Chemical Models, Properties and Structures

Learning Goals:

1. To practice with the different atoms used in Bio 111: to know the number of bonds made by each kind of atom, the structures that they form, and the charges they have.
2. To build molecular models of various bio-molecules.
3. To understand and be able to work with the different representations of molecules used in Bio 111.
4. To experimentally determine hydrophobic and hydrophilic behavior among solutions using both hydrophobic and hydrophilic membranes.

Introduction

Matter is made up of approximately 100 elements. Of these, only carbon, hydrogen, oxygen, nitrogen, sulfur and about a dozen others are found in living organisms. Atoms of these elements can attach to one another by chemical bonds. There are four types of bonds important to us in Bio 111:

1. covalent bonds
2. dipole-dipole interactions (hydrogen bonds)
3. ionic interactions
4. hydrophobic interactions

Today, we will focus on **covalent bonds**, which are the result of a sharing of electrons between two or more atoms. In this case the electrons of the atoms forming the bond occupy the space between each others' nuclei. Molecules can be made up of atoms of different elements, such as the gas methane (CH_4), in which one atom of carbon shares electrons with four atoms of hydrogen, or the molecule can be made up of atoms of the same element (O_2). Carbon atoms are unusual in that they will bond together to form long chains of carbons (-C-C-C-C-) thus making possible very elaborate molecules with carbon "backbones".

Dipole-Dipole interactions (Hydrogen bonds) are weaker than covalent bonds and tend to form between a hydrogen atom covalently bonded to a nitrogen or oxygen atom and another oxygen or nitrogen atom (in the same molecule or in another molecule). These are particularly important in the structure of proteins and nucleic acids, and will be discussed later in the course.

Ionic interactions are the attraction between positive (+) and negative (–) charges. Ionic bonds are the result of the transfer of one or more electrons between atoms. In Bio 111, we will encounter interactions between ions in which "unlike charges attract" and "like charges repel".

Hydrophobic interactions occur between regions of molecules that are not soluble in water (hydrophobic). In water, hydrophobic regions tend to cluster together (like an oil drop on water) to exclude the surrounding water.

Part I: Structures on paper and in 3-d

Using the model kits

The molecular model kits have five different types of atoms. Carbon (black), Oxygen (red), Nitrogen (blue), Chlorine (green), and Hydrogen (light blue sphere). Each of these represents an atom, composed of its nucleus and the surrounding electrons. These atoms can be connected to each other by inserting the white rods into the holes. It will become apparent to you that different atoms have different capacities for bonding with other atoms. The holes in the plastic "atoms" indicate the number of electrons that the atom is able to share with another atom.

[*Note that there may be two types of black atoms in your kits. One type has 4 holes - you should use these, we tried to remove all others but you may find some have 5 holes; don't use them since the geometry will be wrong.]

A reminder of the number of bonds each atom makes & the corresponding charge:

Number of bonds

Element	0	1	2	3	4	5
H	+	neutral				
O		–	Neutral			
N				neutral	+	
C					neutral	
S		–	Neutral			
P						neutral

Also a reminder of the relative electro-negativities of a few relevant elements:

Low: C, S, P, and H

High: N, O and Cl

These properties can all be explained in terms of the electronic structures of the elements involved. You may want to take time to discuss this as a class. See periodic table at the end of this section for details.

The short rods are used to indicate the covalent bond involving hydrogen, since hydrogen, being the smallest atom, has a smaller distance between it and a carbon atom. Similarly, the curved rods are used to show double and triple bonds and have the effect of bringing the atoms closer together, which reflects the true situation. The nuclei of carbon atoms in a C=C bond are closer together than in a C-C, but not so close as in a C≡C bond.

Working in groups of three, build these molecules using the stick models.

<u>1) Simple hydrocarbons.</u>

methane CH_4

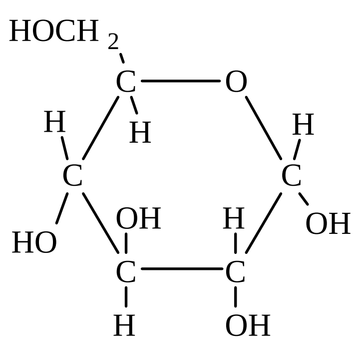
<u>2) Alcohols</u>

butanol C_4H_9-O-H

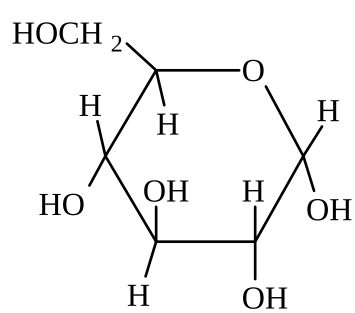
Note: there are 5 isomers of butanol. Three are structural isomers. Two are enantiomers - that is, they are mirror-image isomers (see your course textbook for explanation of the three types of isomers). Draw the three structural isomers and build models of the two enantiomers.

