

Supplementary information:

Integrated chemical profiling of Zhi-Zi-Hou-Po Decoction by liquid chromatography-diode array detector-time of flight mass analyzer and liquid chromatography-triple stage quadrupole mass analyzer combined with chemometrics

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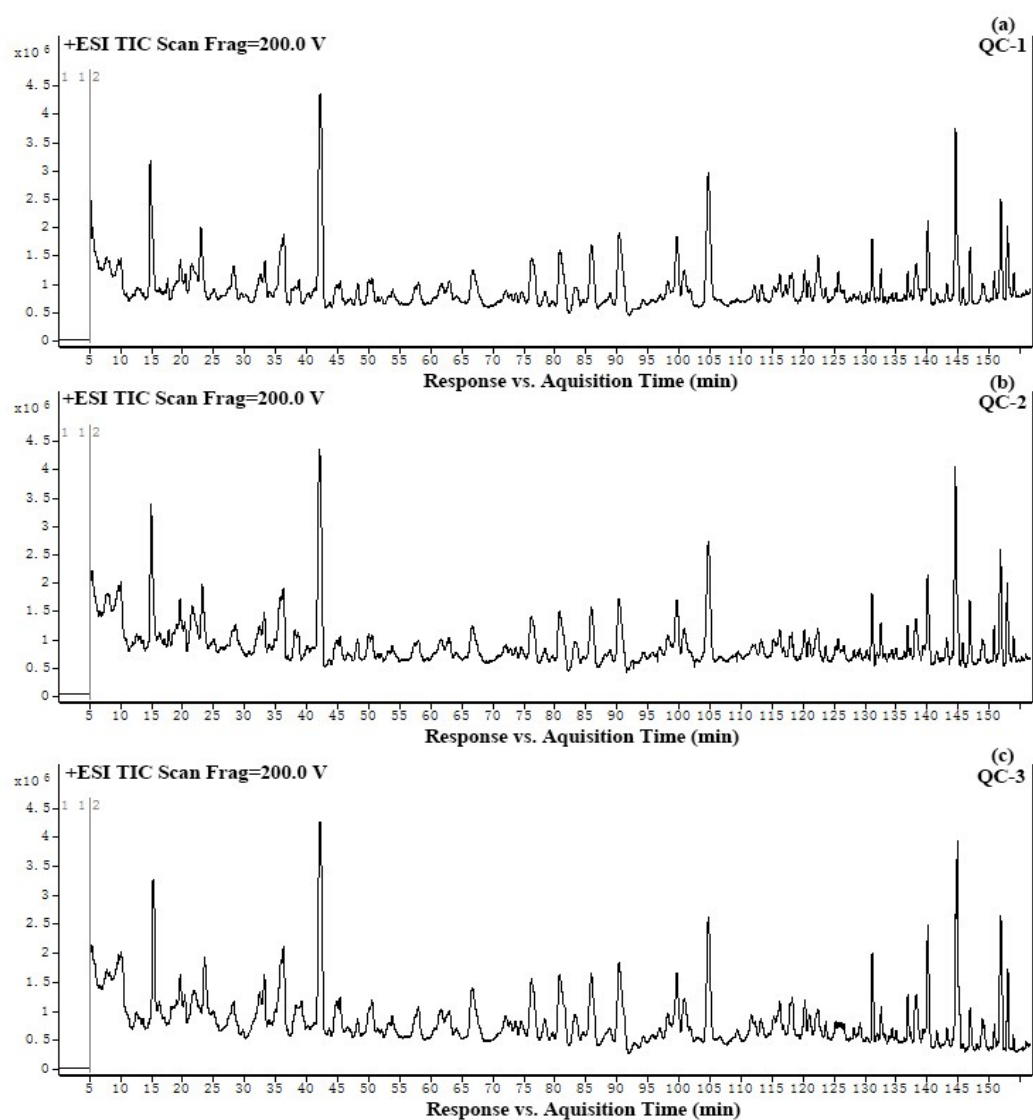


Fig. S1 The total ion chromatograms in positive ion mode of three consecutive runs

