

Supplementary:

Analysis of Volatile Compounds in Pears by HS-SPME-GC×GC-TOFMS

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Table S1. The peak numbers of different classes obtained using 4 SPME fibres.

	50/30 μm		65 μm	
	DVB/CAR/PDMS	85 μm PA	PDMS/PVB	100 μm PDMS
Esters	67	49	62	46
Alkenes	19	3	27	12
Alkanes	19	4	17	14
Arenes	20	2	15	0
Aldehydes	9	6	10	2
Ketones	5	2	4	4
Alcohols	9	7	7	4
Others	15	8	4	2
Total	163	81	146	84

Table S2. Concentrations of volatile compounds in pear cultivars.

No.	Volatile compounds	¹ R.T. (s)	² RI	Longyuanyang li (ng/g)	Packham (ng/g)	D Jules (ng/g)	Clapp (ng/g)	Stark (ng/g)
Esters								
(101)								
1	Methyl acetate	102, 0.630	500.4	³ 16.22±0.56	19.70±3.48	13.97±5.44	13.85±10.19	14.30±0.32
2	Ethyl Acetate	132, 0.810	605.1	66.94±11.81	10.81±5.74	58.90±22.34	48.3±0.79	39.44±41.09
3	Methyl propionate	138, 0.760	614.6	1.55±0.14	⁴ -	-	-	-
4	Ethyl propanoate	198, 0.900	705.3	16.64±5.85	-	-	-	-
5	n-Propyl acetate	201, 0.920	707.9	111.27±3.60	2.87±1.91	95.40±19.72	24.73±1.23	59.64±0.42
6	Methyl butanoate	210, 0.930	715.6	11.59±1.77	0.35±0.13	-	-	0.08±0.02
7	Ethyl-2-methylproanoate	255, 0.930	754.0	0.94±0.70	-	-	-	-
8	Methyl (E)-2-butenate	261, 1.120	759.4	0.69±0.08	-	-	-	-
9	Methyl 2-butenate	264, 1.110	761.9	-	-	-	-	0.03±0.01
10	2-Methylpropyl acetate	273, 0.970	769.4	8.43±0.61	0.46±0.29	5.48±0.75	3.66±0.17	3.64±0.30
11	Methyl 2-methylbutanoate	279, 0.980	774.6	2.62±0.27	0.49±0.03	0.26±0.04	0.50±0.09	0.35±0.08
12	Ethyl butyrate	312, 1.080	802.0	36.37±6.88	-	-	-	-
13	Butyl acetate	330, 1.130	812.7	75.90±53.77	54.69±15.25	17.46±21.05	39.93±9.65	8.90±4.98

14	Methyl valerate	348, 1.100	823.4	0.73±0.08	-	-	-	-
15	Ethyl (Z)-2-butenolate	381, 1.250	843.1	3.66±0.22	-	-	-	-
16	Ethyl 2-methylbutyrate	390, 1.080	848.3	18.01±4.15	0.05±0.01	0.12±0.05	0.13±0.04	-
17	2-Methyl-1-butyl acetate	441, 1.130	878.8	60.23±2.89	-	8.21±1.02	5.19±0.39	4.32±0.33
18	3-Buten-1-ol, 3-methyl-, acetate	450, 1.200	884.2	0.07±0.01	-	-	-	0.19±0.12
19	Propyl butanoate	474, 1.140	898.4	1.50±0.02	-	-	-	-
20	Ethyl pentanoate	477, 1.160	900.2	0.83±0.11	-	-	-	-
21	Butyl propanoate	492, 1.160	908.4	0.08±0.01	-	0.37±0.08	0.36±0.08	0.26±0.02
22	Pentyl acetate	504, 1.190	915.0	68.9±4.11	7.08±5.82	24.91±7.19	21.47±3.87	21.54±2.02
23	Butyrolactone	513, 2.620	920.7	0.22±0.21	-	1.86±0.06	-	-
24	Methyl hexanoate	522, 1.230	924.8	80.75±13.36	1.02±0.27	0.53±0.12	0.61±0.07	1.25±0.17
25	Methyl (E)-3-hexenoate	537, 1.290	933.0	0.05±0.01	-	-	-	-
26	Methyl (Z)-3-hexenoate	543, 1.320	936.3	0.08±0.01	-	-	-	-
27	Ethyl tiglate	549, 1.310	939.6	0.19±0.02	-	-	-	-
28	Propyl 2-methylbutanoate	561, 1.130	946.1	0.55±0.12	-	-	-	-
29	Butyl 2-methylpropanoate	576, 1.120	954.3	-	-	-	0.18±0.04	0.06±0.01
30	2-Methylpropyl butyrate	579, 1.140	955.9	0.12±0.00	-	-	-	-
31	Methyl 2-hexenoate	597, 1.360	965.9	0.28±0.10	-	-	-	-
32	2-Methylpentyl acetate	624, 1.180	980.5	-	-	-	-	0.67±0.09
33	Vinyl caproate	633, 1.270	985.5	0.12±0.04	-	-	-	-
34	Butyl butyrate	654, 1.190	996.9	0.46±0.05	0.06±0.04	0.68±0.09	3.35±0.77	1.84±0.27
35	Ethyl hexanoate	660, 1.270	1000.2	37.76±1.82	-	0.06±0.01	0.08±0.02	0.12±0.02
36	Isobutyl 2-methylbutanoate	669, 1.100	1005.0	-	-	0.02±0.01	0.18±0.02	0.01±0.00
37	(Z)-3-Hexenol acetate	672, 1.280	1006.7	5.41±0.38	1.03±0.13	8.51±0.56	10.98±0.30	6.02±3.89
38	Ethyl (E)-3-hexenoate	681, 1.310	1011.5	0.74±0.05	-	-	-	-
39	Hexyl acetate	690, 1.370	1016.3	9.99±8.97	51.58±7.86	49.52±38.9	44.32±11.96	5.26±3.59
40	(Z)-2-Hexenyl acetate	693, 1.360	1018.0	3.65±2.01	11.46±6.36	2.66±2.61	11.99±0.98	16.84±2.18
41	Methyl 2,4-hexadienoate	693, 1.590	1018.1	0.28±0.08	-	-	-	-
42	(Z)-4-Hexen-1-ol acetate	702, 1.320	1024.4	-	-	0.74±0.07	0.85±0.07	0.56±0.03
43	Methyl heptanoate	708, 1.240	1026.0	1.31±0.18	0.05±0.01	-	0.15±0.02	0.24±0.02
44	Butyl 2-methylbutanoate	741, 1.160	1043.7	0.25±0.07	-	0.41±0.11	3.43±1.45	0.84±0.22
45	Ethyl 2-hexenoate	744, 1.380	1045.4	0.51±0.07	-	-	-	-
46	2-Methylbutyl butanoate	771, 1.180	1059.8	0.31±0.04	-	-	0.06±0.01	-
47	1-Hexanol, 4-methyl-, acetate	816, 1.220	1084.0	0.18±0.02	-	0.07±0.05	-	0.19±0.03
48	(E,E)-Ethyl 2,4-hexadienoate	834, 1.560	1093.9	0.32±0.05	-	-	-	-
49	Butyl pentanoate	834, 1.240	1093.7	-	-	-	0.10±0.01	-
50	Propyl hexanoate	837, 1.240	1095.3	0.96±0.21	-	0.03±0.00	-	0.10±0.00
51	Methyl benzoate	840, 1.850	1097.3	0.16±0.02	-	-	0.05±0.01	0.14±0.07
52	Ethyl heptanoate	843, 1.240	1098.6	1.17±0.12	-	-	-	-
53	Ethyl	849, 1.730	1102.2	0.12±0.02	-	-	-	-

