COSMOS

ADDING VALUE TO CAMELINA AND CRAMBE OIL

Camelina & crambe **O**il crops as **S**ources for **M**edium-chain **O**ils for **S**pecialty oleochemicals

(Grant Agreement No. 635405)

D 6.1 List of molecules that can be used for flavors and fragrances

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Contents

1 Introduction

The objective of this deliverable (D6.1 linked to T6.6) is to identify medium chains functionalized molecules that can be used in flavors and fragrances. The purpose is to valorize long chains or medium chains fatty acids from the Cosmos project into high value marketable products. We have especially focused on the cross-metathesis (T6.2) and oxidative cleavage (T6.3) technologies which are investigated in the project. These technologies are versatile to get acids, esters, aldehydes, alcohols or nitriles derivatives which are well known in the flavors and fragrances industry.

Several of these routes are covered in Arkema's patent applications and granted patents which have been included in the Cosmos accessible background.

2 Flavors and fragrances compounds

Investigations about the existing flavors and fragrances molecules have been carried out principally through the SAFC "Flavors & Fragrances" catalog and the website www.thegoodscentscompany.com.

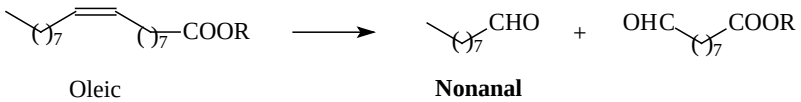
2.1 Aldehydes

A lot of linear aldehydes (saturated or unsaturated) are listed among the commercially available aroma materials.

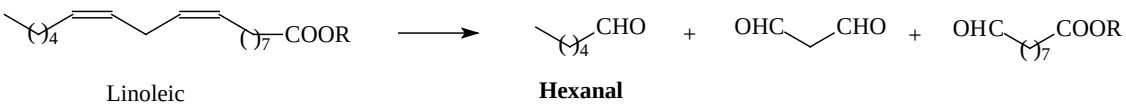
2.1.1. Saturated

Molecule	Formula	Odor/Flavor	Reference
Hexanal	CH_3-$(CH_2)_4$-CHO	Fatty, green	SAFC
Heptanal	CH_3-$(CH_2)_5$-CHO	Oily, fruity, woody, fatty, nutty	SAFC
Octanal	CH_3-$(CH_2)_6$-CHO	Honey, fatty, fruity, citrus	SAFC
Nonanal	CH_3-$(CH_2)_7$-CHO	Apple, coconut, grape, grapefruit, lemon, lime, melon, oily, orange, nutty, citrus, waxy, fatty, peach, rose, vegetable, fishy, meaty	SAFC
Decanal	CH_3-$(CH_2)_8$-CHO	Waxy, floral, citrus, sweet	SAFC
Undecanal	CH_3-$(CH_2)_9$-CHO	Orange, fatty, rose, waxy	SAFC
Dodecanal	CH_3-$(CH_2)_{10}$-CHO	Herbaceous, waxy, floral, sweet	SAFC
Tridecanal	CH_3-$(CH_2)_{11}$-CHO	Fatty, waxy, citrus	SAFC

Saturated aldehydes such as **nonanal** or **hexanal** are accessible from the Cosmos ω9 fatty acids (oleic, eicosenoic, erucic) or ω6 (linoleic) through **oxidative cleavage** or **ozonolysis** (in reductive conditions):

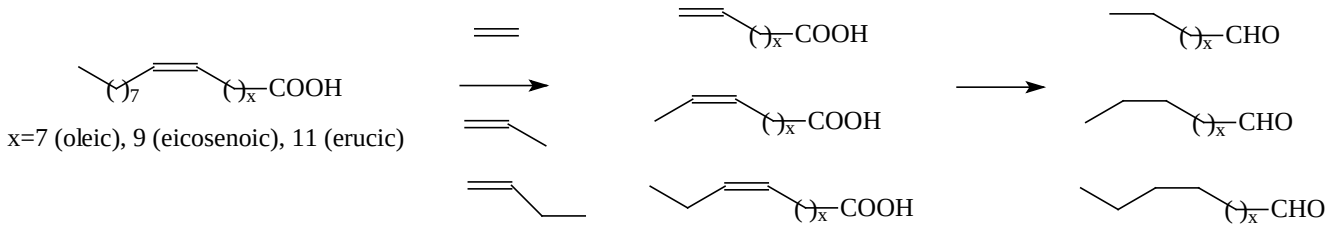


Oleic **Nonanal**



Linoleic **Hexanal**

Medium chains saturated fatty aldehydes (**decanal**, **undecanal**, **dodecanal**, **tridecanal**) could be obtained through alkenolysis (cross-metathesis with ethylene, propene, 1-butene) of the Cosmos fatty acids followed by a selective hydrogenation of the acid function into aldehyde:

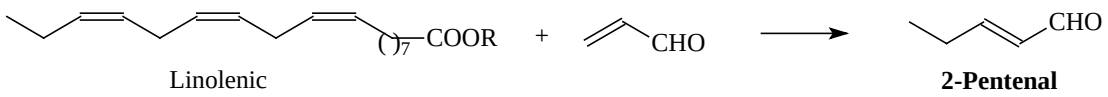


Saturated even numbered aldehydes can also be obtained by direct reduction of the corresponding acids. Technologies from the project are more valuable for odd numbered and/or unsaturated aldehydes.