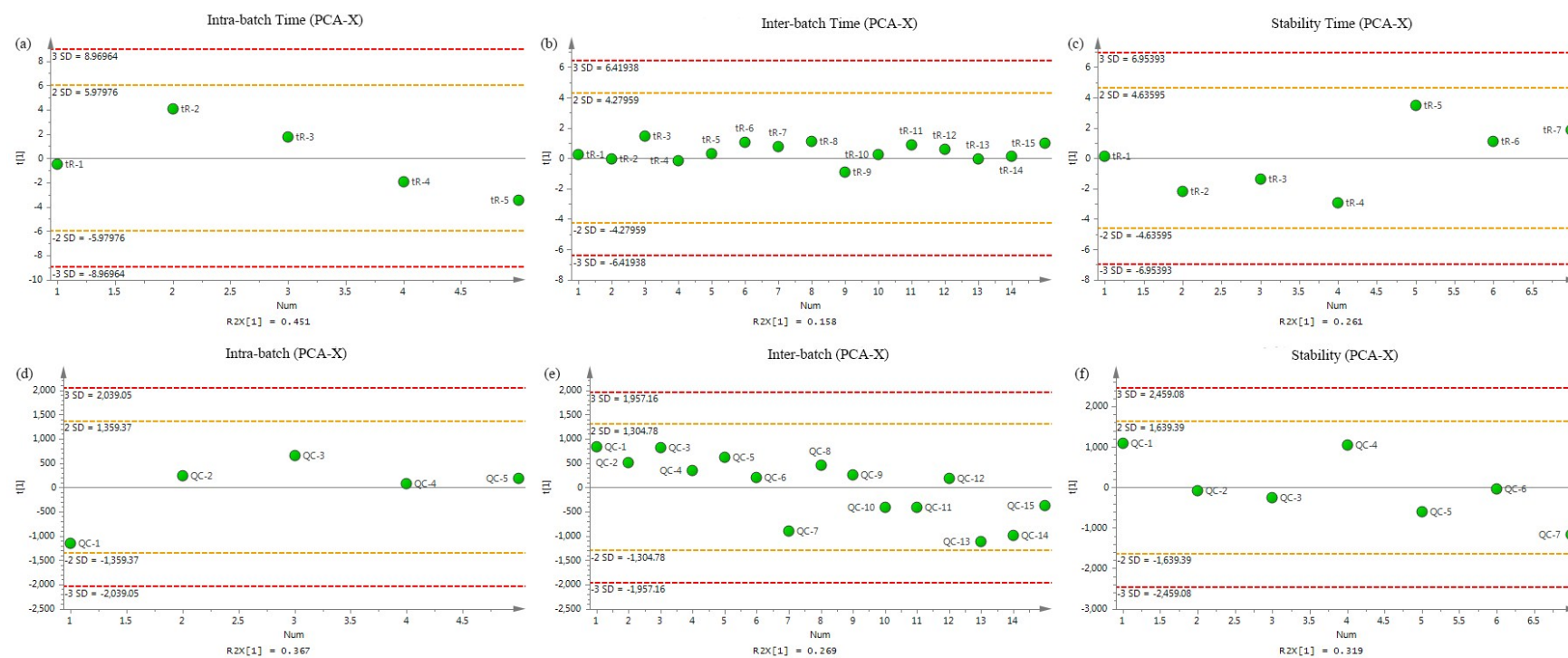


Fig. S2 PCA first component for the QC samples versus time: (a) retention time in intra-batch experiments; (b) retention time in inter-batch experiments; (c) retention time in stability experiments; (d) ion intensity in intra-batch experiments; (e) ion intensity in inter-batch experiments; (f) ion intensity in stability experiments.

