

## Supplemental Materials

**Table S1.** Profiles of volatiles in cherry tomatoes (2021). Values are mean  $\pm$  SD of three independent experiments. ND: not detected; SW: surface water; HNW: hydrogen nanobubble water; SW + F: surface water plus fertilizers; HNW+F: hydrogen nanobubble water plus fertilizers.

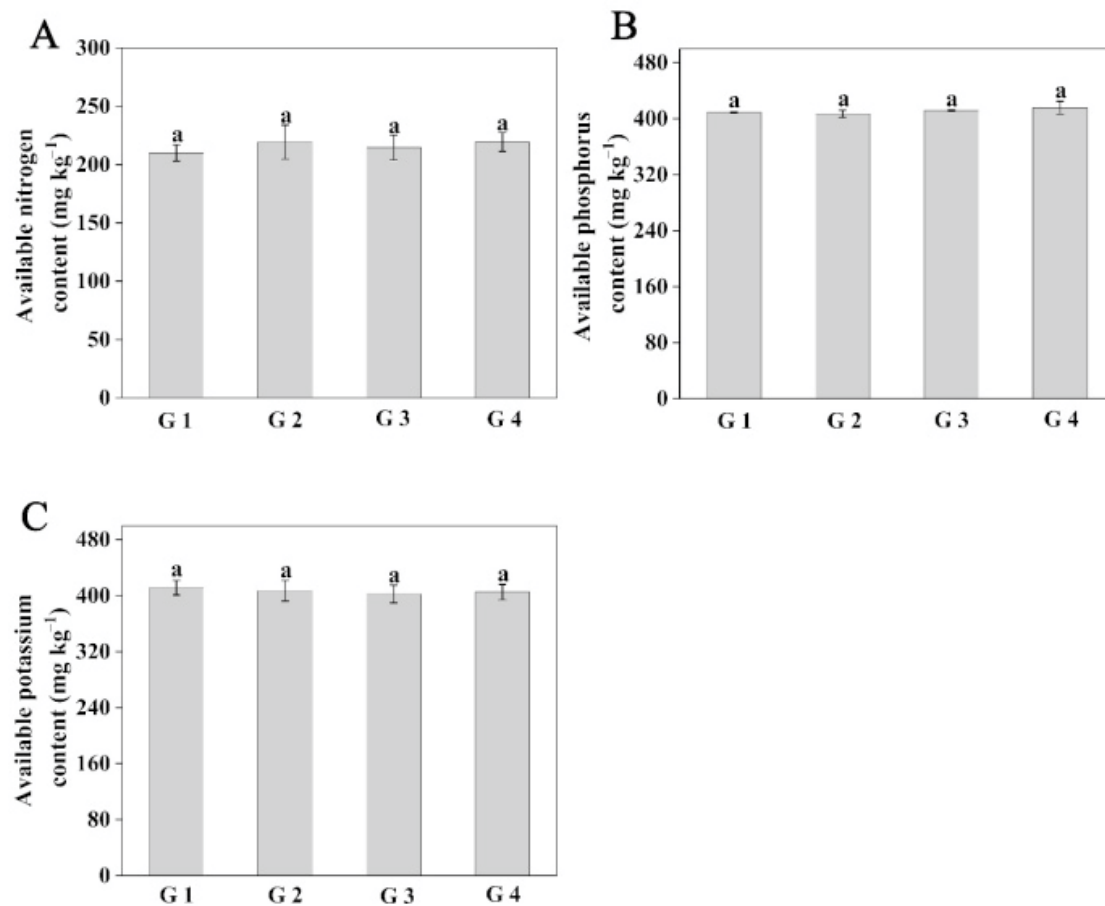
Code	Family	Compound	Concentration (mg kg <sup>-1</sup> )			
			SW	HNW	SW+F	HNW+F
1	Aldehydes (average proportion: 77.1% $\pm$ 1.6%)	Hexanal	0.278 $\pm$ 0.052	0.463 $\pm$ 0.050	0.179 $\pm$ 0.031	0.447 $\pm$ 0.036
2		(E)-2-Hexenal	0.431 $\pm$ 0.049	0.444 $\pm$ 0.000	0.362 $\pm$ 0.014	0.294 $\pm$ 0.094
3		2-Methyl-4-pentenal	0.122 $\pm$ 0.009	0.031 $\pm$ 0.044	0.121 $\pm$ 0.007	0.017 $\pm$ 0.024
4		Methional	0.002 $\pm$ 0.003	0.004 $\pm$ 0.006	0.007 $\pm$ 0.001	0.003 $\pm$ 0.005
5		Benzeneacetaldehyde	0.035 $\pm$ 0.001	0.008 $\pm$ 0.011	0.043 $\pm$ 0.001	0.034 $\pm$ 0.008
6		Decanal	0.004 $\pm$ 0.001	0.002 $\pm$ 0.003	0.005 $\pm$ 0.001	0.006 $\pm$ 0.000
7		(E,E)-2,4-Hexadienal	0.012 $\pm$ 0.001	0.022 $\pm$ 0.019	0.015 $\pm$ 0.002	0.006 $\pm$ 0.001
8		(Z)-2-Heptenal	0.007 $\pm$ 0.001	0.002 $\pm$ 0.003	0.003 $\pm$ 0.004	0.016 $\pm$ 0.007
9		(E)-4-Oxohex-2-enal	0.022 $\pm$ 0.007	0.024 $\pm$ 0.012	0.034 $\pm$ 0.001	0.012 $\pm$ 0.016
10		Nonanal, 3-(methylthio)-	0.002 $\pm$ 0.003	ND	ND	0.002 $\pm$ 0.003
11		Nonanal	ND	0.014 $\pm$ 0.019	ND	0.047 $\pm$ 0.029
12		5-Methyl-hexanal	ND	ND	0.002 $\pm$ 0.003	ND
13		(E)-2-Octenal	ND	ND	ND	0.008 $\pm$ 0.011
14		(E)-2-Nonenal	0.002 $\pm$ 0.003	ND	ND	ND
15	Alcohols (average proportion: 12.3% $\pm$ 4.8%)	trans-1,2-Cyclopentanediol	0.048 $\pm$ 0.004	0.060 $\pm$ 0.006	0.034 $\pm$ 0.013	0.020 $\pm$ 0.002
16		2-Ethyl-1-hexanol	0.010 $\pm$ 0.000	0.004 $\pm$ 0.006	0.007 $\pm$ 0.001	0.004 $\pm$ 0.006
17		Phenylethyl alcohol	0.075 $\pm$ 0.002	0.075 $\pm$ 0.001	0.089 $\pm$ 0.005	0.069 $\pm$ 0.011

