

# **Effects of Varieties, Cultivation Methods, and Origins of *Citrus sinensis* ‘hongjiang’ on Volatile Organic Compounds: HS-SPME-GC/MS Analysis Coupled with OPLS-DA**

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**Table S1. The composition and relative contents of volatile organic compounds (VOCs) among *Citrus sinensis* “hongjiang”**

No	Retention time	Name	CAS#	Molecular formula	CAS #	Retention Index	
						Calculated RIs	Literature values <sup>a</sup>
1	5.684	Hexanal	66-25-1	C <sub>6</sub> H <sub>12</sub> O	100	803	801
2	5.79	ethyl butanoate	105-54-4	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116	784	785
3	7.593	Hex-2-enal	505-57-7	C <sub>6</sub> H <sub>10</sub> O	98	813	814
4	7.772	Hex-3-en-1-ol	928-96-1	C <sub>6</sub> H <sub>12</sub> O	100	866	868
5	8.316	Hexan-1-ol	111-27-3	C <sub>6</sub> H <sub>14</sub> O	102	859	860
6	9.684	Heptanal	111-71-7	C <sub>7</sub> H <sub>14</sub> O	114	906	905
7	10.79	$\alpha$ -Thujene	353-31-3	C <sub>10</sub> H <sub>16</sub>	136	924	927
8	11.053	$\alpha$ -Pinene	80-56-8	C <sub>10</sub> H <sub>16</sub>	136	945	948
9	13.038	Sabinene	3387-41-5	C <sub>10</sub> H <sub>16</sub>	136	896	897
10	14.037	$\beta$ -Myrcene	123-35-3	C <sub>10</sub> H <sub>16</sub>	136	963	958
11	14.627	Octanal	124-13-0	C <sub>8</sub> H <sub>16</sub> O	128	1002	1005
12	14.863	Car-3-ene	13466-78-9	C <sub>10</sub> H <sub>16</sub>	136	945	948
13	15.254	$\alpha$ -Terpinene	99-86-5	C <sub>10</sub> H <sub>16</sub>	136	1014	1018
14	16.582	Limonene	138-86-3	C <sub>10</sub> H <sub>16</sub>	136	1026	1030
15	17.061	$\beta$ -Ocimene	13877-91-3	C <sub>10</sub> H <sub>16</sub>	136	954	976
16	17.498	$\gamma$ -Terpinene	99-85-4	C <sub>10</sub> H <sub>16</sub>	136	967	998
17	18.02	2-Octen-1-ol	18409-17-1	C <sub>8</sub> H <sub>16</sub> O	128	1064	1067
18	18.176	1-Octanol	111-87-5	C <sub>8</sub> H <sub>18</sub> O	130	1058	1059
19	18.36	7-methyloct-3-yne	37050-06-9	C <sub>9</sub> H <sub>16</sub>	124	858	869
20	18.845	$\alpha$ -Terpinolene	586-62-9	C <sub>10</sub> H <sub>16</sub>	136	1043	1052
21	19.657	Linalool	78-70-6	C <sub>10</sub> H <sub>18</sub> O	154	1085	1082
22	19.833	1-Nonanal	124-19-6	C <sub>9</sub> H <sub>18</sub> O	142	1107	1104
23	20.123	<i>p</i> -Mentha-1,5,8-triene	21195-59-5	C <sub>10</sub> H <sub>14</sub>	134	1032	1029
24	20.454	4,8-Dimethylnona-1,3,7-triene	19945-61-0	C <sub>11</sub> H <sub>18</sub>	150	1115	1113
25	20.58	1-methyl-4-(1-methylethenyl)-2-Cyclohexene-1-ol	7212-40-0	C <sub>10</sub> H <sub>16</sub> O	152	1153	1140
26	21.044	Ethyl 3-hydroxyhexanoate	2305-25-1	C <sub>8</sub> H <sub>16</sub> O <sub>3</sub>	160	1126	1129
27	21.087	4-Acetyl-1-methylcyclohexene	1530-61-2	C <sub>9</sub> H <sub>14</sub> O	138	1092	1088
28	21.301	<i>cis-p</i> -Mentha-2,8-dien-1-ol	3886-78-0	C <sub>10</sub> H <sub>16</sub> O	152	1142	1140
29	22.281	Citronellal	106-23-0	C <sub>10</sub> H <sub>18</sub> O	154	1130	1125
30	22.579	6-Nonenal	2277-19-2	C <sub>9</sub> H <sub>16</sub> O	140	1116	1112
31	22.59	2-Nonenal	18829-56-6	C <sub>9</sub> H <sub>16</sub> O	140	1175	1163
32	23.096	2-None-1-ol	31502-14-4	C <sub>9</sub> H <sub>18</sub> O	142	1164	1167
33	23.233	nonan-1-ol	143-08-8	C <sub>9</sub> H <sub>20</sub> O	144	1160	1159
34	23.402	4-methyl-1-(1-methylethyl)-3-Cyclohexen-1-ol	562-74-3	C <sub>10</sub> H <sub>18</sub> O	154	1193	1195
35	23.59	Octanoic acid	124-07-2	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	144	1185	1183
36	23.78	Isogeranial	55722-59-3	C <sub>10</sub> H <sub>16</sub> O	152	1173	1179
37	23.852	Cryptone	500-02-7	C <sub>9</sub> H <sub>14</sub> O	138	1194	1187
38	24.092	$\alpha$ -Terpineol	98-55-5	C <sub>10</sub> H <sub>18</sub> O	154	1198	1195
39	24.573	Ethyl octanoate	106-32-1	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	172	1184	1183
40	24.779	2-methyl-5-(1-methylethenyl)-Cyclohexanone	1478-60-2	C <sub>10</sub> H <sub>16</sub> O	152	1192	1179
41	24.909	Decanal	112-31-2	C <sub>10</sub> H <sub>20</sub> O	156	1206	1204
42	25.276	2,4-Dodecadienal	21662-16-8	C <sub>12</sub> H <sub>20</sub> O	180	1423	1418

