Oleochemistry

Fatty acids

by
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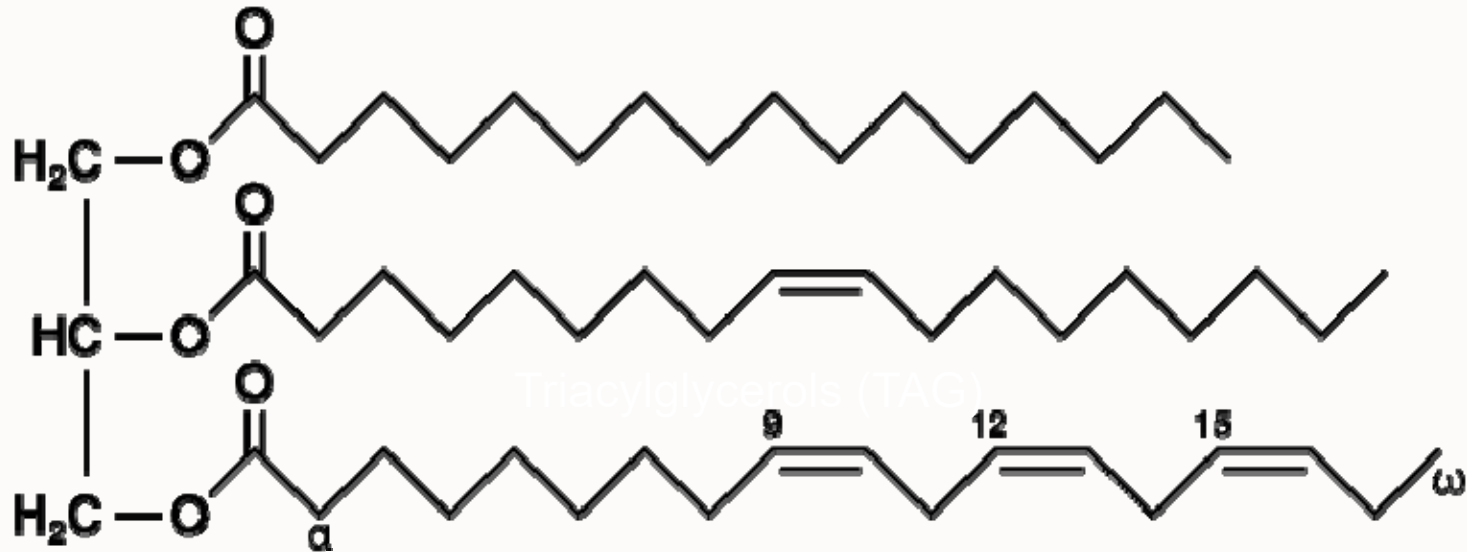**shamsulzakaria@ump.edu.my**

The students should be able to understand:

- The classes of the fatty acids and their structures.

- Isomer of fatty acids

- Naming the fatty acids

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Triacylglycerols (TAG)

Example of an unsaturated fat triglyceride. Left part: glycerol, right part from top to bottom: palmitic acid, oleic acid, alpha-linolenic acid, chemical formula: $C_{55}H_{98}O_6$

