Visualizing Biopolymers and Their Building Blocks

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Living things are primarily composed of carbon-based (organic) polymers. These are made up many small molecules which have been chemically bonded together to form a long chain. Biopolymers can be grouped into 4 main categories: LIPIDS, CARBOHYDRATES, PROTEINS, & NUCLEIC ACIDS. In this exercise, you will use the program VMD to explore the structures and learn more about these molecules and their building blocks.

Loading a Molecule into VMD

1. Click on the "Start" menu, then go to "programs" and then to "VMD 1.8.3". The window labeled "VMD Main" is the control panel and the window labeled "OpenGL" is where the molecule(s) will be displayed.
2. In the VMD Main window, select "file", then "new molecule". Hit the "Browse" button to search for the file you want. They will be stored under your class folder on the "Science on DHS Users" server. Once you select the file you want, you will hit load. The molecule you want should appear in the OpenGL window. If it does not, please see the teacher for help.
3. Once your molecule is loaded, go to the VMD Main menu & select "Representations" under the Graphics menu. On the bottom panel, change the "Drawing Method" to "CPK" to better visualize the molecule.

4. You can use your mouse to manipulate the structure by using the keyboard shortcut commands described below.
5. When you are all finished, go to the VMD main menu and select "molecule" and then "delete molecule" before loading the next structure into VMD.

List of VMD Keyboard Shortcuts (also accessible under the "mouse" menu):

Key pressed	Action Performed
t	Translate, or move entire molecule around
r	Rotate molecule around its center
s	Make the molecule bigger (mouse to left) or smaller (mouse to right)
C	You can select "c" and then click an atom which you would like your structure to rotate around
X	Rotate your molecule about the x axis
Y	Rotate your molecule about the y axis
Z	Rotate your molecule about the z axis
1	Label atoms selected with mouse left click
2	Enters "bond label" mode, which gives the distance between two atoms selected by successive mouse left clicks

CARBOHYDRATES

The basic building block of carbohydrates are sugar monomers, or monosaccharides. Carbohydrates include a wide variety of important and diverse molecules from the starch which is the ultimate food source for most of the biosphere, to cellulose, which is an essential structural component of plant cell walls. In this assignment, you will explore the structure of 2 common monosaccharides as well as one disaccharide, and small starch molecule.

1. First you will explore the structure of glucose. How many carbons, hydrogens and oxygens are present? Write down the chemical formula here:

   Draw a 2-dimensional representation of the glucose structure in the space below:

2. Delete the glucose molecule and load the fructose molecule. How many carbons, hydrogens and oxygens are present? Write down the chemical formula here:

   Compare the chemical formula of glucose and fructose. What is the special relationship between these two sugars (if you can't remember the name, just describe it in your own words)?

All sugars have the same ratio of carbon to hydrogen to oxygen. Write down that ratio here:

Draw a 2-dimensional representation of the fructose structure in the space below:

3. Delete the fructose molecule and load the sucrose molecule. How many carbons, hydrogens and oxygens are present? Write down the chemical formula here:

   Sucrose is a disaccharide. This means that it is made up of two sugar monomers or monosaccharides. Are the two sugars that make up sucrose the same or different?

   Write the sequence of sucrose below (for example, maltose is a homo-disaccharide of glucose, so its sequence is **glucose-glucose**).

   Add the total number of carbons, hydrogens, and oxygens from the two monosaccharides that make up sucrose:

   C= H= O=

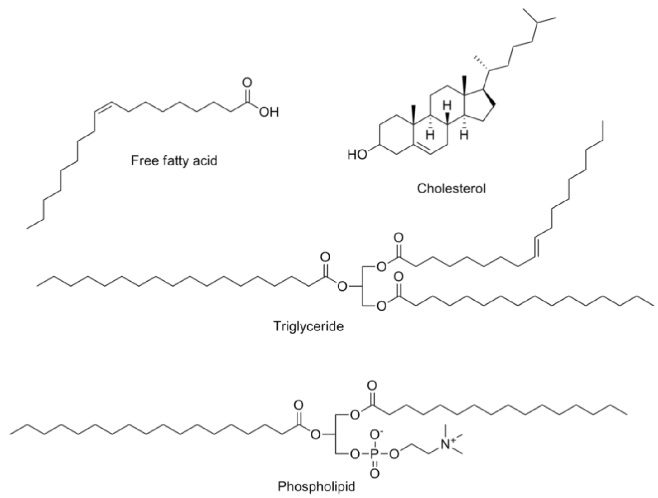
What is lost as a by-product during the formation of sucrose from the two monosaccharides (hint: subtract the formula for sucrose from that of the two monosaccharides above)

4. Delete the sucrose molecule and load the starch molecule. This is much smaller than the average starch molecule in plants, so it is easier to visualize. Which sugar monomer is the building block of starch? (hint: use your drawings from 1 & 2 to help you decide).

   How many sugar monomers are present?