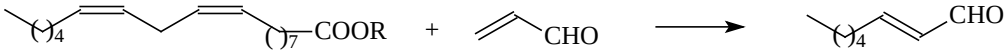
2.1.2. Unsaturated

Molecule	Formula	Odor/Flavor	Reference
2-Pentenal (trans)	CH_3-CH_2-CH=CH-CHO	Apple, orange, green, vegetable	SAFC
2-Hexenal (trans)	CH_3-$(CH_2)_2$-CH=CH-CHO	Almond, apple, green, plum, sweet, vegetable	SAFC
2-Heptenal (trans)	CH_3-$(CH_2)_3$-CH=CH-CHO	Apple, lemon, green, fatty, spicy, vegetable	SAFC
2-Octenal (trans)	CH_3-$(CH_2)_4$-CH=CH-CHO	Spicy, herbaceous, green	SAFC
2-Nonenal (trans)	CH_3-$(CH_2)_5$-CH=CH-CHO	Waxy, fatty	SAFC
2-Decenal (trans)	CH_3-$(CH_2)_6$-CH=CH-CHO	Oily, orange, floral, citrus, fatty, waxy, green, meaty	SAFC
2-Undecenal (trans)	CH_3-$(CH_2)_7$-CH=CH-CHO	Orange, herbaceous, fruity	SAFC
2-Dodecenal (trans)	CH_3-$(CH_2)_8$-CH=CH-CHO	Orange, fatty, herbaceous	SAFC
2-Tridecenal (trans)	CH_3-$(CH_2)_9$-CH=CH-CHO	Waxy, citrus	SAFC
10-Undecenal	CH_2=CH-$(CH_2)_8$-CHO	Fatty, citrus, rose, sweet	SAFC

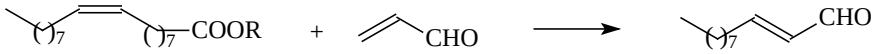
α,β-Unsaturated aldehydes such as **2-pentenal**, **2-octenal**, **2-undecenal** could be obtained from the Cosmos fatty acids (oleic, linoleic, linolenic, eicosenoic, erucic) through **cross-metathesis** with acrolein:



Linolenic **2-Pentenal**



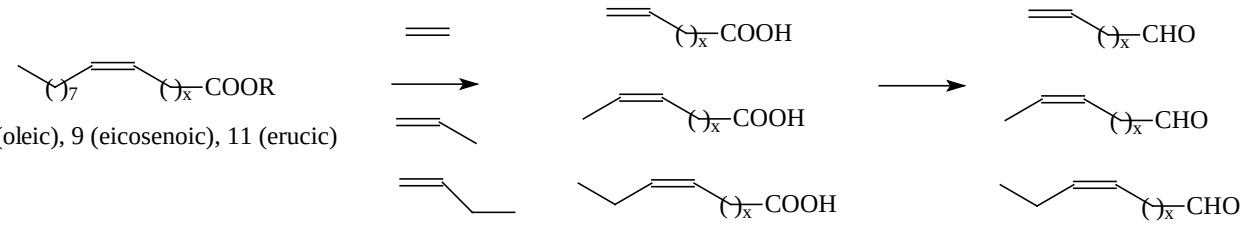
Linoleic **2-Octenal**



Oleic **2-Undecenal**

Eicosenoic acid (ω9 from camelina) and erucic acid (ω9 from crambe) also give 2-undecenal by cross-metathesis with acrolein.

In perfumery, 10-undecenal is currently one essential aldehyde to create the “aldehydic note”. It is industrially produced from undecylenic acid (coming from castor oil cracking). 10-undecenal cannot be obtained directly from camelina or crambe but some similar compounds such as 9-decenal, 9-undecenal, 9-dodecenal, 11-dodecenal, 11-tridecenal... could be synthesized through alkenolysis and the same reduction process used for 10-undecenal (reduction with formic acid):



The molecules which are described in literature are generally the trans isomers since they are obtained through chemical synthesis. It is noteworthy that with the technologies from the project (metathesis), a mixture of cis and trans isomers should be expected. Based on similar cases, we should underline that the odor is most probably different for both isomers.

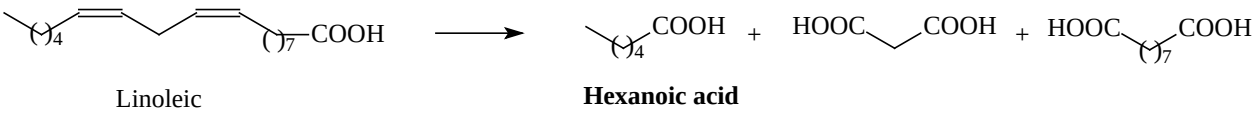
2.2 Acids and esters

2.2.1. Saturated acids

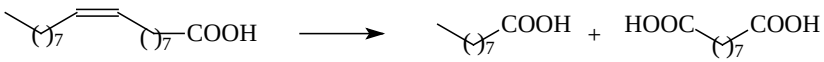
Straight chains saturated fatty acids are already known in aromas:

Molecule	**Formula**	**Odor/Flavor**	**Reference**
Hexanoic acid	CH_3-$(CH_2)_4$-COOH	Cheese, fatty, sour	SAFC
Heptanoic acid	CH_3-$(CH_2)_5$-COOH	Sour	SAFC
Octanoic acid	CH_3-$(CH_2)_6$-COOH	Oily	SAFC
Nonanoic acid	CH_3-$(CH_2)_7$-COOH	Chesse, waxy	SAFC
Decanoic acid	CH_3-$(CH_2)_8$-COOH	Fatty, citrus	SAFC
Undecanoic acid	CH_3-$(CH_2)_9$-COOH	Oily	SAFC
Dodecanoic acid	CH_3-$(CH_2)_{10}$-COOH	Fatty	SAFC
Tridecanoic acid	CH_3-$(CH_2)_{11}$-COOH	Waxy	SAFC
Tetradecanoic acid	CH_3-$(CH_2)_{12}$-COOH	Oily, waxy	SAFC

