

Table S1-1. The flavors detected by HS-SPME-GC-MS (0-16C-L)

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
0-00-0	43,55,91,93,119,145,178	178	1297	1186	Bicyclo[3.1.1]hept-3-ene, 4,6,6-trimethyl-2-vinyloxy-	0.0003	—
0-00-0	27,41,55,83,110,137,166,179,208,250,253,282	282	1986	1989	cis-10-Heptadecenoic acid, methyl ester	0.0005	0.01154
1003-38-9	29,56,85,100	100	711	791	Furan, tetrahydro-2,5-dimethyl-	0.0004	—
100-52-7	39,51,77,106	106	982	964	Benzaldehyde	0.0020	—
104-76-7	29,57,70,98,112	130	995	1014	2-ethyl hexanol	0.0030	0.4288
106-42-3	27,51,77,91	106	907	877	p-Xylene	0.0013	—
107-87-9	27,43,86,87	86	654	677	2-Pentanone	0.0006	—
108-64-5	29,57,85,88,115	130	820	849	Butanoic acid, 3-methyl-, ethyl ester	0.0013	0.0912
108-88-3	39,65,91	92	794	779	Toluene	0.0009	1.5920
109-08-0	26,40,67,94	94	781	801	Pyrazine, methyl-	0.0008	—
110-93-0	27,43,69,108,126	126	938	969	5-Hepten-2-one, 6-methyl-	0.0009	—
111-13-7	27,43,71,95,128	128	952	971	2-Octanone	0.0023	0.1376
111-61-5	27,43,55,88,115,143,157,185,213,241,267,283,312	313	2177	2182	Ethyl stearate	0.0049	0.0775
111-62-6	27,43,55,97,123,137,154,180,222,246,264,284,310	310	2185	2165	Ethyl Oleate	0.0018	0.3299
1120-21-4	29,57,71,85,113,156	156	1115	1099	Undecane	0.0003	—
112-31-2	29,43,70,95,112,138	156	1204	1206	Decanal	0.0040	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
112-54-9	29,41,82,96,110,140	184	1402	1409	Dodecanal	0.0025	—
112-63-0	27,41,67,81,109,150,164,178,220,234,263,294	294	2093	2090	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	0.0015	0.0142
116-53-0	29,57,74,87	102	811	847	Butanoic acid, 2-methyl-	0.0021	1.0929
122-78-1	39,65,91,118,120	120	1081	1059	Benzeneacetaldehyde	0.0014	—
123-51-3	31,55,70,87	88	697	719	1-Butanol, 3-methyl-	0.0114	—
123-86-4	29,43,73,87,115	116	785	796	Acetic acid, butyl ester	0.0052	0.6710
123-92-2	27,43,70,87,115	130	820	836	1-Butanol, 3-methyl-, acetate	0.0003	—
123-96-6	29,45,70,97,115	130	979	973	2-Octanol	0.1225	0.1225
124-10-7	29,55,74,87,129,143,171,199,211,242	242	1680	1704	Methyl tetradecanoate	0.0003	0.0165
124-19-6	29,57,70,98,114,142	142	1104	1104	Nonanal	0.0017	—
137-32-6	29,57,70,87	88	697	723	1-Butanol, 2-methyl-	0.0046	—
142-91-6	43,60,83,102,129,157,185,213,239,256,283,298	298	2013	2025	Isopropyl palmitate	0.0008	—
1565-80-6	29,41,70,87	88	697	663	1-Butanol, 2-methyl-, (S)-	0.0020	—
1632-16-2	27,55,70,112,113	112	784	790	Heptane, 3-methylene-	0.0008	—
20734-29-6	29,41,57,99,128,156	156	1103	1110	2,2-Dimethylheptane-3,5-dione	0.0042	0.0606
2777-58-4	27,41,55,84,110,137,166,180,222,235,264,296	296	2085	2096	6-Octadecenoic acid, methyl ester, (Z)-	0.0021	0.1026
3391-86-4	29,57,72,99,127	128	969	964	1-Octen-3-ol	0.0005	—
431-03-8	15,43,86	86	691	<600	2,3-Butanedione	0.0053	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
513-86-0	45,55,88	88	717	717	Acetoin	0.0316	—
54340-85-1	15,39,77,91,130,145,160	160	1326	1331	Benzene, 1-(2-butenyl)-2,3-dimethyl-	0.0007	—
544-35-4	27,41,67,95,123,150,164,213,220,263,308	308	2193	2107	Linoleic acid ethyl ester	0.0062	0.7132
544-76-3	29,57,71,99,113,141,169,197,226	226	1612	1600	Hexadecane	0.0004	—
558-30-5	27,41,72	72	483	<600	Isobutylene epoxide	0.0016	—
565-69-5	29,57,71,100	100	690	689	3-Pentanone, 2-methyl-	0.0006	—
590-86-3	29,44,71,86	86	643	648	Butanal, 3-methyl-	0.0025	—
5989-27-5	27,41,68,93,136,138	136	1018	1012	D-Limonene	0.0026	—
61142-07-2	39,51,91,106	106	827	859	Cyclopentene, 1-ethenyl-3-methylene-	0.0018	—
623-42-7	27,43,74,87	102	686	723	Methyl butyrate	0.0004	—
628-97-7	27,43,55,88,115,157,158,199,213,239,284	284	1978	1979	Hexadecanoic acid, ethyl ester	0.0060	0.0407
628-97-7	27,43,55,88,115,157,158,199,213,239,284	284	1978	1979	Hexadecanoic acid, ethyl ester	0.0028	—
629-94-7	27,43,57,85,113,141,169,197,211,239,267,296	296	2109	2101	Heneicosane	0.0004	—
64-17-5	31,45	46	463	<600	Ethanol	0.0089	—
66-25-1	27,44,72,87	100	806	802	Hexanal	0.0032	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
7452-79-1	29,57,85,102,115	130	820	837	Butanoic acid, 2-methyl-, ethyl ester	0.0009	—
763-32-6	31,41,68,87	86	728	737	3-Buten-1-ol, 3-methyl-	0.0008	—
78-83-1	31,43,74	74	597	622	1-Propanol, 2-methyl-	0.0023	—
84-69-5	29,57,76,104,121,149, 167,205,223,263,278	278	1908	1850	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	0.0005	0.0084
84-74-2	29,41,76,104,121,149, 167,205,223,278	278	2037	1998	Dibutyl phthalate	0.0014	0.0202
98-01-1	29,39,67,96	96	831	835	Furfural	0.0020	—
116-09-6	31,43,74	74	698	721	2-Propanone, 1-hydroxy-	—	0.6871
123-32-0	27,42,81,108	108	894	916	Pyrazine, 2,5-dimethyl-	—	0.5956
104-62-1	29,65,91,104,122	150	1257	1248	Formic acid, 2-phenylethyl ester	—	0.2189
5308-25-8	28,42,72,99,114	114	1078	1109	N-Ethylpiperazine	—	0.0785
7491-74-9	28,41,70,98,125,142	142	1429	1443	Piracetam	—	0.9098
103-82-2	39,65,91,118,136	136	1249	1261	Benzeneacetic acid	—	1.0366
19780-33-7	43,57,71,97,125,168,196	214	1591	1624	2-Ethyl-1-dodecanol	—	0.4174
0-00-0	43,81,95,109,136,161, 197,212,236,254	254	1723	1755	10-Methyl-E-11-tridece-1-ol acetate	—	0.0654

