

FATTY ACIDS

Nomenclature, Characterization, Properties and Utilization

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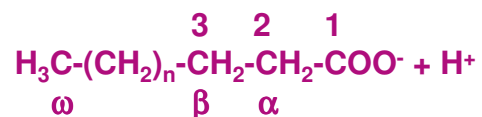
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FATTY ACIDS (FAs)

- Compounds containing a long hydrocarbon chain and a terminal carboxylic group

(i) SATURATED

(ii) UNSATURATED (with double bonds in the hydrocarbon chain)



FATTY ACIDS (FAs)

two major physiological roles:

- (i) building blocks of *phospholipids* and *glycolipids* in *biological membranes*
- (ii) *fuel molecules*

CLASSIFICATION OF FAs

- According to the **chain length**
 - *short-chain fatty acid* - SCFA < 6 carbon atoms
 - *medium-chain fatty acid* - MCFA 6-12 carbon atoms
 - *long-chain fatty acid* - LCFA 14-20 carbon atoms
 - *very-long chain fatty acid* - VLCFA > 20 carbon atoms
- According to the **degree of saturation** (presence or absence of double bonds)
 - *saturated*
 - *unsaturated cis/trans isomers*
- **Branched** (unusual)
- **Hydroxylated** (unusual)

FATTY ACIDS - NOMENCLATURE

Systematic name:

SATURATED: parent hydrocarbon + *oic*
e.g. C18: Octadecan*oic* acid

UNSATURATED: with one double bond: + *enoic*
e.g. C18: Octadec*enoic* acid

with two double bonds: + *dienoic*
e.g. C18: Octadeca*dienoic* acid

with three double bonds: + *trienoic*
e.g. C18: Octadeca*trienoic* acid

FATTY ACIDS - NOMENCLATURE

Common name	Systematic name	Formula
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SATURATED FAs

C16:0 Palmitate	n-Hexadecanoate	$\text{CH}_3(\text{CH}_2)_{14}\text{COO}^-$
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C18:0 Stearate	n-Octadecanoate	$\text{CH}_3(\text{CH}_2)_{16}\text{COO}^-$
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UNSATURATED FAs

C16:1(9) Palmitoleate	cis-9-Hexadecenoate	$\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}(\text{CH}_2)_7\text{COO}^-$
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C18:1(9) Oleate	cis-9-Octadecenoate	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COO}^-$
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C18:2(9,12) Linoleate	all cis-9,12- Octadecadienoate	$\text{CH}_3(\text{CH}_2)_4(\text{CH}=\text{CHCH}_2)_2(\text{CH}_2)_6\text{COO}^-$
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C18:3(9,12,15) Linolenate	all cis-9,12,15- Octadecatrienoate	$\text{CH}_3\text{CH}_2(\text{CH}=\text{CHCH}_2)_3(\text{CH}_2)_6\text{COO}^-$
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C20:4(5,8,11,14) Arachidonate	all cis-5,8,11,14- Eicosatetraenoate	$\text{CH}_3(\text{CH}_2)_4(\text{CH}=\text{CHCH}_2)_4(\text{CH}_2)_2\text{COO}^-$
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FATTY ACIDS - NOMENCLATURE

UNSATURATED

Counting from the carboxy end:

from the methyl (ω) end:

C16:1(9) Palmitoleate

16:1, *n*-7 (ω 7)

C18:1(9) Oleate

18:1, *n*-9 (ω 9)

C18:2(9,12) Linoleate

18:2, *n*-6 (ω 6)

C18:3(9,12,15) Linolenate

18:3, *n*-3 (ω 3)

C20:4(5,8,11,14) Arachidonate

20:4, *n*-6 (ω 6)

C20:5(5,8,11,14,17) EPA (Eicosapentaenoic acid)

