

Supplementary Table S1 The information of volatile compounds identified by GC-IMS.

	Compounds	CAS	Formula	MW	RI	Rt [sec]	Dt [RIPrel]	Odor description
<i>Esters</i>								
1	acetic acid ethyl ester M	141786	C4H8O2	88.1	609.5	152.672	1.09799	Ethereal, fruity, sweet, weedy, green
2	acetic acid ethyl ester D	141786	C4H8O2	88.1	609.5	152.672	1.33578	Ethereal, fruity, sweet, weedy, green
3	2-furanmethanol acetate	623176	C7H8O3	140.1	994.1	577.889	1.41669	Estery, green, banana, peel, nasturtium
4	n-Propyl acetate	109604	C5H10O2	102.1	708.3	200.358	1.16115	
5	Butyl propanoate M	590012	C7H14O2	130.2	908.8	413.855	1.28688	
6	Butyl propanoate D	590012	C7H14O2	130.2	909.1	414.309	1.7168	
7	Propyl butanoate	105668	C7H14O2	130.2	896.3	394.106	1.26291	
8	2-methylpropyl butanoate	539902	C8H16O2	144.2	955.3	496.524	1.32975	
9	Butanoic acid, 3-methyl-, ethyl ester	108645	C7H14O2	130.2	856.5	340.814	1.25746	
10	Butyl formate	592847	C5H10O2	102.1	728.2	215.03	1.20574	
<i>Aldehydes</i>								
11	n-Nonanal	124196	C9H18O	142.2	1106.2	790.28	1.47424	Waxy, aldehydic, rose, fresh, orris, orange, peel, fatty, peely

12	(E)-2-Octenal	2548870	C8H14O	126.2	1066.4	707.8	1.33177	Fresh, cucumber, fatty, green, herbal, banana, waxy, leaf
13	(E,E)-2,4-Heptadienal	4313035	C7H10O	110.2	1022.2	626.31	1.19165	Fat, nut
14	n-Octanal	124130	C8H16O	128.2	1011.5	608.005	1.40253	Aldehydic, waxy, citrus, orange, peel, green, herbal, fresh, fatty
15	Benzaldehyde M	100527	C7H6O	106.1	962.8	511.154	1.14478	Bitter almond, burnt sugar, cherry, malt, roasted
16	Benzaldehyde D	100527	C7H6O	106.1	962.8	511.154	1.47052	Bitter almond, burnt sugar, cherry, malt, roasted
17	(E)-2-Heptenal M	18829555	C7H12O	112.2	957.7	501.096	1.25282	Pungent, green, vegetable, fresh, fatty
18	(E)-2-Heptenal D	18829555	C7H12O	112.2	958.4	502.467	1.66695	Pungent, green, vegetable, fresh, fatty
19	Heptanal M	111717	C7H14O	114.2	902.4	403.64	1.33331	Citrus, fat, green, nut
20	Heptanal D	111717	C7H14O	114.2	902.1	403.186	1.69133	Citrus, fat, green, nut

21	(E)-2-Pentenal M	1576870	C5H8O	84.1	752.6	234.437	1.1044	Pungent, green, fruity, apple, orange, tomato
22	(E)-2-Pentenal D	1576870	C5H8O	84.1	752.1	234.053	1.36164	Pungent, green, fruity, apple, orange, tomato
23	n-pentanal	110623	C5H10O	86.1	698.8	193.755	1.42247	Fermented, bready, fruity, nutty, berry
24	2-methyl Butanal	96173	C5H10O	86.1	661.1	174.192	1.40142	Musty, cocoa, phenolic, coffee, nutty, malty, fermented, fatty, alcoholic
25	3-Methyl butanal D	590863	C5H10O	86.1	646	167.589	1.41009	Ethereal, aldehydic, chocolate, peach, fatty
26	3-Methyl butanal M	590863	C5H10O	86.1	644.9	167.1	1.19088	Ethereal, aldehydic, chocolate, peach, fatty
27	Butanal	123728	C4H8O	72.1	597.5	148.025	1.28872	Pungent, cocoa, musty, green, malty, bready
28	1-hexanal	66251	C6H12O	100.2	796	273.729	1.55951	Apple, fat, fresh, green, oil
29	2-phenylacetaldehyde M	122781	C8H8O	120.2	1053.2	682.409	1.25251	
30	2-phenylacetaldehyde D	122781	C8H8O	120.2	1053.5	682.999	1.53557	

