DRAWING STRUCTURES

SOLVED PROBLEMS

(ANSWERS ON page 6 onwards)

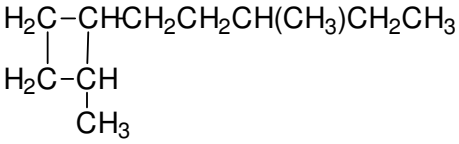
1.- Define the molecular formula of the following compounds, represented here as expanded structural formulas

A) $CH_3CH(C_2H_5)CH_2CH_2OCH_2CH_3$

B) $(CH_3)_2C(C_2H_5)CH_2CH(SCH_3)CH_2CH_2C(CH_3)_3$

C) $CH_3CH(COOH)CH(NH_2)CH_2CH_2CH(C_6H_5)CH_2OCH_3$

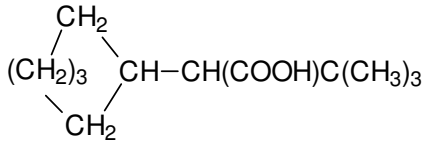
D)



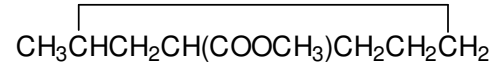
2.- Draw line or abbreviated molecular renderings of compounds of problem 1.

3.- Draw the line molecular structure of the following compounds showing carbon backbone and correct position of substituents of:

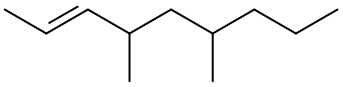
A) $CH_2C(CH_3)CH_2SCH(COOH)CHCHCH_3$

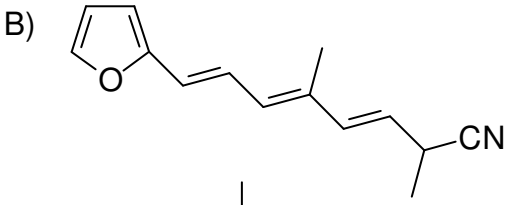
B) 

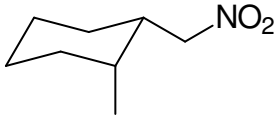
C) $HCCCH_2CH(NHCH_3)CH_2NHCH_2CH_2OCH_3$

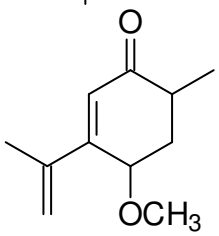
D) 

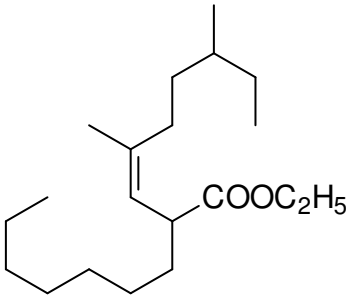
4.- What is the atomic composition (empirical formula) of the following compounds:

A) 

B) 

C) 

D) 

E) 

5.- Ajoene is one of the flavor components of garlic, to which heart-protecting properties have been ascribed. The structure is shown below.

a. Translate this structure into a line molecular drawing
b. Indicate all functional groups and give each one a name

$CH_2CHCH_2S(O)CH_2CHCHSSCH_2CHCH_2$

AJOENE, from Garlic

6.- Glucosinolates are a class of organic compounds frequently found in cauliflowers, broccoli, Brussels sprouts, and cabbage, and contribute to their peculiar aroma. They are produced by these plants as an insecticide although some butterflies have learned to use these compounds to identify those plants where to lay their eggs, which destroy the plants! The structure is given below.

a. Translate this structure into a line molecular drawing
b. Indicate all functional groups and give each one a name

Note: Glu is for glucose, ignore its detailed molecular structure in this problem.

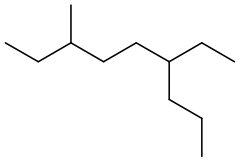
c. Justify the negative charge.

$GluSCHNOSO_3^-$

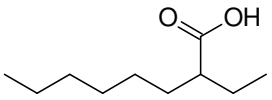
Glucosinolate

7.- Find the mistake(s) in the following translations of molecular rendering. The translated structure is to the right.

