Profiling the ester aroma of fruity beers using comprehensive two-dimensional gas chromatography: a comparison of flow and cryogenic modulators

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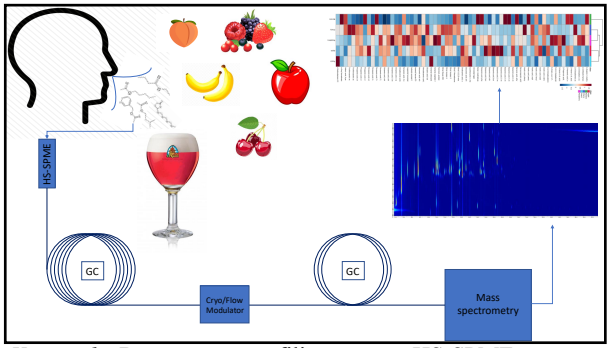
ABSTRACT: Beer aroma results from a complex mixture of volatile compounds that derive mainly from its raw ingredients and during processing. To characterize such a complex gas mixture, comprehensive two-dimensional gas chromatography coupled with mass spectrometry (GCXGC-MS) has proven to be a powerful analytical method. Moreover, this technique can be easily coupled to headspace solid phase micro extraction (HS-SPME), which permits a straightforward and rapid sampling of volatile organic compounds (VOCs). This paper reports on the relative performances of two different types of GCxGC modulator, a flow modulator and a cryogenic modulator, for characterizing the VOC signature of the headspace of five Belgian fruity beers. Particular emphasis is placed on the ester fraction of these volatile compounds. The results demonstrate that the cryogenic modulator permits a better overview of the molecular composition of the beer headspace, detecting nearly three times more molecules than the flow modulator.



Keywords: Beer, aroma profiling, esters, HS-SPME, comprehensive two-dimensional chromatography (GCxGC), flow modulator, cryogenic modulator

1. Introduction

Odors perception is a complex physiological mechanism which involves notably the interaction of volatiles molecules with olfactory receptors located in the nose. The resulting smell of a mixture of aromatic volatiles eventually perceived by the brain depends on several factors, including the concentration of the individual compounds with respect to their odor threshold level as well as their mutual 'interaction', which can result for instance in additive, masking or creative effects [1].

Fermented beverages, such as beer, are considered as 'complex' products by flavor chemists due to the fact that their aroma is formed by at least 25 different aroma compounds present above their corresponding odor threshold. The aroma profile of a given beer is highly dependent on the essential raw ingredients (barley malt, hops and yeast) and the conditions used for brewing it (temperature, fermentation and maturation time, etc.) [2].

The aroma compounds found in beer comprise a family of important organic molecules called esters, which are some of the most important components for determining its flavor [3]. The esters found in beer have different origins but a great majority of them are produced as by-products during yeast fermentation by the enzymatic catalyzed reaction of coenzyme A-activated fatty acids with alcohol precursors (Scheme 1).

$$RCOOH + CoASH + ATP \rightarrow RCO^{-}CoA + AMP + Pi$$

$$RCO^{-}CoA + R'OH \rightarrow RCOOR' + CoASH$$

Scheme 1 Activation of fatty acid RCOOH by coenzyme A CoASH followed by the formation of an ester RCOOR' by condensation with an alcohol precursor R'OH

On account of the aforementioned inherent molecular complexity of the volatile fraction of beer, its aromatic characterization is analytically demanding. In this context, comprehensive two-dimensional gas chromatography coupled to mass spectrometry (GCxGC-MS) comes as a useful analytical tool for studying such a complex gas phase mixture [4] [5].

In this study, the ester fraction of the volatile phase from five different Belgian fruity beers was characterized using GCxGC-MS with HS-SPME sampling. For this purpose, two types of modulators, namely cryogenic and flow modulators, were employed in order to investigate their relative performance. Such a comparison was already addressed in the literature, but mostly with petroleum products [6].

2. Experimental

2.1 Sampling

Five different Belgian fruity beers were analyzed in this study. The different flavors were red berries (Leffe Ruby), cherry (Liedemans Kriek), apple (Liedemans Apple), peach (Pecheresse) and banana (Mongozo Banana). 10 ml of each beer were added to HS vials in replicate of 5 (for both method). 1 g of NaCl was added in each vial. The latter were then capped and sampled automatically via HS-SPME using a DVB-CAR-PDMS fiber and an extraction time of 20 min (at 60 °C).

2.2 Analysis

Following sampling, the SPME fibers were injected onto the injection port in split mode (split ratio of 50:1 and 10:1 for the cryogenic and the flow method, respectively). The first dimension column was a non-polar Rxi5 (30m x 0.25mm x 0.25μm) and the second dimension column was a semi-polar Rxi17 (1m x 0.25mm x 0.25μm). The temperature programming was set as follows: 5 min at 40°C, ramped 5°C/min to 240°C, held 1 min. For the cryogenic modulator, the modulation period was 3 s whereas for the flux modulator, a modulation period of 2 s was chosen. For both methods, gas flow was set to 1 mL/min.

Finally, a time-of-flight mass (TOF) spectrometer was used as a detector for compound identification.

2.3 Data analysis

After raw data processing, the resulting chromatograms were aligned. Statistical methods were performed with the Metaboanalyst 4.0 software.

3. Results & discussions

The chromatograms obtained with the flux and the cryogenic modulator for the analysis of the Leffe Ruby (berry-flavored) are presented in the Supporting Information (Figure S1). A quick look at these chromatograms clearly shows a discrepancy regarding the number of chromatographic peaks. Indeed the latter seems to be higher with the cryogenic method as compared with the valve-based one. Table 1 highlights this difference by comparing the total number of volatile compounds detected with each method in the headspace of all five beers (see also Table S1). If we assume that the combination of both methods enabled the complete characterization of the volatile fraction of the beers, only 36% of the latter could be described with the flow modulator method whereas more than 90% of its components were detected using the cryogenic modulator.

Table 1 Comparison of the number of compounds detected in the headspace of the five beers with both modulators

	Modulator type		
	Flow	Cryogenic	Total
Number of molecules detected (%total)	61 (36%)	151 (90%)	167
Number of esters detected	27	67	70

The difference in sensitivity discussed above can be accounted for by at least two reasons. First, the loss of focusing effect when using a flow modulator instead of a cryogenic modulator [6]. Second, the fact that only part of the material coming out of the first column is sent to the second column with the valve-based modulator that was employed in this study.

Table 1 also displays some figures with regard to the ester fraction of the VOCs detected. 70 different esters were detected in the headspace of the different beers and accounts for the majority (42%) of these VOCs (in terms of chemical identity, see Table S1). Some of these esters are structurally similar and can be grouped in different categories: saturated or unsaturated linear esters, saturated or unsaturated branched esters, "aromatic" esters (ie, esters bearing one aromatic ring not necessarily attached directly to the ester group), lactones and others ester (for more information, please refer to the list of esters in the SI).

As long as odor type is concerned, most of the small chain ($<C_{10}$) saturated branched and linear esters as well as the lactones are characterized by a fruity smell whereas longer chain saturated branched or linear esters and unsaturated branched esters display a waxy and a floral smell, respectively. As for the "aromatic" esters, they have variable types of odor, although most have a floral-like smell. Unsaturated linear chain esters organoleptic properties are not well characterized. Figure 1 shows the structure of a few remarkable esters that have a smell identical to the flavor of the beer they are found in. The markedly distinct ester profiles of each fruity beer emphasize the role of esters in imparting a specific aroma to a given type of beer, although other types of volatiles, such as alcohols and terpenes, also play an important role in this regard (Figure S2).

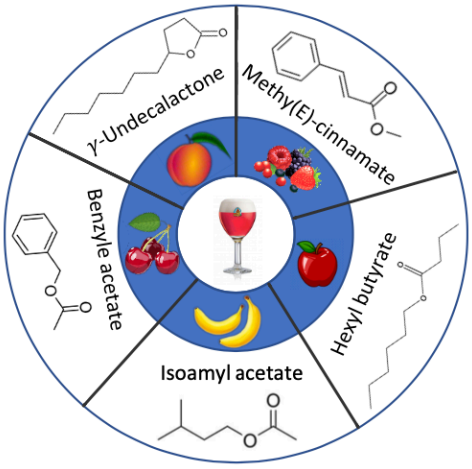


Fig. 1 Representation of the chemical structure of a few esters having an odor analogous to the flavor of the corresponding fruity beer.

4. Conclusion

In this study, we demonstrated that the choice of the modulator turned out to be critical for the HS-SPME and GCxGC-MS analysis of the volatile fraction of five Belgian fruity beers. The lower sensitivity associated with the flow modulator only allowed the identification of a relatively smaller portion of all the volatiles present in the headspace of the beers in contrast with the cryogenic modulator, making the latter a better option for this specific application.

Moreover, a particular focus on the ester fraction revealed that esters composed the majority of the beer volatile compounds with reference to chemical diversity and that they could be gathered into a few groups with similar structure and sometimes similar aroma properties.

ACKNOWLEDGMENT

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Supporting information

Profiling the ester aroma of fruity beers using comprehensive two-dimensional gas chromatography: a comparison of flow and cryogenic modulators

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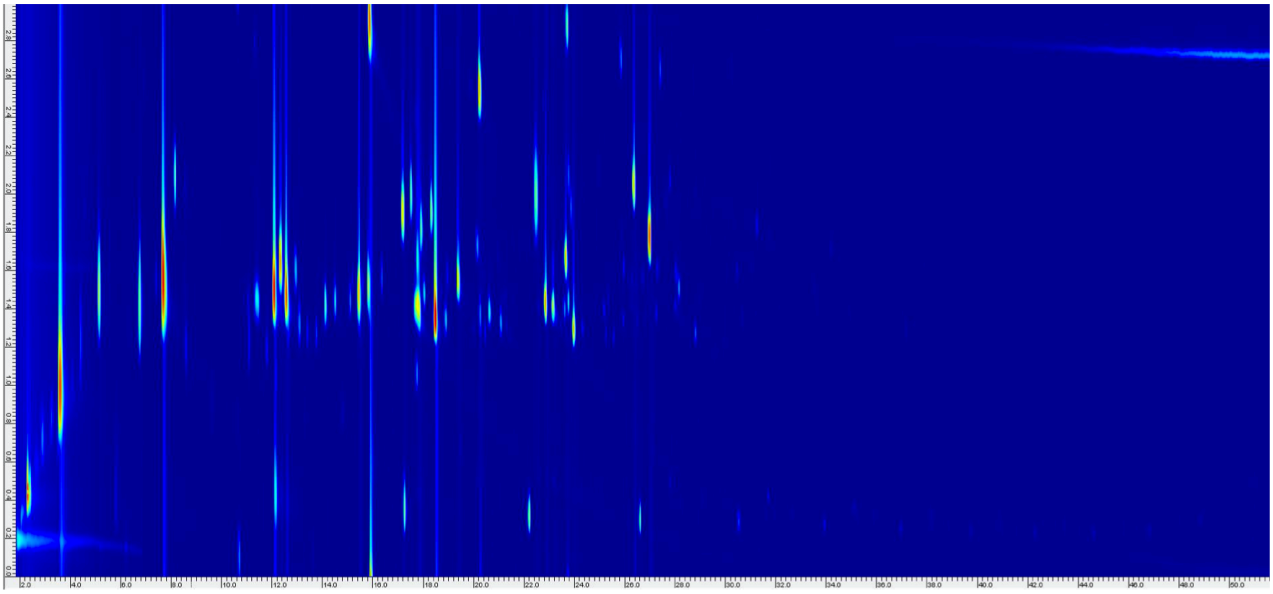
Figure S1: Chromatograms resulting from the HS-SPME and GCxGC-MS analysis of the headspace of the Leffe Rubis beer (berry-flavored). **Top**: Cryogenic modulator. **Bottom**: Flow modulator.



