Additional file 1 Chemical fingerprint of huangqin flavonoids extraction

Preparation of samples

Sample of huangqin flavonoids extraction was diluted with methanol aqueous solution (methanol:pure water = 1:1; V:V), then centrifuged at 8000 r/min for 10 minutes and supernatant was injected for analysis.

LC-MS instruments and operation conditions

Liquid chromatography

An SHIMAZDU 30AD System was used (Shimazdu Corp., Japan) to inject 5 μL aliquots of samples on an Acquity UPLC HSS T3 column (100 × 2.1 mm, i.d., 1.8 mm, Waters, USA) which was maintained at 35℃ in a column oven. The mobile phase was consisting of (A) 0.1% formic acid aqueous solution (prepared using Milli Q water) and (B) acetonitrile at a flow rate of 0.5 mL/min using a gradient elution program showed in **Additional Table 1**.

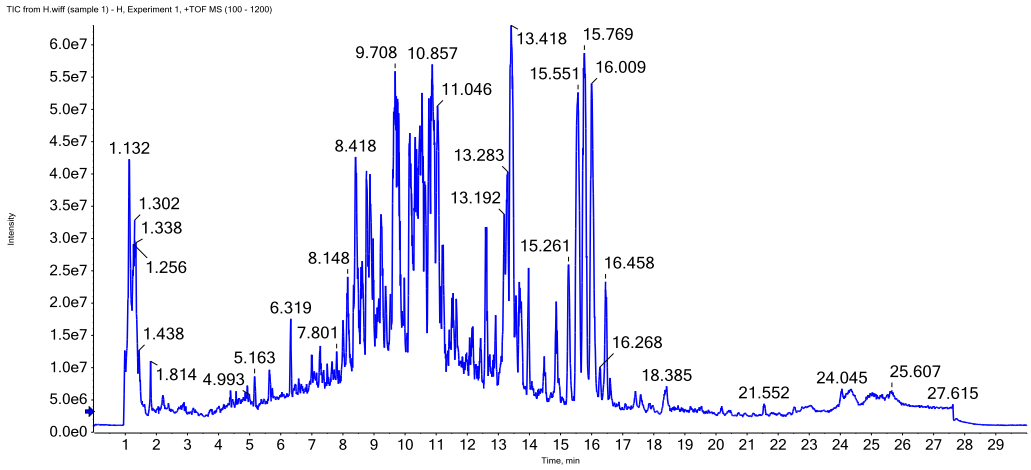
Additional Table 1 Gradient program of liquid chromatography

Time (minute)	Mobile phase B (%)
0	3
1	3
23	95
26	95
26.1	3
30	3

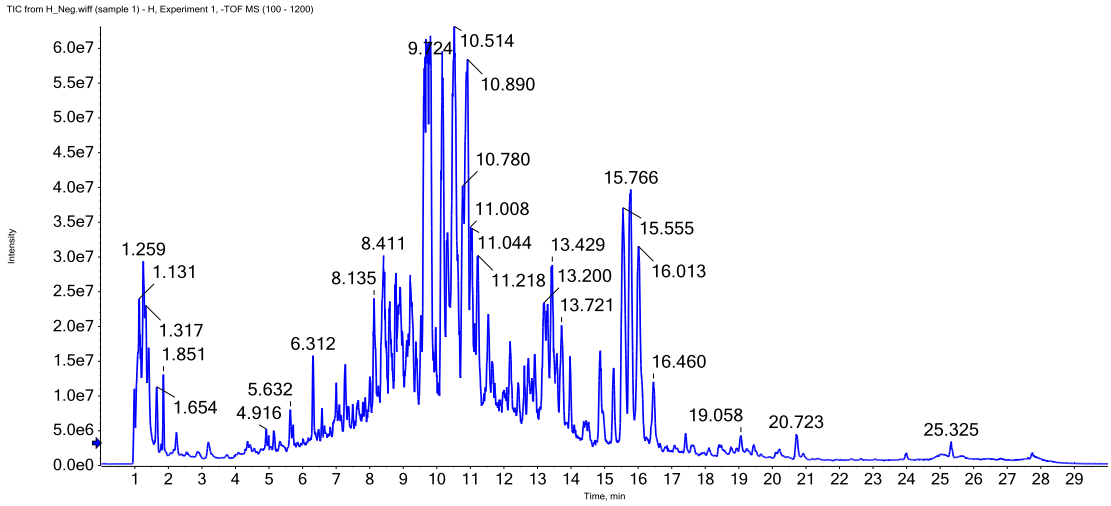
Mass spectrometric conditions

A Triple TOF 5600+ mass spectrometer (AB Sciex Corp., USA) equipped with an electrospray ionization (ESI) interface was used. The operating parameters were as follows: curtain gas, 30 L/h; GS1, 50 L/h; GS2, 60 L/h; ISVF, 5500 V(+), 4500 V(-); desolvation temperature, 500℃. ESI/MS was operated both in positive and negative modes in in TOF-MS-IDA-TOF-MS/MS (n = 8; TOF-MS: 100-1200 Da, TOF-MS/MS: 50-1200 Da).

The chemical fingerprint of huangqin flavonoids extraction in positive mode (ESI+) and negative mode (ESI-) were showed in **Additional Figures 1** and **2**, respectively.



Additional Figure 1 Chemical fingerprint of huangqin flavonoids extraction in positive mode (ESI+)



Additional Figure 2 Chemical fingerprint of huangqin flavonoids extraction in negative mode (ESI-)