31	2-Hexenal M	505577	C6H10O	98.1	852	335.276	1.17693	
32	2-Hexenal D	505577	C6H10O	98.1	851.5	334.661	1.51327	
33	3-Methyl-2-butenal	107868	C5H8O	84.1	793.7	271.429	1.08791	
34	(E,E)-2,4-Hexadienal	142836	C6H8O	96.1	916.1	425.886	1.45165	Green, sweet, fruity, waxy, fatty
35	2-Methylpentanal	123159	C6H12O	100.2	752.7	234.535	1.22271	
	Alcohols							
36	1-Hexanol M	111273	C6H14O	102.2	869.9	357.736	1.32378	Ethereal, fusel oil, fruity, alcoholic, sweet, green
37	1-Hexanol D	111273	C6H14O	102.2	869.4	357.121	1.63998	Ethereal, fusel oil, fruity, alcoholic, sweet, green
38	1,8 Cineole	470826	C10H18O	154.3	1037.5	653.474	1.29356	Mint
39	1-Octen-3-ol M	3391864	C8H16O	128.2	984	555.5	1.1546	Mushroom
40	1-Octen-3-ol D	3391864	C8H16O	128.2	983.8	555.043	1.5982	Mushroom
41	1-Pentanol M	71410	C5H12O	88.1	763	243.254	1.25445	Fusel, sweet
42	1-Pentanol D	71410	C5H12O	88.1	763.4	243.637	1.51334	Fusel, sweet
43	2-Octanol	123966	C8H18O	130.2	984	555.5	1.43615	
44	(Z)-3-hexenol M	928961	C6H12O	100.2	857	341.43	1.23377	
45	(Z)-3-hexenol D	928961	C6H12O	100.2	857.2	341.651	1.50622	
46	2(5H)-Furanone, 3-hydroxy-4,5-dimethyl-	28664359	C6H8O3	128.1	1103.4	784.255	1.22246	
47	3-Methyl-3-buten-1-ol	763326	C5H10O	86.1	728.8	215.52	1.17106	
48	1-butanol 2-methyl	137326	C5H12O	88.1	729.5	216.009	1.23546	
	Ketones							

49	2-Heptanone M	110430	C7H14O	114.2	889.9	384.573	1.25991	Fruity, spicy, sweet, herbal, coconut, woody
50	2-Heptanone D	110430	C7H14O	114.2	890	384.8	1.62842	Fruity, spicy, sweet, herbal, coconut, woody
51	2-Pentanone	107879	C5H10O	86.1	686.6	185.93	1.37045	Sweet, fruity, ethereal, wine, banana, woody
52	2-Butanone	78933	C4H8O	72.1	594.2	146.803	1.24785	Fragrant, fruit, pleasant
53	2-Propanone	67641	C3H6O	58.1	515.9	120.147	1.11781	Solvent, ethereal, apple, pear
54	Cyclohexanone M	108941	C6H10O	98.1	895.4	392.744	1.15206	Mint, cool
55	Cyclohexanone D	108941	C6H10O	98.1	895.5	392.971	1.45765	Mint, cool
56	1-Penten-3-one	1629589	C5H8O	84.1	687.6	186.419	1.30605	Fish, green, mustard, pungent
57	2-Octanone M	111137	C8H16O	128.2	993.4	576.117	1.3346	Dairy, cheese
58	2-Octanone D	111137	C8H16O	128.2	994.3	578.359	1.75534	Dairy, cheese
59	2,3-Butanedione	431038	C4H6O2	86.1	582.3	142.401	1.16487	Creamy, buttery
60	2-Hexanone	591786	C6H12O	100.2	784	262.037	1.5018	
61	5-Hepten-2-one, 6-methyl-	110930	C8H14O	126.2	990.7	570.13	1.17752	
62	2-Cyclopenten-1-one, 3-methyl-	2758181	C6H8O	96.1	976	538.327	1.41227	
63	2-Cyclopenten-1-one, 2-methyl-	1120736	C6H8O	96.1	908.6	413.628	1.41121	

Acids

64	Hexanoic acid	142621	C6H12O2	116.2	993.1	575.527	1.30346	Sour, fatty, sweat, cheese
65	Acetic acid	64197	C2H4O2	60.1	623.1	158.052	1.05712	Sour
66	3-methylbutanoic acid M	503742	C5H10O2	102.1	838.2	318.969	1.2243	
67	3-methylbutanoic acid D	503742	C5H10O2	102.1	838	318.662	1.49076	
Terpenes								
68	β -ocimene	13877913	C10H16	136.2	1037.9	654.064	1.21855	Citrus, woody
69	camphene	79925	C10H16	136.2	956.5	498.81	1.21681	
ethers								
70	1,2-Dimethoxyethane D	110714	C4H10O2	90.1	653.9	171.012	1.30977	
71	1,2-Dimethoxyethane M	110714	C4H10O2	90.1	653.9	171.012	1.10914	
Lactone								
72	γ -Butyrolactone M	96480	C4H6O2	86.1	916.8	427.021	1.08315	Creamy, oily, fatty, caramel
73	γ -Butyrolactone D	96480	C4H6O2	86.1	916.1	425.886	1.29886	Creamy, oily, fatty, caramel
Others								
74	Linalool oxide M	60047178	C10H18O2	170.3	1077.5	730.039	1.26274	Musty, camphor, fenchyl, alcohol
75	Linalool oxide D	60047178	C10H18O2	170.3	1076.8	728.533	1.8066	Musty, camphor, fenchyl, alcohol
76	2-Pentyl furan	3777693	C9H14O	138.2	994.7	579.07	1.25251	Herbal, almond-like, nutty
77	2-Ethyl-6-methylpyrazine	13925036	C7H10N2	122.2	1003	593.833	1.20156	Roasted hazelnut
78	2-Pyridinamine	504290	C5H6N2	94.1	1001.5	591.471	1.34026	

Note: Odor descriptions were from FEMA database.

