quantified features; the dashed line marks the median CV (19.4%) and the dotted line the 30% threshold. The blue cumulative curve (right axis) shows that 74.4% of features have $CV < 30\%$.

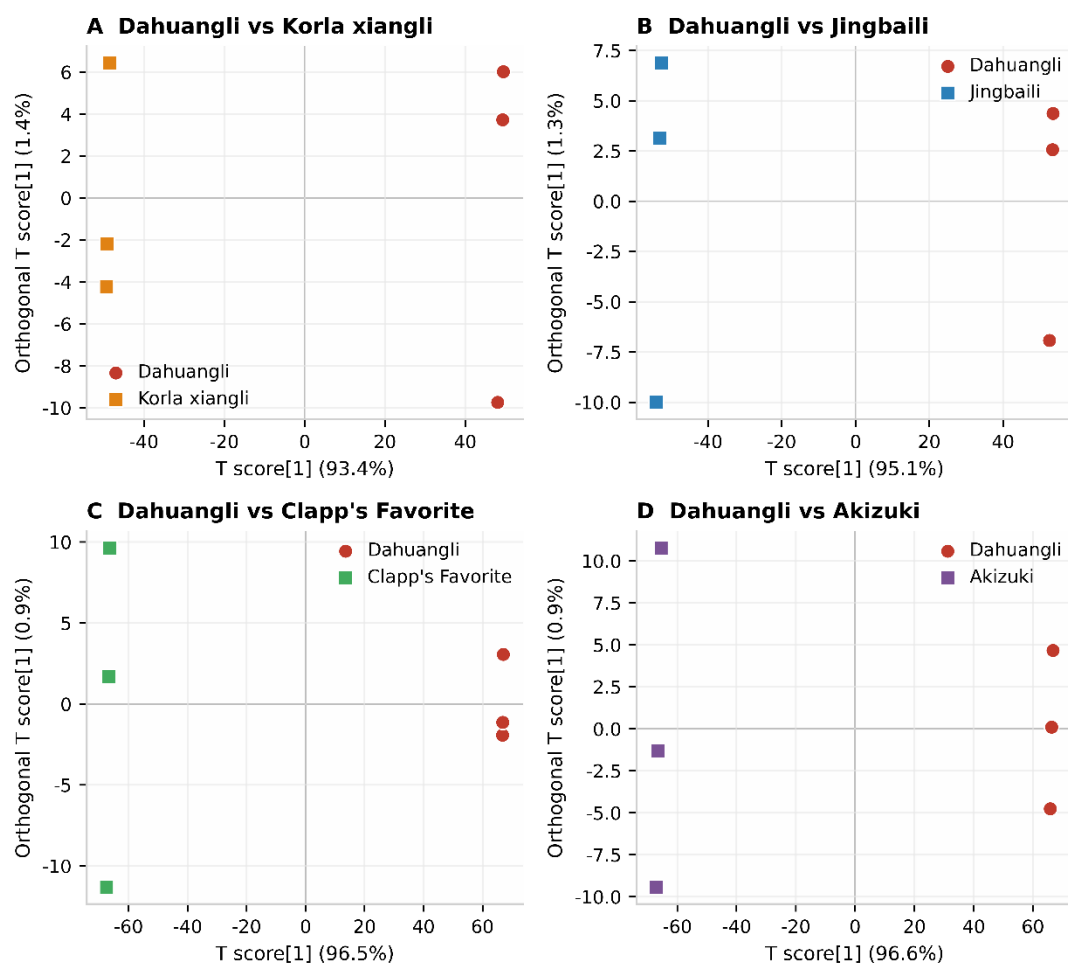


Figure S2: OPLS-DA score plots for the four pairwise comparisons of Dahuangli with each reference variety. (A) Dahuangli vs Korla xiangli; (B) Dahuangli vs Jingbaili; (C) Dahuangli vs Clapp's Favorite; (D) Dahuangli vs Akizuki. Dahuangli replicates (circles) separate completely from each reference cultivar (squares) along the predictive component in all four models.