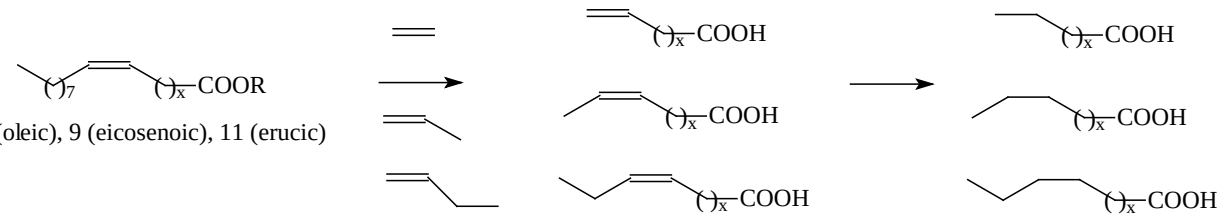
Medium chains fatty acids are the purpose of the Cosmos project. **Hexanoic** and **nonanoic acid** can be obtained by the **oxidative cleavage** technology while the C10-C14 acids (**decanoic, undecanoic, dodecanoic, tridecanoic, tetradecanoic**) are accessible through **cross-metathesis**:



Linoleic **Hexanoic acid**



Oleic **Nonanoic acid**



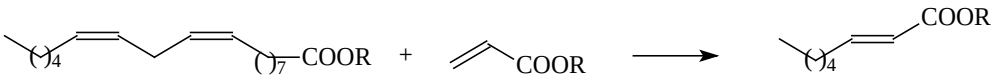
x=7 (oleic), 9 (eicosenoic), 11 (erucic)

Even numbered fatty acids are the natural compounds found in oils and fats. The technologies developed in the project are probably more valuable for the unsaturated and/or odd numbered fatty acids.

2.2.2. Unsaturated acids

Molecule	Formula	Odor/Flavor	Reference
2-Hexenoic acid (trans)	CH_3-$(CH_2)_2$-CH=CH-COOH	Musty, fatty, sweet	SAFC
2-Octenoic acid (trans)	CH_3-$(CH_2)_4$-CH=CH-COOH	Sour, fatty, waxy	SAFC
2-Decenoic acid	CH_3-$(CH_2)_7$-CH=CH-COOH	Fatty	The Good Scents Company
9-Decenoic acid	CH_2=CH-$(CH_2)_7$-COOH	Waxy	The Good Scents Company
10-Undecenoic acid	CH_2=CH-$(CH_2)_8$-COOH	Woody, sweet	SAFC

α,β-Unsaturated acids such **2-octenoic acid** can be obtained by **cross-metathesis** of linoleic acid with an acrylic acid derivative (example methyl acrylate followed by hydrolysis).



Linoleic **2-Octenoic acid**

From oleic acid or eicosenoic acid (camelina) chains, we would get by the same chemistry 2-undecenoic acid or 2-tridecenoic acid which are currently not classified for fragrances use but which could be of interest (similarity with 2-decenoic acid).

ω-Unsaturated acids such as **9-decenoic acid** are accessible through **cross-metathesis** of δ-9 fatty acids (oleic, linoleic, linolenic) with ethylene, propene or 1-butene:

Oleic **9-Decenoic acid**

Metathesis might be a valuable technique to produce these unsaturated fatty acids but it always generate a coproduct for which it would be necessary to find a value.

2.2.3. Saturated esters

The odors and flavors of medium chains fatty esters depends both on the chain length and the nature of the ester function (methyl, ethyl, butyl, amyl, isoamyl…)

Molecule	Formula	Odor/Flavor	Reference
Methyl hexanoate	CH_3-$(CH_2)_4$-$COOCH_3$	Ethereal, pineapple	SAFC
Methyl nonanoate	CH_3-$(CH_2)_7$-$COOCH_3$	Coconut, nutty, wine-like	SAFC
Methyl decanoate	CH_3-$(CH_2)_7$-$COOCH_3$	Oily, wine, fruity	The Good Scents Company
Ethyl undecanoate	CH_3-$(CH_2)_8$-$COOC_2H_5$	Coconut	SAFC
Methyl laurate	CH_3-$(CH_2)_{10}$-$COOCH_3$	Coconut, creamy, soapy, waxy	SAFC
Ethyl laurate	CH_3-$(CH_2)_{10}$-$COOC_2H_5$	Green, fruity, floral	SAFC

Medium chains fatty esters such as **methyl hexanoate** and **methyl nonanoate** can be obtained with the **oxidative cleavage** technology according to the same chemistry as the corresponding acids (see 2.2.1). The C10-C12 esters (**decanoate, undecanoate, laurate**) are accessible through **cross-metathesis** as for the acid derivatives (see 2.2.1).

Even numbered fatty esters can be produced by esterification or transesterification of natural fatty acids or oils and fats.

2.2.4. Unsaturated esters

Molecule	Formula	Odor/Flavor	Reference
Methyl 2-Octenoate (trans)	CH_3-$(CH_2)_4$-CH=CH-$COOCH_3$	Fruity, green	SAFC
Methyl 2-Nonenoate (trans)	CH_3-$(CH_2)_5$-CH=CH-$COOCH_3$	Green, violet	SAFC
Ethyl 2-Decenoate (trans)	CH_3-$(CH_2)_6$-CH=CH-$COOC_2H_5$	Fatty, waxy	SAFC
Methyl 10-undecenoate	CH_2=CH-$(CH_2)_8$-$COOCH_3$	Banana, honey, oily, citrus, rose, earthy, soapy, wine-like	SAFC

α,β-Unsaturated esters such **methyl 2-octenoate** can be obtained by **cross-metathesis** of linoleic acid derivative with methyl acrylate (same chemistry as acids in 2.2.2). The same chemistry applied to oleic acid derivatives would lead to methyl or ethyl 2-undecenoate whose properties should be close to ethyl 2-decenoate.

