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## Final-Dec 12th

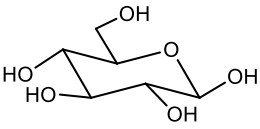
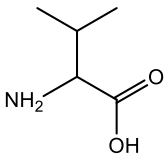
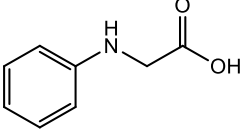
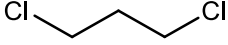
Chem14C-Spring 2020  
Prof. Castillo

Name: \_\_\_\_\_

ID: \_\_\_\_\_

1. Determine the noncovalent intermolecular forces of the following compounds. (10 points)

a. Circle **ALL** the intermolecular forces that applies to each molecule.

<p><b>A</b></p> 	<p><b>B</b></p> 	<p><b>C</b></p> 	<p><b>D</b></p> 
<p>London Dipole-dipole H-bonding Anion-Cation Pi-stacking Ion-dipole Cation-pi</p>	<p>London Dipole-dipole H-bonding Anion-Cation Pi-stacking Ion-dipole Cation-pi</p>	<p>London Dipole-dipole H-bonding Anion-Cation Pi-stacking Ion-dipole Cation-pi</p>	<p>London Dipole-dipole H-bonding Anion-Cation Pi-stacking Ion-dipole Cation-pi</p>

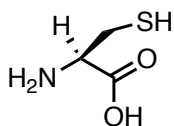
b. Find the molecules on the table on top with the highest and the lowest boiling point

Highest boiling point: \_\_\_\_\_

Lowest boiling point: \_\_\_\_\_

2. Answer the following questions regarding the functional group identification and molecule nomenclature.

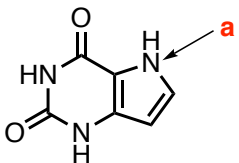
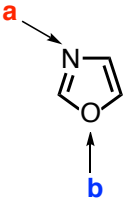
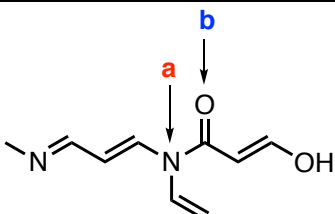
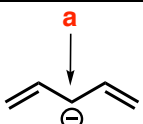
a. There are 3 functional groups existing in the following molecule. Please indicate all of them. (5 points)



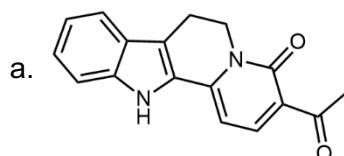
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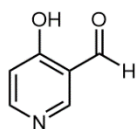
- b. Draw out the bond-line structure of the following two molecules.  
 3,4-dimethylhexanal                      4-chlorobutanoic acid

3. For each of the following molecules, please indicate the number of the pi electrons and indicate the number of the atoms that are involved in the **longest conjugation chain**. Additionally, in each case, for the labeling atoms, indicate which orbital the LP is staying (10 points)

Structure	Number of pi electrons	Number of the atoms in the <b>longest conjugation chain</b>	Indicate which orbital the LPs is staying
			LP on Nitrogen <b>a</b> _____
			LP on Nitrogen <b>a</b> _____ LPs on Oxygen <b>b</b> _____
			LP on Nitrogen <b>a</b> _____ LPs on Oxygen <b>b</b> _____
			LP on Carbon <b>a</b> _____

4. Provide 4 distinct resonance structures for the following molecules. Remember to show the correct formal charges and the atoms that can participate in resonance. (10 points)





b.

-In the above structure what orbital does the lone pair on the Nitrogen occupy? \_\_\_\_\_  
 -Do these electrons participate in resonance \_\_\_\_\_

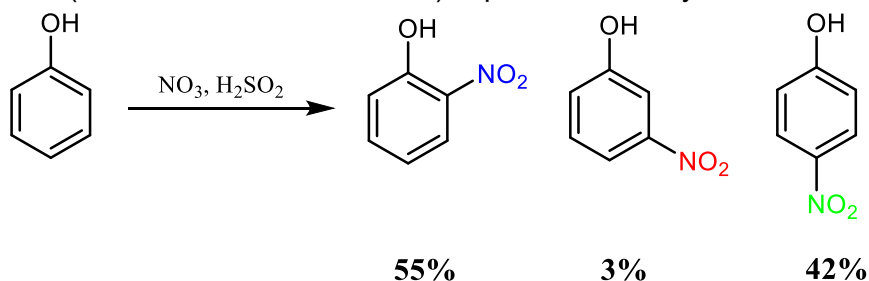
5. As you increase the conjugation of a molecule, the energy between the HOMO- and LUMO orbitals. (5 points)