A) $CH_3CH_2CH(CH_3)CH_2CH(C_2H_5)CH_2CH_2CH_3$

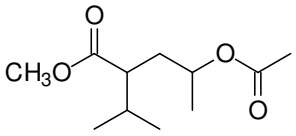


B)

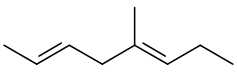


$CH_3(CH_2)_4CH(COOH)CH_3$

C) $CH_3CH(CH_3)CH(OC(CO)CH_3)CH_2CH(OCOCH_3)CH_3$

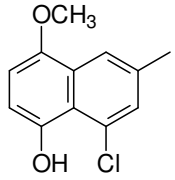
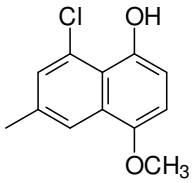


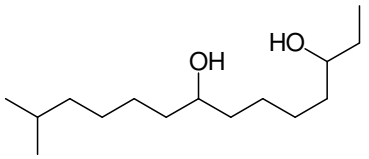
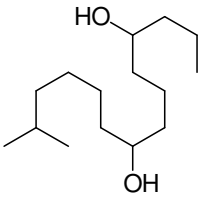
D)

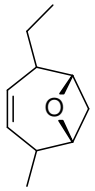
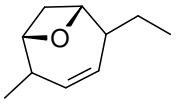


$CH_3CHCHCH_2CH(CH_3)CHCH_2CH_3$

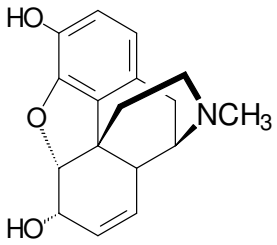
8.- Compare formulas A and B of each pair and test whether they represent the same compound or not.

A)  ...same as...  ?

B)  ...same as...  ?

C)  ...same as...  ?

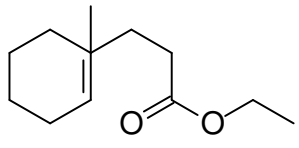
9.- The alkaloid Morphine is a narcotic and pain reliever extensively used to treat severe pain in advanced cancer patients, soldiers wounded in battle and people suffering from untreatable pain. Unfortunately it develops tolerance quickly hence loosing its effects. The structure is given below. Could you tell how many rings are there? Calculate the molecular weight of this compound.

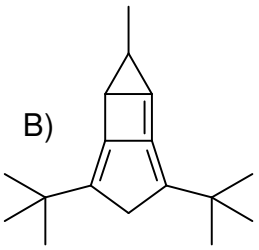


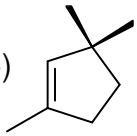
MORPHINE

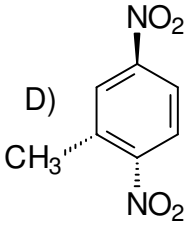
10.- Draw in line structures four different compounds with the empirical formula $C_8H_{16}O_2$.

11) There are a few but serious mistakes in the following structures. Which are they?

A) 

B) 

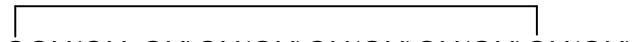
C) 

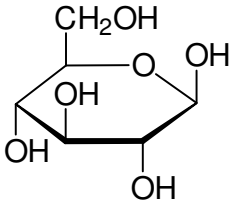
D) 

12) Glucose, one of the most prevalent compounds in living organisms is a fundamental source of chemical energy for metabolism. There are several common ways to represent its molecular structure. Two of them are shown below.

A) Translate rendering (a) into a more informative molecular drawing. Is your answer compatible with rendering (b)?

B) Could you draw the line abbreviated molecular structure from rendering (b) including information about the position of substituents relative to the molecular plane?

