Re-Rolling Treatment in the Fermentation Process Improves the Aroma Quality of Black Tea

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Table S1. Identified volatile compounds and their peak areas in different black tea samples

NO.	Peak	CAS	Tested RI	Referred RI	Category	R1	R1.5	RR1.5	*P*-value
	Alkanes								
1	Dodecane	112-40-3	1199	1200		571422±72491a	516537±55944a	332790±21159b	0.004
2	Farnesane	3891-98-3	1399	1379		152825±13802a	129088±11247a	121800±24703a	0.158
	aromatic hydrocarbons								
3	Toluene	108-88-3	750	759		2816410±429419a	10756413±270611b	6099123±891908c	0.000
4	m-Xylene	108-38-3	854	862		699665±198166a	1666336±152076b	687241±37142a	0.000
5	p-Xylene	106-42-3	861	866		682294±517206a	1552080±136006b	648676±64647a	0.020
6	o-Xylene	95-47-6	886	889		1484518±939061a	3271697±271018b	1616801±80602a	0.015
7	Cumene	98-82-8	920	914		698399±502369a	901719±351893a	441779±64034a	0.350
8	o-Cymene	527-84-4	1022	1021		6233602±56916a	6134748±514593a	5928498±191541a	0.526
9	m-Cymenene	1124-20-5	1087	1084		353720±4521a	347624±33323a	311105±12002a	0.088
10	1,2,4,5-Tetramethylbenzene	95-93-2	1116	1131		126973±2903a	226179±32283b	114747±1107a	0.001
11	2-Methylnaphthalene	91-57-6	1285	1299		11646±1261a	10763±524a	8640±210b	0.009
12	1,1,6-Trimethyl-1,2-dihydronaphthalene	30364-38-6	1348	1355		7303±1846a	8211±2935a	7927±832a	0.862
13	Butylated Hydroxytoluene	128-37-0	1511	1517		74164±7684a	60618±9366ab	53082±2926b	0.030
14	Cadalin	483-78-3	1672	1675		7109±2552a	8172±630a	8181±719a	0.652
	Alkenes								
15	4-Methyl-1,3-pentadiene	926-56-7	596	609		90208±86270a	27340±6647a	87358±30493a	0.329
16	2,6-Dimethyl-1,5-heptadiene	6709-39-3	882	882		45968±2364a	50456±2200ab	54445±3533b	0.026
17	Isocitronellene	85006-04-8	914	926	VT	123238±15707a	79885±5668b	94438±6696b	0.006
18	3,5,5-Trimethyl-2-hexene	26456-76-8	973	985		273924±14054a	263045±43970a	301577±46951a	0.485
19	4-Carene	29050-33-7	988	1009	VT	25681±2414a	32874±977b	31415±245b	0.003
20	α-Fellandrene	99-83-2	1001	1000	VT	1155623±45991a	1254071±140773a	1295110±71172a	0.258
21	α-Terpinene	99-86-5	1013	1003	VT	90403±3963a	104406±13523a	108061±8336a	0.130
22	γ-Terpinene	99-85-4	1015	1030	VT	94351±25955a	66720±10220a	68117±23794a	0.273
23	Limonene	138-86-3	1025	1030	VT	6015561±338482a	6653925±782289a	6824900±54493a	0.187

