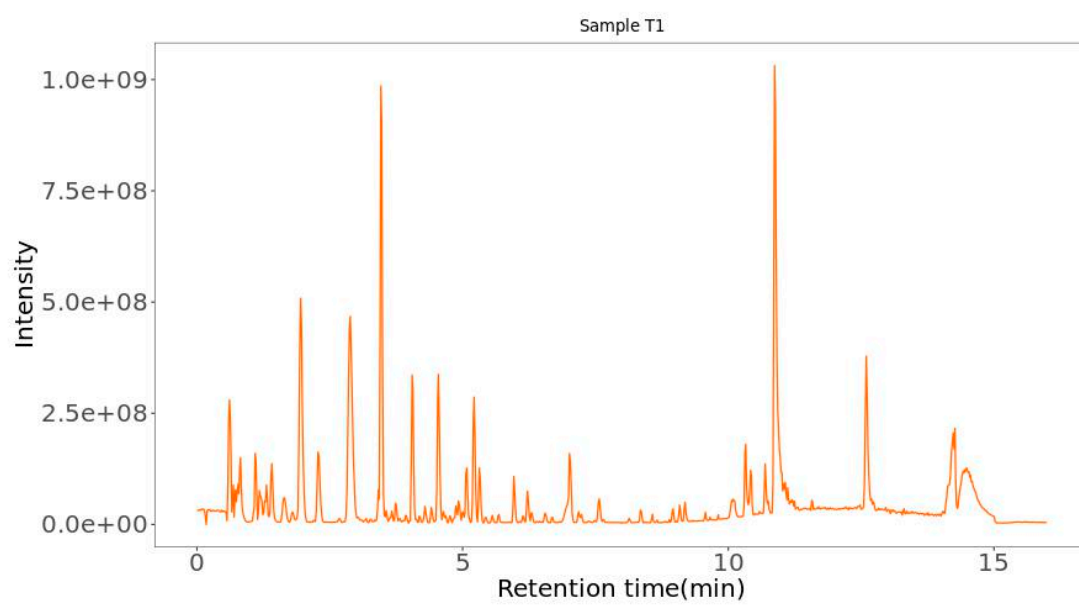
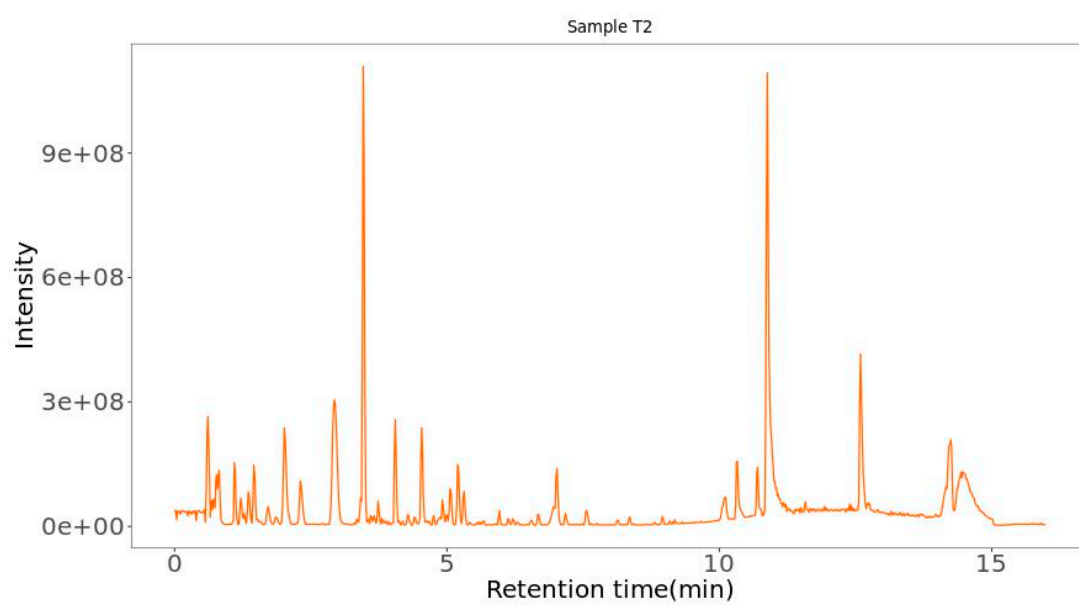