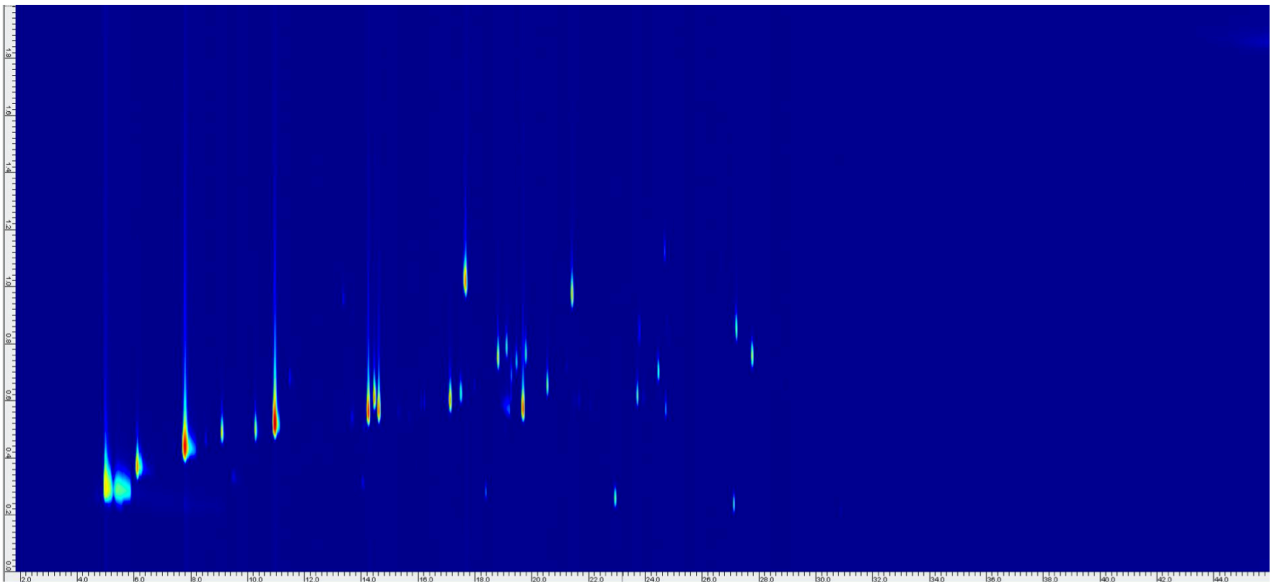
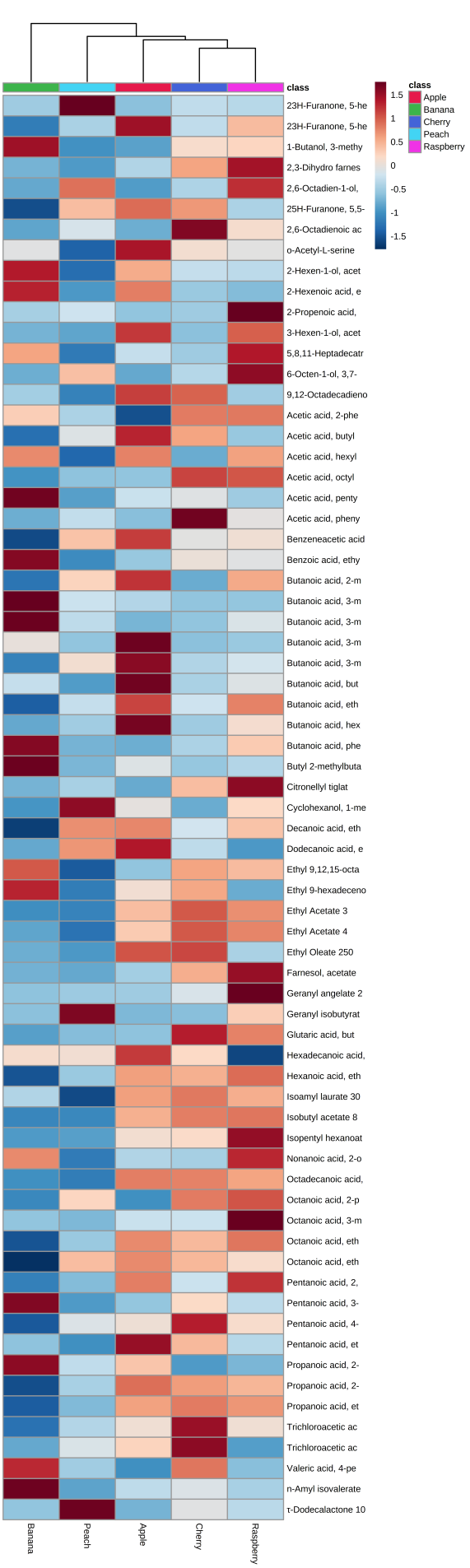


Figure S2: Heat maps for the esters detected in the five fruity beers using the cryogenic (**Left**) and the flow modulator (**Right**). Color scale allows relative comparison of the amount of each ester in the different fruity beers. Each type of beer displays a distinctive ester profile.



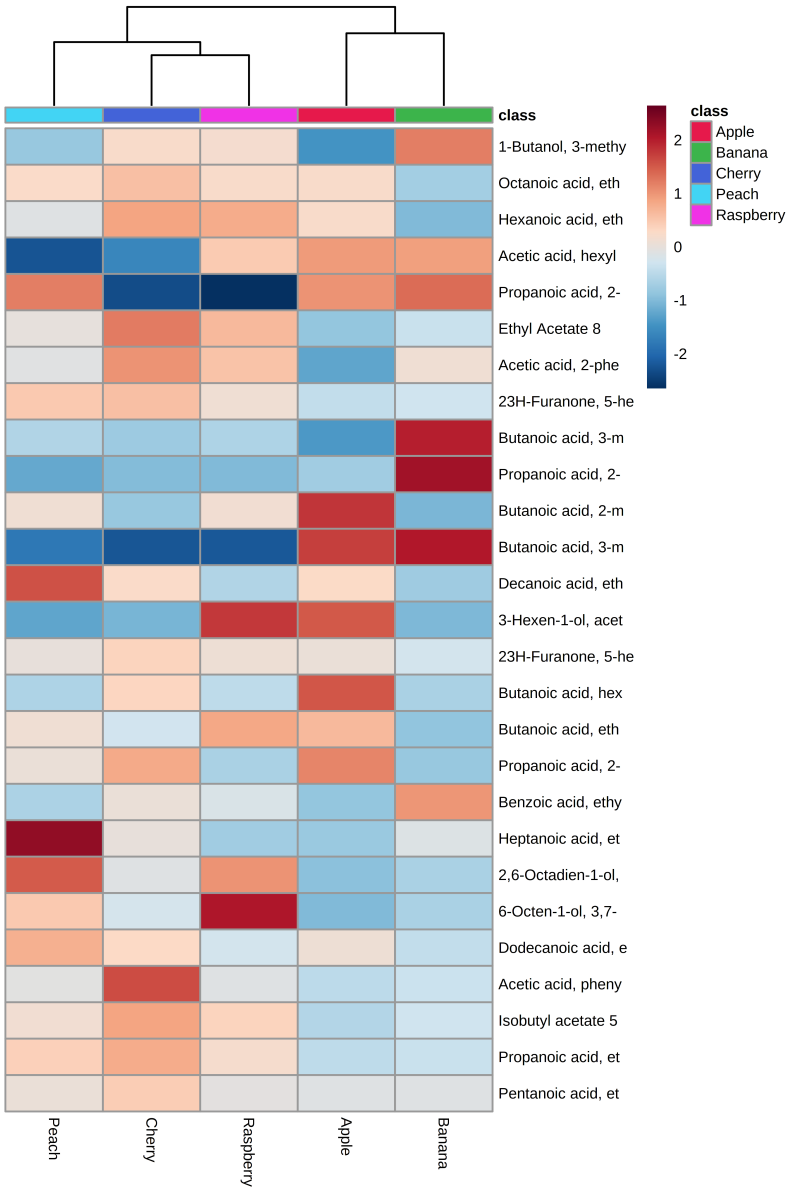


Table S1: List of the compounds detected with the cryogenic and flow method, respectively. The functional group(s) featured in each compound is also given. Ester compounds are highlighted in bold. Numbers in parentheses refer to numbers given in the original data sheets.

Type of modulator		Functional group
Cryogenic	**Flow**	
(E)-a-Famesene (149)		Double bonds
	1,3-Dioxolane, 2-heptyl-4-methyl- (81)	Cyclic Ether
1,3-Dioxolane, 4-methyl-2-pentyl- (151)		Cyclic Ether
	1,3-Hexanediol, 2-ethyl- (20)	Alcohol (x2)
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- (75)		Alcohol + Double bonds
1-Butanol (102)		Alcohol
1-Butanol, 3-methyl- (5)	1-Butanol, 3-methyl- (3)	Alcohol
1-Butanol, 3-methyl-, acetate (2)	**1-Butanol, 3-methyl-, acetate (1)**	**Ester**
1-Buten-3-one, 1-(2-carboxy-4,4-dimethylcyclobutenyl)- (189)		Carboxylic acid + Ketone + Double bonds
1-Decanol (29)	1-Decanol (46)	Alcohol
1-Dodecanol (36)	1-Dodecanol (33)	Alcohol
1-Heptanone, 1-(2-thienyl)- (179)		Ketone + Sulfide
1-Hexanol (27)	1-Hexanol (22)	Alcohol
1-Hexene, 3,5,5-trimethyl- (87)		Alkene
	1-Nonanol (43)	Alcohol
1-Octanol (26)	1-Octanol (61) + (44)	Alcohol
	1-Propanol, 2-methyl- (28)	Alcohol
1-Propanol, 3-(methylthio)- (142)	1-Propanol, 3-(methylthio)- (97)	Alcohol + Sulfide
1H-Indene, 2,3-dihydro-1,1,5,6-tetramethyl- (133)		Aromatic cycle
2(3H)-Furanone, 5-heptyldihydro- (80)	**2(3H)-Furanone, 5-heptyldihydro- (77) + (94)**	**Lactone**
2(3H)-Furanone, 5-hexyldihydro- (65)	**2(3H)-Furanone, 5-hexyldihydro- (56)**	**Lactone**
2(5H)-Furanone, 5,5-dimethyl- (232)		**Lactone** + Double bond
2,3-Butanediol (270)		Alcohol (x2)
2,3-Dihydro farnesyl acetate (293)		**Ester** + Double bonds
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (Z,E)- (243)		Alcohol + Double bonds
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- (74) + (141)	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- (71)	Alcohol + Double bonds
2,6-Octadien-1-ol, 3,7-dimethyl-, acetate (23)	2,6-Octadien-1-ol, 3,7-dimethyl-, acetate (31)	**Ester** + Double bonds
2,6-Octadiene, 2,6-dimethyl- (138) + (242)		Double bonds
2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester (231)		**Ester** + Double bonds
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)- (81)	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)- (57)	Ketone + Double bonds
2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (166)		Ketone + Double bonds

