

Table S1. Identification of volatile constituents in *Rosa* samples.

No.	Compounds	¹ tR ^a (min)	² tR ^b (sec)	CAS	Chemical formula	DMF ^c	RMF ^d	RI _{exp} ^e	RI _{lit} ^f
1	Acetoin	4.09	1.44	513-86-0	C ₄ H ₈ O ₂	848	902	-	690
2	6-Methyl-3,4-dihydro-2H-pyran	4.78	1.47	16015-11-5	C ₆ H ₁₀ O	899	841	-	-
3	1,3-Butanediol	4.99	2.07	107-88-0	C ₄ H ₁₀ O ₂	804	807	-	805
4	Hexanal	5.19	1.71	66-25-1	C ₆ H ₁₂ O	883	932	-	776
5	2-Hexenal	6.29	2.25	505-57-7	C ₆ H ₁₀ O	850	863	-	835
6	(<i>Z</i>)-3-Hexen-1-ol	6.49	1.88	928-96-1	C ₆ H ₁₂ O	811	818	-	839
7	1-Hexanol	6.58	1.82	111-27-3	C ₆ H ₁₄ O	827	828	-	854
8	Styrene	7.18	2.47	100-42-5	C ₈ H ₈	809	935	-	878
9	3-Methylcyclopentyl acetate	7.28	2.08	24070-70-0	C ₈ H ₁₄ O ₂	789	873	901	-
10	Hexanoic acid, methyl ester	7.88	2.08	106-70-7	C ₇ H ₁₄ O ₂	858	871	924	907
11	(<i>E</i>)-3-Hexenoic acid, methyl ester	8.09	2.37	13894-61-6	C ₇ H ₁₂ O ₂	879	853	932	920
12	Benzaldehyde	8.98	3.99	100-52-7	C ₇ H ₆ O	887	888	967	933
13	(<i>E</i>)-2-Hexenoic acid, methyl ester	8.99	2.59	13894-63-8	C ₇ H ₁₂ O ₂	858	836	966	948
14	Hexanal dimethyl acetal	9.29	1.88	1599-47-9	C ₈ H ₁₈ O ₂	814	932	977	964
15	Alpha-Myrcene	9.38	1.81	1686-30-2	C ₁₀ H ₁₆	841	845	981	-
16	6-Methyl-5-hepten-2-one	9.58	2.66	110-93-0	C ₈ H ₁₄ O	834	867	989	964
17	S-sulcatol	9.68	2.26	1569-60-4	C ₈ H ₁₆ O	855	816	993	974
18	beta-Myrcene	9.68	1.85	123-35-3	C ₁₀ H ₁₆	839	847	993	983
19	alpha-Methoxytoluene	9.69	3.16	538-86-3	C ₈ H ₁₀ O	886	901	994	973
20	(<i>E,Z</i>)-2,4-Heptadienal	9.99	3.13	4315-03-5	C ₇ H ₁₀ O	786	819	1005	982
21	alpha-Phellandrene	10.08	2.05	99-83-2	C ₁₀ H ₁₆	845	866	1008	998
22	(<i>Z</i>)-hex-4-enyl acetate	10.09	2.44	42125-17-7	C ₈ H ₁₄ O ₂	892	911	1008	1000
23	<i>E</i> -2-hexenyl acetate	10.29	2.51	2497-18-9	C ₈ H ₁₄ O ₂	874	924	1015	995
24	(+)-4-Carene	10.38	2.07	29050-33-7	C ₁₀ H ₁₆	870	879	1018	998
25	2-methyl-3-methylidenecyclopentane-1-carbaldehyde	10.39	3.20	826337-64-8	C ₈ H ₁₂ O	785	788	1019	-
26	<i>p</i> -Cymene	10.69	2.40	99-87-6	C ₁₀ H ₁₄	832	865	1029	1014
27	<i>D</i> -Limonene	10.79	2.09	138-86-3	C ₁₀ H ₁₆	837	878	1033	1023
28	Benzyl alcohol	10.98	4.21	100-51-6	C ₇ H ₈ O	871	878	1041	1012
29	Benzeneacetaldehyde	11.18	4.60	122-78-1	C ₈ H ₈ O	871	884	1048	1011
30	trans-Ocimen	11.29	2.05	13877-91-3	C ₁₀ H ₁₆	852	865	1050	1038
31	Gamma-terpinene	11.58	2.27	99-85-4	C ₁₀ H ₁₆	869	883	1061	1050
32	Linalool oxide	11.99	2.50	5989-33-3	C ₁₀ H ₁₈ O ₂	850	856	1076	1064
33	(<i>E,E</i>)-3,5-Octadien-2-one	11.99	3.32	30086-02-3	C ₈ H ₁₂ O	819	873	1076	1068
34	4-Isopropenyltoluene	12.48	3.00	1195-32-0	C ₁₀ H ₁₂	837	876	1094	1074
35	trans-Linalool oxide	12.49	2.60	34995-77-2	C ₁₀ H ₁₈ O ₂	827	847	1094	1074
36	Terpinolene	12.49	2.34	586-62-9	C ₁₀ H ₁₆	877	883	1093	1079
37	Linalool	12.68	2.44	78-70-6	C ₁₀ H ₁₈ O	863	864	1101	1086
38	Nonanal	12.88	2.48	124-19-6	C ₉ H ₁₈ O	866	867	1108	1083
39	trans-Rose oxide	13.08	2.49	5258-11-7	C ₁₀ H ₁₈ O	872	916	1115	1115
40	Phenylethyl alcohol	13.28	4.41	60-12-8	C ₈ H ₁₀ O	898	901	1120	1088
41	Octanoic acid, methyl ester	13.38	2.35	111-11-5	C ₉ H ₁₈ O ₂	780	892	1126	1108

