HS-SPME-GC-MS combined with machine learning methods for screening volatile quality indicators in *Hypericum perforatum* L.

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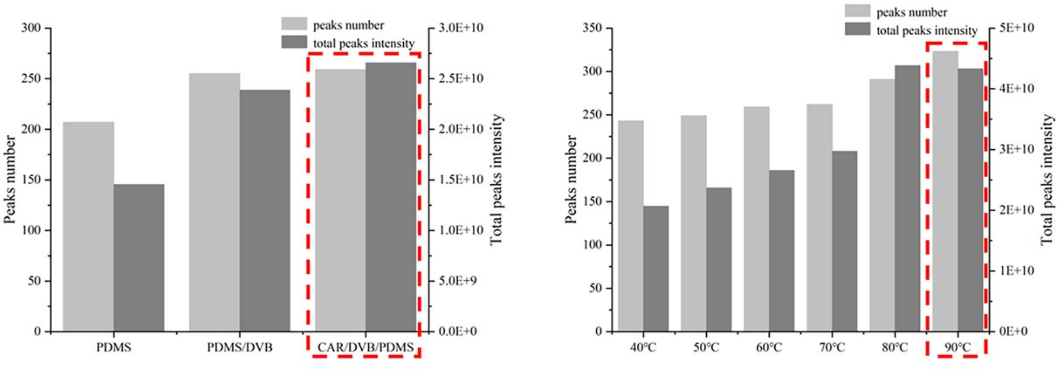
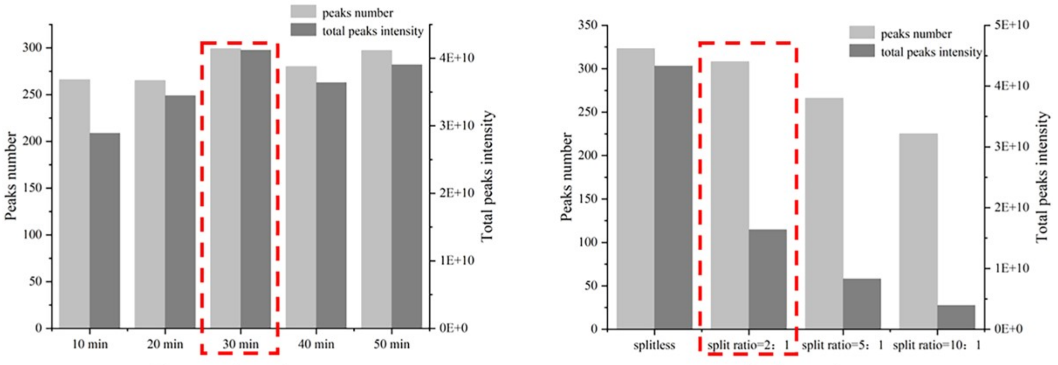
Fig. S1 Optimization of experimental conditions for HS-SPME-GC-MS of Hypericum perforatum L.



SPME fiber **Incubation temperature**



Extraction time **Split ratio**

Fig. S2 The total ion current (TIC) chromatograms of different parts of *Hypericum perforatum* L.(A), Preliminary identification of compounds based on the matching degree of MS fragments (B), calculation of compound RI based on the mixed standard of normal alkane C_8-C_{20} (C).