RI^a:References retention indices from the NIST11 library

RI^b:Retention indices were calculated for the Rtx-5MS capillary column;

Table S1-2. The flavors detected by HS-SPME-GC-MS (0-28C-L)

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
0-00-0	41,55,91,105,133,161,189,204	204	1419	1424	Isoledene	0.0045	—
100-52-7	39,51,77,106	106	982	967	Benzaldehyde	0.0043	—
104-76-7	29,,57,70,98,112	130	995	1029	2-ethyl hexanol	0.0025	—
106-32-1	29,57,88,127,143,172	172	1183	1171	Octanoic acid, ethyl ester	0.0009	0.0415
107-87-9	27,43,86,87	86	654	665	2-Pentanone	0.0010	—
108-88-3	39,65,91	92	794	779	Toluene	0.0009	0.3114
110-93-0	27,43,69,108,126	126	938	970	5-Hepten-2-one, 6-methyl-	0.0012	—
111-11-5	29,43,74,87,127,158	158	1083	1112	Octanoic acid, methyl ester	0.0022	0.1597
111-13-7	27,43,71,95,128	128	952	971	2-Octanone	0.0009	—
111-61-5	27,43,55,88,115,143,157,185,213,241,267,283,312	313	2177	2182	Ethyl stearate	0.0026	0.0423
111-62-6	27,43,55,97,123,137,154,180,222,246,264,284,310	310	2185	2166	Ethyl Oleate	0.0014	0.1082
112-31-2	29,43,70,95,112,138	156	1204	1215	Decanal	0.0088	—
112-54-9	29,41,82,96,110,140	184	1402	1409	Dodecanal	0.0043	—
112-63-0	27,41,67,81,109,150,164,178,220,234,263,294	294	2093	2090	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	0.0044	0.0487