<u>3) Sugars:</u>

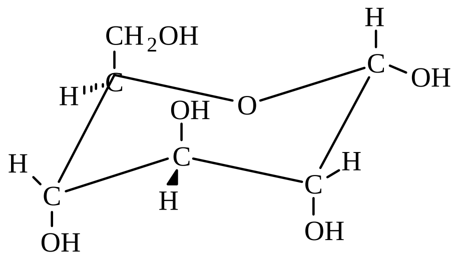
glucose



or:

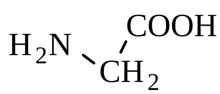


Note that all of the carbons in glucose are chiral – that is, it matters which groups point up from the ring and which point down. A more correct representation would be:

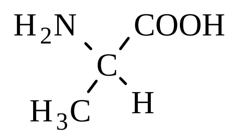


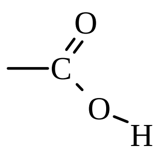
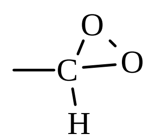
4) Amino acids

glycine



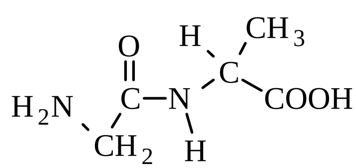
alanine



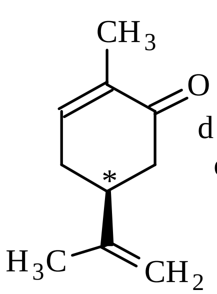
note that -COOH is  not 

Take two amino acids and join them to make a dipeptide, such as the one below: what did you have to remove to make this molecule? You have made a peptide bond.

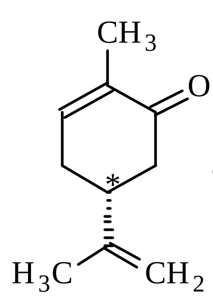
a dipeptide (glycine-alanine)



5) Chirality is a very important feature of biological molecules because their exact 3-dimensional shape determines their function. An interesting example of this is the two forms of the molecule carvone:



d or (+) carvone
oil of caraway
(rye bread)



l or (-) carvone
oil of spearmint
(mint)

Both have the identical formulas ($C_{10}H_{14}O$) and identical structures except for the arrangement of the atoms at the *ed carbon. With the ring of carbons lying flat on the table and the C=O on the right, as shown, the dashed bond points down into the table and the triangle bond points up from the table.

Make one of the forms of carvone and have another group make the other. Convince yourself that they are not the same structure. They are mirror-image isomers, or enantiomers.

Their similar structures lead to them having similar smells, but there is a difference due to the slight difference in shape.

Part II: Molecules on the computer

Learning Goals

• To look at the structures of some important biological molecules and get a feel for their three-dimensional structure.

Background

Jmol is a molecular viewing application. It lets you rotate, highlight, zoom in on, etc. a two-dimensional image of a three-dimensional molecule. It shows molecules in a simplified format, specifically:

• unless noted, hydrogen atoms are not shown
• all covalent bonds are shown as a single rod, whether the bond is single, double, or triple
• atoms are shown as colored spheres; the colors identify each type of atom

Procedure

A) You will work in groups of three people per computer; your worksheet will be a group effort for a group grade. If you are completing this assignment on your own as a make-up, you must submit your own worksheet. You should take turns using the computer, to assure every student gets a try.

B) To find the program, open a browser on the computer and go to www.bio.umb.edu and look for the Summer Bio 111 Labs link and click on it.

C) Once at the web page, click on "Chemical Structures" in order to proceed through this lab. Follow the exercise there and fill in the worksheet.

Briefly, you will:

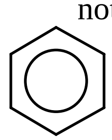
(1) Draw the structures of two sugars, glucose and fructose as well as an amino acid, based on the images on the computer. These images have hydrogen atoms included as a warm-up. You will be asked to find the differences between the sugar structures and identify the amino acid.

(2) Your TA will assign you two randomly-chosen amino acids. You will look at its image in a window using the program RasMol. You will draw the complete structure of each and identify which amino acid each is.

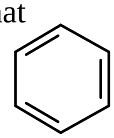
Worksheet

You will turn in the worksheet to your TA at the end of lab to be graded. A copy of this worksheet is at the end of this section of the lab manual.

note that



and



are equivalent representations of a benzene ring

Part III. Artificial Membranes

Artificial membranes can be chemically manufactured. Membranes are useful in the biotechnology field because they can serve as a model for biological membranes. For example, during the drug screening phase in some pharmaceutical companies, artificial membranes serve as models of the digestion system in order to determine if a drug would enter a person's blood stream if digested.

