

Supplementary materials

UPLC-QTOF-MS based metabolomics coupled with diagnostic ion exploration strategy for rapidly evaluating sulfur-fumigation caused holistic quality variation of medicinal herbs, Moutan Cortex as an example

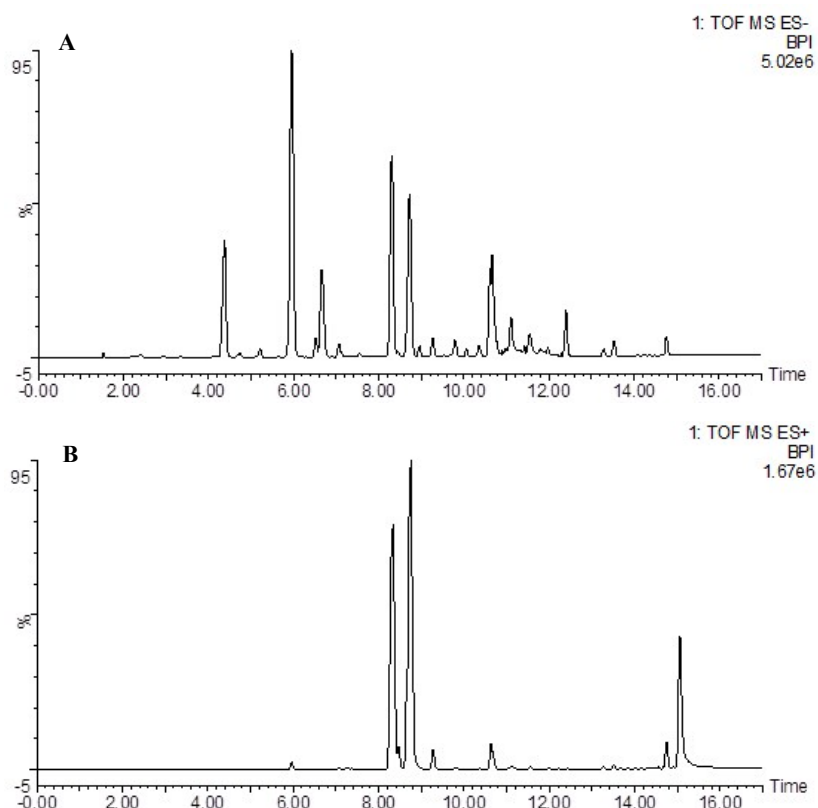
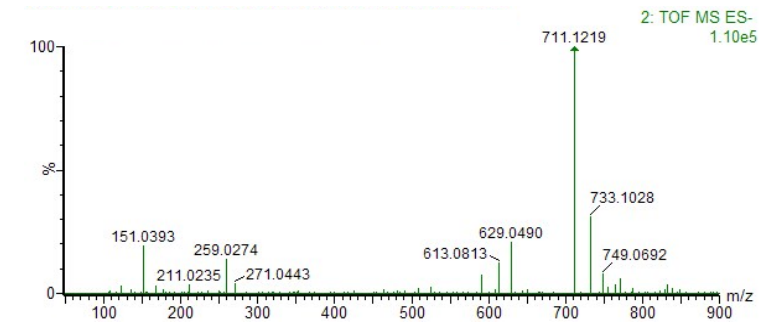
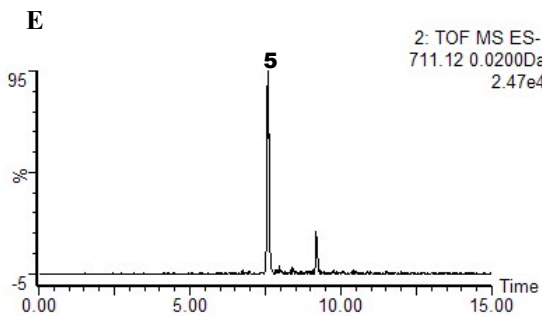
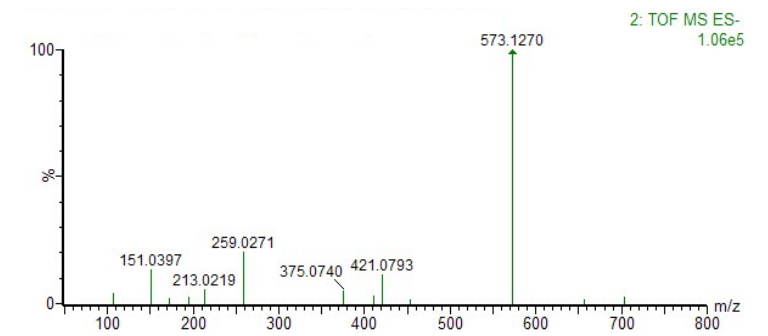