2-Hexen-1-ol, acetate, (Z)- (30)		**Ester** + Double bond
2-Hexenal (96)		Aldehyde
2-Hexenoic acid, ethyl ester (35)		**Ester**
2-Methoxy-4-vinylphenol (154)		Phenol + Ether + Double bond
2-Propenoic acid, 3-phenyl-, methyl ester, (E)- (79)		**Ester** + Double bond
2-Undecanol (114)		Alcohol
2H-Pyran, 2-ethenyltetrahydro-2,6,6-trimethyl- (139)	2H-Pyran, 2-ethenyltetrahydro-2,6,6-trimethyl- (55)	Cyclic Ether + Double bond
2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propenyl)- (71) + (165)		Cyclic Ether + Double bond
3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (54) + (88)	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (42) + (72)	Ketone + Double bonds
3-Decyn-2-ol (187)		Alcohol + Triple bond
	3-Furaldehyde (87)	Aldehyde + Cyclic aromatic ether
3-Hexen-1-ol, (Z)- (94)		Alcohol + Double bond
3-Hexen-1-ol, acetate, (E)- (17)		**Ester** + Double bond
	3-Hexen-1-ol, acetate, (Z)- (16)	**Ester** + Double bond
5,8,11-Heptadecatriynoic acid, methyl ester (168)		**Ester** + Triple bonds
5-Hepten-2-one, 6-methyl- (275)		Ketone + Double bond
6,10-Dodecadien-1-ol, 3,7,11-trimethyl- (217)		Alcohol + Double bonds
6-Octen-1-ol, 3,7-dimethyl-, (R)- (47)		Alcohol + Double bond
6-Octen-1-ol, 3,7-dimethyl-, acetate (34)	6-Octen-1-ol, 3,7-dimethyl-, acetate (36)	**Ester** + Double bond
6-epi-shyobunol (280) + (323)		Alcohol + Double bonds
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin (322)		Ketone + Aromatic cycle
9,12-Octadecadienoic acid, ethyl ester (223)		**Ester** + Double bonds
	10-Undecen-1-ol (27)	Alcohol + Double bond
Acetic acid (51)		Carboxylic acid
Acetic acid, 2-phenylethyl ester (11)	**Acetic acid, 2-phenylethyl ester (9)**	**Ester** + Aromatic cycle
Acetic acid, butyl ester (48)		**Ester**
Acetic acid, hexyl ester (7)	**Acetic acid, hexyl ester (5)**	**Ester**
Acetic acid, octyl ester (59)		**Ester**
Acetic acid, pentyl ester (106)	**Acetic acid, pentyl ester (59)**	**Ester**
Acetic acid, phenylmethyl ester (104)	**Acetic acid, phenylmethyl ester (50)**	**Ester** + Aromatic cycle
Aromadendrene oxide-(1) (147)		Cyclic Ether
Aromadendrene oxide-(2) (296) + (312)		Cyclic Ether
Benzaldehyde (16)	Benzaldehyde (17)	Aromatic aldehyde
Benzene, 1,1'-(1,3-propanediyl)bis- (292)		Aromatic cycle (x2)
Benzene, 1-methyl-3-(1-methylethyl)- (113)		Aromatic cycle
Benzene, 1-methyl-4-(1-methylethenyl)- (253)		Aromatic cycle + Double bond

Benzeneacetic acid, ethyl ester (140)		**Ester** + Aromatic cycle
Benzenebutanal (62)		Aldehyde + Aromatic cycle
Benzofuran, 2,3-dihydro- (235)		Aromatic cycle + Cyclic ether
Benzoic acid, ethyl ester (38)	**Benzoic acid, ethyl ester (25)**	**Ester** + Aromatic cycle
Benzyl alcohol (161)		Alcohol + Aromatic cycle
	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- (51)	Cyclic ketone
	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1α,2α,5α)- (48)	Alcohol
Butanal, 3-hydroxy- (249)		Alcohol + Aldehyde
Butane, 1-methoxy-3-methyl- (66)		Ether
Butanoic acid, 2-methyl-, ethyl ester (19)	**Butanoic acid, 2-methyl-, ethyl ester (13)**	**Ester**
Butanoic acid, 3-methyl- (125)		Carboxylic acid
Butanoic acid, 3-methyl-, butyl ester (28)	**Butanoic acid, 3-methyl-, butyl ester (14)**	**Ester**
Butanoic acid, 3-methyl-, ethyl ester (73)		**Ester**
Butanoic acid, butyl ester (46)		**Ester**
Butanoic acid, ethyl ester (32)	**Butanoic acid, ethyl ester (23)**	**Ester**
Butanoic acid, hexyl ester (43)	**Butanoic acid, hexyl ester (21)**	**Ester**
Butanoic acid, phenylmethyl ester (91)		**Ester** + Aromatic cycle
Butyl 2-methylbutanoate (31)		**Ester**
Butylated Hydroxytoluene (15)	Butylated Hydroxytoluene (19)	Phenol
Caryophyllene oxide (263)		Cyclic Ether + Double bond
	Citronellol (38)	Alcohol + Double bond
Citronellyl tiglate (255)		**Ester** + Double bonds
Cyclohexadecanone (272)		Cyclic ketone
Cyclohexanol, 1-methyl-4-(1-methylethenyl)- (251)		Alcohol + Double bond
Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate (49)		**Ester** + Double bond
Cyclohexanone, 5-methyl-2-(1-methylethyl)- (61) + (78)	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, cis- (32)	Cyclic ketone + Double bond
Cyclohexene, 1-methyl-4-(1-methylethylidene)- (92)		Double bonds
Decanal (105)		Aldehyde
Decanoic acid, ethyl ester (9)	**Decanoic acid, ethyl ester (15)**	**Ester**
Dodecanal (178)		Aldehyde
Dodecanoic acid (41)		Carboxylic acid
Dodecanoic acid, ethyl ester (20)	**Dodecanoic acid, ethyl ester (47)**	**Ester**
Ethanol (37)	Ethanol (10) + (26)	Alcohol
Ethyl 9,12,15-octadecatrienoate (307)		**Ester** + Double bonds
Ethyl 9-hexadecenoate (127)		**Ester** + Double bond
Ethyl Acetate (3) + (4)	**Ethyl Acetate (8)**	**Ester**

Ethyl Oleate (250)		**Ester** + Double bond
	Falcarinol (82)	Alcohol + Double bonds + Triple bonds
Farnesol, acetate (247)		**Ester** + Double bonds
Furan, 2,2'-[oxybis(methylene)]bis- (119)	Furan, 2,2'-[oxybis(methylene)]bis- (62)	Ether + Cyclic aromatic ether (x2)
Furfural (97)		Aldehyde + Cyclic aromatic ether
Geranyl angelate (200)		**Ester** + Double bonds
Geranyl isobutyrate (63)		**Ester** + Double bonds
Geranyl vinyl ether (95)	Geranyl vinyl ether (78)	Ether + Double bonds
Glutaric acid, butyl isobutyl ester (216)		**Ester** (x2)
	Heptanoic acid, ethyl ester (29)	**Ester**
Hexadecanoic acid, ethyl ester (39)		**Ester**
Hexanoic acid (40)		Carboxylic acid
Hexanoic acid, ethyl ester (6)	**Hexanoic acid, ethyl ester (4)**	**Ester**
Ionone (130)	Ionone (70)	Ketone + Double bonds
Isoamyl laurate (309)		**Ester**
Isobutyl acetate (86)	**Isobutyl acetate (58)**	**Ester**
Isopentyl hexanoate (192)		**Ester**
Isopropyl myristate (245)		**Ester**
Levomenthol (68)	Levomenthol (53)	Alcohol
	Limonene (18)	Double bonds
Linalool (10)		Double bonds
Naphthalene, 2,3,6-trimethyl- (156)		Aromatic
Nonane (259)		Alkane
Nonanoic acid, 2-oxo-, methyl ester (76)		**Ester** + Ketone
Octadecanoic acid, ethyl ester (274)		**Ester**
Octanoic acid (13)	Octanoic acid (35)	Carboxylic acid
Octanoic acid, 2-phenylethyl ester (295)		**Ester** + Aromatic cycle
Octanoic acid, 3-methylbutyl ester (184)		**Ester**
Octanoic acid, ethyl ester (1) + (176)	**Octanoic acid, ethyl ester (2)**	**Ester**
Oxime-, methoxy-phenyl-_ (111)		Ether + Oxime
Pentadecanoic acid, 3-methylbutyl ester (197)		**Ester**
Pentadecanoic acid, ethyl ester (313)		**Ester**
Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester (267)		**Ester** (x2)
Pentanoic acid, 3-methylbutyl ester (195)		**Ester**
Pentanoic acid, 4-methyl-, ethyl ester (162)		**Ester**
Pentanoic acid, ethyl ester (143)	**Pentanoic acid, ethyl ester (75)**	**Ester**
	Phenol, 2-methoxy-3-(2-propenyl)- (69)	Phenol + Ether + Double bond

Phenol, 4-ethyl- (123)		Phenol
Phenol, 4-ethyl-2-methoxy- (33)	Phenol, 4-ethyl-2-methoxy- (41)	Phenol + Ether
Phenylethyl Alcohol (8)	Phenylethyl Alcohol (6) + (30)	Alcohol + Aromatic cycle
	Propanoic acid, 2-hydroxy-, ethyl ester (24)	**Ester** + Alcohol
Propanoic acid, 2-methyl-, 3-methylbutyl ester (12)	**Propanoic acid, 2-methyl-, 3-methylbutyl ester (7) + (12)**	**Ester**
Propanoic acid, 2-methyl-, ethyl ester (137)		**Ester**
Propanoic acid, ethyl ester (90)	**Propanoic acid, ethyl ester (65)**	**Ester**
	Styrene (39)	Aromatic cycle + Double bond
Terpinen-4-ol (67)		Alcohol + Double bond
Trichloroacetic acid, hexadecyl ester (199)		**Ester** + Chlorine
Trichloroacetic acid, pentadecyl ester (220)		**Ester** + Chlorine
Undecanal (215)		Aldehyde
Valeric acid, 4-pentenyl ester (194)		**Ester** + Double bond
n-Amyl isovalerate (24) (25) (159)	**n-Amyl isovalerate (11) (66)**	**Ester**
n-Decanoic acid (14)		Carboxylic acid
o-Acetyl-L-serine (316)		**Ester** + Amine + Carboxylic acid
trans-ß-Ocimene (108)		Double bonds
a-Guaiene (288)		Double bonds
a-Myrcene (72)		Double bonds
α-Bisabolol (281)		Alcohol + Double bonds
α-Irone (238)		Ketone + Double bonds
α-Terpineol (18) + (70)	α-Terpineol (52)	Alcohol + Double bond
τ-Dodecalactone (100)		**Lactone**

Table S2: Boiling temperature of the esters listed in the complement.