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
122-78-1	39,65,91,118,120	120	1081	1059	Benzeneacetaldehyde	0.0045	—
123-51-3	31,55,70,87	88	697	719	1-Butanol, 3-methyl-	0.0088	—
123-86-4	29,43,73,87,115	116	785	796	Acetic acid, butyl ester	0.0033	—
123-96-6	29,45,70,97,115	130	979	973	2-Octanol	0.1225	0.1225
124-10-7	29,55,74,87,129,143, 171,199,211,242	242	1680	1704	Methyl tetradecanoate	0.0009	0.0082
124-19-6	29,57,70,98,114,142	142	1104	1105	Nonanal	0.0023	—
13744-15-5	41,55,91,105,133,161, 189,204	204	1339	1370	(3aS,3bR,4S,7R,7aR)-7-methyl-3-methylidene-4-(propan-2-yl)octahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzene	0.0068	—
142-91-6	43,60,83,102,129,157, 185,213,239,256,283, 298	298	2013	2032	Isopropyl palmitate	0.0005	—
17699-14-8	41,55,81,105,119,161, 189,204	204	1344	1348	.alpha.-Cubebene	0.0063	—
19435-97-3	43,55,95,119,121,161, 189,204,222	222	1580	1625	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1R-(1.alpha.,4.beta.,4a.beta.,8a.beta.)]-	0.0043	—
21284-22-0	41,59,93,119,135,161, 189,204	222	1580	1610	Cubenol	0.0030	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
2777-58-4	27,41,55,84,110,137,166,180,222,235,264,296	296	2085	2097	6-Octadecenoic acid, methyl ester, (Z)-	0.0026	0.1827
30021-74-0	41,55,93,105,133,161,189,204	204	1435	1455	.gamma.-Muurolene	0.0010	—
431-03-8	15,43,86	86	691	<600	2,3-Butanedione	0.0024	—
481-34-5	43,79,95,121,137,161,189,204	222	1580	1637	.alpha.-Cadinol	0.0034	—
483-76-1	41,55,81,119,134,161,189,204	204	1469	1459	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	0.0029	—
515-13-9	41,68,81,107,121,147,189,204	204	1398	1439	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1.alpha.,2.beta.,4.beta.)]-	0.0051	—
544-35-4	27,41,67,95,123,150,164,213,220,263,308	308	2193	2107	Linoleic acid ethyl ester	0.0039	0.5767
552-02-3	43,69,81,109,122,161,189,204	222	1530	1608	1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.beta.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-	0.0034	—
556-52-5	31,44,73	74	653	<600	Glycidol	0.0011	—
558-30-5	27,41,72	72	483	<600	Isobutylene epoxide	0.0013	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
565-69-5	29,57,71,100	100	690	689	3-Pentanone, 2-methyl-	0.0008	—
58175-57-8	29,57,70,98,113	130	995	1026	2-Propyl-1-pentanol	0.0012	0.0260
590-86-3	29,44,71,86	86	643	638	Butanal, 3-methyl-	0.0040	—
5986-49-2	41,55,93,111,122,161,179,204,222	222	1530	1563	4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.beta.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-	0.0007	—
623-42-7	27,43,74,87	102	686	715	Butanoic acid, methyl ester	0.0005	—
628-97-7	27,43,55,88,115,157,158,199,213,239,284	284	1978	1979	Hexadecanoic acid, ethyl ester	0.0034	0.0123
628-97-7	27,43,55,88,115,157,158,199,213,239,284	284	1978	1979	Hexadecanoic acid, ethyl ester	0.0019	—
64-17-5	31,45	46	463	<600	Ethanol	0.0026	—
66-25-1	27,44,72,87	100	806	802	Hexanal	0.0070	—
7452-79-1	29,57,85,102,115	130	820	839	Butanoic acid, 2-methyl-, ethyl ester	0.0031	0.0106
78-83-1	31,43,74	74	597	616	1-Propanol, 2-methyl-	0.0017	—
84-66-2	29,50,76,105,121,149,177,194,222	222	1639	1605	Diethyl Phthalate	0.0046	0.4493
84-74-2	29,41,76,104,121,149,167,205,223,278	278	2037	1998	Dibutyl phthalate	0.0022	0.0398