Laboratory Excercise : Hydrophobic and Hydrophilic membranes

****Membranes should NOT be touched. Handle all membranes with FORCEPS**

Depending on the composition of a membrane, it can **wet out**, as can be observed by a slight color change in the membrane. You will determine the "wet-ability" of one hydrophilic and one hydrophobic membrane in water, oil, ethanol, soap, and glycerol.

Question:

Will hydrophilic or hydrophobic membranes wet in water? Oil? Ethanol? Soap? Glycerol?

Step 1) Record your expectations in the hypothesis rows based on the hydrophilic or hydrophobic nature of each solution.

Experimental Design:

Step 2) Place a different piece of **hydrophilic** membrane in water, oil, ethanol, soap, glycerol. Record results in the experimental observation row in the table below.

Step 3) Place a different piece of **hydrophobic** membrane in water, oil, ethanol, soap, glycerol. Record results in the experimental observation row in the table below.

	Water	Oil	Ethanol	Soap	Glycerol
Hypothesis : Hydrophilic membranes will wet? (yes/no)					
Experimental Observations:					
Hypothesis : Hydrophobic membranes will wet? (yes/no)					
Experimental Observations:					

<u>Additional Observations</u>:

<u>Conclusions</u>:

<u>What other questions do the experimental results generate?</u>

Bio 111 Chemical Models, Properties, & Structures Worksheet (Check-Off)

Name_____________________

TA & Sect.____________

<u>This is due at the end of lab today.</u>
<u>The numbers of these questions correspond to the numbers on the web site.</u>

1) Using the image from the web site, draw the structure of the <u>linear form of glucose</u>. You need not indicate the chiral parts of the molecule. (1 pts)

2) Using the image from the web site, draw the structure of the <u>linear form of fructose</u>. You need not indicate the chiral parts of the molecule. (1 pts)

3) On the structure in question (2), indicate the differences between glucose and fructose. (1 pt)

4) Using the image from the web site, draw the structure of the <u>circular form of glucose</u>. You need not indicate the chiral parts of the molecule. (1 pts)

5) On the structure in question (1), indicate which parts of the molecule have been linked to form the ring structure of question 4. (1 pt)

6) Using the image from the web site, draw the structure of the amino acid for part (6). You need not indicate the chiral parts of the molecule. (1 pt)

7)) Using the chart of amino acid structures in the lab manual, identify the amino acid you drew in part (6). (1 pt)

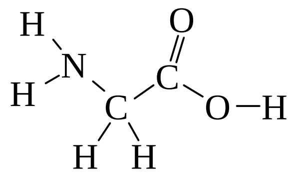
8) Your TA will give you two randomly-selected numbers which corresponds to two amino acids in a protein. One-by-one, choose the number assigned to you by your TA from the list provided on the web site for problem 8. The program will display the amino acid with the hydrogen atoms omitted. It will also show the adjacent two amino acids to help you find the right parts. Draw the complete structure of this amino acid, including the hydrogen atoms. Using the chart in the lab manual, identify the amino acid you have been assigned.

a) Numbers given by TA __________ __________

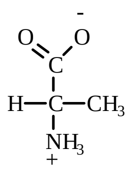
Identities of amino acids __________ __________

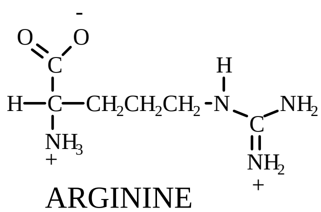
Structures:

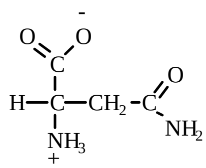
9) Draw several water molecules making hydrogen bonds with the appropriate parts of glycine. (1 pts)

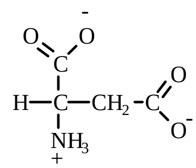


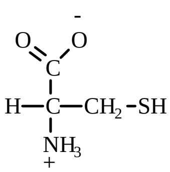
STRUCTURES OF AMINO ACIDS

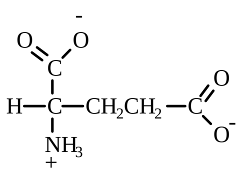

ALANINE
(ala)

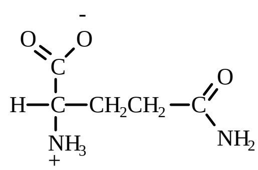

ARGININE
(arg)

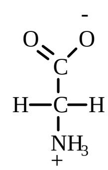

ASPARAGINE
(asN)