	3-(methylsulfanyl)propanoate								
54	2-Methylbutyl 2-methylbutanoate	855, 1.160	1105.2	-	-	-	0.20±0.04	-	
55	3-Hepten-1-ol, acetate	855, 1.330	1105.2	-	-	-	-	0.22±0.04	
56	Hexyl propanoate	858, 1.230	1107.0	-	-	-	1.53±0.28	0.83±0.30	
57	Heptyl acetate	870, 1.260	1113.7	20.98±3.38	0.07±0.04	39.82±6.28	9.68±0.17	21.38±6.14	
58	methyl 4-octenoate	876, 1.350	1117.2	0.47±0.12	-	-	0.05±0.00	0.09±0.01	
59	Methyl octanoate	891, 1.280	1125.6	5.16±1.11	0.07±0.00	0.23±0.04	1.12±0.09	3.45±0.72	
60	3-(Methylthio)propyl acetate	891, 1.810	1125.9	0.27±0.03	-	0.48±0.02	-	-	
61	Methyl (Z)-3-octenoate	900, 1.380	1130.8	0.03±0.01	-	-	-	-	
62	Hexyl 2-methylpropionate	933, 1.180	1149.3	-	-	-	0.15±0.04	-	
63	2-Methylpropyl hexanoate	936, 1.200	1151.0	0.13±0.07	-	-	0.07±0.01	-	
64	3-Methylheptyl acetate	936, 1.200	1152.7	-	-	0.37±0.05	-	1.05±0.31	
65	Methyl (E)-2-octenoate	969, 1.420	1169.8	0.20±0.11	-	-	-	0.03±0.01	
66	Ethyl benzoate	975, 1.800	1173.4	0.07±0.00	-	-	-	-	
67	Methyl benzeneacetate	987, 2.000	1180.3	0.11±0.02	-	-	-	-	
68	Ethyl 3-(methylthio)-(E)-2-propenoate	990, 1.970	1181.9	0.08±0.00	-	-	-	-	
69	(Z)-3-Hexenyl butanoate	999, 1.320	1186.6	-	-	-	0.09±0.00	-	
70	(Z)-Ethyl 4-octenoate	1005, 1.350	1190.1	0.97±0.26	-	-	-	-	
71	Hexyl butanoate	1008, 1.260	1191.7	1.43±0.41	0.07±0.05	5.96±1.20	9.05±1.54	3.97±1.31	
72	Butanoic acid, 2-hexenyl ester, (Z)-	1014, 1.350	1195.1	-	-	-	0.49±0.00	0.32±0.13	
73	Ethyl octanoate	1020, 1.260	1198.5	8.26±2.05	-	0.09±0.01	0.24±0.05	0.43±0.15	
74	(Z)-3-Octen-1-ol acetate	1020, 1.330	1198.5	-	-	0.79±0.13	-	0.11±0.01	
75	Cyclohexylethyl acetate	1038, 1.370	1209.2	0.87±0.17	-	13.44±5.08	1.32±0.09	3.72±0.74	
76	Octyl acetate	1044, 1.270	1212.7	1.04±0.33	-	23.94±10.88	5.24±1.18	14.46±5.34	
77	Methyl nonanoate	1065, 1.280	1225.2	-	-	-	0.05±0.02	-	
78	Hexyl 2-methylbutanoate	1086, 1.210	1237.6	0.42±0.15	0.03±0.00	0.21±0.03	0.55±0.12	0.21±0.08	
79	Hexyl 2-methyl-2-propenoate	1095, 1.410	1243.1	-	-	-	0.02±0.00	0.04±0.01	
80	Ethyl (E)-2-octenoate	1101, 1.410	1246.7	1.42±0.39	-	-	-	-	
81	trans, trans-Octa-2,4-dienyl acetate	1101, 1.500	1246.7	-	-	0.25±0.05	0.18±0.01	0.27±0.12	
82	Ethyl benzeneacetate	1101, 1.910	1247.0	0.32±0.03	-	-	-	-	
83	2-Methylbutyl hexanoate	1113, 1.240	1253.7	0.16±0.04	-	0.03±0.00	0.11±0.01	0.03±0.01	
84	2-Phenethyl acetate	1122, 1.900	1259.5	0.39±0.08	-	0.18±0.01	-	0.02±0.01	
85	Hexyl n-valerate	1173, 1.260	1289.5	-	-	0.05±0.01	0.27±0.23	0.08±0.02	
86	Propyl octanoate	1179, 1.260	1293.0	-	-	-	-	0.06±0.03	
87	Methyl (Z)-4-decenoate	1206, 1.370	1309.9	0.04±0.01	0.04±0.03	-	0.01±0.00	0.02±0.01	

