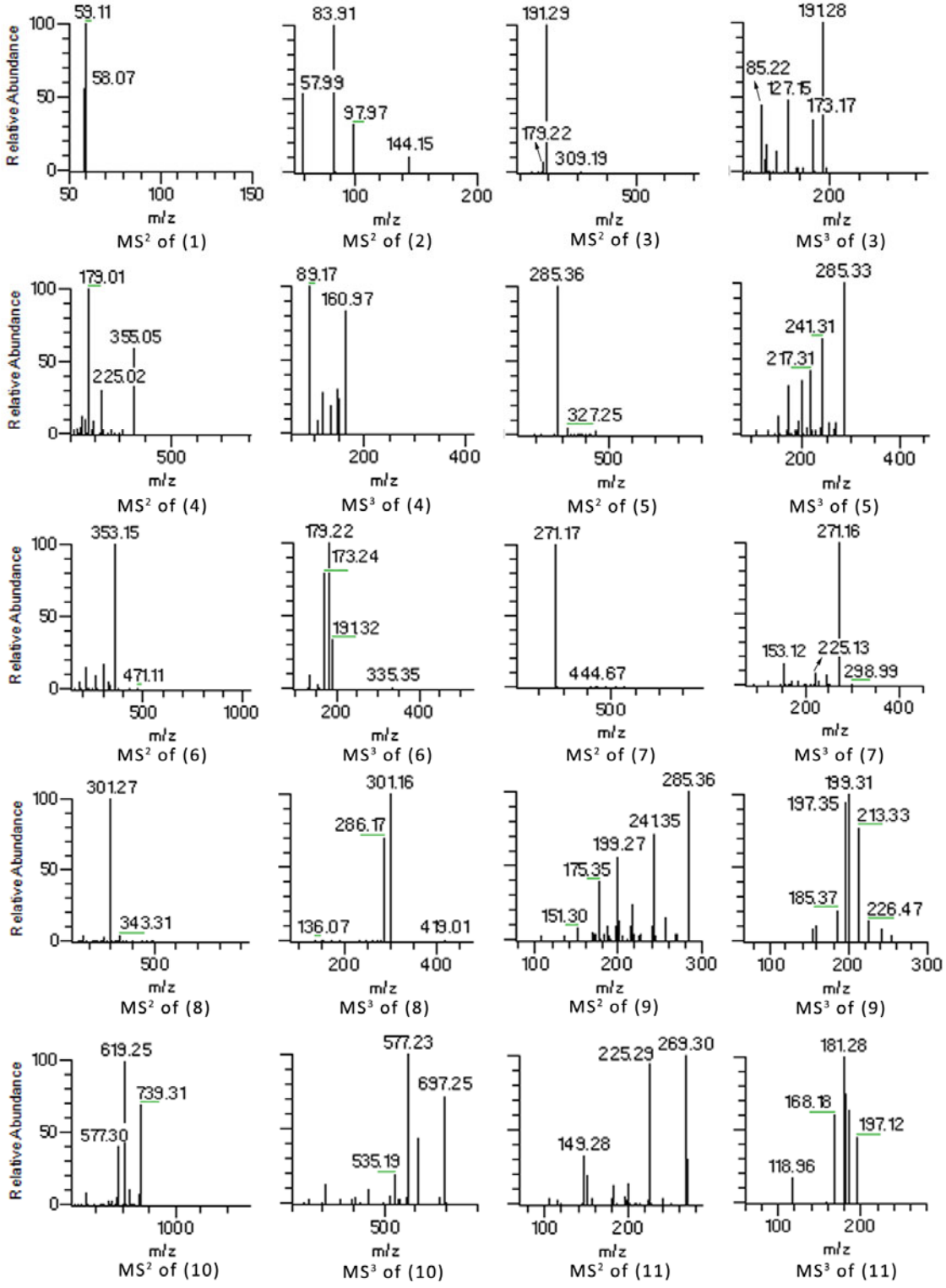
## 1. Identification of 20 constituents in XDKMT by HPLC-PDA/ESI-MS$^n$