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
868-57-5	29,57,85,88,116	116	721	765	Butanoic acid, 2-methyl-, methyl ester	0.0004	—
95-47-6	27,51,77,91	106	907	886	o-Xylene	0.0014	—
96-17-3	29,41,71,86	86	643	645	Butanal, 2-methyl-	0.0039	—
98-01-1	29,39,67,96	96	831	837	Furfural	0.0056	—
5077-67-8	29,57,69,88	88	798	846	1-Hydroxy-2-butanone	—	0.5767
123-32-0	27,42,81,108	108	894	933	Pyrazine, 2,5-dimethyl-	—	0.2139
104-62-1	29,65,91,104,122	150	1257	1193	Formic acid, 2-phenylethyl ester	—	0.0667
24621-61-2	31,45,72,89	90	824	905	1,3-Butanediol, (S)-	—	1.6976
4077-47-8	27,43,71,99,127,142	142	1058	1075	3(2H)-Furanone, 4-methoxy-2,5-dimethyl-	—	1.0127
7491-74-9	28,41,70,98,125,142	142	1429	1442	Piracetam	—	0.0311
13481-95-3	29,55,69,97,123,141, 180,194,222,246,264, 296	296	2085	2050	10-Octadecenoic acid, methyl ester	—	0.3950
877-95-2	30,65,72,104,120,163	163	1492	1527	Acetamide, N-(2-phenylethyl)-	—	0.2217
118452-32-7	43,73,83,111,139,156	156	1023	1043	Octan-2-one, 3,6-dimethyl-	—	0.5389

Table S1-3. The flavors detected by HS-SPME-GC-MS (12-28C-L)

