



## VISUALIZING MACROMOLECULES - Jmol COMPUTER ACTIVITY

Go to the website: <http://www.biotopics.co.uk/JmolApplet/jcontentstable.html>

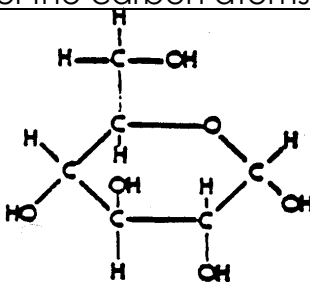
Manipulations of molecules:

- ✓ To rotate the molecule yourself, **left-click and drag** on it. Drag the cursor up and down for x-axis rotation, left-right for y-axis rotation.
- ✓ To translate the molecule yourself, **shift-double-click and drag** on the structure--the molecule will follow the mouse.
- ✓ To zoom the molecule yourself, **shift-click and drag**. Drag the cursor down to zoom in, up to zoom out.
- ✓ TO RESET THE MOLECULE, SHIFT-DOUBLE-CLICK MOUSE

Make sure to view the following molecules and answer the questions below:

Let's start with carbohydrates...

**1. Click GLUCOSE.** Practice zooming in and rotating the glucose molecule. Click the "label glucose" button and label the carbon atoms (C1, C2, etc) on the diagram.



**2. Click on ALPHA-GLUCOSE VS. BETA-GLUCOSE**

Practice zooming in and rotating the alpha glucose molecule.

How does  $\alpha$  (alpha) and  $\beta$  (beta) glucose differ structurally?

**3. Click on GLUCOSE-GALACTOSE COMPARISON**

Galactose and glucose are considered to be \_\_\_\_\_, which means that they both share the same formula  $C_6H_{12}O_6$ .

What is the structural difference between them?

**4. Click on SUCROSE**

Sucrose is a disaccharide - formula \_\_\_\_\_ - consisting of one \_\_\_\_\_ unit combined with one \_\_\_\_\_ unit.

### 5. Click on **AMYLOSE**

Amylose is the name given to linear sections of the starch molecule.

What are the linkages called between the glucose units? (be specific)

\_\_\_\_\_

This model shows 36 glucose units, forming a helical structure - effectively a tube.

Click the appropriate button to **move to the end** to see the structure.

### 6. Click on **CELLULOSE**

This model shows 9 glucose units joined by alternating \_\_\_\_\_ bonds.

Notice the shape of the chain. Describe the difference in shape of the cellulose chain with that of amylose. \_\_\_\_\_

**Let's study lipids now...**

### 7. Click on **GLYCEROL**

What is the functional group in this molecule? \_\_\_\_\_

### 8. Click on **SATURATED AND UNSATURATED FATTY ACIDS**

Locate the **carboxyl group** of stearic acid.

What colour represents the oxygen atoms? \_\_\_\_\_

What is the chemical formula of stearic acid? \_\_\_\_\_

What is the chemical formula of oleic acid? \_\_\_\_\_

Why is there a difference in the number of hydrogen atoms?

### 9. Click on **TRIGLYCERIDES (FATS)**

**Zoom** into the molecule.

What is the bond called between the fatty acids and the central glycerol unit? \_\_\_\_\_

## Let's turn to proteins now...

On to levels of protein structure (General Principles)...

### 10. Click on PRIMARY STRUCTURE

*There are 20 different amino acids.*

For a dipeptide (i.e. 2 amino acids linked together),  
how many different amino acid combinations are possible? \_\_\_\_\_

For a tripeptide, how many different combinations are possible? \_\_\_\_\_

Determine the number of different combinations of amino acid  
sequences that can be possible for a peptide with "n" amino acids. \_\_\_\_\_

*Clearly the number of possible combinations is almost infinite when larger numbers of amino acids are combined to form a polypeptide.*

### Secondary structure

*The polypeptide chain can fold back on itself in a number of ways.  
Click the "**BACKBONE**" button to show the backbone for both secondary structures.*

One way is to fold into a helical structure, \_\_\_\_\_ and the  
other is to fold as a \_\_\_\_\_ sheet.