The sample of XDKMT was analyzed by HPLC-PDA/ESI-MS$^n$ in both negative and positive ionization modes. Mass spectra of the 20 compounds were shown in Fig. S1. By comparing the retention times, UV spectra and MS$^n$ spectra of peaks in sample chromatogram with those of reference standards, 20 peaks were unambiguously identified asstachydrine (**2**), chlorogenic acid (**3**), gentiopicroside (**4**), luteolin-7-*O*-β-D-glucoside (**5**), isochlorogenic acid B (**6**), cosmosiin (**7**), diosmetin-7-*O*-β-D-glucoside (**8**), luteolin (**9**), trifloroside(**10**), apigenin (**11**), diosmetin (**12**), (1*S*, 5*R*, 9*R*)-scabraside (**13**), (1*S*, 5*R*, 9*R*)-deglucosyltrifloroside (**14**), tauroursodeoxycholic acid (**15**), acacetin (**16**), alisol C (**17**), taurochenodeoxycholic acid (**18**), alisol A (**19**), and alisol B-23-acetate (**20**).



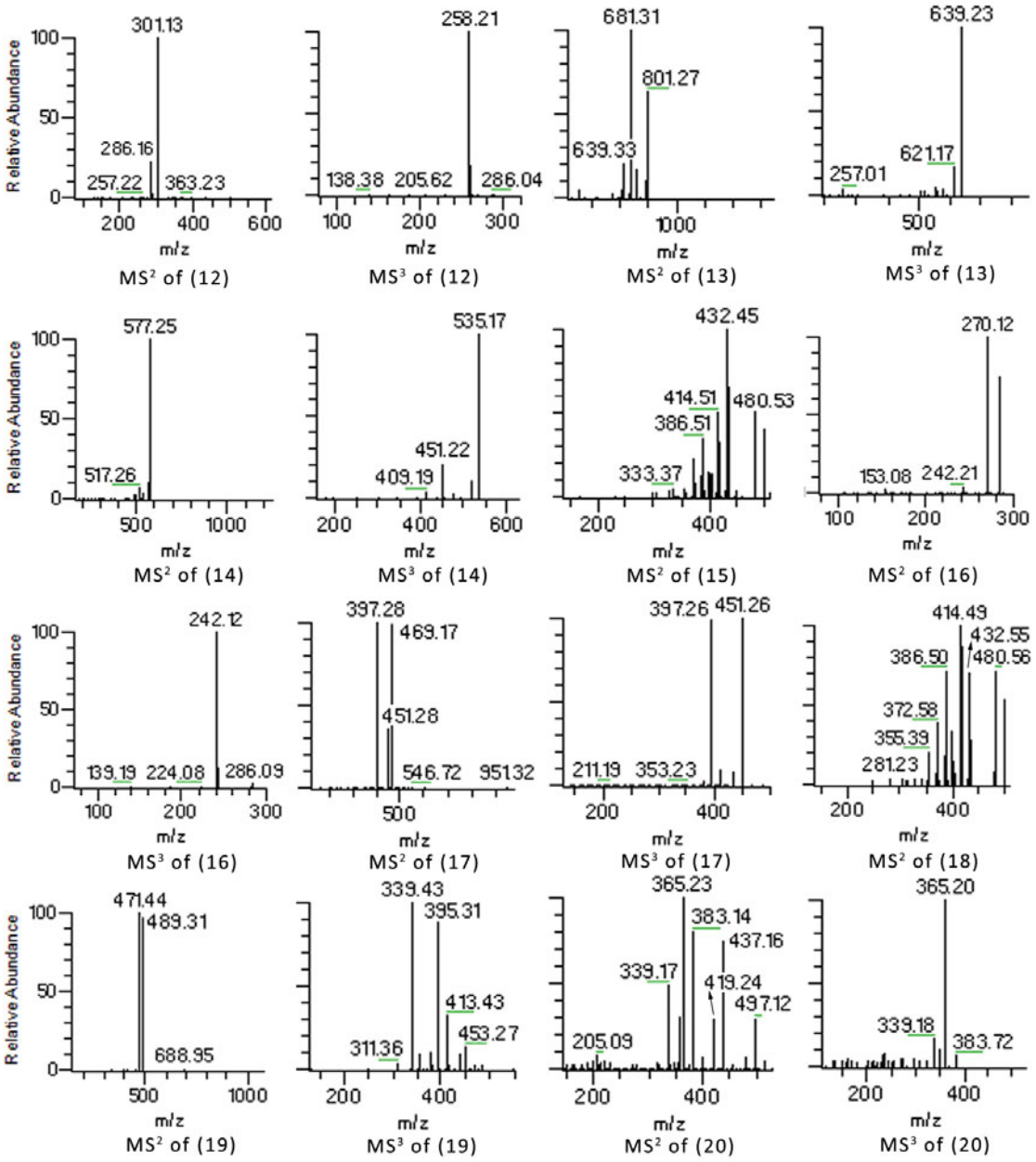



**Fig. S1 Mass spectra of the 20 compounds identified in XDKMT**

## 2. Optimization of sample preparation procedure

2.1 Extraction solvents

In Fig. S2, the vast majority of the compounds reached the maximum extraction rate when extracted by 50% methanol.

2.2 Amount of extraction solvent

In Fig. S3, the extraction rate of all compounds from the points of 20 to 40 ml changed little, and maintained at the highest level. Therefore, to make the operation more convenient and simplify the pre-treatment process (for example avoiding the process of rotary evaporation and making each of the compounds can be detected), we chose 25 ml as the optimal amount.

