Supplementary materials：



Figure S1. Status of *S. miltiorrhiza* at harvesting

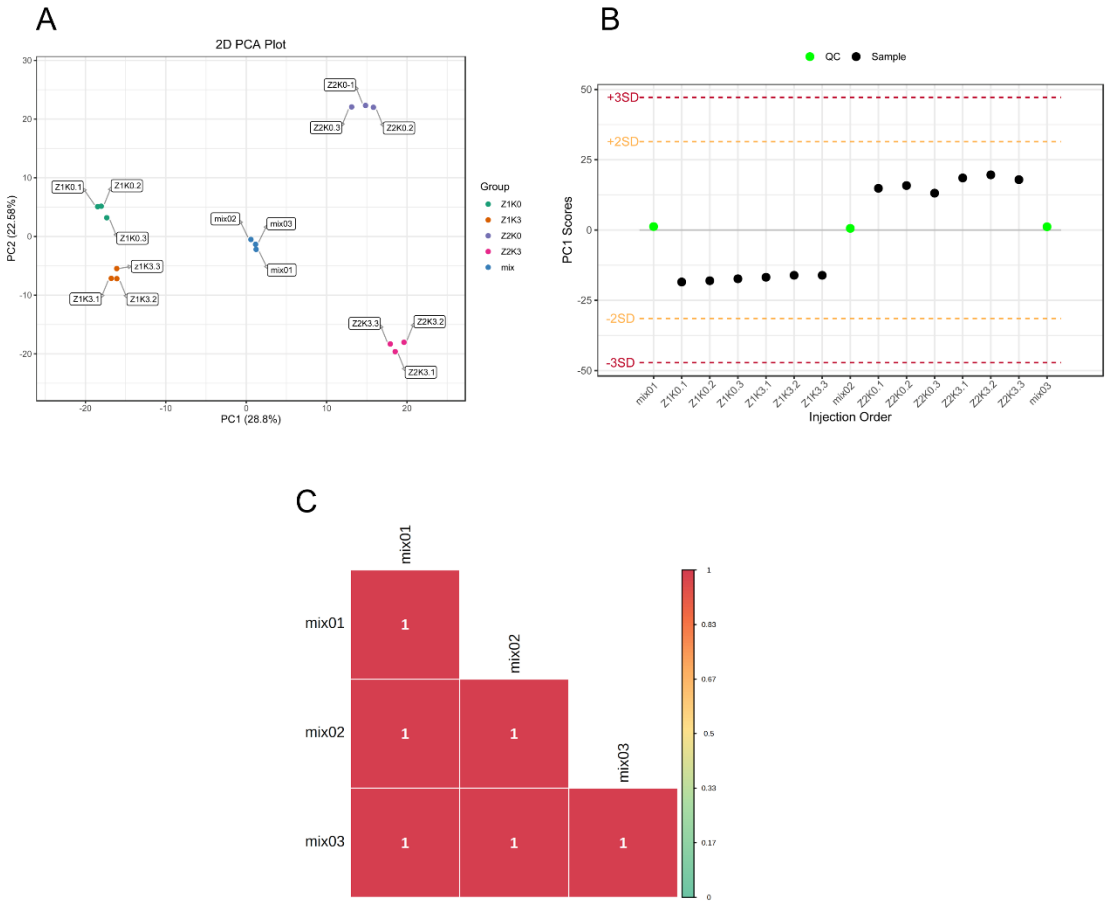


Figure S2. (A) Mass spectral data PCA scores of each group of samples and QC samples (B) Overall sample PC1 control chart (C) Correlation of QC samples