(A)



(B)



(C)

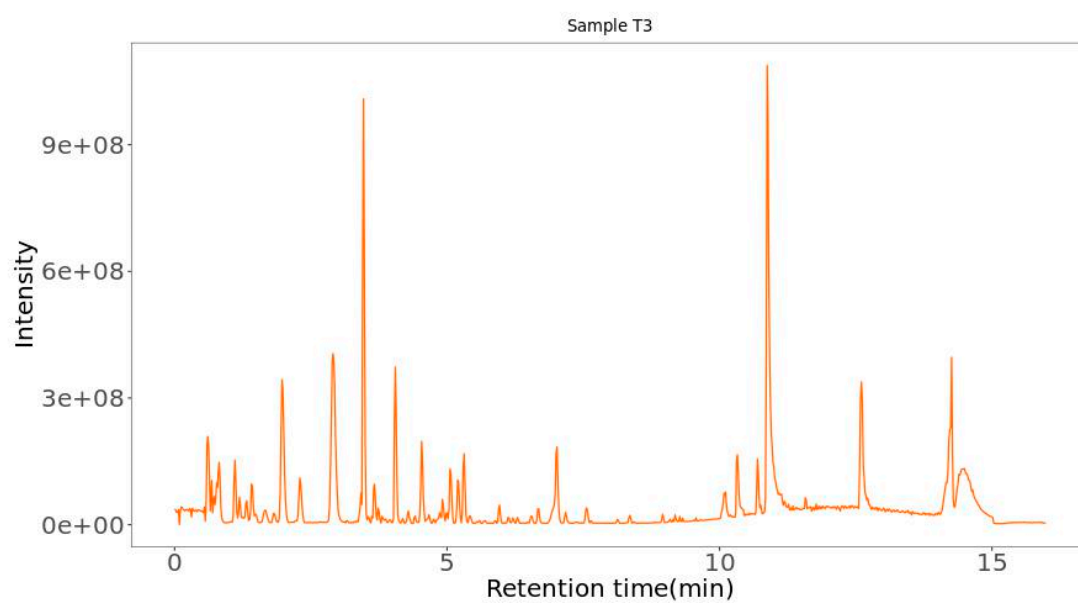
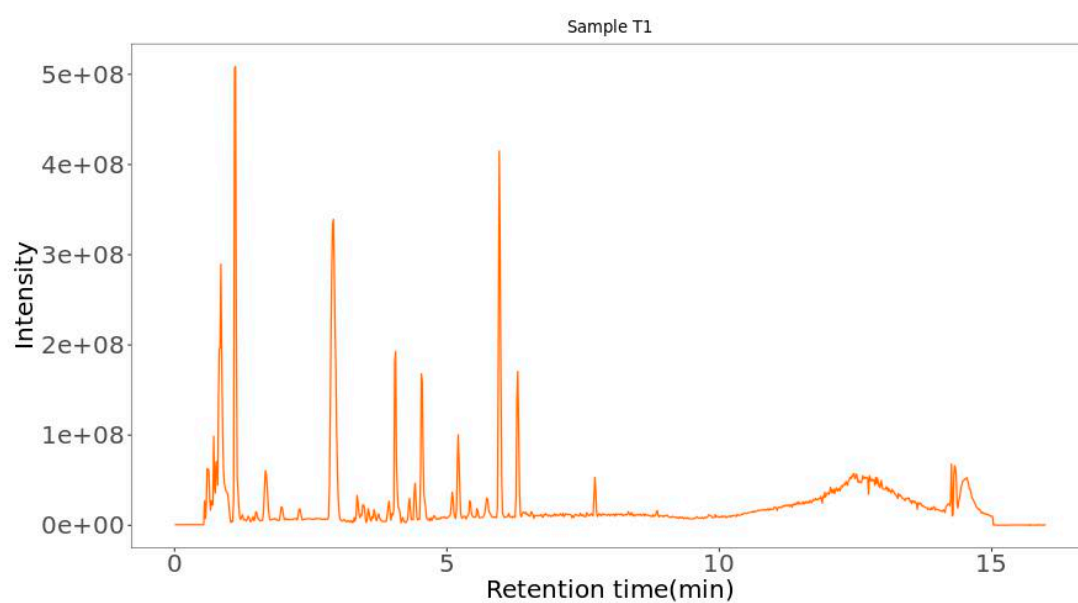


