

## Supplementary Material

### Effects of rootstocks on the flavor quality of Huanglongbing-affected sweet orange juices using targeted flavoromics strategy

Xin Liu <sup>a,b</sup>, Frederick G. Gmitter Jr <sup>a</sup>, Jude W. Grosser <sup>a</sup>, Yu Wang <sup>a,b\*</sup>

<sup>a</sup> *Citrus Research and Education Center, University of Florida, Lake Alfred, Florida  
33850, USA*

<sup>b</sup> *Department of Food Science and Human Nutrition, University of Florida, Gainesville,  
Florida 32611, USA*

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\* Corresponding author

*E-mail address:* [yu.wang@ufl.edu](mailto:yu.wang@ufl.edu) (Yu Wang).

## Reference compounds information

The external standards used for quantitation on Poroshell HILIC-Z column are amino acids (phenylalanine, tryptophan, leucine, isoleucine, methionine, valine, tyrosine, proline, alanine, threonine, glycine, glutamic acid, serine, glutamine, asparagine, aspartic acid, arginine, and theanine), nucleotides and nucleosides (adenine, guanine, xanthine, hypoxanthine, uracil, thymine, cytosine, adenosine, guanosine, 5-methyluridine, uridine, 5-methylcytidine, cytidine, inosine, xanthosine, 2'-deoxyadenosine, 2'-deoxyguanosine, thymidine, 2'-deoxyuridine, 2'-deoxycytidine, 2'-deoxyinosine, adenosine-5'-monophosphate, guanosine-5'-monophosphate, uridine 5'-monophosphate, cytidine-5'-monophosphate, inosine-5'-monophosphate, xanthosine-5'-monophosphate, 2'-deoxyadenosine 5'-monophosphate, 2'-deoxyguanosine 5'-monophosphate, thymidine 5'-monophosphate, 2'-deoxyuridine 5'-monophosphate, 2'-deoxycytidine-5'-monophosphate, 2'-deoxyinosine-5'-monophosphate, adenosine 3',5'-cyclic monophosphate, guanosine 3',5'-cyclic monophosphate, adenosine 5'-diphosphate, guanosine 5'-diphosphate, uridine-5'-diphosphate, cytidine-5'-diphosphate, 2'-deoxyadenosine-5'-diphosphate, 2'-deoxyguanosine 5'-diphosphate, 2'-deoxythymidine-5'-diphosphate, 2'-deoxycytidine 5'-diphosphate, adenosine 5'-triphosphate, guanosine-5'-triphosphate, uridine-5'-triphosphate, cytidine-5'-triphosphate, inosine-5'-triphosphate, 2'-deoxyadenosine-5'-triphosphate, 2'-deoxyguanosine-5'-triphosphate, thymidine-5'-triphosphate, 2'-deoxyuridine-5'-triphosphate, 2'-deoxycytidine-5'-triphosphate), organic acids (quinic acid, shikimic acid, ascorbic acid, pyruvic acid, malonic acid, succinic acid,  $\alpha$ -ketoglutaric acid,

fumaric acid, glutaric acid, ferulic acid, vanillic acid, coumaric acid, cinnamic acid, maleic acid), sugars and sugar alcohols (rhamnose, sucrose, maltose, melibiose, raffinose, sorbitol, mannitol, xylose, arabinose, glucose, fructose, myo-inositol, erythritol, arabitol, xylitol, trehalose, trehalose-6-phosphate, glucose-6-phosphate, and fructose-6-phosphate).

The external standards used for quantitation on Acclaim™ C30 column are amino acids (histidine, lysine, and cysteine), flavonoids, limonoids (taxifolin, rutin, neohesperidin, hesperidin, didymin, naringin, narirutin, diosmetin, neodiosmin, diosmin, eriodictyol, eriocitrin, neoeriocitrin, apigenin, rhoifolin, scutellarein, nobiletin, 5,6,7,3',4',5'-hexamethoxyflavone, sinensetin, tangeretin, luteolin, limonin, and nomilin), and organic acids (cinnamic acid, salicylic acid, benzoic acid, abscisic acid, methyl salicylate, 2,3-dihydroxybenzoic acid, salicylic acid 2-O- $\beta$ -D-glucoside, gentisic acid, tartaric acid, malic acid, isocitric acid, citric acid, oxaloacetic acid, gallic acid, and uric acid).

