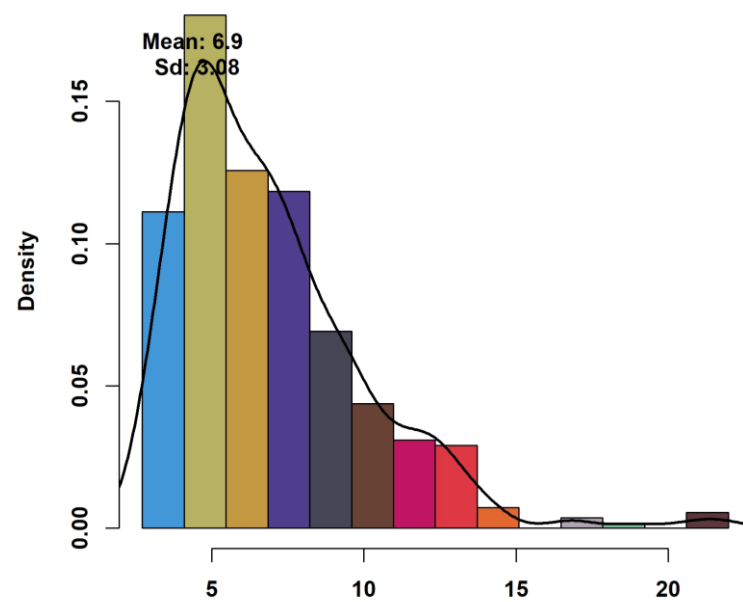
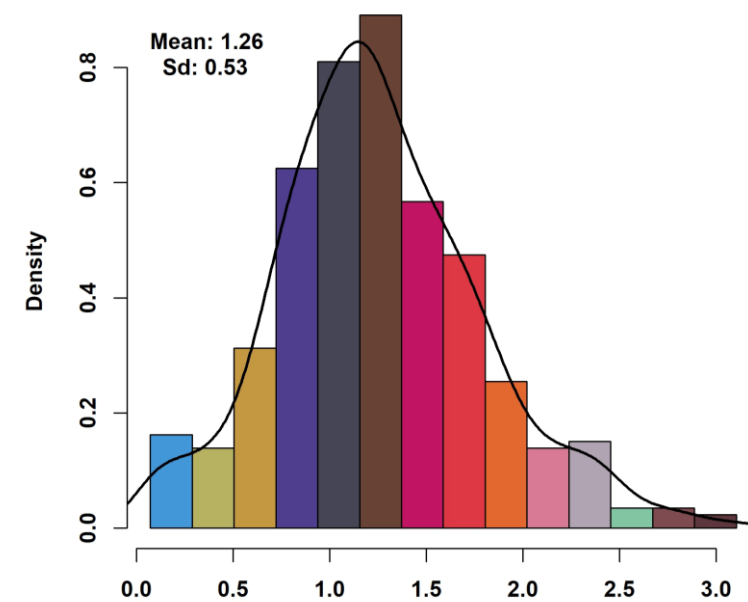


