

Chemical Structures

Objectives

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.

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 five types of bonds important to us in Bio 111:

1. covalent bonds
2. hydrogen bonds
3. ionic bonds
4. Hydrophobic interaction
5. van der Waals interaction

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 ($-\text{C}-\text{C}-\text{C}-\text{C}-$) thus making possible very elaborate molecules with carbon "backbones".

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 are two types of black atoms. One type has 4 holes - you should use these ones. Others have 5 holes; don't use them since the geometry will be wrong.

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

Element	Number of Bonds					
	0	1	2	3	4	5
H	+	neutral				
O		-	neutral			
N				neutral	+	
C					neutral	
S		-	neutral			
P						neutral

Also a reminder of the relative electronegativities 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 an C-C, but not so close as in a C≡C bond.

Working in groups of three, build these molecules using the stick models and have your TA check them off.

1) Simple hydrocarbons

methane CH₄

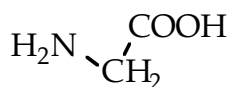
2) Alcohols

butanol C₄H₉-O-H

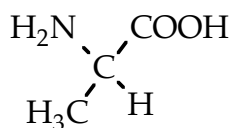
Note: there are 5 isomers of butanol. Three are structural isomers. Two are enantiomers - that is, they are mirror-image isomers (see Campbell Figure 4.7 page 62). Draw the three structural isomers and build models of the two enantiomers.

3) Amino acids

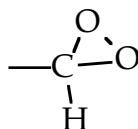
glycine



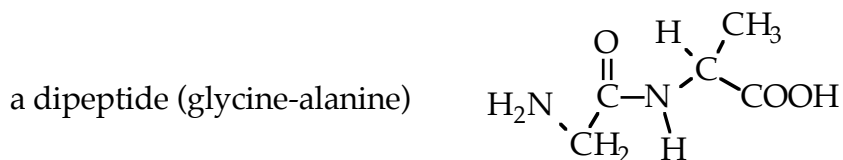
alanine



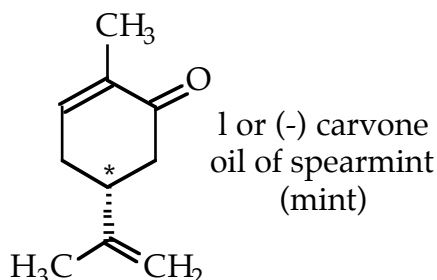
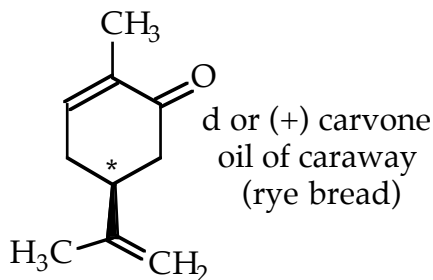
note that -COOH is not



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.



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



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.

Your TA will give you samples of the two carvones to smell. Notice that their similar structures lead to similar smells, but there is a difference due to the slight difference in shape.

Part II: Molecules on the computer

Objectives

- To look at the structures of some important biological molecules and get a feel for their three-dimensional structure.
- To familiarize yourself with the representations of molecules used by the Jmol program, which we will use extensively in future labs.

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

You will follow the exercise on the course web site for this lab and fill in the worksheet described below. You should work in groups of three; your worksheet will be a group effort for a group grade.

- 1) Go back to the dock at the bottom of the screen.
- 2) Click on the "Safari" icon.
- 3) Safari will start up and go to the Biology 111/112 home page.
- 5) Click on the link to the "OLLM" ("On-Line Lab Manual")
- 6) Click on the link to "Chemical Structures Exercises" for this lab.
- 7) Follow the exercise there and fill in the worksheet.

Briefly, you will:

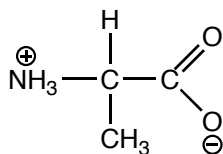
(1) Based on the image on the computer, draw the structures of two sugars, glucose and fructose as well as an amino acid. These images have hydrogen atoms included as a warm-up. You will be asked to find the differences between the sugar structures and identify the amino acid.

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

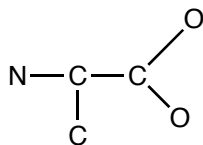
Note: these structures are shown in an unusual way to get you ready for the Protein Structure Lab. There are three important details here:

- hydrogen atoms are not shown
- all covalent bonds, whether single, double, or triple are shown as a single rod connecting two atoms
- the amino acids are part of a larger molecule. The connections to the larger molecule are shown in thinner lines. As a result of this connection, one of the oxygen atoms on the carboxyl (COO^-) group is not shown. This is shown below for the amino acid alanine:

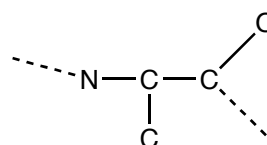
a) alanine as shown on page 11



b) alanine with hydrogens removed and all covalent bonds shown as rods

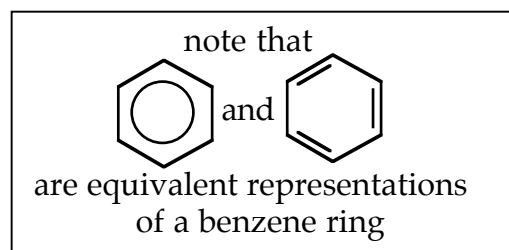


c) alanine as in (b) with adjacent amino acids shown in dotted lines



Lab report

There is no report for this part of the lab. 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.