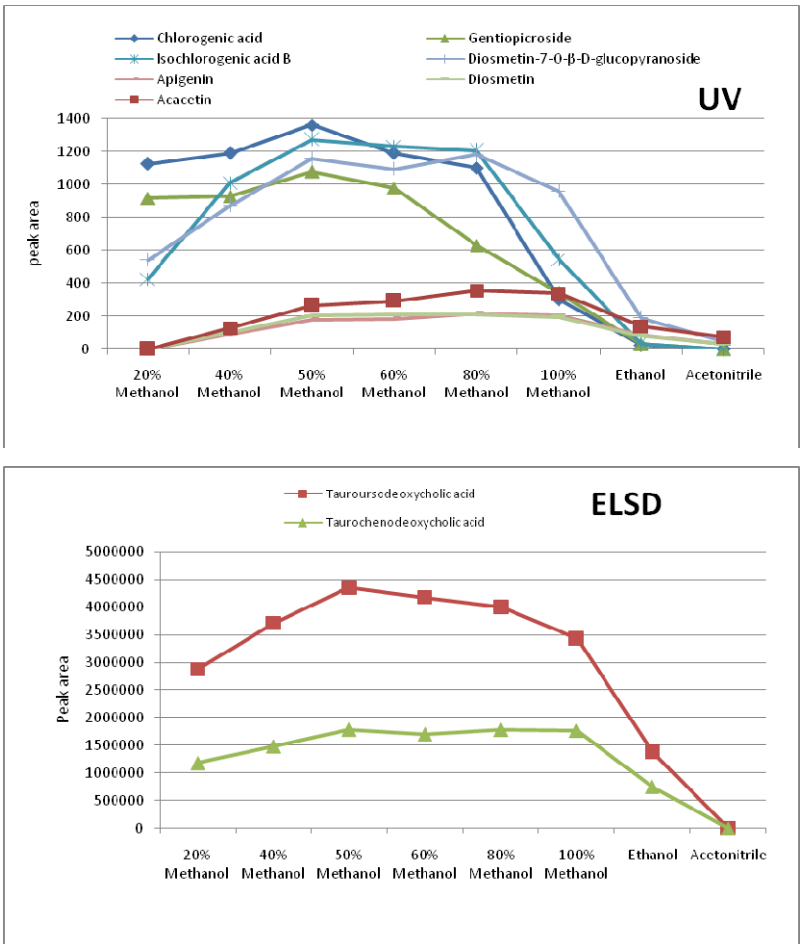



**Fig. S2 Relationship between the peak area and extraction solvent**

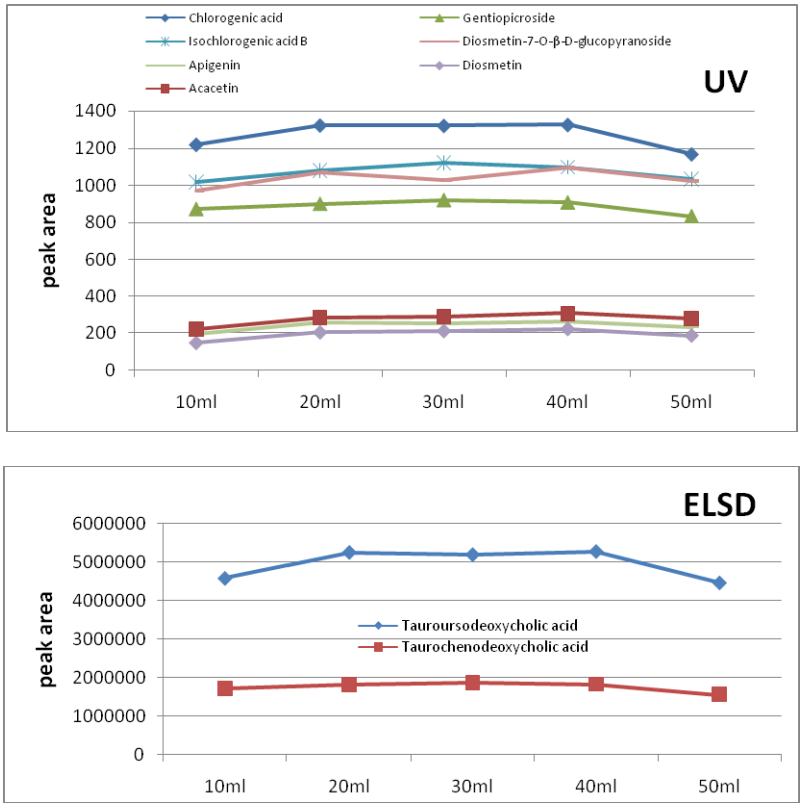



**Fig. S3 Relationship between the peak area and the amount of extraction solvent**

2.3 Extraction time

In Fig. S4, when extracted 40 min, it reached the maximum extraction rate of nine compounds.