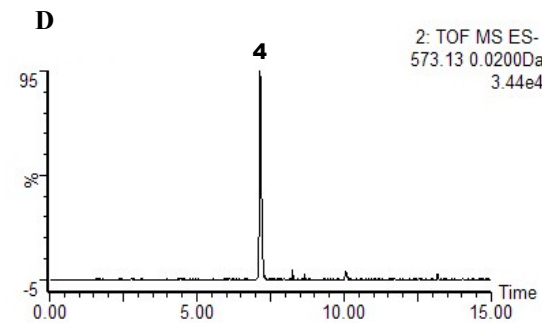
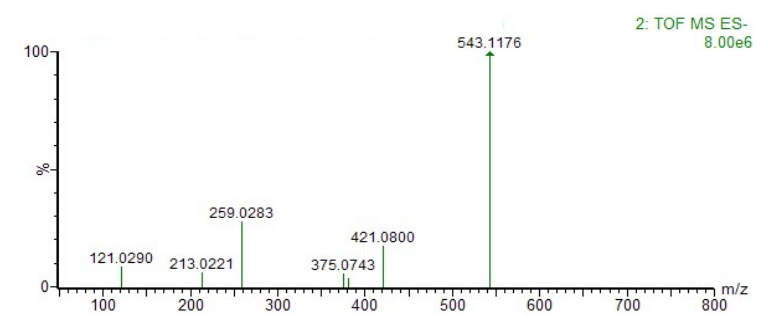
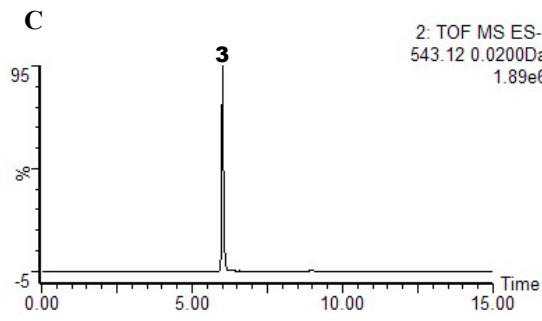
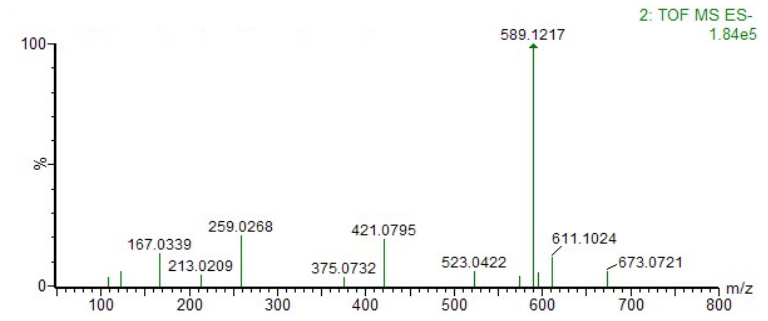
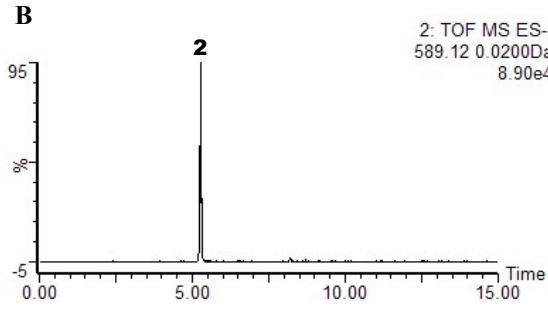
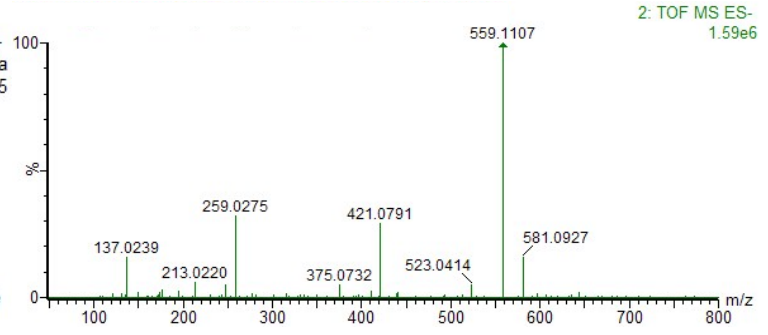
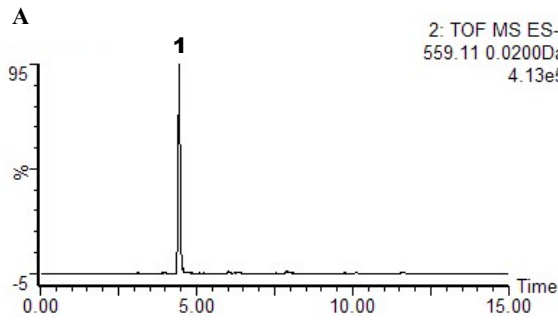


Fig.S1 Base peak ion chromatograms of the S-MC (S26 group) (A) in negative mode and (B) in positive mode.