42	Rose oxide	13.59	2.61	16409-43-1	C ₁₀ H ₁₈ O	795	887	1133	1102
43	(4 <i>E</i> ,6 <i>Z</i>)-allo-Ocimene	13.59	2.28	7216-56-0	C ₁₀ H ₁₆	820	829	1133	1131
44	(-)-trans-Pinocarveol	13.59	3.12	547-61-5	C ₁₀ H ₁₆ O	857	820	1133	1126
45	<i>p</i> -Mentha-1,5,8-triene	13.69	2.53	21195-59-5	C ₁₀ H ₁₄	856	819	1136	1104
46	1,4-Dimethoxybenzene	14.09	4.83	150-78-7	C ₈ H ₁₀ O ₂	772	784	1152	1132
47	Isopinocarveol	14.28	3.22	6712-79-4	C ₁₀ H ₁₆ O	855	792	1158	1176
48	Dill ether	14.39	3.16	74410-10-9	C ₁₀ H ₁₆ O	815	876	1162	1171
49	2-Nonenal	14.48	2.88	18829-56-6	C ₉ H ₁₆ O	837	878	1165	1135
50	Benzyl acetate	14.69	3.24	140-11-4	C ₉ H ₁₀ O ₂	887	887	1173	1151
51	trans-Linalool 3,7-oxide	14.89	3.18	39028-58-5	C ₁₀ H ₁₈ O ₂	821	851	1180	1164
52	Isoneral	15.08	3.04	72203-97-5	C ₁₀ H ₁₆ O	830	864	1187	1151
53	Alpha-Terpineol	15.38	3.17	98-55-5	C ₁₀ H ₁₈ O	850	861	1197	1175
54	Decanal	15.68	2.57	112-31-2	C ₁₀ H ₂₀ O	857	859	1208	1185
55	Cumaldehyde	15.68	3.08	122-03-2	C ₁₀ H ₁₂ O	801	875	1208	1215
56	Benzylacetone	15.69	3.12	2550-26-7	C ₁₀ H ₁₂ O	843	824	1208	1217
57	7-methyl-3-methylene-6-Octen-1-ol	16.09	2.93	13066-51-8	C ₁₀ H ₁₈ O	843	881	1222	-
58	Eucarvone	16.18	3.89	503-93-5	C ₁₀ H ₁₄ O	782	834	1226	-
59	Nonanoic acid, methyl ester	16.18	2.40	1731-84-6	C ₁₀ H ₂₀ O ₂	835	848	1226	1208
60	Levoverbenone	16.19	3.68	1196-01-6	C ₁₀ H ₁₄ O	850	888	1226	1197
61	Alpha-Citronellol	16.29	2.66	6812-78-8	C ₁₀ H ₂₀ O	838	850	1229	1212
62	cis-Geraniol	16.38	3.01	106-25-2	C ₁₀ H ₁₈ O	869	869	1233	1213
63	Citronellol	16.38	2.65	106-22-9	C ₁₀ H ₂₀ O	854	856	1233	1211
64	Nerol	16.39	2.91	106-25-2	C ₁₀ H ₁₈ O	862	862	1233	1213
