Biomolecular Models

Objective:

To construct, using models or diagrams, the three-dimensional organization of Glucose, Ribose, Maltose, Glycerol, a Triglyceride, a phospholipid, Glycine, Glutamate, and Vasopressin at the level of 85% proficiency for each student

In order to achieve this objective, you will need to be able to:

1. Use ball-and-stick models along with computer simulations to examine the three dimensional structure of biomolecules.
2. Construct three dimensional models of the simple sugar Glucose.
3. Explain the effect of changing the orientation of oxygen groups on the biocompatibility of simple sugars.
4. Construct a disaccharide, Maltose, from two molecules of Glucose.
5. Construct models of the simple sugars Ribose and Deoxyribose
6. Construct models of Glycerol and diagram the fatty acid linoleic acid.
7. Construct a Triglyceride from Glycerol and three molecules of short fatty acids.
8. Diagram the structure of the phospholipid Phosphatidylcholine
9. Construct models of the amino acids Glycine and Glutamate.
10. Diagram the structure of the 9-amino acid peptide Vasopressin.

Materials:

Group Supplies

Ball and Stick model kit

Computer with Java and Jmol installed.
https://java.com/en/download/index.jsp
https://sourceforge.net/projects/jmol/files/Jmol/
(These have been pre-installed onto the computers in the physiology lab. Jmol version 14.29.17 or newer is recommended)

You may find exploring these links of interest.
https://cactus.nci.nih.gov
https://pubchem.ncbi.nlm.nih.gov

Methods:

Double click the shortcut named Jmol to open Jmol, an Open-source Java program for viewing chemical structures in 3D.

Files are retrieved online by Jmol by selecting “GetMOL” from the File menu.

When you enter the name of a chemical, Jmol will go to the NCI/NIH chemical identifier resolver,
https://cactus.nci.nih.gov/chemical/structure"structure identifier"/"representation"
If the chemical name is preceded with a colon “**:**”, Jmol will go to PubChem,
https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/"structure identifier"/"representation"

Files can also be viewed offline by Jmol by selecting “Open” from the File menu.

Files for viewing offline are available from my website:
https://www.dgward.com/pdf/physo101/updated_Jmol_biomolecules.zip
Click, and a “.zip” file should download automatically. After downloading, “Open”, select "Extract All", and save to the Desktop.

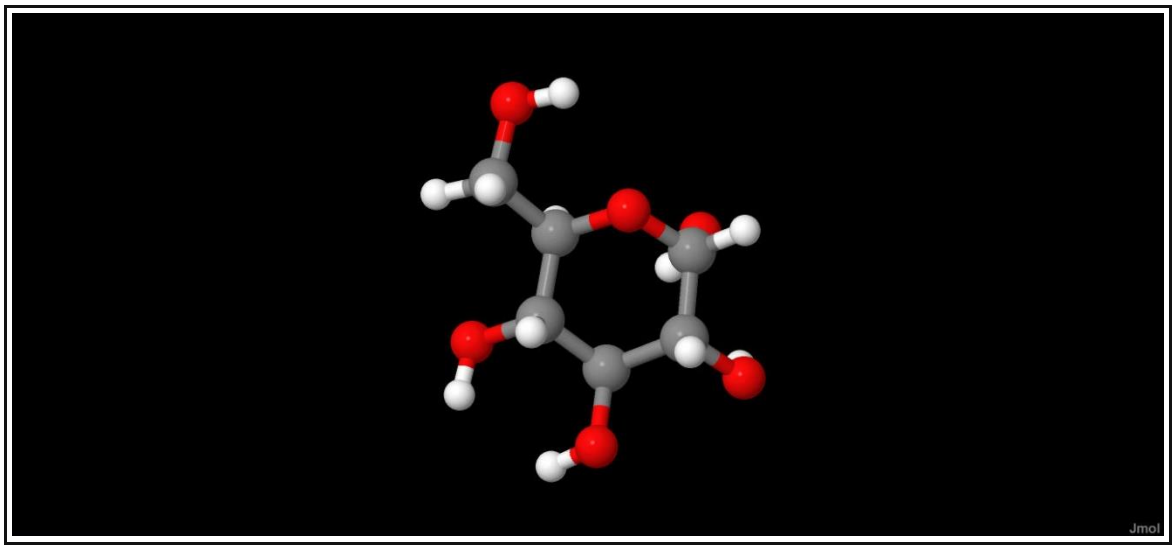
Carbohydrates

Glucose

Within Jmol click on “File”. A dropdown menu will appear. Click on “Get MOL” and type in “alpha-D-glucose” (or “alpha-D-glucopyranose”).