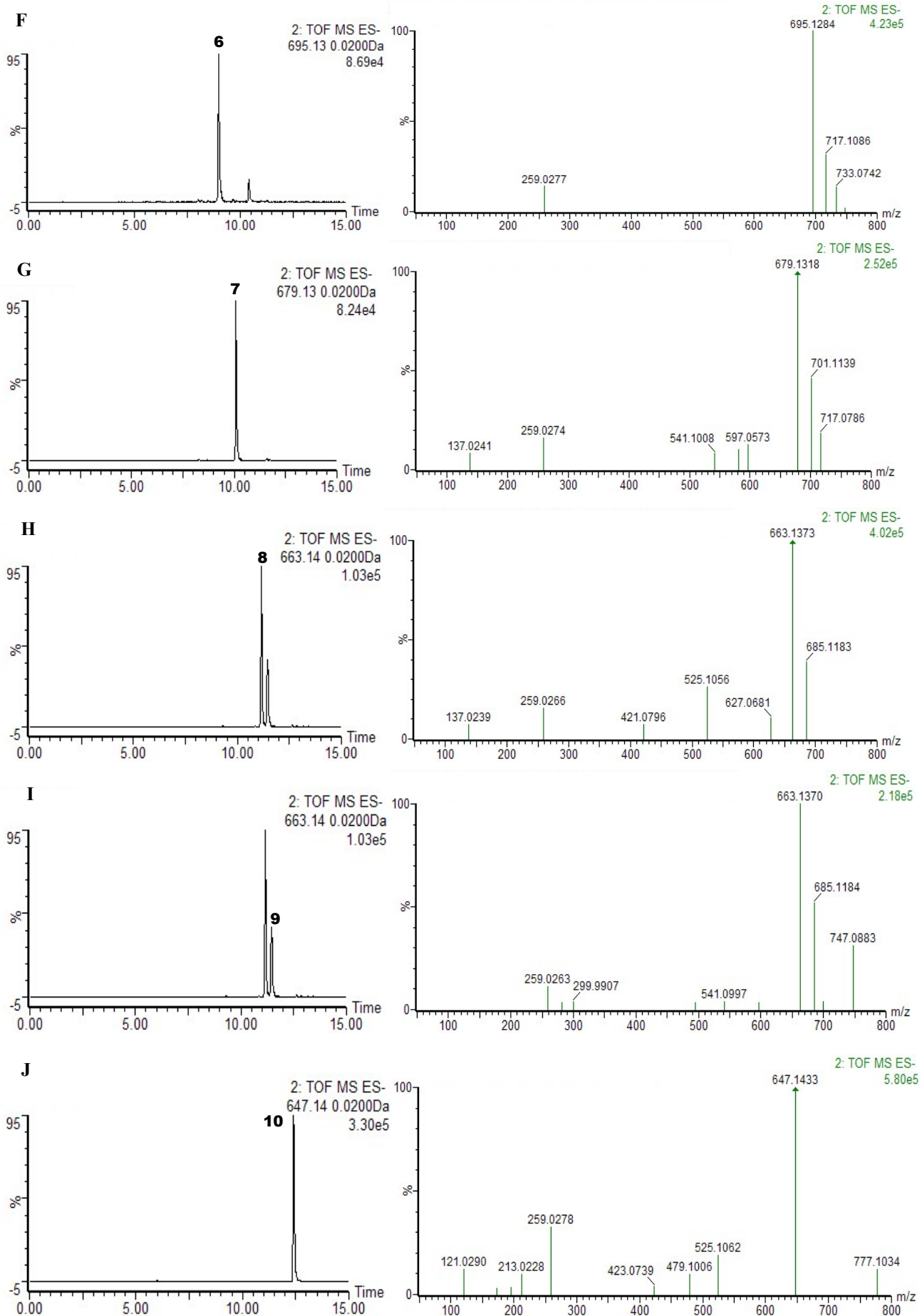


Fig.S2 Extraction ion chromatograms and high energy (30-60V) CID mass spectra of ten newly generated sulfonate derivatives (as summarized in Table.2 and Fig. 6) in S-MC samples (S26) in negative mass mode: (A) oxypaeoniflorin sulfonate; (B) mudanpioside E sulfonate; (C) paeoniflorin sulfonate; (D) mudanpioside D sulfonate; (E) galloyloxypaeoniflorin sulfonate; (F) galloylpaeoniflorin sulfonate; (G) mudanpioside H sulfonate; (H) benzoyloxypaeoniflorin sulfonate; (I) mudanpioside C sulfonate; (J) benzoylpaeoniflorin sulfonate.