65	cis-Citral	16.68	3.38	5392-40-5	C ₁₀ H ₁₆ O	828	855	1244	1241
66	Neral	16.69	3.41	106-26-3	C ₁₀ H ₁₆ O	877	879	1244	1218
67	Isogeraniol	16.78	3.03	5944-20-7	C ₁₀ H ₁₈ O	840	855	1247	1237
68	1,3-Di-tert-butylbenzene	17.08	2.39	1014-60-4	C ₁₄ H ₂₂	898	922	1258	1247
69	Geraniol	17.08	2.99	106-24-1	C ₁₀ H ₁₈ O	843	843	1258	1237
70	2-Phenylethyl acetate	17.19	4.26	103-45-7	C ₁₀ H ₁₂ O ₂	899	907	1262	1228
71	Pulegone	17.28	3.66	89-82-7	C ₁₀ H ₁₆ O	854	766	1266	1249
72	alpha-Citral	17.48	3.47	141-27-5	C ₁₀ H ₁₆ O	867	867	1273	1249
73	3,5-Dimethoxytoluene	17.49	4.33	4179-19-5	C ₉ H ₁₂ O ₂	906	929	1273	1256
74	2-Phenyl-2-butenal	17.69	5.23	4411-89-6	C ₁₀ H ₁₀ O	896	908	1281	1266
75	Geranyl formate	18.38	2.85	105-86-2	C ₁₁ H ₁₈ O ₂	843	847	1305	1282
76	Theaspirane	18.39	2.76	36431-72-8	C ₁₃ H ₂₂ O	857	870	1305	1288
77	Methyl geranoate	18.99	3.00	1189-09-9	C ₁₁ H ₁₈ O ₂	857	894	1328	1302
78	Decanoic acid, methyl ester	18.99	2.36	110-42-9	C ₁₁ H ₂₂ O ₂	853	881	1327	1308
79	Citronellol acetate	19.68	2.53	150-84-5	C ₁₂ H ₂₀ O ₂	871	872	1354	1335
80	alpha-Cubebene	19.69	2.20	17699-14-8	C ₁₅ H ₂₄	874	893	1354	1351
81	Nerol acetate	19.98	2.86	141-12-8	C ₁₂ H ₂₀ O ₂	882	884	1366	1343
82	Megastigma-4,6(<i>Z</i>),8(<i>E</i>)-triene	19.09	2.75	51468-85-0	C ₁₃ H ₂₀	826	847	1332	1340
83	3-Methoxyphenethyl alcohol	20.19	5.33	5020-41-7	C ₉ H ₁₂ O ₂	820	860	1376	1345
84	(<i>E</i>)-2-Butyl-2-octenal	20.28	2.54	13019-16-4	C ₁₂ H ₂₂ O	838	901	1378	1363
85	1,3-Pentanediol,2,2,4-trimethyl-,1-isobutyrate	20.29	2.95	77-68-9	C ₁₂ H ₂₄ O ₃	772	879	1378	1365
86	alpha-Copaene	20.39	2.36	3856-25-5	C ₁₅ H ₂₄	875	879	1381	1376