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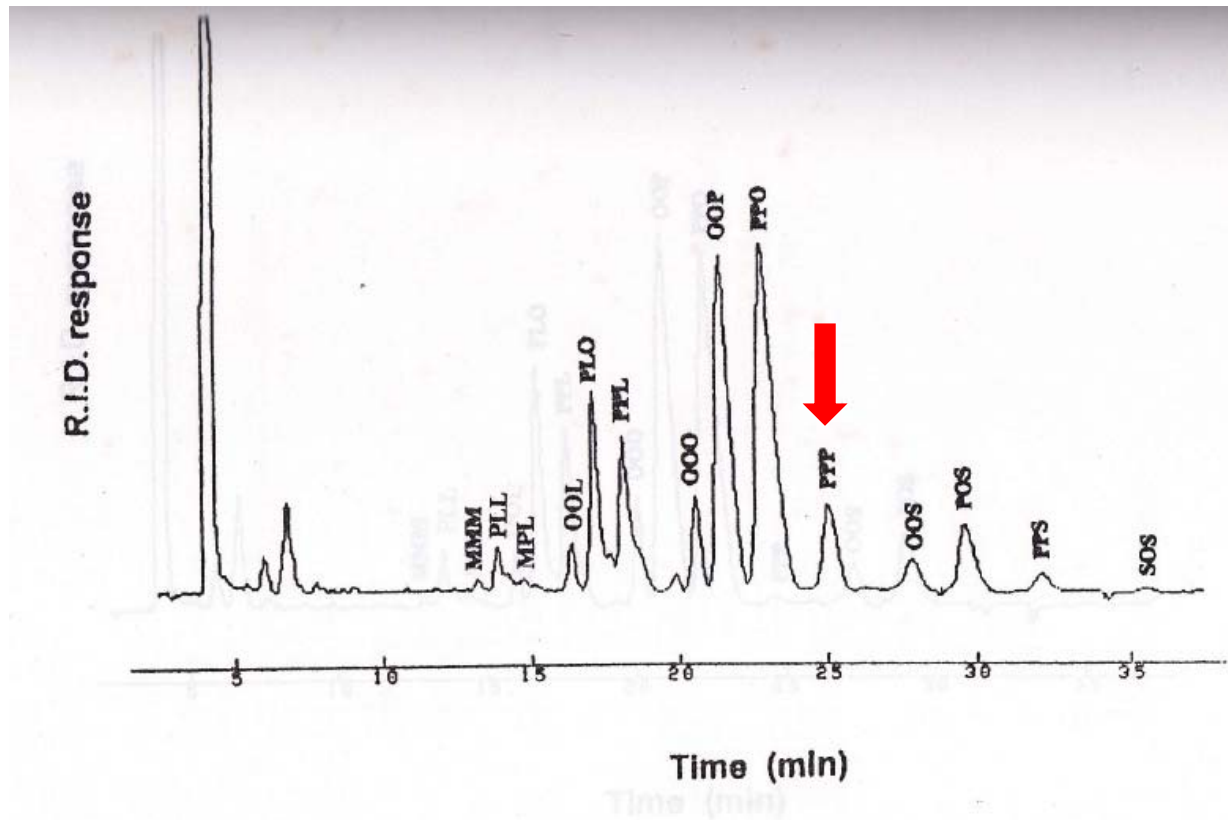
Triglycerides Profile of Palm Oil

Figure 12: HPLC chromatogram of RBD palm oil (M, P, L, O, S refer to Figure 8)
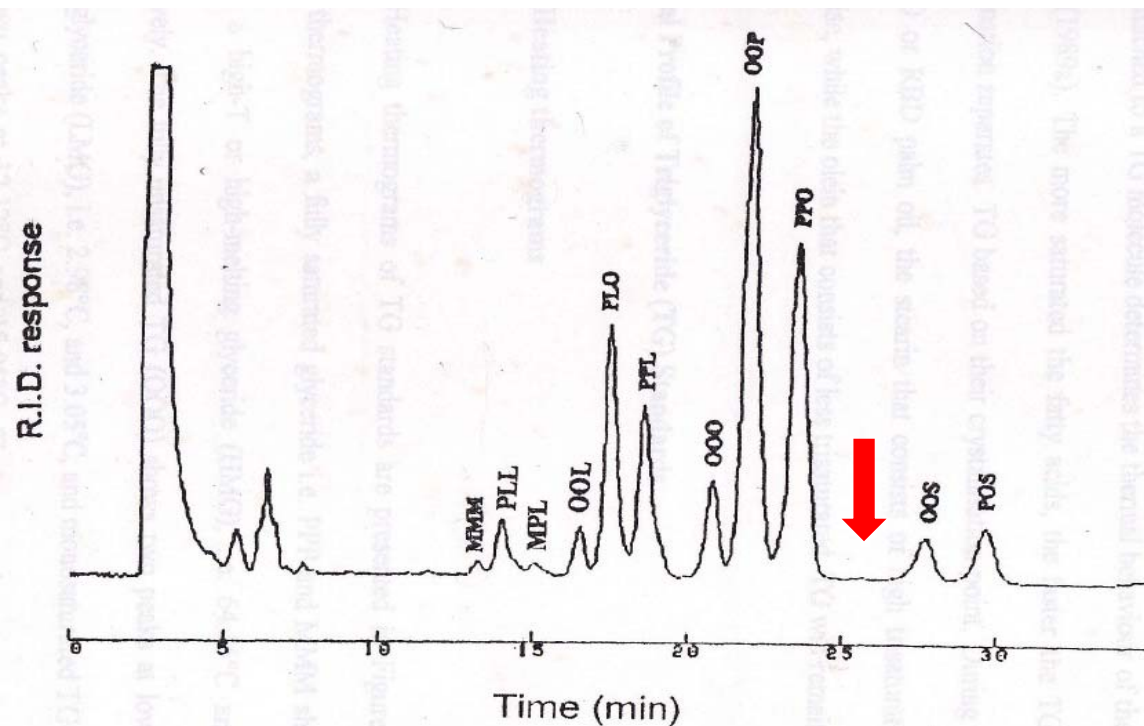
Triglyceride Profile of Palm Olein