- a) Decreases
- b) Increases
- c) Stays the same
- d) Plateaus
- e) C and D

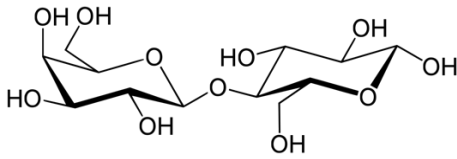
6. List the three criteria (one sentence each) for Aromaticity. Use your own words. (5 points)

Bonus Question (3 points)

During Electrophilic Aromatic Substitution (EAS) reactions, an aromatic compound will attack another (electrophile) molecule to form an addition product with specific regioselectivity at the ortho and para positions indicated in blue and green. Using resonance structures, provide a brief (no more than one sentence) explanation of why this is the case.



7. Please answer the following questions about the displayed molecule (5 points)



a. What type of glycosidic linkage does it have?

- A:  $\beta$  (1-4)
- B:  $\beta$  (1-2)
- C:  $\gamma$  (1-4)
- D:  $\alpha$  (1-4)
- E:  $\alpha$  (1-2)

b. Which disaccharide is it?

- A: sucrose
- B: lactose
- C: maltose
- D: none of the above

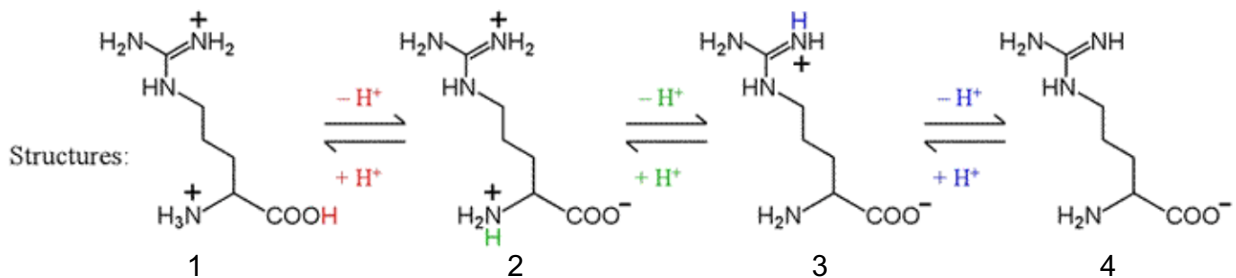
c. Would you expect this molecule to be easy to digest by humans?

- A: Yes
- B: No

d. What are the monosaccharides if this molecule were digested (left to right)?

- A: Glucose, Glucose
- B: Fructose, Glucose
- C: Glucose, Fructose
- D: Glucose, Galactose

8. Arginine  $pK_a$   $\alpha$ -COOH = 2.17,  $pK_a$   $\alpha$ - $NH_3^+$  = 9.04,  $pK_a$  of acidic function in R = 12.48. (5 points)



Please indicate which structure will exist under the conditions at:

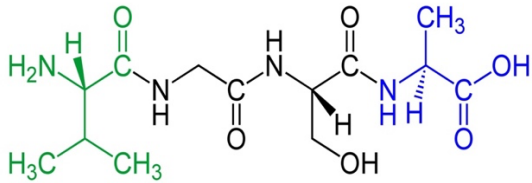
a. pH = 1

b. pH = 6

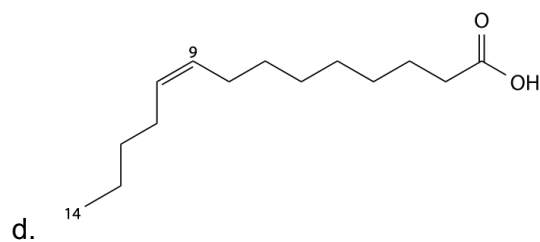
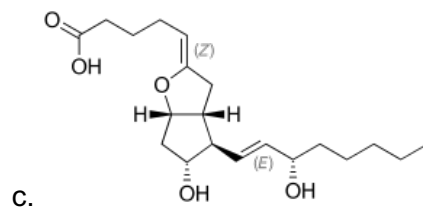
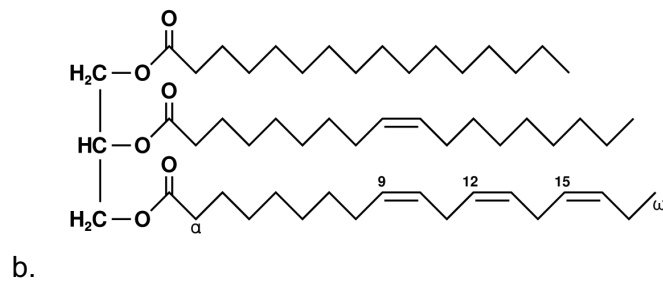
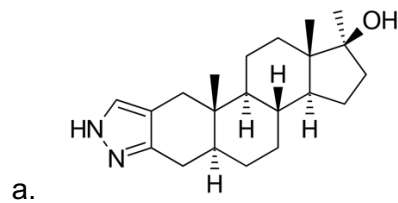
c. pH = 12.5



