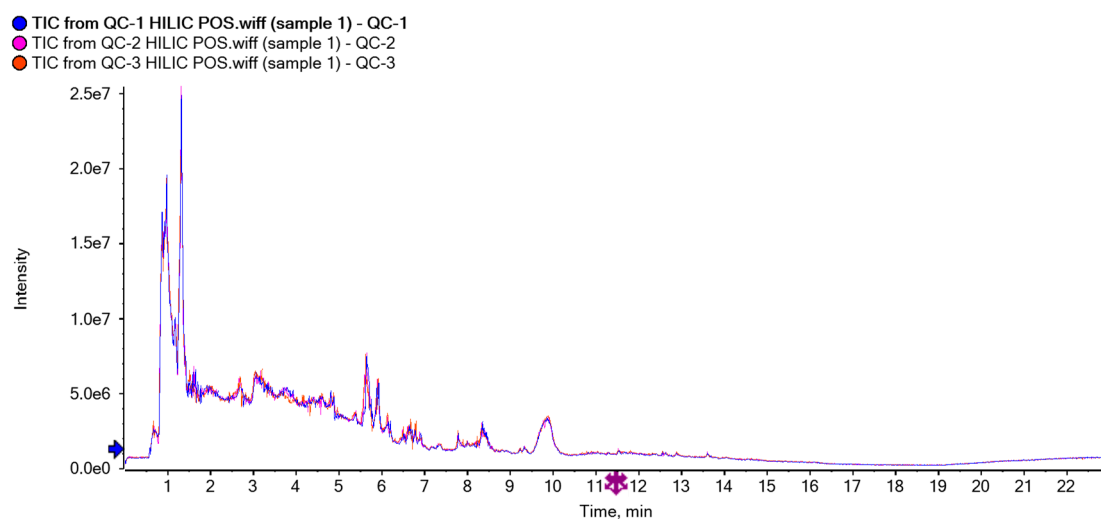
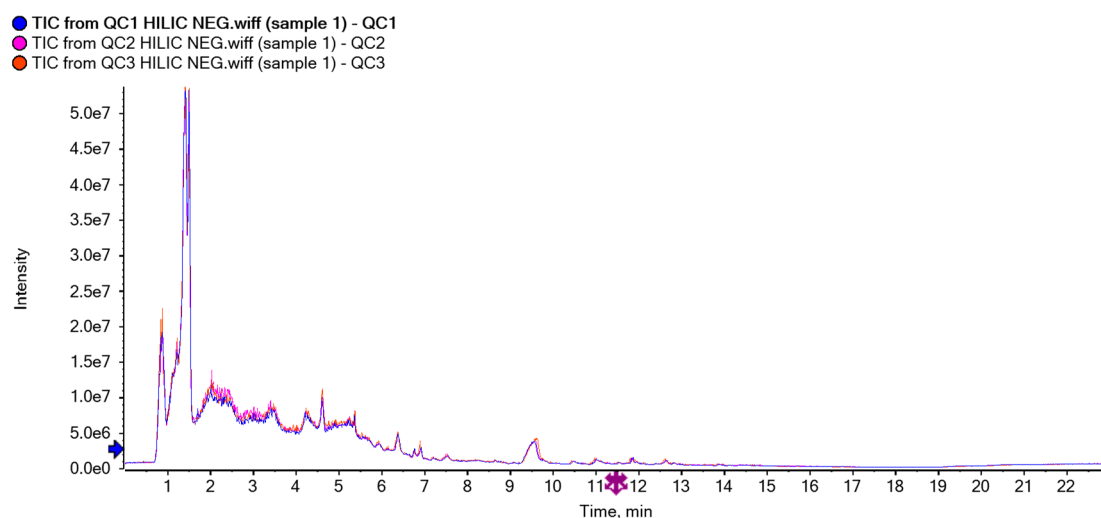


## Supporting figures

**Figure S1&S2. Total ion current (TIC) overlap map of positive and negative ion modes of quality control (QC) samples**



**Figure S1 TIC overlap map of positive ion modes of QC samples**



**Figure S2 TIC overlap map of negative ion modes of QC samples**

**Figure S3 & S4. Orthogonal partial least squares discriminant analysis (OPLS-DA) of fecal metabolites in giant pandas under different dietary conditions**