Fig. S1. Base peak chromatogram of the T1 (A), T2 (B), and T3 (C) samples in positive ESI mode.

(A)



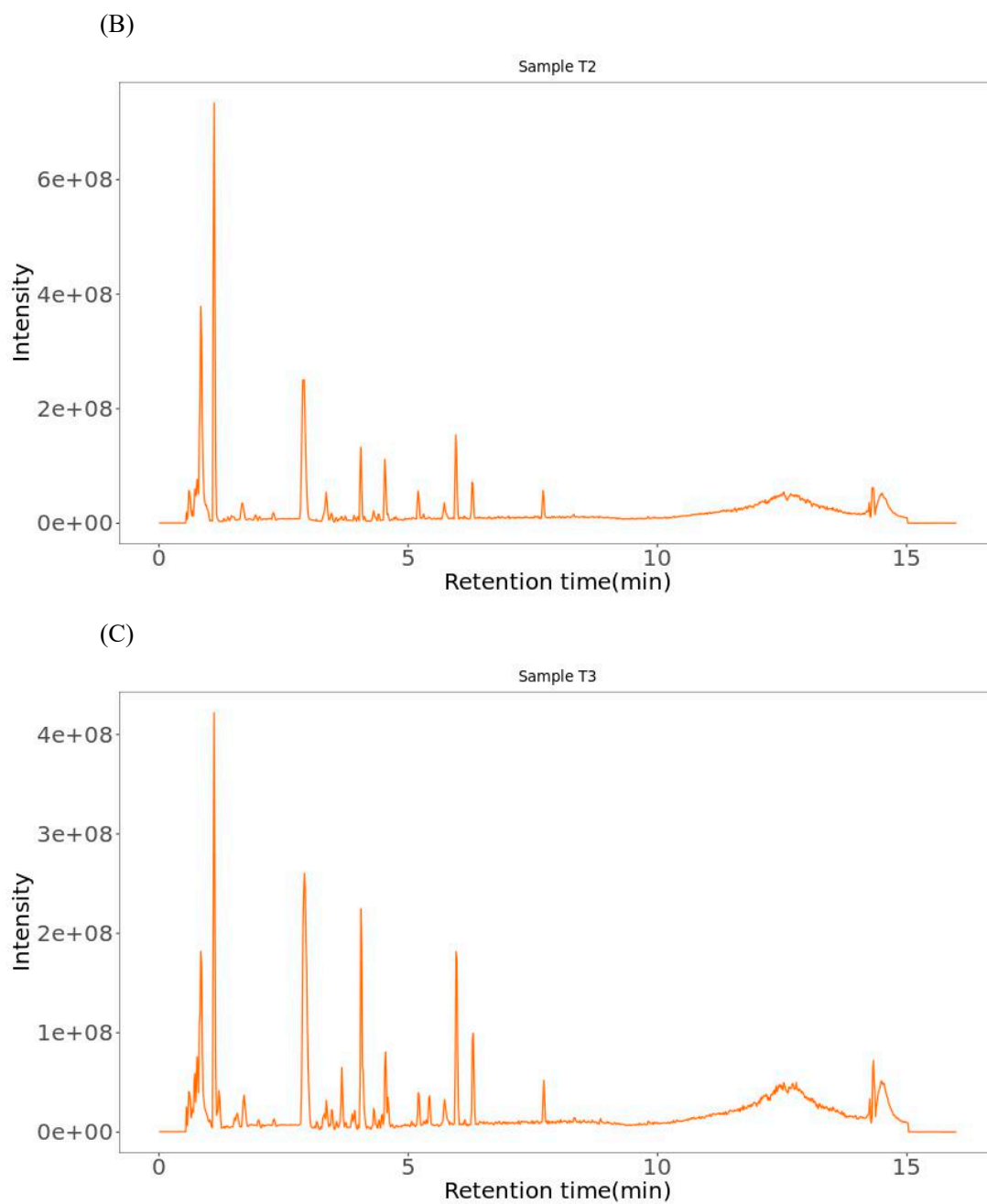


Fig. S2. Base peak chromatogram of the T1 (A), T2 (B), and T3 (C) samples in negative ESI mode.

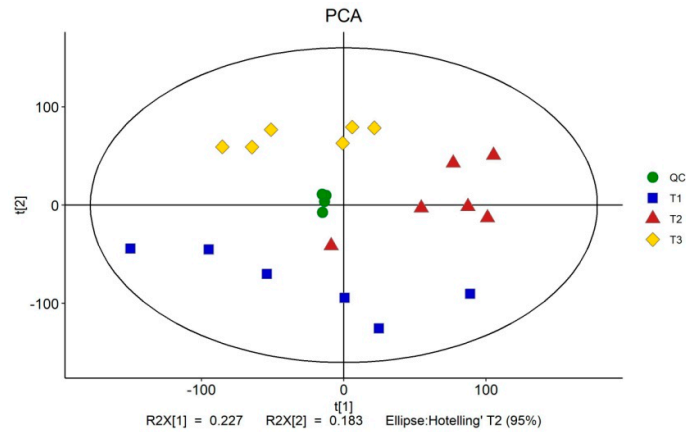


Fig. S3. PCA score scatter plots of LC-MS data from six biological replicates of each *Brassica juncea* sample.