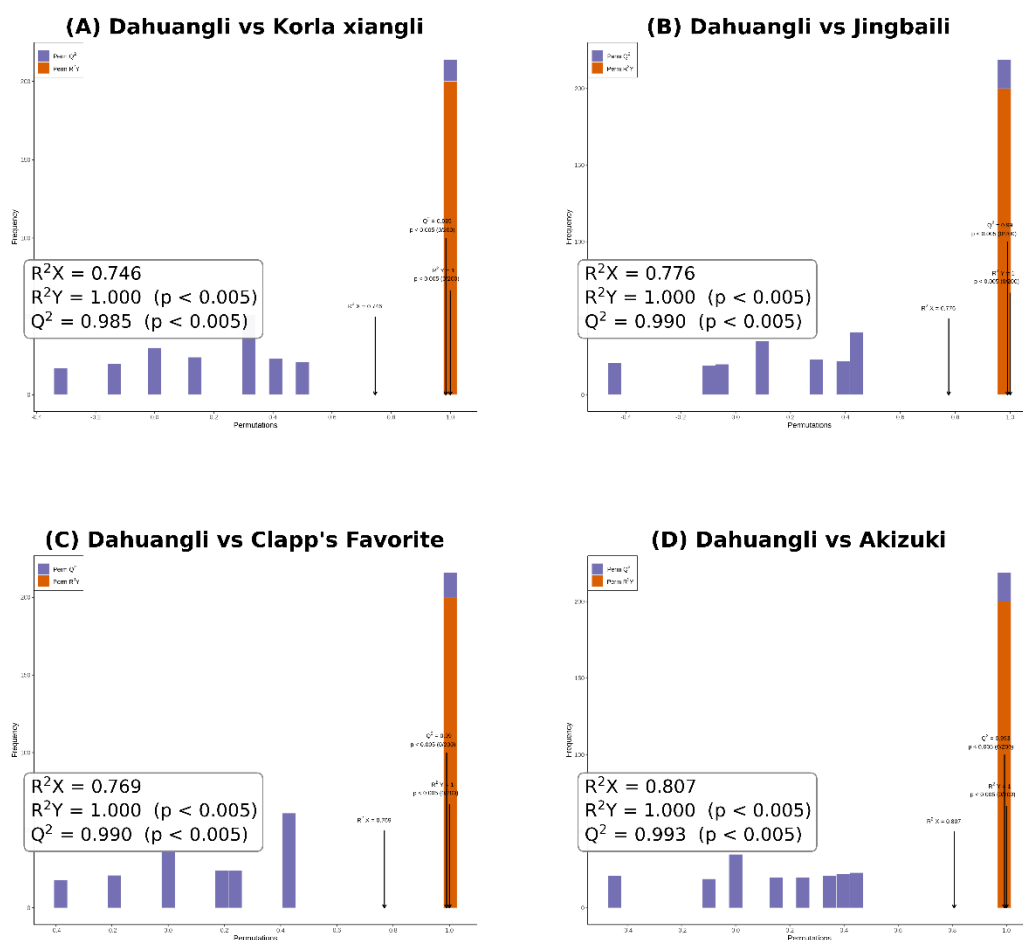


Figure S3: permutation test results (200 permutations) validating the four OPLS-DA models. (A) Dahuangli vs Korla xiangli; (B) Dahuangli vs Jingbaili; (C) Dahuangli vs Clapp's Favorite; (D) Dahuangli vs Akizuki. Histograms show the frequency distribution of permuted R^2Y (orange) and Q^2 (purple) values; the original model statistics (annotated in each panel, $R^2Y = 1.000$, $Q^2 = 0.985\text{--}0.993$) far exceed all permuted values ($p < 0.005$, 0/200), indicating no overfitting.

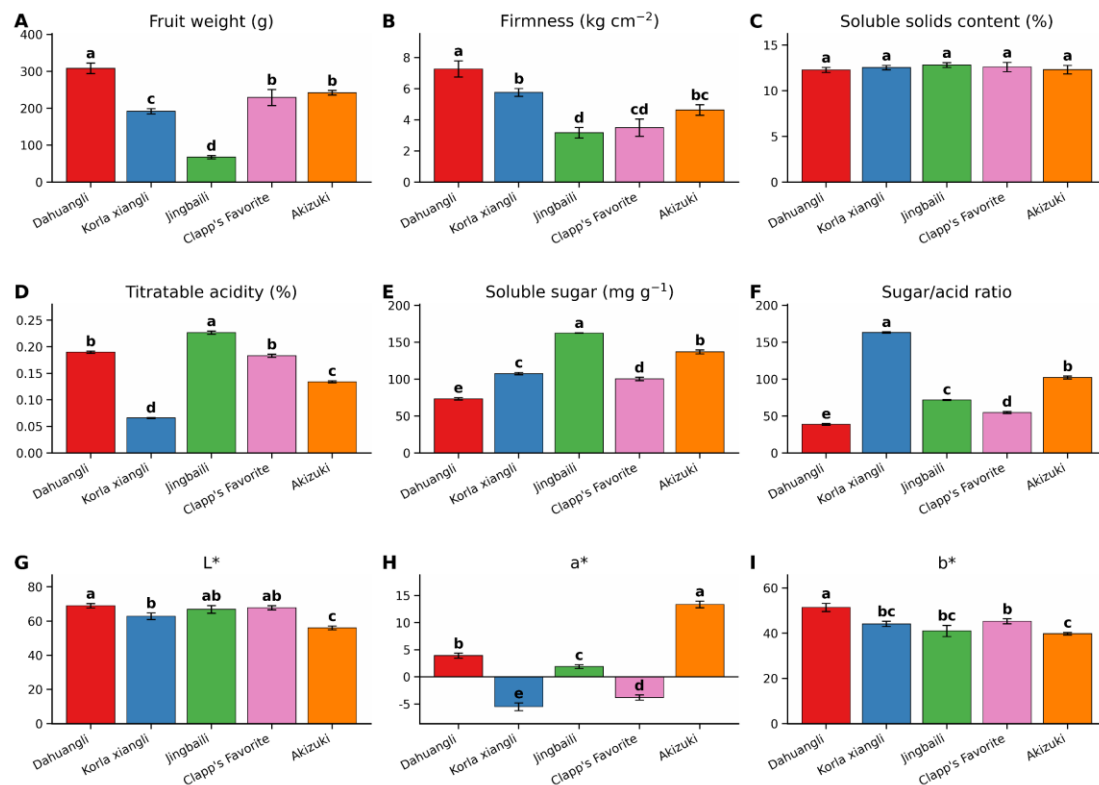


Figure S4: the eight quality traits across the five varieties. (A) Single-fruit weight; (B) firmness; (C) soluble solids content; (D) titratable acidity; (E) soluble sugar; (F) sugar–acid ratio; (G–I) skin colour coordinates L* (lightness), a* (redness) and b* (yellowness). Bars show the mean $\pm$ SE; different lowercase letters above bars indicate significant differences among cultivars.