In order to obtain a higher level of group separation and a better understanding of the variables responsible for group classification, OPLS-DA was applied. Seven-fold

cross validation was used to estimate the optimal component number of the model and avoid the over-fitting. At positive ion mode, the  $R^2Y$  and  $Q^2$  accumulation were  $R^2Y=0.999$ ,  $Q^2=0.984$  (Culm vs Shoot);  $R^2Y=0.996$ ,  $Q^2=0.981$  (Leaf vs Shoot);  $R^2Y=0.989$ ,  $Q^2=0.963$  (Leaf vs Culm). At negative ion mode, the  $R^2$  and  $Q^2$  intercept values were  $R^2Y=0.998$ ,  $Q^2=0.986$  (Culm vs Shoot);  $R^2Y=0.994$ ,  $Q^2=0.982$  (Leaf vs Shoot);  $R^2Y=0.986$ ,  $Q^2=0.965$  (Leaf vs Culm). The values of  $R^2Y$  and  $Q^2$  accumulation were close to 1, indicate the models were stable and reliable. The  $R^2$  and  $Q^2$  intercept values after 200 permutations were shown in figure. The low values of the  $Q^2$  intercept indicate the robustness of the models, and thus show a low risk of over fitting and reliability.

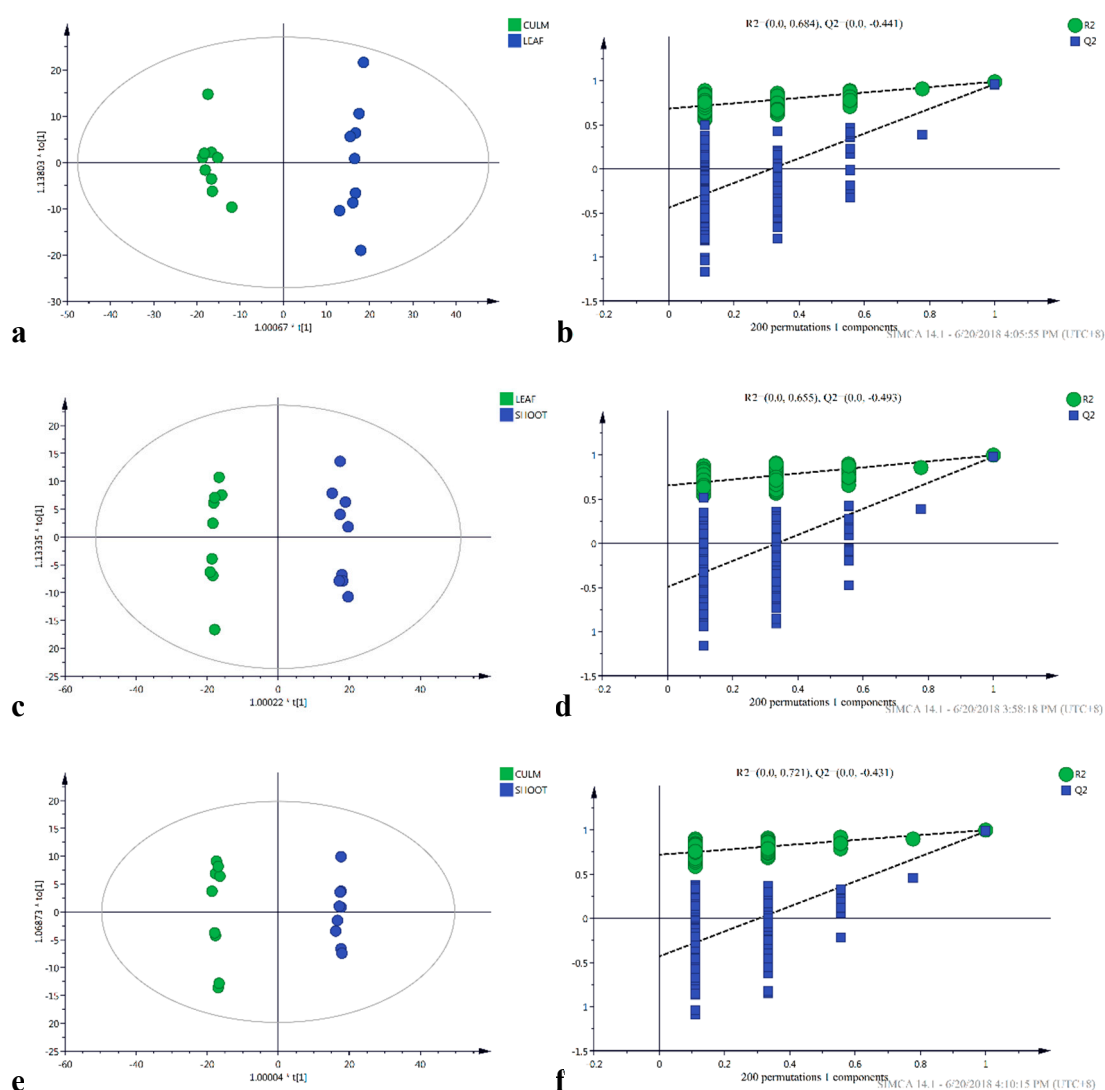


Figure S3 Positive ion pattern OPLS-DA score diagram and permutations test.