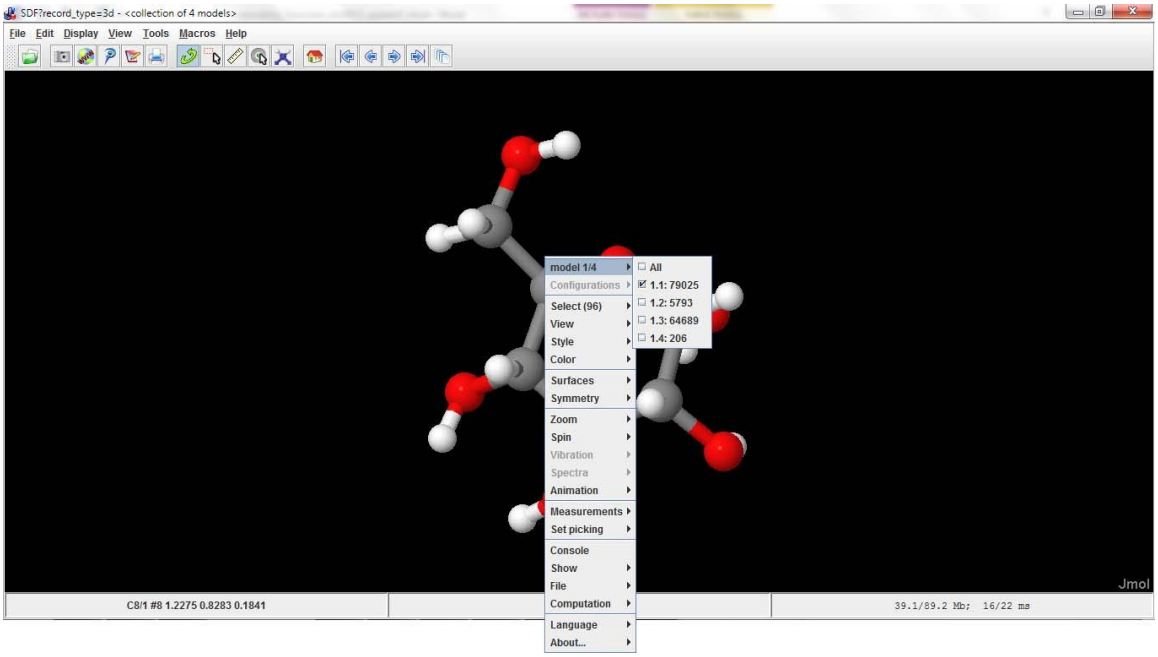
> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “alpha-D-glucose_CID_79025“.

A 3D model of alpha-D-Glucose will appear, as shown below.



Hold down the left button on the mouse (or touchpad) and move the cursor to rotate the molecule.

Right click on the molecule to change options for display.



Use the three-dimensional image of alpha-D-Glucose to construct a physical model of alpha-D-Glucose using the ball and stick kit.

Then, change the orientation of the hydroxyl and the hydrogen at the first carbon to make beta-D-Glucose.

To check how you did, Click on “Get MOL” and type in “beta-D-Glucose” (or “beta-D-glucopyranose”).

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “beta-D-glucose_CID_5793“.

Maltose

Click on “Get MOL” and type in “alpha-maltose”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “alpha-maltose_CID“.

Use the three-dimensional image of alpha-Maltose as a guide to construct a physical model of alpha-Maltose using the ball and stick kit.

The two groups at your table will work together. If necessary, change your model so that each group at your table has alpha-D-Glucose. Working together, combine these two models of alpha-D-Glucose to make a molecule of alpha-maltose. In doing this you will be performing dehydration synthesis.

Ribose and Deoxyribose

Click on “Get MOL” and type in “beta-D-ribose” (or “beta-D-ribofuranose”).

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “beta-D-ribofuranose_CID_447347“.

Use the three-dimensional image of beta-D-Ribose to construct a physical model of beta-D-Ribose using the ball and stick kit. Make certain that all oxygen atoms are oriented in the correct direction.

At the second carbon, remove the hydroxyl (OH) and replace with hydrogen (H) to make 2-deoxyribose (the form of deoxyribose found in DNA).

To check how you did, Click on “Get MOL” and type in “2-deoxyribofuranose”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “beta-D-deoxyribofuranose_CID_447347_modified“.

Lipids

Glycerol and Fatty Acids

Click on “Get MOL” and type in “glycerol”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “glycerol_CID_753“.

Use the three-dimensional images of glycerol to guide you in the construction of a physical model of glycerol, using the ball and stick kit

Click on “Get MOL” and type in “linoleic acid”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”, ”CID”, and “linoleic_acid_CID_5280450 “.

Examine the three-dimensional images of linoleic acid, a typical fatty acid. This fatty acid is too complex to construct a physical model.

The two groups at your table will work together, using linoleic acid as a guide, to construct three (3) short fatty acids, each with three (3) carbons.

Triglycerides

The two groups at your table will work together to construct a small triglyceride, by combining your model of glycerol and your three (3) models of short fatty acids. In constructing this small triglyceride, you will be performing dehydration syntheses.

Phospholipids

Click on “Get MOL” and type in “phosphatidylcholine”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “phosphatidylcholine_CID“.

Examine the three-dimensional images of phosphatidylcholine, a very common phospholipid. This phospholipid is too complex to construct a physical model.

Amino Acids and Proteins

Glycine

Click on “Get MOL” and type in “glycine”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “glycine_CID_750“.

Use the three-dimensional images of glycine to guide you in the construction of a physical model of glycine, using the ball and stick kit.

Glutamate

Click on “Get MOL” and type in “glutamate”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”,” CID”, and “glutamate_CID_33032“.

Use the three-dimensional images of glutamate to guide you in the construction of a physical model of glutamate, using the ball and stick kit. Pay particular attention to the difference between glycine and glutamate

Vasopressin

Click on “Get MOL” and type in “arginine vasopressin”.

> Alternately, click on “File”, “Open”, “Look In: Desktop”, select “updated_Jmol_biomolecules”, ”CID”, and “arginine_vasopressin_modified“.

Examine the three-dimensional images of vasopressin, a 9-amino acid peptide. Focus specifically on the presence of the amino acids. This peptide is too complex to construct a physical model.

Discussion:

1. Compare and contrast the composition and general structure of carbohydrates, lipids, and proteins.
2. Compare and contrast dehydration synthesis and hydrolysis of carbohydrates, lipids, and proteins.
3. Speculate on whether a carbohydrate, a lipid, or a protein would make a better chemical messenger.