88	Methyl decanoate	1230, 1.290	1325.2	0.12±0.03	0.10±0.08	0.23±0.07	0.09±0.01	0.19±0.08
89	6-Octen-1-ol, 3,7-dimethyl-, acetate	1275, 1.340	1354.1	-	-	0.14±0.01	-	-
90	Butyl benzoate	1311, 1.750	1377.4	-	-	-	0.01±0.00	-
91	Hexyl hexoate	1326, 1.270	1386.7	0.25±0.08	-	1.63±0.32	8.13±3.39	2.55±1.55
92	Ethyl decanoate	1341, 1.270	1396.3	0.11±0.03	-	-	-	-
93	Methyl (E,Z)-2,4-decadienoate	1344, 1.510	1398.4	0.09±0.02	0.53±0.32	-	-	-
94	Decyl acetate	1365, 1.270	1412.2	-	-	0.37±0.12	-	-
95	Ethyl (E,Z)-2,4-decadienoate	1452, 1.490	1470.3	0.12±0.04	0.05±0.05	-	-	-
96	Methyl dodecanoate	1533, 1.290	1525.7	-	-	0.22±0.08	0.15±0.03	0.34±0.16
97	Hexyl octylate	1614, 1.280	1583.2	-	-	-	0.11±0.05	0.05±0.02
98	Methyl (6E)-6-nonenoate	1770, 1.380	1698.0	-	-	0.09±0.03	-	-
99	Methyl tetradecanoate	1806, 1.300	1726.4	0.03±0.01	-	0.09±0.03	-	0.13±0.05
100	Methyl hexadecanoate	2052, 1.110	1933.5	0.04±0.01	-	0.12±0.05	0.16±0.06	0.12±0.05
101	Methyl (Z)-9-octadecenoate	2181, 0.840	2063.8	0.03±0.02	-	0.04±0.03	0.02±0.01	0.03±0.03
	Subtotal			692.72	162.66	378.94	273.54	241.03
Alkenes								
(30)								
102	1,4-Pentadiene	108, 0.580	522.4	-	0.23±0.05	-	0.17±0.03	0.14±0.02
103	(Z),(Z)-2,4-Hexadiene	144, 0.660	623.9	-	0.28±0.11	-	-	-
104	1-Methyl-1,4-cyclohexadiene	255, 0.880	754.0	-	-	0.28±0.12	-	0.08±0.01
105	Styrene	459, 1.370	891.4	0.46±0.03	-	0.29±0.06	0.06±0.02	0.08±0.01
106	β-myrcene	645, 1.060	991.9	0.02±0.00	-	-	-	-
107	L-Limonene	714, 1.140	1030.8	0.31±0.03	-	-	-	-
108	1-Propenylbenzene	729, 1.550	1037.5	0.13±0.01	-	-	-	-
109	(Z)-β-ocimene	753, 1.130	1050.1	-	-	0.03±0.00	-	-
110	1-Ethenyl-3-ethylbenzene	822, 1.460	1087.4	0.06±0.02	-	0.24±0.08	0.05±0.01	-
111	1-Ethenyl-4-ethylbenzene	834, 1.480	1093.8	0.17±0.09	-	0.26±0.04	0.06±0.00	0.07±0.01
112	1,3-Diethenylbenzene	873, 1.610	1115.6	-	-	0.07±0.02	-	-
113	1,4-Diethenyl benzene	894, 1.660	1127.5	0.02±0.00	-	0.06±0.01	-	-
114	(Z)-3-Tetradecene	1176, 1.010	1291.1	-	-	0.04±0.01	-	-
115	α-Cubenene	1275, 1.180	1354.0	-	0.01±0.00	-	0.09±0.03	-
116	Copaene	1320, 1.240	1382.8	-	0.39±0.05	0.26±0.02	-	0.05±0.02
117	1-Tetradecene	1335, 1.040	1396.2	-	-	0.06±0.03	-	-
118	Aromandendrene	1368, 1.370	1414.2	0.07±0.02	-	-	0.03±0.00	-
119	(5Z)-2,6,10-Trimethyl-1,5,9-undecatrien	1431, 1.170	1456.1	-	-	0.14±0.03	-	-
120	(E)-β-Farnesene	1437, 1.240	1460.1	0.34±0.03	-	0.39±0.06	0.11±0.01	0.10±0.05
121	α-Humulene	1440, 1.410	1462.3	-	0.02±0.00	-	0.04±0.01	-
122	2,3,5,8-Tetramethyl-1,5,9-de	1446, 1.190	1466.1	0.16±0.03	-	0.27±0.10	-	-

