
Table S1. Aroma descriptor reference.

No.	Aroma descriptors	Reference standards
1	nut	<i>Le Nez du Vin</i> - prune,
2	tropical fruit	<i>Le Nez du Vin</i> - pineapple and banana
3	apricot	<i>Le Nez du Vin</i> - apricot or peach
4	honey	<i>Le Nez du Vin</i> - honey
5	caramel	<i>Le Nez du Vin</i> - caramel
6	rose	<i>Le Nez du Vin</i> - rose

Table S2. Information on 156 compounds with aroma characteristics ($\mu\text{g}\cdot\text{L}^{-1}$).

Name	CAS	K1	EC1118	ST	R2	Odor
1-Nonanol	143-08-8	9.49 ± 0.33	7.77 ± 0.02	16.53 ± 1.96	6.95 ± 0.00	fat, green
(Z)-2-Penten-1-ol	1576-95-0	2.88 ± 0.02	2.33 ± 0.14	3.79 ± 0.43	3.10 ± 0.28	green, plastic, rubber
3-Octanol	589-98-0	86.48 ± 8.71	94.11 ± 5.83	261.55 ± 16.17	218.14 ± 4.76	chemical, metal, burnt
1-Octanol	111-87-5	57.68 ± 1.48	59.09 ± 2.67	56.72 ± 4.68	55.05 ± 2.31	moss, nut, mushroom
(E)- 2-Octen-1-ol	18409-17-1	63.06 ± 3.02	58.51 ± 6.35	56.50 ± 3.93	34.47 ± 2.76	mushroom
3-Heptanol	589-82-2	1.86 ± 0.14	2.36 ± 0.12	1.84 ± 0.09	2.66 ± 0.21	chemical, green
3-ethoxy- 1-Propanol	111-35-3	12.02 ± 1.05	18.63 ± 0.83	11.93 ± 1.26	9.06 ± 0.02	fruit
2-Nonanol	628-99-9	31.01 ± 2.39	29.84 ± 1.58	25.41 ± 1.72	28.93 ± 0.38	cucumber
1-Undecanol	112-42-5	0.33 ± 0.01	0.77 ± 0.08	0.45 ± 0.02	0.67 ± 0.08	mandarin
1-Decanol	112-30-1	3.06 ± 0.18	2.98 ± 0.23	2.04 ± 0.15	1.88 ± 0.13	fat
3-methyl-1-Butanol	123-51-3	508.32 ± 50.59	18.01 ± 1.14	657 ± 19.36	1488.75 ± 23.63	whiskey, malt, burnt
1-octen-3-ol	3391-86-4	41.40 ± 0.97	111.92 ± 12.86	69.78 ± 1.66	114.08 ± 0.98	soap, plastic
2-Butanol	78-92-2	2.64 ± 0.00	4.21 ± 0.42	2.02 ± 0.00	4.51 ± 0.00	medicine, fruit
1-Propanol	71-23-8	100.97 ± 13.63	113.23 ± 8.01	100.32 ± 13.18	169.14 ± 5.24	alcohol, pungent
isobutyl alcohol	78-83-1	366.78 ± 16.74	426.04 ± 18.44	393.49 ± 13.08	533.37 ± 8.43	wine, solvent, bitter
3-Pentanol	584-02-1	19.66 ± 0.96	25.83 ± 2.20	16.47 ± 1.14	29.33 ± 2.23	balsamic