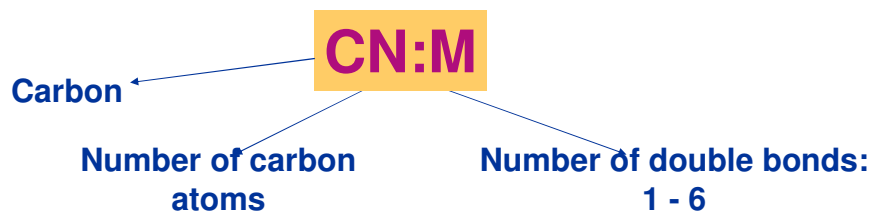
20:5, *n*-3 (ω 3)

C22:6(4,7,10,13,16,19) DHA (Docosahexaenoic acid)

22:6, *n*-3 (ω 3)

“Telegraphic” nomenclature of FAs (1)

SATURATED FAs:



SATURATED FAs WITH A SHORT CHAIN

- If free smell badly
- Fluid
- Present in milk fat (C4-C10)
- Easily digestible

Common name	Systematic name	Formula
C4:0 Butyric acid	Butanoic acid	$\text{CH}_3(\text{CH}_2)_2\text{COOH}$
C6:0 Capronic acid	Hexanoic acid	$\text{CH}_3(\text{CH}_2)_4\text{COOH}$
C8:0 Caprylic acid	Octanoic acid	$\text{CH}_3(\text{CH}_2)_6\text{COOH}$
C10:0 Caprinic acid	Decanoic acid	$\text{CH}_3(\text{CH}_2)_8\text{COOH}$

SATURATED FAs WITH A LONG CHAIN

- Solid at room temperature
- Most common in animal and plant fats
- Less easily digestible

Common name	Systematic name	Formula
C14:0 Myristic acid	Tetradecanoic acid	$\text{CH}_3(\text{CH}_2)_{12}\text{COOH}$
C16:0 Palmitic acid	Hexadecanoic acid	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$
C18:0 Stearic acid	Octadecanoic acid	$\text{CH}_3(\text{CH}_2)_{16}\text{COOH}$
C20:0 Arachidic acid	Eicosanoic acid	$\text{CH}_3(\text{CH}_2)_{18}\text{COOH}$

“Telegraphic” nomenclature of FAs (2)

UNSATURATED FAs:

position of the double bond

- **Numbering from the carboxyl end** - carboxyl C is No 1



CN:M Δ^{a,b,c}

CN:M (a,b,c)

CN:M; a,b,c

The Nos of the double-bonded carbon atoms; counting from the carboxy end

- **Numbering from the methyl end** - methyl C is marked ω or n



CN:M ω a

The No of the first double-bonded carbon atom; counting from the methyl (ω, n) end

UNSATURATED FAs - classes

- With one double bond - **monounsaturated fatty acids - MUFA**
- With more than one double bond – **polyunsaturated fatty acids - PUFA**

The double bonds tend to occur at every third carbon atom toward the CH₃ terminus of the molecule (such as -CH=CH-CH₂-CH=CH-).

3 6

The double bonds are almost never conjugated. Triple bonds are rare. Two important classes of PUFA are denoted n-3 (or ω-3) and n-6 (or ω-6) fatty acids.

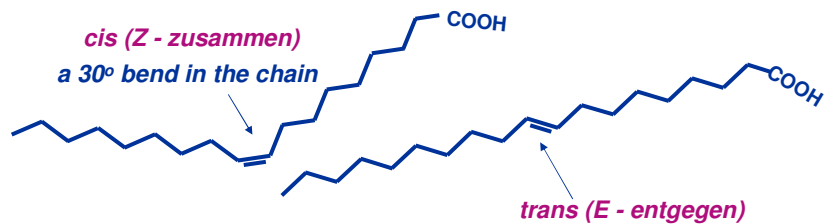
MONOUNSATURATED FAs

16:1(9) Palmitooleic a. acid	<i>cis</i> -9-Hexadecenoic
18:1(9) Oleic a.	<i>cis</i> -9-Octadecenoic acid
18:1(9) Elaidic a.	<i>trans</i> -9-Octadecenoic acid
22:1(13) Erucic a.	<i>cis</i> -13-Docosenoic acid