18		2,4,6-Trimethyl-1,6-heptadien-4-ol	0.023±0.000	0.009±0.012	0.006±0.009	0.007±0.010
19		Benzene-1,2-diol, 4-(2-guanidinothiazol-4-yl)-	0.005±0.000	0.003±0.004	0.004±0.000	ND
20		3-Hepten-1-ol	0.001±0.002	0.008±0.004	ND	ND
21		cis-1,3-Cyclopentanediol	0.004±0.006	ND	ND	ND
22		cis-2-Methylcyclohexanol	0.004±0.001	ND	ND	ND
23		5-Methyl-5-hexen-2-ol	0.002±0.003	ND	ND	ND
24		E,E-2,6-Dimethyl-3,5,7-octatriene-2-ol	0.001±0.002	ND	ND	0.003±0.001
25	Esters	Carbamic acid, (2-methylphenyl)methyl ester	0.019±0.003	0.009±0.002	0.020±0.002	0.026±0.005
26	(average proportion: 1.9% ± 1.5%)	Decanoic acid, ethyl ester	0.004±0.000	ND	0.002±0.004	0.005±0.000
27		Isobutyl acrylate	ND	0.002±0.003	ND	0.001±0.002
28		Oxalic acid, isohexyl neopentyl ester	ND	ND	ND	0.001±0.001
29	Phenols (average proportion: 2.1% ± 1.2%)	2,4-Bis(1,1-dimethylethyl)-phenol	0.020±0.002	0.022±0.006	0.030±0.011	0.022±0.001
30	Others (average proportion: 6.6% ± 2.9%)	L-Isoleucine	0.012±0.016	0.042±0.031	ND	ND
31		1,6-Anhydro-3,4-dideoxy-.beta.-D-manno-hexapyranose	0.013±0.018	ND	ND	0.012±0.006
32		Benzene, 1-(1-hydroxyheptyl)-3-[1-(tetrahydropyran-2-yloxy)heptyl]-	ND	0.006±0.008	0.005±0.007	ND
33		Oxetane, 2-methyl-4-propyl-	0.006±0.000	0.003±0.004	0.002±0.003	0.002±0.003
34		Benzyl nitrile	0.014±0.000	0.004±0.005	0.011±0.000	0.022±0.011
35		Octyl-oxirane	0.005±0.000	ND	ND	0.004±0.005
36		Propanoic acid, 3-hydroxy-, hydrazide	ND	ND	0.009±0.012	0.002±0.003
37		4-(2,2,6-Trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-3-buten-2-one	0.003±0.004	ND	ND	0.003±0.001
38		Bis(3-methylbutyl) fluorene-2,7-disulfonate	0.004±0.000	ND	0.004±0.000	0.004±0.005