N°	Compound	Boiling point (760 mm Hg)	N°	Compound	Boiling point (760 mm Hg)
1	Ethyl acetate	77°C	41	Methyl (E)-cinnamate	254°C
2	Butyl acetate	126°C	42	γ-Decalactone	304°C
3	Pentyl acetate	149°C	43	γ-Undecalactone	297°C
4	Hexyl acetate	171°C	44	γ-Dodecalactone	361°C
5	Octyl acetate	207°C	45	2(5H)-Furanone, 5,5-dimethyl	202°C
6	Ethyl propionate	99°C	46	cis-2-Hexenyl acetate	165°C
7	Ethyl butyrate	120°C	47	cis-3-Hexenyl acetate	120°C
8	Butyl butyrate	166°C	48	trans-3-Hexenyl acetate	174°C
9	Hexyl butyrate	204°C	49	4-Pentenyl pentanoate	/
10	Ethyl pentanoate	144°C	50	Ethyl 2-hexenoate	167°C
11	Ethyl hexanoate	166°C	51	Ethyl 9-hexadecenoate	354°C
12	Ethyl heptanoate	188°C	52	Ethyl oleate (Z)	205°C
13	Ethyl octanoate	206°C	53	Ethyl-9,12-octadecadienoat	374°C
14	Ethyl decanoate	241°C	54	Ethyl linolenate	397°C
15	Ethyl laurate	269°C	55	Methyl 5,8,11-heptadecatriynoate	/
16	Ethyl Pentadecanoate	312°C	56	Citronellyl acetate	229°C
17	Ethyl palmitate	303°C	57	Ethyl tiglate	148°C
18	Ethyl stearate	442°C	58	Geranyl isobutyrate	240°C
19	Isobutyl acetate	116.5°C	59	Geranyl acetate	240°C
20	Isoamyl acetate	142°C	60	Farnesyl acetate	394°C
21	Isoamyl butyrate	179°C	61	Methyl geranate (Z)	247°C
22	Isopentyl pentanoate	185°C	62	Citronellyl tiglate	/
23	Isopentyl hexanoate	225°C	63	Farnesol acetate	/
24	Isopentyl octanoate	267°C	64	Geranyl Angelate	/
25	Isopentyl decanoate	286°C	65	Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate	236°C
26	Isoamyl laurate	311°C	66	Glutaric acid, butyl isobutyl ester	/
27	Isopropyl myristate	344°C	67	Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester	/

28	Ethyl isobutyrate	112°C	68	Ethyl lactate	154°C
29	Ethyl 2-methylbutyrate	132°C	69	Methyl 9-oxononanoate	249°C
30	Butyl 2-methylbutyrate	179°C	70	O-Acetylserine	736°C
31	Ethyl isovalerate	131°C			
32	Ethyl isohexanoate	160°C			
33	Isopentyl isobutyrate	168°C			
34	Isoamyl isovalerate	212°C			
35	Benzyl acetate	238°C			
36	Phenethyl acetate	238°C			
37	Benzyl butyrate	238°C			
38	Phenethyl octanoate	295°C			
39	Ethyl benzoate	212°C			
40	Ethyl phenylacetate	227°C			

Complement: List of the 70 different esters detected in this study.

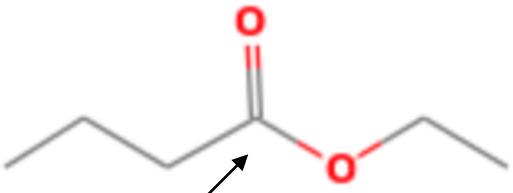
How to interpret this list?

Common name (informal)

IUPAC name (formal)

7) **Ethyl butyrate** (Butanoic acid, ethyl ester)

Background color refers to the type of fruity beer which has the highest heat map intensity for the given ester. When the ester is detected with both the cryogenic and the flow modulator, the intensity of the cryogenic heat map is taken into account.
Color code: Yellow = Banana; Red = Cherry; Violet = Berry; Green = Apple; Cyan = Peach; White = Compound absent from the heat map



2D Chemical structure

Corresponding numeration in initial data sheets. Red = Flow ; Blue = Cryogenic

[23] [32]

Odor type: FRUITY (Pineapple)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1004792.html
Signal: R_{Cryo} Medium R_{Flow} Very High
A_{Cryo} High

Organoleptic information

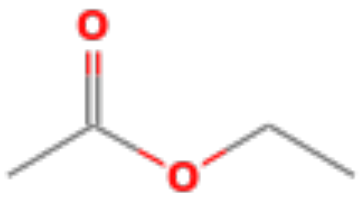
- Strong, medium & low refer to the odor strength
- The internet link gives more information about the compound
- All organoleptic properties are from the Perflavory™ database
- 'nd' means that the information is not available ; '/' means that the compound of interest could not be retrieved in the database

Relative intensity in the Heat maps of Figure S2

- B = Banana; C = Cherry; R = Raspberry (berry); A = Apple; P = Peach
- 'Cryo' and 'Flow' refer to the cryogenic and the flow heat maps, respectively
- Very Low = Color scale 0
  Low = Color scale 0.5
  Medium = Color scale 1.0
  High = Color scale 1.5
  Very high = Color scale > 1.5

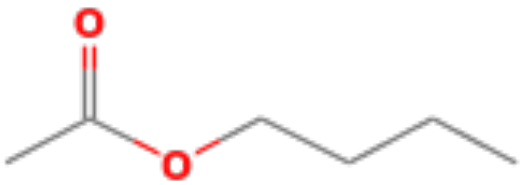
Saturated linear esters

1) **Ethyl acetate** (Ethyl Acetate) [8] [3] [4]



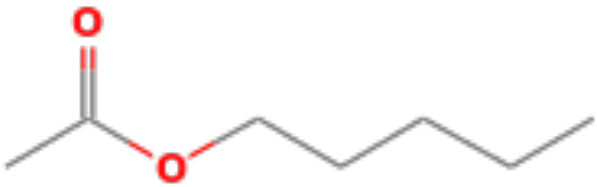
Odor type: ETHEREAL (Grape)
Flavour: ETHEREAL (Cherry nuance)
Strong
http://www.perflavory.com/docs/doc1004691.html
Signal: B_{Flow} Very Low
C_{Cryo} Medium C_{Flow} Medium - High
R_{Cryo} Low R_{Flow} Low
A_{Cryo} Very Low

2) **Butyl acetate** (Acetic acid, butyl ester) [48]



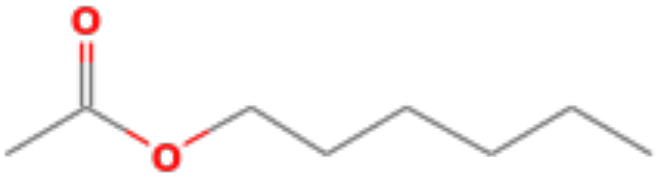
Odor type: ETHEREAL (Banana)
Flavour: ETHEREAL
Strong
http://www.perflavory.com/docs/doc1019351.html
Signal: C_{Cryo} Low
A_{Cryo} High

3) **Pentyl acetate** (Acetic acid, pentyl ester) [59] [106]



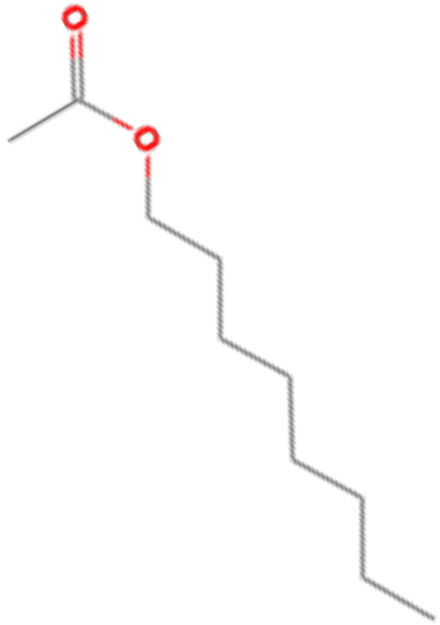
Odor type: FRUITY (Banana, Pear, Apple)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1040001.html
Signal: B_{Cryo} Very High

4) **Hexyl acetate** (Acetic acid, hexyl ester) [5] [7]



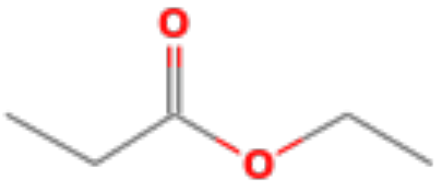
Odor type: FRUITY (Pear, Apple, Berry, Banana)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1003201.html
Signal: B_{Cryo} Low - Medium B_{Flow} Very High
R_{Cryo} Low - Medium R_{Flow} Very Low
A_{Cryo} Medium

5) **Octyl acetate** (Acetic acid, octyl ester) **[59]**



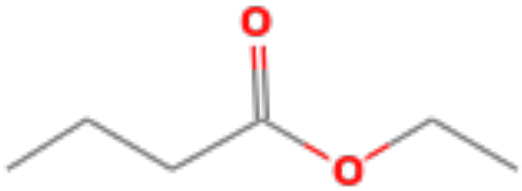
Odor type: FLORAL (Apple)
Flavour: WAXY
Medium
http://www.perflavory.com/docs/doc1003462.html
Signal: C_{Cryo} High
R_{Cryo} Medium

6) **Ethyl propionate** (Propanoic acid, ethyl ester) **[65] [90]**



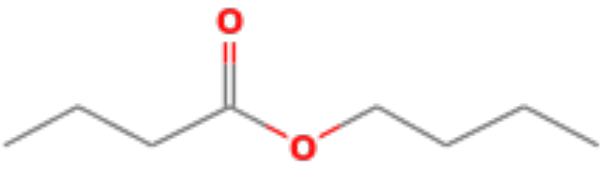
Odor type: FRUITY (Pineapple, Grape)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1004931.html
Signal: B_{Flow} Very Low
C_{Cryo} Low C_{Flow} Medium
R_{Cryo} Low R_{Flow} Very Low
A_{Cryo} Very Low

7) **Ethyl butyrate** (Butanoic acid, ethyl ester) **[23] [32]**



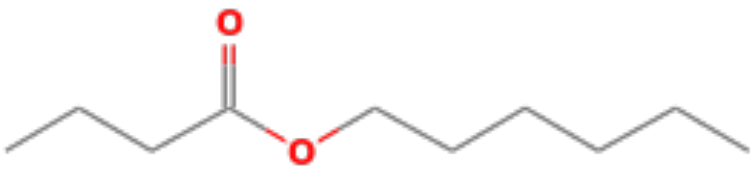
Odor type: FRUITY (Pineapple)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1004792.html
Signal: R_{Cryo} Medium R_{Flow} Very High
A_{Cryo} High

8) **Butyl butyrate** (Butanoic acid, butyl ester) **[46]**



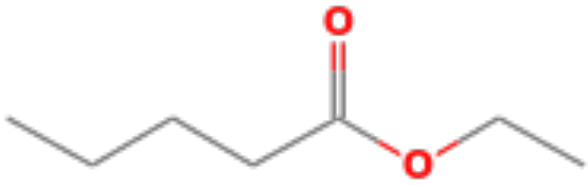
Odor type: FRUITY (Banana, Berry, Pineapple, Apple)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1014091.html
Signal: A_{Cryo} Very High

9) **Hexyl butyrate** (Butanoic acid, hexyl ester) **[21] [43]**



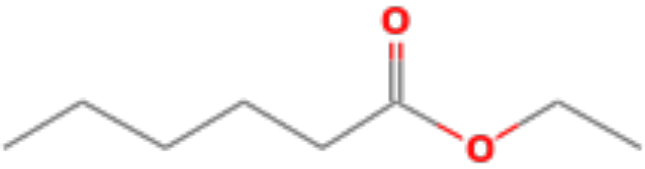
Odor type: GREEN (Apple)
Flavour: GREEN
Medium
http://www.perflavory.com/docs/doc1023951.html
Signal: C_{Flow} Low
R_{Cryo} Very Low
A_{Cryo} Very High A_{Flow} High

10) **Ethyl pentanoate** (Pentanoic acid, ethyl ester) **[75] [143]**



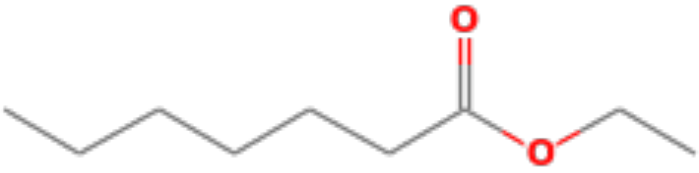
Odor type: FRUITY (Apple, Pineapple, Berry)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1000701.html
Signal: B_{Flow} Medium - High
C_{Cryo} Low C_{Flow} Low - Medium
A_{Cryo} High - Very High