Bio 111 Small Molecules Worksheet

Name _____ TA & Sect. _____
Name _____
Name _____ Score _____ / 20

This is a
group effort
for a group
grade.

This is due at the end of lab today.

The numbers of these questions correspond to the numbers on the web site.

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

2) Using the image from the web site, draw the structure of the linear form of fructose. You need not indicate the chiral parts of the molecule. (2 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 circular form of glucose. You need not indicate the chiral parts of the molecule. (2 pts)

5) On the structure in question (1), indicate which parts of the molecule have been linked to form ring structure. (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 question (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 hydrogens 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 hydrogens. Using the chart in the lab manual, identify the amino acid you have been assigned.

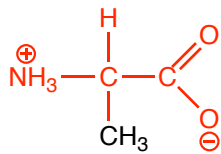
a) Number given by TA _____ Identity of amino acid _____ (2 pts)

Structure: (3 pts)

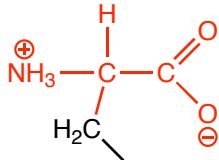
b) Number given by TA _____ Identity of amino acid _____ (2 pts)

Structure: (3 pts)

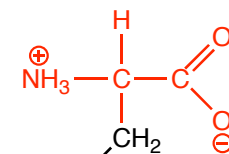
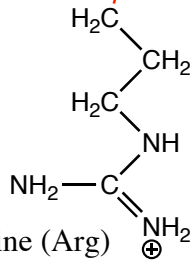
Structures of Amino Acids



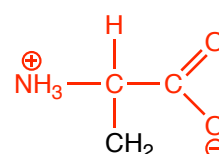
Alanine (Ala)



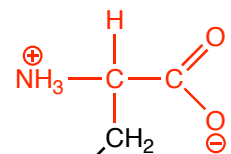
Arginine (Arg)



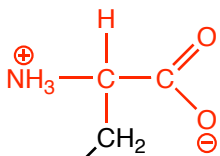
Asparagine (Asn)



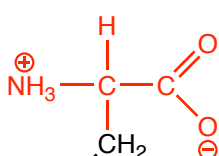
Aspartic Acid (Asp)



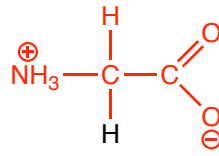
Cysteine (Cys)



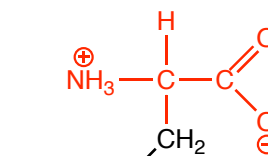
Glutamic Acid (Glu)



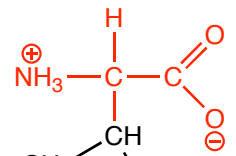
Glutamine (Gln)



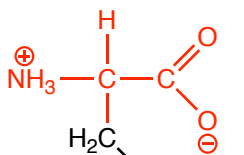
Glycine (Gly)



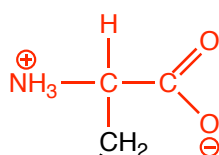
Histidine (His)



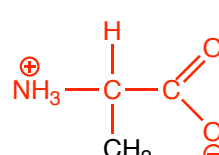
Isoleucine (Ile)



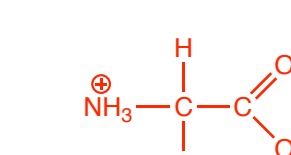
Leucine (Leu)



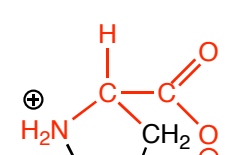
Lysine (Lys)



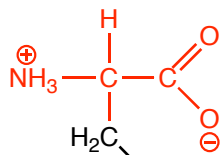
Methionine (Met)



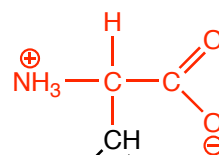
Phenylalanine (Phe)



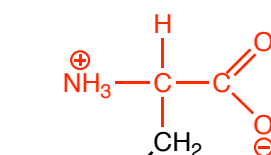
Proline (Pro)



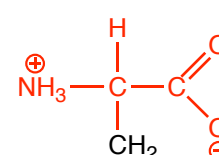
Serine (Ser)



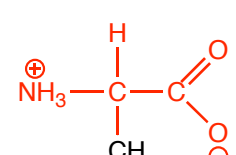
Threonine (Thr)



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)	

