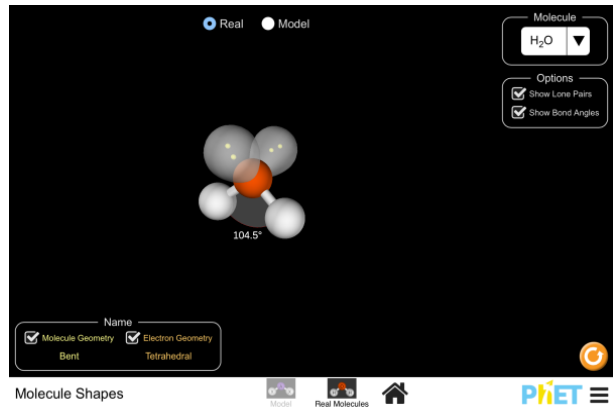
Understanding Chemistry in 3D



1. Click on the image to launch the simulation
2. Choose "Real Molecules"
3. Click on "Show Bond Angles"
    - you may also de-select "Show Lone Pairs"
4. Drag the atoms to understand the 3-D shape
5. Choose CH_4 from the drop-down menu of molecules
    - CH_4 is methane, the simplest organic molecule
    - notice the restraints on the physical space occupied by the atoms as you drag the atoms around
    - remember these bond angles and constraints when we explore organic chemistry
    - toggling between "Model" and "Real" will illustrate if the position of the atoms are influenced by other factors we don't see
6. Choose NH_4 from the drop-down menu
    - NH_4 is ammonia, a polar solvent
    - NH_4 is **NOT** an organic molecule
    - Toggle the lone pairs to see how these electrons play a role in the positioning of atoms
7. Choose CO_2 from the drop-down
    - explore this non-organic molecule to visualize the effects of double bonds on geometry

Organic Chemistry

Living things are composed of **organic molecules** primarily made up of the elements carbon and hydrogen. Molecules of hydrogen and carbon (referred to as **hydrocarbons**) have the property of being **non-polar**. Yet 70- 90% of cells are composed of water (a **polar** compound). Polar substances mix with other polar substances. Likewise, non-polar substances interact with other non-polar compounds. Polar and non-polar compounds are immiscible (unable to mix).

So how do cells keep from falling apart in a water environment?

Functional groups are clusters of atoms in a group that impart a new “function” to the compound they are attached to. Hydrocarbons in cells have functional groups attached to them that permit them to interact with the water environment of the cell. These functional groups also define the type of molecule it is based on the characteristics of those groups.

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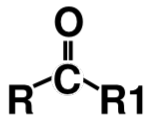
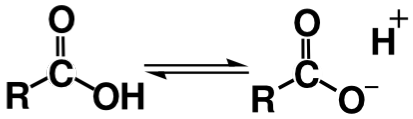
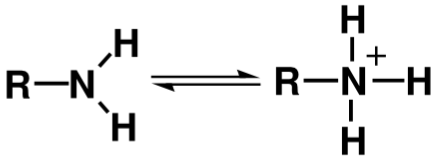
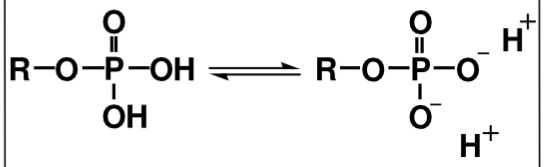
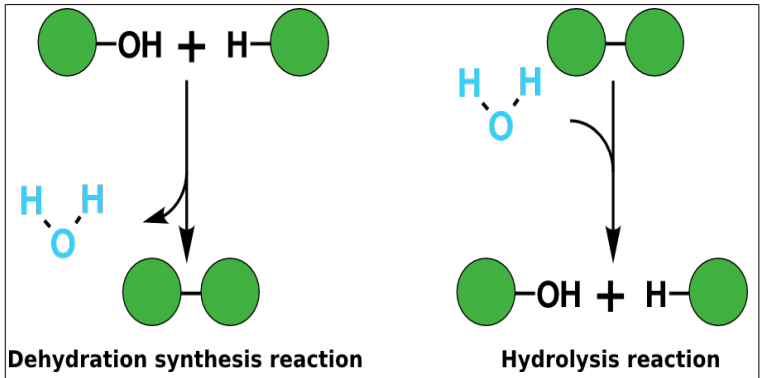
Group Name	Structure	Compound Name	Property
Hydroxyl	R—OH	alcohol	polar
Carbonyl		Aldehyde (R1=H) Ketone (R1=C)	polar
Carboxyl		acid	polar acidic
Amino		amine	polar basic
Sulfhydryl	R—SH	thiol	polar
Phosphate			polar acidic

Functional Groups. *Functional groups commonly found in organic compounds. R is a placeholder chemical that can be anything (like a hydrocarbon chain). The functional groups in this table are those that add polar or charged properties to the hydrocarbon chains. Bi-directional arrows indicate that those functional groups dynamically ionize and reach an equilibrium in solution.*

How are macromolecules assembled?