Table S1. Relative concentration of nonvolatile compounds in six different rootstocks groups (mg/L)

Compound	1804	Blue	CH	FG	SW	Volk
phenylalanine	977.18 ± 37.95 <sup>abc</sup>	935.75 ± 55.54 <sup>abd</sup>	1024.55 ± 38.91 <sup>ac</sup>	889.75 ± 18.51 <sup>d</sup>	920.35 ± 36.58 <sup>d</sup>	999.77 ± 46.76 <sup>abc</sup>
tryptophan	75.33 ± 1.2 <sup>a</sup>	66.62 ± 1.47 <sup>b</sup>	90.23 ± 1.97 <sup>c</sup>	64.98 ± 2.24 <sup>b</sup>	77.27 ± 2.65 <sup>a</sup>	83.4 ± 4.06 <sup>d</sup>
leucine	70.37 ± 1.84 <sup>a</sup>	66.7 ± 2.41 <sup>b</sup>	82.05 ± 1.75 <sup>c</sup>	63.9 ± 2.18 <sup>b</sup>	82.13 ± 2.62 <sup>c</sup>	73.78 ± 2.49 <sup>d</sup>
methionine	30.28 ± 1.06 <sup>a</sup>	25.92 ± 1.06 <sup>b</sup>	33.32 ± 0.48 <sup>c</sup>	28.92 ± 1.04 <sup>d</sup>	31.93 ± 1.24 <sup>e</sup>	34.4 ± 1.18 <sup>c</sup>
valine	5.95 ± 0.19 <sup>a</sup>	6.33 ± 0.21 <sup>b</sup>	10.33 ± 0.23 <sup>c</sup>	5.42 ± 0.19 <sup>d</sup>	7.65 ± 0.19 <sup>e</sup>	6.45 ± 0.19 <sup>b</sup>
tyrosine	25.08 ± 0.96 <sup>a</sup>	19.52 ± 1.13 <sup>b</sup>	27.25 ± 1.16 <sup>c</sup>	18.5 ± 0.98 <sup>b</sup>	23.47 ± 1.1 <sup>d</sup>	25.42 ± 1.01 <sup>a</sup>
proline	421.88 ± 65.24 <sup>a</sup>	400.68 ± 49.13 <sup>a</sup>	682.68 ± 34.94 <sup>c</sup>	368.44 ± 50.76 <sup>ad</sup>	505.92 ± 73.61 <sup>ae</sup>	383.48 ± 54.32 <sup>a</sup>
alanine	12.25 ± 0.45 <sup>a</sup>	10.7 ± 0.35 <sup>b</sup>	21.27 ± 0.72 <sup>c</sup>	12.97 ± 0.64 <sup>d</sup>	14.68 ± 0.44 <sup>e</sup>	14 ± 0.41 <sup>f</sup>
threonine	1.05 ± 0.54 <sup>a</sup>	1.42 ± 0.5 <sup>ab</sup>	3.1 ± 0.13 <sup>c</sup>	0.97 ± 0.05 <sup>bd</sup>	1.68 ± 0.08 <sup>b</sup>	1.57 ± 0.39 <sup>abd</sup>
glutamic acid	26.25 ± 0.69 <sup>a</sup>	23.08 ± 0.66 <sup>b</sup>	33.67 ± 1.28 <sup>c</sup>	24.72 ± 1.01 <sup>d</sup>	28.08 ± 1.34 <sup>e</sup>	27.07 ± 1.09 <sup>ae</sup>
serine	14.35 ± 0.31 <sup>a</sup>	14.28 ± 0.42 <sup>ab</sup>	21.5 ± 0.51 <sup>c</sup>	13.18 ± 0.5 <sup>d</sup>	16.07 ± 0.76 <sup>e</sup>	13.57 ± 0.48 <sup>d</sup>
glutamine	5.22 ± 0.17 <sup>a</sup>	5.4 ± 0.15 <sup>a</sup>	6.03 ± 0.18 <sup>b</sup>	4.6 ± 0.2 <sup>c</sup>	6.5 ± 0.21 <sup>d</sup>	5.75 ± 0.1 <sup>e</sup>
asparagine	46.12 ± 0.97 <sup>a</sup>	40.62 ± 1.02 <sup>b</sup>	81.75 ± 3.16 <sup>c</sup>	33.05 ± 1.44 <sup>d</sup>	53.58 ± 2.12 <sup>e</sup>	38.48 ± 0.92 <sup>f</sup>
aspartic acid	25.35 ± 0.9 <sup>a</sup>	25.67 ± 1.67 <sup>ab</sup>	41.58 ± 2.25 <sup>c</sup>	22.78 ± 1.28 <sup>d</sup>	28.07 ± 2.06 <sup>be</sup>	22.63 ± 0.85 <sup>d</sup>
arginine	459.22 ± 55.32 <sup>a</sup>	517.94 ± 49.15 <sup>ab</sup>	778.08 ± 97.9 <sup>c</sup>	437.06 ± 18.71 <sup>a</sup>	591.23 ± 25.23 <sup>bc</sup>	463.96 ± 41.05 <sup>ab</sup>
lysine	3.13 ± 0.12 <sup>a</sup>	3.22 ± 0.12 <sup>a</sup>	5.9 ± 0.18 <sup>b</sup>	2.47 ± 0.1 <sup>c</sup>	4.13 ± 0.16 <sup>d</sup>	3.5 ± 0.13 <sup>e</sup>
histidine	0.58 ± 0.15	0.7 ± 0.17	0.78 ± 0.3	0.67 ± 0.23	0.73 ± 0.21	0.77 ± 0.2
adenine	2.8 ± 0.06 <sup>a</sup>	2.35 ± 0.1 <sup>b</sup>	3.42 ± 0.12 <sup>c</sup>	2.32 ± 0.1 <sup>b</sup>	3.08 ± 0.22 <sup>d</sup>	2.85 ± 0.16 <sup>ad</sup>
cytosine	17.97 ± 0.61 <sup>a</sup>	16.27 ± 0.61 <sup>b</sup>	9.9 ± 0.24 <sup>c</sup>	15.5 ± 0.67 <sup>bd</sup>	15.35 ± 4.7 <sup>abde</sup>	13.32 ± 2.29 <sup>e</sup>
adenosine	116.6 ± 9.55 <sup>a</sup>	91.42 ± 3.96	93.75 ± 7.6	93.13 ± 3.76	120.67 ± 14.47 <sup>a</sup>	94.1 ± 9.06
guanosine	5.72 ± 2.82 <sup>a</sup>	5.27 ± 0.15 <sup>b</sup>	7.15 ± 0.33 <sup>a</sup>	4.47 ± 0.21 <sup>c</sup>	8.85 ± 0.46 <sup>d</sup>	5.38 ± 0.95 <sup>b</sup>
uridine	12.55 ± 0.37 <sup>a</sup>	9.65 ± 0.36 <sup>b</sup>	9.42 ± 4.62 <sup>c</sup>	9.22 ± 0.46 <sup>b</sup>	14.52 ± 1.52 <sup>d</sup>	9.92 ± 0.67 <sup>b</sup>
cytidine	21.7 ± 0.64 <sup>a</sup>	18.3 ± 0.51 <sup>b</sup>	20.62 ± 0.27 <sup>c</sup>	17.05 ± 0.73 <sup>d</sup>	23.68 ± 0.67 <sup>e</sup>	16.92 ± 0.62 <sup>d</sup>
quinic acid	519.1 ± 27.97 <sup>a</sup>	279.06 ± 21.32 <sup>b</sup>	342.6 ± 25.68 <sup>b</sup>	465.57 ± 33.7 <sup>a</sup>	281.12 ± 24.96 <sup>b</sup>	342.97 ± 35.48 <sup>b</sup>

