Food Oils and Fats: Chemistry & Technology Professor H N Mishra Agricultural and Food Engineering Department Indian Institute of Technology Kharagpur Week 1: Course Overview and Introduction Lecture 08: Glycerides – Type, Structure and Function



Hello everybody. Namaskar. Now, we are in the eight lecture of this course.



In this lecture today, we will discuss about glycerides, their types, structure and function. The concepts that are covered in today's lecture include glycerides and its classification, chemical synthesis of glycerides in the biological materials, then triglycerides structure and function and then triglycerides as an energy source. So, these we will cover.



So, the glycerides as was also briefly told in earlier classes that they are the fatty acids esters of glycerol, ok. They are non-polar hydrophobic molecule that are insoluble in water because of the polar hydroxyl of glycerol and they are polar carboxyls of the fatty acids are bound in ester linkages. Lipids have lower specific gravities than water. They may be mono, di- or triglycerides depending upon the number of fatty acids present, ok.

See here in this reaction, it is shown that the glycerol and then the fatty acids. It joins with this molecule that is fatty acid OH, the OH here and this OH in the carboxylic group fatty acid, ok. So, from this one water molecule goes out, alright, and there is a linkage between CH2O-COOR, yes. So, that becomes a easter linkage. So, depending upon whether 1 or 2 or all the 3, they are esterified, it will become a monoglyceride, diglyceride or finally, triglycerides, ok.



The glycerol molecules has 3 carbon atoms, 5 hydrogen atoms and 3 hydroxyl groups. So, there are 4 bonds or linkages to each of the 3 carbon atoms. It is I hope you all know that is carbon contains 4 bond that is 4 hydrogen can join to the single carbon atom, ok. Then esterification is the reaction of an alcohol with a carboxylic acid to give a ester and water like for example, here you see a fatty acid plus alcohol. So, if it is esterification process it undergoes, then it gives the ester like R we take as a fatty acids. So, R-COOR1. So, this becomes here this is one is fatty acid and there is alcohol. So, it is fatty group and alcoholic group reaction between carboxylic and alcohol it becomes a ester, ok. So, this shows you the general and in the process and water molecule is released, ok.

This gives you a general description of the esterification process and mind it when it is hydrolyzed then ester linkage can be broken and one will get again the fatty acids and the alcohol may be glycerol. So, the other in this lower reaction it is shown esterification of a glycerol with a fatty acid to form triglyceride. That is where three molecules of fatty acids are esterified with the three hydroxyl group of the glycerol, then it becomes a triglyceride and in the process three molecules of water get released, ok.

Given Structure of glycerides

- Glycerol and common fatty acids are achiral compounds with no chiral centres in the molecule.
- An achiral molecule has a plane of symmetry and superimposable mirror images.
- When the middle carbon in glycerol has four different substituent groups, it becomes chiral with mono-, di-, and mixed TAGs having a chiral carbon.
- A chiral molecule has neither a plane nor a centre of symmetry and has non-superimposable mirror images, which are called enantiomers or optical isomers.
- · Optical isomerism is a type of stereoisomerism.
- To distinguish the configuration of the fatty acids in TAGs, the carbon atoms of glycerol are numbered stereo specifically.

So, if we discuss the structure of glycerides, this glycerol and common fatty acids are achiral compounds with no chiral centers in the molecule. An achiral molecule has a plane of symmetry and it has superimposable mirror image. When the middle carbon in glycerol has four different substituent groups, it becomes chiral with mono, di and mixed triacylglycerols having a chiral carbon atoms. A chiral molecule has neither a plane nor a center of symmetry and has non superimposable mirror images which are called enantiomers or optical isomers. Optical isomerism is a type of stereoisomerism. To distinguish the configuration of the fatty acid in triacylglycerols, the carbon atoms of glycerol are numbered stereospecifically, ok. That is the from the top is the number one that is stereospecific numbering that is Sn stand for stereospecific numbering.



And here in this if you keep that carbon atom like in the top from the top to bottom the top carbon atom is known as Sn1 stereospecific number 1, then middle is the Sn2 stereospecifically numbered 2 carbon atom and the bottom one is the Sn3. So, that is called stereospecific numbering of the carbon that is a Fischer projection must drawn with hydroxyl group at C2 to the left. The carbon atom at the top of the structure is C1 and at the bottom it is C3. And in this case the prefix Sn that is stereospecific numbering is used and in that way it is possible to differentiate between the positioning of the fatty acid. That is a stereospecific numbering of triglyceride is used to designate the configuration of triglycerides.