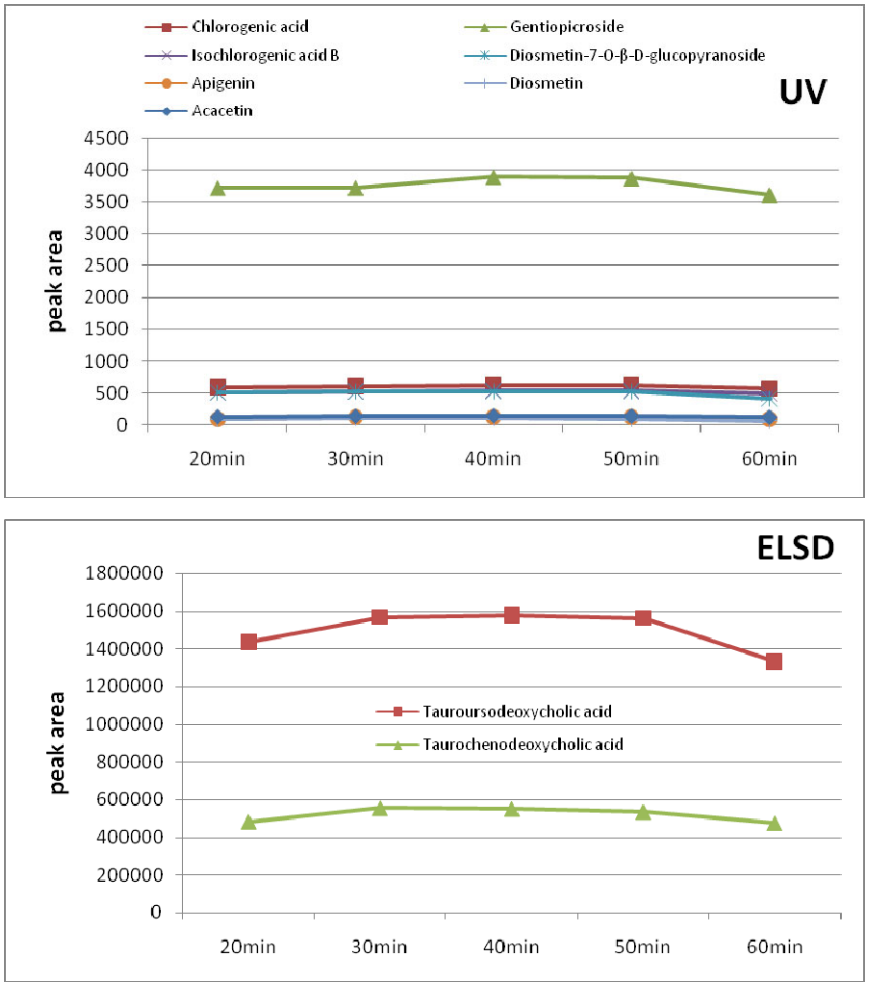



**Fig. S4 Relationship between the peak area and the extraction time**

2.4 Extraction number of times

In Fig. S5, when the number of extraction increased, peak area almost ceased to increase. Therefore, to simplify the pre-treatment process, we selected extracted once.

## 3. Optimization of the HPLC chromatographic conditions

3.1 Columns

To optimize the condition of separation, different reverse-phase HPLC columns were compared to separate the target compounds, such as Zorbax SB-C18 (4.6 mm×250 mm, 5 μm) and Zorbax Eclipse Plus C18 (4.6 mm×100 mm, 1.8 μm). In Fig. S6, the latter had a shorter analysis time but a poor resolution. The better separation efficiency and peak shape were achieved by Zorbax SB-C18.