**A**

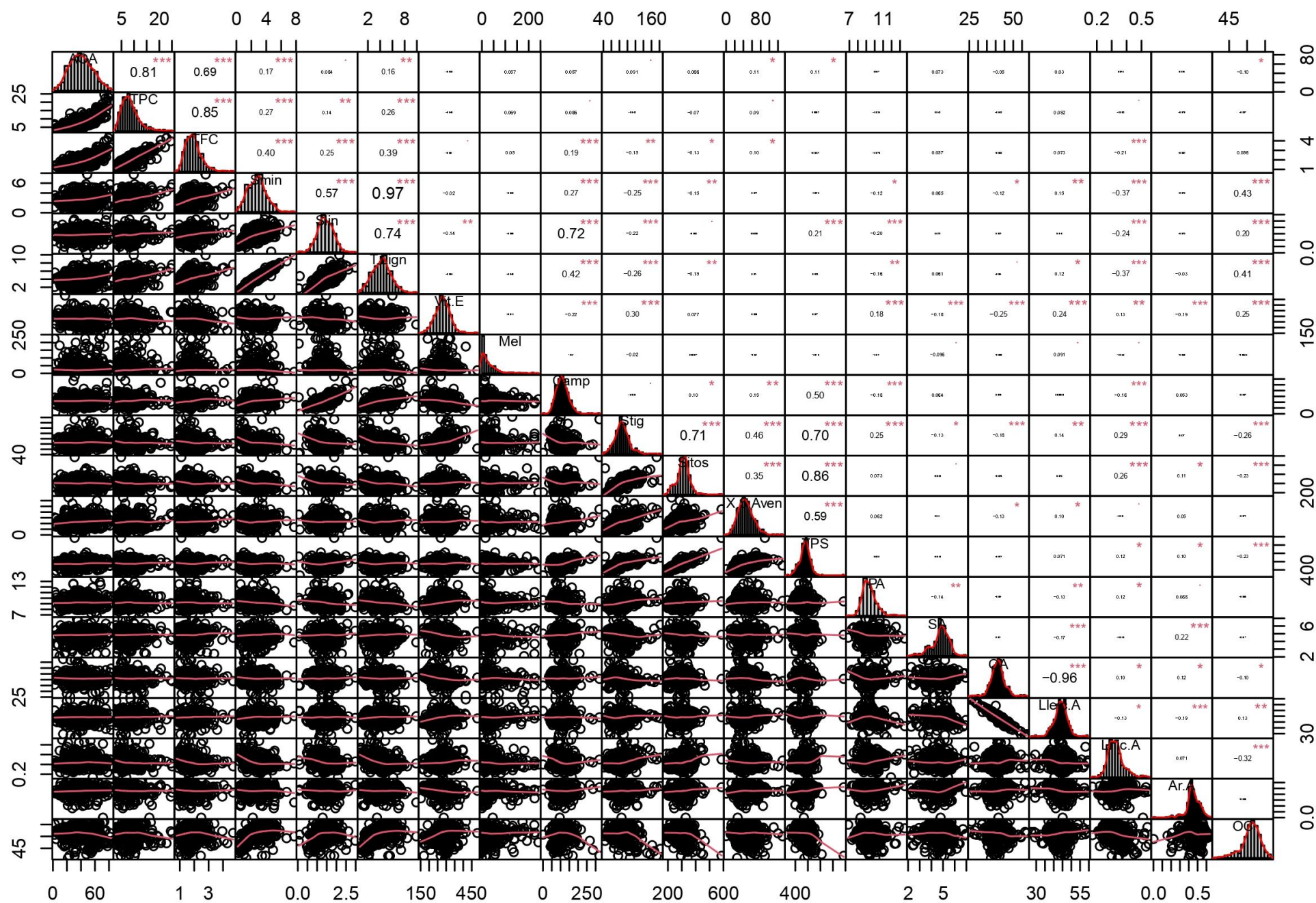


**B**

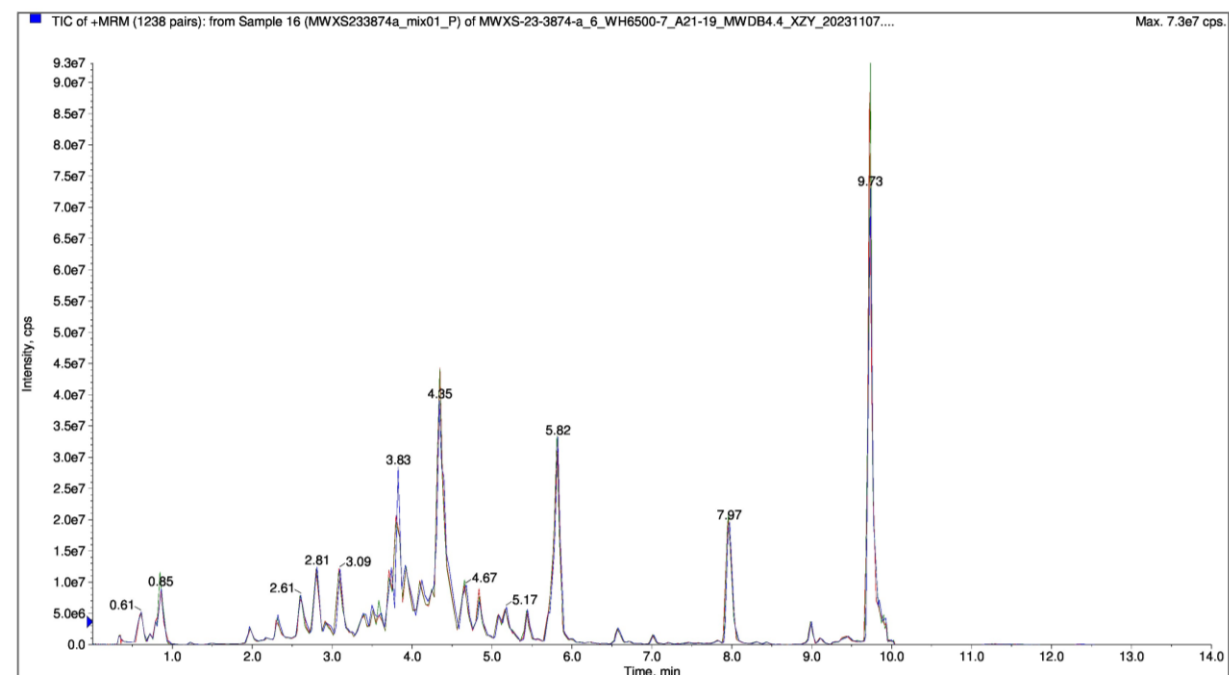
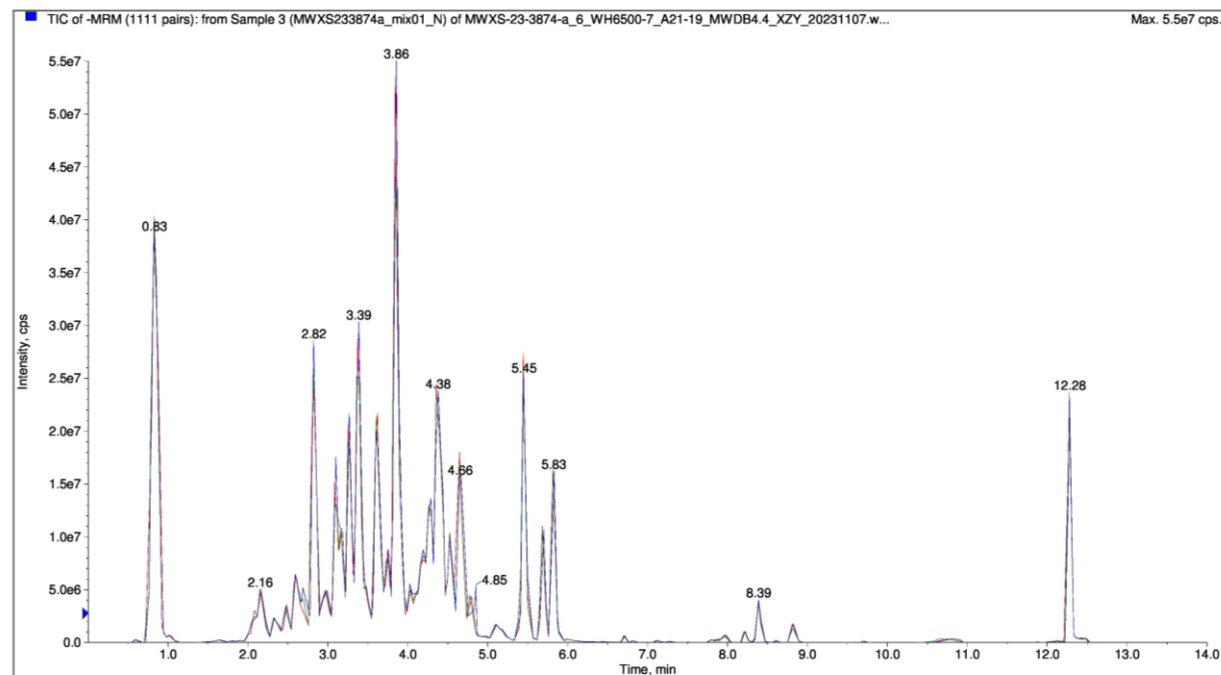