1-Butanol, 3-methyl-, acetate	123-92-2	128.35 ± 2.07	142.25 ± 7.41	88.78 ± 4.37	209.13 ± 15.61	banana
2-Pentanol	6032-29-7	24.29 ± 0.02	24.14 ± 0.17	23.9 ± 0.00	27.55 ± 2.80	green
1-Butanol	71-36-3	127.26 ± 3.18	143.79 ± 16.1	89.89 ± 0.59	152.22 ± 1.16	wine
1-Penten-3-ol	616-25-1	23.29 ± 0.08	23.94 ± 1.72	13.25 ± 0.40	26.16 ± 0.78	butter, pungent
1-Pentanol	71-41-0	77.81 ± 0.23	82.36 ± 7.91	85.55 ± 2.21	100.91 ± 0.88	fruit
1-Hexanol	111-27-3	211.3 ± 2.13	279.92 ± 20.48	200.79 ± 12.61	284.22 ± 16.93	resin, flower, green
3-hexen-1-ol	928-97-2	35.31 ± 3.10	40.57 ± 1.85	20.65 ± 1.80	67.91 ± 1.82	moss, fresh
(Z)-2-Hexen-1-ol	928-94-9	2.37 ± 0.07	2.27 ± 0.05	-	2.73 ± 0.20	leaf, green, wine, fruit

1-heptanol	111-70-6	135.31 ± 3.10	140.57 ± 10.85	120.65 ± 7.80	167.91 ± 10.82	herb
2-methyl-Propanoic acid,	79-31-2	59.91 ± 0.29	67.36 ± 0.51	37.81 ± 3.15	67.98 ± 0.63	rancid, butter, cheese
2,3-Butanediol	513-85-9	704.98 ± 68.43	614.67 ± 56.74	76.66 ± 6.38	1262.81 ± 36.77	fruit, onion
Undecanal	112-44-7	1.00 ± 0.08	0.88 ± 0.06	0.78 ± 0.01	1.36 ± 0.04	oil, pungent, sweet
(E,Z)-3,6-Nonadien-1-ol	56805-23-3	1.83 ± 0.13	2.94 ± 0.28	1.12 ± 0.12	3.21 ± 0.17	fish
Acetic acid,2-phenylethyl ester	103-45-7	289.29 ± 14.27	115.32 ± 10.86	396.14 ± 10.4	145.99 ± 14.34	rose, honey, tobacco
Benzoic acid, methyl ester	93-58-3	1.00 ± 0.11	0.80 ± 0.09	1.04 ± 0.02	0.75 ± 0.00	prune, lettuce, herb, sweet
Benzoic acid, ethyl ester	93-89-0	29.57 ± 2.20	34.33 ± 1.24	37.56 ± 3.58	22.91 ± 0.00	camomile, flower, celery, fruit
Acetic acid, phenylmethyl ester	140-11-4	0.45 ± 0.03	0.51 ± 0.02	0.94 ± 0.08	0.49 ± 0.05	fresh, boiled vegetable
Benzeneacetic acid, ethyl ester	101-97-3	114.67 ± 4.79	42.83 ± 3.50	150.64 ± 3.26	93.18 ± 0.34	fruit, sweet
Benzenemethanol	100-51-6	7.00 ± 0.76	7.40 ± 0.38	14.34 ± 1.70	6.23 ± 0.17	sweet, flower
2-Propenoic acid, 3-phenyl-, ethyl ester	103-36-6	0.44 ± 0.03	0.46 ± 0.03	0.54 ± 0.00	0.26 ± 0.01	honey, cinnamon