(a) 

(b) 

ANSWERS TO PROBLEMS

1)

A) $C_8H_{18}O$ B) $C_{14}H_{30}S$ C) $C_{15}H_{22}NO_3$ D) $C_{11}H_{22}$

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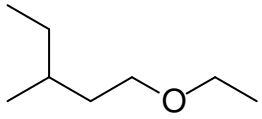
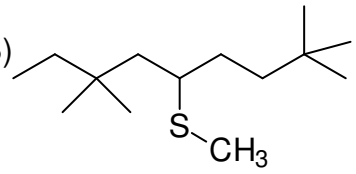
2)

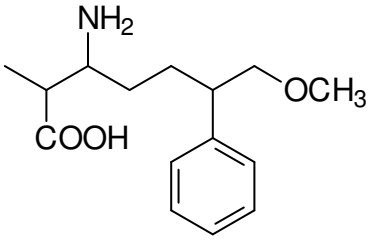
A)



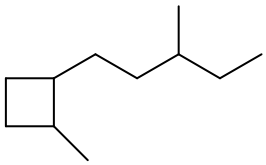
B)



C)

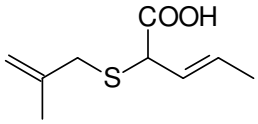


D)

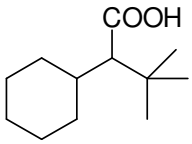


3)

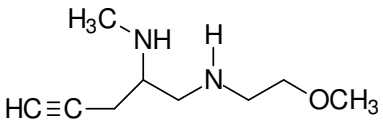
A)



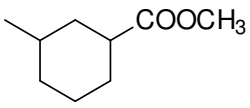
B)



C)

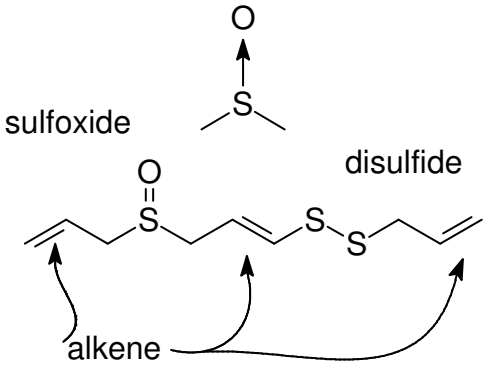


D)



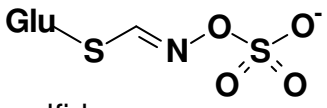
4) **A)** $C_{11}H_{22}$ **B)** $C_{14}H_{15}NO$ **C)** $C_8H_{15}NO_2$ **D)** $C_{11}H_{16}O_2$ **E)** $C_{20}H_{38}O_2$

5)



6)

Glucosinolate



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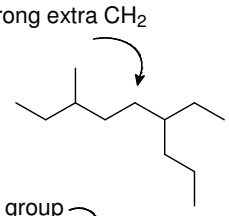
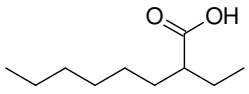
7)

A) $CH_3CH_2CH(CH_3)CH_2CH(C_2H_5)CH_2CH_2CH_3$



B)

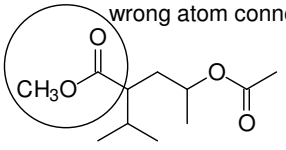


misplaced group

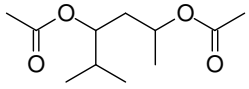
$CH_3(CH_2)_4CH(COOH)CH_3$

need one additional CH_2

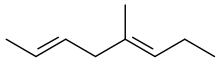
C) $CH_3CH(CH_3)CH(OC(CO)CH_3)CH_2CH(OCOCH_3)CH_3$



should be:



D)

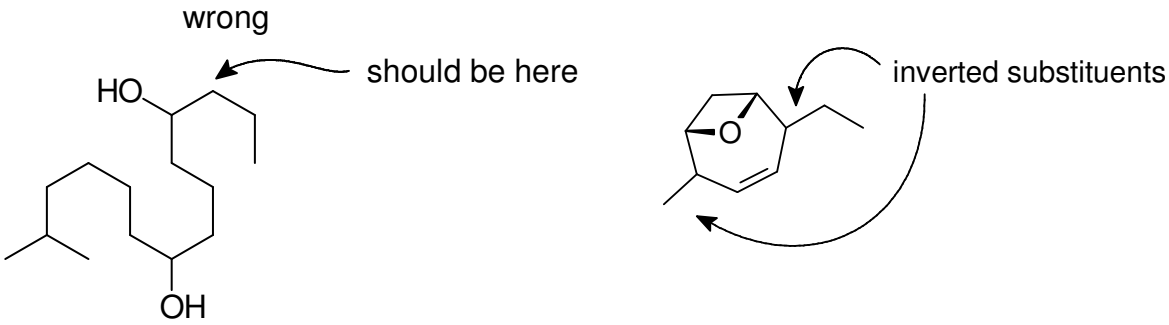


wrong extra H

$CH_3CHCHCH_2CH(CH_3)CHCH_2CH_3$

8)

A) Yes **B) No, OH in wrong position** **C) No:**



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9) There are 5 rings, two of them in a bicyclic arrangement.