**C**

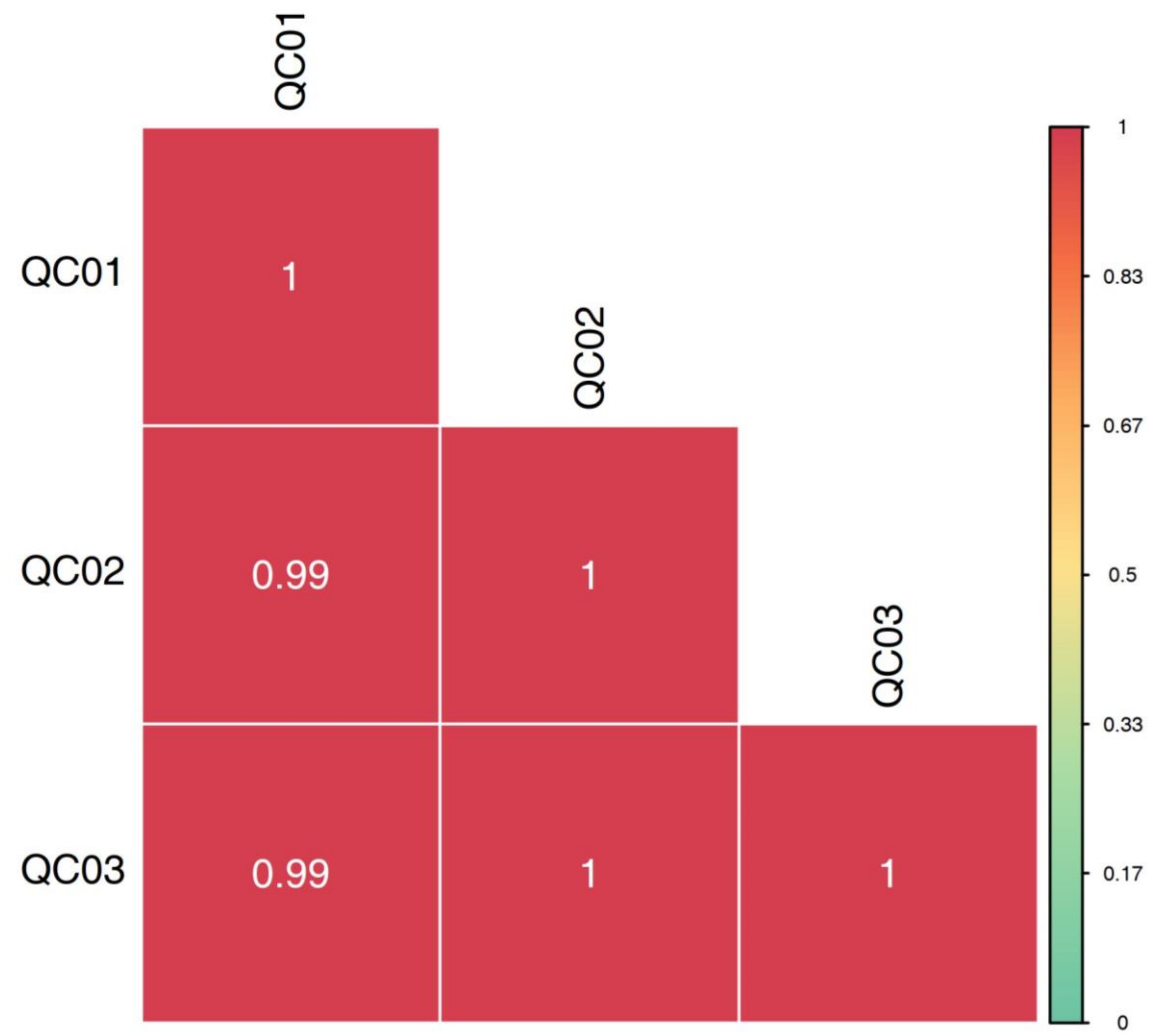
**Figure S1.** Frequency distribution of antioxidant activity (A), total phenolic content (B), and total flavonoid content (C) of the 400 seeds from different accessions.



