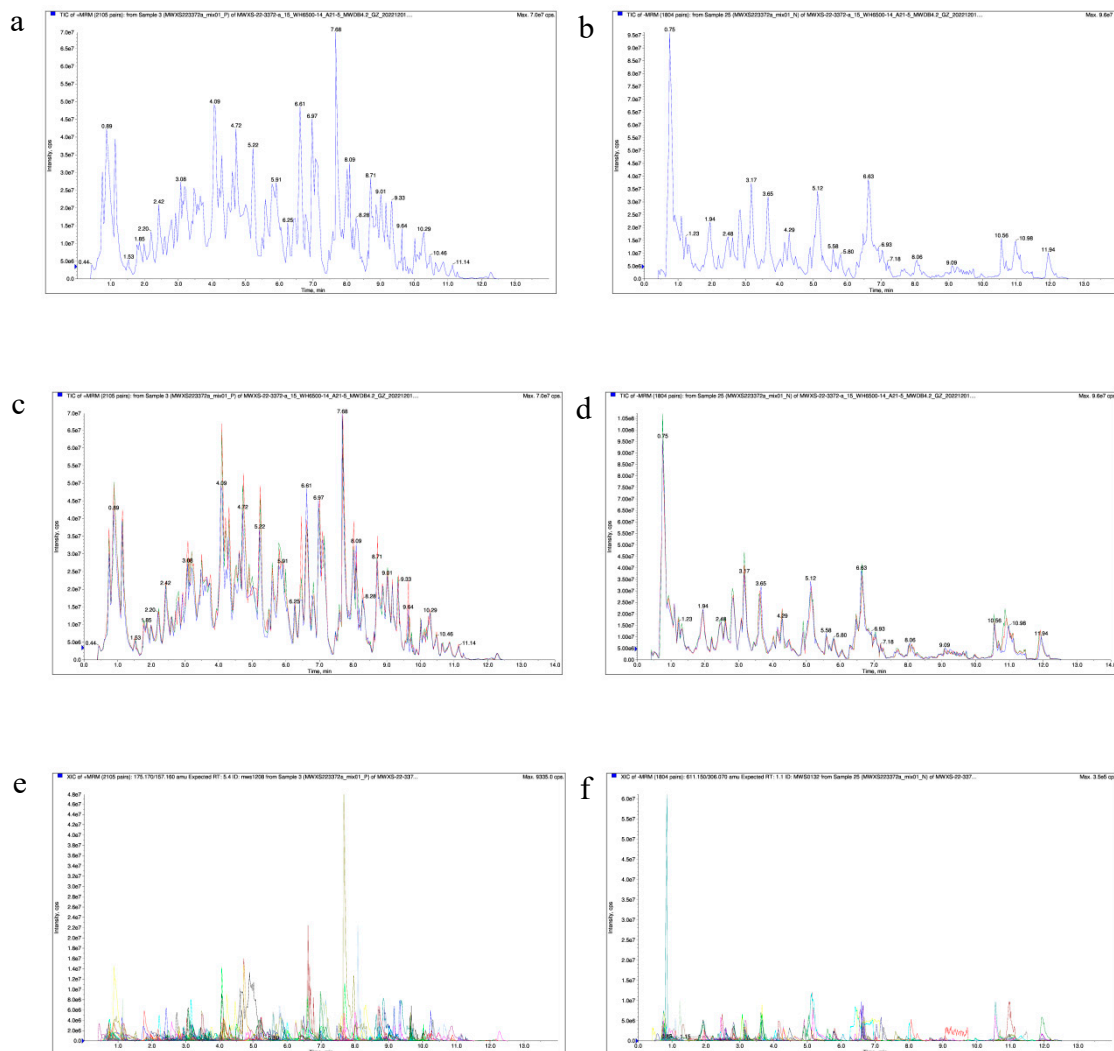
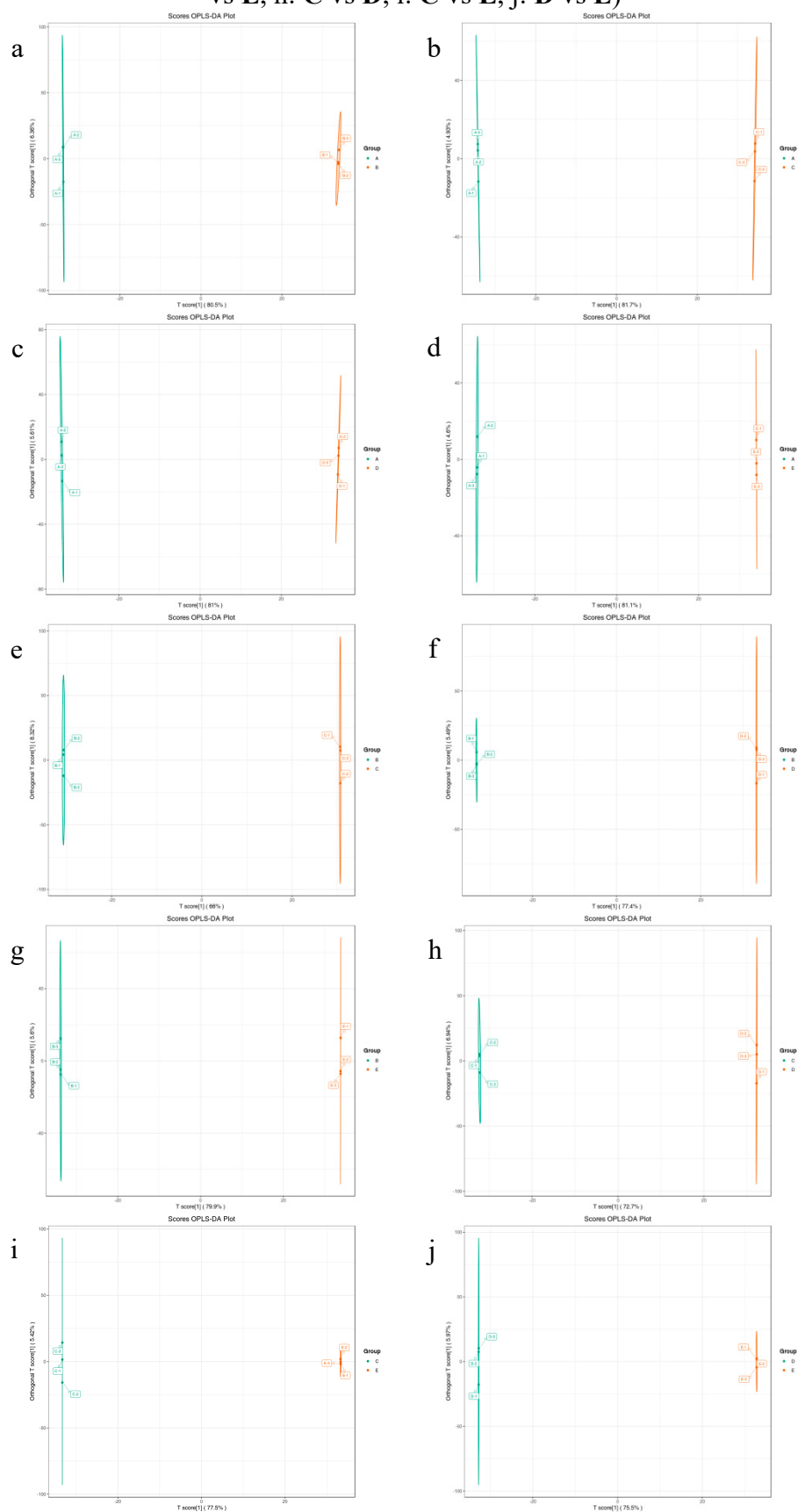


**Figure S1** TIC plots of mass spectrometry detection of QC samples (a: positive ion mode, b: negative ion mode) and their TIC overlaps (c: positive ion mode, d: negative ion mode), TIC plots of multi-peak detection of metabolites in MRM mode (e: positive ion mode, f: negative ion mode)



**Figure S2** Plot of two-by-two comparison of OPLS-DA scores of different parts of Shatian pomelo (a: **A** vs **B**, b: **A** vs **C**, c: **A** vs **D**, d: **A** vs **E**, e: **B** vs **C**, f: **B** vs **D**, g: **B** vs **E**, h: **C** vs **D**, i: **C** vs **E**, j: **D** vs **E**)



**Figure S3** The  $R^2Y$  and  $Q^2$  scores of the two-by-two comparison of OPLS-DA model validation for different parts of Shatian pomelo (a: **A** vs **B**, b: **A** vs **C**, c: **A** vs **D**, d: **A** vs **E**, e: **B** vs **C**, f: **B** vs **D**, g: **B** vs **E**, h: **C** vs **D**, i: **C** vs **E**, j: **D** vs **E**)