The common organic compounds of living organisms are **carbohydrates**, **proteins**, **lipids**, and **nucleic acids**. Each of these are macromolecules or **polymers** made of smaller subunits called **monomers**. The bonds between these subunits are formed by a process called **dehydration synthesis**. This process requires energy; a molecule of water is removed (dehydration) and a covalent bond is formed between the subunits. Because a new water molecule is formed, this is also referred to as *condensation*. The opposite where water and energy are used to break apart polymers into simpler monomers is called **hydrolysis** (***hydro***- water, ***lysis***- to break or split).



Polymer formation. *Dehydration reactions join monomers. Hydrolysis splits polymers.*

Where do we find macromolecules?

Sample label for Macaroni & Cheese

Nutrition Facts

Serving Size 1 cup (228g)
Servings Per Container 2

Amount Per Serving	
Calories 250	Calories from Fat 110
	% Daily Value*
Total Fat 12g	18%
Saturated Fat 3g	15%
Trans Fat 3g	
Cholesterol 30mg	10%
Sodium 470mg	20%
Total Carbohydrate 31g	10%
Dietary Fiber 0g	0%
Sugars 5g	
Protein 5g	
Vitamin A	4%
Vitamin C	2%
Calcium	20%
Iron	4%

* Percent Daily Values are based on a 2,000 calorie diet. Your Daily Values may be higher or lower depending on your calorie needs.

	Calories	2,000	2,500
Total Fat	Less than	65g	80g
Sat Fat	Less than	20g	25g
Cholesterol	Less than	300mg	300mg
Sodium	Less than	2,400mg	2,400mg
Total Carbohydrate		300g	375g
Dietary Fiber		25g	30g

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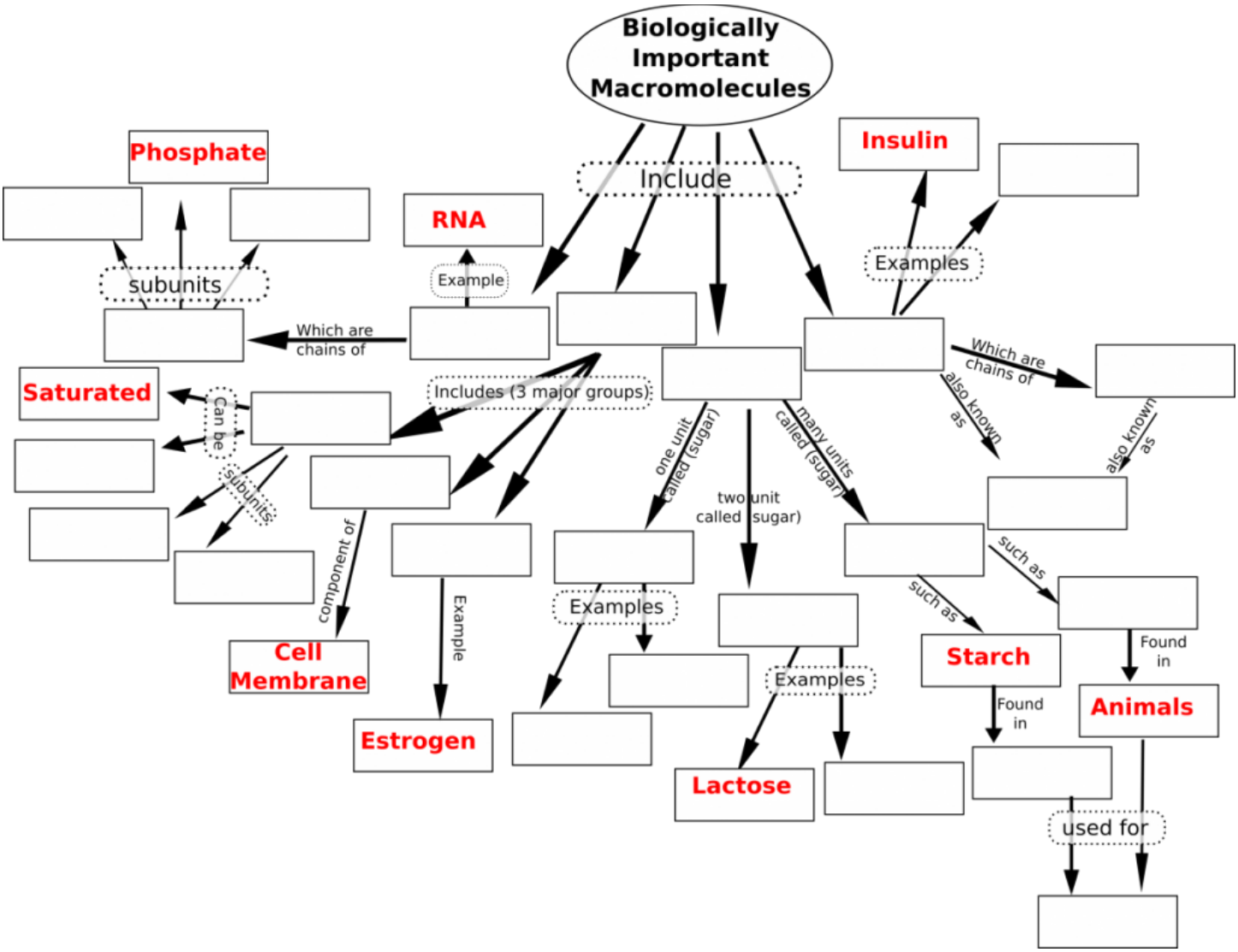
Additional Resources