So, here you see that is to be a specific numbering that is the chiral objects in this figure that if you look at our left hand and right hand that mirror image they cannot be superimposed. They do not have a plane of symmetry. Whereas, if this there are two flask of identical nature they are a chiral object they can be superimposed each other they have the plane of symmetry. So, this is the that mixed triglyceride they are normally chiral there is no plane of symmetry in this. Whereas, glycerol it is a it has a plane of symmetry. It is achiral ok. So, that is the concept.

- ✓ A Fischer projection must be drawn with the hydroxyl group at C-2 to the left.
- ✓ The carbon atom at the top of the structure is C-1 and at the bottom is C-3.
- ✓ In this case, the prefix Sn (Stereospecific numbering) is used and in that way, it is possible to differentiate the positioning of the fatty acid(s).



So, this is used in fact, for this numbering also that these stereospecific numbering I already discussed this.



Then you can see let us see stereospecific numbering of and test of chirality of some of the common triglycerides, monoglycerides and diglycerides. So, here if you look at the monoacylglycerol, monoglyceride. It has a that is the 1 SN1 acylglycerol means at the first one the fatty acid. So, this indicates that the symbol is star indicates that the chiral center that is the other second one in all these three ok. It is the chiral center because they are all chiral compounds and in this whether the SN2 acylglycerol or SN1 acylglycerol or SN3 acylglycerol that is it is just shows that the number of that the fatty acid positioning of fatty acid whether it is first carbon atom in this case second carbon atom or in third carbon atom ok.



Then becomes similarly stereospecific numbering and test of chirality for the diacylglycerols. Diacylglycerol may be SN12 diacylglycerol or 23 diacylglycerol or 13 SN diacylglycerol ok. That is 12 means that is the ester linkage is the top carbon atom and middle carbon atom that is these are 12. Whereas, the 23 it is the middle carbon atom are 31, 13 it is the top carbon and bottom carbon ok. That the also that is they are the in the second carbon is the see that is superimposable structure it is a chiral from chiral center ok that is star in all these cases.



Then it is a triacylglycerol you see that is where there are a simple triglyceride and we say the mixed triglyceride ok. Simple triglyceride means where all the three fatty acids are the same fatty acid and it is triglyceride obviously, so 1, 2, 3 all the three are there are same fatty acids. So, it is a achiral compound whereas, the mixed triglyceride it is a R1, R2 and R3. There are all these three fatty acid different fatty acid it is a chiral compound chiral center is at 2. Whereas, in the mixed triglyceride where R1 and R2 there are two fatty acids same there is R2 and R2 at second and third carbon atom and at first carbon atom it is R1. So, this is achiral. Similarly if there is a R1, R1 and R2 at the second position R1 at first position and second third last position there is same carbon and the second. So, it is also that is the presence of the chiral centers in R1 and R2 can make these triacylglycerols as chiral.

Types of glycerides Glyceride, or glyceryl ester, is a monoacylglycerol, diacylglycerol, or triacylglycerol, depending on whether one, two, or three of the alcohol groups (-OH) of glycerol are esterified with fatty acid(s) (ROOH).



Then types of triglyceride if you discuss that is the glyceride or glycerol ester is a monoacylglycerol, diacylglycerol or triacylglycerol depending upon whether 1, 2 or 3 of the alcohol groups of glycerol are esterified with fatty acids. So, see that these are the mono esters of glycerol, di esters of glycerol, tri esters of glycerol. Monoglycerides, diglycerides or triglycerides there are three types of glycerides.



Then monoglycerides may be either 1 or alpha monoglyceride or 2 or beta monoglyceride depending upon whether the terminal or middle hydroxyl groups have been esterified respectively. Like you see that alpha monoglyceride it is the terminal hydroxyl and beta monoglyceride that esterified at a middle one, but it is a monoglyceride. So, both here in the beta monoglyceride that both the terminal hydroxyl are there only esterified in the middle one 2 SN2 and when in the alpha means that is either of the terminal hydroxyl is esterified.



Then diglycerides can be further described as a 1, 2 diglyceride or 1, 3 diglyceride depending upon the position of the fatty acids on the glycerol molecule ok. 1, 2 diglyceride that is 1, 2 means esterified at carbon number 1 and 2 fatty acids are there whereas, 1, 3 esterified is carbon atom number 1 and 3 ok.



The triglycerides are the simplest lipids constructed from the fatty acids. They are also referred to as triacylglycerol or natural fats. Plants, particularly cereal grains, usually store lipids as triacylglycerol. Triglycerides are the main lipids stored in all cereals, endosperm and in wheat the endosperm contributes about 12 percent of the total in the grain. Mixed triglycerides are most naturally occurring triglycerides. They are important as emulsifiers in food proteins.