	catriene							
123	(Z,E)- α -Farnesene	1494, 1.290	1498.2	3.64 \pm 1.41	-	5.50 \pm 0.96	0.73 \pm 0.04	1.02 \pm 0.28
124	α -Muurolene	1506, 1.400	1506.7	-	0.07 \pm 0.00	0.02 \pm 0.00	-	-
125	α -Farnesene	1518, 1.350	1512.9	15.78 \pm 12.87	0.04 \pm 0.03	15.07 \pm 3.89	15.10 \pm 2.94	17.47 \pm 2.99
126	(Z,Z)- α -Farnesene	1539, 1.290	1530.0	1.18 \pm 0.70	-	0.23 \pm 0.03	0.08 \pm 0.07	0.09 \pm 0.06
127	(+)- δ -Cadinene	1539, 1.420	1530.1	-	0.10 \pm 0.00	0.16 \pm 0.02	0.15 \pm 0.05	0.04 \pm 0.02
128	cis-Calamenene	1539, 1.570	1530.1	-	0.02 \pm 0.00	-	-	-
129	α -Calacorene	1569, 1.670	1551.5	-	0.01 \pm 0.00	0.03 \pm 0.00	-	-
130	(E)- γ -Bisabolene	1578, 1.340	1557.7	0.55 \pm 0.21	-	0.36 \pm 0.05	0.08 \pm 0.01	0.07 \pm 0.00
131	(Z)- γ -Bisabolene	1602, 1.360	1574.7	0.64 \pm 0.25	-	0.37 \pm 0.04	0.10 \pm 0.01	0.09 \pm 0.02
	Subtotal			23.53	1.17	24.13	16.85	19.3
Alkanes								
	(12)							
132	Undecane	846, 0.890	1100.0	0.06 \pm 0.02	0.05 \pm 0.01	0.78 \pm 0.18	0.04 \pm 0.01	0.06 \pm 0.00
133	Dodecane	1023, 0.930	1200.0	0.17 \pm 0.04	-	0.19 \pm 0.04	0.05 \pm 0.00	0.06 \pm 0.01
134	2-Methyldodecane	1131, 0.930	1264.3	0.07 \pm 0.02	-	0.04 \pm 0.01	-	-
135	Tridecane	1191, 0.960	1300.0	0.91 \pm 0.26	0.05 \pm 0.01	0.55 \pm 0.17	0.15 \pm 0.04	0.16 \pm 0.02
136	2-Methyltridecane	1290, 0.960	1363.4	0.24 \pm 0.07	-	0.12 \pm 0.02	-	-
137	3-Methyltridecane	1302, 0.970	1371.1	0.24 \pm 0.06	-	0.12 \pm 0.03	0.03 \pm 0.01	0.03 \pm 0.00
138	Tetradecane	1347, 0.980	1400.0	1.87 \pm 0.67	0.17 \pm 0.04	1.54 \pm 0.22	0.58 \pm 0.17	0.43 \pm 0.13
139	3-Methyltetradecane	1455, 0.990	1472.0	0.16 \pm 0.04	-	-	-	-
140	Pentadecane	1497, 1.000	1500.0	0.88 \pm 0.32	0.13 \pm 0.07	1.91 \pm 0.55	0.33 \pm 0.03	0.36 \pm 0.08
141	2-Methylpentadecane	1587, 0.990	1563.8	0.16 \pm 0.06	-	-	0.05 \pm 0.00	-
142	Hexadecane	1638, 1.010	1600.0	0.65 \pm 0.21	0.06 \pm 0.03	0.81 \pm 0.20	0.22 \pm 0.02	0.19 \pm 0.06
143	Heptadecane	1773, 1.020	1700.0	0.12 \pm 0.05	-	0.15 \pm 0.04	0.05 \pm 0.01	0.11 \pm 0.02
	Subtotal			5.53	0.46	6.21	1.5	1.4
Arenes								
	(19)							
144	Benzene	165, 0.800	657.4	-	-	0.28 \pm 0.12	-	-
145	Toluene	285, 0.990	761.8	0.85 \pm 0.15	0.35 \pm 0.35	0.76 \pm 0.11	0.40 \pm 0.03	0.36 \pm 0.04
146	Ethylbenzene	408, 1.190	859.2	0.87 \pm 0.04	-	-	0.05 \pm 0.02	0.06 \pm 0.01
147	p-Xylene	420, 1.200	866.3	10.74 \pm 3.68	0.30 \pm 0.20	8.22 \pm 0.28	2.99 \pm 0.33	2.77 \pm 0.61
148	1,3-Dimethylbenzene	462, 1.270	891.3	4.11 \pm 0.36	-	-	0.06 \pm 0.02	0.04 \pm 0.03
149	o-Xylene	468, 1.100	894.8	0.27 \pm 0.20	-	-	0.06 \pm 0.02	-
150	1-Ethyl-4-methylbenzene	591, 1.270	962.5	0.54 \pm 0.23	-	0.35 \pm 0.03	0.17 \pm 0.05	0.10 \pm 0.02
151	3-Ethyl-1-methylbenzene	603, 1.250	969.1	0.23 \pm 0.05	-	0.28 \pm 0.02	-	-
152	1,2,4-Trimethylbenzene	648, 1.330	993.7	0.30 \pm 0.01	-	0.10 \pm 0.02	-	-
153	1,2,3-Trimethylbenzene	705, 1.410	1024.5	0.60 \pm 0.06	-	-	-	-
154	p-Cymene	708, 1.280	1026.0	0.15 \pm 0.02	-	-	-	-
155	1-Methyl-3-propylbenzene	756, 1.300	1051.8	0.11 \pm 0.00	-	-	-	-
156	1-Methyl-2-propylbenzene	771, 1.320	1059.9	0.08 \pm 0.01	-	-	-	-
157	1,2-Dimethyl-4-ethylbenzene	819, 1.370	1085.7	0.08 \pm 0.03	-	-	-	-