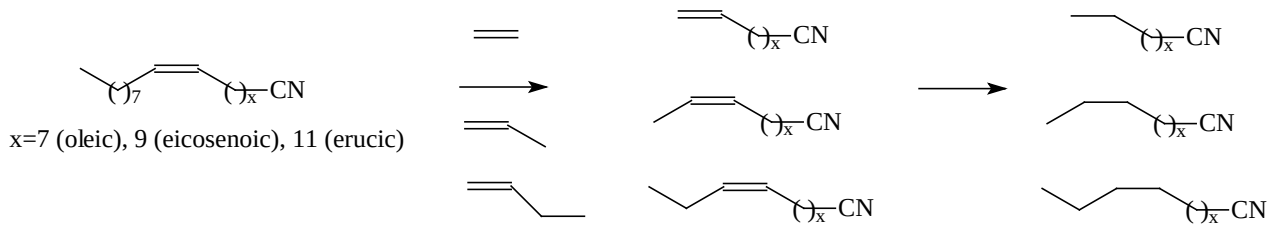
ω-Unsaturated esters such as methyl 9-decenoate are accessible through cross-metathesis of δ-9 fatty esters (oleic, linoleic, linolenic) with ethylene, propene or 1-butene. Properties of these molecules should be of interest with regards to existing methyl 10-undecenoate.

2.3 Nitriles

A few linear nitriles are described for perfumes applications. These compounds are less affected than aldehydes in acid, basic or oxidizing conditions, and exhibit aldehydic and hesperidic notes with floral aspects which are similar to aldehydes.

Molecule	Formula	Odor/Flavor	Reference
Octane nitrile	CH_3-$(CH_2)_6$-CN	Fatty, green	The Good Scents Company
Decane nitrile	CH_3-$(CH_2)_8$-CN	Fatty	The Good Scents Company
Dodecane nitrile	CH_3-$(CH_2)_{10}$-CN	Citrus	The Good Scents Company
Tretadecane nitrile	CH_3-$(CH_2)_{12}$-CN	Fresh, orange, green	The Good Scents Company
9-Undecenitrile	CH_3-CH=CH-$(CH_2)_7$-CN	Fresh, floral, fruity	EP1174117
10-Undecenitrile	CH_2=CH-$(CH_2)_8$-CN	Fresh, floral, fruity	EP1174117

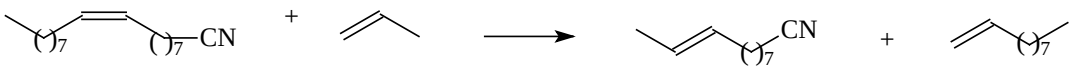
Medium chains saturated fatty nitriles such as **decanitrile**, **dodecanenitrile** and **tetradecanitrile** can be obtained from fatty acids or nitriles (oleic, eicosenoic, erucic) by cross-metathesis:



From ω9 fatty acids (oleic, eicosenoic, erucic), we could obtain by oxidative cleavage nonanenitrile whose properties should be close to known octanenitrile and decanenitrile.

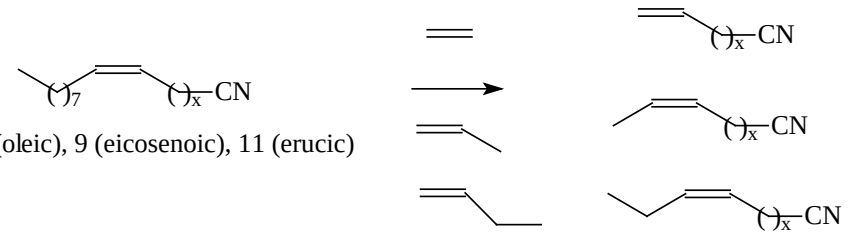
Saturated nitriles with even numbers can also be obtained by direct conversion of the acids to the nitriles. The technologies developed in the project would be more valuable for odd numbered and unsaturated nitriles.

Medium chains unsaturated fatty nitriles such as **9-undecenitrile** can be obtained by cross-metathesis of δ9 fatty acids/nitriles (oleic, linoleic…) with propene:



Oleic **9-Undecenitrile**

More generally, cross-metathesis from unsaturated fatty acids (oleic, eicosenoic, erucic) with different olefins (ethylene, propene, 1-butene) gives the opportunity to get a range of medium chains unsaturated nitriles with structures close to 9-undecenitrile and 10-undecenitrile:



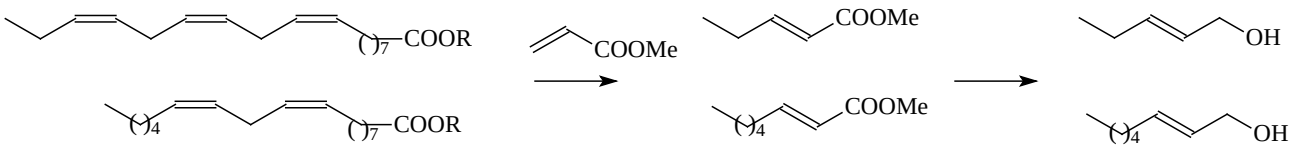
x=7 (oleic), 9 (eicosenoic), 11 (erucic)

2.4 Alcohols

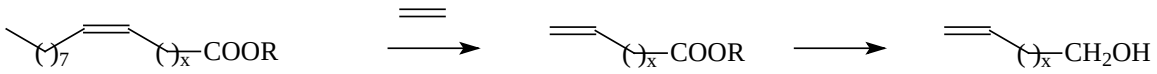
Fatty alcohols are used in the fragrances industry (as such or on the ester form such as acetate). They are generally produced by reduction of the corresponding fatty esters (copper-chromium catalyst or Bouveault-Blanc reduction with sodium). Unsaturated alcohols are also used for specific aromas.