Figure 15: HPLC chromatogram of super olein (M, P, L, O, S refer to Figure 8)

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Diglycerides profile of Palm Oil

Figure 15: HPLC chromatogram of super olein (M, P, L, O, S refer to Figure 8)

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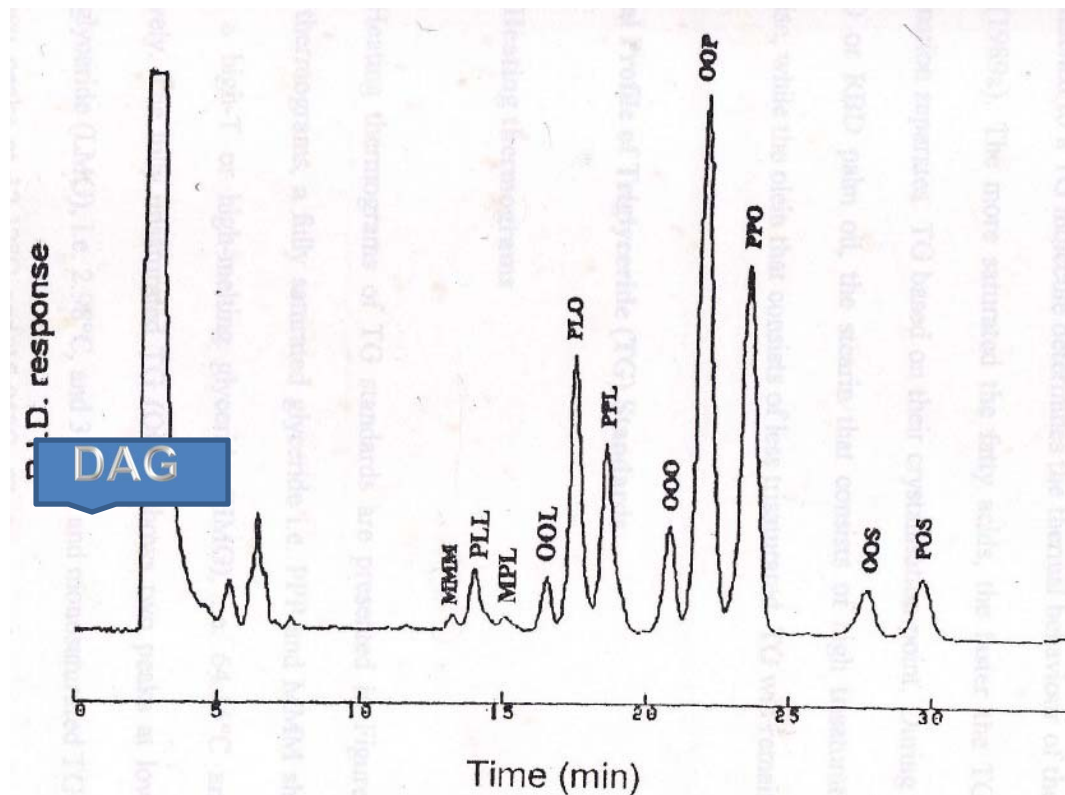
Type of Fatty Acids

Saturated fatty acid (e.g.: $C_{18:0}$ stearic acid)

1. Have no double bonds between the individual carbon atoms of the fatty acid chain.
2. That is, the chain of carbon atoms is fully "saturated" with hydrogen atoms.

Unsaturated fatty acid (e.g.: $C_{18:1}$ oleic acid)

1. At least one double bond within the fatty acid chain
2. monounsaturated = contains one double bond
3. polyunsaturated = contains more than one double bond
4. Where double bonds are formed, hydrogen atoms are eliminated.