24	5-Ethyl-1-formylcyclopentene	36431-60-4	1028	1026		149667±7057a	135392±10480ab	123917±7423b	0.027
25	(E)-β-Ocimene	3779-61-1	1039	1040	VT	264748±14290a	324590±41659ab	333873±14917b	0.039
26	β-Ocimene	13877-91-3	1048	1046	VT	2471437±203674a	2933632±454402a	3088188±64831a	0.091
27	Terpinolene	586-62-9	1085	1088	VT	503357±14271a	536388±64080a	535063±22311a	0.553
28	4,8-Dimethyl-1,3,7-nonadiene	19945-61-0	1117	1117		138444±5321a	154689±9361a	180711±16518b	0.011
29	1,3,8-p-Menthatriene	18368-95-1	1121	1119	VT	71978±4575a	81911±6425a	83192±3732a	0.065
30	allo-Ocimene	7216-56-0	1129	1131	VT	275826±9813a	320363±26641b	322809±13332b	0.033
31	(4E,6E)-Allocimene	3016-19-1	1140	1131	VT	199404±24486a	231433±36347a	243094±9537a	0.182
32	α-Terpineol	10482-56-1	1188	1187	VT	488758±26545a	488022±54704a	466501±33293a	0.752
33	α-Cubebene	17699-14-8	1347	1351	VT	106810±9320a	113392±10121a	129116±7193a	0.055
34	cis-β-Farnesene	28973-97-9	1415	1428	VT	55570±1849a	60934±17586a	61038±6868a	0.790
35	Humulene	6753-98-6	1449	1452	VT	108653±4588a	121781±28889a	126050±3393a	0.472
36	β-Farnesene*	77129-48-7	1456	1455	VT	36568±1077a	45829±2512a	56132±7162b	0.005
37	Germacrene D	23986-74-5	1473	1480	VT	13314±3069a	16268±2590a	16145±4061a	0.504
38	α-Muurolene	10208-80-7	1497	1497	VT	65453±1218a	71938±5776ab	74723±1870b	0.047
39	α-Farnesene	502-61-4	1507	1505	VT/CDV	23833±2092a	22426±3778a	25286±2003a	0.487
40	Calamenene	483-77-2	1520	1527	VT	874274±44186a	968173±58264a	981115±30230a	0.055
41	δ-Cadinene	483-76-1	1521	1524	VT	300089±12849a	342430±32581ab	362303±12535b	0.031
42	Cubenene	29837-12-5	1529	1513	VT	21586±1177ab	18042±1942a	22318±1590b	0.036
43	α-Calacorene	21391-99-1	1540	1542	VT	12719±705a	11706±1492a	13939±1731a	0.220
44	Neophytadiene	504-96-1	1842	1838	VT	7740±1521a	7954±1228a	9606±2028a	0.369
	Alcohols								
45	3-Methyl-1-butanol	123-51-3	720	726	AADV	57719±9406a	43794±3609a	21433±6936b	0.002
46	1-Pentanol	71-41-0	753	763	FADV	1490178±270186a	1588054±111403a	1280679±162469a	0.218
47	(Z)-2-pentenol	1576-95-0	760	769	FADV	2114798±477328a	1772285±131585ab	1169151±198488b	0.025
48	(Z)-3-Hexenol*	928-96-1	852	851	FADV	11115041±1864685a	8145185±944450b	6195826±616019b	0.009
49	(E)-2-Hexenol	928-95-0	863	852	FADV	1830113±660838a	1251113±349826a	999029±129982a	0.136
50	1-Hexanol*	111-27-3	866	865	FADV	9765593±247595a	5994946±371294b	4794893±315483c	0.000

51	Linalool-3,7-oxide	7392-19-0	969	971	VT	110312±9670a	115730±16036a	115716±6114a	0.804
52	1-Heptanol	111-70-6	971	967	FADV	896333±50030a	907862±87858a	892328±58942a	0.958
53	1-Octen-3-ol*	3391-86-4	979	986	FADV	4241123±233661a	5071255±306378b	5165420±340258b	0.016
54	cis-Anhydrolinalool	54750-69-5	1005	1007	VT	53372±4269a	53793±11191a	57570±3529a	0.746
55	2-Ethyl-1-hexanol	104-76-7	1030	1031		1684512±78834a	1392400±157246b	1199253±42531b	0.004
56	Benzyl alcohol	100-51-6	1034	1045	AADV	3252497±1847742a	7717482±5168190a	11074733±1520219a	0.070
57	cis-Linalool oxide (furanoid)*	5989-33-3	1071	1064	VT	6806606±183026a	5154254±192801b	4333389±229804c	0.000
58	1-Octanol	111-87-5	1072	1068	FADV	1421472±59098a	1499777±115702a	1564331±62611a	0.190
59	trans-Linalool oxide (furanoid)*	34995-77-2	1087	1087	VT	11633708±461899a	8748930±310685b	7356637±379121c	0.000
60	Linalool*	78-70-6	1102	1098	VT	51622770±2601166a	44142686±3478152b	40246694±1110780b	0.005
61	Hotrienol	29957-43-5	1105	1108	VT	8464733±419660a	8168068±1051234a	8705896±259738a	0.638
62	Phenylethyl Alcohol	60-12-8	1111	1121	AADV	29285710±1739404a	28603892±1868901a	27435221±2225251a	0.539
63	(Z)-3-Nonen-1-ol	10340-23-5	1154	1156		167605±11468a	165627±25718a	184931±9776a	0.380
64	cis-Linalol oxide (pyranoid)*	14009-71-3	1168	1173	VT	1042967±70189a	909868±58601a	762209±56684b	0.004
65	1-Nonanol	143-08-8	1172	1186	FADV	861614±24686a	810378±59477a	827536±65323a	0.521
66	trans-Linalol oxide (pyranoid)*	39028-58-5	1168	1171	VT	2515503±87601a	2488640±233195a	2131985±26710b	0.031
67	4-Terpinenol	562-74-3	1174	1172	VT	38231±4249a	33682±6419a	32429±1397a	0.323
68	γ-Isogeraniol	13066-51-8	1218	1222	VT	694495±32837a	656186±59330a	672353±166117a	0.903
69	Nerol	106-25-2	1227	1229	VT	1047911±65944a	886533±121827a	919345±85561a	0.165
70	Geraniol*	106-24-1	1256	1259	VT	25769711±1090887a	21431450±1657520b	19606191±471063b	0.002
71	Nerolidol*	40716-66-3	1563	1565	VT	488503±72886a	361807±30178b	395544±22759ab	0.040
72	Phytol	150-86-7	2115	2116		27732±7796a	26763±5835a	24144±3967a	0.765
	Aldehydes								
73	2-Methylpropanal	78-84-2	533	537	AADV	1557107±1015817a	1431389±624624a	2729304±1363561a	0.316
74	3-Methylbutanal	590-86-3	611	649	AADV	6569875±5107068a	6643096±4374612a	8104601±240058a	0.865
75	2-Methylbutanal	96-17-3	625	646	AADV	14850268±9777461a	16454979±10400634a	19861537±765478a	0.759
76	(E)-2-Butenal	123-73-9	610	615		146155±41625a	1246082±112670b	1082990±71888b	0.000
77	Pentanal	110-62-3	674	698	FADV	4762169±624255a	5662566±1779847a	6317962±591540a	0.316