shikimic acid	16.8 ± 0.74 <sup>a</sup>	16.63 ± 0.33 <sup>ab</sup>	17.4 ± 0.7 <sup>ac</sup>	14.67 ± 1.24 <sup>d</sup>	13.12 ± 0.38 <sup>e</sup>	17.2 ± 0.76 <sup>abc</sup>
ferulic acid	4.67 ± 0.85 <sup>a</sup>	2.6 ± 0.59 <sup>b</sup>	3.27 ± 0.37 <sup>c</sup>	4.27 ± 0.3 <sup>ad</sup>	5.12 ± 0.52 <sup>ae</sup>	5.37 ± 0.56 <sup>ade</sup>
maleic acid	2.77 ± 0.12 <sup>a</sup>	2.77 ± 0.27 <sup>ab</sup>	3.37 ± 0.18 <sup>c</sup>	2.48 ± 0.26 <sup>b</sup>	3.05 ± 0.33 <sup>abc</sup>	3.42 ± 0.39 <sup>abce</sup>
malonic acid	17.18 ± 0.67 <sup>a</sup>	20.47 ± 0.78 <sup>b</sup>	17.87 ± 0.54 <sup>ac</sup>	16.7 ± 0.62 <sup>ad</sup>	20.25 ± 3.35 <sup>abc</sup>	21.4 ± 0.81 <sup>b</sup>
benzoic acid	0.33 ± 0.15 <sup>ab</sup>	0.38 ± 0.1 <sup>a</sup>	0.4 ± 0.09 <sup>a</sup>	0.37 ± 0.05 <sup>a</sup>	0.5 ± 0.09 <sup>b</sup>	0.32 ± 0.04 <sup>c</sup>
pyruvic acid	84.58 ± 19.98 <sup>a</sup>	98.4 ± 28.19 <sup>b</sup>	106.48 ± 34.2 <sup>b</sup>	78.47 ± 21.23 <sup>b</sup>	89.55 ± 27.52 <sup>ac</sup>	85.28 ± 25.28 <sup>c</sup>
abscisic acid	10.15 ± 1.52 <sup>a</sup>	13.6 ± 3.51 <sup>ab</sup>	14.37 ± 2.63 <sup>b</sup>	14.42 ± 1.4 <sup>b</sup>	15.52 ± 0.83 <sup>b</sup>	15.67 ± 2.55 <sup>b</sup>
tartaric acid	2.2 ± 0.34	3.33 ± 1.07	4.47 ± 0.77 <sup>a</sup>	2.88 ± 0.84	2.12 ± 0.65	2.47 ± 0.77
ascorbic acid	2104.23 ± 115.04	2208.95 ± 185.37	2056.37 ± 153.58	1825.98 ± 177.99	1896.58 ± 163.68	1972.88 ± 150.81
malic acid	13508.42 ± 384.09	12381.83 ± 530.56	10137.62 ± 121.11	10731.07 ± 74.6	11472.12 ± 479.59	12908.87 ± 879.55
isocitric acid	23038.97 ± 563.52	22785.97 ± 738.85	31811.7 ± 1852.7	17598.88 ± 931.63 <sup>a</sup>	23811.7 ± 518.7	23392.73 ± 699.45
citric acid	60449.28 ± 1718.98	72651.43 ± 4010.59	67830.65 ± 5211.14	74543.42 ± 2338.04	72270.18 ± 2493.72	66771.77 ± 2020.95
oxaloacetic acid	1.90 ± 0.58 <sup>ab</sup>	1.80 ± 0.89 <sup>ab</sup>	3.4 ± 1.8 <sup>abc</sup>	1.42 ± 0.35 <sup>a</sup>	1.37 ± 0.49 <sup>a</sup>	1.52 ± 0.34 <sup>a</sup>
uric acid	28.00 ± 5.62 <sup>a</sup>	23.5 ± 7.31 <sup>ab</sup>	27.85 ± 7.02 <sup>a</sup>	19.65 ± 5.29 <sup>b</sup>	32.2 ± 7.87 <sup>a</sup>	33.3 ± 9.87 <sup>a</sup>
rhamnose	2.03 ± 0.36 <sup>ad</sup>	1.87 ± 0.27 <sup>abd</sup>	2.62 ± 0.54 <sup>ac</sup>	1.82 ± 0.23 <sup>a</sup>	2.27 ± 0.42 <sup>ad</sup>	1.77 ± 0.05 <sup>a</sup>
sucrose	13459.32 ± 439.66	12547.3 ± 502.51	14898.85 ± 863.42	15023.48 ± 654.61	13568.07 ± 678.69	15219.8 ± 631.44
raffinose	23.02 ± 4.08 <sup>a</sup>	28.65 ± 4.8 <sup>abc</sup>	32.93 ± 5.79 <sup>b</sup>	18.42 ± 3.06 <sup>ad</sup>	31.47 ± 6.02 <sup>bc</sup>	23.97 ± 3.12 <sup>ab</sup>
sorbitol	7.83 ± 0.51 <sup>a</sup>	9.18 ± 0.51 <sup>b</sup>	13.32 ± 0.55 <sup>c</sup>	7.33 ± 0.42 <sup>ad</sup>	9.4 ± 0.39 <sup>b</sup>	8.95 ± 0.38 <sup>b</sup>
xylose	8.02 ± 0.43 <sup>a</sup>	8.43 ± 0.41 <sup>a</sup>	10.22 ± 0.82 <sup>b</sup>	6.25 ± 0.3 <sup>c</sup>	9.43 ± 0.43 <sup>b</sup>	8.42 ± 0.69 <sup>a</sup>
glucose	1628.98 ± 92.89 <sup>a</sup>	1780.62 ± 130.31 <sup>b</sup>	2285.1 ± 121.02 <sup>c</sup>	1540.28 ± 101.98 <sup>a</sup>	1780.1 ± 83.52 <sup>b</sup>	1650.72 ± 175.08 <sup>ab</sup>
fructose	1309.3 ± 148.52 <sup>a</sup>	1697.58 ± 123.12 <sup>b</sup>	1282.93 ± 123.02 <sup>c</sup>	1480.77 ± 106.61 <sup>a</sup>	1034.25 ± 85.16 <sup>d</sup>	1043.25 ± 94.01 <sup>d</sup>
myo-inositol	539.63 ± 92.5 <sup>a</sup>	922.65 ± 31.95 <sup>b</sup>	1232.88 ± 29.99 <sup>c</sup>	616.43 ± 57.82 <sup>a</sup>	869.83 ± 48.7 <sup>d</sup>	837.55 ± 59.27 <sup>d</sup>
arabitol	2.4 ± 0.71 <sup>a</sup>	3.2 ± 0.09 <sup>b</sup>	3.68 ± 0.1 <sup>c</sup>	2.1 ± 1.06 <sup>a</sup>	3.8 ± 0.21 <sup>c</sup>	3.17 ± 0.41 <sup>d</sup>
glucose-6-phosphate	44.7 ± 3.49 <sup>a</sup>	42.62 ± 2.04 <sup>a</sup>	41.85 ± 2.6 <sup>a</sup>	35.08 ± 4.18 <sup>b</sup>	46.38 ± 7.3 <sup>ac</sup>	51.37 ± 3.15 <sup>cd</sup>
rutin	4.5 ± 0.24	4.37 ± 0.84	4.83 ± 0.48	4.88 ± 0.29	4.67 ± 0.23	4.7 ± 0.27
hesperidin	355.78 ± 24.68 <sup>a</sup>	408.52 ± 40.37 <sup>a</sup>	553.78 ± 21.2 <sup>b</sup>	455.78 ± 37.31 <sup>ab</sup>	440.52 ± 35.17 <sup>ab</sup>	461.63 ± 43.97 <sup>ab</sup>