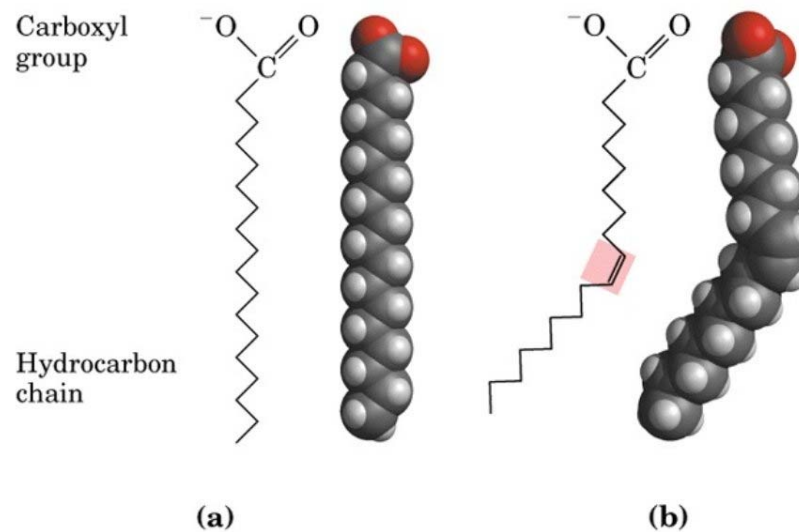Communitising Technology

Type of Fatty Acids

- FA can also be divided into saturated or unsaturated

- Unsaturated FA contain double bonds.

Fatty Acid Structure

Carboxyl group

Hydrocarbon chain

(a)   (b)

acid

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Fatty Acids (FA)

- **It is not attach to the glycerol molecule**
- **Usually even number of carbon atoms (eg 4, 6, 8 C atoms)**
- **Short chain FA – C4 - 10 carbon**
- **Medium chain FA –C 12-14 carbon**
- **Long chain FA - > C16 carbons**

(see Table 1)

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Fatty Acids Alkyl Chain

Common Name	Short Name	MW	MP (°C)
Butyric acid	4:0	88.11	-4.5
Caproic acid	6:0	116.16	-2.0
Caprylic acid	8:0	144.21	16.5
Capric acid	10:0	72.27	31.5
Lauric acid	12:0	200.32	44.0
Myristic acid	14:0	228.38	58.0
Palmitic acid	16:0	256.43	63.0
Palmitoleic acid	16:1	254.41	33.0
Stearic acid	18:0	284.48	71.0
Oleic acid	18:1	282.47	16.3
Elaidic acid	18:1 (tr)	282.47	45.0
Linoleic acid	18:2	280.45	-5.0
Linolenic acid	18:3	278.44	-11.3
Arachidic acid	20:0	312.54	77.0
Arachidonic acid	20:4	304.47	-49.5

Short chain

medium chain

Long chain

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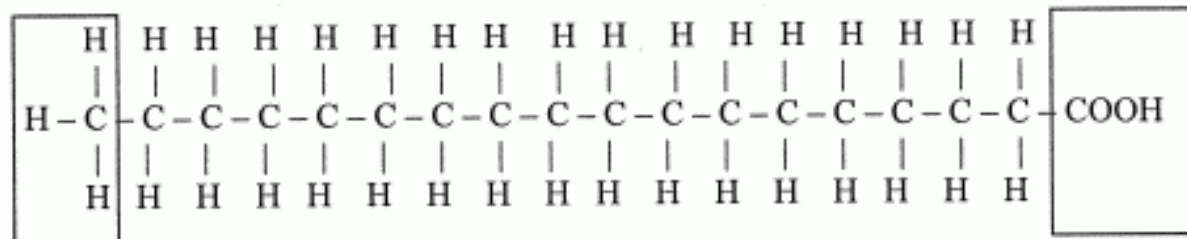
Saturated Fatty Acid
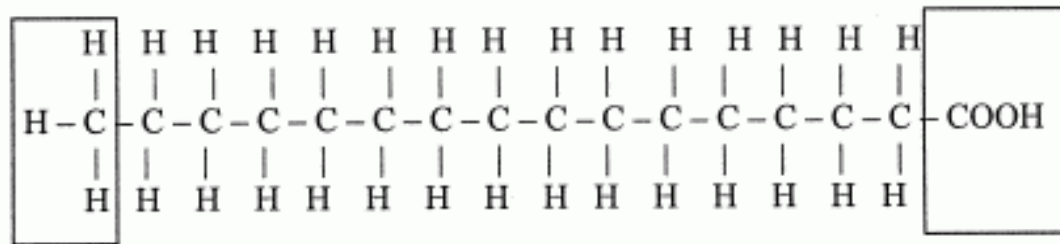
Methyl
Oil-Soluble

PALMITIC ACID
16 carbons

Carboxyl
Water-Soluble

OMEGA (ω) END

DELTA (Δ) END

Methyl
Oil-Soluble

STEARIC ACID
18 carbons

Carboxyl
Water-Soluble

OMEGA (ω) END

DELTA (Δ) END

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Saturated Fatty Acid (Example)