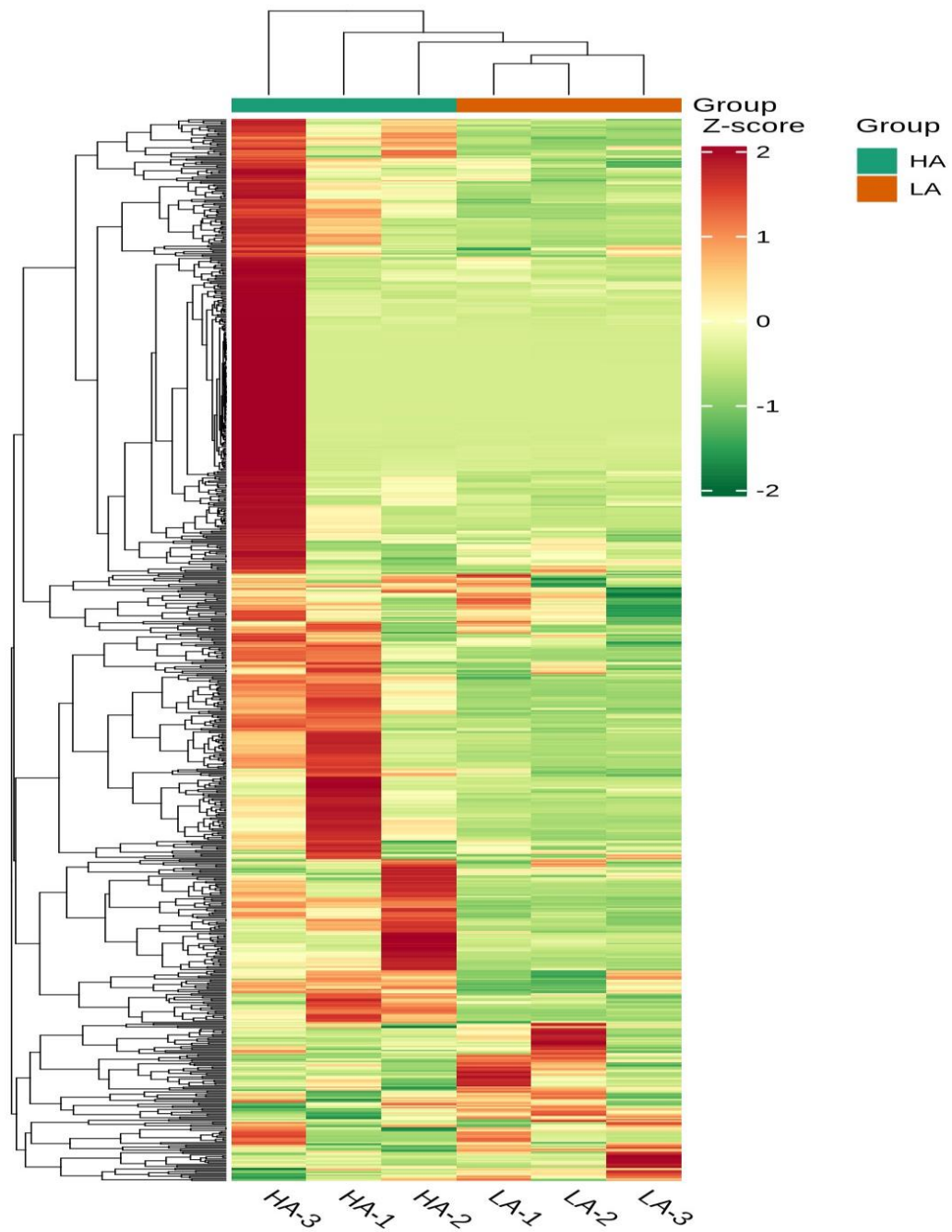
**Figure S2.** Other correlation plot of AOA with seed phytochemical components. AOA, antioxidant activity; TPC, total phenolic content; TFC, total flavonoid content; Smin, sesamin; Slin, sesamol; Tlign, total lignan; Camp, campesterol; 5-Aven, 5-avenasterol; Sitos, sitosterol; Stig, stigmasterol; TPS, total sterols; Vit E, vitamin E (tocopherol); OC, oil content; OA, oleic acid; Lnic A, linolenic acid; SA, stearic acid; Lneic A, linoleic acid; PA, palmitic acid; Mel, melatonin. \*, \*\*, and \*\*\* indicate significant correlations at  $P < 0.05$ ,  $0.01$ , and  $0.001$ , respectively.



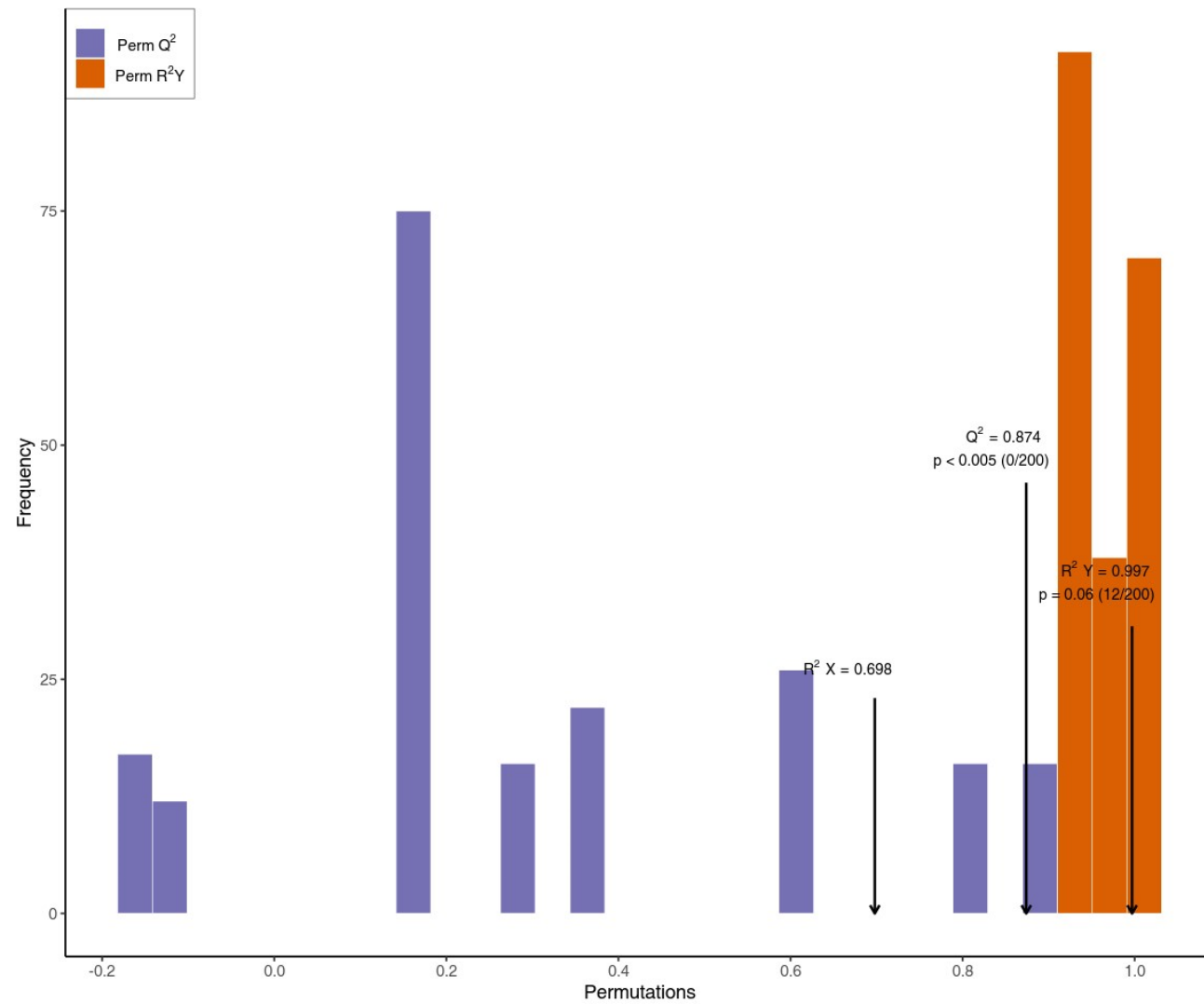
**Figure S3.** Multiple reaction monitoring (MRM) graphs of QC samples showing the total Ions Current (TIC) of some identified metabolites at the negative and positive ionization, respectively.