2-Hydroxybenzoic acid methyl ester	119-36-8	3.32 ± 0.07	3.48 ± 0.24	2.64 ± 0.18	1.97 ± 0.06	peppermint
Benzoic acid	65-85-0	5.84 ± 0.45	6.90 ± 0.47	4.80 ± 0.57	4.15 ± 0.45	urine
Ethyl vanillate	617-05-0	0.23 ± 0.01	0.43 ± 0.02	0.13 ± 0.01	0.28 ± 0.01	flower, fruit, sweet, vanilla
4-ethyl-Benzaldehyde	4748-78-1	1.18 ± 0.03	1.39 ± 0.06	0.70 ± 0.04	1.57 ± 0.17	sweet
1-methyl-4-(1-methylethenyl)-Benzene	1195-32-0	180.47 ± 2.03	133.08 ± 9.31	120.44 ± 10.64	202.62 ± 6.81	citrus, pine
Benzaldehyde	100-52-7	353.87 ± 7.70	350.62 ± 32.99	391.22 ± 36.37	498.43 ± 12.74	almond, burnt sugar
Benzenacetaldehyde	122-78-1	42.59 ± 1.20	42.56 ± 3.88	32.79 ± 3.95	47.59 ± 0.29	hawthorne, honey, sweet
1-(4-methylphenyl)- Ethanone	122-00-9	0.24 ± 0.01	0.28 ± 0.02	0.46 ± 0.03	2.31 ± 0.20	bitter almond
Benzoic acid, 2-hydroxy-, ethyl ester	118-61-6	3.75 ± 0.31	2.09 ± 0.14	3.46 ± 0.19	12.47 ± 0.92	wintergreen, mint
Ethyl 3-phenylpropionate	2021-28-5	8.38 ± 0.61	5.82 ± 0.14	3.95 ± 0.19	12.33 ± 2.92	flower
5-methyl-2-Furancarboxaldehyde	620-02-0	2.35 ± 0.08	3.19 ± 0.01	4.18 ± 0.08	2.62 ± 0.33	almond, caramel, burnt sugar
2-Furanmethanol	98-00-0	-	0.44 ± 0.00	0.74 ± 0.01	-	burnt
2-pentyl-Furan	3777-69-3	42.20 ± 1.67	48.05 ± 0.39	12.21 ± 0.90	52.91 ± 3.64	green bean, butter
1-(2-furanyl)- Ethanone	1192-62-7	3.95 ± 0.14	4.91 ± 0.30	4.05 ± 0.42	5.17 ± 0.59	balsamic

Trimethyl-Pyrazine	14667-55-1	0.36 ± 0.00	0.27 ± 0.01	0.28 ± 0.00	0.36 ± 0.01	roast, potato, must
Pyridine	110-86-1	0.24 ± 0.02	0.41 ± 0.01	0.24 ± 0.01	3.84 ± 0.11	rancid
2-Methylpyrazine	109-08-0	0.46 ± 0.03	0.72 ± 0.05	1.24 ± 0.02	0.83 ± 0.07	popcorn
Disulfide, dimethyl	624-92-0	6.34 ± 0.39	6.02 ± 0.04	5.47 ± 0.52	6.37 ± 0.13	onion, cabbage, putrid
Benzothiazole	95-16-9	1.64 ± 0.18	2.21 ± 0.18	2.34 ± 0.17	2.31 ± 0.26	gasoline, rubber
Trisulfide, dimethyl	3658-80-8	1.20 ± 0.17	2.26 ± 0.17	2.09 ± 0.18	1.81 ± 0.19	sulfur, fish, cabbage
3-(methylthio)-1-Propanol	505-10-2	8.17 ± 0.14	10.26 ± 0.41	5.83 ± 0.48	5.50 ± 0.10	sweet, potato