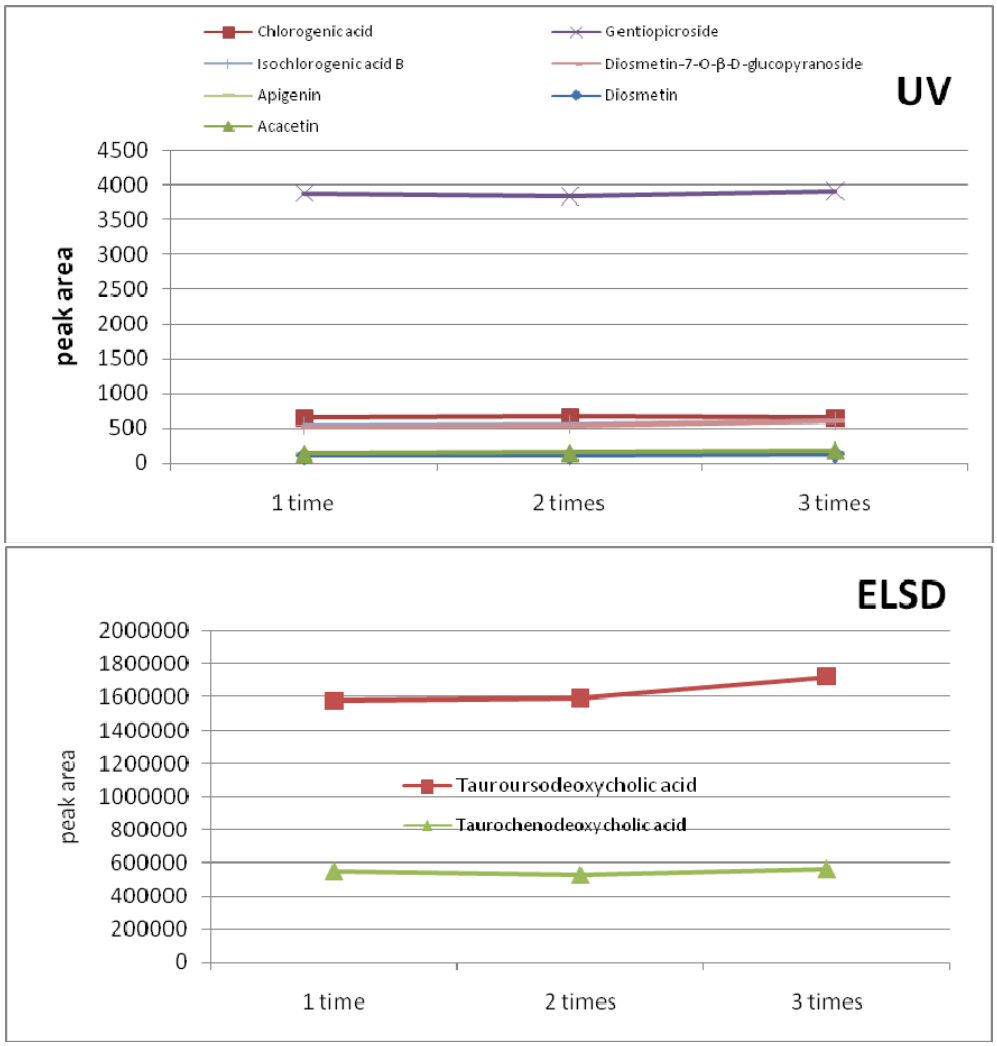



**Fig. S5 Relationship between the peak area and the number of extraction**

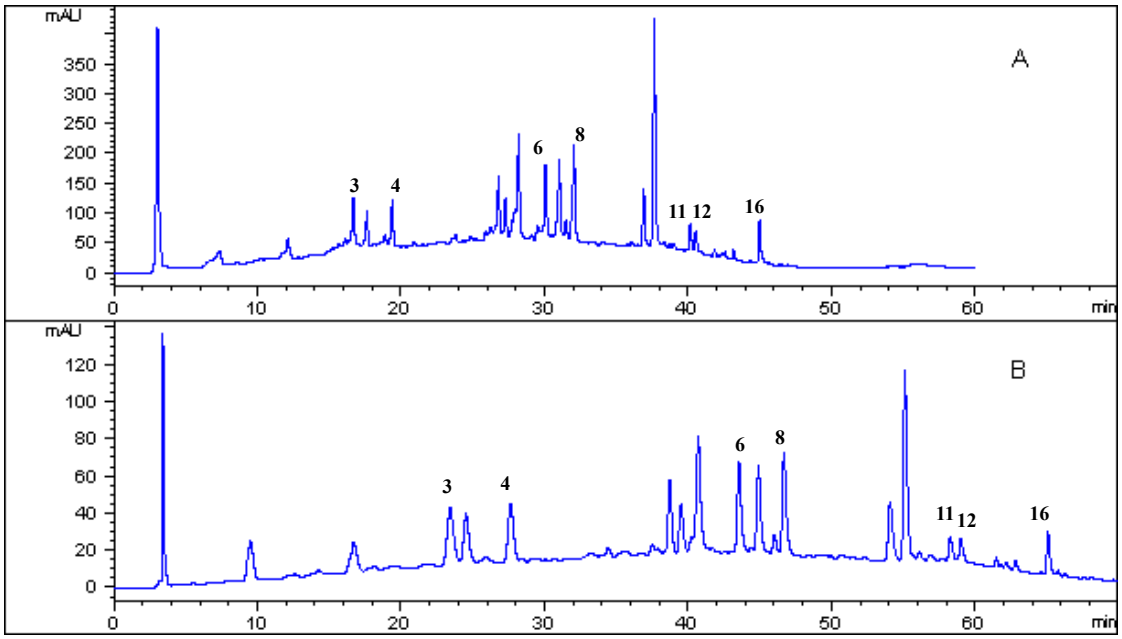



**Fig. S6 Comparison of two types of columns**

A. Zorbax Eclipse Plus C18 (4.6 mm×100 mm, 1.8 μm); B. Zorbax SB-C18 (4.6 mm×250 mm, 5 μm)

3.2 Column temperature

Column temperature had a great effect on the resolution. So temperatures between 20 and 40 °C were tested, and 39 °C was