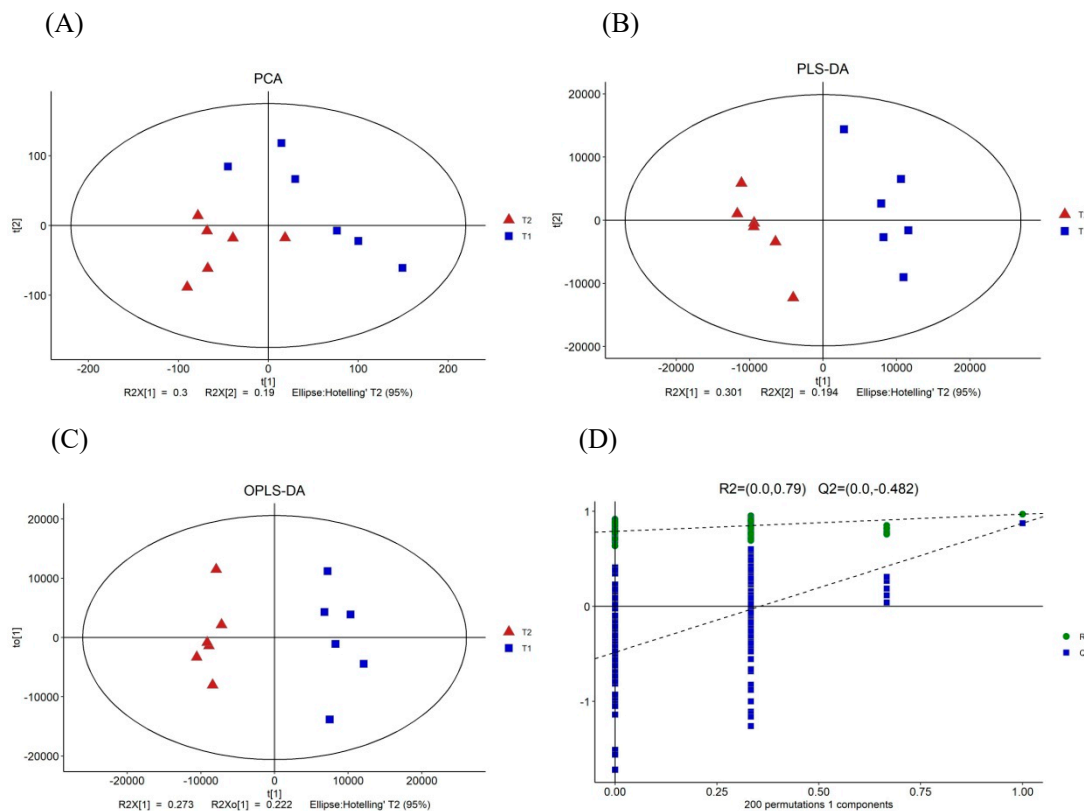


Fig. S4. Multivariate statistical score scatter plots and permutation test between T2 and T1. (A) PCA; (B) PLS-DA; (C) OPLS-DA; (D) permutation test of the OPLS-DA model.