78	2-Methyl-2-butenal	1115-11-3	728	730		418154±72367a	361863±57492a	347124±31195a	0.333
79	(E)-2-Pentenal	1576-87-0	740	754	FADV	875833±86954a	2252363±379855b	2113131±68104b	0.001
80	2-Methylpentanal	123-15-9	745	758		302624±30975a	211069±7622b	192307±3532b	0.001
81	Hexanal*	66-25-1	795	801	FADV	9100569±803361a	17689571±751896b	16983313±989890b	0.000
82	(E)-2-Hexenal*	6728-26-3	841	850	FADV	11485375±3319958a	24223696±1450802b	27827075±993717b	0.000
83	(Z)-4-Heptenal	6728-31-0	898	904	FADV	107774±13458a	142380±2715b	162360±14924b	0.004
84	Heptanal	111-71-7	900	903	FADV	8154933±71523a	8714515±272733a	9344194±358112b	0.004
85	(E,E)-2,4-Hexadienal*	142-83-6	908	915	FADV	25725±14564a	118903±62068ab	205824±43728b	0.008
86	(Z)-2-Heptenal	57266-86-1	954	958	FADV	790759±19360a	948708±42674b	1068360±47044c	0.000
87	Benzaldehyde	100-52-7	955	961	AADV	24805558±899084a	26175437±2309837a	26046351±1459430a	0.568
88	2,4-Heptadienal	5910-85-0	995	1007	FADV	3044277±411930a	4192485±339107b	4103731±316573b	0.014
89	Octanal*	124-13-0	1002	1004	FADV	508426±20523a	597753±43687b	714702±14643c	0.000
90	(E,E)-2,4-Heptadienal*	4313-03-5	1009	1002	FADV	6496582±512012a	7794333±558681b	8194534±469419b	0.016
91	Phenylacetaldehyde*	122-78-1	1041	1051	AADV	56823231±2044326a	66991480±1025440b	68054420±3320279b	0.002
92	Melonal*	106-72-9	1053	1044		97092±16613a	120797±1979a	152643±17645b	0.008
93	(E)-2-Octenal*	2548-87-0	1057	1063	FADV	1559265±39619a	1843570±85621b	2142355±96235c	0.000
94	(E,E)-2,4-Octadienal	30361-28-5	1109	1111	FADV	127651±6036a	132196±13234a	144056±8882a	0.190
95	α-Cyclocitral	432-24-6	1114	1123	CDV	212973±10244a	193063±13038a	202078±10374a	0.177
96	(E)-2-Nonenal*	18829-56-6	1159	1162	FADV	208979±9964a	219917±10542a	260125±21139b	0.012
97	2,4-Dimethylbenzaldehyde	15764-16-6	1171	1181		326760±7415a	307131±18876a	332756±19649a	0.212
98	Safranal	116-26-7	1196	1201	CDV	722187±36118a	703980±45905a	701820±9517a	0.737
99	Decanal	112-31-2	1205	1205	FADV	568381±28238a	548891±29861a	640998±19928b	0.012
100	1-p-Menthen-9-al	29548-14-9	1214	1217		75039±3328a	78173±7239a	81945±5198a	0.367
101	β-Cyclocitral	432-25-7	1217	1226	CDV	2038359±82487a	2154588±158494a	2294881±30805a	0.064
102	Neral	106-26-3	1240	1242	VT	88951±4489a	79587±6217a	90291±7851a	0.159
103	β-Cyclohomocitral	472-66-2	1254	1251	CDV	571796±30634a	611633±32245ab	640414±6585b	0.047
104	(E)-2-Decenal	3913-81-3	1261	1250		151559±10150a	176071±11288a	202867±13350b	0.005
105	Geranial	141-27-5	1270	1279	VT	1191126±35482a	1201364±136140a	1306873±40739a	0.256