appropriate. As shown in Fig. S7B, it had a better resolution of peaks **3**, **6**, **11**, **12**, **16** at 39 °C.

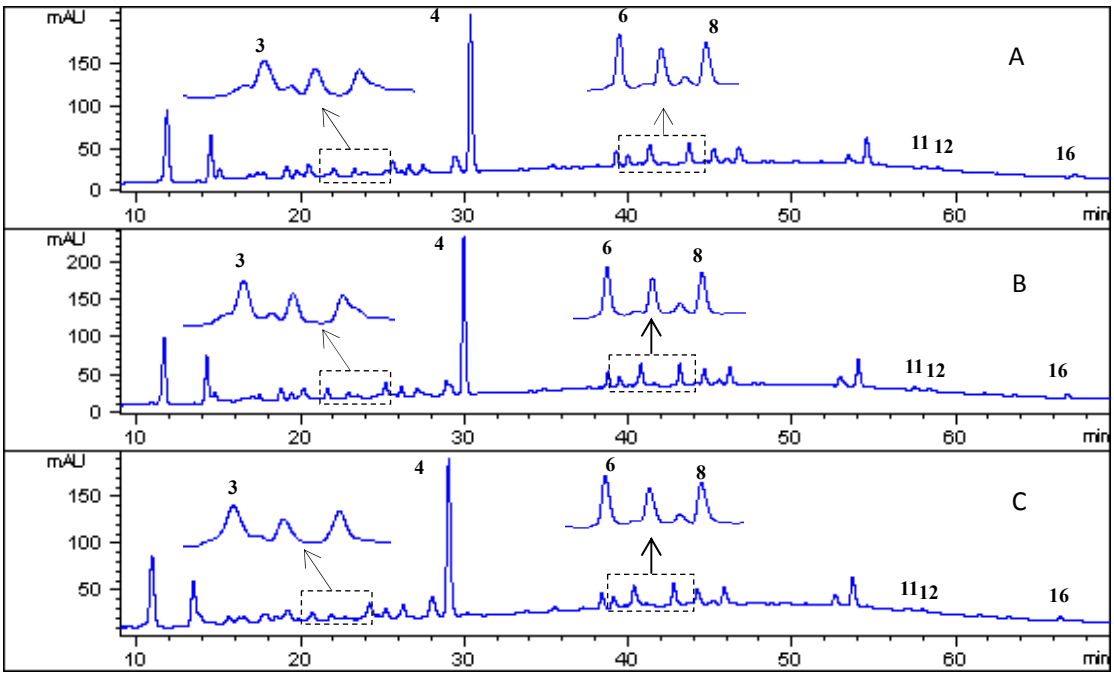



**Fig. S7 Comparison of different column temperatures: A. 38 °C; B. 39 °C; C. 40 °C**

3.3 Optimization of the ELSD conditions

As for ELSD, the drift tube temperature, flow rate of nebulizing gas and detector gain are crucialto improve the signal-to-noise (S/N) ratio.HPLC-ELSD analysisof thesample solution at different drift tube temperatures (110, 100, 90 °C), different gas flow rates (2.5, 2.0, 1.5 L/min) and different detector gains (3, 2, 1) were performed respectively and optimal parameters were then selected for obtaining the optimal sensitivity. Finally, we found that when the drift tube temperature was set to 100 °C at gain 1 and the nitrogen flow rate was 2 L/min, the S/N ratio achieved the maximum values (Fig. S8).