   Write the chemical equation for synthesis of this starch molecule below:

LIPIDS



Lipids are a diverse category of molecules, made up of non-polar molecules, which are unable to be dissolved well or at all in water. These include many molecules made of fatty acids and steroid-alcohols such as cholesterol. The diagram on your right shows the structure of cholesterol, a mono-unsaturated fatty acid, a mono-unsaturated triglyceride (fat), and a saturated phospholipid (primary component of the cell membrane).

1. Load the palmitic acid molecule. This is a 16-carbon fatty acid which is a building block of many fats and phospholipids present in plant and animal cells. Fatty acids all contain a long carbon chain terminated with a carboxylic acid. Draw the palmitic acid molecule below and circle the carboxylic acid group in your structure.

2. Fatty acids can be saturated or unsaturated. An unsaturated fatty acid has a double bond between two of the carbon atoms in its tail. A mono-unsaturated fatty acid has one double bond, while a poly-unsaturated fatty acid has two or

more. Which type is palmitic acid, saturated, mono-unsaturated, or poly-unsaturated? (hint: To determine double bond positions, count the number of atoms bound to each carbon. If it is 4, then there cannot be a double bond. The first carbon, bound to the oxygens does not count for this).

3. Delete the palmitic acid molecule and now load the oleic acid. This is an 18-carbon fatty acid that is also common to many fats and phospholipids. Draw the structure of this molecule below. What is the main difference in the structure, other than the length, between oleic acid and palmitic acid? The difference is the result of a carbon-carbon double bond in one of these molecules but not the other.

4. Now delete the oleic acid and load the glycerol molecule. This very simple molecule forms the basis for linking fatty acid chains together into triglycerides (fats) or together with polar and charged "headgroups" in phospholipids. Draw the glycerol molecule below, making sure to point out the 3 alcohol groups (where the fatty acid chains or headgroups would be attached).

5. Now delete the glycerol molecule and load the POPC molecule. This phospholipid is the most common constituent of cell membranes. You should notice that it is basically just the glycerol molecule you have just looked at, only with two fatty acid chains and one headgroup attached where the alcohol

groups were. Draw the molecule, making sure to point out the glycerol unit, the two fatty acids, and the headgroup.

6. The POPC has one saturated and one unsaturated fatty acid chain. In your drawing above, point out which one is unsaturated and indicate the position of the double bond (hint: count the number of atoms bound to each carbon as before – but don't include the carbons bound to oxygen).
7. One of the chains is palmitic acid and the other oleic acid. Use your answers and drawings from 1 & 2 above to determine which is which and label each chain in the above drawing.
8. Which fatty acid has a more kinked structure, the saturated, or unsaturated one?

Extra Credit:

Load the structure of cholesterol into VMD. There are 3 important regions of the cholesterol molecule, the alcohol group, the 4-ring structure that is characteristic of all steroid hormones, and the hydrocarbon tail. Draw the structure of cholesterol below. Circle and label each of these regions in your drawing.

NUCLEIC ACIDS

Nucleic acids are the genetic information storing molecules present in every known life form and they are even required for viruses to be infectious. They are made from primary building blocks called nucleotides. The nucleotides with guanine, cytosine, adenine and, thymine bases are found in deoxyribonucleic acid, or DNA. In ribonucleic acid, or RNA, thymine is replaced by another nucleotide called uracil. Each nucleic acid building block also has a sugar and phosphate group attached. This sugar-phosphate-sugar-phosphate sequence is referred to as the "backbone" of the nucleic acid and does not change throughout the molecule. The backbone is different in DNA and RNA, however, since the RNA backbone contains a ribose sugar, while DNA contains a deoxy-ribose sugar. The entire nucleotide-sugar-phosphate unit is referred to as a nucleoside.

1. Load the thymine nucleotide into VMD. This structure contains a phosphate group, a 2-deoxyribose sugar, and the thymine base. Draw this molecule in the space below, labeling these three parts of the DNA building block.

2. Delete the thymine molecule and load the uracil nucleotide into VMD. Draw this structure below, pointing out the phosphate, sugar, and uracil base. Also, indicate the two major differences between uracil & thymine (hint: one difference is in the base itself and the other is in the sugar).

3. Delete uracil molecule and load the adenosine nucleoside (the nucleotide base + phosphate + sugar). Draw the molecule below and indicate whether it is from DNA or RNA building block. How do you know?

4. Delete the adenosine molecule and load the DNA molecule. In the presence of magnesium and calcium, DNA is rarely found as a single polymer strand, but instead forms a so-called double helix structure which is held together by hydrogen bonding between the nucleotides (bases). Each base can only hydrogen bond with its complimentary base, so that each strand is an exact compliment of the other one. You can imagine how this could prove useful for storing important genetic information, since there is always a backup copy of the code available in the second strand. Use the label function to determine which nucleotides hydrogen bond to which in DNA (just give the two pairs). To enter label mode, press the number 1 on your keyboard. You can then left click on individual atoms in the structure to determine which nucleotide they are from (DT means DNA-thymine, DC means DNA-cytosine, DG means DNA-guanine, and DA means DNA-adenine).