43	25.283	2,4-Nonadienal	1771-49-0	C9H14O	138	1125	1120
44	25.533	Carveol	1197-07-5	C10H16O	152	1222	1206
45	26.056	$\beta$ -Citronellol	106-22-9	C10H20O	156	1224	1179
46	26.626	Z-Citral	106-26-3	C10H16O	152	1176	1174
47	26.707	Carvone	6485-40-1	C10H14O	150	1121	1190
48	27.299	Geraniol	106-24-1	C10H18O	154	1236	1228
49	27.611	7-methoxy-3,7-dimethyl-Octanal	3613-30-7	C11H22O2	186	1233	1230
50	28.078	3,7-dimethyl-2,6-Octadienal	141-27-5	C10H16O	152	1175	1174
51	28.961	<i>p</i> -Mentha-1(7),8(10)-dien-9-ol	29548-13-8	C10H16O	152	1260	1256
52	29.111	2,4-Decadienal	25152-83-4	C10H16O	152	1233	1220
53	29.768	Undecanal	112-44-7	C11H22O	170	1314	1309
54	30.592	Methyl geranate	1189-09-9	C11H18O2	182	1330	1320
55	31.246	1-methyl-4-(1-methylethenyl)-1,2-Cyclohexanediol	1946-00-5	C10H18O2	170	1355	1346
56	31.702	$\alpha$ -Copaene	138874-68-7	C15H24	204	1380	1375
57	31.941	Citronellyl acetate	150-84-5	C12H22O2	198	1374	1350
58	32.382	2-Undecenal	2463-77-6	C11H20O	168	1311	1311
59	32.385	8-undecen-1-al	147159-49-7	C11H20O	168	1373	1365
60	32.434	Neryl acetate	141-12-8	C12H20O2	196	1352	1352
61	32.62	<i>n</i> -Decanoic acid	334-48-5	C10H20O2		1374	1372
62	33.655	$\beta$ -Element	515-13-9	C15H24	204	1398	1398
63	33.88	Ethyl decanoate	110-38-3	C12H24O2	200	1340	1399
64	34.403	Dodecanal	112-54-9	C12H24O	184	1345	1402
65	34.845	<i>trans</i> -Caryophyllene	87-44-5	C15H24	204	1496	1494
66	34.875	Caryophyllene	13877-93-5	C15H24	204	1425	1424
67	35.285	Germacrene D	23986-74-5	C15H24	204	1217	1216
68	35.913	1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-azulene	3691-11-0	C15H24	204	1451	1490
69	36.22	decahydro-1,1,7-trimethyl-4-methylene-1H-Cycloprop-azulene	25246-27-9	C15H24	204	1387	1386
70	36.377	6,10-dimethyl-5,9-Undecadien-2-one	689-67-8	C13H22O	194	1422	1420
71	36.382	linalyl acetate	115-95-7	C12H20O2	196	1276	1272
72	36.581	Farnesene	18794-84-8	C15H24	204	1451	1440
73	36.869	Eremophila-1(10),8,11-triene	190327-38-9	C15H22	202	1508	1507
74	36.875	Farnesene epoxide	83637-40-5	C15H24O	220	1542	1540
75	36.901	8-Cedren-13-ol	18319-35-2	C15H24O	220	1647	1646
76	37.036	4a-dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene	823810-22-6	C15H24	204	1475	1473
77	37.294	$\alpha$ -selinene	473-13-2	C15H24	204	1478	1474
78	37.715	Selina-4,11-diene	17627-30-4	C15H24	204	1479	1476
79	37.732	decahydro-1,1,3a-trimethyl-7-methylene-1H-Cyclopropa-naphthalene	20071-49-2	C15H24	204	1489	1398
80	38.445	Valencene	997-29-7	C15H24	204	1578	1474
81	38.63	$\alpha$ -Bulnesene	489-81-6	C15H24	204	1506	1505
82	39.188	$\alpha$ -Panasinsen	56633-28-4	C15H24	204	1418	1416
83	39.369	$\delta$ -Cadinene	483-76-1	C15H24	204	1522	1518