4-methyl-Phenol	106-44-5	2.64 ± 0.09	2.06 ± 0.16	2.64 ± 0.29	1.77 ± 0.14	medicine, phenol, smoke
2-methyl-Phenol	95-48-7	4.02 ± 0.15	6.56 ± 0.00	3.62 ± 0.18	4.00 ± 0.29	phenol
Phenol	108-95-2	18.09 ± 2.26	30.65 ± 1.09	20.56 ± 1.55	15.41 ± 0.91	phenol
4-ethyl-2-methoxy-Phenol	2785-89-9	2.58 ± 0.05	2.35 ± 0.17	2.16 ± 0.23	2.71 ± 0.14	spice, clove
2-methoxy-4-(2-propenyl)-Phenol	97-53-0	0.45 ± 0.01	0.40 ± 0.02	0.32 ± 0.01	0.45 ± 0.03	clove, honey
3-ethyl-Phenol	620-17-7	1.78 ± 0.05	2.13 ± 0.07	1.18 ± 0.05	1.18 ± 0.04	must
2-Methoxy-4-vinylphenol	7786-61-0	5.42 ± 0.39	7.53 ± 0.29	3.22 ± 0.29	4.82 ± 0.11	clove, curry
2,6-dimethoxy-4-(2-propenyl)-Phenol	6627-88-9	0.23 ± 0.00	0.23 ± 0.03	0.12 ± 0.01	0.23 ± 0.01	sweet, flower
2-ethyl-4-hydroxy-5-methyl-3-(2H)furanone	27538-09-6	0.78 ± 0.02	0.67 ± 0.06	0.81 ± 0.01	0.60 ± 0.00	cotton candy, sweet
Dihydro-2(3H)-Furanone	96-48-0	0.79 ± 0.07	0.91 ± 0.09	0.78 ± 0.04	0.67 ± 0.00	Hexanoic acid
5-ethyl-2(5H)-Furanone	2407-43-4	0.63 ± 0.03	0.89 ± 0.03	0.60 ± 0.01	0.57 ± 0.06	spice
Tetrahydro-6-pentyl-2H-Pyran-2-one	705-86-2	2.39 ± 0.02	2.99 ± 0.31	1.09 ± 0.02	1.99 ± 0.01	peach
6-heptyltetrahydro-2H-Pyran-2-one	713-95-1	0.69 ± 0.04	0.20 ± 0.00	0.12 ± 0.01	-	fruit, sweet
(Z)-dihydro-5-(2-octenyl)-2(3H)-Furanone	18679-18-0	0.93 ± 0.03	0.82 ± 0.03	0.62 ± 0.01	0.57 ± 0.06	peach, sweet
5-hexyldihydro-2(3H)-Furanone	706-14-9	0.54 ± 0.01	0.28 ± 0.02	0.31 ± 0.03	0.15 ± 0.10	peach, fat
5-ethyldihydro-2(3H)-Furanone	695-06-7	46.31 ± 3.54	46.03 ± 2.63	48.99 ± 2.51	51.38 ± 1.19	coumarin, sweet
Dihydro-5-propyl-2(3H)-Furanone	105-21-5	1.90 ± 0.13	2.12 ± 0.13	2.16 ± 0.07	2.89 ± 0.27	nut, fat, fruit
2-methyl-2-Butenal	1115-11-3	0.24 ± 0.00	-	0.15 ± 0.01	0.33 ± 0.01	green, fruit
Pentanal	110-62-3	0.37 ± 0.04	1.42 ± 0.13	1.66 ± 0.00	2.60 ± 0.00	almond, malt, pungent

2-octenal	2548-87-0	0.75 ± 0.08	0.90 ± 0.02	0.40 ± 0.01	1.43 ± 0.02	green, nut, fat