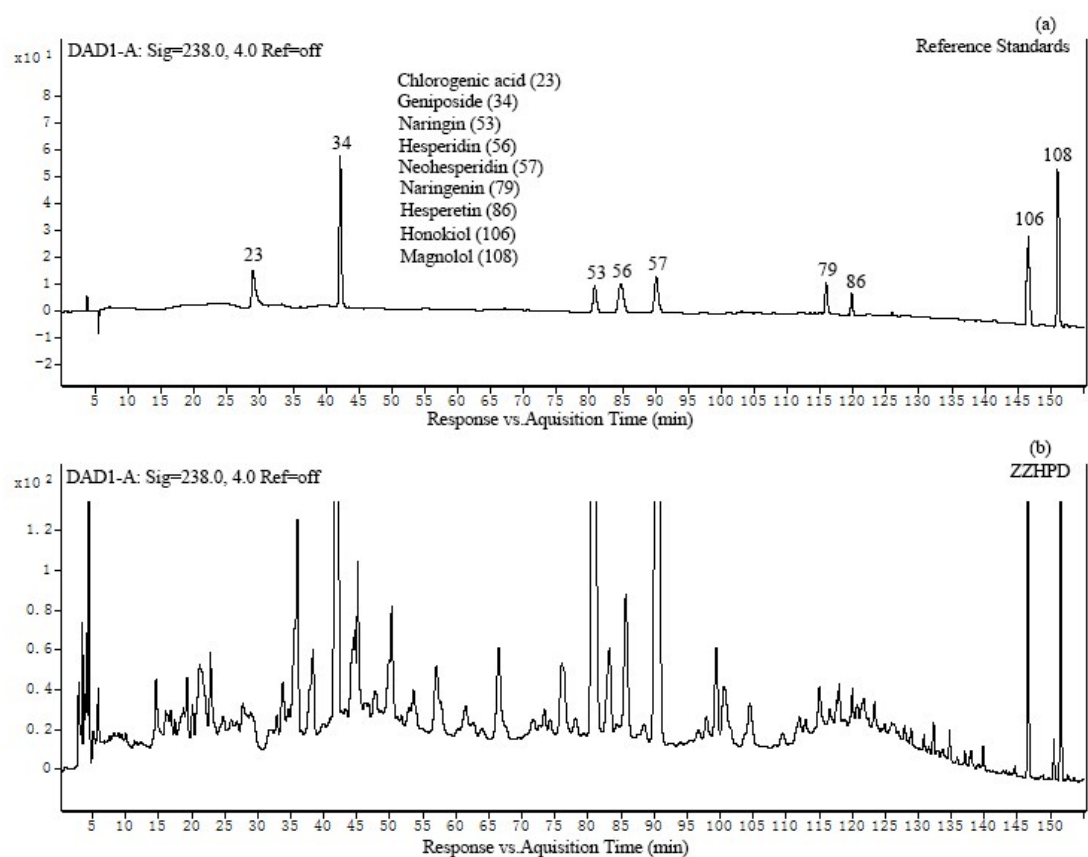


Fig. S3 HPLC-DAD chromatograph of 9 reference standards (a) and ZZHPD extract (b) monitored at 238 nm.

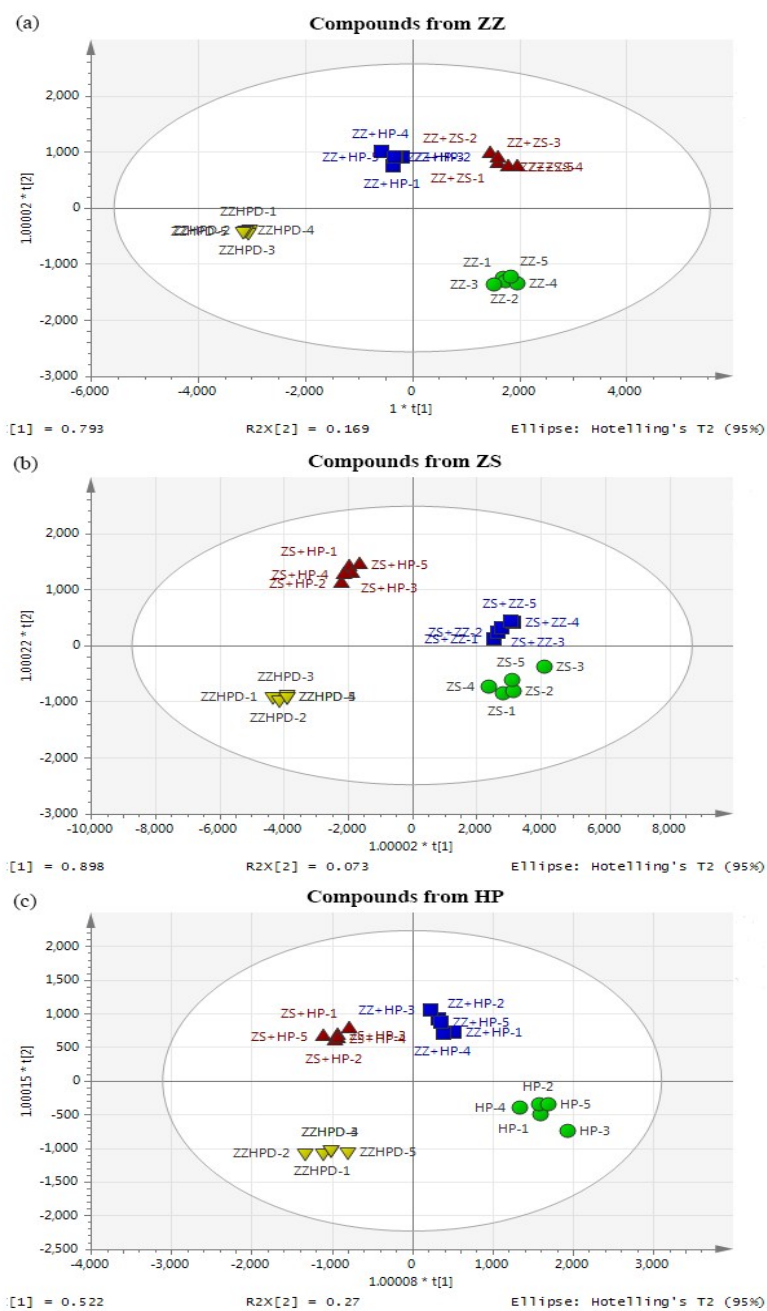


Fig. S4 Scores plots of OPLS-DA models for components in ZZ, ZS and HP with the statistical parameters as follows: (a) $R^2X=0.988$, $R^2Y=0.986$, $Q^2=0.962$; (b) $R^2X=0.989$, $R^2Y=0.973$, $Q^2=0.957$; (c) $R^2X=0.944$, $R^2Y=0.981$, $Q^2=0.944$.