Molecule	Formula	Odor/Flavor	Reference
2-Hexen-1-ol (trans)	CH_3-$(CH_2)_2$-CH=CH-CH_2OH	Apple, banana, orange, green, fatty, wine-like, fruity, raspberry, strawberry, vegetable, minty, herbaceous	SAFC
9-Decen-1-ol	CH_2=CH-$(CH_2)_7$-CH_2OH	Floral	The Good Scents Company
10-Undecen-1-ol	CH_2=CH-$(CH_2)_8$-CH_2OH	Fresh, floral,citrus	The Good Scents Company

α,β-Unsaturated alcohols can be obtained by cross-metathesis of fatty acids with methyl acrylate followed by reduction or by direct cross-metathesis with allyl alcohol (not in the scope of the project). We could target 2-Penten-1-ol from linolenic derivative or 2-octen-1-ol from linoleic derivative that could be interesting with regards to 2-hexen-1-ol:



ω-Unsaturated alcohols such 9-decen-1-ol, 11-dodecen-1-ol or 13-tetradecen-1-ol could be obtained by ethenolysis of fatty acids/esters followed by a selective reduction of the acid/ester function (or the same reaction sequence in the reversed order). These products could have similar properties than 10-undecen-1-ol. The challenge for the process is to find catalysts and conditions that enable to keep the terminal double bond (T6.4 in the project).



x=7 (oleic), 9 (eicosenoic), 11 (erucic)

3 Conclusions

Many molecules that can be obtained from camelina and crambe fatty acids through cross-metathesis (CM) or oxidative cleavage (OC) technologies are already classified as potential flavors and fragrances ingredients.

Molecule	**Odor/Flavor**	**Fatty acid source**	**Techno.**
Aldehydes			
Hexanal	Fatty, green	Linoleic	OC
Nonanal	Apple, coconut, grape, grapefruit, lemon, lime, melon, oily, orange, nutty, citrus, waxy, fatty, peach, rose, vegetable, fishy, meaty	Oleic	OC
Decanal	Waxy, floral, citrus, sweet	Oleic	CM
Undecanal	Orange, fatty, rose, waxy	Oleic	CM
Dodecanal	Herbaceous, waxy, floral, sweet	Oleic, eicosenoic	CM
Tridecanal	Fatty, waxy, citrus	Oleic, eicosenoic	CM
2-Pentenal	Apple, orange, green, vegetable	Linolenic	CM
2-Octenal	Spicy, herbaceous, green	Linoleic	CM
2-Undecenal	Orange, herbaceous, fruity	Oleic, eicosenoic, erucic	CM
Acids			
Hexanoic acid	Cheese, fatty, sour	Linoleic	OC
Nonanoic acid	Cheese, waxy	Oleic, eicosenoic, erucic	OC
Decanoic acid	Fatty, citrus	Oleic	CM
Undecanoic acid	Oily	Oleic	CM
Dodecanoic acid	Fatty	Oleic, eicosenoic	CM
Tridecanoic acid	Waxy	Eicosenoic	CM
Tetradecanoic acid	Oily, waxy	Eicosenoic, erucic	CM
2-Octenoic acid	Sour, fatty, waxy	Linoleic	CM
9-Decenoic acid	Waxy	Oleic, linoleic, linolenic	CM

Esters			
Methyl hexanoate	Ethereal, pineapple	Linoleic	OC
Methyl nonanoate	Coconut, nutty, wine-like	Oleic, eicosenoic, erucic	OC
Methyl decanoate	Oily, wine, fruity	Oleic	CM
Ethyl undecanoate	Coconut	Oleic	CM
Methyl laurate	Coconut, creamy, soapy, waxy	Oleic, eicosenoic	CM
Ethyl laurate	Green, fruity, floral	Oleic, eicosenoic	CM
Methyl 2-Octenoate	Fruity, green	Linoleic	CM
Nitriles			
Decanenitrile	Fatty	Oleic	CM
Dodecanenitrile	Citrus	Oleic, eicosenoic	CM
Tetradecanenitrile	Fresh, orange, green	Eicosenoic, erucic	CM
9-Undecenitrile	Fresh, floral, fruity	Oleic, linoleic, linolenic	CM

Other molecules that could be issued from the project could also be of interest for flavors and fragrances with respect to similar structures:

- 9-Decenal *(analogy 10-undecenal – fatty, citrus, rose, sweet)*
- 9-Undecenal *(analogy 10-undecenal)*
- 9-Dodecenal *(analogy 10-undecenal)*
- 11-Dodecenal *(analogy 10-undecenal)*
- 11-Tridecenal *(analogy 10-undecenal)*
- 2-Undecenoic acid *(analogy 2-decenoic acid – waxy)*
- 2-Tridecenoic acid *(analogy 2-decenoic acid)*
- Ethyl 2-undecenoate *(analogy ethyl 2-decenoate – fatty, waxy)*
- Methyl 9-decenoate *(analogy methyl 10-undecenoate – banana, honey, oily, citrus)*
- Nonanenitrile *(analogy octanitrile and decanitrile – fatty, green)*
- 9-Decenitrile *(analogy 10-undecenitrile – fresh, floral, fruity)*
- 11-Dodecenitrile *(analogy 10-undecenitrile)*
- 13-Tetradecenitrile *(analogy 10-undecenitrile)*
- 2-Penten-1-ol *(analogy 2-hexen-1-ol – apple, banana, orange, green...)*
- 2-Octen-1-ol *(analogy 2-hexen-1-ol)*
- 9-Decen-1-ol *(analogy 10-undecen-1-ol – fresh, floral, citrus)*
- 11-Dodecen-1-ol *(analogy 10-undecen-1-ol)*
- 13-Tetradecen-1-ol *(analogy 10-undecen-1-ol)*

Samples of these different molecules could be supplied for research purpose under conditions to be agreed.