didymin	36.08 ± 1.95 <sup>a</sup>	51.3 ± 9.82 <sup>b</sup>	74.55 ± 4.7 <sup>c</sup>	46.75 ± 2.03 <sup>b</sup>	44.43 ± 2.49 <sup>b</sup>	47.28 ± 1.39 <sup>b</sup>
narirutin	68.52 ± 5.21 <sup>a</sup>	114.13 ± 16.63 <sup>b</sup>	137.9 ± 10.21 <sup>c</sup>	83.93 ± 8.46 <sup>d</sup>	86.32 ± 7.37 <sup>d</sup>	60.92 ± 6.53 <sup>a</sup>
eriocitrin	12.02 ± 1.82	9.82 ± 2.24	10.78 ± 1.41	11.28 ± 2.4	10.92 ± 0.96	11.02 ± 2.66
nobiletin	26.33 ± 8.37	30.82 ± 7.49	26.45 ± 8.92	31.6 ± 11.2	29.72 ± 8.08	32.18 ± 6.96
sinensetin	17.85 ± 5.53	22.1 ± 4.29	17.22 ± 6.37	18.12 ± 9.46	18.18 ± 5.32	24.08 ± 6.52
tangeretin	9.42 ± 3.23	8.82 ± 2.13	7.8 ± 2.98	11.08 ± 4.16	10.03 ± 3.52	11.8 ± 3.67
limonin	33.23 ± 2.15 <sup>a</sup>	38.24 ± 1.89 <sup>a</sup>	40.23 ± 3.74 <sup>a</sup>	37.26 ± 2.25 <sup>ab</sup>	49.87 ± 3.75 <sup>c</sup>	32.67 ± 4.02 <sup>a</sup>