To calculate the molecular weight of morphine you need its atomic composition first. This is: $C_{17}H_{19}NO_3$. Thus the molecular weight is:

12 x 17 + 19 + 14 + 16 x 3 = 185

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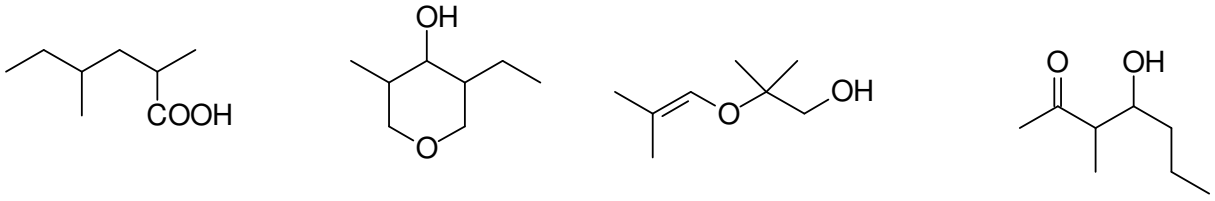
10)



same atomic composition, different connections : these are called isomers

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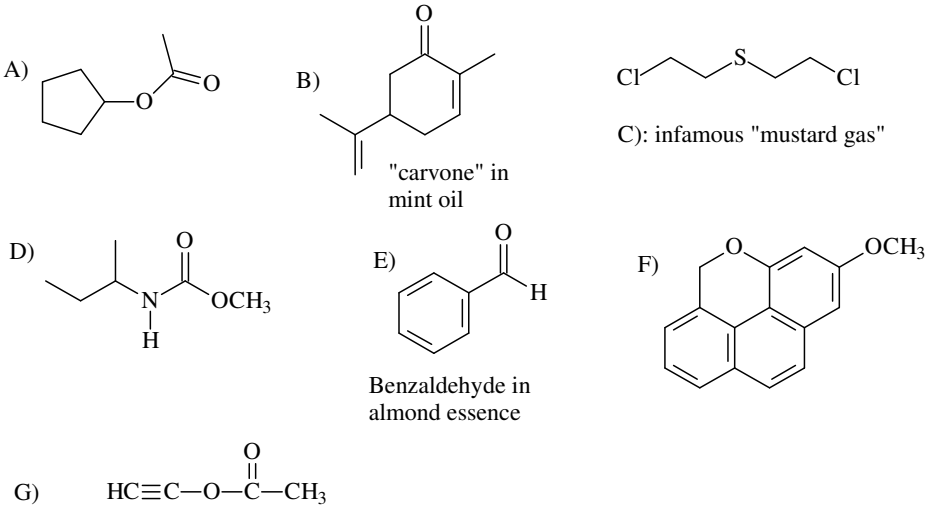
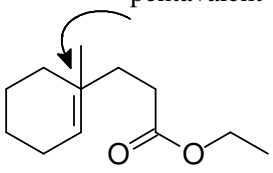
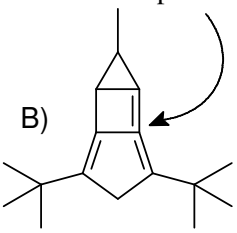
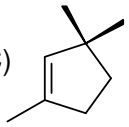
11)

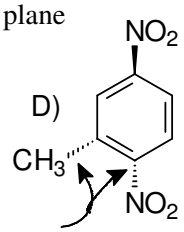


12)

A) 

B) 

C) 

D) 

benzene is planar.
Wrong to specify
stereochemistry

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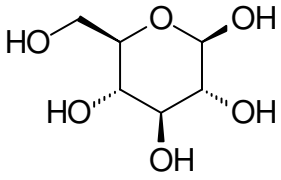
13) B)



END OF PROBLEM SHEET