UNSATURATED FAs:

isomerism of the double bond

- ***cis*-configuration** – a 30° bend in the hydrocarbon chain
(„L“ shaped)
 - *natural occurrence*
 - *the melting point is lower than that of saturated FAs*
- ***trans*-configuration** – straight chain (similar as in the saturated FAs)



cis-UNSATURATED FAs:

position of the first double bond from the methyl (ω) end:

C18:1(9) Oleate:

ω 9 (*n*-9) class

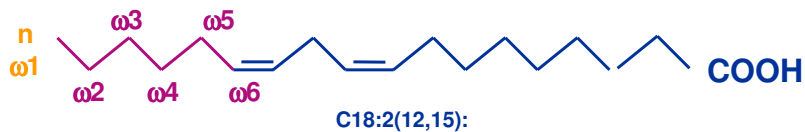
The first double-bonded carbon atom is carbon atom 9



C18:2(9,12) Linoleate:

ω 6 (*n*-6) class

The first double-bonded carbon atom is carbon atom 6



C18:2(12,15):

ω 3 (*n*-3) class

The first double-bonded carbon atom is carbon atom 3



FATTY ACIDS

- Over half of the fatty acid residues of plant and animal lipids are unsaturated and are often polyunsaturated.
- Bacterial fatty acid residues are rarely polyunsaturated but are commonly branched, hydroxylated, or contain cyclopropane rings.
- Unusual fatty acids also occur as components of the oils and waxes (esters of FAs and long chain alcohols) produced by certain plants.

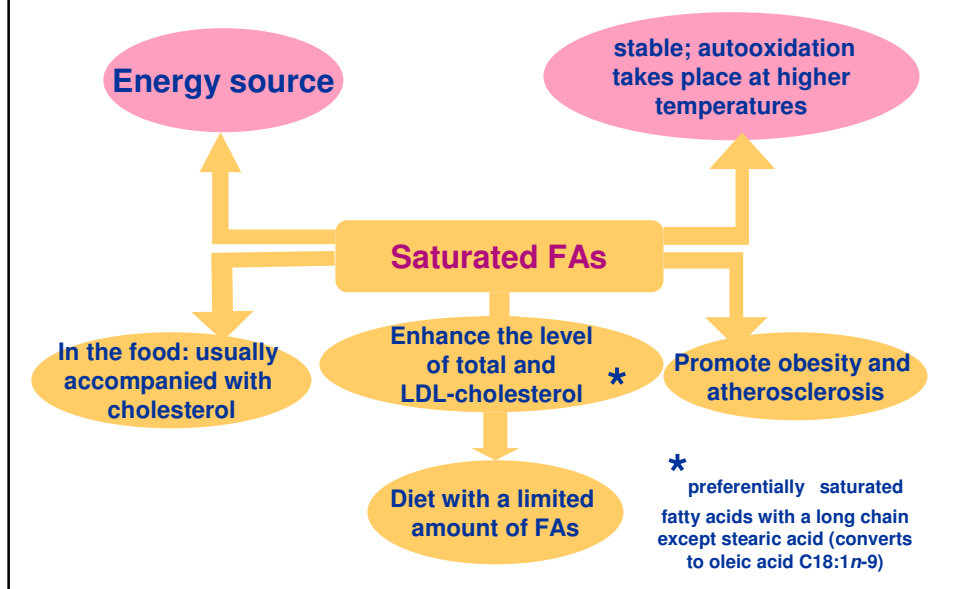
FATTY ACIDS

- more than 100 different FAs in nature
- most FAs have an *even* number of carbon atoms (mainly due to the mechanism of biosynthesis-the concatenation of C₂ units)
- mainly present in the form of *esters* (not free)
- in higher plants and animals, the predominant FA residues are those of the *C16 and C18 species* (palmitic, oleic, linoleic, and stearic acids).
- FAs with less than 14 and more than 20 carbon atoms are uncommon

FATTY ACIDS

EFFECTS

SATURATED FAs



UNSATURATED FAs

- **Mainly in plant fats**

90 % (rape-seed oil) ← → 10 % (coco-nut oil)

- **Less in animal fats except for fish oils**

– **Fish oils contain ω -3 FAs** (mostly originating from microalgae in the sea plankton) with 4-6 double bonds e.g.