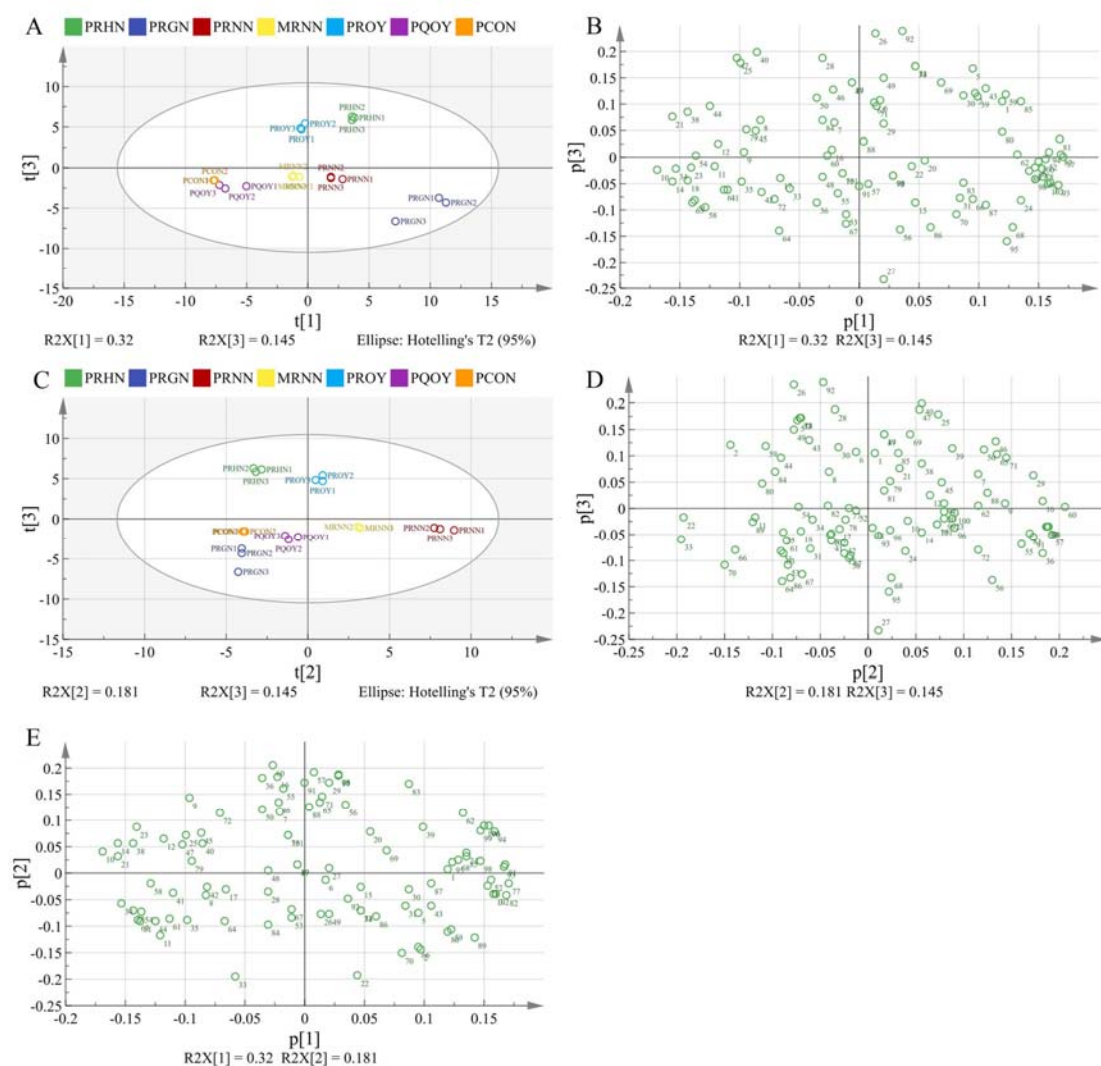
84	39.739	11-Tridecyn-1-ol	33925-75-6	C13H24O	196	1576	1574
85	40.984	Nerolidol	40716-66-3	C15H26O	222	1568	1561
86	42.268	Diethyl phthalate	84-66-2	C12H14O4	222	1594	1592
87	42.834	Caryophyllene oxide	1139-30-6	C15H24O	220	1589	1587
88	42.995	Neointermedeol	5945-72-2	C15H26O	222	1688	1668
89	43.22	13-nor-Eremophil-1(10)-en-11-one	54275-21-7	C14H22O	206	1592	1581
90	43.246	Labdadienedial	104263-85-6	C20H30O2	302	1591	1490
91	43.605	cadin-4-en-1 $\beta$ -ol	73365-77-2	C15H26O	222	1616	1614
92	43.616	Himbaccol	552-02-3	C15H26O	222	1535	1530
93	43.998	11,11-dimethyl-, 4,8-bis(methylene)-Bicyclo [7.2.0] undecan-3-ol	79580-01-1	C15H24O	220	1647	1636
94	44.216	Viridiflorol	19078-39-8	C15H26O	222	1598	1594
95	44.791	Intermedeol	6168-59-8	C15H26O	222	1670	1668
96	46.065	decahydro-1,5,5,8a-tetramethyl-1,4-Methanoazulen-9-one	465-26-9	C15H24O	220	1579	1576
97	48.299	1,5-diethenyl-2,3-dimethyl-Cyclohexane	68779-12-4	C12H20	164	1145	1143
98	48.65	$\alpha$ -Cyperone	473-08-5	C15H22O	218	1674	1673
99	50.272	Nootkatone	91416-23-8	C15H22O	218	1837	1834
100	50.55	Solavetivone	54878-25-0	C15H22O	218	1746	1645
101	51.085	geranylgeranyl acetate	61691-98-3	C22H36O2	332	2319	2316
102	51.638	Corymbolone	97094-19-4	C15H24O2	236	1788	1785