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4 Annexes

SAFC references

Aldehydes (saturated)

Hexanal

Caproaldehyde; Aldehyde C_6; Hexyl aldehyde
[66-25-1] FEMA 2557 Flavis 5.008 $CH_3(CH_2)_4CHO$
$C_6H_{12}O$ FW 100.16
Arc. 1592; *Fen.* 326; *Fen.* 328

▶ **≥97%, FCC, FG**
CoE Nr 96
Organoleptic: fatty; green
Halal, Kosher, NI

W255718-SAMPLE-K

Heptanal

Heptaldehyde; Enanthaldehyde; Oenanthaldehyde; 1-Heptanal; Aldehyde C_7
[111-71-7] $CH_3(CH_2)_5CHO$ $C_7H_{14}O$ FW 114.19
Arc. 1494; *Fen.* 312

▶ **≥92%, FCC**
FEMA 2540 Flavis 5.031 CoE Nr 117
Organoleptic: oily; fruity; woody; fatty; nutty
Halal, NI

W254002-SAMPLE

Octanal

Octyl aldehyde; Caprylic aldehyde; Aldehyde C_8
[124-13-0] FEMA 2797 Flavis 5.009 CoE Nr 97
$CH_3(CH_2)_6CHO$ $C_8H_{16}O$ FW 128.21
Arc. 2397; *Fen.* 611

▶ **≥92%, FCC**
Organoleptic: honey; fruity; fatty; citrus
Halal, Kosher, NI

W279706-SAMPLE-K

Nonanal

Pelargonaldehyde; Nonyl aldehyde; Aldehyde C_9
[124-19-6] $CH_3(CH_2)_7CHO$ $C_9H_{18}O$ FW 142.24
Arc. 2343; *Fen.* 598

▶ **≥95%, FCC**
FEMA 2782 Flavis 5.025 CoE Nr 114
Natural occurrence: Apple, avocado, balck currants, cooked beef, cucumber, fish, grapefruit, lemon, lime, mandarin, orange and peach.
Organoleptic: apple; coconut; grape; grapefruit; lemon; lime; melon; oily; orange; nutty; citrus; waxy; fatty; peach; rose; vegetable; fishy; meaty
Halal, Kosher, NI
contains tocopherol as stabilizer

W278203-SAMPLE-K

Decanal

Caprinaldehyde; Decyl aldehyde
[112-31-2] FEMA 2362 Flavis 5.01 $CH_3(CH_2)_8CHO$
$C_{10}H_{20}O$ FW 156.27
Arc. 833; *Fen.* 393

▸ **≥95%, FCC**
CoE Nr 98
Organoleptic: waxy; floral; citrus; sweet
Kosher, NI

W236209-SAMPLE-K

Undecanal

Undecyl aldehyde
[112-44-7] $CH_3(CH_2)_9CHO$ $C_{11}H_{22}O$ FW 170.29
Arc. 3028; *Fen.* 781

▸ **≥96%, FCC**
FEMA 3092 Flavis 5.034 CoE Nr 121
Organoleptic: orange; fatty; rose; waxy
Kosher, NI
contains 0.025% BHT as stabilizer

W309206-SAMPLE-K

Lauric aldehyde

Dodecyl aldehyde; Laurinaldehyde; Dodecanal; Lauraldehyde; Aldehyde C_{12}
[112-54-9] FEMA 2615 Flavis 5.011
$CH_3(CH_2)_{10}CHO$ $C_{12}H_{24}O$ FW 184.32
Arc. 1105; *Fen.* 427

▸ **≥95%, FCC**
CoE Nr 99
Organoleptic: herbaceous; waxy; floral; sweet
Halal, Kosher, NI

W261505-SAMPLE-K

Tridecanal NEW

Tridecyl aldehyde
[10486-19-8] $CH_3(CH_2)_{11}CHO$ $C_{13}H_{26}O$ FW 198.34

▸ **≥95%**
FEMA 4335
Kosher

W433500-SAMPLE-K

Aldehydes (unsaturated)

trans-2-Pentenal

2-Ethylacrylic aldehyde
[1576-87-0] $C_2H_5CH=CHCHO$ C_5H_8O FW 84.12
Fen. 640

▸ **≥95%, FG**
FEMA 3218 CoE Nr 10375
Organoleptic: apple; orange; green; vegetable
Halal, Kosher, NI

W321818-SAMPLE-K

trans-2-Hexen-1-al

Leaf aldehyde; *trans*-2-Hexenal
[6728-26-3] FEMA 2560 Flavis 5.073 CoE Nr 748
$CH_3CH_2CH_2CH=CHCHO$ $C_6H_{10}O$ FW 98.14
Arc. 1599; *Fen.* 789

▸ **≥95%, FCC, FG**
Organoleptic: almond; apple; green; plum; sweet; vegetable
Halal, Kosher, NI
hexenoic acid ..... <3%

W256005-SAMPLE-K

trans-2-Heptenal

[18829-55-5] $CH_3(CH_2)_3CH=CHCHO$ $C_7H_{12}O$
FW 112.17
Arc. 1506; *Fen.* 317

▸ **≥95%**
FEMA 3165 Flavis 5.15 CoE Nr 730
Organoleptic: apple; lemon; green; fatty; spicy; vegetable
Kosher, NI
contains 0.1-0.5% alpha-tocopherol as antioxidant

W316504-SAMPLE-K

trans-2-Octenal

[2548-87-0] $CH_3(CH_2)_4CH=CHCHO$ $C_8H_{14}O$
FW 126.20
Arc. 124; *Fen.* 617

▸ **≥94%**
FEMA 3215 Flavis 5.19 CoE Nr 663
Organoleptic: spicy; herbaceous; green
Kosher, NI

W321508-SAMPLE-K

trans-2-Nonenal

[18829-56-6] $CH_3(CH_2)_5CH=CHCHO$ $C_9H_{16}O$
FW 140.22
Arc. 2356; *Fen.* 603

▶ **≥93%**

FEMA 3213 Flavis 5.072 CoE Nr 733
Organoleptic: waxy; fatty
Kosher, NI

W321303-SAMPLE-K

trans-2-Decenal

[3913-81-3] $CH_3(CH_2)_6CH=CHCHO$ $C_{10}H_{18}O$
FW 154.25
Arc. 842

▶ **≥92%, FCC**

Flavis 5.191 CoE Nr 2009
Organoleptic: oily; orange; floral; citrus; fatty; waxy; green; meaty
Kosher, NI
Fen. 398