### Tertiary structure

The 3-dimensional structure of a protein's polypeptide chain or chains may be locked in place by **other stronger bonds**. These bonds are formed between components of the \_\_\_\_\_ groups of the amino acid residues.

*Click on "**Trace the chain**" and "**show backbone**".*

Notice the different amino acids that form the primary structure and the two types of secondary structures.

### Quaternary structure

*Not all proteins have a quaternary level of structure.*

A protein with a quaternary structure consists of more than one practically identical sub-unit, not joined by strong bonds like those above.

### 11. Click on AMYLASE (enzyme)

Name the two structures that can be identified in the molecule.

How many amino acids make up this enzyme? \_\_\_\_\_

Finally, a look at nucleic acids...

Recall from Gr. 11 Biology, the structure of a general nucleotide.

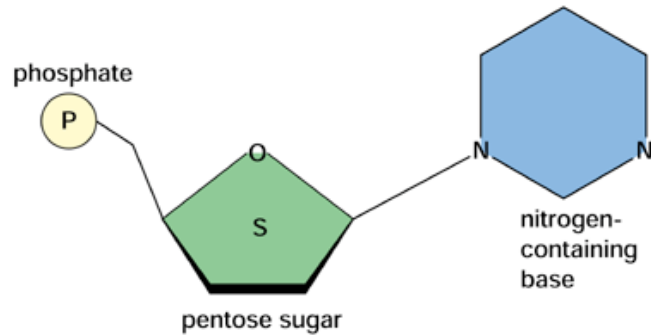
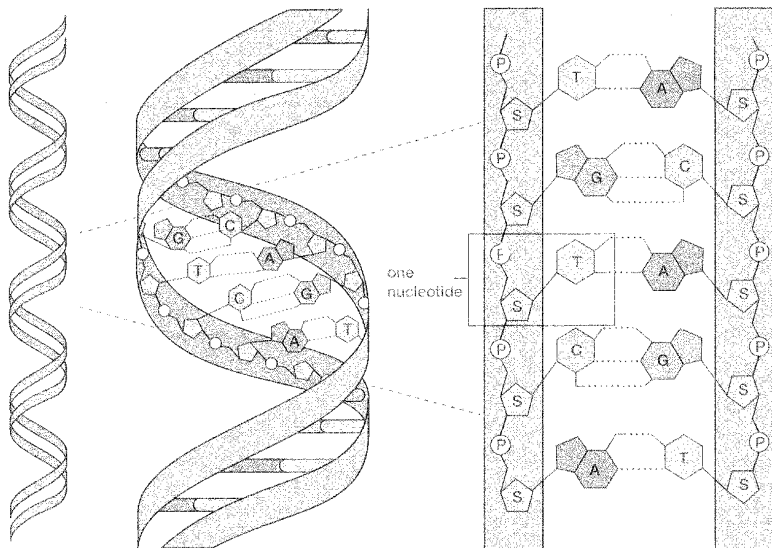


Figure 1.20. Generalized nucleotide. Nucleotides consist of a five-carbon simple sugar (ribose in the case of RNA and deoxyribose in DNA), a nitrogen base, and a phosphate group.

## 12. Click on DNA

The outside edges of the DNA double helix are composed of alternating

\_\_\_\_\_ and \_\_\_\_\_ groups.

Click the appropriate button to see the **sugar-phosphate backbone**.

What element does the orange atom represent? \_\_\_\_\_

Across the middle of the molecule are the nitrogenous bases, showing the nitrogen atoms in blue. In each case the bases do not directly contact their partner on the opposite strand, to which they are held by \_\_\_\_\_ bonds.

Click the appropriate button to see the **hydrogen bonds**.

## 13. Click on DNA Bases

Which nitrogenous bases are purines? \_\_\_\_\_

Which nitrogenous bases are pyrimidines? \_\_\_\_\_

What is the structural difference between purines and pyrimidines? \_\_\_\_\_

How many hydrogen bonds are between A-T? \_\_\_\_\_ C-G? \_\_\_\_\_

**You have now completed your task. Make sure you keep this sheet for future reference.**