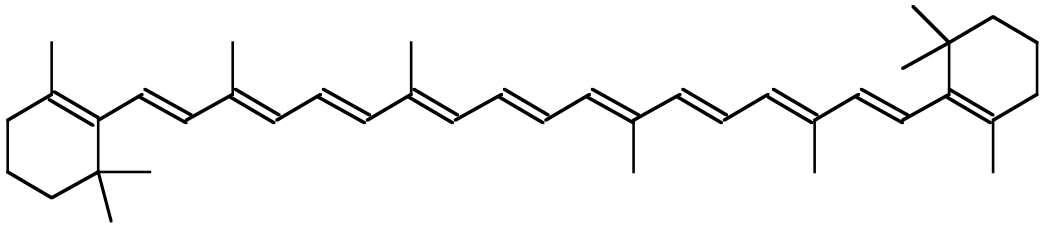
Chemical Properties

Objectives:

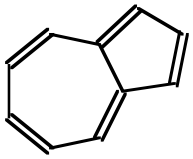
- to get a clearer understanding of hydrophobic/hydrophilic molecules
  - how to 'read' structures
  - the effects of various groups of atoms on the properties of a molecule
- to learn how to use a software program that you can use at home to strengthen your understanding of hydrophobic/hydrophilic molecules

Part I: Questions for Discussion:

1) Consider the four dye molecules:

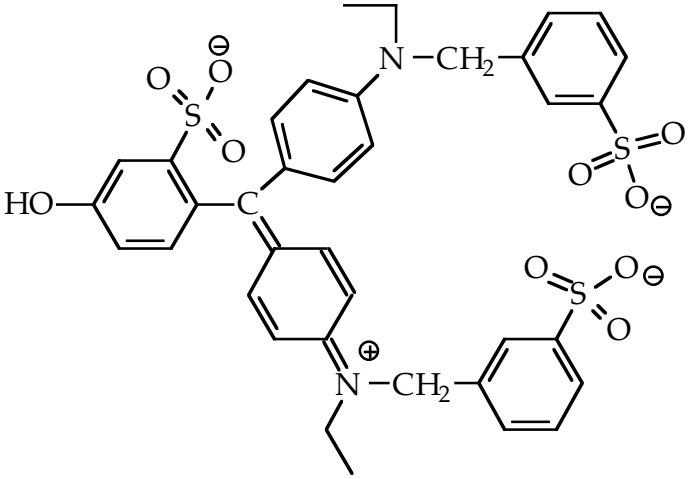


β–carotene (orange-red; present in carrots, etc.)

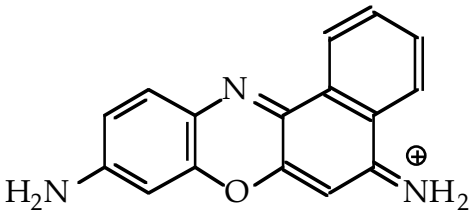


azulene
(deep purple)

fast green FCF
(blue-green)



cresyl violet
(red-purple)



For each of the molecules above, indicate the parts that are hydrophobic and those that are hydrophilic.

2) Two of these dyes are soluble in water and two are not. Predict which is which in terms of the bonds that each molecule can make with water and their hydrophobicity/hydrophilicity.

3) Your TA will demonstrate this solubility as follows. He/she will have prepared tubes with water on the bottom layer and hexane ($H_3CCH_2CH_2CH_2CH_2\ CH_3$ – very hydrophobic) on the top layer (remember that oils like hexane float on water). He/she will then add a small amount of a solution of each dye to the test tubes.

- Hydrophilic dyes will make favorable interactions with water, leaving the water colored and the hexane colorless.
- Hydrophobic dyes will not make favorable interactions with water and the hydrophobic effect will drive them to be in the hexane. Thus they will color the hexane and not the water.

Based on your predictions in part (2), predict which dyes will be found in water or hexane.

4) Work through problem 1.2.5 from Chapter 2 of APAIB.

Part II: Exercises on the Computer

The exercises in this lab can be found in *A Problems Approach to Introductory Biology* chapter 2.

Begin by working through problem C1 (page 86).