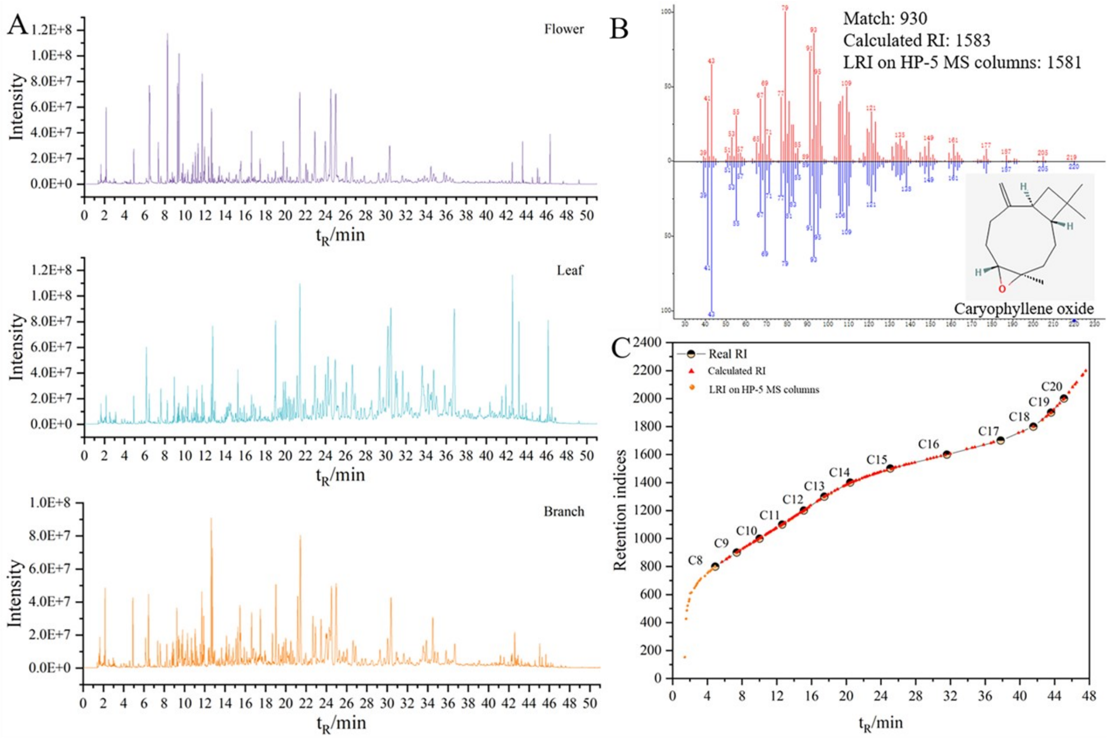


Fig. S3 Screening of differential compounds in different parts of *Hypericum perforatum* L. (a-c: Volcano plots; d-f, OPLS-DA model)