- Carbohydrates http://www.visionlearning.com/en/library/Biology/2/Carbohydrates/61
- Lipids http://www.visionlearning.com/en/library/Biology/2/Lipids/207/reading
- Fats and Proteins http://www.visionlearning.com/en/library/Biology/2/Fats-and-Proteins/62

Vocabulary

- carbohydrates
- reducing sugar
- polymer
- monomer
- monosaccharide
- disaccharide
- polysaccharide
- aldehyde
- ketone
- lipid
- Dehydration synthesis
- hydrolysis
- reduction
- oxidation

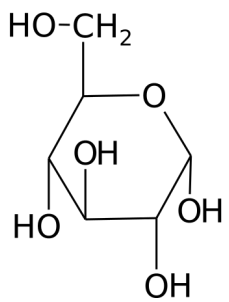

Biologically Important Macromolecules
Include
Phosphate
RNA
Insulin
subunits
Example
Examples
Which are chains of
Which are chains of
Saturated
Can be
Includes (3 major groups)
also known as
also known as
subunits
one unit called (sugar)
two unit called (sugar)
many units called (sugar)
component of
Example
Examples
such as
such as
Cell Membrane
Estrogen
Starch
Found in
Found in
Animals
Examples
Lactose
used for

Introduction: Carbohydrates

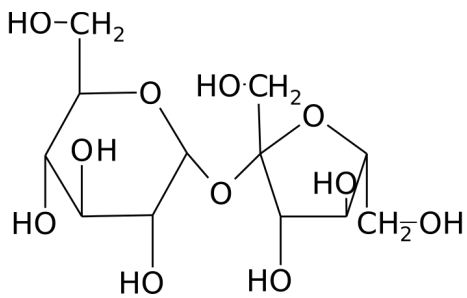
Carbohydrates serve 2 major functions: energy and structure. As energy, they can be simple for fast utilization or complex for storage. Simple sugars are monomers called **monosaccharides**. These are readily taken into cells and used immediately for energy. The most important monosaccharide is glucose (**$C_6H_{12}O_6$**), since it is the preferred energy source for cells. The conversion of this chemical into cellular energy can be described by the equation below:

$$C_6H_{12}O_6\ (s) + 6\ O_2\ (g) \rightarrow 6\ CO_2\ (g) + 6\ H_2O\ (l) + \text{energy}$$

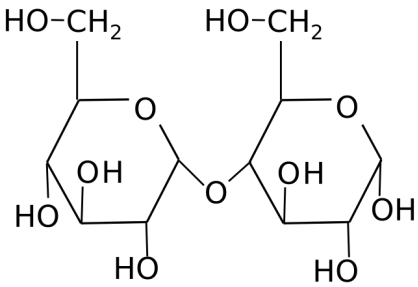
Long polymers of carbohydrates are called **polysaccharides** and are not readily taken into cells for use as energy. These are used often for energy storage. Examples of energy storage molecules are: amylose or **starch** (plants) and **glycogen** (animals). Some polysaccharides are so long and complex that they are used for structure like **cellulose** in the cell walls of plants. Cellulose is very large and practically indigestible, making it unsuitable as a readily available energy source for cells.