Data are expressed as means ± the standard error (n = 6); values with each sample marked by different letters within the same row are significant different ( $P < 0.05$ ).

Table S2. Relative concentrations of volatile compounds in six different orange juices (mg/L)

Compound	RI (FFAP)	1804	Blue	CH	FG	SW	Volk
Alcohol							
2-octenol	1155	0.6739 ± 0.084 <sup>a</sup>	0.4153 ± 0.1115 <sup>b</sup>	0.3723 ± 0.0495 <sup>c</sup>	0.5665 ± 0.0878 <sup>a</sup>	0.7627 ± 0.109 <sup>a</sup>	0.8217 ± 0.0271 <sup>d</sup>
1-hexanol	868	0.0219 ± 0.0042 <sup>a</sup>	0.0312 ± 0.0066 <sup>b</sup>	0.0512 ± 0.0081 <sup>c</sup>	0.0148 ± 0.0015 <sup>d</sup>	0.0185 ± 0.0074 <sup>d</sup>	0.0169 ± 0.0053 <sup>ad</sup>
linalool	1099	12.8762 ± 0.3339 <sup>a</sup>	9.5226 ± 0.7756 <sup>c</sup>	7.9941 ± 0.6572 <sup>c</sup>	12.0111 ± 1.3631 <sup>a</sup>	11.9784 ± 1.0647 <sup>a</sup>	13.4538 ± 0.6397 <sup>a</sup>
1-octanol	1071	1.0392 ± 0.1844 <sup>a</sup>	1.0878 ± 0.1759 <sup>a</sup>	0.8887 ± 0.0857 <sup>a</sup>	0.5769 ± 0.1676 <sup>b</sup>	0.9952 ± 0.3096 <sup>a</sup>	0.5686 ± 0.0987 <sup>b</sup>
terpinen-4-ol	922	3.0136 ± 1.4673 <sup>a</sup>	1.9255 ± 0.1341 <sup>b</sup>	1.2227 ± 0.1415 <sup>c</sup>	3.2534 ± 0.4068 <sup>a</sup>	2.9355 ± 0.1635 <sup>a</sup>	3.0788 ± 0.1827 <sup>a</sup>
dihydrocarveol	1192	0.1089 ± 0.0261 <sup>a</sup>	0.1395 ± 0.0512 <sup>ab</sup>	0.1063 ± 0.0176 <sup>a</sup>	0.0857 ± 0.0648 <sup>a</sup>	0.1165 ± 0.0372 <sup>a</sup>	0.1566 ± 0.0301 <sup>b</sup>
carveol	1219	0.0964 ± 0.0173 <sup>a</sup>	0.0902 ± 0.018 <sup>a</sup>	0.0891 ± 0.0226 <sup>a</sup>	0.0459 ± 0.0232 <sup>b</sup>	0.0883 ± 0.0242 <sup>a</sup>	0.088 ± 0.0124 <sup>a</sup>
carotol	1594	0.2945 ± 0.0626 <sup>a</sup>	0.3912 ± 0.0726 <sup>b</sup>	0.3932 ± 0.0759 <sup>b</sup>	0.1928 ± 0.0992 <sup>a</sup>	0.4 ± 0.0853 <sup>b</sup>	0.3657 ± 0.0428 <sup>b</sup>
terpineol	1189	1.4207 ± 0.0809 <sup>a</sup>	1.2357 ± 0.0721 <sup>b</sup>	0.8933 ± 0.1127 <sup>b</sup>	1.3799 ± 0.2096 <sup>b</sup>	1.2308 ± 0.1038 <sup>b</sup>	1.5525 ± 0.1381 <sup>b</sup>
<i>trans</i> -isopiperitenol	1210	0.1286 ± 0.0752	0.1371 ± 0.0488	0.1195 ± 0.0222	0.0835 ± 0.0938	0.0899 ± 0.0628	0.1528 ± 0.0364