2-methyl-Butanal	96-17-3	1.67 ± 0.00	1.55 ± 0.15	0.89 ± 0.06	2.78 ± 0.25	malt
3-methyl-Butanal	590-86-3	0.49 ± 0.02	1.10 ± 0.02	0.76 ± 0.00	1.67 ± 0.01	cocoa, almond
Octanal	124-13-0	4.80 ± 0.20	6.03 ± 0.74	3.84 ± 0.28	16.95 ± 1.89	fat, soap, lemon, green
Decanal	112-31-2	9.31 ± 0.48	10.02 ± 1.05	7.84 ± 0.13	10.43 ± 0.39	soap, orange peel, tallow
(E,E)-2,4-Octadienal	30361-28-5	0.34 ± 0.03	0.36 ± 0.01	0.43 ± 0.02	0.13 ± 0.00	green, seaweed, cucumber
Dodecanal	112-54-9	2.77 ± 0.40	2.52 ± 0.17	3.55 ± 0.01	3.03 ± 0.01	lily, fat, citrus
Nonanal	124-19-6	56.35 ± 5.71	77.32 ± 0.62	26.42 ± 2.42	57.79 ± 4.92	fat, citrus, green
trans-4,5-Epoxy-2(E)-decenal	134454-31-2	0.07 ± 0.00	0.28 ± 0.01	0.02 ± 0.00	0.28 ± 0.01	metal, green
Acetic acid	64-19-7	1191.14 ± 122.03	1216.82 ± 108.67	1297.73 ± 113.08	1476.64 ± 134.34	sour
Pentanoic acid	109-52-4	30.36 ± 0.34	32.55 ± 1.51	28.56 ± 2.63	36.73 ± 0.62	sweat
Nonanoic acid	112-05-0	-	9.05 ± 0.90	24.34 ± 0.21	0.90 ± 0.00	green, fat
Decanoic acid	334-48-5	27.87 ± 1.00	18.10 ± 1.77	31.36 ± 2.92	13.92 ± 1.49	rancid, fat
Hexanoic acid	142-62-1	112.94 ± 12.63	282.66 ± 22.23	108.40 ± 5.68	197.12 ± 8.54	sweat
Octanoic acid	124-07-2	0.99 ± 0.08	2.69 ± 0.02	0.73 ± 0.05	0.45 ± 0.02	sweat, cheese
Butanoic acid	107-92-6	84.59 ± 1.33	88.94 ± 0.18	58.78 ± 5.18	135.39 ± 2.89	rancid, cheese, sweat
β-Citral	106-26-3	0.06 ± 0.00	-	0.38 ± 0.01	0.19 ± 0.02	lemon
à-Calacorene	21391-99-1	0.93 ± 0.05	0.74 ± 0.04	0.44 ± 0.05	1.47 ± 0.15	wood
Nerol	106-25-2	1.93 ± 0.05	1.82 ± 0.05	1.55 ± 0.10	2.02 ± 0.13	oil, flower
β-Cyclocitral	432-25-7	2.98 ± 0.32	2.61 ± 0.09	1.75 ± 0.03	3.07 ± 0.05	mint
α-Terpinolene	586-62-9	11.58 ± 0.00	-	8.21 ± 0.52	13.72 ± 1.68	pine, plastic
1,4-Cineole	470-67-7	5.64 ± 0.43	5.58 ± 0.40	4.79 ± 0.33	7.53 ± 0.21	pine
γ-Terpinene	99-85-4	61.45 ± 1.32	55.28 ± 6.47	33.43 ± 1.15	78.67 ± 7.60	gasoline, turpentine
β-Damascenone	23726-93-4	71.61 ± 1.19	54.99 ± 0.39	30.98 ± 3.86	85.43 ± 2.50	apple. rose, honey