158	1,2,3,4-Tetramethylbenzene	882, 1.440	1120.6	0.06±0.02	-	-	-	-
159	Naphthalene	996, 2.030	1185.4	0.58±0.09	-	0.34±0.06	0.22±0.03	0.21±0.03
160	2-Methylnaphthalene	1185, 2.000	1297.0	0.12±0.02	-	0.10±0.02	0.04±0.00	0.04±0.01
161	1-Methylnaphthalene	1212, 2.080	1314.2	0.05±0.01	-	0.04±0.01	0.01±0.00	0.02±0.01
162	1-(1,5-Dimethylhexyl)-4-methylbenzene	1422, 1.320	1452.0	0.09±0.02	-	-	0.03±0.00	-
	Subtotal			19.83	0.65	10.47	4.03	3.6

Aldehydes

(28)								
163	Acetaldehyde	78, 2.100	417.2	23.71±8.76	5.01±2.71	4.81±1.91	13.10±3.36	10.19±5.33
164	Butanal	120, 0.720	567.3	0.52±0.05	0.23±0.05	1.58±1.23	0.52±0.13	0.38±0.06
165	(E)-2-Butenal	159, 0.910	648.1	-	-	0.60±0.71	-	-
166	Pentanal	192, 0.910	700.2	-	0.14±0.02	0.09±0.03	0.21±0.02	-
167	(E)-2-Methyl-2-butenal	237, 1.120	738.8	0.28±0.10	-	-	-	-
168	3-Methyl-2-butenal	291, 1.340	787.7	0.04±0.01	-	0.07±0.01	0.03±0.01	-
169	Hexanal	309, 1.160	800.2	12.46±8.42	5.63±0.77	2.07±0.16	2.68±0.48	2.78±0.05
170	3-Hexenal	312, 1.150	802.0	-	-	-	0.10±0.05	0.17±0.02
171	(Z)-2-hexenal	384, 1.310	846.7	-	-	-	0.06±0.01	1.98±2.57
172	(E)-2-Hexenal	393, 1.370	850.4	6.27±2.56	5.27±0.90	1.60±0.07	4.84±2.07	2.73±1.88
173	Heptanal	480, 1.240	901.9	-	0.03±0.01	0.07±0.01	0.08±0.02	0.04±0.01
174	(E,E)-2,4-Hexadienal	495, 1.630	910.3	0.10±0.02	0.13±0.01	-	0.06±0.00	0.10±0.02
175	(E)-2-Heptenal	579, 1.420	957.7	0.03±0.01	-	0.23±0.01	0.21±0.02	0.13±0.05
176	Benzaldehyde	588, 1.910	961.2	0.29±0.04	0.04±0.01	0.25±0.10	0.08±0.00	0.08±0.01
177	Octanal	666, 1.290	1003.5	0.27±0.13	0.04±0.01	0.34±0.15	0.24±0.12	-
178	(Z)-2-Octenal	717, 1.180	1030.8	0.38±0.25	-	0.44±0.06	0.64±0.05	0.37±0.03
179	Benzeneacetaldehyde	744, 2.040	1045.8	0.10±0.01	-	-	-	-
180	(E)-2-Octenal	768, 1.450	1058.4	0.13±0.03	0.03±0.01	0.61±0.05	0.43±0.05	0.31±0.12
181	Nonanal	855, 1.310	1105.3	-	0.07±0.00	-	1.14±0.55	-
182	(E,Z)-2,6-Nonadienal	942, 1.560	1154.6	-	-	-	0.05±0.01	-
183	(E)-2-Nonenal	954, 1.450	1161.3	-	0.06±0.02	0.88±0.18	1.10±0.80	0.53±0.28
184	cis-4-Decenal	1014, 1.410	1195.2	-	-	0.08±0.03	0.04±0.00	-
185	Decanal	1032, 1.330	1205.6	0.05±0.01	0.02±0.00	0.09±0.02	0.04±0.00	0.04±0.01
186	(E,E)-2,4-Nonadienal	1047, 1.630	1214.7	-	-	0.10±0.01	0.09±0.01	0.08±0.04
187	4-Methoxybenzaldehyde	1119, 2.420	1258.0	-	-	-	0.02±0.00	0.05±0.01
188	(Z)-2-Decenal	1128, 1.450	1262.8	-	-	0.02±0.00	0.01±0.00	-
189	Citral	1143, 1.630	1271.8	-	-	0.05±0.01	-	-
190	2,4-Decadienal	1182, 1.550	1295.0	-	-	0.24±0.04	0.13±0.01	0.10±0.06
	Subtotal			44.63	16.7	14.22	25.90	20.06

Ketones

(8)								
191	Acetone	102, 0.600	500.3	-	0.29±0.02	1.35±1.02	-	1.12±0.99
192	Methyl vinyl ketone	120, 0.740	567.3	0.61±0.28	-	-	-	-
193	3-Octanone	636, 1.270	987.1	0.29±0.19	-	0.34±0.02	0.35±0.04	0.13±0.02