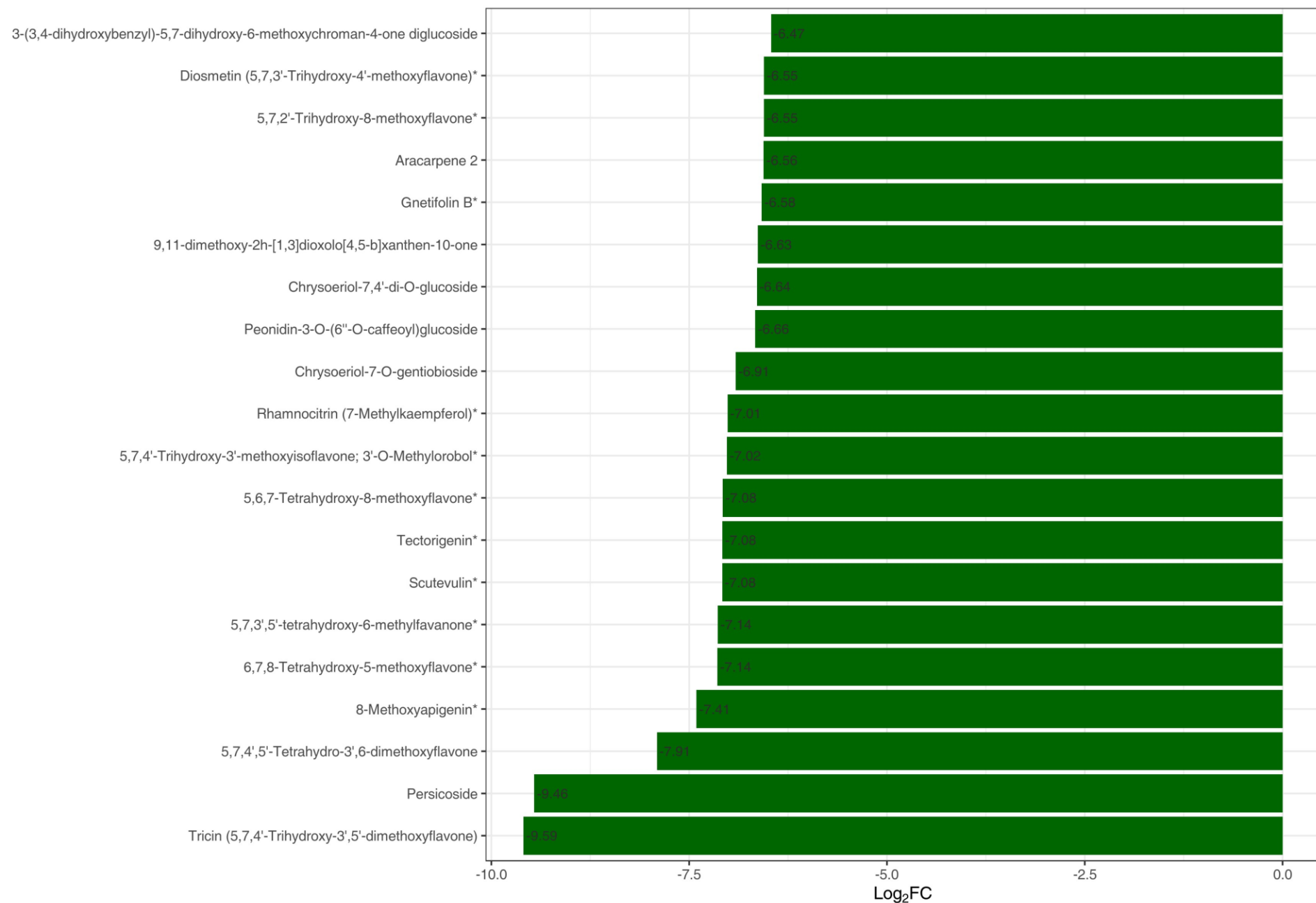
**Figure S4.** Correlations analysis between QC samples.



**Figure S5.** Hierarchical clustering analysis (HCA) of the polyphenol profiles of high (HA) and low (LA) antioxidant seeds.



**Figure S6.** Permutation plot of OPLS-DA results of pairwise comparison between high (HA) and low (LA) antioxidant seeds.

