Table S1. Mass spectrometer parameters

Parameters	Positive ion	Negative ion
Spray Voltage (V)	3800	-3000
Capillary Temperature (℃)	320	320
Aux gas heater temperature (℃)	350	350
Sheath Gas Flow Rate (Arb)	40	35
Aux gas flow rate (Arb)	10	8
S-lens RF level	50	50
Mass range(m/z)	100 ~1200	100 ~1200
Full ms resolution	70000	70000
MS/MS resolution	17500	17500
NCE/stepped NCE	10, 20, 40	10, 20, 40

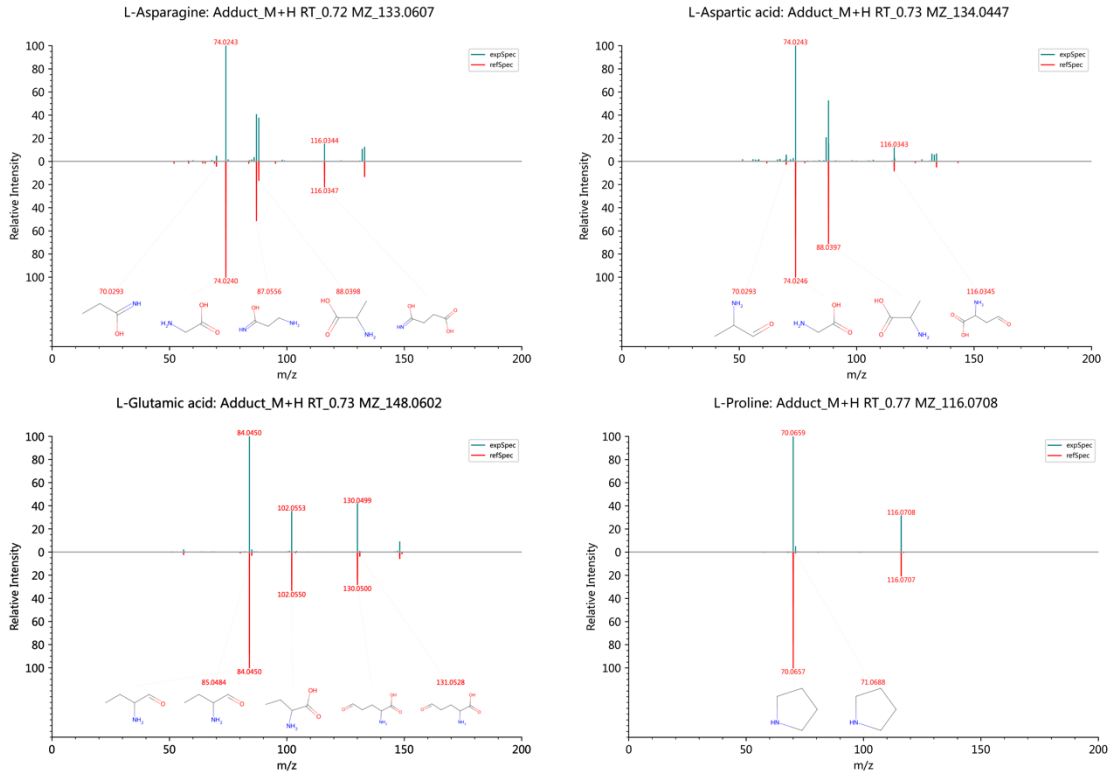


Figure S1. Representative MS/MS fragmentation spectra of four key metabolites (L-Asparagine, L-Aspartic acid, L-Glutamic acid, and L-Proline).

