

Supporting Information

Metabolomic elucidation of the effect of sucrose on the secondary metabolite profiles in *Melissa officinalis* by ultra-performance liquid chromatography-mass spectrometry

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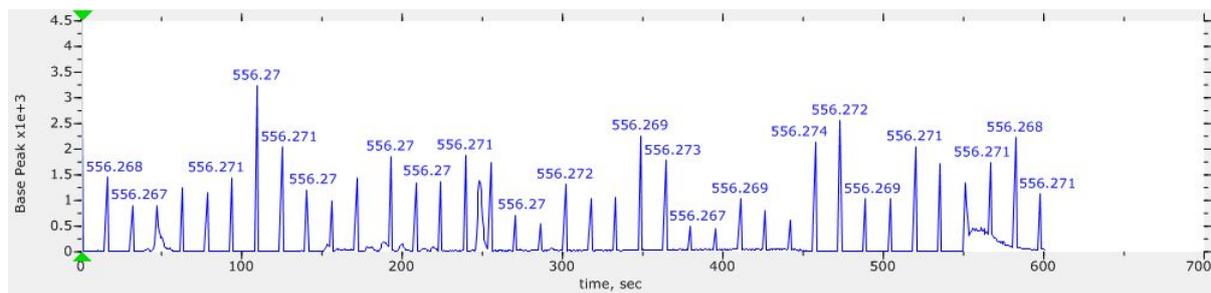
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Figure S2. Validation of the PLS-DA model using the 100 permutation test. The Y-intercept of R^2 and Q^2 indicate 0.719 and -0.248 , respectively.

Table S1. Number of peaks detected, peak-groups, IP-clusters, and predictions in negative and positive modes.

(A)



(B)

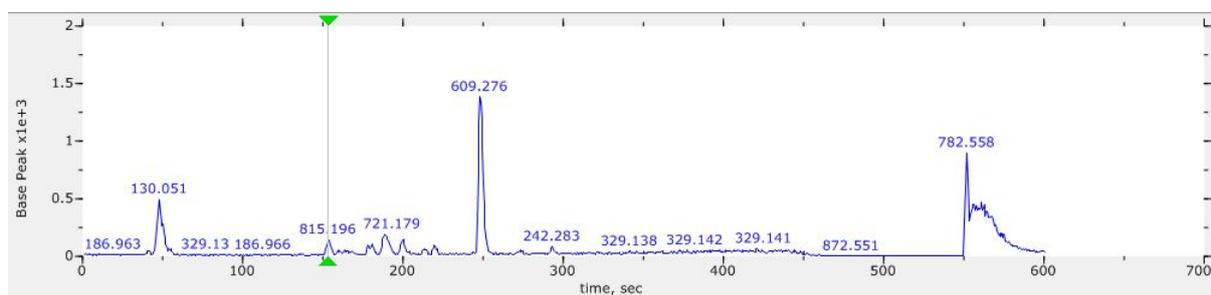


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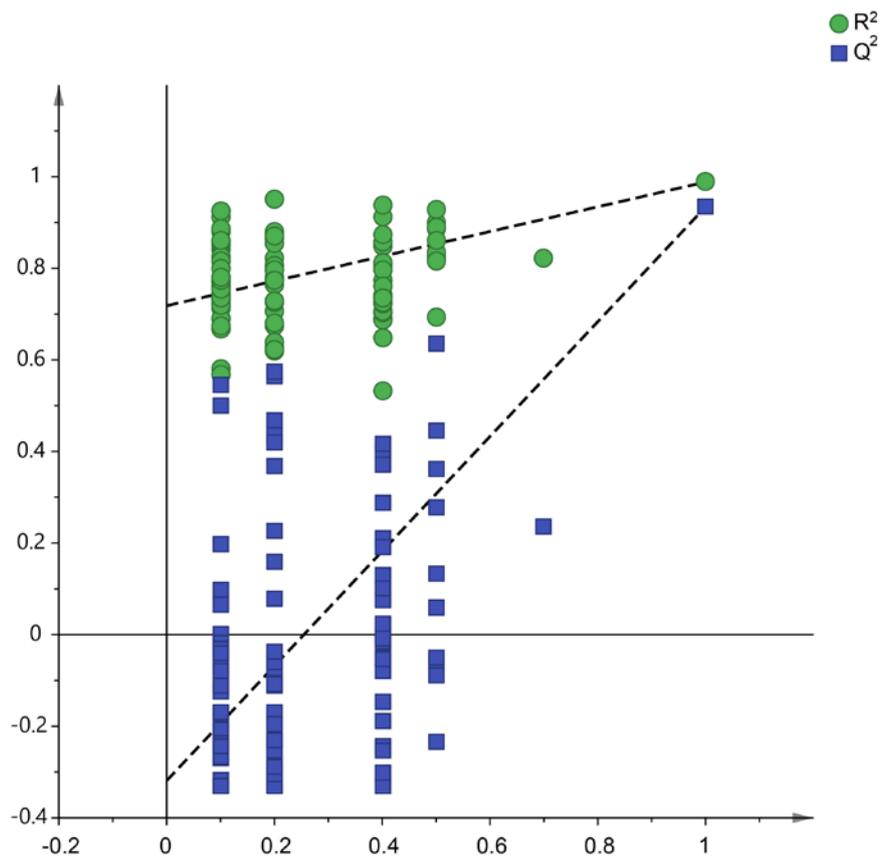


Figure S2. Validation of the PLS-DA model using the 100 permutation test. The Y-intercept of R^2 and Q^2 indicate 0.719 and -0.248, respectively.

Table S1. Number of peaks detected, peak-groups, IP-clusters, and predictions in negative and positive modes.

Feature	Negative	Positive
Peaks detected	21754	11705
Peak-groups with minimum SNR >2	736	376
IP-Clusters	515	251
Predictions	613	286