9. Identify the amino acid sequence of the following peptide using the one letter codes in the format of (A-B-C-D): (5 points)



10. Classify the following molecules by filling the box with A (fatty acid), B (wax), C (triglyceride), D (Phospholipid), E (steroid), or F (prostaglandins) (5 points)



11. Fill in the main biological function for the lipids below with A (antioxidant), B (cell membranes), C (energy storage), or D (signaling) (5 points)

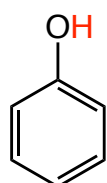
a. Triacylglycerols

b. Phospholipids

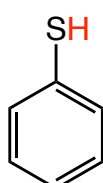
c. Steroids

d. Vitamins

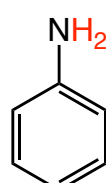
12. Rank the acidity of the following species from the strongest to the weakest. (the proton is highlighted in red) Remember to use the stability of the conjugate base to determine your answer (resonance>size>EN>inductive effect) (10 points)



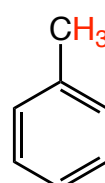
**A**



**B**

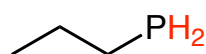


**C**

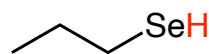


**D**

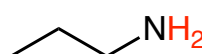
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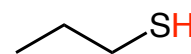
**A**



**B**

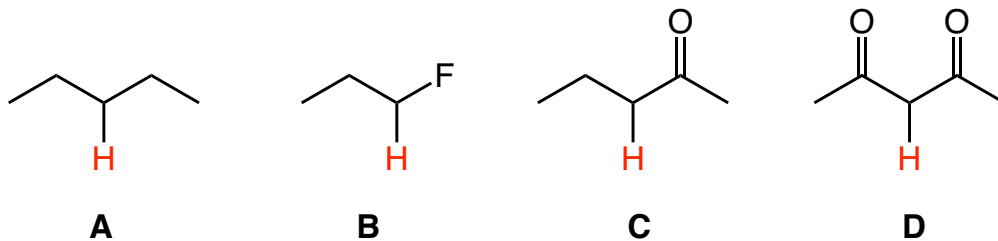


**C**

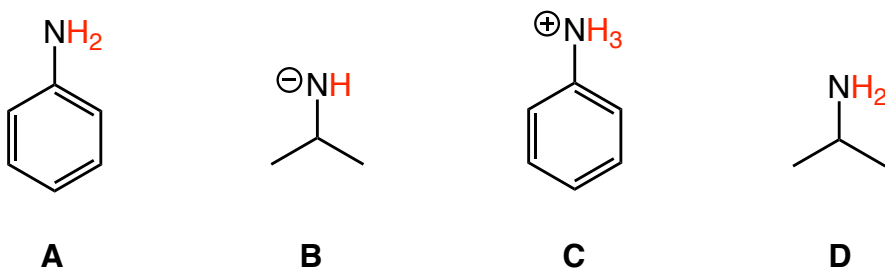


**D**

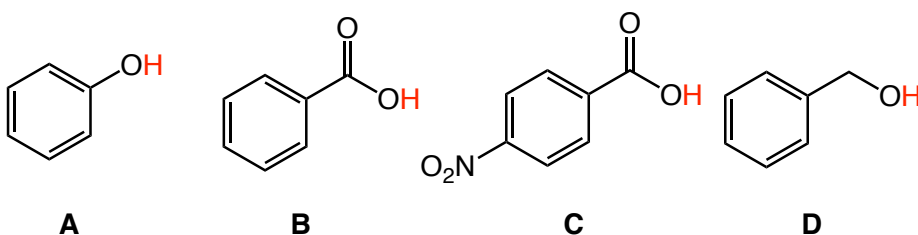
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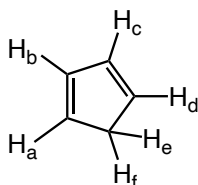


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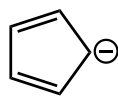
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13. Cyclopentadiene is a hydrocarbon compound. It can be deprotonated easily, and its anion is a very important ligand in organometallic chemistry. Here is the structure of cyclopentadiene. (10 points)



- a. How many signals do you expect to see in the  $^1\text{H}$  NMR spectrum of cyclopentadiene?

- b. Here is the anion of cyclopentadiene after it is treated with base. Answer the following questions.