citronellol	1228	0.0798 ± 0.0071 <sup>a</sup>	0.0904 ± 0.0215 <sup>a</sup>	0.0561 ± 0.0222 <sup>b</sup>	0.0402 ± 0.0169 <sup>b</sup>	0.0724 ± 0.0162 <sup>a</sup>	0.0878 ± 0.0109 <sup>a</sup>
nerol	1235	0.1256 ± 0.0227 <sup>a</sup>	0.0778 ± 0.0222 <sup>b</sup>	0.0441 ± 0.0199 <sup>c</sup>	0.0573 ± 0.0383 <sup>bc</sup>	0.1144 ± 0.0215 <sup>a</sup>	0.1014 ± 0.0229 <sup>ab</sup>
<i>cis</i> -carveol	1230	0.1197 ± 0.0381 <sup>a</sup>	0.1284 ± 0.0504 <sup>a</sup>	0.1152 ± 0.0338 <sup>ab</sup>	0.0718 ± 0.0344 <sup>b</sup>	0.1217 ± 0.0389 <sup>a</sup>	0.158 ± 0.0369 <sup>a</sup>
Aldehyde							
hexanal	800	0.2437 ± 0.0126 <sup>a</sup>	0.2892 ± 0.0246 <sup>b</sup>	0.3205 ± 0.0747 <sup>b</sup>	0.1857 ± 0.0268 <sup>c</sup>	0.2414 ± 0.0196 <sup>a</sup>	0.3333 ± 0.0122 <sup>b</sup>
octanal	1071	1.5269 ± 0.2469 <sup>a</sup>	0.9043 ± 0.1101 <sup>b</sup>	0.4336 ± 0.0646 <sup>c</sup>	1.4903 ± 0.1798 <sup>a</sup>	1.3019 ± 0.1024 <sup>a</sup>	1.353 ± 0.104 <sup>a</sup>
nonanal	1104	0.2682 ± 0.0523 <sup>a</sup>	0.1941 ± 0.0566 <sup>b</sup>	0.1129 ± 0.0466 <sup>c</sup>	0.1933 ± 0.0763 <sup>a</sup>	0.3043 ± 0.0404 <sup>a</sup>	0.2989 ± 0.0575 <sup>a</sup>
decanal	1206	0.8756 ± 0.1696 <sup>a</sup>	0.4872 ± 0.1236 <sup>b</sup>	0.2943 ± 0.0721 <sup>c</sup>	0.545 ± 0.2171 <sup>b</sup>	0.674 ± 0.1491 <sup>a</sup>	0.6953 ± 0.0902 <sup>a</sup>
perilla aldehyde	1272	0.8943 ± 0.1199 <sup>a</sup>	0.331 ± 0.0682 <sup>b</sup>	0.2237 ± 0.0858 <sup>c</sup>	0.6932 ± 0.1912 <sup>a</sup>	0.6515 ± 0.112 <sup>a</sup>	0.766 ± 0.0918 <sup>a</sup>
citral	1276	0.0826 ± 0.0235 <sup>a</sup>	0.0705 ± 0.0298 <sup>ab</sup>	0.0638 ± 0.0187 <sup>ac</sup>	0.0458 ± 0.0217 <sup>c</sup>	0.0767 ± 0.0447 <sup>a</sup>	0.1078 ± 0.0315 <sup>a</sup>
Ester							
methyl butyrate	772	0.0204 ± 0.0021 <sup>a</sup>	0.0326 ± 0.0036 <sup>b</sup>	0.0383 ± 0.011 <sup>c</sup>	0.0094 ± 0.0015 <sup>a</sup>	0.0411 ± 0.0091 <sup>d</sup>	0.0279 ± 0.0039 <sup>d</sup>
ethyl butyrate	802	0.1363 ± 0.011 <sup>a</sup>	0.1884 ± 0.0241 <sup>b</sup>	0.176 ± 0.0411 <sup>ac</sup>	0.1216 ± 0.0289 <sup>ac</sup>	0.1234 ± 0.0208 <sup>d</sup>	0.1937 ± 0.0168 <sup>abc</sup>