106	α-Ethylidene-phenylacetaldehyde	4411-89-6	1270	1284		253293±7118a	241802±24602a	268121±13732a	0.236
107	(2E,4Z)-Decadienal	25152-83-4	1292	1312	FADV	114326±15077a	138565±5474ab	164699±16353b	0.010
108	(E,E)-2,4-Decadienal	25152-84-5	1314	1312	FADV	209565±31087a	268749±21704ab	314146±27444b	0.009
109	2-Undecenal	2463-77-6	1363	1368		59504±6230a	63783±4335a	78554±8102b	0.025
	Ketones								
110	3-Methyl-2-butanone	563-80-4	658	645		1717302±691361a	1296829±1141386a	978215±66930a	0.536
111	1-Penten-3-one	1629-58-9	659	678	FADV	356856±24534a	301826±8375a	329265±40119a	0.223
112	3-Penten-2-one	625-33-2	727	733		71464±4617a	82762±17806a	146189±50246a	0.051
113	2-Methyl-3-pentanone	565-69-5	735	742		63334±5887a	58307±3845a	58866±2934a	0.372
114	2-Methyl-1-penten-3-one	25044-01-3	755	748		66010±3329a	61692±2591a	51314±463b	0.001
115	2,3-Hexanedione	3848-24-6	774	786		214348±45273a	268128±19633a	265458±7945a	0.108
116	2-Heptanone	110-43-0	889	884	FADV	2418638±125970a	2631224±196698a	2837011±304036a	0.147
117	1-Octen-3-one*	4312-99-6	978	979	FADV	560822±43623a	701995±46764b	791889±16814c	0.001
118	2,3-Octanedione	585-25-1	985	987		1145000±121236a	1457002±58751b	1662807±8066c	0.001
119	3-Octanone	106-68-3	986	984		356980±12595a	437711±43605b	439124±28270b	0.027
120	6-Methyl-5-hepten-2-one	110-93-0	987	985	CDV	1486219±91022a	1279058±136207a	1315618±103764a	0.130
121	2,2,6-Trimethylcyclohexanone*	2408-37-9	1031	1023	CDV	2440672±29870a	2228902±81284b	2369612±6807a	0.006
122	3-Octen-2-one*	1669-44-9	1039	1037		1156988±132335a	1614664±130321b	1677405±91054b	0.003
123	γ-Caprolactone	695-06-7	1059	1056	FADV	172278±13558a	278932±65791a	375750±159874a	0.119
124	Ipsenone	19860-68-5	1066	1083	VT	90304±28821a	60674±23909a	190953±46949b	0.009
125	Isophorone	78-59-1	1118	1126	CDV	48006±5622a	50446±3257a	55158±7634a	0.369
126	3-Nonen-2-one	14309-57-0	1140	1136		153542±13899a	166551±15338a	199307±5251b	0.010
127	5-Ethyl-6-methyl-3E-hepten-2-one	57283-79-1	1146	1144		1417613±70830a	1587395±165591a	1893314±53429b	0.005
128	3-Methylacetophenone	585-74-0	1181	1192		36047±1392a	34034±4961a	35467±2299a	0.749
129	β-Damascenone*	23726-93-4	1382	1388	CDV	500084±31353a	534153±40448ab	591220±34308b	0.048
130	Pseudoionone	1604-34-8	1405	1407	CDV	22103±2582a	22627±1423a	26970±1518b	0.039
131	α-Ionone*	127-41-3	1426	1429	CDV	285101±21431a	362749±33931b	439720±29115c	0.002
132	Geranylacetone	3796-70-1	1452	1445	CDV	224779±19186a	201611±19881a	240363±27156a	0.183