C20:5 (5,8,11,14,17) = Eicosapentaenoic acid, EPA

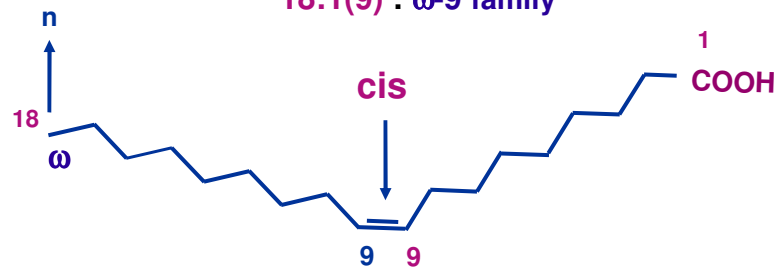
C22:6 (4,7,10,13,16,19) = Docosahexaenoic acid, DHA
(Cervonic acid)

Oleic acid

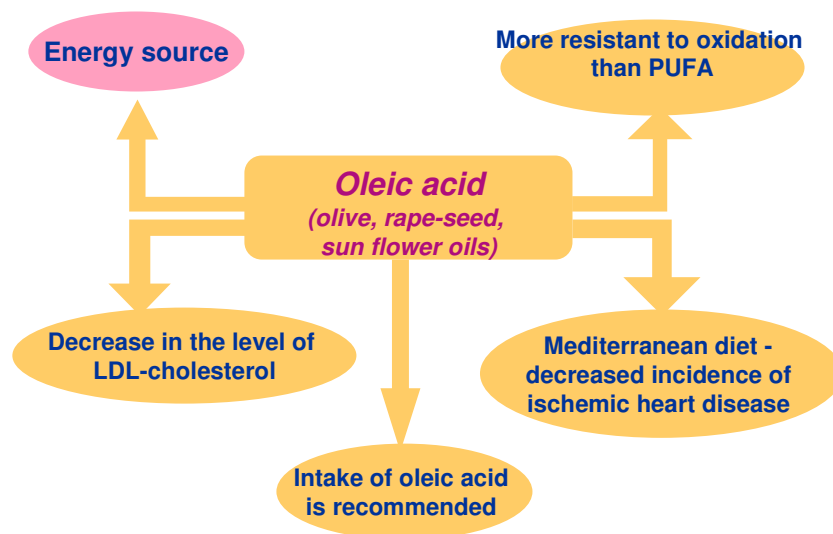
MONOUNSATURATED FA

cis-9-Octadecenoic acid

18:1(9) : ω -9 family



Oleic acid (ω -9)



POLYUNSATURATED FAs: ω -6 FAMILY

Linoleic acid
acid

cis,cis-9,12- Octadecadienoic
C18:2 (9,12) ω -6,9
essential FA

γ -Linolenic acid
acid

all *cis*-6,9,12-Octadecatrienoic
C18:3 (6,9,12) ω -6,9,12

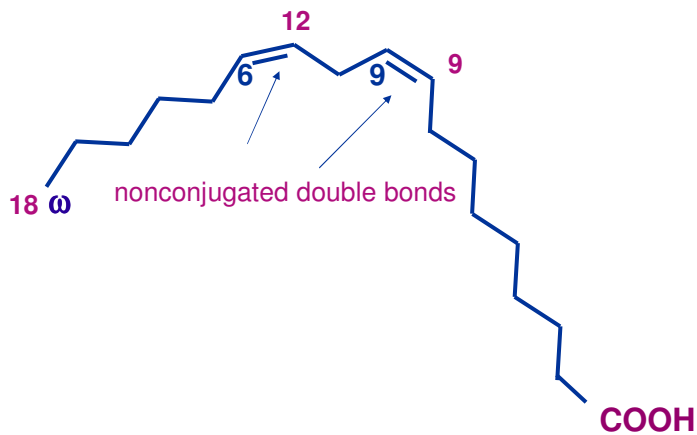
Arachidonic acid

all-*cis*-5,8,11,14-Eicosatetraenoic acid
C20:4 (5,8,11,14) ω -6,9,12,15
(*Eicosanoids*)