Common name	Chemical structure	*C:D*
Caprylic acid	$CH_3(CH_2)_6COOH$	8:0
Capric acid	$CH_3(CH_2)_8COOH$	10:0
Lauric acid	$CH_3(CH_2)_{10}COOH$	12:0
Myristic acid	$CH_3(CH_2)_{12}COOH$	14:0
Palmitic acid	$CH_3(CH_2)_{14}COOH$	16:0
Stearic acid	$CH_3(CH_2)_{16}COOH$	18:0
Arachidic acid	$CH_3(CH_2)_{18}COOH$	20:0
Behenic acid	$CH_3(CH_2)_{20}COOH$	22:0
Lignoceric acid	$CH_3(CH_2)_{22}COOH$	24:0
Cerotic acid	$CH_3(CH_2)_{24}COOH$	26:0

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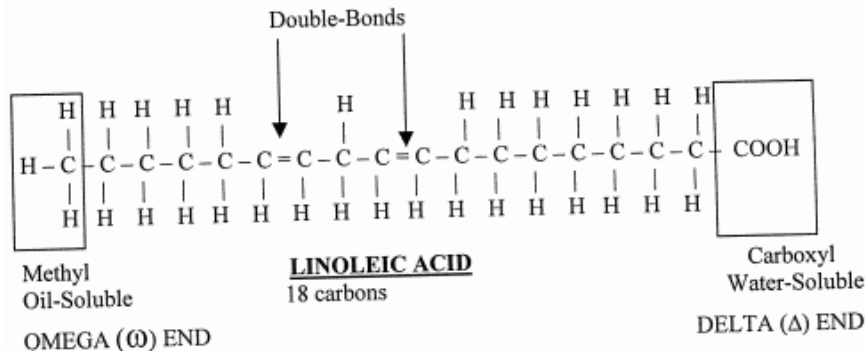
Unsaturated Fatty Acid (Example)

Monounsaturated (1 double bond)
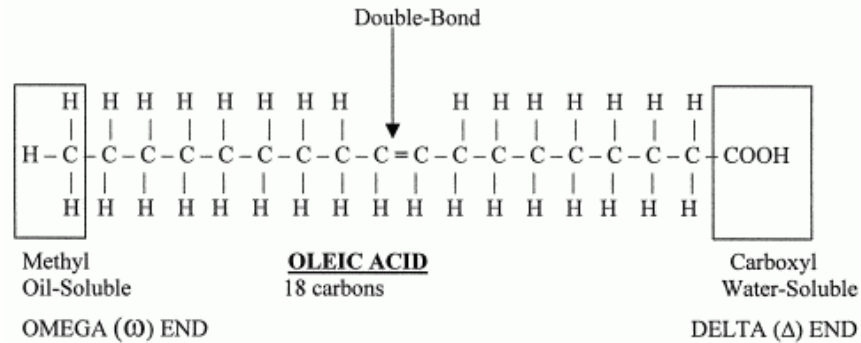
Diunsaturated (2 double bond)

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Unsaturated Fatty Acid (Example)

- ▣ FA with 2 or more double bonds are also called polyunsaturated fatty acid (PUFA)
- ▣ Eg: linoleic, linolenic (essential FA that are not synthesised but needed in body from diet), EPA (20:5) and DHA (22:6)

Example of Unsaturated FA

Common Name	Systematic Name	# of Carbon Atoms	# of Double Bonds	Structure	Typical Fat Source
Common Unsaturated Fatty Acids					
Palmitoleic Acid	Hexadecenoic Acid	16	1	$CH_3(CH_2)_5CH=CH(CH_2)_7COOH$	Some Fish Oils, Beef Fat
Oleic Acid	9-Octadecenoic Acid	18	1	$CH_3(CH_2)_7CH=CH(CH_2)_7COOH$	Olive, Canola Oils
*Linoleic Acid	9, 12 Octadecadienoic Acid	18	2	$CH_3(CH_2)_4(CH=CHCH_2)_2(CH_2)_6COOH$	Soybean, Corn Oils
*Alpha-Linolenic Acid	9,12,15 Octadecatrienoic Acid	18	3	$CH_3CH_2(CH=CHCH_2)_3(CH_2)_6COOH$	Soybean, Canola Oils
Arachidonic Acid	5, 8,11,14 Eicosatetraenoic Acid	20	4	$CH_3(CH_2)_4(CH=CHCH_2)_4(CH_2)_2COOH$	Lard
EPA	5, 8, 11, 14, 17 Eicosapentaenoic Acid	20	5	$CH_3CH_2(CH=CHCH_2)_5(CH_2)_2COOH$	Some Fish Oils
DHA	Docosohexaenoic Acid	22	6	$CH_3CH_2(CH=CHCH_2)_6(CH_2)COOH$	Some Fish Oils