87	Geranyl acetate	20.48	2.92	105-87-3	C ₁₂ H ₂₀ O ₂	878	883	1386	1361
88	beta-Cubebene	20.79	2.44	13744-15-5	C ₁₅ H ₂₄	844	877	1397	1385
89	Ethyl geranate	20.79	2.97	32659-21-5	C ₁₂ H ₂₀ O ₂	811	852	1397	-
90	Isoeugenol	20.99	4.64	5912-86-7	C ₁₀ H ₁₂ O ₂	897	903	1406	1381
91	Methyleugenol	21.08	4.54	93-15-2	C ₁₁ H ₁₄ O ₂	871	889	1410	1372
92	1,3,5-Trimethoxybenzene	21.18	5.36	621-23-8	C ₉ H ₁₂ O ₃	870	874	1415	1385
93	alpha-Gurjunene	21.29	2.53	489-40-7	C ₁₅ H ₂₄	812	838	1417	1406
94	beta-Caryophyllene	21.58	2.68	87-44-5	C ₁₅ H ₂₄	890	892	1430	1419
95	beta-Copaene	21.79	2.61	18252-44-3	C ₁₅ H ₂₄	881	882	1438	1426
96	Tetrahydroionone	22.09	3.05	60761-23-1	C ₁₃ H ₂₄ O	801	813	1451	1427
97	(+)-epi-Bicyclosesquiphellandrene	22.19	2.73	54274-73-6	C ₁₅ H ₂₄	851	858	1455	-
98	Geranylacetone	22.28	3.02	3796-70-1	C ₁₃ H ₂₂ O	868	881	1459	1429
99	Calarene	22.59	2.80	17334-55-3	C ₁₅ H ₂₄	841	859	1472	1450
100	gamma-Muurolene	22.99	2.72	30021-74-0	C ₁₅ H ₂₄	881	883	1488	1472
101	Germacrene D	23.09	2.87	23986-74-5	C ₁₅ H ₂₄	874	885	1493	1477
102	beta-Ionone	23.09	3.58	79-77-6	C ₁₃ H ₂₀ O	874	874	1493	1466
103	Isohomogenol	23.49	4.78	93-16-3	C ₁₁ H ₁₄ O ₂	835	887	1511	1487
104	alpha-Muurolene	23.49	2.81	10208-80-7	C ₁₅ H ₂₄	871	872	1509	1494
105	Butylated Hydroxytoluene	23.79	3.14	128-37-0	C ₁₅ H ₂₄ O	862	863	1522	1494
106	gamma-Cadinene	23.89	2.94	39029-41-9	C ₁₅ H ₂₄	869	870	1526	1507
107	Methyl laurate	23.99	2.38	111-82-0	C ₁₃ H ₂₆ O ₂	859	862	1530	1508
108	Calamenene	24.08	3.33	483-77-2	C ₁₅ H ₂₂	882	889	1535	1510
109	beta-Cadinene	24.09	2.87	523-47-7	C ₁₅ H ₂₄	846	846	1534	1522
110	alpha-Cubebene	24.29	3.03	29837-12-5	C ₁₅ H ₂₄	840	898	1543	1525
111	alpha-Cadinene	24.39	2.97	24406-05-1	C ₁₅ H ₂₄	818	892	1547	1528
112	alpha-Calacorene	24.59	3.61	21391-99-1	C ₁₅ H ₂₀	885	906	1556	1531
113	alpha-Corocalene	26.39	3.98	20129-39-9	C ₁₅ H ₂₀	850	868	1632	1607
114	gamma-Eudesmol	26.58	3.60	1209-71-8	C ₁₅ H ₂₆ O	875	878	1641	1618
115	Cedrelanol	26.79	3.60	5397-11-1	C ₁₅ H ₂₆ O	858	873	1649	1627
116	alpha-Cadinol	26.89	3.53	481-34-5	C ₁₅ H ₂₆ O	818	826	1654	1642
117	beta-Eudesmol	27.08	3.81	473-15-4	C ₁₅ H ₂₆ O	857	864	1662	1636
118	alpha-Eudesmol	27.18	3.66	473-16-5	C ₁₅ H ₂₆ O	878	887	1667	1643
119	Cadalene	27.59	4.38	483-78-3	C ₁₅ H ₁₈	894	894	1685	1654
120	Methyl tetradecanoate	28.59	2.39	124-10-7	C ₁₅ H ₃₀ O ₂	830	850	1729	1708
121	Isobutyl phthalate	31.59	4.47	84-69-5	C ₁₆ H ₂₂ O ₄	879	883	1874	1850
122	Dibutyl phthalate	33.48	4.73	84-74-2	C ₁₆ H ₂₂ O ₄	899	901	1971	1924

NOTE:

^a ¹t_R: retention times of 1D.

^b ²t_R: retention times of 2D.

^c DMF: direct match factor—similarity of the deconvoluted mass spectra of unknowns to those in the NIST mass spectral library.

^d RMF: reverse match factor—a reverse search matching factor between the library and deconvoluted mass spectra of unknown.

^e RI_{exp}: experimental retention index.

^f RI_{lit}: retention index of the literature.