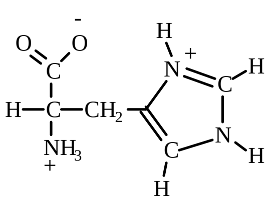

ASPARTIC ACID
(asp)

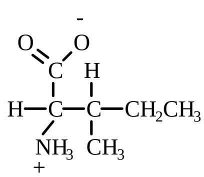

CYSTEINE
(cys)

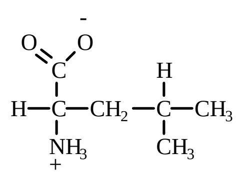

GLUTAMIC ACID
(glu)

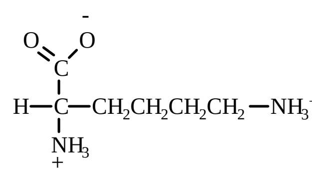

GLUTAMINE
(glN)

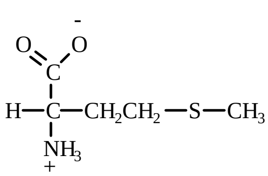

GLYCINE
(gly)

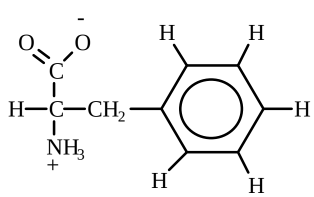

HISTIDINE
(his)

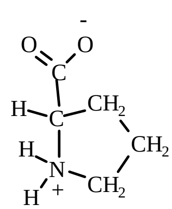

ISOLEUCINE
(ile)

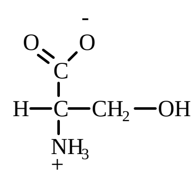

LEUCINE
(leu)

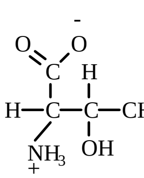

LYSINE
(lys)

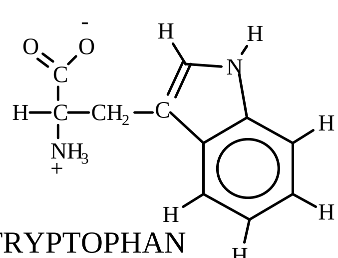

METHIONINE
(met)

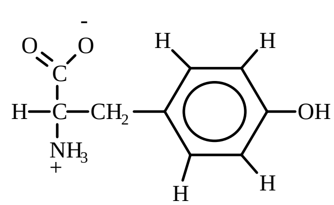

PHENYLALANINE
(phe)

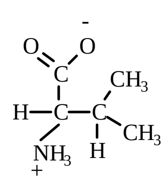

PROLINE
(pro)


SERINE
(ser)


THREONINE
(thr)


TRYPTOPHAN
(trp)


TYROSINE
(tyr)


VALINE
(val)

Partial Periodic Table

H Hydrogen $1p^+$ $0n^0$ $1e^-$ 1(1 open) En=2.1							**He** Helium $2p^+$ $2n^0$ $2e^-$ 2(full) En=none
Li Lithium $3p^+$ $4n^0$ $3e^-$ 2(full) 1(7 open) En=1.0	**Be** Beryllium $4p^+$ $5n^0$ $4e^-$ 2(full) 2(6 open) En=1.5	**B** Boron $5p^+$ $6n^0$ $5e^-$ 2(full) 3(5 open) En=2.0	**C** Carbon $6p^+$ $6n^0$ $6e^-$ 2(full) 4(4 open) En=2.5	**N** Nitrogen $7p^+$ $7n^0$ $7e^-$ 2(full) 5(3 open) En=3.0	**O** Oxygen $8p^+$ $8n^0$ $8e^-$ 2(full) 6(2 open) En=3.5	**F** Fluorine $9p^+$ $10n^0$ $9e^-$ 2(full) 7(1 open) En=4.0	**Ne** Neon $10p^+$ $10n^0$ $10e^-$ 2(full) 8(full) En=none
				P Phosphorus $15p^+$ $16n^0$ $15e^-$ 2(full) 8(full) 5(3 open) En=2.1	**S** Sulfur $16p^+$ $16n^0$ $16e^-$ 2(full) 8(full) 6(2 open) En=2.5		

Elements in this column do not form any covalent bonds (at least, not in Bio 111) ↑

P ← Symbol

Phosphorus ← Name

$15p^+$ $16n^0$ ← Contents of nucleus: p^+ = proton (+1 charge) n^0 = neutron (0 charge)

$15e^-$ ← Total number of electrons (e^-; (-1 charge). Balances protons.

2 (full) ← # electrons in innermost shell

8 (full) ← # electrons in next shell out

5 (3 open) ← # electrons in outer (valence) shell ("# open" = # required to fill outer shell)

En = 2.1 ← Electronegativity. Increases as you go ⇑ and ⇒