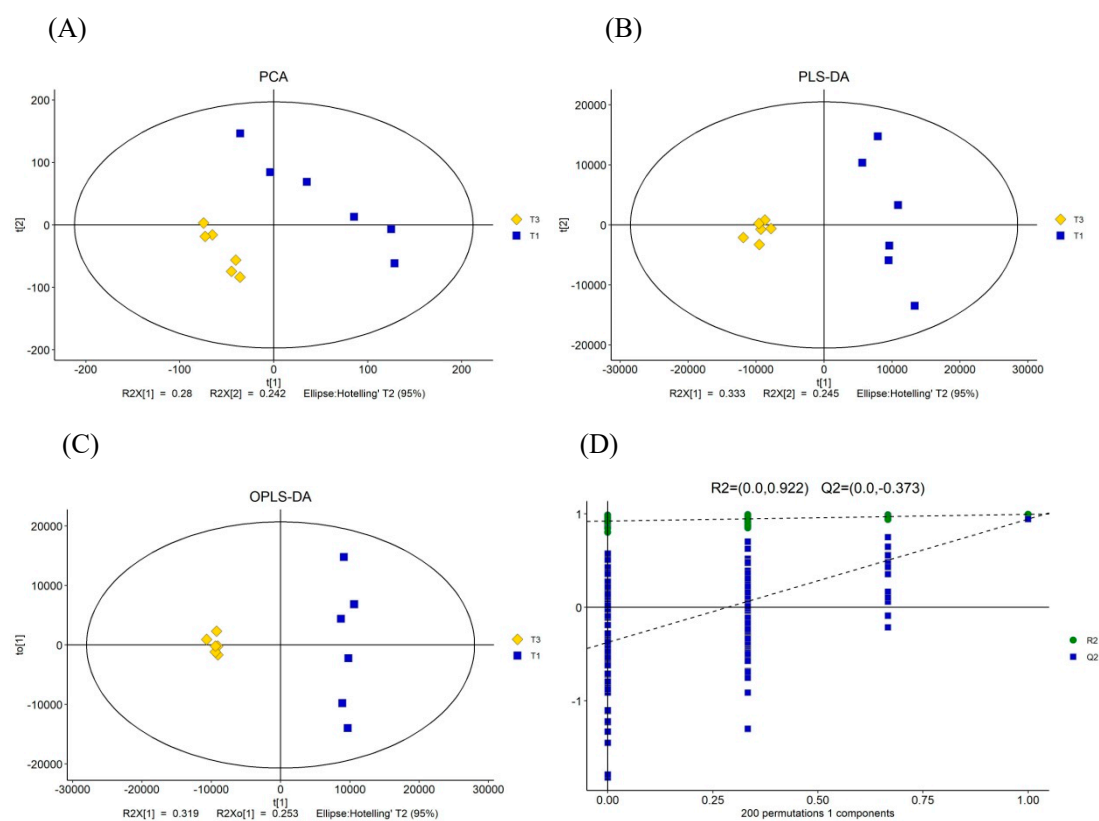


Fig. S5. Multivariate statistical score scatter plots and permutation test between T3 and T1. (A) PCA; (B) PLS-DA; (C) OPLS-DA; (D) permutation test of the OPLS-DA model.