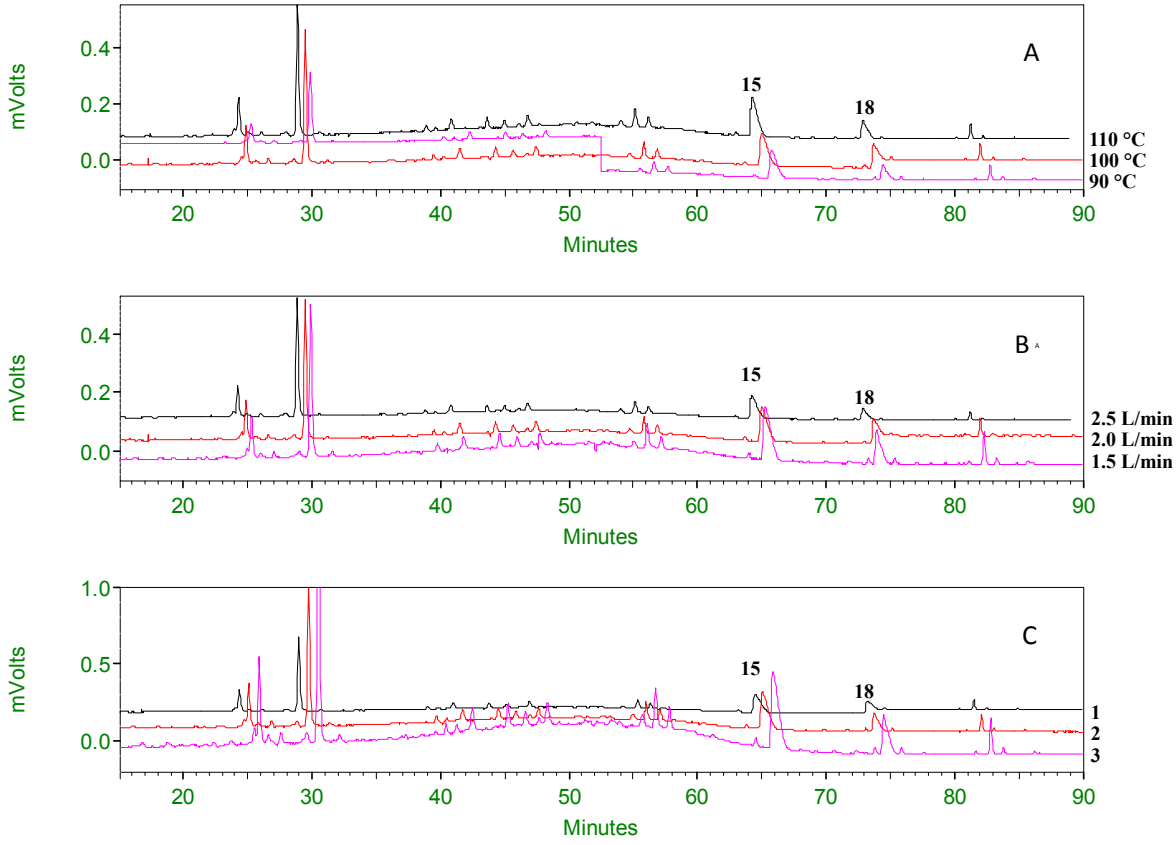



**Fig. S8 Optimization of the ELSD conditions**

A. Tube temperatures (110, 100, 90 °C); B. Gas flow rates (2.5, 2.0, 1.5 L/min); C. Detector gains (1, 2, 3)