a. the data were from NIST Chemical Structures Library (USA Database of Standards Institute, 2014 edition), Wiley Library (William Atlas Library, 9th edition).

**Table S2.** the differences in VOCs in 'hongjiang' obtained from different factors were analyzed by

VIP analysis and heat map analysis in OPLS-DA

No	VIP value	No	VIP value	No	VIP value
1	0.959186	35	1.20053	69	0.707304
2	0.990339	36	1.07735	70	1.01253
3	0.943815	37	1.17301	71	1.11464
4	1.1721	38	0.958761	72	1.01737
5	1.02816	39	1.05897	73	1.08372
6	0.717722	40	1.05021	74	1.11093
7	1.17921	41	1.03707	75	1.18045
8	0.919489	42	1.25436	76	1.08912
9	0.925623	43	1.05368	77	0.907922
10	0.90578	44	0.917137	78	0.983413
11	1.00441	45	1.07168	79	1.13552
12	0.777899	46	1.18342	80	0.97246
13	1.10488	47	1.00776	81	0.924352
14	0.890596	48	1.03303	82	0.916278
15	0.434662	49	1.16439	83	1.01064
16	0.951232	50	1.1993	84	0.742262
17	1.09365	51	0.95244	85	0.946582
18	0.918413	52	0.950733	86	0.859058
19	1.17095	53	0.743983	87	0.771121
20	1.17351	54	1.00333	88	0.844081
21	0.933587	55	1.09626	89	0.929089
22	1.03961	56	0.971896	90	1.09131
23	0.977287	57	1.07311	91	1.06074
24	0.841294	58	1.00257	92	1.03756
25	1.02435	59	0.970501	93	0.904177
26	1.06594	60	1.03263	94	0.918559
27	1.00836	61	0.960167	95	0.989988
28	1.17296	62	0.914333	96	0.924141
29	1.0793	63	0.963771	97	1.07991
30	0.72771	64	0.871637	98	0.812826
31	0.645616	65	1.12163	99	0.874442
32	1.11097	66	1.03231	100	0.902154
33	0.969324	67	1.24131	101	1.18013
34	0.937454	68	0.95051	102	0.929052



**Figure S1.** Scores plot of PC1/PC3 (A) and PC2/PC3 (C), loading plot of PC1/PC2 (E), PC1/PC3 (B) and PC2/PC3 (D) for VOCs among *Citrus sinensis*. 'hongjiang'.