Names: _____ *Section_____*

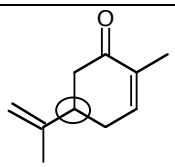
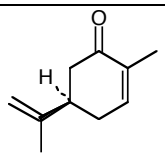
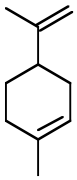
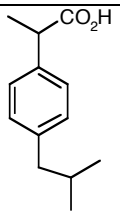
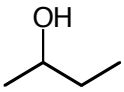
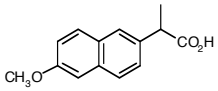
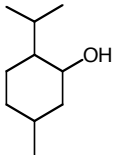
Chem 226/ Fall 2008 *Dr. Rusay*

Optical Rotation: PART 2

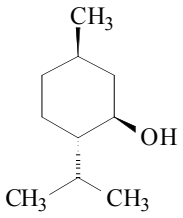
Structure & Configuration; Refer to:

http://chemconnections.org/organic/chem226/Labs/opt-rotation/opt-rot-II.html

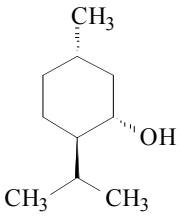
In PART 2, you will examine several chiral molecules using *jmol*. Some of the molecules are NSAIDs and the others are odorants whose olfactory properties have been studied by smell panels. Complete the following table. Carvone is given as an example. Circle all of the chiral atoms in the general structure. Under comments, if it is an NSAID, indicate if the stereochemistry of the Web molecule is the correct absolute configuration of the active drug (ACTIVE) or its enantiomer (NOT ACTIVE). If it is an odorant, list the type of smell, eg. MINT. For smell information refer to the handout: M. Laska and P. Teubner, *Chemical Senses*, 24, 161-170 (1999) and M. Laska, *Chemical Senses*, 29, 143-152 (2004).

	Name	General Structure	Stereo Structure	Funct-ion(s)	Abs. Config	Rel. Config + or -	Comments
A	l-carvone			ketone; alkene	R-	(-)	MINT
B							
C			Fisher Drawing:				
D			Fisher:				
E			Fisher:				
F							

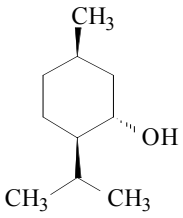
(-)-Menthol is a naturally occurring compound found in peppermint leaves and other plants in the mint family. It is widely used in cough drops, lip balms, nasal inhalers, liqueurs, perfumery, and cigarettes. Since menthol has three stereocenters, there are eight possible stereoisomers in total. Unlabeled samples were found, which contained four of the eight isomers: (-)-menthol, (+)-menthol, (+)-isomenthol, and (+)-neomenthol. Compound F is among the four. The four compounds include a pair of enantiomers and two diastereomers. In the structures below circle the chiral carbons in each and provide the absolute configuration (R-) or (S-) for each chiral carbon.



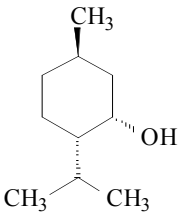
(-)-menthol



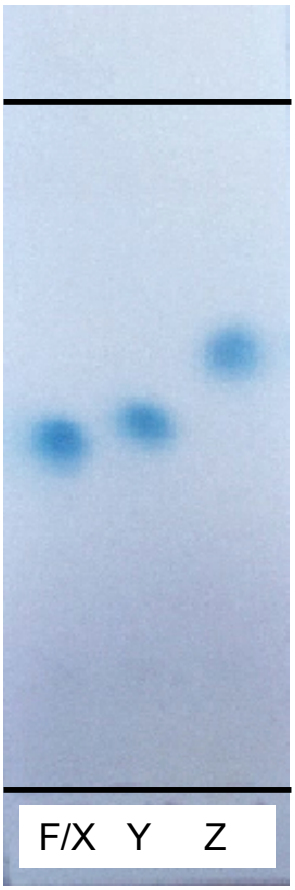
(+)-menthol



(+)-isomenthol



(+)-neomenthol



TLC plate of the four stereoisomers
4:1 hexanes:EtOAc

F /X were spotted on top of each other.
F and X melt at 43-45 °C
Y is a liquid at room temperature
Z melts at 77-83 °C

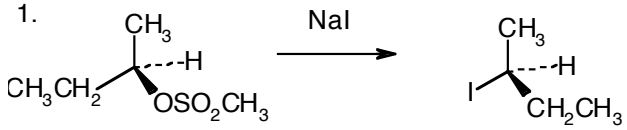
Identify the stereoisomers.
F: _____ X: _____

Y: _____ Z: _____
Briefly explain the reasons for your assignments.

Bonus Question: Briefly describe how menthol relates to the leading U.S. cigarette brand "Newport" and the marketing of this brand to teenagers.

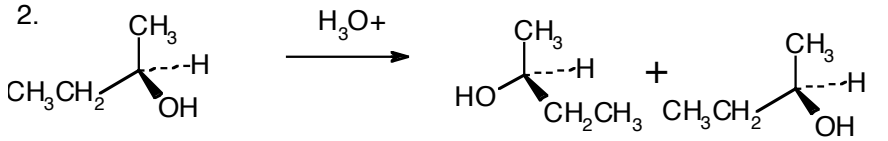
Circle each chiral carbon atom in both the reactant and product(s). Indicate the absolute configuration (R- or S-) next to each. An additional chiral carbon is introduced in #3; circle all of the chiral carbons and indicate R- or S- for each. In #2 and #3 identify the pair as enantiomers or diastereomers. For #1, #2, & #4 consider the stereochemistry of the reactant and compare it to the product(s): does the chiral center of the reactant remain the same (retention), change to the other configuration (inversion) or racemize (i.e., give a 50:50 mixture of both enantomers)?

1.



retention or inversion or racemization

2.



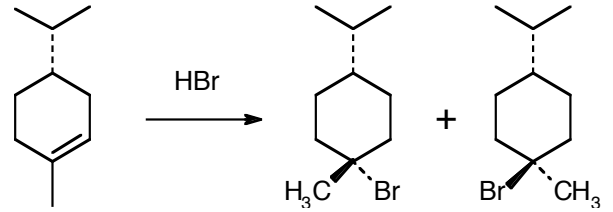
$[\alpha] = 0^o$

$[\alpha] = -13.52^o$

retention or inversion or racemization

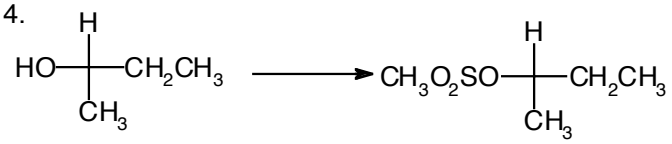
enantomers or diasteroemers

3.



enantomers or diasteroemers

4.



retention or inversion or racemization

5. Is chiral recognition by smell universal?, i.e., is it possible for anyone to distinguish between the enantiomers of any chiral odor molecule? Briefly explain your answer on the basis of the published abstracts provided in the handout.