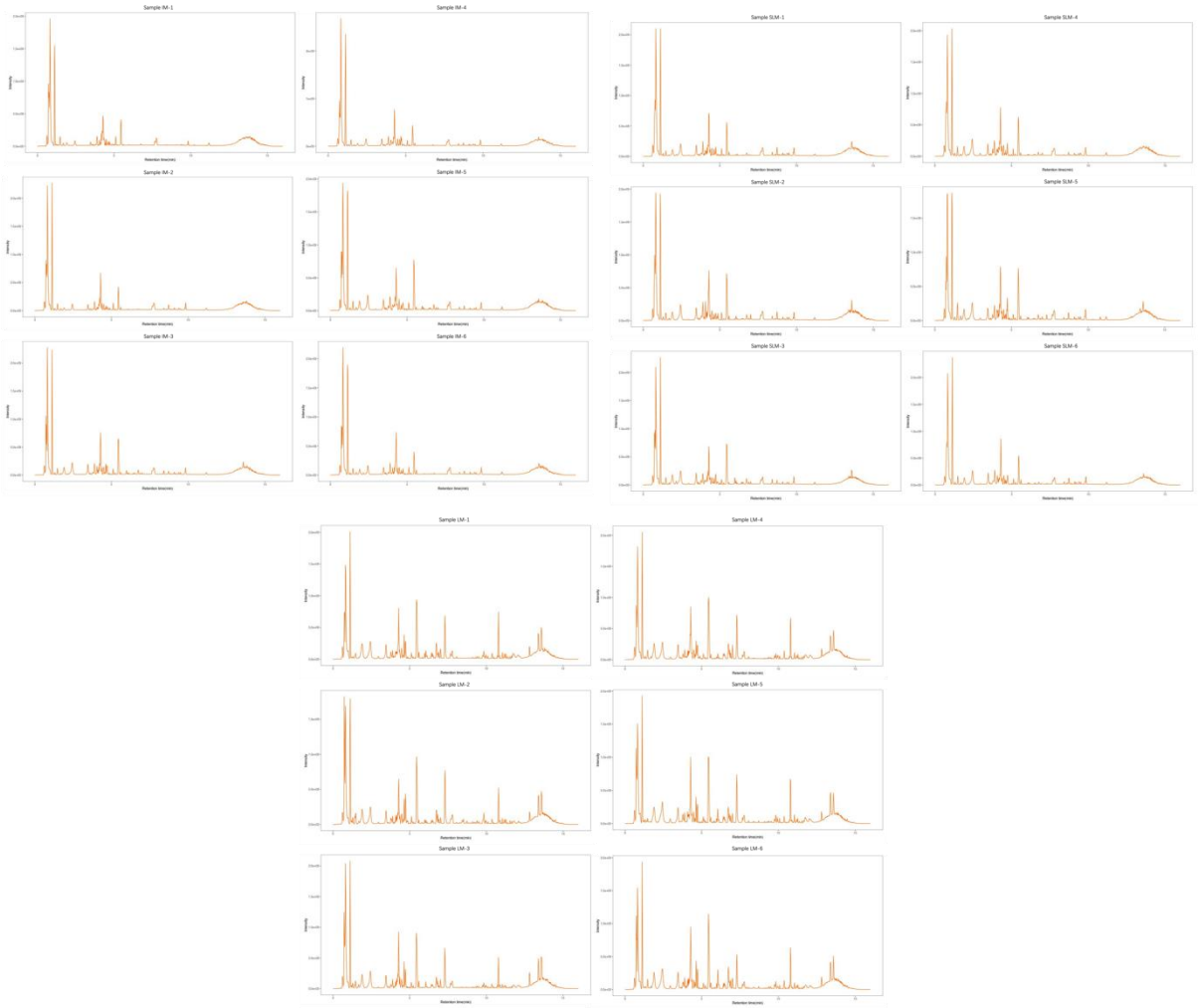


Figure S2. Representative base peak chromatograms of Q. acutissima seed samples in positive ionization mode. Each chromatogram represents an individual biological replicate across the three moisture content groups (IM, SLM, and LM)