133	β-Ionone*	14901-07-6	1484	1488	CDV	752448±38784a	906992±35734b	1005997±52380c	0.001
134	Dihydroactinidiolide*	17092-92-1	1523	1525	CDV	93215±3414a	121389±3309b	126872±4814b	0.000
	Esters								
135	Pentyl formate	638-49-3	823	827		259127±66505a	501681±12003b	525623±48440b	0.001
136	Methyl caproate	106-70-7	925	938	FADV	474851±48950a	454970±28470a	458212±17180a	0.757
137	Hexyl formate	629-33-4	928	927	FADV	109160±3118a	135800±10475b	163402±13730c	0.002
138	3-Methyl-4-penten-1-ol acetate	71487-16-6	1008	1006		657143±64274a	537279±97966ab	418209±86961b	0.037
139	Benzyl formate	104-57-4	1075	1082	AADV	96363±5282a	123776±21600a	94294±9840a	0.075
140	(Z)-3-Hexenyl isobutanoate	41519-23-7	1145	1143	FADV	134511±4709a	140098±14815a	155284±1772a	0.071
141	(E)-3-Hexenyl butanoate	53398-84-8	1187	1186	FADV	1948656±81477a	1912644±208818a	2085532±72931a	0.329
142	Methyl salicylate*	119-36-8	1191	1199	AADV	11328008±152147a	9740791±605279b	9029901±436991b	0.002
143	Hexyl butyrate	2639-63-6	1193	1184	FADV	143198±6854a	145781±10547a	165555±14466a	0.091
144	(E)-2-Hexenyl butanoate	53398-83-7	1196	1195	FADV	654350±16433ab	574413±66504a	676202±10782b	0.046
145	(Z)-3-Hexenyl-α-methylbutyrate	53398-85-9	1233	1233	FADV/AADV	3204437±160701a	3595800±284190ab	4046202±120078b	0.006
146	(Z)-3-Hexenyl isovalerate*	35154-45-1	1237	1245	FADV/AADV	605793±17831a	695421±58578ab	728231±32280b	0.023
147	Hexyl 2-methylbutyrate	10032-15-2	1238	1227	FADV/AADV	324285±18970a	330497±22082a	395996±5029b	0.004
148	(E)-2-Hexenyl isovalerate	68698-59-9	1240	1245	FADV/AADV	412003±23496a	383539±55677a	470344±17304a	0.065
149	(Z)-2-Hexenyl isovalerate		1246	1245	FADV/AADV	107795±6319a	102149±13305a	142505±7213b	0.004
150	β-Octalactone*	698-76-0	1283	1288		31772±5297a	36088±6604ab	46619±4554b	0.041
151	Pentyl hexanoate	540-07-8	1289	1288	FADV	55020±596a	60678±4689a	70004±3663b	0.005
152	Methyl geranate	1189-09-9	1324	1321	VT	219693±14783a	179694±20308a	209242±16000a	0.068
153	cis-3-Hexenyl hexanoate*	31501-11-8	1382	1380	FADV	4791843±95104a	4599033±450493a	5660186±326154b	0.015
154	Hexyl hexanoate*	6378-65-0	1387	1385	FADV	320920±12899a	338163±22918a	387174±21543b	0.015
155	(E)-2-Hexenyl hexanoate	53398-86-0	1390	1391	FADV	340337±11048ab	297972±35746a	382884±23705b	0.019
156	cis-3-Hexenyl trans-2-hexenoate	53398-87-1	1433	1401	FADV	23334±1702ab	20405±2060a	25984±2430b	0.046
157	(Z)-3-Hexenyl benzoate	25152-85-6	1568	1565	FADV/AADV	94765±7121ab	86667±4655a	114608±12901b	0.022
158	(E)-2-Hexenyl benzoate	76841-70-8	1583	1590	FADV/AADV	25787±2998a	23440±1803a	32423±5175a	0.053
	Acids								

159	2-Methylbutyric acid	116-53-0	877	894	AADV	15057±968a	22835±4415ab	29001±7818b	0.046
160	Hexanoic acid	142-62-1	1005	1013	FADV	5978366±1431306ab	2721934±277423a	9319470±3742702b	0.036
161	(E)-3-Hexenoic acid	1577-18-0	1023	1021	FADV	283771±5298a	680949±136019b	837363±131156b	0.002
162	(E)-2-Hexenoic acid	13419-69-7	1045	1041	FADV	22536±6206a	35017±21290a	35847±11458a	0.491
163	Levulinic acid	123-76-2	1060	1063		182445±39815a	302460±111112a	247356±52166a	0.223
164	Nonanoic acid	112-05-0	1276	1281	FADV	1070712±204888a	1053283±155982a	1078096±323599a	0.992
165	trans-Geranic acid	4698-08-2	1356	1355	VT	466567±196526a	465080±57513a	515235±99031a	0.871
	Oxygen heterocyclic compounds								
166	2-Methylfuran	534-22-5	569	590		30492±13922a	39746±4203a	70866±15315b	0.016
167	2-Ethyl-furan	3208-16-0	679	702		12912661±1931188a	19559460±1393131b	20008958±417828b	0.001
168	2-Butylfuran	4466-24-4	888	889		1465334±94862a	1528276±102703a	1965421±141570b	0.003
169	Pentyl-oxirane	5063-65-0	903	905		535872±24469a	352430±132486a	456470±106758a	0.156
170	(Z)-2-(2-Pentenyl)furan	70424-13-4	1000	1001		490464±6621a	571532±41344b	620708±8880b	0.002
171	2-Methyl-2-cyclohexylbutane	31797-64-5	1152	1130		160457±6909a	162754±10318a	184146±11602a	0.047
172	Theaspirane isomer1	36431-72-8	1294	1305	CDV	488258±23286a	506516±29833a	568110±2267b	0.010
173	Theaspirane isomer2	36431-72-8	1312	1305	CDV	470615±26019a	488685±26027a	542935±8385b	0.016
	Sulfur compounds								
174	Dimethyl sulfide	75-18-3	518	532	AADV	2799808±2469068a	4020864±343221a	4911749±1902674a	0.413
175	Dimethyl trisulfide	3658-80-8	962	972	AADV	86971±2348a	69468±13024a	70381±9858a	0.113
	Nitrogen compounds								
176	1-Ethyl-1H-pyrrole-2-carboxaldehyde*	2167-14-8	1046	1046		66322±4049a	75465±3374a	95074±6856b	0.001
	Other compounds								
177	Benzyl nitrile	140-29-4	1137	1143		242611±6819a	222717±16161ab	207489±9159b	0.026
178	4-sec-Butylphenol	99-71-8	1314	1315		32152±2180a	33346±3014a	40919±2638b	0.013
179	Caffeine	58-08-2	1846	1841		424826±182534a	624819±120658a	413377±98904a	0.191