194	6-Methyl-5-heptene-2-one	639, 1.380	988.8	0.44±0.30	0.07±0.02	1.48±0.14	0.19±0.22	0.80±0.08
195	Acetophenone	786, 2.040	1068.4	0.13±0.01	-	0.20±0.02	-	-
196	(E)-4-Phenylbut-3-en-2-one	1200, 2.150	1306.5	-	-	0.03±0.00	-	-
197	(E)-6,10-dimethyl-5,9-undecadien-2-one	1431, 1.500	1456.3	-	-	0.59±0.03	0.11±0.02	0.36±0.13
198	4,4-Dimethyl-3-phenyl-2,5-cyclohexadien-1-one	1614, 1.830	1583.5	0.10±0.03	-	-	0.03±0.00	-
	Subtotal			1.57	0.36	3.99	0.68	2.41
Alcohols								
(20)								
199	Ethanol	90, 0.600	456.0	26.06±10.27	12.34±1.25	27.35±8.83	24.15±7.38	16.15±5.27
200	1-Propanol	108, 0.670	522.7	0.42±0.19	-	0.55±0.03	0.27±0.04	0.29±0.05
201	2-Methylpropanol	144, 0.750	624.1	-	-	-	0.18±0.03	-
202	1-Butanol	159, 0.820	648.0	2.66±0.25	1.50±0.54	8.80±1.02	10.20±0.94	5.55±0.50
203	2-Methylbutanol	234, 0.920	731.0	4.06±0.44	0.03±0.01	0.44±0.07	0.61±0.04	0.21±0.04
204	1-Pentanol	270, 0.990	766.9	-	0.11±0.03	0.43±0.12	0.38±0.04	0.19±0.03
205	1-Hexanol	420, 1.180	866.3	9.84±7.29	11.26±2.67	26.97±4.90	14.30±1.13	13.31±2.54
206	trans-2-Hexen-1-ol	420, 1.210	866.3	-	0.50±0.09	-	-	-
207	1-Heptanol	606, 1.200	970.7	0.16±0.02	0.02±0.00	0.25±0.04	0.17±0.01	0.13±0.03
208	2-Ethylhexanol	717, 1.190	1030.8	-	0.06±0.03	-	-	-
209	1-Octanol	792, 1.260	1071.2	0.57±0.18	-	0.99±0.38	0.44±0.04	0.43±0.13
210	2-Nonanol	846, 1.200	1100.2	-	0.08±0.02	0.19±0.05	-	-
211	Linalool	846, 1.260	1100.2	-	-	0.05±0.00	-	-
212	(E)-2-Nonen-1-ol	969, 1.340	1171.4	-	-	-	0.08±0.01	-
213	1-Nonanol	972, 1.290	1169.7	-	-	0.25±0.08	0.23±0.06	-
214	3,4,5-Trimethyl-4-heptanol	1044, 1.380	1212.7	0.90±0.21	-	-	-	-
215	Citronellol	1071, 1.370	1228.8	-	-	0.08±0.03	0.09±0.03	0.06±0.01
216	(Z)-4-Decen-1-ol	1119, 1.380	1257.4	-	-	0.03±0.01	-	-
217	1-Decanol	1143, 1.290	1271.6	-	-	0.05±0.00	-	-
218	2,3-Dihydrofarnesol	1764, 1.460	1693.6	-	-	-	0.09±0.02	0.07±0.02
	Subtotal			44.67	25.90	66.43	51.19	36.39
Others								
(23)								
219	Dimethyl sulfide	108, 0.600	522.4	-	0.19±0.04	-	0.53±0.51	0.23±0.08
220	2,3-Dihydrofuran	120, 0.640	567.2	0.04±0.01	0.03±0.01	-	0.10±0.01	0.16±0.04
221	Acetic acid	123, 0.690	578.2	-	-	-	0.06±0.01	0.07±0.00
222	2-Methylfuran	132, 0.690	609.7	0.48±0.50	-	0.65±0.22	-	0.11±0.04
223	Thioacetic acid	213, 0.680	718.0	1.40±0.13	-	-	-	-
224	Anisole	507, 1.550	918.4	0.02±0.00	-	0.05±0.01	0.03±0.00	0.03±0.01
225	Benzonitrile	633, 2.050	987.5	0.23±0.02	-	0.38±0.08	-	-
226	Phenol	639, 1.610	993.8	0.07±0.01	-	0.10±0.03	-	0.04±0.00
227	2-Pentylfuran	645, 1.160	993.6	0.26±0.04	0.33±0.07	4.86±0.32	4.45±0.88	2.61±0.39
228	1-Methoxy-4-methylbenzen	702, 1.580	1023.0	-	-	0.06±0.01	0.03±0.00	0.05±0.02