*Essential Fatty Acids
Prepared by the International Food Information Council Foundation http://www.ific.org

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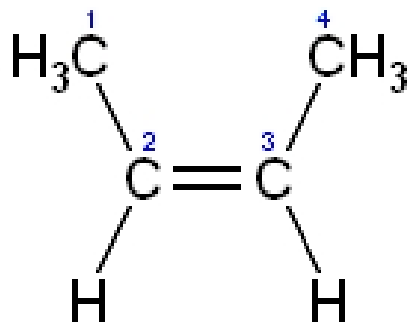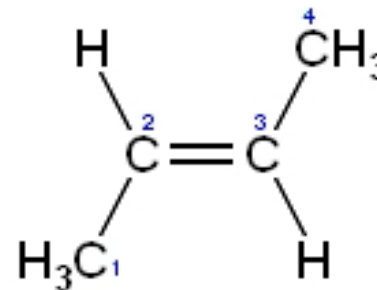
Isomers in FA

- FA can also appear in isomers of *cis* or *trans* form.
- Isomers are 2 compounds that have the same empirical formula but different physical and chemical properties.

cis configuration

trans configuration

Nomenclature

System	Example	Explanation
Trivial nomenclature	Oleic acid	**Trivial names** (or **common names**) 1. are non-systematic historical names 2. most frequent naming system used in literature. 3. frequently do not follow any pattern, but they are concise and often unambiguous.
Systematic nomenclature	(9Z)-Octadecenoic acid	**Systematic names** (or **IUPAC names**) 1. Counting begins from the carboxylic acid end. 2. Double bonds are labelled with cis-/trans- notation or E-/Z- notation, where appropriate.
Δ^x nomenclature	cis-Δ^9-Octadecenoic acid	**Δ^x (or delta-x) nomenclature** 1. each double bond is indicated by Δ^x, where the double bond is located on the xth carbon–carbon bond, counting from the carboxylic acid end. 2. Each double bond is preceded by a cis- or trans- prefix, indicating the conformation of the molecule around the bond.
$n-x$ nomenclature	α-Linolenic acid $n-3$	**$n-x$ (n minus x; also ω-x or omega-x) nomenclature** 1. A double bond is located on the xth carbon–carbon bond, counting from the terminal methyl carbon (designated as n or ω) toward the carbonyl carbon. 2. For example, α-Linolenic acid is classified as a $n-3$ or omega-3 fatty acid.
Lipid numbers	18:3 18:3, $n-6$ 18:3, cis,cis,cis-$\Delta^9,\Delta^{12},\Delta^{15}$	**Lipid numbers** take the form $C{:}D$, where C is the number of carbon atoms in the fatty acid; D is the number of double bonds in the fatty acid. This notation can be ambiguous, as some different fatty acids can have the same numbers. Consequently, when ambiguity exists this notation is usually paired with either a Δ^x or $n-x$ term.

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Systematic nomenclature

- based on hydrocarbon molecule with the same number and arrangement of carbon atoms
- saturated = anoic; octanoic acid (octa = 8)
- unsaturated = enoic; octadecenoic acid (octa = 8 and deca = 10, thus 18)
- carbon atoms; # from carboxyl (acid group) carbon (#1)
- adjacent carbon known as α-carbon (#2)
- terminal methyl carbon (CH_3) as n-carbon or ω-carbon

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Systematic nomenclature

- for unsaturated: where is/are double bond(s)?
    - a. Δ^9 = double bond between carbon atoms 9 and 10
        $\Delta^{9,12}$ = double bonds between 9 and 10, 12 and 13
        i.e. all-*cis*-9,12-octadecadienoic acid
    - b. omega (ω) = indicates first or only double bond counting from the methyl (last) carbon (n or ω)

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Conclusion

- Fatty acid is devided into two classes which are saturated fatty acid and unsaturated fatty acid

- Unsaturated fatty acid has isomer for examples cis and trans

- Nomenclature are based on the chemical structure of the fatty acids

Chapter description

All pictures/photographs/diagrams/figures used in this chapter is subjected to common creative that for education purposes

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