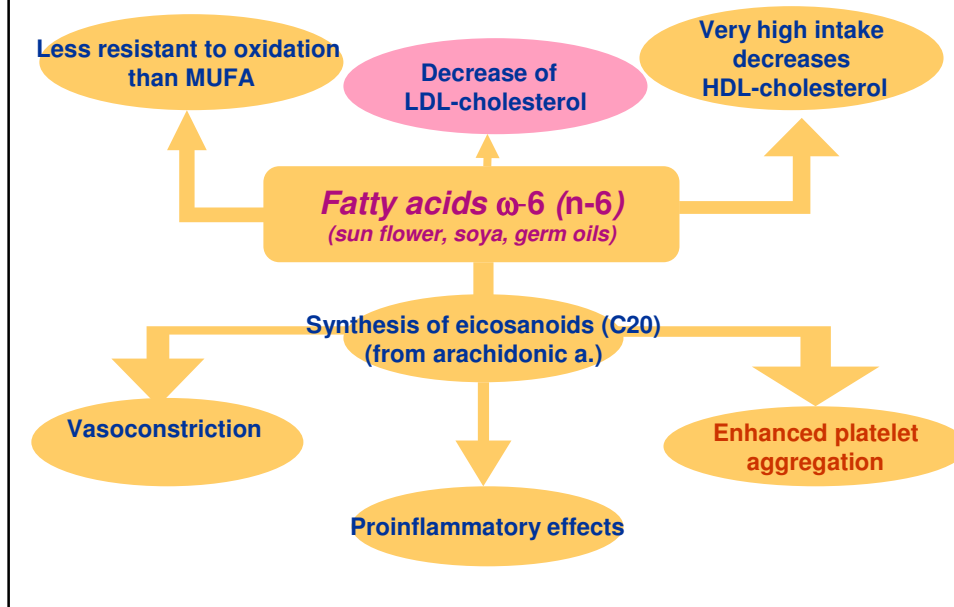
Linoleic acid (ω -6 family)

essential FA
arachidonic acid precursor

18:2 (9,12) ω -6, 9



POLYUNSATURATED FAs: ω -6 (n-6)



