

Table. Total aroma-active compounds identified in three samples and their relative concentration, threshold and r-OAV.

Aroma Compounds ^a	RI ^b	NIST RI ^c	Relative Concentration(µg/kg)						Perception ^d	Identificati on ^e	Threshold (wat er, mg/kg) ^f	r-OAV		
			LF		MF		HF					LF	MF	HF
			AVE	SD	AVE	SD	AVE	SD						
3,7,11-trimethyl-1,6,10-dodecatrien-3-ol	201	2034-P	986.9	68.5	929.1	70.0	770.3	39.7	floral	1D/2D/S	0.01-0.1	99	93	77
	3		3	6	1	2	8	6						
3,7-dimethyl-1,5,7-octatrien-3-ol	158	1613-P	748.4	26.6	432.6	18.6	217.5	10.8	mouldy	1D/2D/S	-	-	-	-
	0		6	2	9	7	9	6						
benzaldehyde	149	1520-P	434.4	13.8	462.4	22.1	495.1	18.6	almond	1D/2D/S	0.35	1	1	1
	9		1	8	4	4	8	7						
<i>(E,E)</i> -2,4-heptadienal	146	1495-P	391.2	83.5	338.8	14.8	48.92	9.65	fatty	1D/2D/S	0.057 (in air)	7	6	1
	8		7	7	3	5								
hexanoic acid (<i>Z</i>)-3-hexenyl ester	163	1645-P	330.6		303.8		407.8	68.4	fruity	1D/2D	-	-	-	-
	4		9	7.63	8	1.55	8	9						
<i>(E,E)</i> -3,5-octadien-2-one	154	1570-P	321.8		157.3		18.71	1.54	fruity green	1D/2D	-	-	-	-
	5		0	8.12	9	1.17								
linalool	151	1547-P	320.3	31.5	290.7	17.5	167.1	12.7	floral woody	1D/2D/S	0.0006	534	485	279
	8		7	0	6	5	2	8						
<i>(E)</i> -β-ionone	191	1940-P	270.0	12.5	226.2	13.2	214.0		floral woody	1D/2D/S	0.000007	3857	3231	3058
	2		3	8	3	1	8	9.79						
indole	240	2445-P	263.5		181.8	13.2			floral fecal	1D/2D/S	0.33 (in alcohol)	1	1	-
	2		2	8.04	7	4	92.68	4.46						
<i>cis</i> -5-ethenyltetrahydro-α,α,5-trimethyl-2-furanmethanol	142	1444-P	230.6	23.2	345.2	21.7	398.2	34.0	earthy floral	1D/2D/S	0.1	2	3	4
	2		8	3	2	5	5	2						
2,6,6-trimethyl-1-cyclohexene-1-carboxaldehyde	159	1611-P	219.1		229.1		283.0	48.2	tobacco fruity	1D/2D	0.003	73	76	94
	9		6	5.30	2	6.55	6	6						
furfural	143	1461-P	214.2	35.1	494.6	26.6	738.5		sweet bread	1D/2D/S	3	-	-	-
	7		4	4	6	6	7	7.32						
α-ionone	182	1840-P	202.6	10.3	195.4		181.5		sweet woody floral	1D/2D/S	0.0106	19	18	17
	7		6	2	4	8.68	1	0.96						
benzeneacetaldehyde	161	1640-P	185.3		195.8		185.9	13.7	floral honey	2D/S	0.0063	29	31	30
	3		2	8.25	8	8.09	1	8						
hexanal	105	1083-P	176.8	2.99	79.80	2.07	35.80	4.23	grassy	1D/2D/S	0.0024	74	33	15