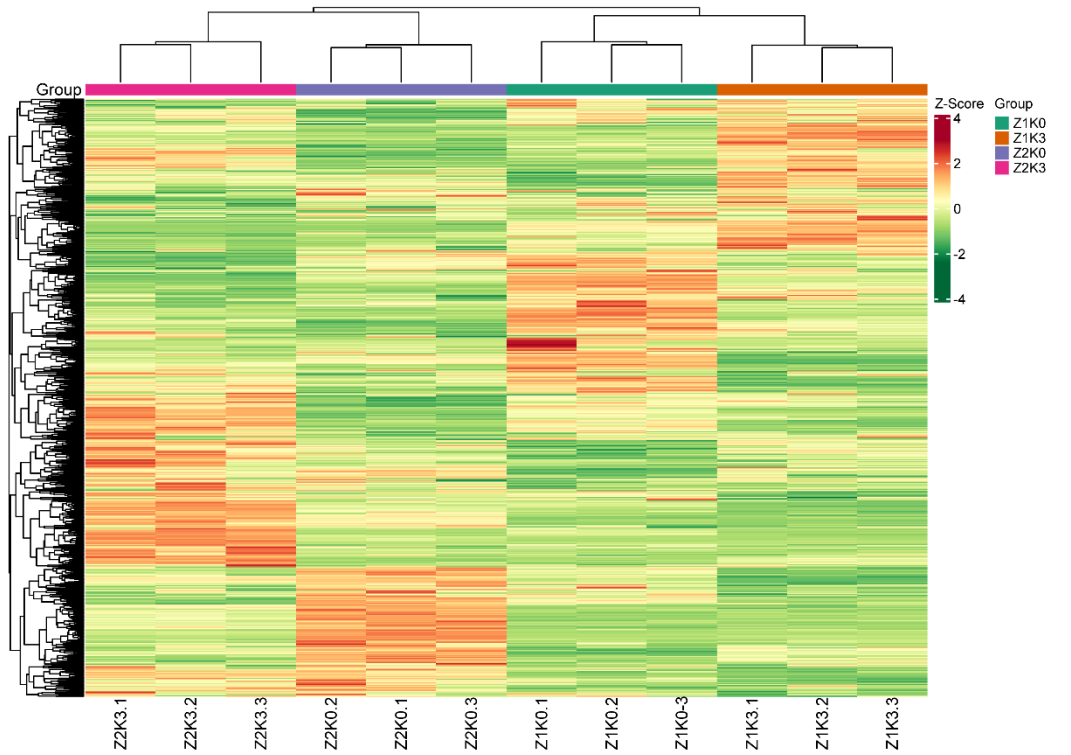


Figure S3. Overall clustering chart of samples

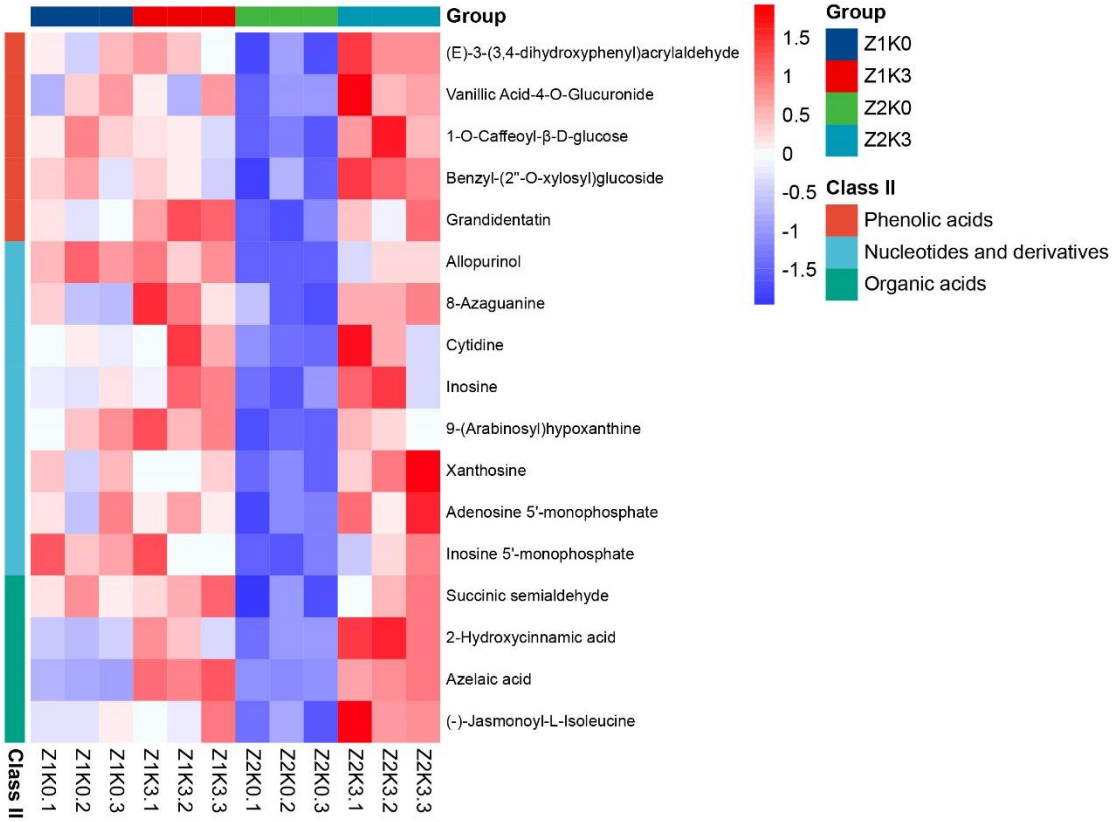


Figure S4. Subclass5 Top 3 classes of differential metabolites

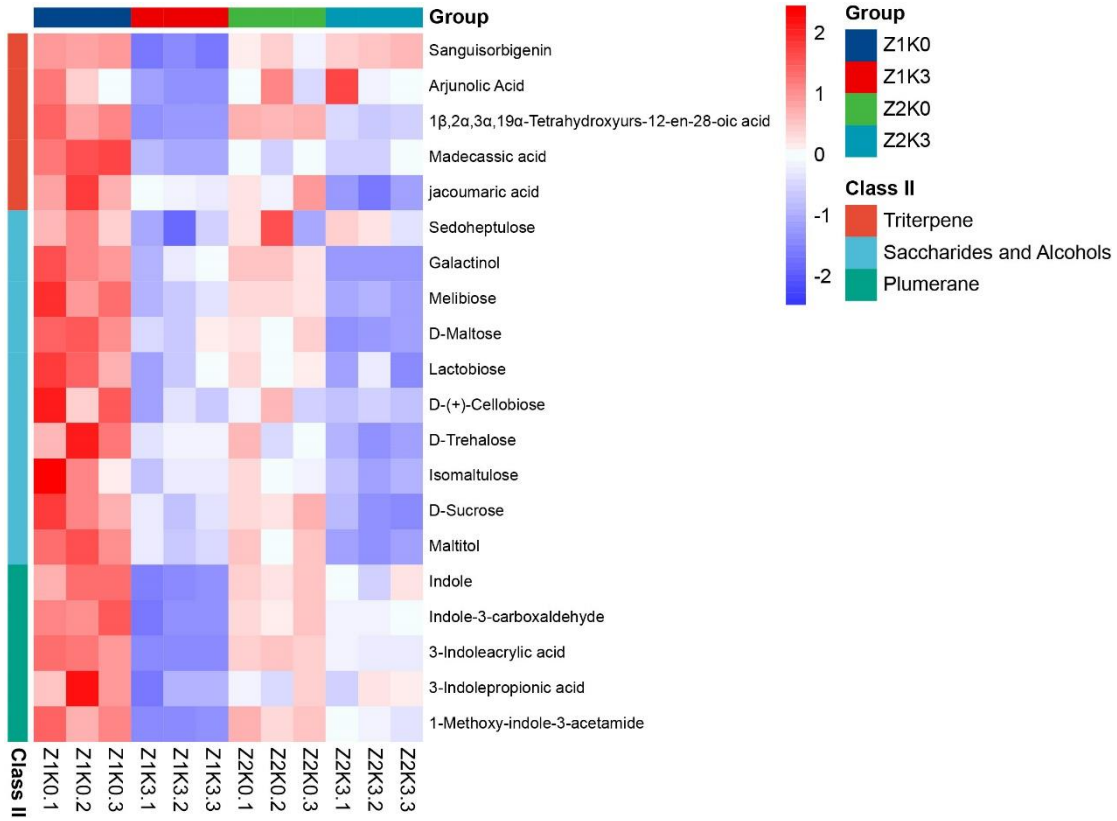


Figure S5. Subclass8 Top 3 classes of differential metabolites

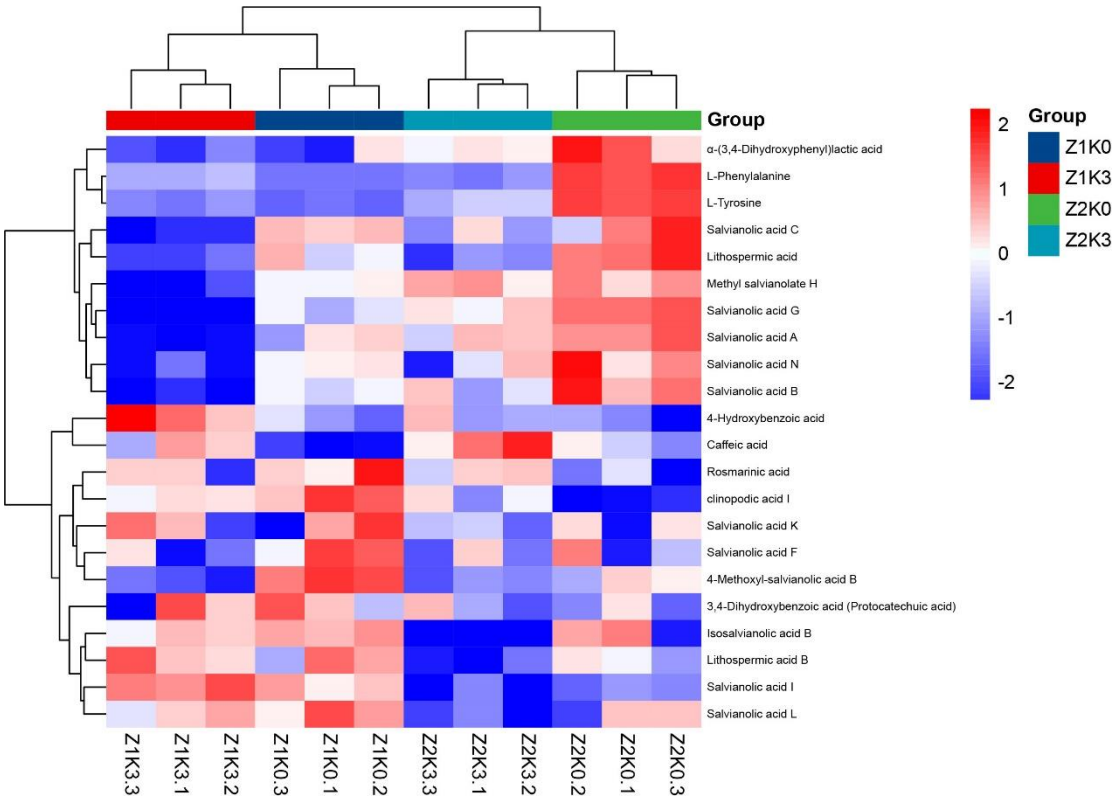


Figure S6. Heat map of differential metabolites associated with salvianolic acid