Note: The data was shown as mean ± SD with peak area (n=3); *: the compound was confirmed by the authentic standard; a, b, c: $P < 0.05$ for the changes with different letters (Tukey s-b (K) test).

Table S2. The fold changes (FC) and *P*-values of differential volatile compounds in the R1 vs R1.5 group

	R1	**R1.5**	**FC**	***P*-values**
(E)-2-Butenal	146155	1246082	8.53	0.000
Toluene	2816410	10756413	3.82	0.000
(E)-2-Pentenal	875833	2252363	2.57	0.004
(E)-3-Hexenoic acid	283771	680949	2.40	0.007
m-Xylene	699665	1666336	2.38	0.003
p-Xylene	682294	1552080	2.27	0.048
o-Xylene	1484518	3271697	2.20	0.034
(E)-2-Hexenal	11485375	24223696	2.11	0.004
Hexanal	9100569	17689571	1.94	0.000
Pentyl formate	259127	501681	1.94	0.003
1,2,4,5-Tetramethylbenzene	126973	226179	1.78	0.006
2-Methylbutyric acid	15057	22835	1.52	0.041
2-Ethyl-furan	12912661	19559460	1.51	0.008
3-Octen-2-one	1156988	1614664	1.40	0.013
2,4-Heptadienal	3044277	4192485	1.38	0.020
(Z)-4-Heptenal	107774	142380	1.32	0.012
Dihydroactinidiolide	93215	121389	1.30	0.001
4-Carene	25681	32874	1.28	0.009
2,3-Octanedione	1145000	1457002	1.27	0.016
α-Ionone	285101	362749	1.27	0.029
β-Farnesene	36568	45829	1.25	0.004
1-Octen-3-one	560822	701995	1.25	0.019
Hexyl formate	109160	135800	1.24	0.013
3-Octanone	356980	437711	1.23	0.037
β-Ionone	752448	906992	1.21	0.007
(E,E)-2,4-Heptadienal	6496582	7794333	1.20	0.041
(Z)-2-Heptenal	790759	948708	1.20	0.004
1-Octen-3-ol	4241123	5071255	1.20	0.020
(E)-2-Octenal	1559265	1843570	1.18	0.006
Phenylacetaldehyde	56823231	66991480	1.18	0.002
Octanal	508426	597753	1.18	0.033
(Z)-2-(2-Pentenyl)furan	490464	571532	1.17	0.028
(E)-2-Decenal	151559	176071	1.16	0.049
1-Ethyl-1H-pyrrole-2-carboxaldehyde	66322	75465	1.14	0.040
Heptanal	8154933	8714515	1.07	0.026
2,2,6-Trimethylcyclohexanone	2440672	2228902	0.91	0.013
Methyl salicylate	11328008	9740791	0.86	0.012
Linalool	51622770	44142686	0.86	0.041
Geraniol	25769711	21431450	0.83	0.019
2-Ethyl-1-hexanol	1684512	1392400	0.83	0.045

cis-Linalool oxide (furanoid)	6806606	5154254	0.76	0.000
trans-Linalool oxide (furanoid)	11633708	8748930	0.75	0.001
2-Methylpentanal	302624	211069	0.70	0.008
Isocitronellene	123238	79885	0.65	0.011
1-Hexanol	9765593	5994946	0.61	0.000
Hexanoic acid	5978366	2721934	0.46	0.018

Note: The difference significances were calculated by ANOVA.

Table S3. The fold changes (FC) and *P*-values of differential volatile compounds in the R1 vs RR1.5 group

