

Table S2-1 Volatile organic compounds originating from 5 major pathways (shikimate pathway (red), MEP pathway (green), mevalonate pathway (purple), leucine and isoleucine biosynthesis (blue), and lipoxygenase (LOX) pathway (black)). Each column represents an enzyme, which is involved in the biosynthesis of one or more compounds listed in column 2. Enzymes involved in the biosynthesis of compounds are denoted with a black bar in the line of the compound. Visual inspection of matrix allows to identify the core parts of the pathway and the terminal steps of each compound. For a more detailed table including substrates, enzyme names, and products see Notes S3.

#	name	pathway	functional group
1	2-methylbutyraldoxime	aliphatics	N-containing
2	3-methylbutyraldoxime	aliphatics	N-containing
3	isomylalcohol	aliphatics	alcohol
4	isovaleric acid	aliphatics	acid
5	methyl-2-methylbutyrate	aliphatics	ester
6	methyl-3-methylbutyrate	aliphatics	ester
7	2-oxo-2-phenylacetaldehyde	aromatics	aldehyde
8	2-phenylacetaldehyde	aromatics	aldehyde
9	2-phenylethanol	aromatics	alcohol
10	2-phenylethylformate	aromatics	ester
11	3-methylbutanoic acid-phenylmethyl-ester	aromatics	ester
12	acetophenone	aromatics	ketone
13	anisaldehyde	aromatics	aldehyde
14	benzaldehyde	aromatics	aldehyde
15	benzoic acid	aromatics	acid
16	benzylalcohol	aromatics	alcohol
17	benzylbenzoate	aromatics	ester
18	benzylpyridate	aromatics	N-containing
19	benzylformate	aromatics	ester
20	benzylmethyl ether	aromatics	ether
21	benzylbiglate	aromatics	ester
22	cinamaldehyde	aromatics	aldehyde
23	cinnamylalcohol	aromatics	alcohol
24	dimethylalkylate	aromatics	alcohol
25	estragal	aromatics	ether
26	eugenol	aromatics	alcohol
27	indole	aromatics	N-containing
28	isomylbenzoate	aromatics	ester
29	methoxyphenole	aromatics	alcohol
30	methyl phenylacetate	aromatics	ester
31	methylaminobenzaldehyde	aromatics	aldehyde
32	methylbenzoate	aromatics	ester
33	methylkinamate	aromatics	ester
34	methylsalicylate	aromatics	ester
35	metoxybenzaldehyde	aromatics	aldehyde
36	phenylbenzoate	aromatics	ester
37	veratrole	aromatics	ether
38	methylpalmitate	fatty acid derived	ester
39	1-hexanol	fatty acid derived	alcohol
40	(E)-3-hexenylacetate	fatty acid derived	ester
41	hexylacetate	fatty acid derived	ester
42	nonanal	fatty acid derived	aldehyde
43	nonenal	fatty acid derived	aldehyde
44	octanal	fatty acid derived	aldehyde
45	octenal	fatty acid derived	aldehyde
46	octanol	fatty acid derived	alcohol
47	(Z)-2-hexenylacetate	fatty acid derived	acetate
48	(Z)-3-hexenylacetate	fatty acid derived	acetate
49	(Z)-heexanol	fatty acid derived	alcohol
50	(Z)-jasmone	fatty acid derived	ketone
51	6-methyl-5-heptene-2-one	monoterpenoid	ketone
52	(E,E)-TMTT	monoterpenoid	hydrocarbon
53	2-methyl-6-methylene-1,7-octadien-3-one	monoterpenoid	ketone
54	6-3-carene	monoterpenoid	hydrocarbon
55	α-pinene	monoterpenoid	hydrocarbon
56	allo-ocimene	monoterpenoid	hydrocarbon
57	α-phellandrene	monoterpenoid	hydrocarbon
58	arbusculone	monoterpenoid	ketone
59	α-terpinene	monoterpenoid	hydrocarbon
60	α-terpinol	monoterpenoid	alcohol
61	α-thujene	monoterpenoid	hydrocarbon
62	β-cymene	monoterpenoid	hydrocarbon
63	β-myrcene	monoterpenoid	hydrocarbon
64	bornol	monoterpenoid	alcohol
65	bornylacetate	monoterpenoid	ester
66	β-phellandrene	monoterpenoid	hydrocarbon
67	β-pinene	monoterpenoid	hydrocarbon
68	camphene	monoterpenoid	hydrocarbon
69	camphor	monoterpenoid	ketone
70	1,8-cineole	monoterpenoid	epoxy
71	β-citronellol	monoterpenoid	alcohol
72	(E)-linaloolbide(l)uranoid	monoterpenoid	alcohol
73	(Z)-linaloolbide(l)uranoid	monoterpenoid	alcohol
74	(E)-linaloolbide(l)uranoid	monoterpenoid	alcohol
75	γ-terpinene	monoterpenoid	hydrocarbon
76	hottienol	monoterpenoid	alcohol
77	isobornylbutyrate	monoterpenoid	ester