The classification of triglycerides we discussed earlier also they may be simple triglyceride or mixed triglycerides. Simple triglycerides are mono acid triglycerides where all the 3 fatty acids are the same ok. Whereas, the mixed triglyceride here there are 2 may be different it will be 2 fatty acid joining the 3 ester linkages, it will be 3 different fatty acids and so on.

Nomenclature of triglycerides

- Triacylglycerols can be named by several different systems.
- Triacylglycerols are often named using the common names of the fatty acids.

Simple triglycerides



Let us discuss nomenclature of triglycerides. They can triglycerides can be named by several different systems like triacylglycerols are often named using the common names of fatty acids. Simple triglycerides they contain like let us say if they contain all the 3 fatty acids or the stearic acid, then different way of naming like they can be renamed as a tristearin or tristearate, glycerol tristearate, tristearylglycerol or simply StStSt or 18:0-18:0 18:0 that is for the stearic acid. If there is similarly other like if oleic acid is everywhere, then it can be the triolein, trioleate, glycerol trioleate, triacylglycerol, OOO that is abbreviation for and then it will be 18:1-18:1-18:1 because it has a 1 double bond. Similarly, if there are only oleic acids, simple triglyceride depending upon whether what are the if they are having a stearic acid, palmitic acid, oleic acid etcetera, all the 3 fatty acids are same. So, accordingly you can name it tripalmitin, tripalmitate, glycerol tripalmitate and so on.

Mixed triglycerides Nomenclature depends on whether the stereospecific location of each fatty acid is known. The nomenclature for these heterogeneous triacylglycerols replaces the -ic at the end of the fatty acid name with -oyl. Stereospecific location is not known A triacylglycerol-containing palmitic acid (P), oleic acid (O), and stearic acid (St) Palmito-oleoyl-stearoyl-glycerol. Palmito-oleo stearit Glycerol-palmito-oleo stearate POSt (abbreviated names) 16:0-18:1-18:0 (abbreviated names)

In the case of mixed glyceride, nomenclature depends upon whether the stereo specific location of each fatty acid is known. The nomenclature of these heterogeneous triacylglycerols replaces the IC at the end of the fatty acid with OYL like that triglyceride containing palmitic acid that is IC is there in the last case that is T oleic acid that is OIC is there and stearic acid IC. In all these cases suppose if triglyceride has all these 3 acids. So, in the IC will be is replaced with OYL. So, palmitoyl-oleoyl-stearoyl-glycerol or simply it can be named as palmito-oleo stearin or glycerol-palmito-oleo stearate or simply P for palmito, O for oleo, St for stearate that is the POSt. It shows that simply that is this glycerol these are the 3 fatty acids like first is P, second is oleic acid and the third is Sn3 stearate the POSt are 16:0, 18:1, 18:0 these are abbreviated name. So, in this way they can be named.



Then other case when the stereo specific location is known that is stereo specific location of the fatty acid is if it is known then Sn is added to the name like 1 palmitoyl, 2 oleoyl, 3 stearoyl, Sn glycerol. So, it clearly indicate that is that palmitic acid is at Sn1 position, oleic acid is at Sn2 position and stearic acid is Sn3 position. It can also be said that is Sn1-palmito-2-oleo-3-stearin or Sn-glycerol-1-palmito, 2-oleo-3-stearate or Sn POSt or Sn-16:0-18:1-18:0. So, these are the different ways.



Also if two of the fatty acids are identical the naming other than the abbreviated names can be shortened like suppose here in the structure you see that first and second they are the palmitic acid and at the third position it is a stearic acid. So, these fatty acids can be named diglyceride can be named like 1,2-dipalmitoyl-3-stearoyl- -Sn-glycerol means 1, 2 di palmitoyl means 1 and second position there are each palmitic acid and total there are 2 palmitoyl the di palmitoyl or Sn2 di palmito-3-stearate, Sn-glycerol-1,2-dipalmito-3-stearate or PPSt or 16:0-16:0-18:0 that is ok. So, that in that way it can be named.



Then fats as energy source they are we consume the fat or major energy source in the body, but in the fats and carbohydrates and nutritionist recommend that approximately 30 percent or so, but not more than 30 percent of the total intake of body energy should come from the fat sources. So, cells can obtain fatty acids or fuels from three sources like fats which are consumed in the diet, fats which are stored in the cell as lipid droplets or fats synthesized in one organ for export to another. Some species use all three sources under various circumstances, other use one or two. Vertebrates, for example, obtained fats in the diet they like they also mobilize fats stored in a specialized tissues like adipose tissue which consists of cell that is called adipocytes. Then in the also they have the fats in the liver that is which converts excess dietary carbohydrate to fats for export to other tissues ok. So, if this is the you see in the left this figure is adipose and here adipocyte is in the right. So, in the adipose you see that the fat globules how their membrane as well as fat reservoir they are in the adipocyte stese fats are present in the body cells.