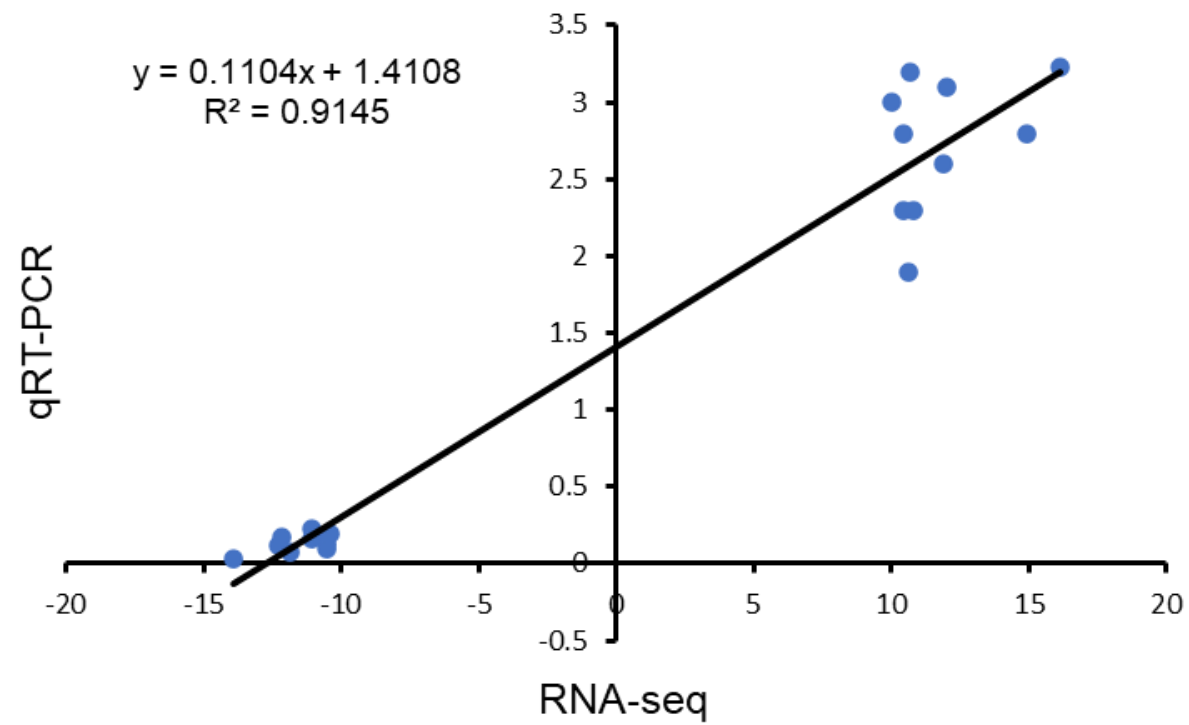


**Figure S7.** Top 20 highly accumulated phenolic compounds in high