We will then work through problem C4 (page 105). You can use the software on the APAIB CD-ROM or from the course website; go to the page for this lab in the On-Line Lab Manual.

You should do part (1) in your book; part (2) should be done on the attached worksheet.

Bio 111 Chemical Properties Worksheet

Name_____

Name_____

Name_____

TA & Sect._____

Score_____/30

This is due at the end of lab this week.

Use the computer program to answer the questions below.

1) In organic chemistry "R" is shorthand used to represent "the rest of the molecule" - **this must be the same in all the molecules you use in this part!**. To answer this question, you can use the "R group" of your choice; just be sure that you use the same "R group for all four molecules.

Consider the following 4 molecules:

$R\text{-}CH_3$ R-OH R-SH $R\text{-}NH_2$

For a given R-group, two of these have high logP values and two have low logP values.

a) Choose an R group of your own design, draw it, draw the four variations of this molecule ($R\text{-}CH_3$, R-OH, R-SH, and $R\text{-}NH_2$), and give their logP values. (4 pts)

b) In terms of the bonds involved, explain why the two molecules with high logP are more hydrophobic and why the two with low logP are more hydrophilic. (6 pts)

2) Ethanol (H_3CCH_2OH) and di-methyl-ether (H_3COCH_3) have the same number of carbons, hydrogens, and oxygens (C_2H_6O) but differ in the following important way: in ethanol, the O is bonded to a carbon and a hydrogen, but in di-methyl-ether, the O is bonded to two carbons.

Create a similar pair of molecules (DO NOT USE THE SAMPLES GIVEN ABOVE).

- Both members of this pair should have the same number of carbons and hydrogens (check this using the formula that jlogp calculates).
- Both members should have only one oxygen (check this using the formula)
- One member should have the oxygen bonded to a carbon and a hydrogen; the other should have the oxygen bonded to two <u>different</u> carbon atoms.

a) Draw **<u>your own</u>** two molecules. (3 pts)

b) In terms of their capability of forming bonds with water, predict which will be more hydrophobic and explain your reasoning. (5 pts)

c) Give the logP values for your two molecules. Do they agree with your prediction? (2 pts)

3) Adding an -OH (hydroxyl) group makes a molecule more hydrophilic; adding a $-CH_3$ or $-CH_2-$ (methyl) makes a molecule more hydrophobic. Approximately how many "$-CH_3$"s (or "$-CH_2-$"s) are required to counterbalance the effect of an -OH? Note that this will depend on many factors and will not be the same for all molecules. (3 pts)

a) Start with a molecule of your choosing. Draw it below & calculate it's logP:_____

b) Add an -OH to the molecule from part (3a). Draw it below & calculate it's logP:_____

c) Keep adding $-CH_3$'s to the molecule from part (3b) until it has approximately the same logP as the original molecule (3a). Draw the molecule below, fill in the number of $-CH_3$'s you had to add, and give the logP. Discuss the results with your classmates.

of "$-CH_3$"s or "$-CH_2-$"s required_____

logP_____

4) Adding a charged group $-O^-$ or $-NH_3^+$ group makes a molecule much more hydrophilic; adding a $-CH_3$ (methyl) makes a molecule more hydrophobic. Approximately how many $-CH_3$'s are required to counterbalance the effect of a charged group? Note that this will depend on many factors and will not be the same for all molecules. (3 pts)

a) Start with a molecule of your choosing. Draw it below & calculate it's logP:_____

b) Add a charged group to the molecule from part (4a).
Draw it below & calculate it's logP:_____

c) Keep adding $-CH_3$'s to the molecule from part (4b) until it has approximately the same logP as the original molecule (4a). Draw the molecule below, fill in the number of $-CH_3$'s you had to add, and give the logP. Discuss the results with your classmates.

of "$-CH_3$"s or "$-CH_2-$"s required_____

logP_____

5) The shape of a molecule can also have an effect on it's hydrophobicity. Create a pair of isomeric molecules. (4 pts)

- Both members of this pair should have the same formula (the same number of carbons hydrogens, nitrogens, etc.); check this with the formula that jlogp calculates.
- One member should have a 'long and thin' shape; the other should be 'short and fat'; this makes them structural isomers.

Draw your two molecules and label them with their logP values. Discuss the results with your classmates.