	9		6												
(E)- β -farnesene	164	1664-P	175.2	13.6	156.7	3.64	149.8	25.5	woody herbal	1D/2D	-	-	-	-	
	5		8	5	8		5	8	sweet						
(E)-hexanoic acid 2-hexenyl ester	164	1662-P	160.8	7.28	137.8	1.73	219.6	58.4	green waxy	1D/2D	0.781-3.13	-	-	-	
	5		4		2		4	0							
geraniol	181	1847-P	153.8	3.13	124.5	0.47	53.64	2.24	sweet floral	1D/2D/S	0.0032	48	39	17	
	4		0		6				citrus						
phenylethyl alcohol	188	1906-P	146.7	7.79	150.5	17.1	136.6	14.3	floral	1D/2D/S	0.14	1	1	1	
	0		1		7	8	5	6							
nonanal	137	1391-P	112.4	3.00	90.94	1.57	60.30	13.0	waxy fatty	1D/2D/S	0.0058	19	16	10	
	0		5					9							
(E)-2-octenal	140	1429-P	90.59	1.00	82.18	0.75	28.40	3.27	cucumber green	1D/2D/S	0.003	30	27	9	
	7								leaf						
1-octanol	153	1557-P	85.08	7.21	65.11	1.20	73.87	8.86	waxy	1D/2D/S	0.1258	1	1	1	
	1														
5-methyl-2-furancarboxaldehyde	154	1570-P	77.38	5.95	292.8	14.9	591.4	17.4	spice caramel	1D/2D/S	0.5	-	1	1	
	5				3	9	8	8							
D-limonene	117	1201-P	68.20	11.3	141.5	29.9	357.7	99.1	citrus	1D/2D/S	0.034	2	4	11	
	5			3	4	8	0	9							
acetic acid 2-phenylethyl ester	178	1813-P	61.82	2.18	77.44	5.48	125.9	11.6	floral honey	1D/2D	0.25	-	-	1	
	7						0	3	fruity						
β -phenylethyl butyrate	193	1958-P	58.35	1.61	59.76	5.10	83.98	12.4	musty sweet	1D/2D	-	-	-	-	
	4							2	floral						
benzylalcohol	184	1870-P	50.27	2.14	58.35	5.82	50.17	5.50	floral rose	1D/2D/S	2.5	-	-	-	
	5														
acetophenone	162	1647-P	48.29	2.78	84.41	1.65	143.1	12.0	sweet pungent	1D/2D/S	0.065	1	1	2	
	5						6	6							
(E)-2-pentenal	110	1127-P	44.95	1.48	32.59	9.79	5.98	0.18	pungent fruity	1D/2D/S	0.31	-	-	-	
	8														
2-methylbutanal	895	914-P	41.84	6.67	50.58	1.76	31.85	3.75	cocoa coffee	1D/2D/S	0.001	42	51	32	
β -myrcene	113	1161-P	39.69	4.04	68.01	14.6	184.9	10.0	woody,	1D/2D/S	0.0012	33	57	154	
	8					5	5	9	vegetative, citrus						
3-octen-2-one	138	1411-P	38.32	2.69	-	-	-	-	sweet blueberry	1D/2D	0.0067	6	-	-	

	5														
(E)-2-nonenal	151 3	1534-P	34.79	1.98	46.46	0.23	61.91	12.1 2	fatty cucumber	1D/2D/S	0.00019	183	245	326	
(R)-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone	231 8	2331-P	34.26	9.07	31.51	4.50	34.03	1.70	musk coumarin	1D/2D	-	-	-	-	
(E,Z)-2,6-nonadienal	156 1	1584-P	33.89	0.48	26.87	5.07	25.41	1.58	fatty	1D/2D/S	0.0008	42	34	32	
octanal	126 7	1289-P	33.40	0.58	13.38	0.95	-	-	waxy fatty	1D/2D/S	0.000587	57	23	-	
3-nonen-2-one	148 9	1515-P	31.07	1.36	26.45	2.40	15.60	0.91	weedy spicy	1D/2D	0.8	-	-	-	
2-pentylfuran	120 6	1231-P	29.19	6.42	51.15	9.73	108.6 8	32.0 8	green earthy beany	1D/2D/S	0.0058	5	9	19	
1-(1H-pyrrol-2-yl)-ethanone	193 7	1973	28.44	3.51	47.06	6.60	51.40	7.33	musty nut	1D/2D	58.58	-	-	-	
pentanal	956	979-P	26.08	1.85	16.75	1.38	-	-	fermented	1D/2D/S	0.012	2	1	-	
(Z)-4-heptenal	121 8	1240-P	25.17	1.02	25.77	1.90	-	-	fatty green	2D/S	0.00006	419	430	-	
p-cymene	124 8	1272-P	24.18	2.87	70.56	18.4 3	212.9 0	71.8 4	fresh woody	1D/2D	0.00501	5	14	42	
(E,E)-2,4-hexadienal	137 7	1400-P	22.44	0.79	15.03	0.26	8.28	0.91	green spicy	1D/2D/S	0.0018 (in air)	12	8	5	
butanoicacid 2-methyl-hexyl ester	141 0	1433-P	21.40	0.83	17.12	2.21	34.29	9.45	fruity apple	1D/2D	0.086-0.43	-	-	-	
1-pentanol	122 9	1250-P	20.79	4.50	22.72	1.01	22.54	2.37	oil	1D/2D/S	0.1502	-	-	-	
1-(2-furanylmethyl)-1H-pyrrole	179 6	1824-P	20.78	1.65	91.28	1.41	147.4 9	16.2 4	plastic waxy coffee vegetable	1D/2D/S	0.1	-	1	1	
α -phellandrene	113 8	1167-P	20.23	2.55	18.52	4.31	36.72	11.5 1	herbal green woody	2D	0.04	1	-	1	
3-methylbutanal	899	918-P	19.29	3.43	24.99	1.53	16.53	1.80	chocolate	1D/2D/S	0.00035-0.0004	55	71	47	
2-ethylfuran	934	950-P	19.23	1.42	26.08	1.67	26.87	2.84	earthy	1D/2D	8(in coconut oil)	-	-	-	