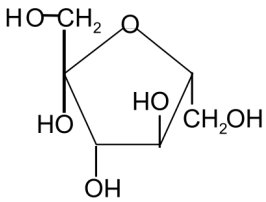
Glucose, a monosaccharide



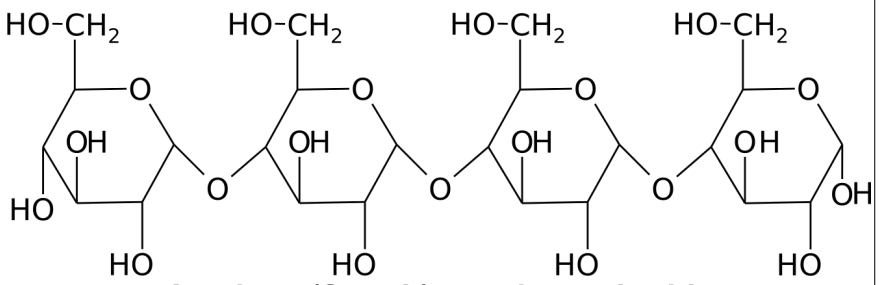
Sucrose, a disaccharide



Maltose, a disaccharide



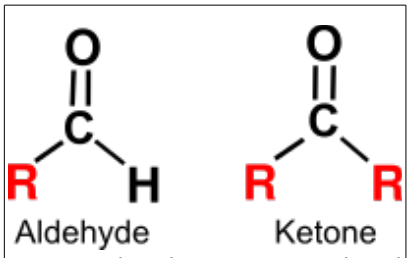
Fructose, a monosaccharide



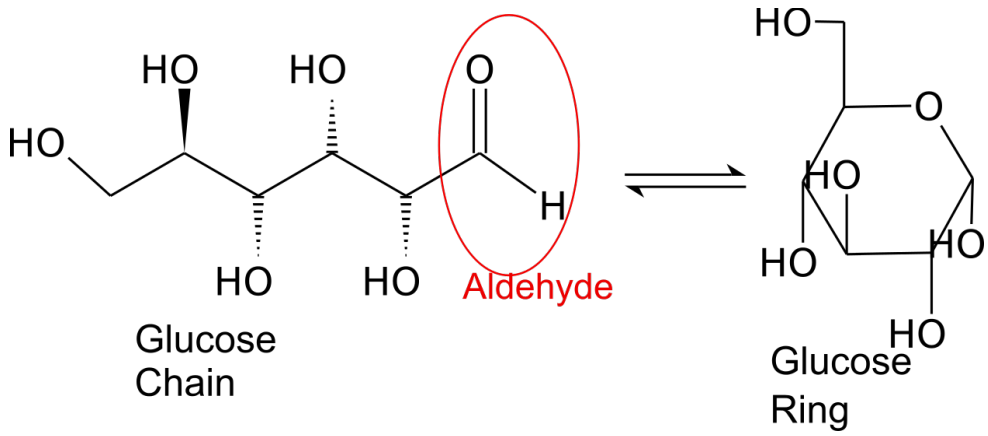
Amylose (Starch), a polysaccharide

***Carbohydrates**: Carbohydrates are composed of sugar units referred to as -saccharides.*

Many monosaccharides such as glucose and fructose are **reducing sugars,** meaning that they possess free **aldehyde** or **ketone** groups that reduce weak oxidizing agents such as the copper in Benedict's reagent. The double bond in the carbonyl group is a source of electrons that can be donated to something else. That is to say, those electrons can be "*lost*" by the sugar and "*gained*" by another chemical. **Benedict's reagent** contains cupric (copper) ion complexed with citrate in alkaline solution. Benedict's test identifies reducing sugars based on their ability to reduce the cupric (Cu^{2+}) ions to cuprous oxide (Cu^{+}) at basic (high) pH. Cuprous oxide is green to reddish orange. Roughly speaking, **reduction** is a type of chemical reaction that is paired with **oxidation**. In oxidation/reduction reactions (**RedOx**), some chemical loses electrons (oxidized) to another chemical that gains them (reduced). We remember whether a compound is reduced or gained by using the pnemonic: LEO goes GER or **L**oss of **E**lectrons is **O**xidation & **G**ain of **E**lectrons is **R**eduction.