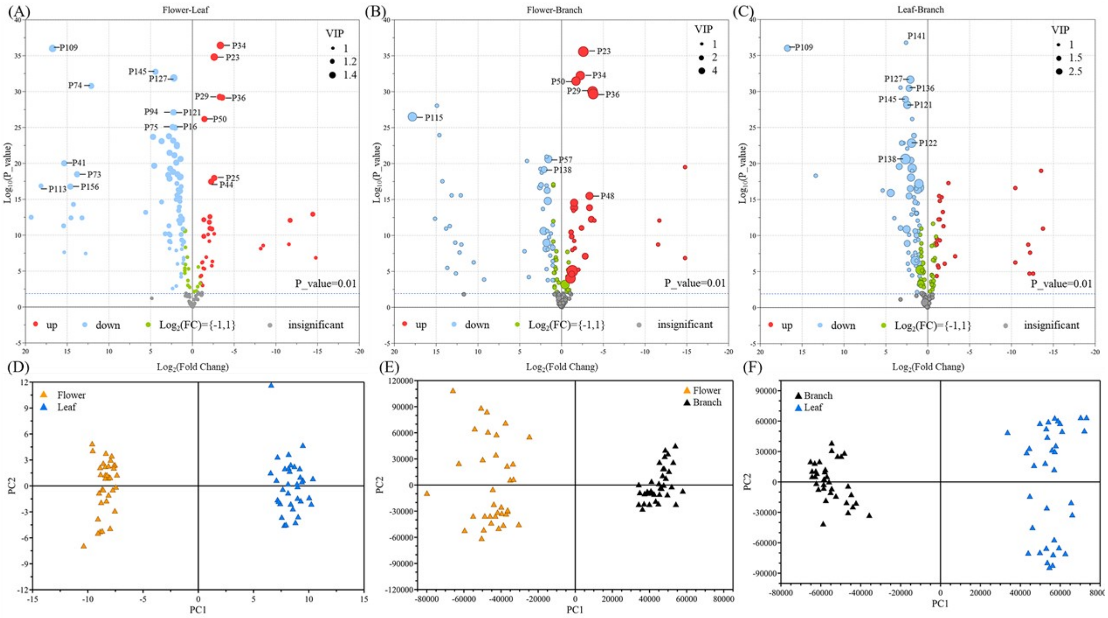


Fig. S4 PPI network of total gene target

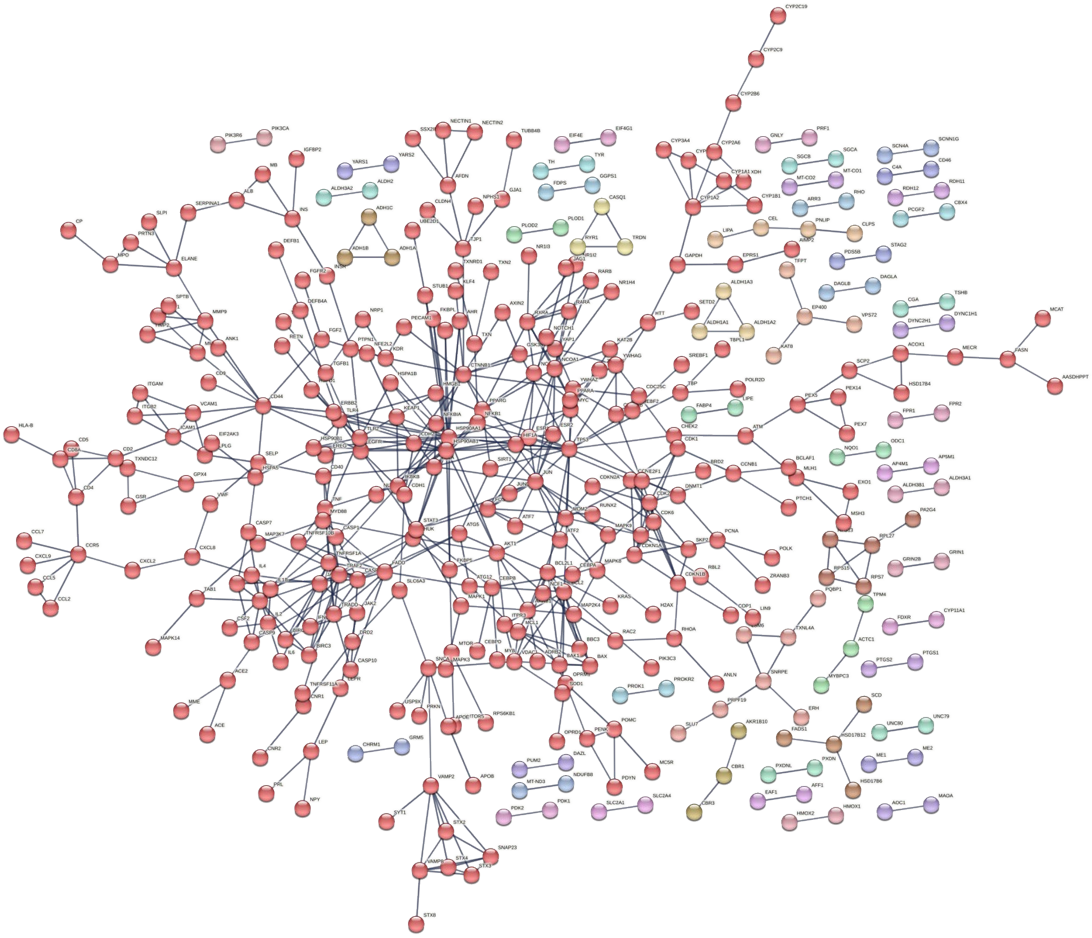


Fig. S5 PPI network of core gene target

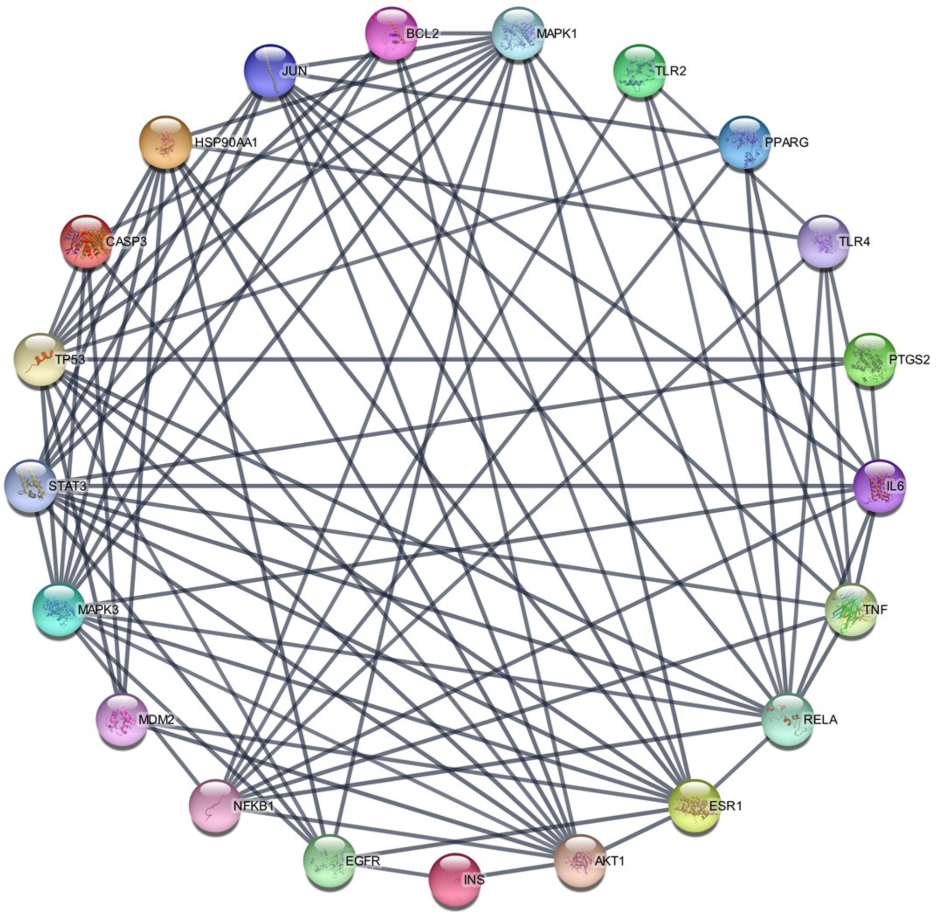


