

Supporting Information

Description of supplementary data:

Table S1. List of *Carthamus tinctorius* L. samples used in this study

Table S2. Supplementary file of Secondary Metabolome data(xlsx)

Table S3. Supplementary file of Volatile Metabolome data(xlsx)

Figure S1. Identification of secondary metabolites of Sichuan *C. tinctorius*. (The left picture shows negative ion mode, and the right picture shows positive ion mode.) The multi-peak chromatogram of metabolite detection by MRM (multi-substance extracted ion current (XIC)).

Figure S2. Identification of secondary metabolites of Henan *C. tinctorius*. (The left picture shows negative ion mode, and the right picture shows positive ion mode.) The multi-peak chromatogram of metabolite detection by MRM (multi-substance extracted ion current (XIC)).

Figure S3. Identification of secondary metabolites of Xinjiang *C. tinctorius*. (The left picture shows negative ion mode, and the right picture shows positive ion mode.) The multi-peak chromatogram of metabolite detection by MRM (multi-substance extracted ion current (XIC)).

Figure S4. Identification of secondary metabolites of Yunnan *C. tinctorius*. (The left picture shows negative ion mode, and the right picture shows positive ion mode.) The multi-peak chromatogram of metabolite detection by MRM (multi-substance extracted ion current (XIC)).

Figure S5. Identification of volatile metabolites. (A)TIC (Total ionscurrent) of the QC samples for mixed samples. (B)The multi-peak chromatogram of metabolite detection by MRM (multi-substance extracted ion current (XIC)).

Figure S6. PPI (protein-protein-interaction) network of differential metabolites of *C. tinctorius* from Sichuan(others VS Sichuan, fold change ≤ 0.5 or ≥ 2 , VIP ≥ 1). (A) PPI network of secondary differential metabolites. (A) PPI network of volatile differential metabolites.

Figure S7. Molecular docking results of differential metabolites in *C. tinctorius* from different producing areas (CA2 and PTGS2).