β-Myrcene	123-35-3	3.13 ± 0.18	4.62 ± 0.23	2.86 ± 0.21	7.68 ± 0.66	balsamic, must, spice
α-Phellandrene	99-83-2	13.07 ± 1.01	13.12 ± 0.95	9.55 ± 1.50	17.25 ± 0.76	turpentine, mint, spice

α -Terpinene	99-86-5	0.38 \pm 0.00	50.98 \pm 4.50	38.59 \pm 2.06	68.72 \pm 5.65	lemon
Dill ether	74410-10-9	10.49 \pm 0.64	13.61 \pm 1.07	8.76 \pm 0.67	15.09 \pm 1.51	dill
Linalool	78-70-6	49.61 \pm 3.23	72.12 \pm 2.08	50.55 \pm 5.11	103.33 \pm 3.81	lavender, wood
β -Citronellol	106-22-9	16.4 \pm 1.73	14.86 \pm 1.43	12.21 \pm 1.29	18.67 \pm 0.44	rose
Geraniol	106-24-1	4.30 \pm 0.13	3.90 \pm 0.30	3.05 \pm 0.35	7.10 \pm 0.29	rose, geranium
4-methyl-1-(1-methylethyl)-3-Cyclohexen-1-ol	562-74-3	203.48 \pm 12.29	161.88 \pm 14.28	288.12 \pm 21.51	53.42 \pm 5.24	turpentine, nutmeg, must
D-Fenchyl alcohol	1632-73-1	0.19 \pm 0.02	-	0.34 \pm 0.03	0.13 \pm 0.00	camphor
Piperitone	89-81-6	3.37 \pm 0.07	3.48 \pm 0.29	2.62 \pm 0.18	1.97 \pm 0.06	mint, fresh
Geranyl acetone	3796-70-1	5.54 \pm 0.67	16.52 \pm 0.93	4.97 \pm 0.35	6.40 \pm 0.03	magnolia, green
1,8-Cineole	470-82-6	0.79 \pm 0.02	0.91 \pm 0.09	0.78 \pm 0.04	0.67 \pm 0.02	mint, sweet
2,3-Pentanedione	600-14-6	1.10 \pm 0.10	1.34 \pm 0.17	0.49 \pm 0.01	1.50 \pm 0.03	cream, butter
1-Hexen-3-one	1629-60-3	0.84 \pm 0.03	1.00 \pm 0.09	0.54 \pm 0.01	1.64 \pm 0.08	cooked vegetable, metal
2,3-Butanedione	431-03-8	2.58 \pm 0.11	3.27 \pm 0.29	1.32 \pm 0.19	3.43 \pm 0.28	butter
1-Penten-3-one	1629-58-9	0.57 \pm 0.03	0.89 \pm 0.08	0.40 \pm 0.00	1.10 \pm 0.02	fish, pungent
4-methyl-3-Penten-2-one	141-79-7	-	0.74 \pm 0.00	0.41 \pm 0.02	0.79 \pm 0.01	sweet, chemical
3-Octanone	106-68-3	7.97 \pm 0.23	6.77 \pm 0.00	6.65 \pm 0.42	8.07 \pm 0.17	soap, gasoline
2-Octanone	111-13-7	5.09 \pm 0.63	4.81 \pm 0.08	4.85 \pm 0.22	7.41 \pm 0.20	herb, butter, resin
1-Octen-3-one	4312-99-6	9.96 \pm 1.14	10.83 \pm 0.91	7.71 \pm 0.35	14.55 \pm 0.68	mushroom, metal