octyl acetate	1210	0.0168 ± 0.0054 <sup>a</sup>	0.0421 ± 0.01 <sup>b</sup>	0.0223 ± 0.0066 <sup>ab</sup>	0.0266 ± 0.0109 <sup>a</sup>	0.0219 ± 0.012 <sup>a</sup>	0.0278 ± 0.0094 <sup>ab</sup>
perilla acetate	1436	0.0579 ± 0.018 <sup>a</sup>	0.0256 ± 0.0058 <sup>b</sup>	0.0147 ± 0.0049 <sup>c</sup>	0.0296 ± 0.0196 <sup>b</sup>	0.0427 ± 0.0239 <sup>a</sup>	0.0531 ± 0.0173 <sup>a</sup>
Ketone							
carvone	1204	0.445 ± 0.0657 <sup>a</sup>	0.5955 ± 0.0555 <sup>b</sup>	0.5988 ± 0.0742 <sup>c</sup>	0.4325 ± 0.1476 <sup>a</sup>	0.4041 ± 0.0362 <sup>a</sup>	0.7778 ± 0.0549 <sup>d</sup>
Terpene							
$\alpha$ -pinene	937	0.164 ± 0.0159 <sup>a</sup>	0.1463 ± 0.0183 <sup>a</sup>	0.0801 ± 0.0157 <sup>b</sup>	0.1388 ± 0.0329 <sup>a</sup>	0.1538 ± 0.0111 <sup>a</sup>	0.1508 ± 0.0124 <sup>a</sup>
$\beta$ -pinene	979	0.2482 ± 0.132 <sup>a</sup>	0.4069 ± 0.0647 <sup>b</sup>	0.0716 ± 0.0371 <sup>c</sup>	0.3419 ± 0.0494 <sup>ab</sup>	0.0513 ± 0.022 <sup>c</sup>	0.0264 ± 0.0075 <sup>d</sup>
$\beta$ -myrcene	991	1.5293 ± 0.3877 <sup>a</sup>	0.8814 ± 0.0986 <sup>b</sup>	0.9481 ± 0.1882 <sup>c</sup>	1.0143 ± 0.4163 <sup>abc</sup>	1.8391 ± 0.1094 <sup>a</sup>	1.7749 ± 0.1216 <sup>a</sup>
limonene	1030	133.0555 ± 27.0634 <sup>a</sup>	115.1254 ± 5.4412 <sup>a</sup>	64.4849 ± 4.6203 <sup>b</sup>	113.3053 ± 22.7497 <sup>a</sup>	111.5866 ± 8.8735 <sup>a</sup>	108.4767 ± 11.2714 <sup>a</sup>
cosmene	1131	0.1124 ± 0.0136 <sup>a</sup>	0.081 ± 0.0152 <sup>b</sup>	0.0538 ± 0.009 <sup>c</sup>	0.0874 ± 0.0261 <sup>ab</sup>	0.0974 ± 0.0126 <sup>ab</sup>	0.1004 ± 0.0114 <sup>a</sup>
terpinolene	1088	0.0896 ± 0.0227 <sup>a</sup>	0.0598 ± 0.0082 <sup>b</sup>	0.0358 ± 0.0071 <sup>c</sup>	0.0607 ± 0.0196 <sup>b</sup>	0.0663 ± 0.0112 <sup>a</sup>	0.0713 ± 0.017 <sup>a</sup>
<i>p</i> -cymenene	1090	0.0392 ± 0.0113 <sup>a</sup>	0.0419 ± 0.0116 <sup>a</sup>	0.0395 ± 0.0084 <sup>a</sup>	0.0264 ± 0.0145 <sup>ab</sup>	0.0557 ± 0.0288 <sup>a</sup>	0.0452 ± 0.0091 <sup>ac</sup>
valencene	1698	1.2423 ± 0.4116 <sup>a</sup>	1.2121 ± 0.2048 <sup>a</sup>	1.6646 ± 0.3225 <sup>b</sup>	0.6433 ± 0.4077 <sup>c</sup>	1.2203 ± 0.4175 <sup>a</sup>	0.7317 ± 0.2564 <sup>c</sup>
Data are expressed as means ± the standard error (n = 6); values with each sample marked by different letters within the same row are significant different ( $P < 0.05$ ).							