11) **Ethyl hexanoate** (Hexanoic acid, ethyl ester) **[4] [6]**



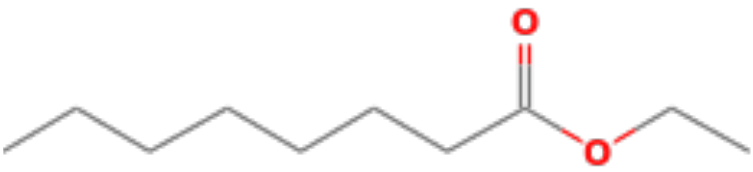
Odor type: FRUITY (Banana, Pineapple, Apple, Strawberry)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1004811.html
Signal: C_{Cryo} Very Low
R_{Cryo} Low-Medium
A_{Cryo} Low

12) **Ethyl heptanoate** (Heptanoic acid, ethyl ester) **[29]**



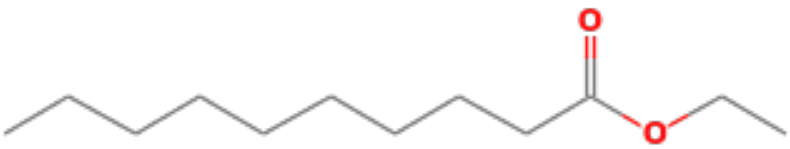
Odor type: FRUITY (Pineapple, Berry, Banana, Apple)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1009172.html
Signal: B_{Flow} Very Low - Low
P_{FLow} High

13) **Ethyl octanoate** (Octanoic acid, ethyl ester) **[2] [1] [176]**



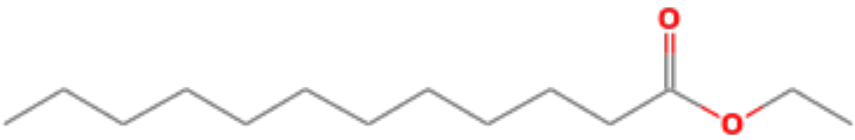
Odor type: WAXY (Banana, Pineapple, Apple, Apricot)
Flavour: WAXY
Medium
http://www.perflavory.com/docs/doc1056351.html
Signal: C_{Cryo} Very Low C_{FLow} High
R_{Cryo} Low-Medium R_{Flow} Low
A_{Cryo} Low

14) **Ethyl decanoate** (Decanoic acid, ethyl ester) **[15] [9]**



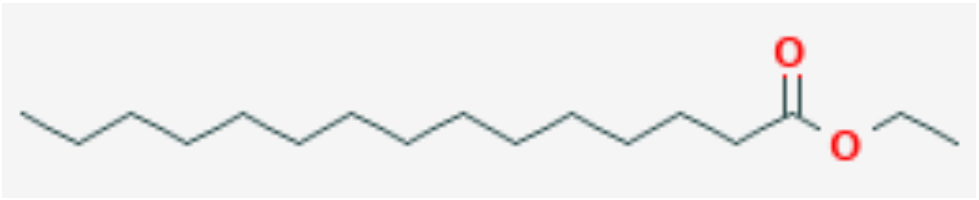
Odor type: WAXY (Apple)
Flavour: WAXY
Medium
http://www.perflavory.com/docs/doc1015411.html
Signal: C_{Flow} Low
R_{Cryo} Very Low
A_{Cryo} Low
P_{Cryo} Medium P_{Flow} High

15) **Ethyl laurate** (Dodecanoic acid, ethyl ester) **[47] [20]**



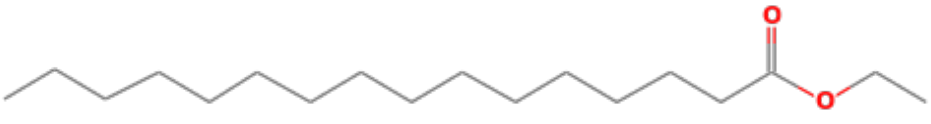
Odor type: WAXY
Flavour: WAXY
Medium
http://www.perflavory.com/docs/doc1012432.html
Signal: B_{Flow} Very Low
C_{Flow} Medium
A_{Cryo} High
P_{Cryo} Low - Medium P_{Flow}

16) **Ethyl Pentadecanoate** (Pentadecanoic acid, ethyl ester) **[313]**



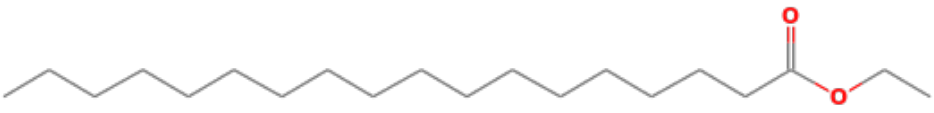
Odor type: SWEET
Flavour: nd
Medium
http://www.perflavory.com/docs/doc1434491.html

17) **Ethyl palmitate** (Hexadecanoic acid, ethyl ester) **[39]**



Odor type: WAXY
Flavour: WAXY
Low
http://www.perflavory.com/docs/doc1008251.html
Signal: C_{Cryo} Low
A_{Cryo} High

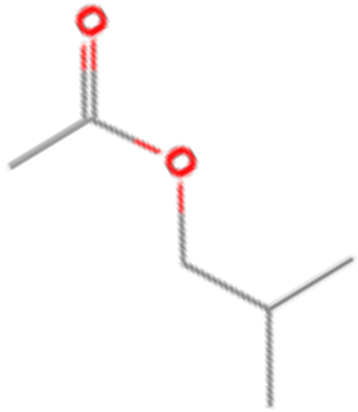
18) **Ethyl stearate** (Octadecanoic acid, ethyl ester) **[274]**



Odor type: WAXY
Flavour: nd
Low
http://www.perflavory.com/docs/doc1022961.html
Signal: C_{Cryo} Medium
R_{Cryo} Low
A_{Cryo} Low

Saturated branched esters

19) **Isobutyl acetate** (Isobutyl acetate) **[58] [86]**



Odor type:
Flavour:

Medium

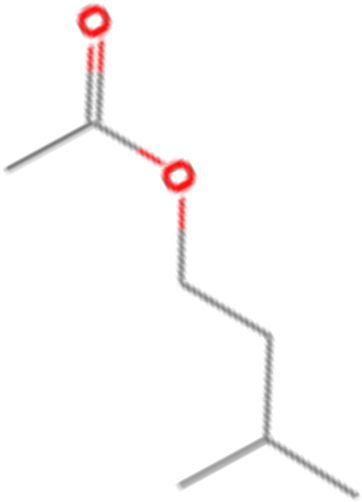
Signal:

B_{Flow} Very Low
C_{Cryo} Low C_{Flow} Medium
R_{Cryo} Low R_{Flow} Very Low - Low
A_{Cryo} Very Low

FRUITY (Banana, Apple, Pear)
FRUITY

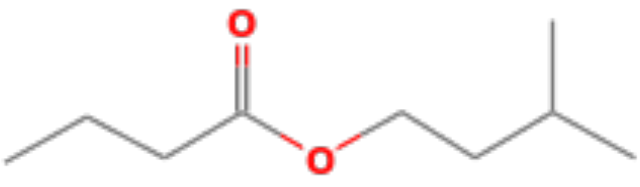
http://www.perflavory.com/docs/doc1013631.html

20) **Isoamyl acetate** (1-Butanol, 3-methyl-, acetate) **[1] [2]**



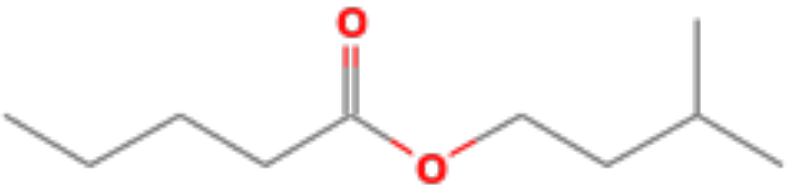
Odor type: FRUITY (Banana)
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1006711.html
Signal: B_{Cryo} High - Very High B_{Flow} Very High
C_{Cryo} Very Low
R_{Cryo} Very Low

21) **Isoamyl butyrate** (Butanoic acid, 3-methyl-, butyl ester) **[14] [28]**



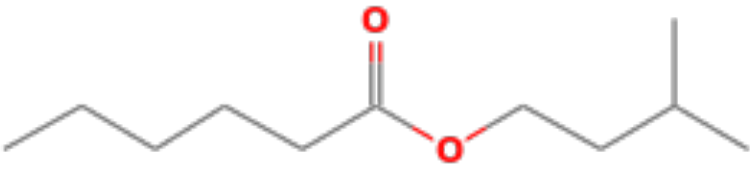
Odor type: FRUITY (Apricot, Banana, Pineapple, Pear)
Flavour: WAXY
Medium
http://www.perflavory.com/docs/doc1006752.html
Signal: B_{Flow} Very High
A_{Cryo} Very High A_{Flow} Very Low

22) **Isopentyl pentanoate** (Pentanoic acid, 3-methylbutyl ester) **[195]**



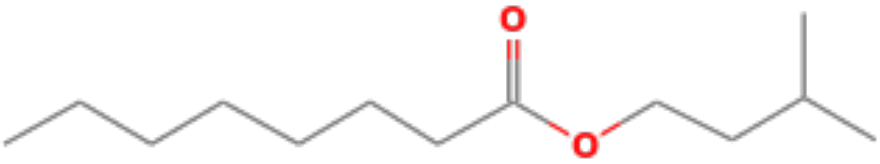
Odor type: FRUITY (Apple)
Flavour: FRUITY (Strawberry)
Medium
http://www.perflavory.com/docs/doc1045091.html
Signal: B_{Cryo} Very High
C_{Cryo} Very Low

23) **Isopentyl hexanoate** (Isopentyl hexanoate) **[192]**



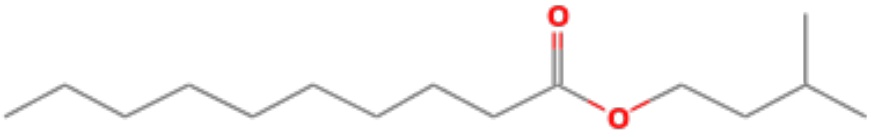
Odor type: FRUITY (Banana, Pineapple, Apple)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1019751.html
Signal: P_{Cryo} Very High

24) **Isopentyl octanoate** (Octanoic acid, 3-methylbutyl ester) **[184]**



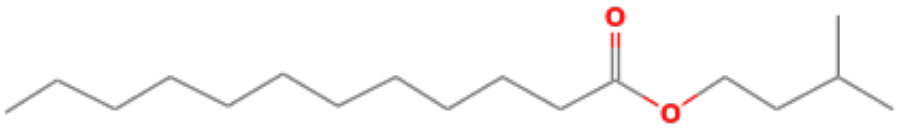
Odor type: FRUITY (Pineapple, Coconut)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1019811.html
Signal: R_{Cryo} Very high

25) **Isopentyl decanoate** (Pentadecanoic acid, 3-methylbutyl ester) **[197]**



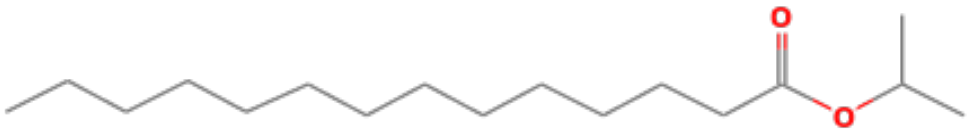
Odor type: WAXY (Banana, Coconut)
Flavour: WAXY
Medium
http://www.perflavory.com/docs/doc1001591.html