Monosaccharides contain a carbonyl group. The carbonyl is a source of electrons (the double bond on the oxygen). These electrons can be donated (or lost and oxidized) to reduce another compound (that gains those electrons)



Monosaccharides are capable of **isomerizing**. This means they alternate in structure from a linear chain to a ring form in solution. In the chain form, the aldehyde is free to donate (lose) electrons to reduce another compound. When monosaccharides undergo dehydration synthesis to form polymers, they can no longer isomerize into chains with free aldehydes and are unable to act as reducing sugars. Green color indicates a small amount of reducing sugars, and reddish orange color indicates an abundance of reducing sugars. Non-reducing sugars produce no change in color (i.e., the solution remains blue).

Oxidized Benedict's reagent (Cu^{2+}) + Reducing sugar (R-C=O)
(blue)

Heat
High pH

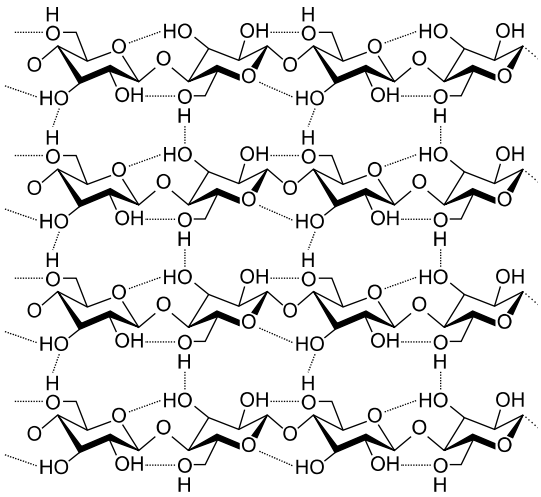
Reduced Benedict's reagent (Cu^{+}) + Oxidized sugar (R-COOH)
(green to reddish orange)

Note: Cu^{2+} has fewer electrons than Cu^{+}.

Structural Carbohydrates

In food, more complex carbohydrates are derived from larger polysaccharides. These larger carbohydrates are fairly insoluble in water. Dietary fiber is name given to indigestible materials in food most often derived from the complex carbohydrates from vegetable material. Some of this material serves the plants as a structural component of the cells and is completely insoluble. **Cellulose** is the major structural carbohydrate found in plant cell walls. Similarly, animals and fungi have structural carbohydrates that are composed of the indigestible compound called **chitin**. We will not be testing for these items.

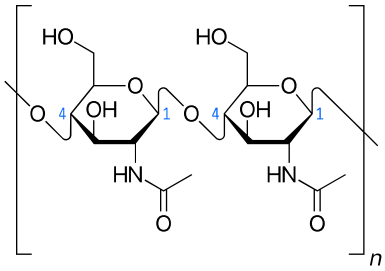
Cellulose (plant structural)



Cellulose is a complex carbohydrate of glucose molecules. It is the major structural component of plant cell walls. It's structural durability is enhanced by intramolecular hydrogen bonds.

A cicada molting from it's shell made of chitin.
Credit: Jodelet / Lépinay (CC BY-SA 2.0)

Chitin (animal and fungi)



Chitin is a structural carbohydrate found in animal shells or fungi cell walls. The polymer contains amide groups that differentiates it from other carbohydrates composed of glucose.

Test your knowledge

- http://www.visionlearning.com/en/library/Biology/2/Carbohydrates/61/quiz

Materials

• potato juice • apple juice • urine sample 1 • urine sample 2 • reducing sugar solution • starch solution • Benedict's Reagent	• Sucrose solution • glucose solutions • distilled water • hot plates • beakers of water • test tubes • test tube rack

Stop and Think:

- Use your senses and previous observations/experiences about the qualities of the experimentals.
- Formulate some hypotheses about the carbohydrate content of the experimentals or unknowns.
    - Identify if the sample is experimental or control before making hypothesis

QUESTION: Are there simple reducing sugars in my juice? Are there simple reducing sugars in my urine?