	R1	**RR1.5**	**FC**	***P*-values**
(E,E)-2,4-Hexadienal	25725	205824	8.00	0.002
(E)-2-Butenal	146155	1082990	7.41	0.000
(E)-3-Hexenoic acid	283771	837363	2.95	0.002
(E)-2-Hexenal	11485375	27827075	2.42	0.001
(E)-2-Pentenal	875833	2113131	2.41	0.000
2-Methylfuran	30492	70866	2.32	0.028
Toluene	2816410	6099123	2.17	0.005
Ipsenone	90304	190953	2.11	0.034
Pentyl formate	259127	525623	2.03	0.005
2-Methylbutyric acid	15057	29001	1.93	0.037
Hexanal	9100569	16983313	1.87	0.000
Melonal	97092	152643	1.57	0.017
2-Ethyl-furan	12912661	20008958	1.55	0.003
α-Ionone	285101	439720	1.54	0.002
β-Farnesene	36568	56132	1.53	0.009
(Z)-4-Heptenal	107774	162360	1.51	0.009
(E,E)-2,4-Decadienal	209565	314146	1.50	0.012
Hexyl formate	109160	163402	1.50	0.003
β-Octalactone	31772	46619	1.47	0.021
2,3-Octanedione	1145000	1662807	1.45	0.002
3-Octen-2-one	1156988	1677405	1.45	0.005
(2E,4Z)-Decadienal	114326	164699	1.44	0.017
1-Ethyl-1H-pyrrole-2-carboxaldehyde	66322	95074	1.43	0.003
1-Octen-3-one	560822	791889	1.41	0.001
Octanal	508426	714702	1.41	0.000
(E)-2-Octenal	1559265	2142355	1.37	0.001
Dihydroactinidiolide	93215	126872	1.36	0.001
(Z)-2-Heptenal	790759	1068360	1.35	0.001
2,4-Heptadienal	3044277	4103731	1.35	0.024
2-Butylfuran	1465334	1965421	1.34	0.007
(E)-2-Decenal	151559	202867	1.34	0.006
β-Ionone	752448	1005997	1.34	0.003

5-Ethyl-6-methyl-3E-hepten-2-one	1417613	1893314	1.34	0.001
Pentanal	4762169	6317962	1.33	0.035
(Z)-2-Hexenyl isovalerate	107795	142505	1.32	0.003
2-Undecenal	59504	78554	1.32	0.032
4,8-Dimethyl-1,3,7-nonadiene	138444	180711	1.31	0.013
3-Nonen-2-one	153542	199307	1.30	0.006
4-sec-Butylphenol	32152	40919	1.27	0.010
Pentyl hexanoate	55020	70004	1.27	0.002
(Z)-2-(2-Pentenyl)furan	490464	620708	1.27	0.000
(Z)-3-Hexenyl-α-methylbutyrate	3204437	4046202	1.26	0.002
(E,E)-2,4-Heptadienal	6496582	8194534	1.26	0.013
(E)-β-Ocimene	264748	333873	1.26	0.004
β-Ocimene	2471437	3088188	1.25	0.008
(E)-2-Nonenal	208979	260125	1.24	0.019
3-Octanone	356980	439124	1.23	0.010
4-Carene	25681	31415	1.22	0.015
Hexyl 2-methylbutyrate	324285	395996	1.22	0.003
Pseudoionone	22103	26970	1.22	0.048
(4E,6E)-Allocimene	199404	243094	1.22	0.045
1-Octen-3-ol	4241123	5165420	1.22	0.018
α-Cubebene	106810	129116	1.21	0.030
δ-Cadinene	300089	362303	1.21	0.004
Hexyl hexanoate	320920	387174	1.21	0.010
(Z)-3-Hexenyl isovalerate	605793	728231	1.20	0.005
Phenylacetaldehyde	56823231	68054420	1.20	0.008
α-Terpinene	90403	108061	1.20	0.030
β-Damascenone	500084	592318	1.18	0.025
2,6-Dimethyl-1,5-heptadiene	45968	54445	1.18	0.026
cis-3-Hexenyl hexanoate	4791843	5660186	1.18	0.011
allo-Ocimene	275826	322809	1.17	0.008
Theaspirane isomer1	488258	568110	1.16	0.004
Humulene	108653	126050	1.16	0.006
1,3,8-p-Menthatriene	71978	83192	1.16	0.030
(Z)-3-Hexenyl isobutanoate	134511	155284	1.15	0.002
Theaspirane isomer2	470615	542935	1.15	0.010
2-Methyl-2-cyclohexylbutane	160457	184146	1.15	0.038
Heptanal	8154933	9344194	1.15	0.005
α-Muurolene	65453	74723	1.14	0.002
(E)-2-Hexenyl isovalerate	412003	470344	1.14	0.026
Limonene	6015561	6824900	1.13	0.015
Decanal	568381	640998	1.13	0.022
β-Cyclocitral	2038359	2294881	1.13	0.007
(E)-2-Hexenyl hexanoate	340337	382884	1.13	0.048