Score plot of OPLS model obtained from Culm vs Leaf (a); Leaf vs Shoot (c); Culm vs Shoot (e).

Permutation analysis of OPLS-DA models from Culm vs Leaf (b); Leaf vs Shoot (d); Culm vs

Shoot (f). Two hundred permutations were performed, and the resulting R2 and Q2 values were

plotted. (Green triangle): R2; (blue square): Q2. The green line represents the regression line for

R2 and the blue line for Q2.

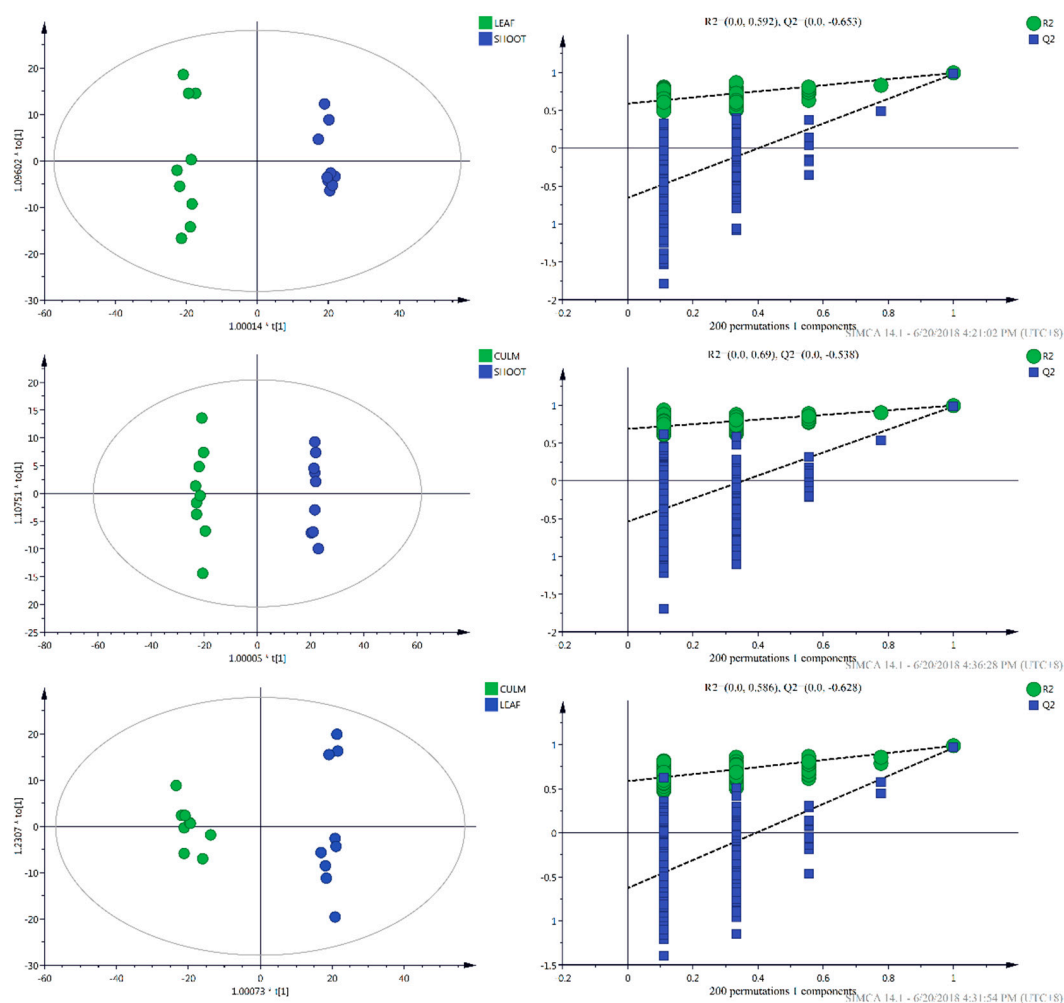


Figure S4 Negative ion pattern OPLS-DA score diagram and permutations test. Details

were described in figure s3.