Diabetes mellitus is a disease that refers to the inability of the cells to take in glucose. The word diabetes refers to urination and mellitus refers to sweetness. Since the cells of diabetics cannot remove glucose from the blood, there is an excess of glucose circulating that is eliminated in the urine. The traditional method of diagnosing someone with diabetes mellitus was to taste the sweetness of the patient's urine. Let's use Benedict's test for the detection process instead of the unhygienic alternative.

Make a hypothesis and ask what we would predict from a Benedict's test if testing a urine sample of someone with diabetes mellitus.

Benedict's Test For Reducing Sugars

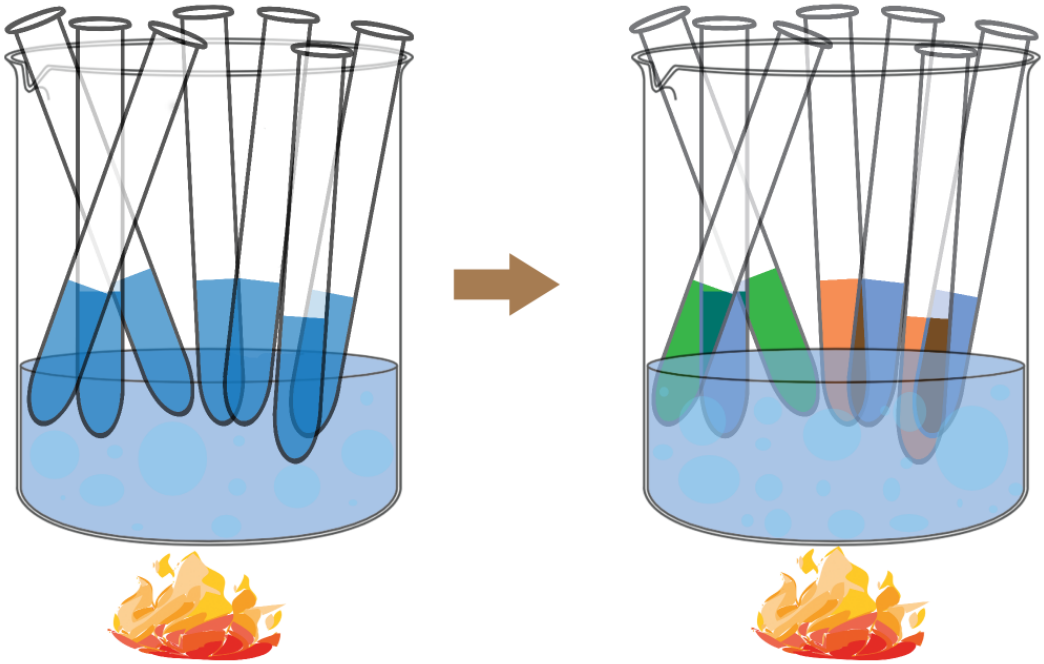
1. Obtain 9 test-tubes and number them 1-9.
2. Add to each tube the materials to be tested. Your instructor may ask you to test some additional materials. If so, include additional numbered test tubes.
3. Indicate in the table whether the the sample you are testing is positive control, a negative control or an experimental.
4. Before you begin the heating of the samples, use predict the color change (if any) for each sample. (use the sample type to aid in your prediction)
5. Add 40 drops (or 2 ml) Benedict's solution to each tube.
6. Place all of the tubes in a boiling water bath for 3 min or until a noticeable color change and observe colors during this time.

7. After 3 min, remove the tubes from the water bath and let them cool to room temperature. Record the color of their contents in the Table.

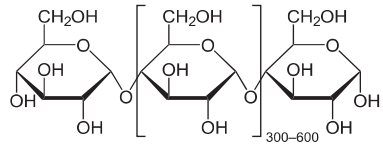
Table:Solution And Color Reactions For Benedict's Test For Reducing Sugars

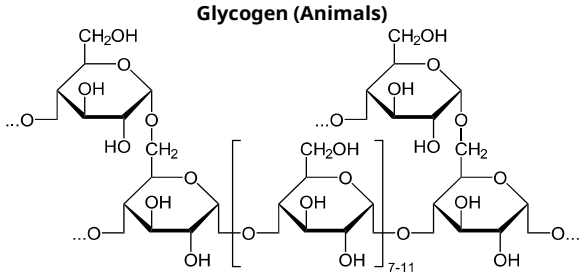
Tube	Solution	Type of Sample (unknown, + control, - control)	Hypothesized Color	Benedict's Test Color
1	10 drops apple juice			
2	10 drops potato juice			
3	10 drops sucrose solution			
4	10 drops glucose solution			
5	10 drops distilled water	- **Control**	**Blue**	
6	10 drops reducing sugar	+ **Control**	**Red**	
7	10 drops starch solution			
8	10 drops Urine sample 1			
9	10 drops Urine sample 2			