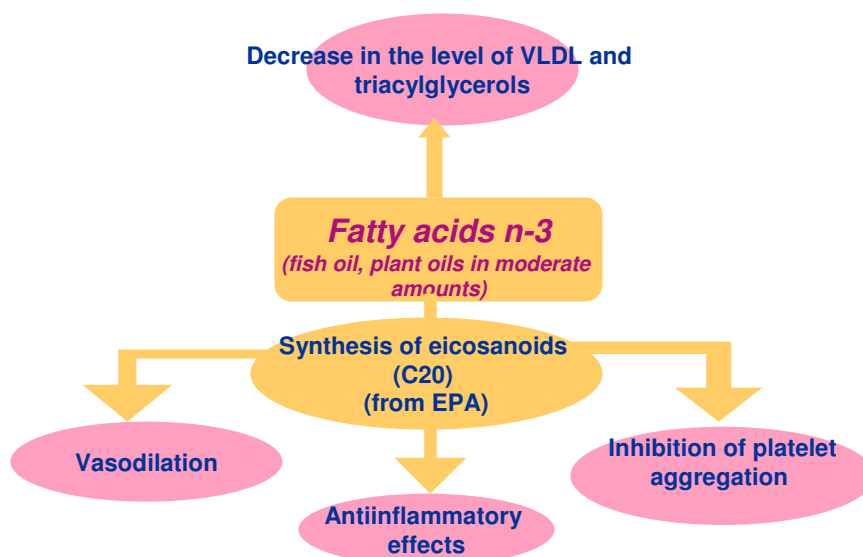
CLA - conjugated linoleic acids

- **Isomers of linoleic acid** – double bonds are conjugated
 - C18:2 CLA most frequent configuration: cis-9, trans-11, and trans-10, cis-12
- **Origins of CLA**
 - *in vivo* – in the intestine of cattle (isomerase of linoleic a.)
 - (not in humans)
 - *in vitro* – thermal processing of dairy products
- **Effects on laboratory animals**
 - antioxidative
 - anticancerogenic
 - antiatherogenic
 - antidiabetic
 - weight loss
 - immunomodulatory

POLYUNSATURATED FAs: ω -3 (n-3) Class

α -Linolenic acid <i>essential FA</i>	all cis-9,12,15 - Octadecatrienoic a. 18:3 (9,12,15) ω -3 (6,9) 18:3 n-3, 18:3 ω -3	mp -17°C
EPA	all cis-5,8,11,14,17- Eicosapentaenoic a. 20:5 (5,8,11,14,17) ω -3,6,9,12,15 20:5 n-3, 20:5 ω -3	-54°C
DHA	all cis-4,7,10,13,16,19 - Docosahexaenoic a. 22:6 (4,7,10,13,16,19) ω -3,6,9,12,15,18 22:6 n-3, 22:6 ω -3	

POLYUNSATURATED FAs: ω -3 (n-3)



UNSATURATED FAs – *trans* isomers

At least one double bond is in *trans* configuration
The configuration is similar to that of saturated FAs



trans
straight hydrocarbon chain



Saturated FA
Straight hydrocarbon chain



ORIGINS OF *TRANS* UNSATURATED FAs

in nature

- milk, dairy products and other animal fats (2-7%) – produced by **microorganisms** in the stomach of cattle
- in some **plants** (pomegranate)

artificially – industrial processing of plant oils

- during the process of **artificial hydrogenation** of unsaturated FAs in food industry (originally as much as 40 %; more advanced technologies: the yield of *trans* FAs is low)
- **long term fat frying**

The *trans* unsaturated FAs can be deposited in the human adipose tissue.

EFFECTS OF TRANS UNSATURATED FAs

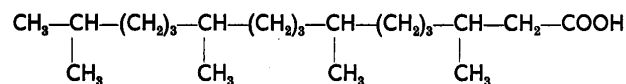
- Increased intake 

INCREASED LEVEL OF LDL CHOLESTEROL

INCREASED RISK OF ATHEROSCLEROSIS

BRANCHED FAs

- *Of plant origin, not synthesized in mammalian organisms*
- **Phytanic acid (in cow milk) – oxidation product of phytol**
(part of chlorophyll)



3,7,11,15 Tetramethylhexadecanoic acid

- In sebaceous glands
- Failure to degrade phytanic acid - **Refsum disease:**
- deposits of the phytanic acid can be found in the nervous system –*neurological disorders of cerebellum, peripheral nerves, eyes*
- Prevention: phytanic acid-free food

HYDROXYDERIVATIVES OF FAs

- *Components of sphingolipids in animals* - typically
OH groups attached to C₂
 - In the CNS – C24:0 Cerebronic a. (2-hydroxytetracosanoic a.)
$$\text{CH}_3-(\text{CH}_2)_{21}-\underset{\text{OH}}{\text{CH}}-\text{COOH}$$
- *Ricin oil* – C18:1 Ricinoleic a. (12-hydroxy-9-Octadecenoic a.)
 - $\text{CH}_3-(\text{CH}_2)_5-\underset{\text{OH}}{\text{CH}}-\text{CH}_2-\text{CH}=\text{CH}-(\text{CH}_2)_7-\text{COOH}$
- *Precursors of leukotrienes*
 - hydroxy(OH) and hydroperoxy(OOH) derivatives of C20 PUFAs