Fig. S6 KEGG pathway enrichment analysis of 24 core gene

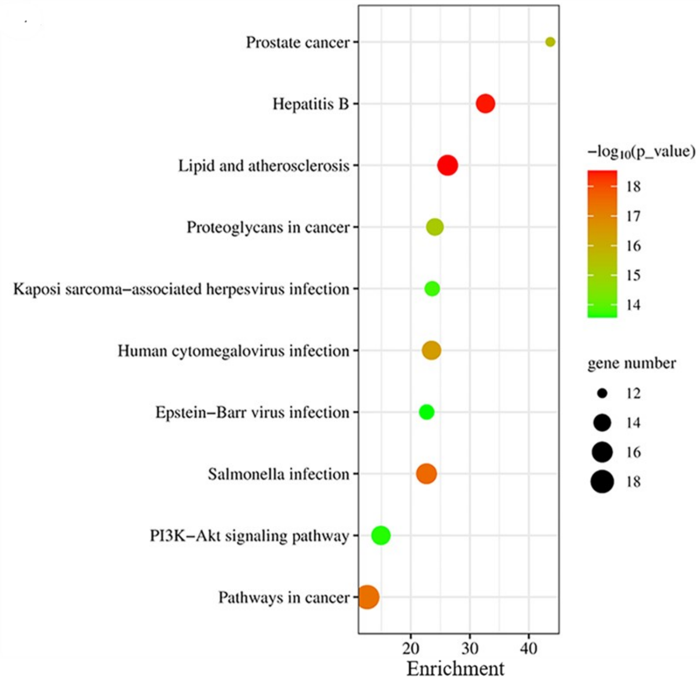


Fig. S7 Division of datasets. (A: Kennard Stone; B, Stratified sampling)