Boil solutions until color changes



Iodine Test for Starch





Carbohydrates that are used for energy storage are not reducing sugars since they are polymers that lack free aldehydes. Plant cells store energy in the form of starches like amylose or pectin. Since these molecules are larger than monosaccharides or disaccharides, they are not sweet to the taste and are not very soluble in water. **Iodine** (iodine-potassium iodide, I_2KI) staining distinguishes starch from monosaccharides, disaccharides, and other polysaccharides. The basis for this test is that starch is a coiled polymer of glucose --- iodine interacts with these coiled molecules and becomes bluish black. Iodine does not react with other carbohydrates that are not coiled, and remains yellowish brown. Therefore, a bluish black color is a positive test for starch, and a yellowish brown color (i.e., no color change) is a negative test for starch. Notably, glycogen, a common energy storage polysaccharide in animals, has a slightly different structure than does starch and produces only an intermediate color reaction.

Activity: Iodine Test For Starch

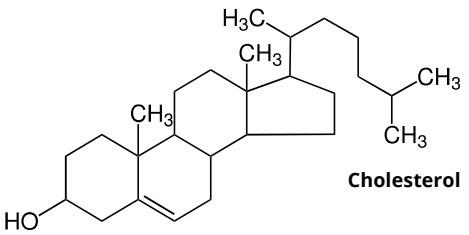
1. Obtain 7 test-tubes and number them 1-7.
2. Hypothesis Testing: Indicate in the table if the sample is experimental or control. Predict your expected color changes for each sample.
3. Add to each tube the materials to be tested as indicated in the table below. Your instructor may ask you to test some additional materials. If so, include additional numbered test tubes.
4. Add 10 drops of iodine to each tube. This test does **NOT** require boiling.
5. Record the color of the tubes' contents in the table below.

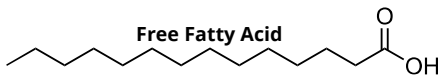
Table: Solution And Color Reactions For Iodine Test For Starch

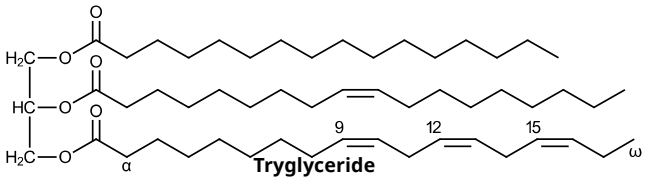
Tube	Solution	Type of Sample (unknown, + control, - control)	Hypothesized Color	Iodine Test Color
1	20 drops apple juice			
2	20 drops potato juice			
3	20 drops sucrose solution			
4	20 drops glucose solution			
5	20 drops distilled H_2O	**- Control**	**Yellow**	
6	20 drops reducing sugar			
7	20 drops starch solution	**+ Control**	**Black-Purple**	

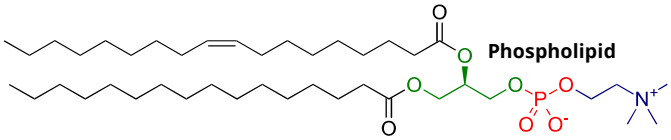
Questions for Reflection

1. In the Benedict's test, which of the solutions is a positive control? Which is a negative control?
2. Which is a reducing sugar, sucrose or glucose?
3. Which contains more reducing sugars, potato juice or onion juice?
4. Is there a difference between the storage of sugars in onions and potatoes?
5. Which patient sample likely comes from a diabetic patient and how do we know this?
6. In the Iodine test, which of the solutions is a positive control? Which is a negative control?
7. Which is more positive for the iodine test: onion juice or potato juice?
8. What can you infer about the storage of carbohydrates in onions? In potatoes?
9. Describe the half reaction $\mathbf{Cu^{2+} \rightarrow Cu^{+}}$ as oxidation or reduction.
10. Describe the half reaction $\mathbf{Cu^{+} \rightarrow Cu}$ as oxidation or reduction.