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
1003-38-9	29,56,85,100	100	711	791	Furan, tetrahydro-2,5-dimethyl-	0.0023	—
100-52-7	39,51,77,106	106	982	966	Benzaldehyde	0.0015	—
104-76-7	29,,57,70,98,112	130	995	1029	1-Hexanol, 2-ethyl-	0.0030	0.3514
107-87-9	27,43,86,87	86	654	678	2-Pentanone	0.0012	—
108-88-3	39,65,91	92	794	773	Toluene	0.0007	0.9237
110-93-0	27,43,69,108,126	126	938	970	5-Hepten-2-one, 6-methyl-	0.0010	—
111-13-7	27,43,71,95,128	128	952	977	2-Octanone	0.0004	—
111-61-5	27,43,55,88,115,143,1 57,185,213,241,267,2 83,312	313	2177	2180	Ethyl stearate	0.0028	0.1546
111-62-6	27,43,55,97,123,137,1 54,180,222,246,264,2 84,310	310	2185	2166	Ethyl Oleate	0.0020	0.0995
111-71-7	29,41,70,96,114	114	905	906	Heptanal	0.0006	—
1120-21-4	29,57,71,85,113,156	156	1115	1099	Undecane	0.0002	—
112-39-0	27,43,74,87,115,143,1 71,185,227,239,270	270	1878	1915	Hexadecanoic acid, methyl ester	0.0005	0.0199
116-53-0	29,57,74,87	102	811	847	Butanoic acid, 2-methyl-	0.0198	1.2423
1192-62-7	15,39,67,95,110	110	878	899	Ethanone, 1-(2-furanyl)-	0.0040	0.0709
122-78-1	39,65,91,118,120	120	1081	1042	Benzeneacetaldehyde	0.0015	—
123-51-3	31,55,70,87	88	697	719	1-Butanol, 3-methyl-	0.0132	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
123-86-4	29,43,73,87,115	116	785	796	Acetic acid, butyl ester	0.0046	—
123-96-6	29,45,70,97,115	130	979	973	2-Octanol	0.1225	0.1225
124-19-6	29,57,70,98,114,142	142	1104	1105	Nonanal	0.0010	—
142-91-6	43,60,83,102,129,157, 185,213,239,256,283, 298	298	2013	2025	Isopropyl palmitate	0.0007	—
1632-16-2	27,55,70,112,113	112	784	790	Heptane, 3-methylene-	0.0011	—
18409-18-2	29,57,67,95,110,138	156	1266	1242	2-Decen-1-ol, (E)-	0.0008	—
3391-86-4	29,57,72,99,127	128	969	969	1-Octen-3-ol	0.0003	—
526-73-8	27,39,77,105,120	120	1020	1000	Benzene, 1,2,3-trimethyl-	0.0003	—
544-35-4	27,41,67,95,123,150,1 64,213,220,263,308	308	2193	2110	Linoleic acid ethyl ester	0.0047	0.1514
583-60-8	27,41,68,112,113	112	952	971	Cyclohexanone, 2-methyl-	0.0008	—
590-86-3	29,44,71,86	86	643	633	Butanal, 3-methyl-	0.0016	—
60-12-8	31,39,65,91,122	122	1136	1088	Phenylethyl Alcohol	0.0095	0.4267
60-33-3	27,41,67,81,110,137,1 68,182,210,237,264,2 80	280	2183	2146	9,12-Octadecadienoic acid (Z,Z)-	0.0008	0.0224
61142-07-2	39,51,91,106	106	827	856	Cyclopentene, 1-ethenyl-3-methylene-	0.0016	—
623-42-7	27,43,74,87	102	686	715	Butanoic acid, methyl ester	0.0005	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
628-97-7	27,43,55,88,115,157,158,199,213,239,284	284	1978	1979	Hexadecanoic acid, ethyl ester	0.0044	0.0110
64-17-5	31,45	46	463	<600	Ethanol	0.0033	—
66-25-1	27,44,72,87	100	806	804	Hexanal	0.0017	—
6754-66-1	41,55,91,105,133,161,176,203,218	218	1694	1712	5(1H)-Azulenone, 2,4,6,7,8,8a-hexahydro-3,8-dimethyl-4-(1-methylethylidene)-, (8S-cis)-	0.0016	—
689-67-8	43,69,93,107,125,151,194	194	1420	1451	5,9-Undecadien-2-one, 6,10-dimethyl-	0.0027	0.1726
71-36-3	31,56,73	74	662	655	1-Butanol	0.0023	—
7452-79-1	29,57,85,102,115	130	820	837	Butanoic acid, 2-methyl-, ethyl ester	0.0043	0.4410
78-83-1	31,43,74	74	597	622	1-Propanol, 2-methyl-	0.0043	—
78-84-2	27,43,72	72	543	<600	Propanal, 2-methyl-	0.0005	—
78-93-3	29,43,72	72	555	<600	2-Butanone	0.0008	—
84-66-2	29,50,76,105,121,149,177,194,222	222	1639	1605	Diethyl Phthalate	0.0040	0.3203
84-69-5	29,57,76,104,121,149,167,205,223,263,278	278	1908	1887	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	0.0004	0.0134
84-74-2	29,41,76,104,121,149,167,205,223,278	278	2037	1995	Dibutyl phthalate	0.0034	0.0275
868-57-5	29,57,85,88,116	116	721	765	Butanoic acid, 2-methyl-, methyl ester	0.0005	—

CAS	Qualitative ions	Molecular weight	RI ^a	RI ^b	Name	HS-SPME	Liquid-liquid extraction
						Content (mg/l)	Content (mg/l)
96-22-0	29,57,86,87	86	654	678	3-Pentanone	0.0009	—
98-01-1	29,39,67,96	96	831	804	Furfural	0.0030	—
109-08-0	26,40,67,94	94	781	812	Pyrazine, methyl-	—	0.4165
108-50-9	28,42,67,108	108	894	915	Pyrazine, 2,6-dimethyl-	—	0.1396
505-10-2	31,61,106	106	912	937	1-Propanol, 3-(methylthio)-	—	0.7826
10522-34-6	43,71,89,126,144,171,214	214	1417	1448	Propanoic acid, 2-methyl-, nonyl ester	—	0.1420
103-82-2	39,65,91,118,136	136	1249	1268	Benzeneacetic acid	—	0.6366
301-00-8	27,41,67,79,108,135,163,228,236,292	292	2101	2068	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	—	0.4634
0-00-0	43,81,95,109,136,161,197,212,236,254	254	1723	1752	10-Methyl-E-11-tridece-1-ol acetate	—	0.0101
118452-32-7	43,73,83,111,139,156	156	1023	1039	Octan-2-one, 3,6-dimethyl-	—	0.0538