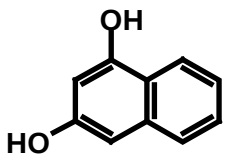
BASIC PHARMACEUTICAL SCIENCE FOR THE PRACTICING PHARMACIST
MEDC 527, Fall 2008
Quiz #1, Dr. Desai, 100 points; September 9, 2008

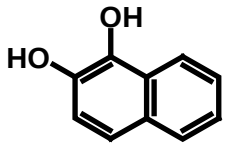
STUDENT NAME (in CAPITAL Letters ONLY) **VCU ID #**

	IV	V	VI	VII
2	C	N	O	F
3	Si	P	S	Cl
4	Ge	As	Se	Br
5				I

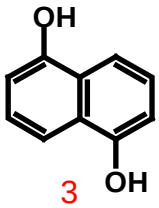
1. Rank the molecules according to their expected mp/bp. Use 1 for least and 3 for highest mp/bp. (6 pts)



2



1

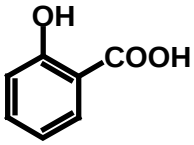


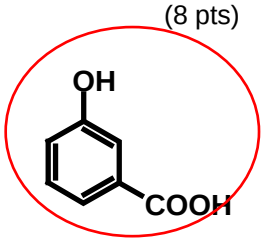
3

2. Circle the molecule in the pair that is expected to have higher boiling/melting point. (8 pts)

a) CH_3CH_2F; **HF**

b)





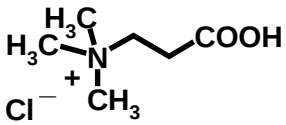
3. Write the Henderson – Hasselbach equation for the following equilibrium. Define the terms involved. (12 pts)

$$PhCOOH + H_2O \Longleftrightarrow PhCOO^- + H_3O^+$$

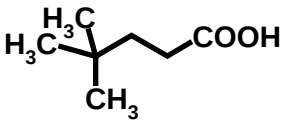
$$\log \frac{[PhCOO^-]}{[PhCOOH]} = pH - pKa$$

where pKa = -logKa (or negative log of the acid dissociation constant); pH = -log [H+] (or a measure of the concentration of protons); [PhCOO-] is the concentration of the conjugate base and [PhCOOH] is the concentration of the acid at equilibrium.

4. In few sentences, explain why **I** is expected to have lower pKa than **II**. (6 pts)



I



II

1) The positive charge on the nitrogen induces a withdrawal of electrons from the carbon of the carboxylic acid resulting in easier release of the proton in I as compared to that in II;

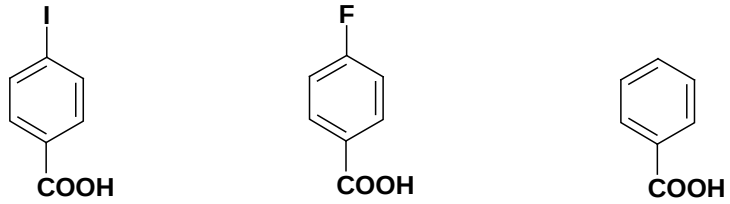
Alternative explanation: the negative charge of the carboxylate is stabilized more by the positive charge of nitrogen in I than in II.

5. Rank the molecules/ions in each series according to their pKa values. Use 1 for the least pKa value, 2 for the next higher and so on. (18 pts)

a) $-CH_2-CH_2-COOH$ | $CH_3-CH(NO_2)-COOH$ | $CH_3-CH(COOH)-COOH$

3 | 1 | 2

b)

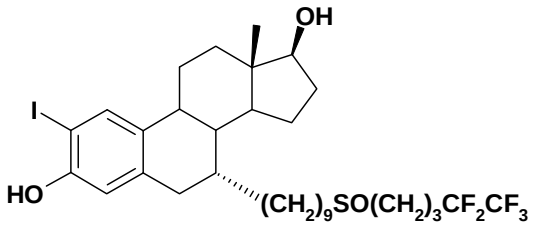


2 | 1 | 3

c) $F-CH_2-COOH$ | CH_3-COOH | $Br-CH_2-COOH$

1 | 3 | 2

6. The molecule underneath is potential diagnostic marker for an anti-estrogenic agent. Indicate the Kier-Hall electronegativity values of the following atoms. (8 pts)