antioxidant sesame seeds.

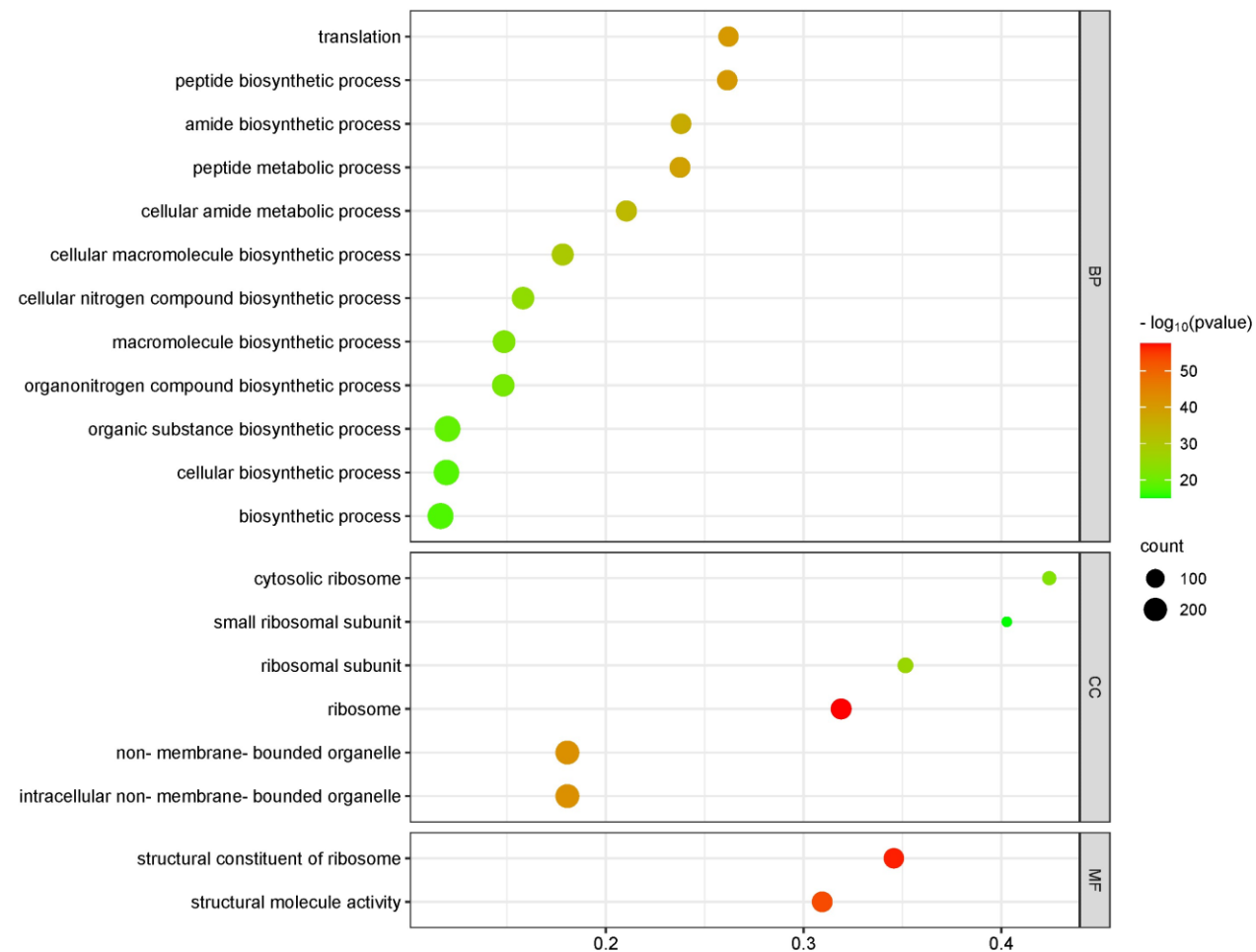
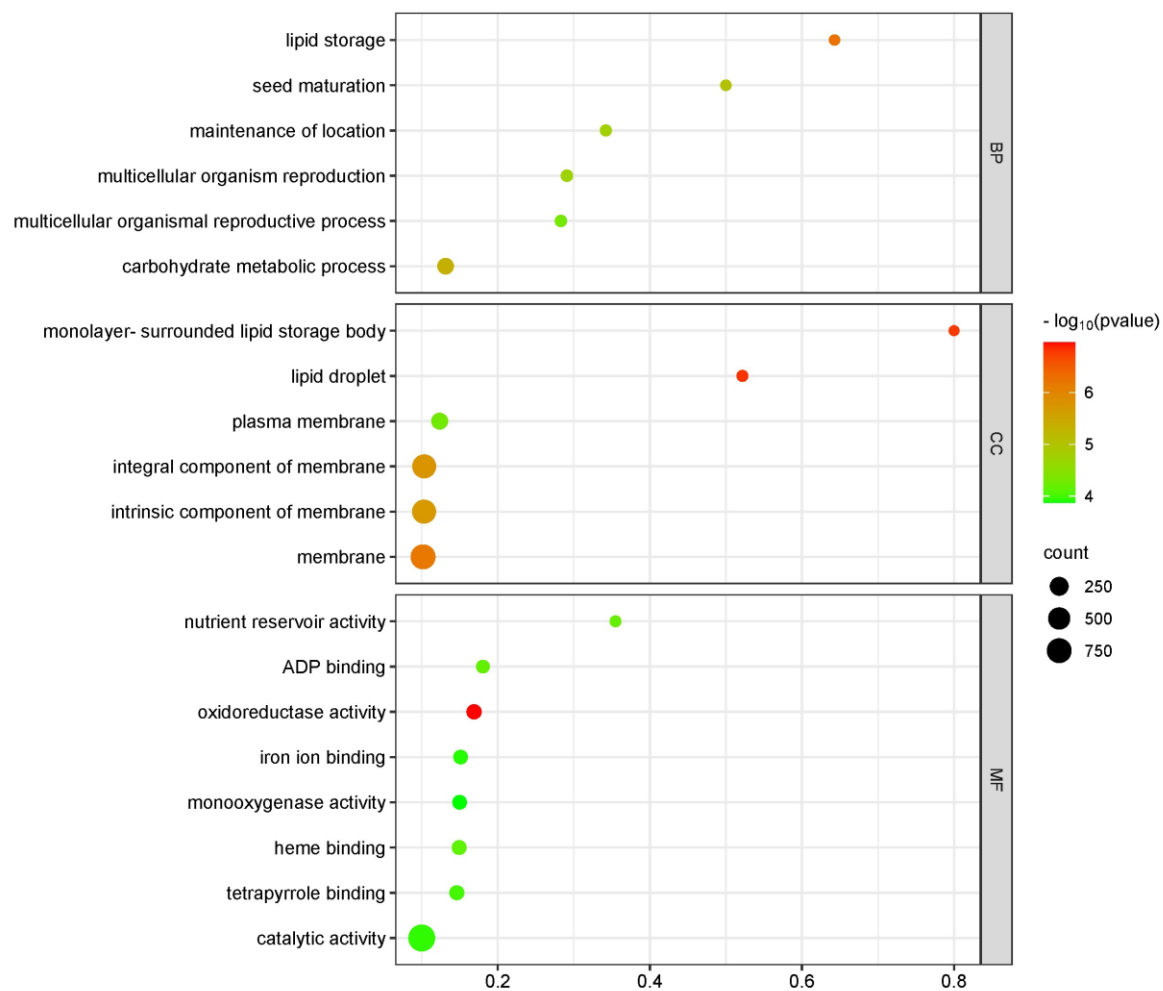