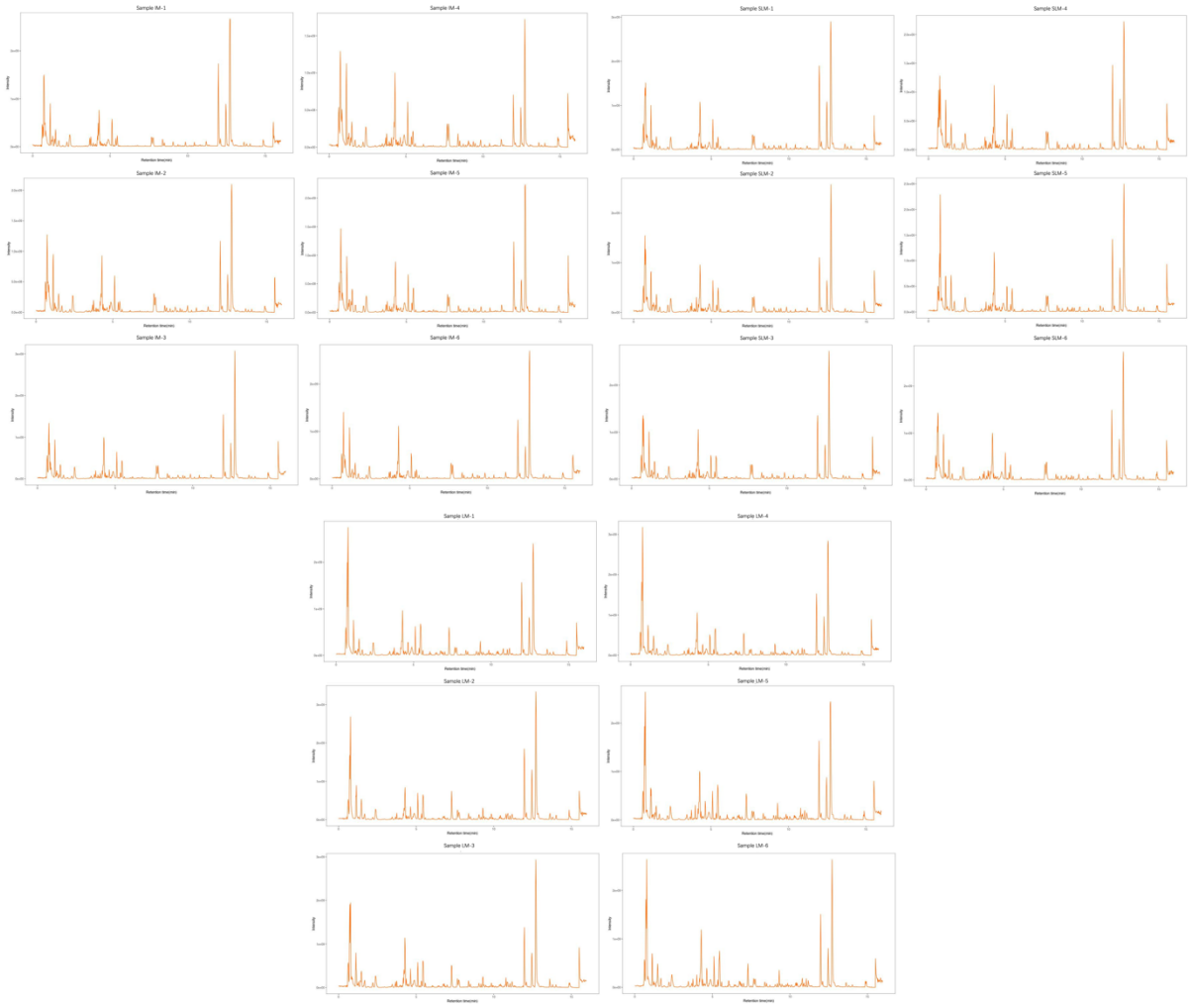


Figure S3. Representative base peak chromatograms of Q. acutissima seed samples in negative ionization mode. Each chromatogram represents an individual biological replicate across the three moisture content groups (IM, SLM, and LM)