Calamenene	874274	981115	1.12	0.026
α-Fellandrene	1155623	1295110	1.12	0.046
β-Cyclohomocitral	571796	640414	1.12	0.019
1-Octanol	1421472	1564331	1.10	0.045
Geranial	1191126	1306873	1.10	0.021
2,2,6-Trimethylcyclohexanone	2440672	2369612	0.97	0.016
1,2,4,5-Tetramethylbenzene	126973	114747	0.90	0.002
m-Cymenene	353720	311105	0.88	0.005
Benzyl nitrile	242611	207489	0.86	0.006
trans-Linalol oxide (pyranoid)	2515503	2131985	0.85	0.002
5-Ethyl-1-formylcyclopentene	149667	123917	0.83	0.012
Dimethyl trisulfide	86971	70381	0.81	0.047
Methyl salicylate	11328008	9029901	0.80	0.001
Linalool	51622770	40246694	0.78	0.002
2-Methyl-1-penten-3-one	66010	51314	0.78	0.002
Isocitronellene	123238	94438	0.77	0.043
Geraniol	25769711	19606191	0.76	0.001
2-Methylnaphthalene	11646	8640	0.74	0.015
cis-Linalol oxide (pyranoid)	1042967	762209	0.73	0.006
Butylated Hydroxytoluene	74164	53082	0.72	0.011
2-Ethyl-1-hexanol	1684512	1199253	0.71	0.001
cis-Linalool oxide (furanoid)	6806606	4333389	0.64	0.000
3-Methyl-4-penten-1-ol acetate	657143	418209	0.64	0.019
2-Methylpentanal	302624	192307	0.64	0.004
trans-Linalool oxide (furanoid)	11633708	7356637	0.63	0.000
Dodecane	571422	332790	0.58	0.005
(Z)-3-Hexenol	11115041	6195826	0.56	0.012
(Z)-2-pentenol	2114798	1169151	0.55	0.034
1-Hexanol	9765593	4794893	0.49	0.000
3-Methyl-1-butanol	57719	21433	0.37	0.006

Note: The difference significances were calculated by ANOVA.

Table S4. The fold changes (FC) and *P*-values of differential volatile compounds in the R1.5 vs RR1.5 group

	R1.5	**RR1.5**	**FC**	***P*-values**
Hexanoic acid	2721934	9319470	3.42	0.038
4-Methyl-1,3-pentadiene	27340	87358	3.20	0.029
Ipsenone	60674	190953	3.15	0.013
2-Methylfuran	39746	70866	1.78	0.027
(Z)-2-Hexenyl isovalerate	102149	142505	1.40	0.010
(E)-2-Hexenyl benzoate	23440	32423	1.38	0.047
(Z)-3-Hexenyl benzoate	86667	114608	1.32	0.024
2-Butylfuran	1528276	1965421	1.29	0.012

(E)-2-Hexenyl hexanoate	297972	382884	1.28	0.027
cis-3-Hexenyl trans-2-hexenoate	20405	25984	1.27	0.039
Melonal	120797	152643	1.26	0.036
1-Ethyl-1H-pyrrole-2-carboxaldehyde	75465	95074	1.26	0.011
Cubenene	18042	22318	1.24	0.042
cis-3-Hexenyl hexanoate	4599033	5660186	1.23	0.030
4-sec-Butylphenol	33346	40919	1.23	0.031
α-Ionone	362749	439720	1.21	0.041
Hexyl 2-methylbutyrate	330497	395996	1.20	0.007
3-Nonen-2-one	166551	199307	1.20	0.025
Octanal	597753	714702	1.20	0.012
5-Ethyl-6-methyl-3E-hepten-2-one	1587395	1893314	1.19	0.038
Pseudoionone	22627	26970	1.19	0.022
(E)-2-Nonenal	219917	260125	1.18	0.042
Isocitronellene	79885	94438	1.18	0.045
Decanal	548891	640998	1.17	0.011
(E)-2-Octenal	1843570	2142355	1.16	0.016
(E)-2-Hexenal	24223696	27827075	1.15	0.024
2,3-Octanedione	1457002	1662807	1.14	0.004
1-Octen-3-one	701995	791889	1.13	0.035
(Z)-2-Heptenal	948708	1068360	1.13	0.031
Theaspirane isomer1	506516	568110	1.12	0.023
Theaspirane isomer2	488685	542935	1.11	0.026
2,2,6-Trimethylcyclohexanone	2228902	2369612	1.06	0.040
2-Methylpentanal	211069	192307	0.91	0.018
trans-Linalool oxide (furanoid)	8748930	7356637	0.84	0.008
cis-Linalool oxide (furanoid)	5154254	4333389	0.84	0.009
cis-Linalol oxide (pyranoid)	909868	762209	0.84	0.035
2-Methyl-1-penten-3-one	61692	51314	0.83	0.002
2-Methylnaphthalene	10763	8640	0.80	0.003
1-Hexanol	5994946	4794893	0.80	0.013
(Z)-3-Hexenol	8145185	6195826	0.76	0.040
(Z)-2-Pentenol	1772285	1169151	0.66	0.012
Dodecane	516537	332790	0.64	0.006
Toluene	10756413	6099123	0.57	0.001
1,2,4,5-Tetramethylbenzene	226179	114747	0.51	0.004
o-Xylene	3271697	1616801	0.49	0.001
3-Methyl-1-butanol	43794	21433	0.49	0.008
p-Xylene	1552080	648676	0.42	0.000
m-Xylene	1666336	687241	0.41	0.000

Note: The difference significances were calculated by ANOVA.