**Figure S1. Total Ions Chromatograph (TIC) of five Quality Control Samples (A), 5 Internal Standards in QC samples (B), and Blank sample (C).**

**Figure S2. Principal Component Analysis plot of the peaks in 5 QC samples and 24 test samples. Green spots indicate the QC samples, while blue spots indicate the test samples.**

**Figure S3.** **High concordance among the peaks in five QC samples (r2 ≥ 0.941).**

**Figure S4. Score scatter plot of OPLS-DA model for metabolites (peaks) in leaves of Fucaishu18 (A) and Baisheng (B) under different growing patterns.**

**Figure S5. Pathway analysis for different metabolites in leaves of Baisheng (A) and Fucaishu18 (B) under different growing patterns.**