6-Methyl-5-Hepten-2-one	110-93-0	31.79 \pm 2.94	29.65 \pm 1.16	27.72 \pm 2.13	49.30 \pm 1.65	pepper, mushroom, rubber
2-Nonanone	821-55-6	4.15 \pm 0.20	4.07 \pm 0.13	3.90 \pm 0.41	4.17 \pm 0.21	hot milk, soap, green
2-Undecanone	112-12-9	1.06 \pm 0.02	1.39 \pm 0.15	2.20 \pm 0.21	1.23 \pm 0.13	orange, fresh, green
2-Hexanone	591-78-6	0.63 \pm 0.04	1.52 \pm 0.15	0.30 \pm 0.01	1.12 \pm 0.01	ether, grape
3-hydroxy-2-Butanone	513-86-0	49.04 \pm 4.25	49.89 \pm 3.12	46.76 \pm 0.95	47.14 \pm 0.13	butter, cream
Octanoic acid, ethyl ester	106-32-1	151.46 \pm 10.63	763.81 \pm 20.32	81.16 \pm 8.58	790.81 \pm 58.84	fruit, fat
Hexanoic acid, ethyl ester	123-66-0	442.56 \pm 27.68	633.02 \pm 15.37	227.37 \pm 3.45	747.76 \pm 30.14	apple peel, fruit
Butanoic acid,3-methyl-, ethyl ester	108-64-5	12.23 \pm 0.45	9.21 \pm 1.05	9.60 \pm 0.56	15.00 \pm 0.09	fruit

Hexanoic acid, methyl ester	106-70-7	29.50 ± 2.67	27.50 ± 2.04	21.54 ± 1.87	35.81 ± 1.05	fruit, fresh, sweet
Acetic acid ethyl ester	141-78-6	313.15 ± 17.29	292.49 ± 33.81	374.83 ± 15.88	841.98 ± 30.65	pineapple
ethyl isobutyrate	97-62-1	94.52 ± 3.43	73.74 ± 1.89	57.28 ± 5.22	96.80 ± 2.01	sweet, rubber
Butanoic acid, methyl ester	623-42-7	0.99 ± 0.04	1.07 ± 0.08	0.75 ± 0.03	1.52 ± 0.08	ether, fruit, sweet
Acetic acid, 2-methylpropyl ester	110-19-0	225.18 ± 3.38	247.11 ± 24.9	131.01 ± 6.64	271.01 ± 15.04	fruit, apple, banana
Butanoic acid, ethyl ester	105-54-4	145.24 ± 10.61	238.62 ± 24.70	233.70 ± 10.23	308.32 ± 26.61	apple
Propanoic acid, propyl ester	106-36-5	0.34 ± 0.03	0.40 ± 0.03	0.44 ± 0.01	1.26 ± 0.01	pineapple
Acetic acid, butyl ester	123-86-4	44.38 ± 0.25	26.46 ± 2.53	21.34 ± 1.95	55.62 ± 3.98	pear
Acetic acid,hexyl ester	142-92-7	32.23 ± 2.49	29.48 ± 0.69	22.96 ± 1.92	58.06 ± 2.08	fruit, herb
Propyl hexanoate	626-77-7	1.21 ± 0.10	1.00 ± 0.07	1.05 ± 0.13	1.81 ± 0.19	fruit
Heptanoic acid, ethyl ester	106-30-9	213.31 ± 11.11	252.87 ± 11.04	234.26 ± 19.59	261.87 ± 24.87	fruit