W236608-SAMPLE-K

trans-2-Undecenal

[53448-07-0] $CH_3(CH_2)_7CH=CHCHO$ $C_{11}H_{20}O$
FW 168.28
Arc. 3033; *Fen.* 785

▶ **≥90%**

FEMA 3423 Flavis 5.184 CoE Nr 11827
Halal, Kosher, NI
Organoleptic: orange; herbaceous; fruity
contains 0.50% alpha-tocopherol, synthetic as additive

cis-2-undecenal 0.1-3.5%

W342300-SAMPLE-K

trans-2-Dodecenal

[20407-84-5] $CH_3(CH_2)_8CH=CHCHO$ $C_{12}H_{22}O$
FW 182.30
Arc. 1110; *Fen.* 207

▶ **≥93%, FCC**

FEMA 2402 Flavis 5.144 CoE Nr 124
Organoleptic: orange; fatty; herbaceous
Kosher, NI

W240206-SAMPLE-K

trans-2-Tridecenal

[7774-82-5] $CH_3(CH_2)_9CH=CHCHO$ $C_{13}H_{24}O$
FW 196.33
Arc. 2987; *Fen.* 766

▶ **≥92%, FCC**

FEMA 3082 Flavis 5.078 CoE Nr 2011
Organoleptic: waxy; citrus
Kosher, NI
contains 0.50% alpha-tocopherol, synthetic as anti-oxidant

W308218-SAMPLE-K

10-Undecenal

Undecylenic aldehyde
[112-45-8] $H_2C=CH(CH_2)_8CHO$ $C_{11}H_{20}O$
FW 168.28

▶ **≥90%**

FEMA 3095 Flavis 5.035 CoE Nr 122
Organoleptic: fatty; citrus; waxy; rose; sweet
Kosher
Arc. 3035; *Fen.* 786

W309508-SAMPLE-K

Acids (saturated)

Hexanoic acid

Caproic acid; Acid C_6

[142-62-1] FEMA 2559 Flavis 8.009
$CH_3(CH_2)_4COOH$ $C_6H_{12}O_2$ FW 116.16
Organoleptic: cheese; fatty; sour
Arc. 1596; *Fen.* 331

▶ **≥98%, FCC, FG**
CoE Nr 9
Halal, Kosher, NI

W255904-SAMPLE-K

Heptanoic acid

Oenanthic acid; Enanthic acid

[111-14-8] FEMA 3348 Flavis 8.028
$CH_3(CH_2)_5COOH$ $C_7H_{14}O_2$ FW 130.18
Arc. 1500; *Fen.* 314

▶ **97%**
CoE Nr 28
Organoleptic: sour
NI

W334804-SAMPLE

Octanoic acid

Caprylic acid; Acid C_8

[124-07-2] FEMA 2799 Flavis 8.01
$CH_3(CH_2)_6COOH$ $C_8H_{16}O_2$ FW 144.21
Arc. 2400; *Fen.* 613

▶ **≥98%, FG**
CoE Nr 10
Organoleptic: oily
Halal, Kosher, NI

W279900-SAMPLE-K

Nonanoic acid

Pelargonic acid; Acid C_9

[112-05-0] $CH_3(CH_2)_7COOH$ $C_9H_{18}O_2$ FW 158.24
Arc. 2347; *Fen.* 600

▶ **≥96%**
FEMA 2784 Flavis 8.029 CoE Nr 29
Organoleptic: cheese; waxy
Halal, Kosher, NI

W278408-SAMPLE-K

Decanoic acid

Capric acid; Acid C_{10}

[334-48-5] FEMA 2364 Flavis 8.011 CoE Nr 11
$CH_3(CH_2)_8COOH$ $C_{10}H_{20}O_2$ FW 172.26
Fen. 395
Arc. 840

▸ **≥98%, FCC, FG**

Organoleptic: fatty; citrus
Halal, Kosher, NI

W236403-SAMPLE-K

Undecanoic acid

Hendecanoic acid

[112-37-8] $CH_3(CH_2)_9COOH$ $C_{11}H_{22}O_2$ FW 186.29
Arc. 3051; *Fen.* 782

▸ **≥97%**

FEMA 3245 Flavis 8.042 CoE Nr 696
Organoleptic: oily
NI

W324507-SAMPLE

Lauric acid

Dodecanoic acid; ABL

[143-07-7] FEMA 2614 Flavis 8.012
$CH_3(CH_2)_{10}COOH$ $C_{12}H_{24}O_2$ FW 200.32
Organoleptic: fatty
Arc. 1107; *Fen.* 427

▸ **≥98%, FCC, FG**

CoE Nr 12
Halal, Kosher, NI

W261408-SAMPLE-K

Tridecanoic acid NEW

[638-53-9] $CH_3(CH_2)_{11}CO_2H$ $C_{13}H_{26}O_2$ FW 214.34

▸ **≥98%**

FEMA 4336

W433600-SAMPLE

Myristic acid

Tetradecanoic acid

[544-63-8] FEMA 2764 Flavis 8.016
$CH_3(CH_2)_{12}COOH$ $C_{14}H_{28}O_2$ FW 228.37
Arc. 2288; *Fen.* 586

▸ **FCC, FG**

CoE Nr 16
Organoleptic: oily; waxy
Halal, Kosher, NI

W276405-SAMPLE-K

Acids (unsaturated)

trans-2-Hexenoic acid

[13419-69-7] $CH_3CH_2CH_2CH=CHCO_2H$ $C_6H_{10}O_2$
FW 114.14
Arc. 1603; *Fen.* 335

▶ **≥98%, FG**

FEMA 3169 Flavis 8.054 CoE Nr 11777
Organoleptic: musty; fatty; sweet
Halal, Kosher, NI