26) **Isoamyl laurate** (Isoamyl laurate) **[309]**



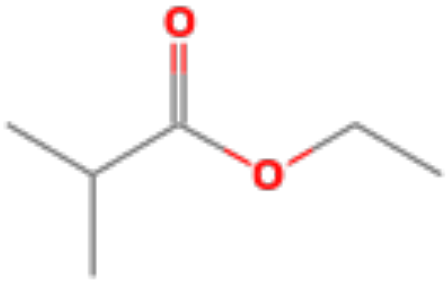
Odor type: WAXY (Peach)
Flavour: FATTY
Medium
http://www.perflavory.com/docs/doc1003691.html
Signal: C_{Cryo} Medium
R_{Cryo} Low
A_{Cryo} Very Low

27) **Isopropyl myristate** (Isopropyl myristate) **[245]**



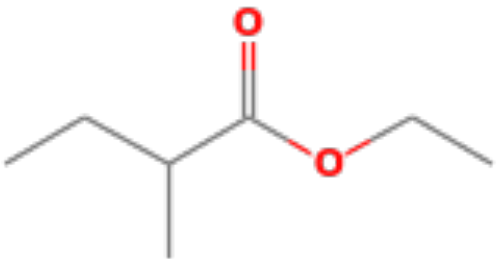
Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1019332.html

28) **Ethyl isobutyrate** (Propanoic acid, 2-methyl-, ethyl ester) **[137]**



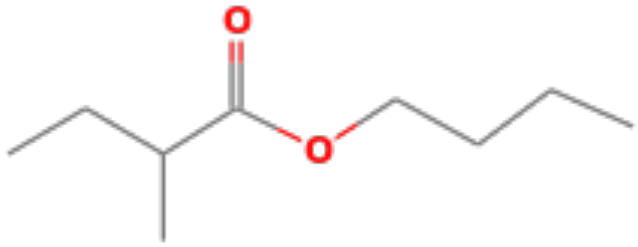
Odor type: FRUITY (Citrus, Cherry, Strawberry)
Flavour: ETHEREAL
High
http://www.perflavory.com/docs/doc1000751.html
Signal: C_{Cryo} Low
R_{Cryo} Very Low
A_{Cryo} Low

29) **Ethyl 2-methylbutyrate** (Butanoic acid, 2-methyl-, ethyl ester) **[13] [19]**



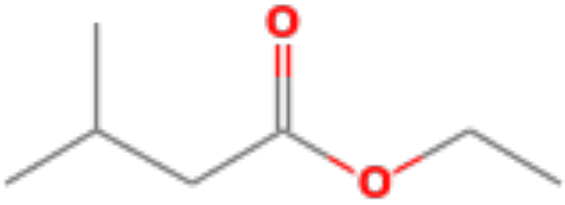
Odor type: FRUITY (Apple, Strawberry, Berry)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1004871.html
Signal: R_{Cryo} Low R_{Flow} Very Low - Low
A_{Cryo} Medium - High A_{Flow} Very High
P_{Cryo} Very Low

30) **Butyl 2-methylbutyrate** (Butyl 2-methylbutanoate) **[31]**



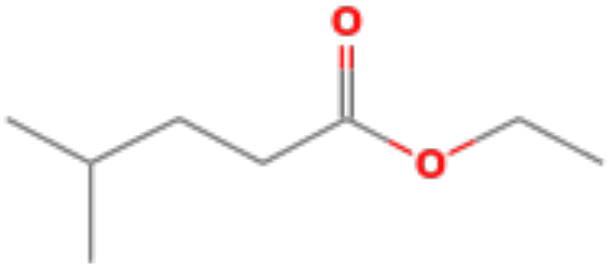
Odor type: GREEN (Cocoa, Pineapple, Apple)
Flavour: nd
Medium
http://www.perflavory.com/docs/doc1007621.html
Signal: B_{Cryo} Very High

31) **Ethyl isovalerate** (Butanoic acid, 3-methyl-, ethyl ester) **[73]**



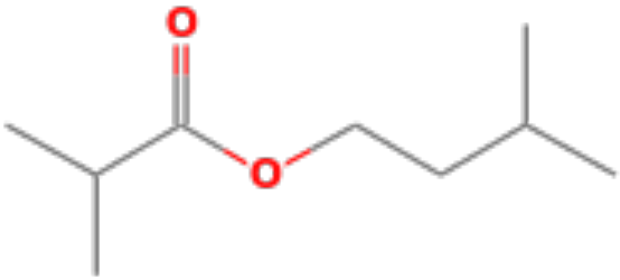
Odor type: FRUITY (Apple, Pineapple, Banana, Orange)
Flavour: FRUITY
High
http://www.perflavory.com/docs/doc1007041.html
Signal: A_{Cryo} Very High
P_{Cryo} Very Low

32) **Ethyl isohexanoate** (Pentanoic acid, 4-methyl-, ethyl ester) **[162]**



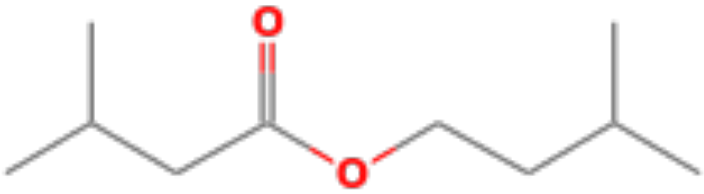
Odor type: FRUITY
Flavour: nd
Medium
http://www.perflavory.com/docs/doc1477041.html
Signal: C_{Cryo} High

33) **Isopentyl isobutyrate** (Propanoic acid, 2-methyl-, 3-methylbutyl ester) **[7] [12] [7] [12]**



Odor type: FRUITY (Banana, Pineapple, Apricot)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1003311.html
Signal: B_{Cryo} Very High B_{Flow} Very High
A_{Cryo} Very Low - Low
P_{Flow} Very Low

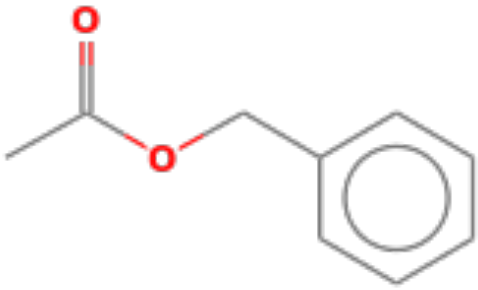
34) **Isoamyl isovalerate** (Butanoic acid, 3-methyl-, 3-methylbutyl ester **or** n-Amyl isovalerate)
[11] [66] [24] [25] [159]



Odor type: FRUITY (Apple, Banana, Apricot, Mango)
Flavour: GREEN
Medium
http://www.perflavory.com/docs/doc1003562.html
Signal: B_{Cryo} Very High B_{Flow} Very High

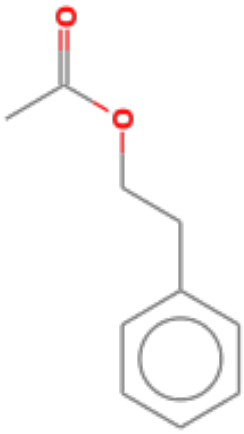
Unsaturated "aromatic" esters

35) **Benzyl acetate** (Acetic acid, phenylmethyl ester) **[50] [104]**



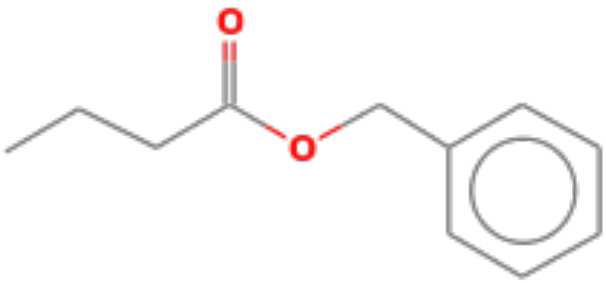
Odor type: FLORAL (Cherry, Apple, Apricot)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1001612.html
Signal: B_{Flow} Very Low
C_{Cryo} Very High C_{Flow} High

36) **Phenethyl acetate** (Acetic acid, 2-phenylethyl ester) **[9] [11]**



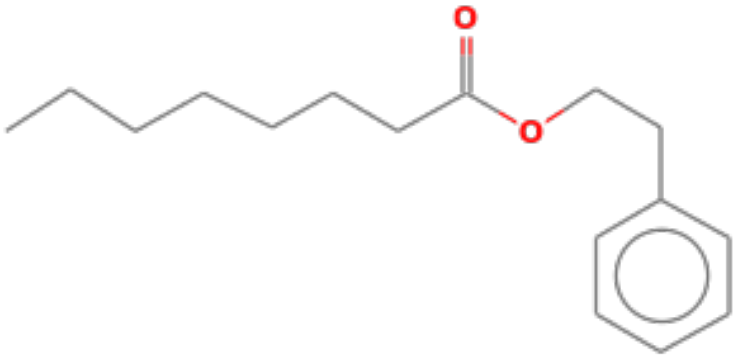
Odor type: Flavour: Medium Signal: B_{Cryo} Low C_{Cryo} Medium R_{Cryo} Medium	 B_{Flow} Low- Medium C_{Flow} Low - Medium R_{Flow} Low	FLORAL HONEY http://www.perflavory.com/docs/doc1010032.html

37) **Benzyl butyrate** (Butanoic acid, phenylmethyl ester) **[91]**



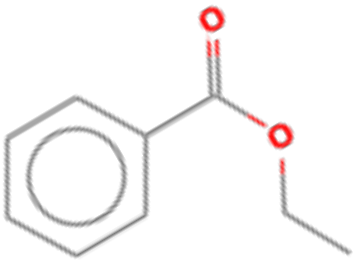
Odor type: FRUITY (Apricot, Berry)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1022171.html
Signal: B_{Cryo} Very High
R_{Cryo} Very Low -Low

38) **Phenethyl octanoate** (Octanoic acid, 2-phenylethyl ester) **[295]**



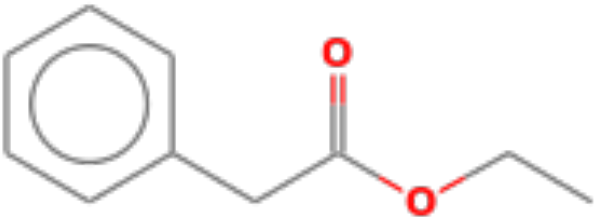
Odor type: WAXY
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1035571.html
Signal: C_{Cryo} Low - Medium
R_{Cryo} Low - Medium
P_{Cryo} Low

39) **Ethyl benzoate** (Benzoic acid, ethyl ester) **[25] [38]**



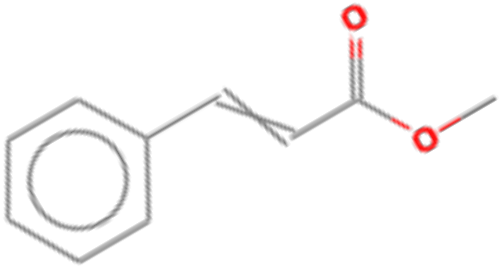
Odor type: MINTY (Cherry, Grape)
Flavour: MEDICINAL
Medium
http://www.perflavory.com/docs/doc1004771.html
Signal: B_{Cryo} Very High B_{Flow}