Hexanoic acid, butyl ester	626-82-4	0.84 ± 0.04	0.63 ± 0.06	1.04 ± 0.06	1.93 ± 0.05	fruit
3-Hydroxy-butanoic acid ethyl ester	5405-41-4	0.67 ± 0.01	0.92 ± 0.08	1.53 ± 0.07	2.29 ± 0.03	marshmallow
Propanedioic acid, diethyl ester	105-53-3	14.56 ± 0.00	15.33 ± 0.26	11.29 ± 1.03	17.79 ± 0.74	apple
Hexanoic acid, hexyl ester	6378-65-0	0.37 ± 0.01	0.48 ± 0.01	0.36 ± 0.04	0.46 ± 0.02	apple peel, peach
Butanedioic acid, diethyl ester	123-25-1	144.71 ± 5.13	148.74 ± 12.04	474.16 ± 50.26	456.84 ± 27.19	wine, fruit
Nonanoic acid, methyl ester	1731-84-6	1.82 ± 0.13	1.90 ± 0.16	2.51 ± 0.22	1.73 ± 0.09	coconut
Decanoic acid,methyl ester	110-42-9	13.26 ± 1.37	11.57 ± 1.42	13.99 ± 0.23	6.09 ± 0.71	wine
Dodecanoic acid, methyl ester	111-82-0	0.66 ± 0.05	0.61 ± 0.04	0.75 ± 0.04	0.37 ± 0.02	fat, coconut
Dodecanoic acid, ethyl ester	106-33-2	80.84 ± 2.40	39.45 ± 2.19	109.28 ± 7.22	27.85 ± 0.19	leaf
Pentadecanoic acid, ethyl ester	539-82-2	82.71 ± 1.75	96.35 ± 3.71	127.84 ± 6.05	59.69 ± 3.03	yeast, fruit
Hexadecanoic acid, ethyl ester	628-97-7	100.90 ± 0.85	67.98 ± 4.99	116.98 ± 11.57	60.52 ± 4.21	wax
Butylcaprylate	589-75-3	0.47 ± 0.01	1.10 ± 0.10	0.64 ± 0.04	0.88 ± 0.09	fruit
ethyl 2-methylbutyrate	7452-79-1	27.61 ± 0.69	28.94 ± 1.37	16.39 ± 0.93	19.67 ± 0.81	apple
Undecanoic acid, ethyl ester	627-90-7	0.65 ± 0.05	0.75 ± 0.02	0.46 ± 0.01	0.71 ± 0.05	cognac, coconut
Hexyl octanoate	1117-55-1	0.28 ± 0.01	0.55 ± 0.04	0.29 ± 0.03	0.46 ± 0.04	herb, green, oil

Decanoic acid, ethyl ester	110-38-3	100.98 ± 8.58	54.82 ± 3.36	63.82 ± 4.18	59.32 ± 3.68	grape
Octanoic acid, methyl ester	111-11-5	287.00 ± 15.12	173.23 ± 5.08	147.68 ± 1.72	179.84 ± 17.92	orange

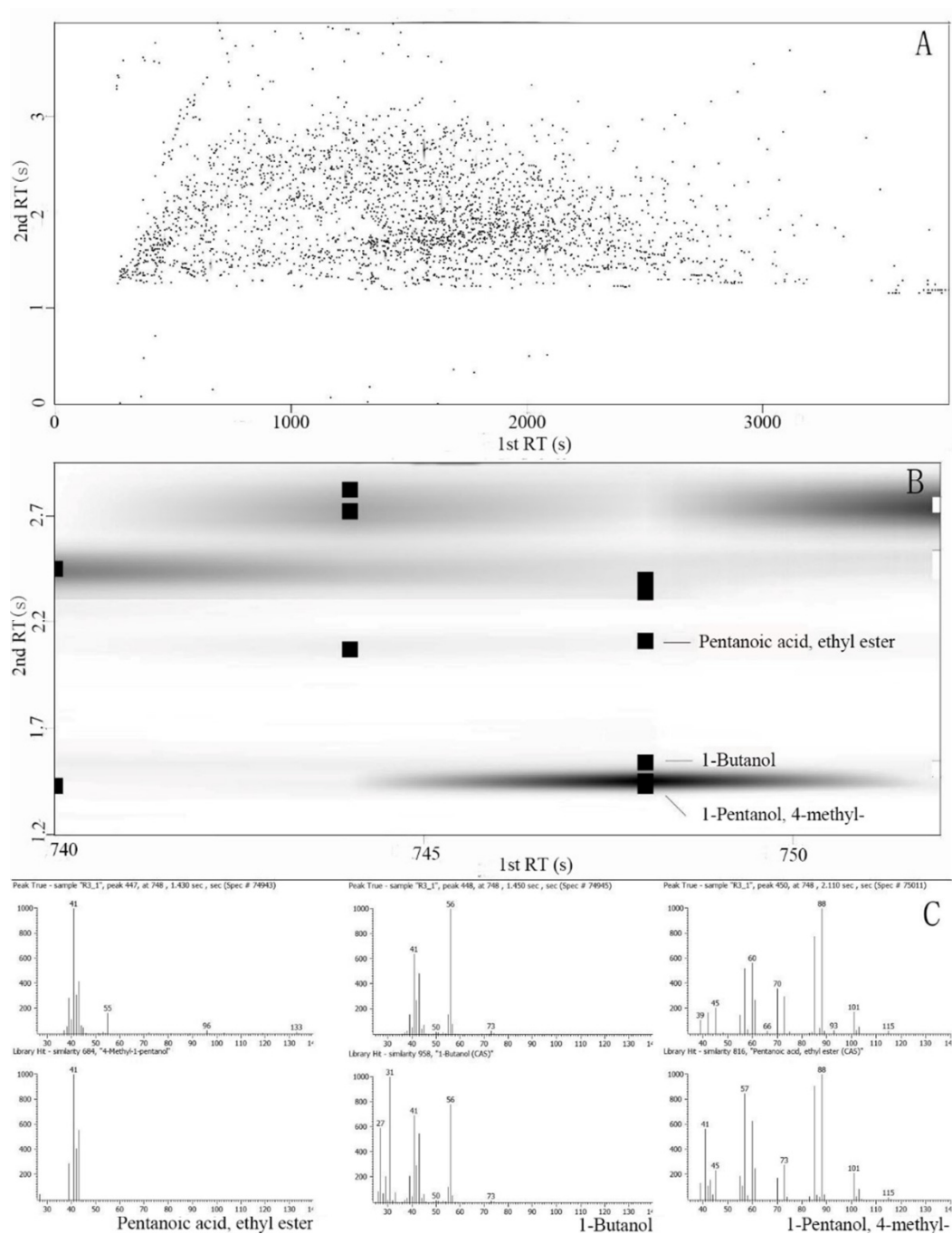


Figure S1. Analytical ion chromatogram contour plot analysis of volatile components in icewine fermented R2 yeast (A) and modulated peaks of 3 compounds found in icewine (B) and deconvoluted mass spectra of 3 compounds (C) .