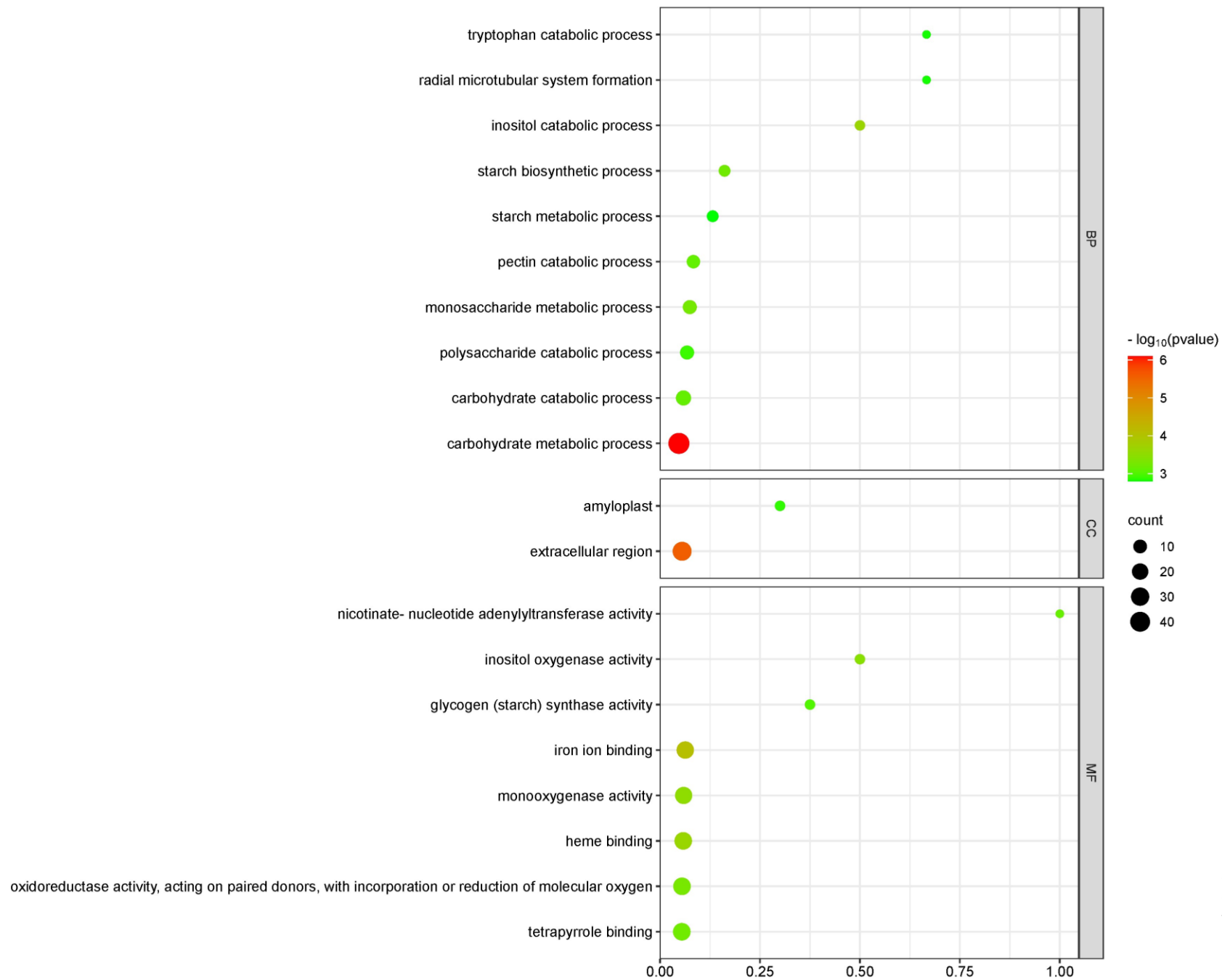




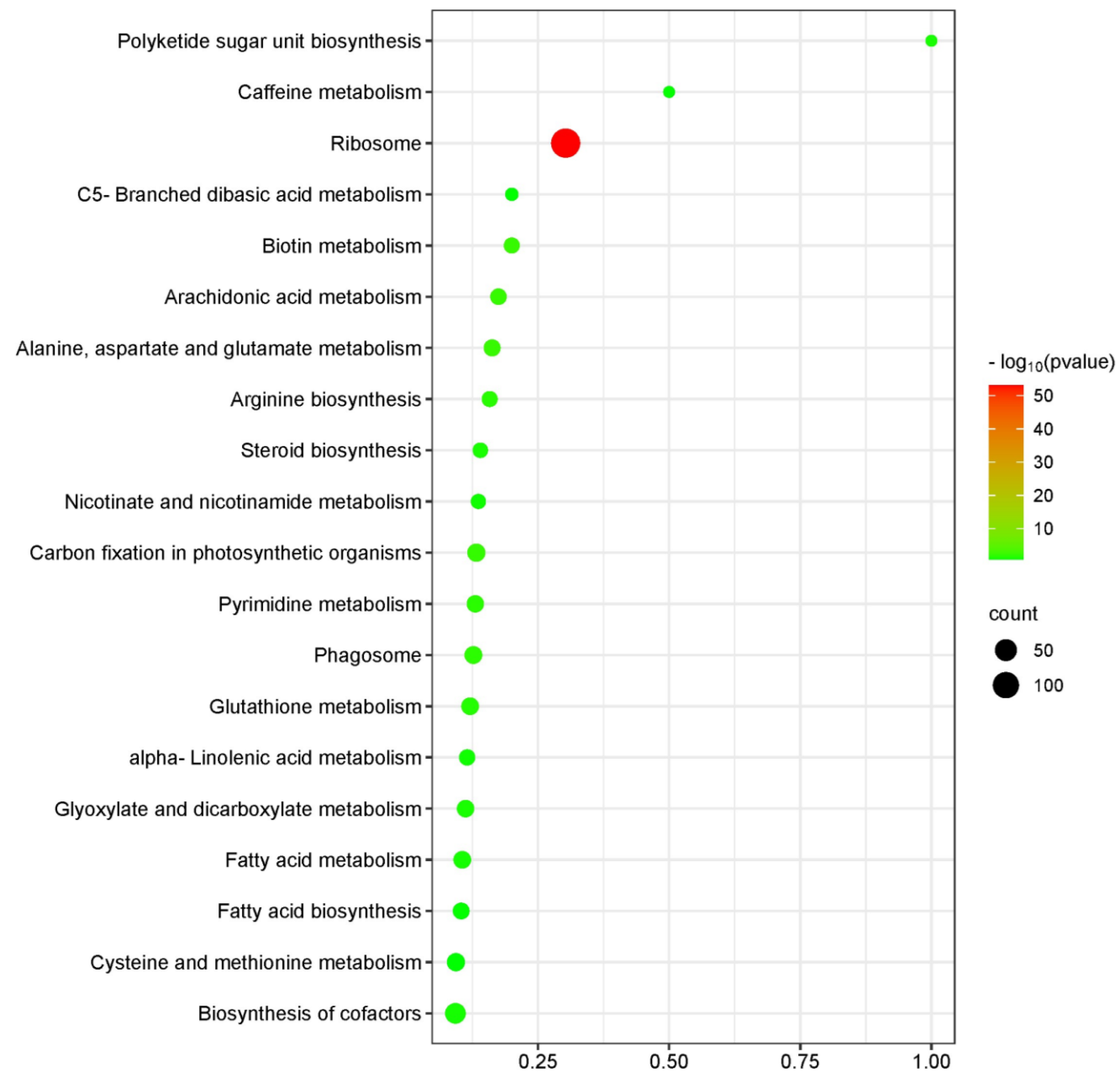
**Figure S9.** qRT-PCR validation of the RNA-seq data.



**Figure S10.** (A) and (B) GO analysis results of DEGs between LA and HA varieties at 10 and 20DPA, respectively.



**Figure S11.** GO analysis results of DEGs between LA and HA varieties at 30DPA.



**Figure S12.** KEGG analysis results of DEGs between LA and HA varieties at 20DPA.