Kier-Hall eN Value

-O- of phenolic OH = 1.0

I- = 6/25 or 0.24

S = 1/3 or 0.33

F of CF_2 = 1.5 or 6/4

7. In few sentences, explain why the **bp** of **I** is expected to be higher than that of **II**. (6 pts)

I **II**

The COOH group of I introduces both inter- and intra-molecular H-bonds, which are completely absent in II. This raises the BP of I in comparison to that of II.

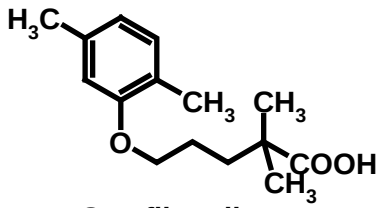
8. Amyl nitrite is a nitrovasodilator. The structure of amyl nitrite is $(CH_3)_2CHCH_2CH_2$-O-N=O. Write the electronic structure of its nitrogen and the double bonded oxygen atoms and indicate their hybridization states. (8 pts)

The electronic structure of **N** is 1s2 2s2 2px1 2py1 2pz1 (some may write the hybridized form. If correct give full pts)
The hybridization state of **N** is sp2

The electronic structure of **=O** is 1s2 2s2 2px2 2py1 2pz1
The hybridization state of **=O** is sp2

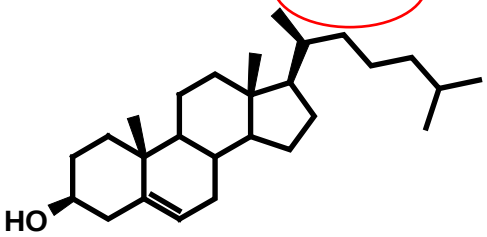
9. Indicate whether the following drugs or biological molecules will exhibit good water solubility at pH 7.2-7.4. Circle the correct answer. (16 pts)

A) Soluble OR Insoluble



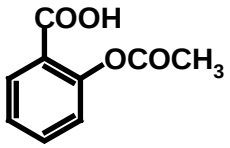
Gemfibrozil

B) Soluble OR Insoluble



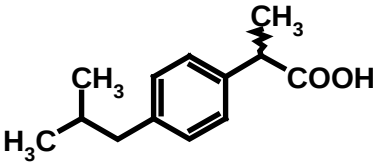
Cholesterol

C) Soluble OR Insoluble



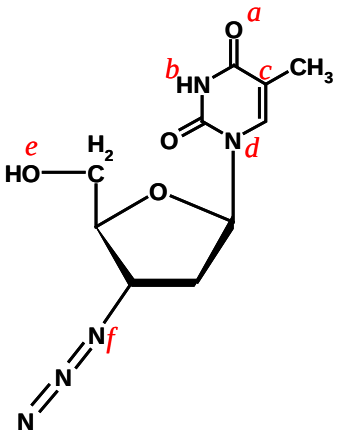
Aspirin

D) Soluble OR Insoluble



Ibuprofen

10. Azidothymidine (below) is an inhibitor of HIV reverse transcriptase enzyme. Write the hybridization state of non-hydrogen atoms marked '***a***' (oxygen), '***b***' (nitrogen), '***c***' (carbon), '***d***' (nitrogen), '***e***' (oxygen) and '***f***' (nitrogen). Also indicate the type of geometry corresponding to the hybridization. (12 pts)



	Hybridization state	Type of Geometry
a =	sp2	planar
b =	sp3	tetrahedral
c =	sp2	planar
d =	sp3	tetrahedral
e =	sp3	tetrahedral
f =	sp2	planar