acetic acid methyl ester	808	828-P	18.99	0.22	49.21	1.36	154.8 4	9.06	fruity	1D/2D	1.5-47	-	-	-
1-(2-furanyl)ethanone	147 8	1499-P	15.61	13.5 4	74.37	9.64	90.80	3.77	cocoa caramel coffee	1D/2D/S	15	-	-	-
2-methylpropanal	<80 0	819-P	15.26	0.97	19.62	0.79	-	-	pungent, malty	1D/2D/S	0.0015	10	13	-
(Z)-3-hexen-1-ol	136 0	1382-P	12.63	2.29	15.42	0.30	24.36	2.20	fresh green grass	2D	0.0039	3	4	6
dihydro-5-pentyl-2(3H)-furanone	199 9	2024-P	11.95	0.93	15.39	1.52	15.36	0.98	coconut creamy	2D	0.0097	1	2	2
tetrahydro-6-pentyl-2H-pyran-2-one	216 4	2194-P	9.28	1.43	13.12	2.75	11.02	0.12	fresh sweet	1D/2D	0.066	-	-	-
1-penten-3-one	999	1019-P	8.56	0.17	11.14	0.82	-	-	mustard	1D/2D	0.023	-	-	-
β -phellandrene	118 4	1211-P	8.17	0.97	10.18	2.18	21.02	7.22	mint terpentine	1D/2D	0.036	-	-	1
(E,E)-2,6-dimethyl-2,4,6-octatriene	135 1	1379-P	6.83	0.60	12.35	1.70	-	-	terpene sweet fresh floral	1D/2D	-	-	-	-
2-methylbutanenitrile	106 3	1091-P	5.80	1.37	8.42	0.41	13.47	2.54	gasoline	1D/2D	-	-	-	-
2,3-pentanedione	103 5	1058-P	2.65	0.15	8.27	0.51	9.37	0.74	toasted	1D/2D	0.02	-	-	-
methyl jasmonate	229 5	2338-P	2.60	0.61	2.60	0.58	2.72	0.54	floral fresh	2D	0.07	-	-	-
p-cresol	204 3	2080-P	1.70	0.14	4.74	0.30	11.47	1.08	floral	2D	0.0039	-	1	3
1-ethyl-1H-pyrrole-2-carboxaldehyde	158 5	1610-p	-	-	331.9 1	18.6 3	424.2 5	14.1 3	burnt roasted smoky	1D/2D	-	-	-	-
methyl salicylate	175 0	1765-P	-	-	270.9 4	1.99	566.5 6	42.8 6	mint	2D	0.04	-	7	14
hexanoic acid hexyl ester	159 1	1602-P	-	-	190.9 0	3.09	315.7 5	72.5 1	fruity	1D/2D	6.4	-	-	-
2,6,6-trimethyl-1,3-cyclohexadiene-1-carboxaldehyde	162 5	1616-P	-	-	147.6 7	3.65	193.1 8	29.3 7	fresh herbal	1D/2D	-	-	-	-