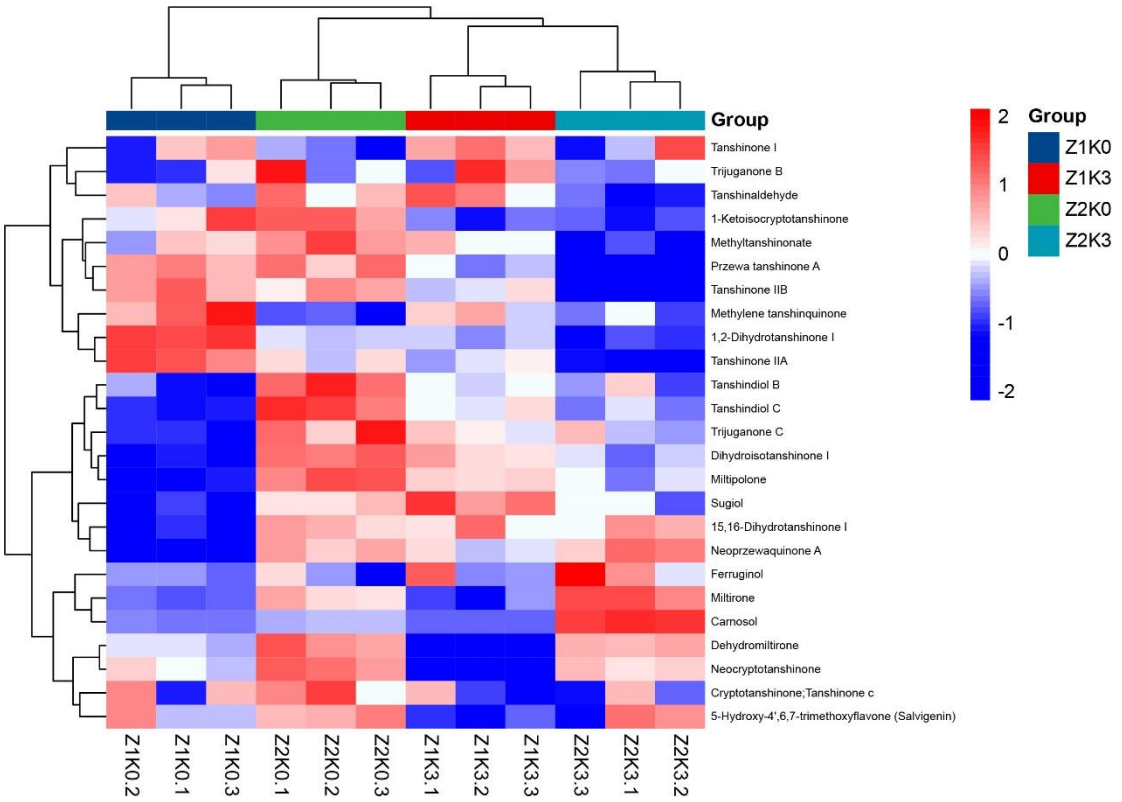


Figure S7. Heat map of differentially metabolized substances associated with tanshinone.

Table S1. Calibration curves of 6 standard chemicals.

Standard chemicals	Equations	R^2	Linear range（μg/ml）
Rosmarinic acid	y=1.379E+9x+2.274E+7	0.9938	0.5–50
Salvia acid B	y=1.171E+8x−2.881E+7	0.9973	0.5–500
Salvianolic acid A	y=5.938E+8x−4.048E+7	0.9987	0.5-50
Cryptotanshinone	y=1.872E+10x+1.184E+10	0.9935	0.5-50
Tanshinone I	y=3E+8x+2E+9	0.9946	0.5-25
Tanshinone IIA	y=1.094E+10x+1.096E+10	0.9928	0.1-10

Table. S2. Statistical table of the number of differential metabolites.

group name	All sig diff	down regulated	up regulated
Z1K0-Z1K3	123	84	39
Z2K0-Z2K3	154	62	92

Table. S3. Secondary classification statistics of SubClass differential metabolites for each experimental treatment.

Class II	Sub Class8	Sub Class5
Organic acids	1	4
Nucleotides and derivatives	1	8
Amino acids and derivatives	2	3
Plumerane	5	0
Alkaloids	1	0
Saccharides and Alcohols	10	1
Phenolic acids	4	5
Coumarins	1	0
Flavones	4	0
Quinones	0	1
Sesquiterpenoids	1	0
Free fatty acids	1	1
Flavonols	2	0
Flavanones	1	0
Triterpene	5	1
Others	1	3