78	isobornylpropionate	monoterpenoid	ester
79	lavandulol	monoterpenoid	alcohol
80	linalcolol	monoterpenoid	alcohol
81	linalcoldehyde	monoterpenoid	aldehyde
82	linalcol degradation	monoterpenoid	aldehyde
83	limonene	monoterpenoid	hydrocarbon
84	limonenebioxide	monoterpenoid	epoxy
85	limonenebide	monoterpenoid	epoxy
86	linalool	monoterpenoid	alcohol
87	linaloolbide(l)ketone	monoterpenoid	ketone
88	1,5,9-p-mentatriene	monoterpenoid	hydrocarbon
89	(Z)-ocimene	monoterpenoid	hydrocarbon
90	(E)-β-ocimene	monoterpenoid	hydrocarbon
92	p-cymene	monoterpenoid	hydrocarbon
93	pinocarvone	monoterpenoid	ketone
94	piperitol	monoterpenoid	alcohol
95	piperitone	monoterpenoid	ketone
96	sabinene	monoterpenoid	hydrocarbon
97	terpinene	monoterpenoid	hydrocarbon
98	terpinene-4-ol	monoterpenoid	alcohol
99	terpinolene	monoterpenoid	hydrocarbon
100	thuj-2-(10)-diene	monoterpenoid	hydrocarbon
101	thujol	monoterpenoid	alcohol
102	tricyclene	monoterpenoid	hydrocarbon
103	verbeneone	monoterpenoid	ketone
104	(Z)-linaloolbide(l)uranoid	monoterpenoid	alcohol
105	(Z)-linaloolbide(l)uranoid	monoterpenoid	alcohol
106	4-methyl-3-penten-2-one	monoterpenoid	ketone
107	6-methyl-5-hepten-2-one	monoterpenoid	ketone
108	epoxy oxaisophorone	monoterpenoid	ketone
109	geranylacetate	monoterpenoid	ketone
110	(E)-DMNT	sesquiterpenoid	hydrocarbon
111	(Z)-DMNT	sesquiterpenoid	hydrocarbon
112	7-epi-silphiperfol-5-ene	sesquiterpenoid	hydrocarbon
113	7-silphiperfol-5-ene	sesquiterpenoid	hydrocarbon
114	α-cadinene	sesquiterpenoid	hydrocarbon
115	α-cedrene	sesquiterpenoid	hydrocarbon
116	α-copaene	sesquiterpenoid	hydrocarbon
117	α-cubebene	sesquiterpenoid	hydrocarbon
118	(E,E)-α-farnesene	sesquiterpenoid	hydrocarbon
119	α-humulene	sesquiterpenoid	hydrocarbon
120	α-muurolene	sesquiterpenoid	hydrocarbon
121	β-bourbonene	sesquiterpenoid	hydrocarbon
122	β-cedrene	sesquiterpenoid	hydrocarbon
123	β-chamigrene	sesquiterpenoid	hydrocarbon
124	β-copaene	sesquiterpenoid	hydrocarbon
125	β-elemene	sesquiterpenoid	hydrocarbon
126	(E)-α-bergamotene	sesquiterpenoid	hydrocarbon
127	bicyclogermaene	sesquiterpenoid	hydrocarbon
128	bourbonene	sesquiterpenoid	hydrocarbon
129	β-selinene	sesquiterpenoid	hydrocarbon
130	β-sesquiphellandrene	sesquiterpenoid	hydrocarbon
131	γ-ylangene	sesquiterpenoid	hydrocarbon
132	C15H24-119,105,79	sesquiterpenoid	hydrocarbon
133	caryophyllenebide(l)	sesquiterpenoid	alcohol
134	caryophyllenebide(l)	sesquiterpenoid	alcohol
135	δ-cadinene	sesquiterpenoid	hydrocarbon
136	(E,E)-α-farnesene	sesquiterpenoid	hydrocarbon
137	(E)-α-bergamotene	sesquiterpenoid	hydrocarbon
138	(E)-β-caryophyllene	sesquiterpenoid	hydrocarbon
139	(E)-β-farnesene	sesquiterpenoid	hydrocarbon
140	germacreneB	sesquiterpenoid	hydrocarbon
141	germacreneD	sesquiterpenoid	hydrocarbon
142	longicyclene	sesquiterpenoid	hydrocarbon
143	longifolene	sesquiterpenoid	hydrocarbon
144	nerolidol	sesquiterpenoid	alcohol
145	thujopsene	sesquiterpenoid	hydrocarbon
146	unidentified sesquiterpene hydrocarbon	sesquiterpenoid	hydrocarbon
147	(Z,E)-α-farnesene	sesquiterpenoid	hydrocarbon
148	(Z,Z)-β-farnesene	sesquiterpenoid	hydrocarbon
149	(Z)-α-bergamotene	sesquiterpenoid	hydrocarbon
150	(Z)-β-farnesene	sesquiterpenoid	hydrocarbon

Fig. S2-1 Biosynthetic similarity of volatile organic compounds. Tree is based on Sørensen distances between compounds regarding the number of shared enzymes involved in their biosynthesis. Small Sørensen distances indicate a large proportion of shared enzymes required in the biosynthesis of the compounds whereas large Sørensen distances indicate few or no shared enzymes. Major pathways are colour coded: shikimate pathway (red), MEP pathway (green), mevalonate pathway (purple), leucine and isoleucine biosynthesis (blue), and lipoxygenase (LOX) pathway (black).