e

229	Eucalyptol	720, 1.230	1032.4	0.89±0.49	-	-	-	-
230	1-Methoxymethyl-2-methyl benzene	831, 1.640	1092.3	-	-	0.05±0.00	-	-
231	(Z)-Rose oxide	867, 1.290	1112.1	-	-	-	0.06±0.01	0.03±0.00
232	(E)-Rose oxide	897, 1.310	1129.0	-	-	-	0.05±0.00	-
233	β-Citronellol, methyl ether	984, 1.140	1178.1	-	-	-	0.11±0.01	0.06±0.02
234	Estragole	1023, 1.730	1200.5	2.03±0.45	-	0.41±0.20	0.02±0.00	0.07±0.02
235	(Z)-1-Methoxy-4-(prop-1-en-1-yl)benzene	1116, 1.810	1255.9	0.02±0.00	-	-	-	-
236	Anethole	1170, 1.870	1288.0	0.11±0.01	-	0.03±0.02	0.02±0.00	0.02±0.00
237	(E)-3-Octenoic acid	1320, 1.350	1382.9	-	-	-	0.11±0.01	0.08±0.02
238	Methyleugenol	1359, 1.990	1408.7	0.09±0.02	-	0.66±0.16	-	-
239	(Z)-1,2-Dimethoxy-4-(prop-1-en-1-yl)benzene	1497, 2.100	1500.8	-	-	0.05±0.02	-	-
240	Sesquirosefuran	1578, 1.440	1557.7	-	-	0.09±0.01	0.06±0.00	0.05±0.03
241	(E)-3-(4,8-Dimethylnona-3,7-dien-1-yl)furan	1605, 1.420	1576.9	-	-	0.09±0.03	0.40±0.04	0.22±0.04
	Subtotal			5.64	0.55	7.48	6.03	3.83
	Total			838.12	208.45	511.87	379.72	328.02

¹R.T. refers to the retention time. ²RI refers to the calculated retention index. ³Data are means±SD of three replications. ⁴"-" represents no data.

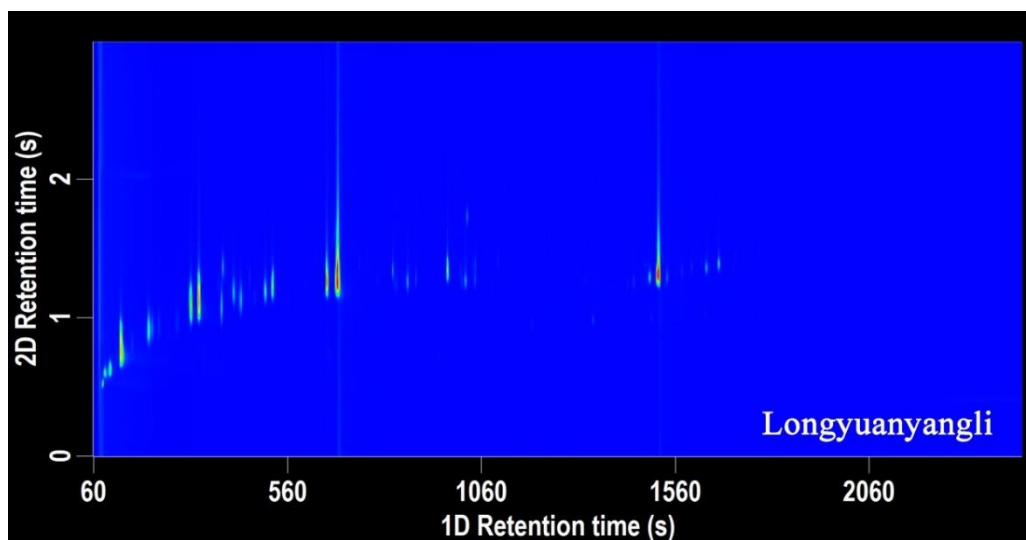


Figure S1. 2D chromatogram (total ion chromatography) of Longyuanyangli.

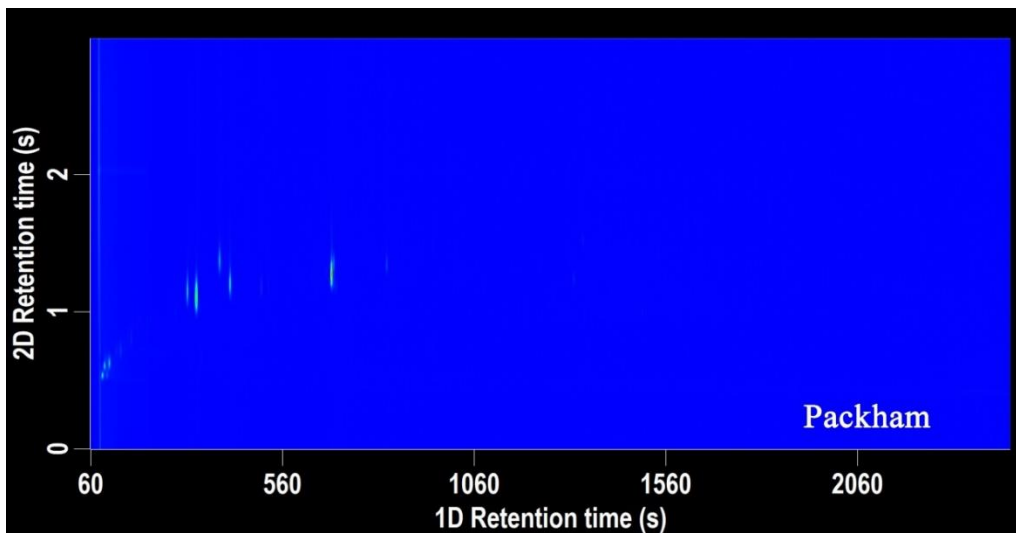


Figure S2. 2D chromatogram (total ion chromatography) of Packham.