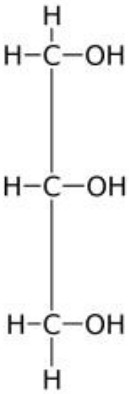




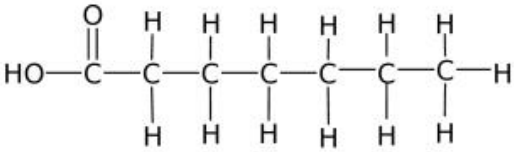


Lipids are the class of macromolecules that mostly serve as long-term energy storage. Additionally, they serve as signaling molecules, water sealant, structure and insulation. Lipids are insoluble in polar solvents such as water, and are soluble in nonpolar solvents such as ether and acetone.

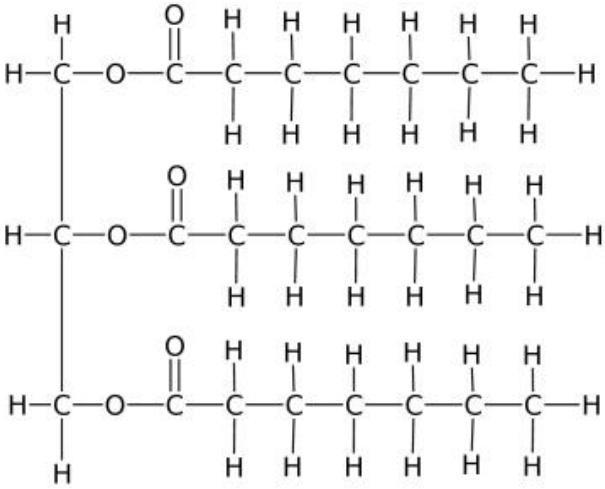
Fats or triglycerides are made of glycerol and three fatty acid chains. They form through 3 dehydration synthesis reactions between a hydroxyl of the glycerol and the carboxyl group of the fatty acid.



Glycerol

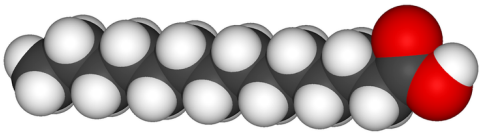


Fatty Acid

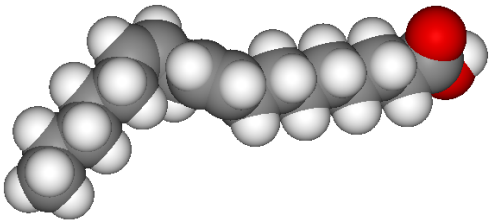


Triglyceride

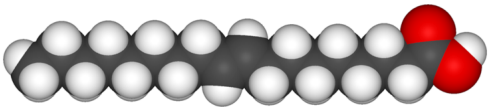
Saturated versus Unsaturated fats



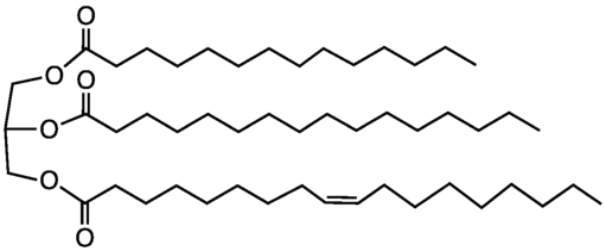
A saturated fatty acid. The molecule takes up little space in three dimensions. Many molecules can stack upon each other. Saturated fats are solid at room temperature.



A polyunsaturated fatty acid. A kink from the double bond increases the amount of three dimensional space that the molecule fills. Unsaturated fats tend to be liquid at room temperature.



A trans fatty acid. Despite an unsaturated bond, the molecule fills as much space as a saturated fatty acid and is solid at room temperature. Trans fats usually arise from artificial saturation techniques.



Butterfat is almost completely saturated. Notice how molecules can stack very closely. Because butterfat can stack together very closely, it is dense and found as a solid at room temperature.

Because butterfat can stack together very closely, it is dense and found as a solid at room temperature.
Credit: Steve Karg (CC BY 2.5)

Testing for Lipids

Tests for lipids are based on a lipid's ability to selectively absorb pigments in fat-soluble dyes such as Oil Red O or Sudan IV.

Tube	Solution	Control (+/-) or Experimental	Reaction Description
1	1 ml vegetable oil + water		
2	1 ml vegetable oil + Oil Red O		
3	1 ml water + Oil Red O		
4	1 ml Lipid Solution + Oil Red O		

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