So, on an average 40 percent or more of the daily energy requirement of human in highly industrialized countries is supplied by dietary triacylglycerols, but as I told you the nutritional guidelines recommend no more than 30 percent of daily calorie intake from fats it should be restricted. Triacylglycerols provide more than half the energy requirements of some organs particularly the liver, heart and resting skeletal muscle. Stored triacylglycerols are virtually the sole source of energy in hibernating animals and migrating birds. Protists obtain fat by consuming organisms lower in food chain ok and some also store fats as cytosolic lipid droplets cytosolic lipid droplets. Vascular plants mobilize fats stored in seeds during germination, but do not otherwise depend on the fats for energy.



The energy value of foods is currently predominantly expressed in kilo calories it may be written as k small c a l or capital C a l capital C a l this indicates that kilo calorie ok. The energy value of a single food or nutrients can be directly measured by determining the amount of heat released upon its ignition and total combustion in a bomb calorimeter ok. And in this way when the food is burnt in the bomb calorimeter. So, the energy which is measured in this is this not take does not take into consideration the amount lost by the digestive and metabolic processes that is excretion in the faces, sweat, and urine etcetera what happen when we are taking the fat inside our body then fat goes into a system specific metabolism and where the energy is released.

But in the body whatever energy is released that energy utilized by a part of the various body functions various purposes, but some of the energy it is not utilized that also is a it goes out is excreted from the body in the form of faeces in the form of sweat urine etcetera. So, the total energy that is obtained from the fat in the body it may be that the one after whatever you are getting the calorific value from the bomb calorimeter if you minus it from the energy that is not utilized by the body that is excreted released through excreta, sweats, urine, etcetera that becomes. So, that is the they do not correspond to the amount of the energy utilized by the body that is bomb calorimeter it gives energy it will give you a total energy value of the fat, but not necessarily that the energy value which is utilized by the body.

Food or nutrient	Kcal/g	KJ/g	
Starch	4.18	17.49	
Glycogen	4.19	17.53	
Dextrins	4.11	17.20	
Disaccharides	3.95	16.53	
Monosaccharides	3.74	15.65	
Glycerol	4.31	18.03	
Butyric acid	5.95	24.89	
Dleic acid	9.41	39.37	
stearic acid	9.53	39.87	
Butter	9.20	38.49	
Olive oil	9.33	39.04	
Rapeseed oil	9.49	39.71	
Peanuts oil	9.47	39.62	
Beef tallow	9.50	39.75	
ard	9.59	40.12	
Caseine	5.86	24.52	
Gelatine	5.25	21.97	
Ovoalbumine	5.69	23.81	
Wheat Gluten	5.95	24.89	
Ethanol	7.11	29.75	

So, the physical energy values of common foods and nutrients is given in this table. Like you see that starch, glycogen, dextrins, disaccharides, monosaccharides, glycerol they gives us to the tune of that is 4 kilo calorie per gram. Generally, the carbohydrate polysaccharides etcetera of course, disaccharide monosaccharides they have little less, but all most all together close. Butyric acid 5.95, then oleic acid, stearic acid, butter, olive oil, rapeseed oil all these there is a beef tallow, lard they all to the tune of 9 kilo calorie somewhere 9.4, 9.5, 9.2 and so on. Then gelatin has 5.25 kilo calorie or 21.97 kilo joule ok. Ovalalbumin 5.69 kilo calorie or 23.81 kilo joule, wheat gluten it gives 5.95 kilo calorie energy or 24.8. Ethanol gives almost 7.11 kilo calorie energy or 29.75 kilo joule ok. So, these were the total calories.