40) **Ethyl phenylacetate** (Benzeneacetic acid, ethyl ester) **[140]**



Odor type: FLORAL (Apple, Apricot, Cherry, Pineapple, Raspberry)
Flavour: HONEY
High
http://www.perflavory.com/docs/doc1015111.html
Signal: A_{Cryo} Medium - High
P_{Cryo} Low

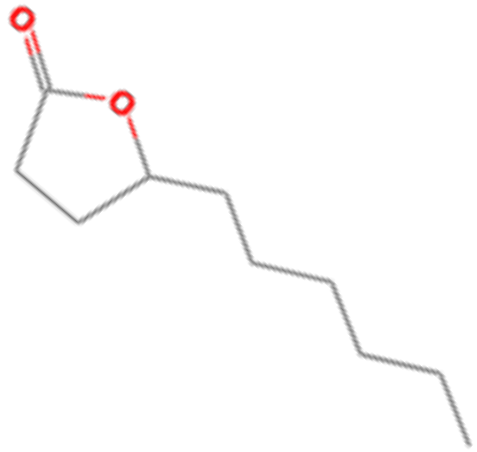
41) **Methyl (E)-cinnamate** (2-Propenoic acid, 3-phenyl-, methyl ester, (E)-) **[79]**



Odor type: BALSAMIC (Strawberry, Cherry)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1008271.html
Signal: R_{Cryo} Very High

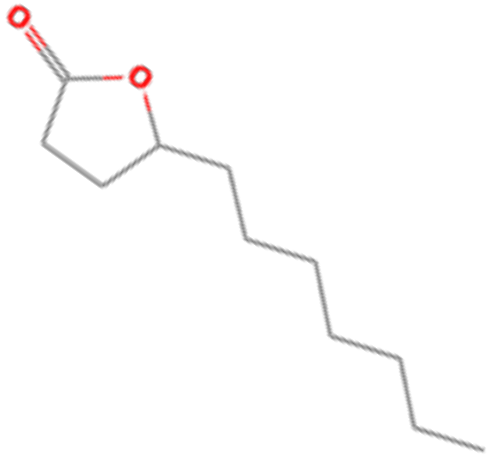
Lactones

42) γ-**Decalactone** (2(3H)-Furanone, 5-hexyldihydro-) **[56] [65]**



Odor type: FRUITY (Peach, Coconut)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1012281.html
Signal: B_{Flow} Low, C_{Flow} Medium, R_{Flow} Very Low, R_{Cryo} Low, A_{Cryo} High

43) γ-**Undecalactone** (2(3H)-Furanone, 5-heptyldihydro-) **[77] [94] [80]**

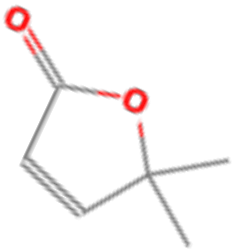


Odor type: FRUITY (Peach, Apricot, Coconut)
Flavour: CREAMY
Medium
http://www.perflavory.com/docs/doc1000822.html
Signal: B_{Flow} Low, C_{Flow} Medium, R_{Flow} Very Low, P_{Cryo} Very High

44) γ-**Dodecalactone** (τ-Dodecalactone) **[100]**

Odor type: FRUITY (Peach)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1013371.html
Signal: P_{Cryo} Very High

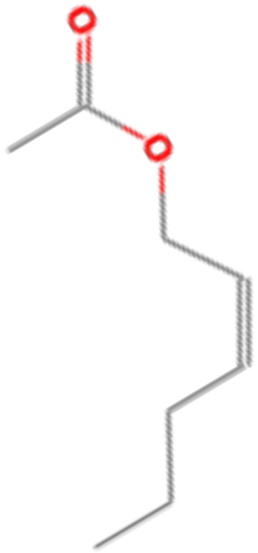
45) **2(5H)-Furanone, 5,5-dimethyl-** (2(5H)-Furanone, 5,5-dimethyl-) **[232]**



Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1428431.html
Signal: C_{Cryo} Medium
A_{Cryo} Medium - High
P_{Cryo} Low

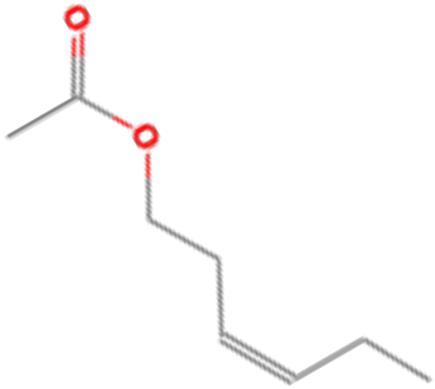
Unsaturated linear esters

46) **cis-2-Hexenyl acetate** (2-Hexen-1-ol, acetate, (Z)-) **[30]**



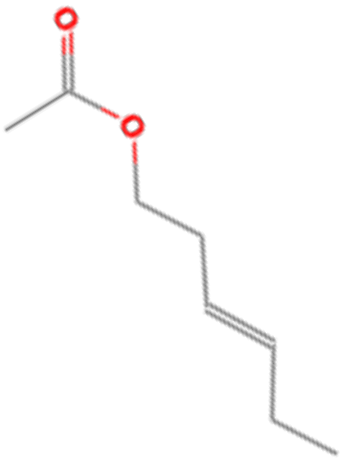
Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1400051.html
Signal: B_{Cryo} High
A_{Cryo} Low

47) **cis-3-Hexenyl acetate** (3-Hexen-1-ol, acetate, (Z)-) **[16]**



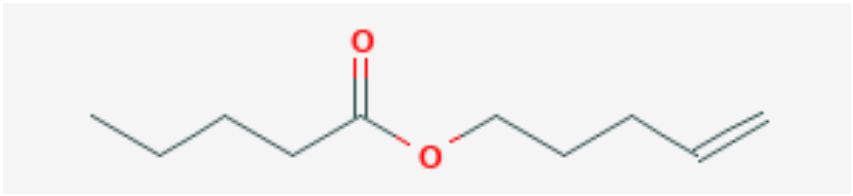
Odor type: GREEN (Pineapple)
Flavour: GREEN
Strong
http://www.perflavory.com/docs/doc1004792.html
Signal: R_{Flow} High
A_{Flow} Low

48) **trans-3-Hexenyl acetate** (3-Hexen-1-ol, acetate, (E)-) **[17]**



Odor type: FRUITY (Banana, Pear)
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1130931.html
Signal: R_{Cryo} Medium
A_{Cryo} Medium - Strong

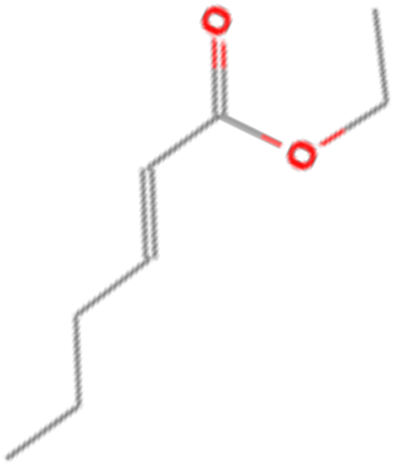
49) **4-Pentenyl pentanoate** (Valeric acid, 4-pentenyl ester [194]) **[194]**



/

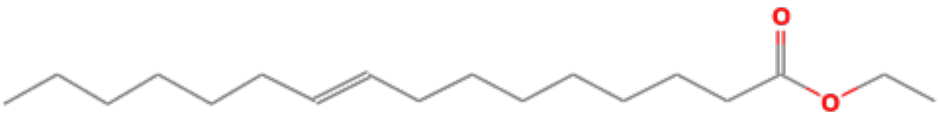
B_{Cryo} High
C_{Cryo} Medium

50) **Ethyl 2-hexenoate** (2-Hexenoic acid, ethyl ester) **[35]**



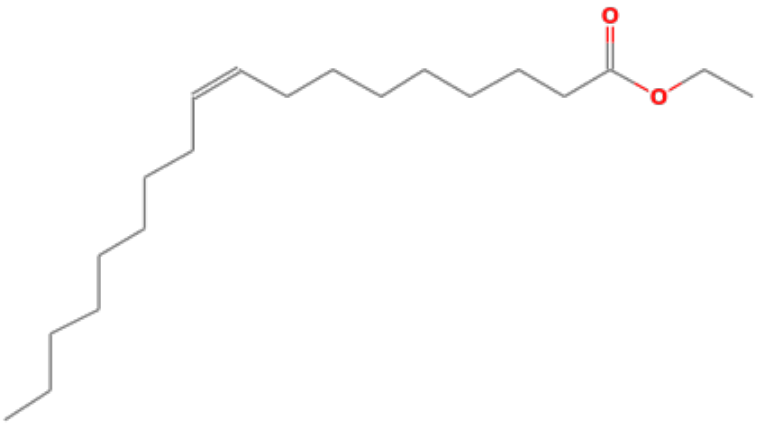
Odor type: FRUITY
Flavour: FRUITY
Medium
http://www.perflavory.com/docs/doc1385771.html
Signal: B_{Cryo} High
A_{Cryo} Medium

51) **Ethyl 9-hexadecenoate** (Ethyl 9-hexadecenoate) **[127]**



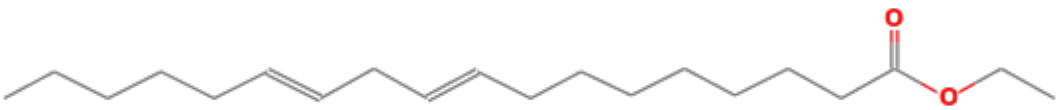
Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1587311.html
Signal: B_{Cryo} High
C_{Cryo} Low - Medium

52) **Ethyl oleate** (Ethyl Oleate) **[250]**



Odor type (Z): FATTY
Odor type (E): nd
Flavour (Z): FATTY
Flavour (E): nd
Low
Z: http://www.perflavory.com/docs/doc1023041.html
E: http://www.perflavory.com/docs/doc1433821.html
Signal: C_{Cryo} Medium - High
A_{Cryo} Medium

53) **Ethyl-9,12-octadecadienoate** (9,12-Octadecadienoic acid, ethyl ester) **[223]**



/

C_{Cryo} Medium - High
A_{Cryo} Medium

54) **Ethyl linolenate** (Ethyl 9,12,15-octadecatrienoate) **[307]**

Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1043721.html
Signal: B_{Cryo} Medium
C_{Cryo} Medium
R_{Cryo} Low

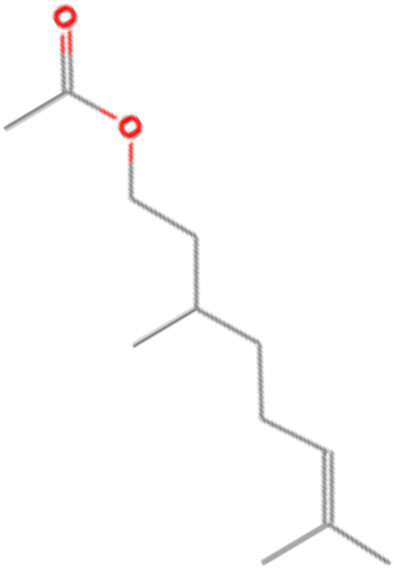
55) **Methyl 5,8,11-heptadecatriynoate** (5,8,11-Heptadecatriynoic acid, methyl ester) **[168]**