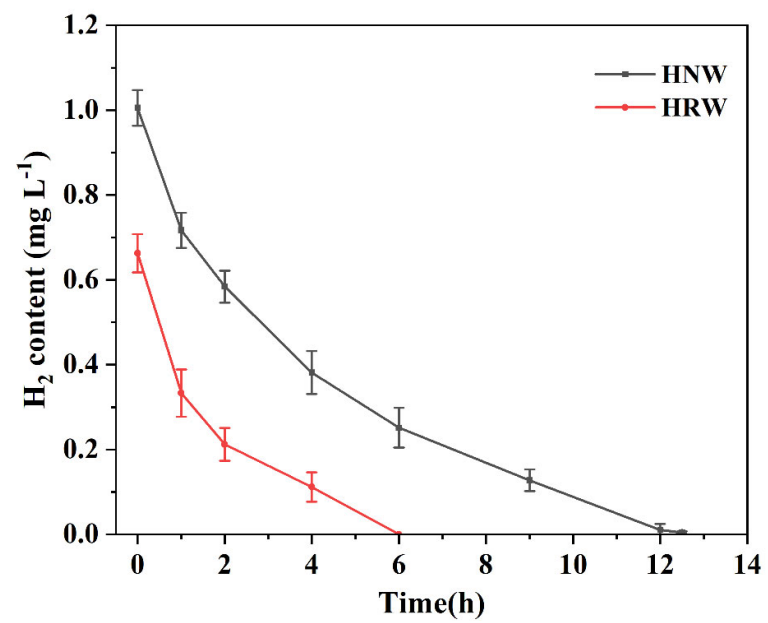
39	Hydroxylamine, O-decyl-	0.006±0.001	ND	0.005±0.001	0.003±0.004
40	Decane, 6-ethyl-2-methyl-	ND	ND	ND	0.001±0.001
41	trans- $\beta$ -Ionone	ND	ND	ND	0.003±0.000
42	1H-Pyrrole, 2,5-dihydro-1-nitroso-	0.007±0.010	ND	0.036±0.011	ND
43	2-Isobutylthiazole	ND	ND	ND	0.022±0.022
44	Thieno[2,3-c]furan-3-carbonitrile, 2-amino-4,6-dihydro-4,4,6,6-tetramethyl-	ND	ND	0.003±0.005	ND
45	1,2-Epoxyundecane	ND	ND	0.008±0.000	ND
46	Valeric acid hydrazide	ND	ND	0.004±0.000	ND
47	Methyl 2-methoxypropenoate	0.005±0.007	ND	ND	ND
48	4-Hydroxybutyric acid hydrazide	ND	ND	0.001±0.002	ND
49	Hydrazinecarboxamide	ND	ND	ND	0.007±0.010

**Table S2.** Primers of qPCR used in this study.

Gene	Forward primer (5'–3')	Reverse primer (5'–3')
<i>SLACT</i> (NM_001330119.1)	CGGTGACCACTTTCCGATCT	TCCTCACCGTCAGCCATTTT
<i>18S rRNA</i> (XM_004241429.4)	GGGCATTCGTATTTTCATAGTCAGA	GTTCTTGATTAATGAAAACATCCT
<i>SIPSY1</i> (NM_001347838.1)	TGGCCCAAACGCATCATATA	CACCATCGAGCATGTCAAATG
<i>SIPDS</i> (NM_001247166.2)	TGCCAAACCACCACAAATTTCA	CCAATTTGAGGCATTTTACTCGGA
<i>LeAMT2</i> (NM_001247324.2)	TTGTACCGCCGCTCTGACAACTTT	CATGGCTCAACAACCTGCACAACCT
<i>LePT2</i> (NM_001247114.1)	CATTGGACACTGGAGGCTAACC	ATAAGAACCCATACGCTCCCA
<i>LePT5</i> (XM_004240903.4)	GGCGAATGAAGATGCCTGAAAC	TACCAATTAAGTGATGTCCGTG
<i>SIHKT1,1</i> (NM_001308344.1)	TGTTTTGTGCTTTGGAGTGGA	GGGGGTGAAAGAGTGGAGAT



**Figure S1.** The contents of available nitrogen (A), available phosphorus (B), and available potassium (C) in soil of four greenhouses before fertilizing (Shanghai, 2021). The different letters indicate significant differences at  $p < 0.05$  (one-way ANOVA; Duncan's multiple range tests). G 1: greenhouse 1; G 2: greenhouse 2; G 3: greenhouse 3; G 4: greenhouse 4.



**Figure S2.** Changes in H<sub>2</sub> content of fresh HRW and HNW. HRW: hydrogen-rich water; HNW: hydrogen nanobubble water.



**Figure S3.** The design and location information of the four greenhouses (Shanghai, 2021). 1#: Irrigation with surface water (SW) and normal fertilization; 2#: Irrigation with SW and free of fertilization; 3#: Irrigation with hydrogen nanobubble water (HNW) and normal fertilization; 4#: Irrigation with HNW and free of fertilization.