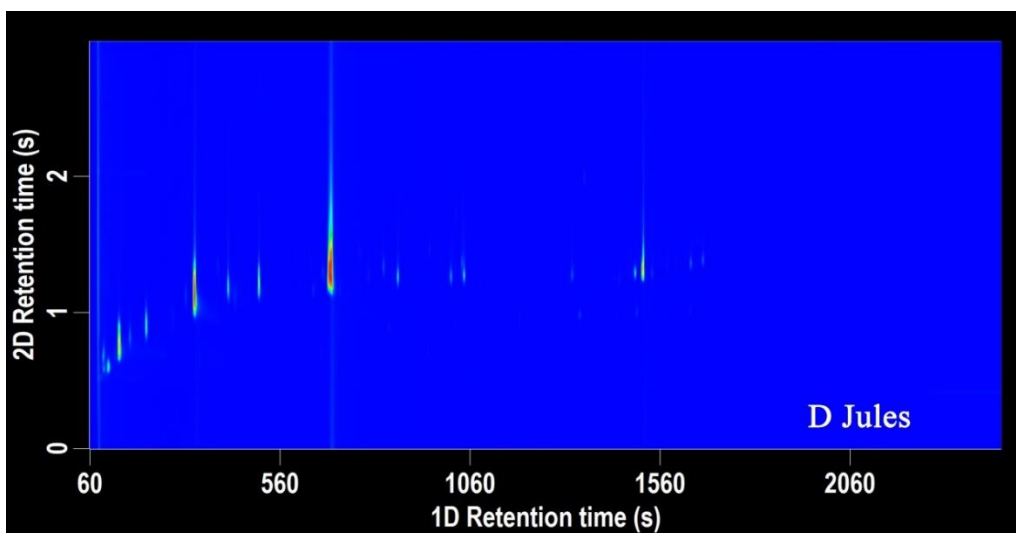


Figure S3. 2D chromatogram (total ion chromatography) of D Jules.

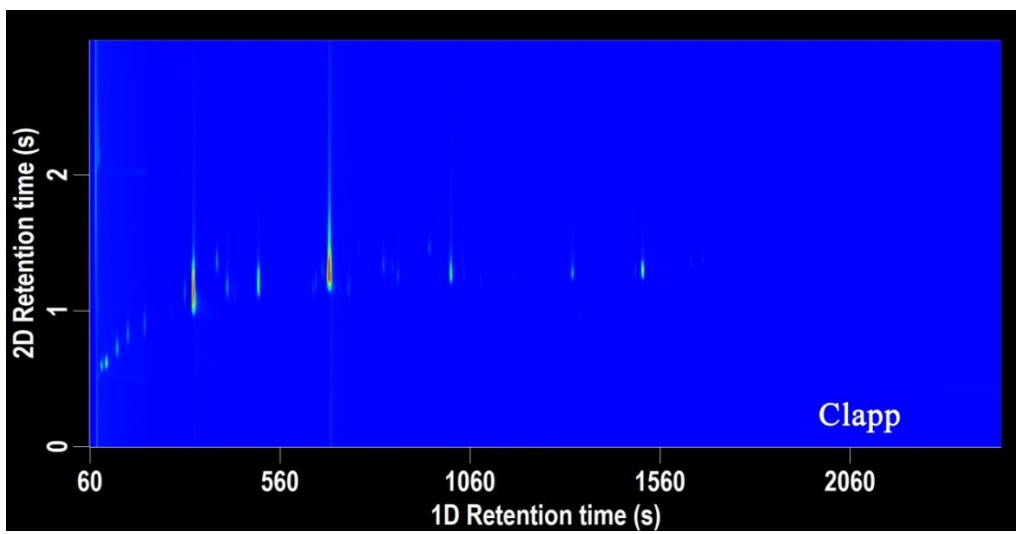


Figure S4. 2D chromatogram (total ion chromatography) of Clapp.

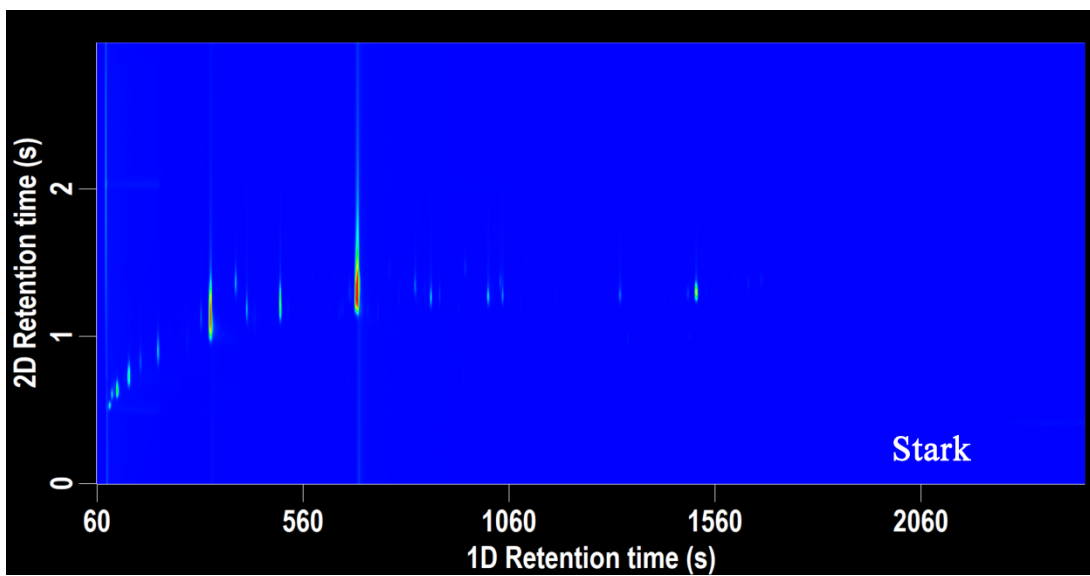


Figure S5. 2D chromatogram (total ion chromatography) of Stark.