Table S3. VIP scores of metabolites in OPLS-DA model for discrimination

Nonvolatile compounds			
Compound	VIP Score	Compound	VIP Score
tyrosine	1.37	ferulic acid	1.12
abscisic acid	1.36	lysine	1.11
shikimic acid	1.33	maleic acid	1.11
alanine	1.27	sorbitol	1.10
tryptophan	1.27	guanosine	1.09
xylose	1.22	glucose 6-phosphate	1.08
cytidine	1.22	valine	1.08
arabitol	1.22	cytosine	1.08
methionine	1.22	phenylalanine	1.06
malonic acid	1.20	aspartic acid	1.05
didymine	1.20	uridine	1.05
glutamine	1.18	threonine	1.05
glutamic acid	1.17	adenosine	1.05
rutin	1.15	benzoic acid	1.04
hesperidin	1.14	glucose	1.03
asparagine	1.13	serine	1.02
Volatile compounds			
Compound	VIP Score	Compound	VIP Score
1-octanol	1.32	citronellol	1.12
$\beta$ -pinene	1.22	octyl acetate	1.09
carvone	1.21	decanal	1.06
$\beta$ -myrcene	1.16	methyl butyrate	1.03
valencene	1.15	carveol	1.01
1-hexanol	1.13	butanoic acid, ethyl ester	1.01
nerol	1.13	<i>p</i> -cymenene	1.00