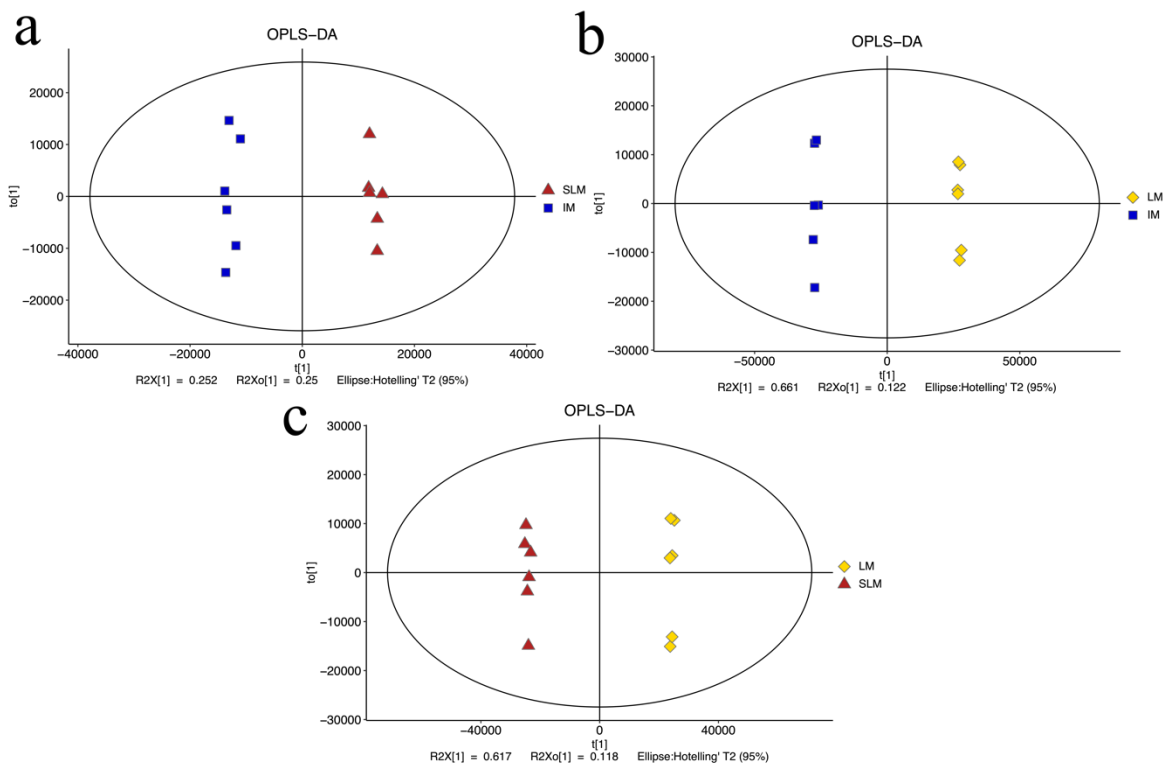


Figure S4. OPLS-DA score plots for pairwise comparisons of Q. acutissima seeds during desiccation. (a) SLM vs IM, (b) LM vs IM, (c) LM vs SLM.

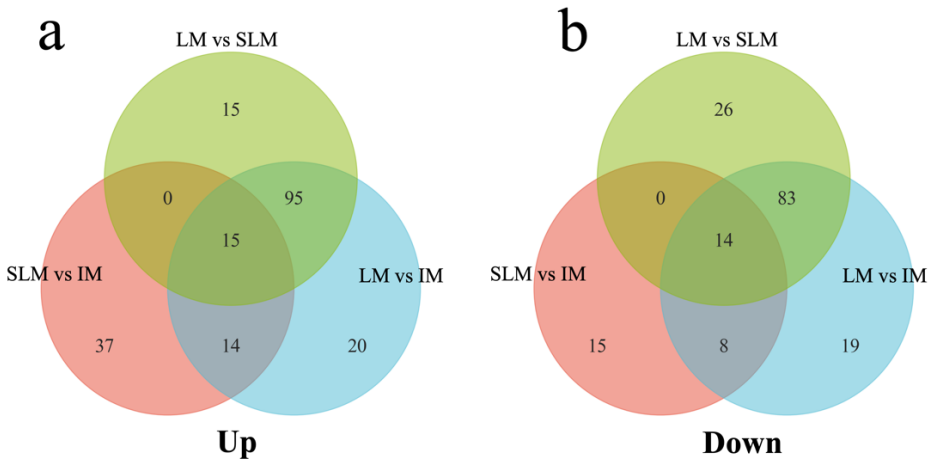


Figure S5. Venn diagrams of DEMs in *Q. acutissima* seeds during desiccation. (a) Upregulated DEMs across different moisture content comparisons; (b) Downregulated DEMs across different moisture content comparisons.