-How many electrons are in the largest conjugation of this anion?

-Is this molecule aromatic?

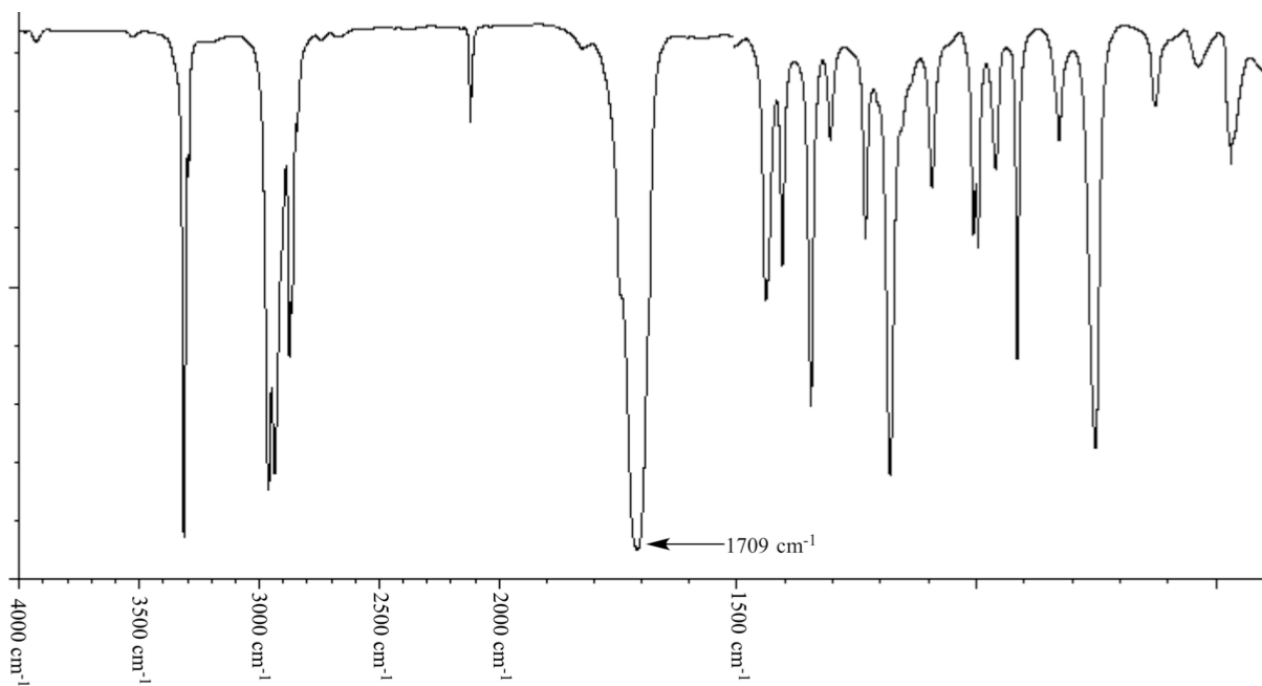
-The pKa of cyclopentadiene is 16. For regular alkanes, C–H bond pKa is ~50. Explain why cyclopentadiene is much more acidic than regular alkanes.

14. Predict the molecule using the following MS, IR,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  spectra. Show all your work in the spaces provided. (15 points)

**Mass spec:**  $m/z = 172$  (M; 100%),  $m/z = 173$  (10.4%), and  $m/z = 174$  (32.6%).

**MS workspace.** Propose possible molecular formula with the information given from MS. Show all work to receive full credit.





IR workspace: What functional groups are present? (Please provide the region in the IR with its respective bond type)

What is the molecular formula?

Degrees of unsaturation: \_\_\_\_\_

<b><sup>1</sup>H-NMR chemical shift</b>	<b>Splitting</b>	<b>Integral</b>	<b>#H</b>	<b>Implications</b>
3.54 ppm	Triplet	2.0		
3.45 ppm	Singlet	1.0		
1.76 ppm	Pentet	2.0		
1.56 ppm	Triplet	2.0		
0,95 ppm	Singlet	6.0		

<b><sup>13</sup>C-NMR chemical shift</b>	<b>Splitting</b>	<b>Implications</b>
195 ppm	Singlet	
81 ppm	Singlet	
79 ppm	Doublet	
47 ppm	Triplet	
45 ppm	Singlet	
37 ppm	Triplet	
34 ppm	Triplet	
24 ppm	Quartet	

Propose the structure of the molecule in the box to the right.  
Only one structure is graded. You may use this space to  
work out the problem. This space will not be graded

**Proposed structure:**



15. Identify the chiral center on the following drugs and define the stereochemical configuration (R/S) (15 points)