/

B_{Cryo} Low
R_{Cryo} Very High

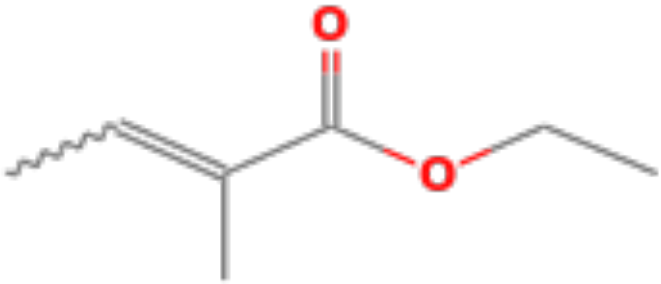
Unsaturated branched esters

56) **Citronellyl acetate** (6-Octen-1-ol, 3,7-dimethyl-, acetate) **[36] [36]**



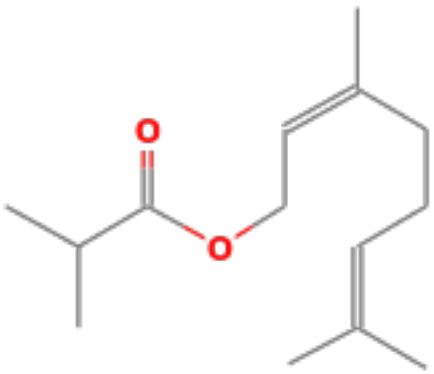
Odor type: FLORAL (Pear)
Flavour: FLORAL
Medium
http://www.perflavory.com/docs/doc1012172.html
Signal: R_{Cryo} High R_{Flow} High - Very High
P_{Cryo} Low

57) **Ethyl tiglate** (2-Butenoic acid, 2-methyl-, ethyl ester) **[300]**



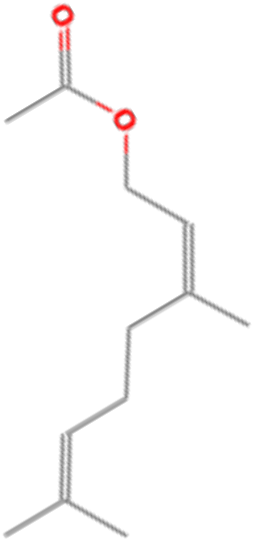
Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1052991.html

58) **Geranyl isobutyrate** (Geranyl isobutyrate) **[63]**



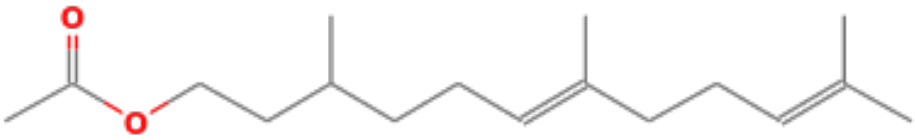
Odor type: FLORAL
Flavour: FLORAL
Medium
http://www.perflavory.com/docs/doc1016431.html
Signal: C_{Cryo} Very low
R_{Cryo} High

59) **Geranyl acetate** (if trans) (2,6-Octadien-1-ol, 3,7-dimethyl-, acetate) **[31] [23]**



Odor type: FLORAL
Flavour: GREEN
Medium
http://www.perflavory.com/docs/doc1030092.html
Signal: R_{Cryo} High R_{Flow} Medium - High
P_{Cryo} Medium P_{Flow} Low - Medium

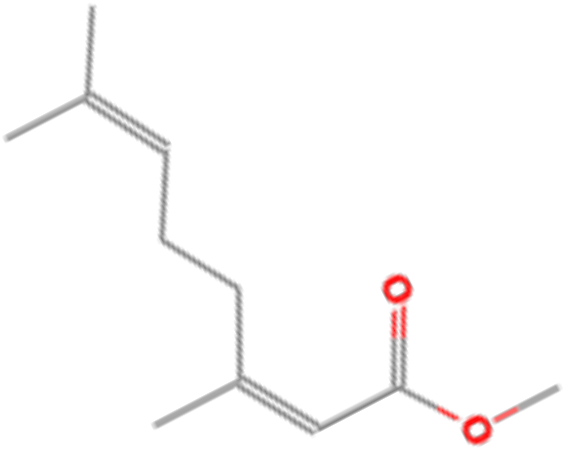
60) **2,3-Dihydro Farnesyl acetate** (2,3-Dihydro farnesyl acetate) **[293]**



/

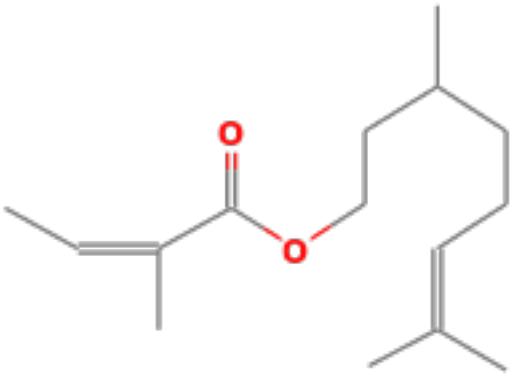
Signal: C_{Cryo} Low
R_{Cryo} High

61) **Methyl geranate** (if Trans) (2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester) **[231]**



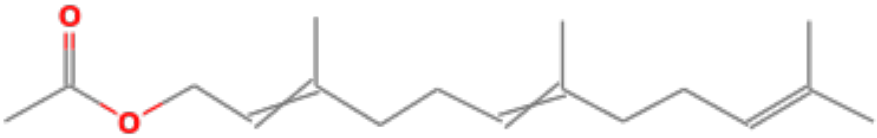
Odor type (Z): FLORAL
Odor type (E): WAXY
Flavour: nd
Medium
Z: http://www.perflavory.com/docs/doc1050841.html
E: http://www.perflavory.com/docs/doc1046801.html
Signal: C_{Cryo} Very High

62) **Citronellyl tiglate** (Citronellyl tiglate) **[225]**



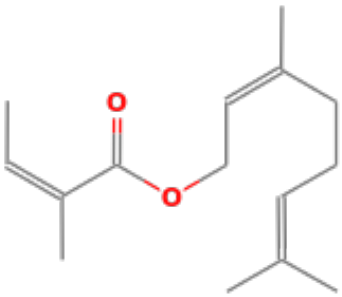
Odor type: FLORAL
Flavour: GREEN
Medium
http://www.perflavory.com/docs/doc1004481.html
Signal: C_{Cryo} Low
R_{Cryo} High

63) **Farnesol acetate** (Farnesol, acetate) **[247]**



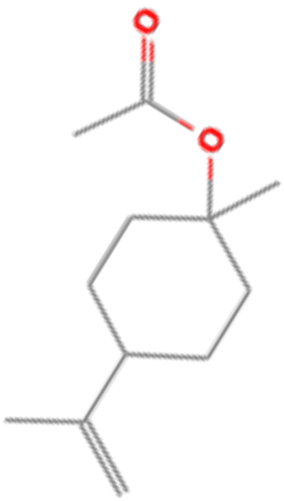
Odor type: FLORAL
Flavour: FLORAL
Medium
http://www.perflavory.com/docs/doc1023681.html
Signal: C_{Cryo} Low
R_{Cryo} High

64) **Geranyl Angelate** (Geranyl Angelate) **[200]**



/
R_{Cryo} Very High

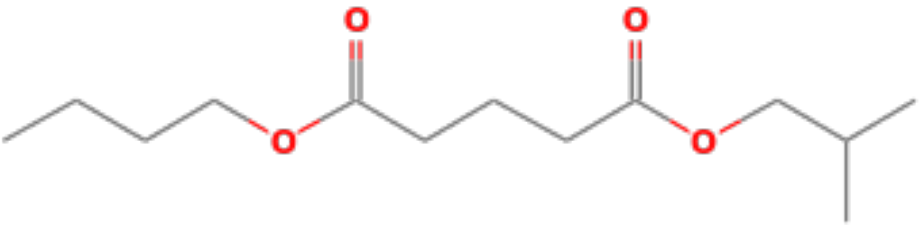
65) **Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate** (Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate) **[49]**



Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1382861.html
Signal: R_{Cryo} Very Low
P_{Cryo} Very High

Di-esters

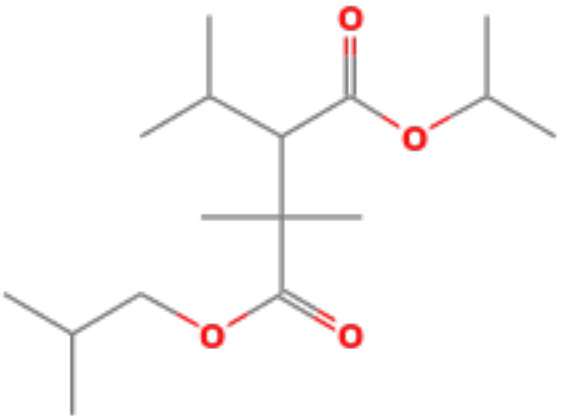
66) **Glutaric acid, butyl isobutyl ester** (Glutaric acid, butyl isobutyl ester) **[216]**



/

C_{Cryo} High
R_{Cryo} Low

67) **Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester** (Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester) **[267]**

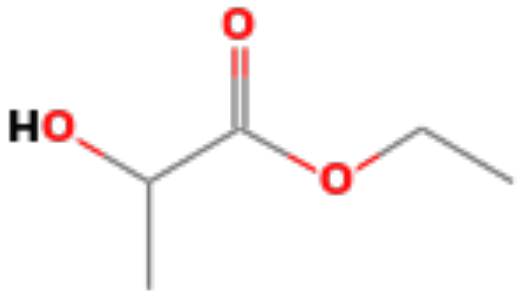


/

R_{Cryo} High
A_{Cryo} Low - Medium

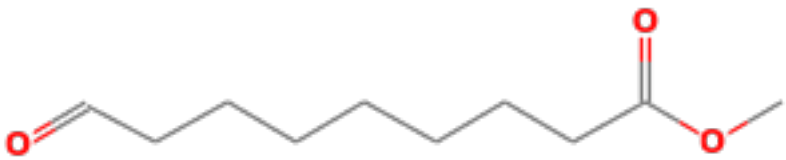
Esters with other functional groups

68) **Ethyl lactate** (Propanoic acid, 2-hydroxy-, ethyl ester) **[24]**



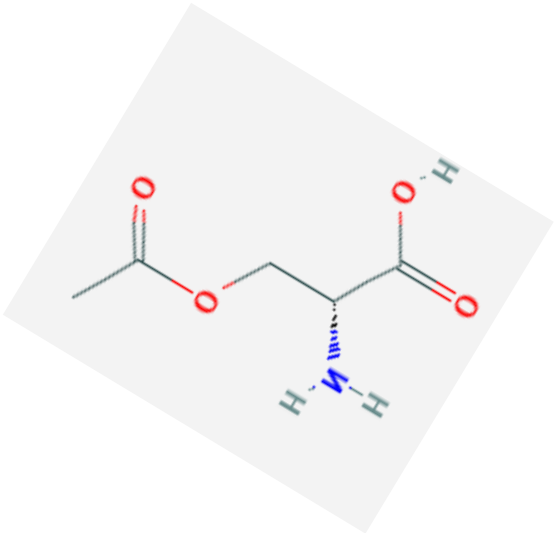
Odor type: FRUITY
Flavour: FRUITY
Strong
http://www.perflavory.com/docs/doc1032431.html
Signal: C_{Flow} High
A_{Flow} Low - Medium

69) **Methyl 9-oxononanoate** (Nonanoic acid, 2-oxo-, methyl ester) **[76]**



Odor type: nd
Flavour: nd
nd
http://www.perflavory.com/docs/doc1625811.html
Signal: B_{Cryo} Medium
R_{Cryo} High - Very High

70) **O-Acetylserine** (o-Acetyl-L-serine) **[316]**



/

A_{Cryo} High