W316903-SAMPLE-K

2-Octenoic acid

[1871-67-6] $CH_3(CH_2)_4CH=CHCO_2H$ $C_8H_{14}O_2$
FW 142.20
predominantly *trans*

▶ **85%**

FEMA 3957 Flavis 8.114
Possible uses: lamb, mutton, goat, ripe cheeses, shell fish, meaty chicken.[1]
Natural occurrence: strawberry, capsicum frutescens, chicken fat, boiled mutten[1]
Lit. cited: 1. Mosciano, Gerard, *Perfum. Flavor.* 3rd ed., **33**, 50 (2008)

W395701

Undecylenic acid

10-Undecenoic acid
[112-38-9] CI 42650 $CH_2=CH(CH_2)_8COOH$
$C_{11}H_{20}O_2$ FW 184.28
Arc. 3049; *Fen.* 786

▶ **≥95%**

FEMA 3247 Flavis 8.039 CoE Nr 689
Organoleptic: woody; sweet
Halal, NI

W324701-SAMPLE

Esters (saturated)

Methyl hexanoate

Methyl caproate; Caproic acid methyl ester
[106-70-7] FEMA 2708 Flavis 9.069
$CH_3(CH_2)_4COOCH_3$ $C_7H_{14}O_2$ FW 130.18
Arc. 1945; *Fen.* 500; *Fen.* 509

▸ **≥99%, FG**

CoE Nr 319
Organoleptic: ethereal; pineapple
Halal, NI

W270806-SAMPLE

Methyl nonanoate

Methyl pelargonate; Nonanoic acid methyl ester
[1731-84-6] $CH_3(CH_2)_7COOCH_3$ $C_{10}H_{20}O_2$
FW 172.26
Arc. 2128; *Fen.* 531

▸ **≥97%**

FEMA 2724 Flavis 9.108 CoE Nr 389
Organoleptic: coconut; nutty; wine-like
Kosher, NI

W272418-SAMPLE-K

Ethyl undecanoate

Undecanoic acid ethyl ester
[627-90-7] $CH_3(CH_2)_9CO_2C_2H_5$ $C_{13}H_{26}O_2$
FW 214.34
Arc. 1359; *Fen.* 271

▸ **≥97%**

FEMA 3492 Flavis 9.274 CoE Nr 10633
Organoleptic: coconut
NI

W349208-SAMPLE

Methyl laurate

Methyl dodecanoate; Lauric acid methyl ester
[111-82-0] $CH_3(CH_2)_{10}CO_2CH_3$ $C_{13}H_{26}O_2$
FW 214.34
Arc. 2095; *Fen.* 520

▸ **≥98%**

FEMA 2715 Flavis 9.101 CoE Nr 377
Organoleptic: coconut; creamy; soapy; waxy
NI

W271500-SAMPLE

Ethyl laurate

Ethyl dodecanoate; Lauric acid ethyl ester
[106-33-2] FEMA 2441 Flavis 9.099
$CH_3(CH_2)_{10}COOC_2H_5$ $C_{14}H_{28}O_2$ FW 228.37
Arc. 1277; *Fen.* 244

▸ **≥98%, FCC, FG**

CoE Nr 375
Organoleptic: green; fruity; floral
Halal, Kosher, NI

W244104-SAMPLE-K

Esters (unsaturated)

Methyl *trans*-2-octenoate

[7367-81-9] $CH_3(CH_2)_4CH=CHCO_2CH_3$ $C_9H_{16}O_2$
FW 156.22
Arc. 2143; *Fen.* 536

▶ **≥96%**

FEMA 3712 Flavis 9.299 CoE Nr 11800
Organoleptic: fruity; green
Kosher, NI

W371203-SAMPLE-K

Methyl *trans*-2-nonenoate

Methyl 2-nonenoate
[111-79-5] $CH_3(CH_2)_5CH=CHCO_2CH_3$ $C_{10}H_{18}O_2$
FW 170.25
Arc. 2139; *Fen.* 532

▶ **≥97%**

FEMA 2725 Flavis 9.234 CoE Nr 2099
Organoleptic: green; violet
Halal, Kosher

W272507-SAMPLE-K

Ethyl *trans*-2-decenoate

trans-2-Decenoic acid ethyl ester
[7367-88-6] $CH_3(CH_2)_6CH=CHCO_2C_2H_5$ $C_{12}H_{22}O_2$
FW 198.30
Fen. 226

▶ **≥95%**

FEMA 3641 Flavis 9.283 CoE Nr 10577
Organoleptic: fatty; waxy
Kosher
contains 0.10% alpha-tocopherol, synthetic as anti-oxidant

W364118-SAMPLE-K

Methyl 10-undecenoate

Undecylenic acid methyl ester; 10-Undecenoic acid methyl ester
[111-81-9] $CH_2=CH(CH_2)_8CO_2CH_3$ $C_{12}H_{22}O_2$
FW 198.30

▶ **96%**

FEMA 4253
Organoleptic: banana; honey; oily; citrus; rose; earthy; soapy; wine-like

W425301-SAMPLE

Alcohols

trans-2-Hexen-1-ol

[928-95-0] $CH_3CH_2CH_2CH{=}CHCH_2OH$ $C_6H_{12}O$
FW 100.16
Arc. 1606; *Fen.* 336

▶ **≥96%, FCC, FG**

FEMA 2562 CoE Nr 69
Natural occurrence: Raspberry, orange, apple, green tea, kiwi, peach, strawberry and tomato.
Organoleptic: apple; banana; orange; green; fatty; wine-like; fruity; raspberry; strawberry; vegetable; minty; herbaceous
Halal, Kosher, NI

W256218-SAMPLE-K