Carbohydrates	Fats	Proteins	1
4.1 kcal/g	9.3 kcal/g	5.65 kcal/g	-
97%	95%	91%	
Carbon dioxide and Water	Carbon dioxide and Water	Urine (urea, creatinine, uric acid, and other nitrogenous compounds)	
		1.25 kcal/g	
4.1 * 0.97 = 4 kcal/g	9.3 * 0.95 = 9 kcal/g	(5.65 - 1.25) * 0.91 = 4 kcal/g	
	Carbohydrates 4.1 kcal/g 97% Carbon dioxide and Water 4.1 * 0.97	Carbohydrates Fats 4.1 kcal/g 9.3 kcal/g 97% 95% 200 25% Carbon dioxide and Water Carbon dioxide and Water 4.1 *0.97 9.3 *0.95 - 4.1 *0.97 - 9 kcal/g	CarbohydratesFatsProteins4.1 kcal/g9.3 kcal/g5.65 kcal/g97%95%91%97%95%91%Carbon dioxide and WaterCarbon dioxide and WaterUrine (urea, creatinine, uric acid, and other nitrogenous compounds)L1.25 kcal/g4.1 * 0.97 = 9 kcal/g9.3 * 0.95 = 4 kcal/g

That physiological energy values if you see that there are certain parameter. That is the carbohydrate, fat and protein. Physical energy value of the carbohydrate is 4.1 kilo calorie per gram, that is from the fat it is 9 or 9.3 kilo calorie and proteins 5.65 kilo calorie. Digestibility coefficient that is the how much the fat is actually utilized that is digested in the body if you see that that is the digestibility coefficient is for the energy is energy intake minus energy in faeces divided by energy intake multiplied by 100 that is what is the total energy you are taking ok. And how much is released from the body through excreta etcetera is a then in the case of carbohydrate it is 97 percent fats 95 percent and proteins 91 percent. So, if this is a physiological energy value whatever final that is 4.1 if it takes that is a multiplied by 0.97 it gives 4 kilo calorie per gram. So, normally we consume in our calculations etcetera food calculation energy value calculation food formulation we should take this that is a we should account the carbohydrate 4 kilo calorie. Similarly, for the fats 9.3 multiplied by 0.95 that is 9 kilo calorie. For the protein that is the 5.65 minus 1.25 into 0.91 because this 1.25 comes energy value of the final metabolic product because in the protein it is urea that is a urine it also goes urine in the form of urea, creatine, uric acid and other nitrogenous compounds. But in the carbohydrate and fats the final metabolic products are carbon dioxide and water carbon dioxide water.

So, the normally there is no energy lost in this it is only through the excreta after the undigested energy which goes through excreta. So, in this way total energy energy value can be calculated in the case of protein that is from 5.65 it is also subtracted this final metabolic product which goes 1.25 energy value of the final metabolic products ok then 0.91 is 4 kilo calorie. So, carbohydrate and protein 4 kilo calorie and fats 9 kilo calorie. So, this is the data it can be used for food formulation. Normally the protein is not taken as a input formulation input calculation it is not taken as a source for energy ok.



So, with this I will summarize this lecture by saying that glycerides are esters of glycerol and fatty acids and can be classified as mono, tri, and diglycerides. Triglycerides are the major components of the fats and oil in fact, they are all fats and oils are basically chemically if you say they are all triglycerides only. Monoglycerides and diglycerides are minor component that are used as emulsifiers in food products etcetera. Glycerides exhibit stereoisomerism and their stereospecific structure is important for the nomenclatures. Fats are an important source of energy and energy reserves for the human body ok.

References

- · Lehninger, AL, Nelson, DL, & Cox, MM (2005). Lehninger principles of biochemistry . Macmillan.
- Scrimgeour, C., Gao, Y., Oh, W.Y. and Shahidi, F. (2023). Chemistry of Fatty Acids. In Bailey's Industrial Oil and Fat Products, F. Shahidi (Ed.). https://doi.org/10.1002/047167849X.bio005.pub2
- Flickinger, B.D. and Matsuo, N. (2005). Diacylglycerols. In Bailey's Industrial Oil and Fat Products, F. Shahidi (Ed.). https://doi.org/10.1002/047167849X.bio069
- Julian McClements, D., and Decker, E.A. (2007) Fennema's Food Chemistry. Damodaran, S., Parkin, K., and Fennema, O. (Ed.). CRC Press.
- Lawson, H. W. (1995). Food oils and fats: technology, utilization and nutrition. Springer Science & Business Media.
- O'brien, R. D. (2008). Fats and oils: formulating and processing for applications. CRC press.
- Gunstone, F. (2009). Oils and fats in the food industry. John Wiley & Sons.
- O'Keefe, Sean & Sarnoski, Paul. (2017). 1 Nomenclature and Classification of Lipids: Chemistry, Nutrition, and Biotechnology, Fourth Edition. 10.1201/9781315151854-2.
- Tomassi, G., & Merendino, N. (2006). Energy values of foods. Cachexia and Wasting: A Modern Approach, 47-52.



-IIT Kharagpur

These are the references which are used in this lecture this.



Thank you very much.