(2-nitroethyl)-benzene	208 5	2064-P	-	-	109.9 2	3.24	98.06	5.69	flower spice	1D/2D/S	0.002	-	55	49
2,5-dimethyl-3-ethylpyrazine	142 7	1443-P	-	-	88.94	6.04	151.7 3	9.05	potato cocoa roasted nutty	2D/S	0.0086	-	10	18
6-methyl-3,5-heptadiene-2-one	156 7	1602-P	-	-	80.98	1.70	69.34	8.27	cinnamon spice woody weedy	1D/2D	-	-	-	-
4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-3-buten-2-one	196 7	1962-P	-	-	52.27	2.99	34.31	0.90	fruity sweet berry woody	1D/2D	-	-	-	-
6-methyl-2-ethylpyrazine	136 5	1386-p	-	-	50.94	16.5 2	15.37	4.23	roasted potato	1D/2D	0.04	-	1	-
4-methyl-3-penten-2-one	111 3	1127-P	-	-	42.64	1.19	32.84	4.84	pungent earthy vegetable	1D/2D	0.20 (in air)	-	-	-
3-methyl-2-ethylpyrazine	138 5	1407-P	-	-	39.55	2.04	35.89	5.05	peanut musty	2D	0.5	-	-	-
citral	170 5	1718-P	-	-	30.33	3.64	25.58	5.85	lemon	2D	0.032	-	1	1
4-ethylbenzaldehyde	168 2	1721-P	-	-	29.61	5.08	58.13	3.37	almond	1D/2D	0.04	-	1	1
butanoic acid hexyl ester	139 5	1414-P	-	-	26.70	3.85	-	-	green fruity	1D/2D	0.203	-	-	-
2,4-decadienal	173 8	1797-P	-	-	13.37	0.10	-	-	fatty	2D	0.0003	-	45	-
1H-pyrrole-2-carboxaldehyde	198 9	2030-P	-	-	10.65	2.02	20.89	4.12	musty beefy coffee	1D/2D	65	-	-	-
1-methyl-1H-pyrrole-2-carboxaldehyde	159 3	1626-p	-	-	10.32	0.76	29.58	0.52	roasted nutty	2D	0.037	-	-	1
trans-Isoeugenol	230 2	2354-P	-	-	9.41	1.21	-	-	sweet spicy floral	1D/2D	0.978 (in oil)	-	-	-
5-butylidihydro-2(3H)-furanone	188 9	1910-P	-	-	8.65	0.89	12.03	2.81	coconut	2D/S	0.012	-	1	1
1-propen-2-ol,acetate	<80 0	-	-	-	2.40	0.10	18.22	2.56	grape	2D	-	-	-	-
dimethyl disulfide	105	1077-P	-	-	1.38	0.70	5.84	0.51	cabbage	1D/2D/S	0.09	-	-	-

	2														
(E)-2-methyl-2-butenal	107 1	1092-P	-	-	-	-	9.24	1.37	strong green fruit	1D/2D	0.4589	-	-	-	
4,5-dimethyl-2-isobutyloxazole	132 9	1330-P	-	-	-	-	26.16	6.53	burnt roasted	2D	-	-	-	-	
5-methyl-2-ethylpyrazine	137 2	1387-P	-	-	-	-	64.34	19.5 1	coffee bean nutty	2D	0.016	-	-	4	
2-nonanone	136 8	1390-P	-	-	-	-	35.77	0.77	green weedy	1D/2D/S	0.041-0.082	-	-	1	
2-nonen-4-one	145 8	1468-P	-	-	-	-	15.22	7.23	0	2D	0.02 (in air)	-	-	1	
cyclopentanol	956	1299-P	-	-	-	-	17.79	2.52	0	2D	0.1251	-	-	-	
5-methyl-2-(1-methylethenyl)-4-hexen-1-ol	107 1	-	-	-	-	-	63.09	12.5 3	floral	2D	-	-	-	-	
trans-linalooloxide(furanoid)	145 0	1452-P	-	-	-	-	173.7 3	8.25	floral	1D/2D	0.06	-	-	3	
(Z)-3,7-dimethyl-1,3,6-octatriene	122 7	1235-P	-	-	-	-	169.2 1	11.1 1	floral herb	1D/2D	0.034	-	-	5	
1-octen-3-one	132 2	1300-P	-	-	-	-	-	-	mushroom	1D/2D/S	-	-	-	-	
unknown	109 8		-	-	-	-	-	-	garlic	1D/2D	-	-	-	-	
unknown	122 1		-	-	-	-	-	-	popcorn	1D	-	-	-	-	
unknown	134 1		-	-	-	-	-	-	popcorn	1D/2D	-	-	-	-	
unknown	200 6	□	-	-	-	-	-	-	roasty	1D	-	-	-	-	

^a Totally aroma-active compounds were identified as the aroma-active compounds.

^b The RI values that calculated on DB-WAX column in 2D mode; "P" represent for polar column.

^c The NIST RI values were referred from the NIST 14 library.

^d The aroma depiction of each compound was obtained at the sniffer port.

^e The identified mode of each compounds. "S" represented the verification by authentic reference standards.

^f The thresholds listed in the table were referred the book: Gemert L.J.v, Compilations of odour threshold values in air, water & other media and compilations of flavour threshold values in water & other media, 2011 1st ed. Oliemans Punter & Partners BV, Netherlands (2003).