

3.S: ORGANIC COMPOUNDS- ALKANES AND THEIR STEREOCHEMISTRY (SUMMARY)

CONCEPTS & VOCABULARY

3.1: Functional Groups

- Functional groups** are atoms or small groups of atoms (two to four) that exhibit a characteristic reactivity.
- Functional groups have characteristic names that often carry over into the naming of compounds.
- The most common organic functional groups that will be encountered in this course are: alkanes, alkenes, alkynes, arenes, (alkyl and aryl) halides, alcohols, ethers, aldehydes, ketones, esters, carboxylic acids, acid chlorides, amides, amines, nitriles, nitro compounds, sulfides and sulfoxides.

3.2: Alkanes and Alkane Isomers

- Hydrocarbons are a common class of organic molecules that contain only carbon and hydrogen atoms.
- Alkanes are one type of hydrocarbon that contains only carbon-carbon and carbon hydrogen single bonds.
- Straight chain and branched alkanes have the generic formula C_nH_{2n+2} , where n is equal to the number of carbons. Cycloalkanes have the generic formula C_nH_{2n} .
- Structural isomers are molecules with the same molecular formula, but different structures.

3.3: Alkyl Groups

- Alkyl groups** are small hydrocarbon chains attached to the parent alkane chain. The names of alkyl groups use the same prefixes to indicate the number of carbons (meth-, eth-, etc.), but use "-yl" as the ending, instead of "-ane".

3.4: Naming Alkanes

- The IUPAC System of nomenclature provides a set of rules for assigning every molecule a unique name.

3.5: Properties of Alkanes

- The boiling point of an alkane depends upon molecular weight and number of branches in the chain. Boiling points tend to increase with increasing molecular weight. Boiling points tend to decrease within a set of isomers as the number of branches increases.
- Alkanes and cycloalkanes are generally more soluble in organic solvents than in water.

3.6: Conformations of Ethane

- Rotation about the carbon-carbon sigma bonds in ethane results in different **rotational isomers** (also known as **conformational isomers** or **conformers**). **Newman projections** are a very common way of depicting conformers.
- The two most common conformers of ethane are called **staggered** and **eclipsed**. The staggered conformer is lower in energy (more stable) than the eclipsed conformer, because it has less **torsional strain**.

3.7: Conformations of Other Alkanes

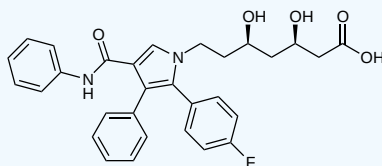
- Alkanes more complex than ethane, will have a greater variety of possible conformers. The **anti** and **gauche** conformers of butane are specific types of staggered conformations.

3.8: Gasoline - A Deeper Look

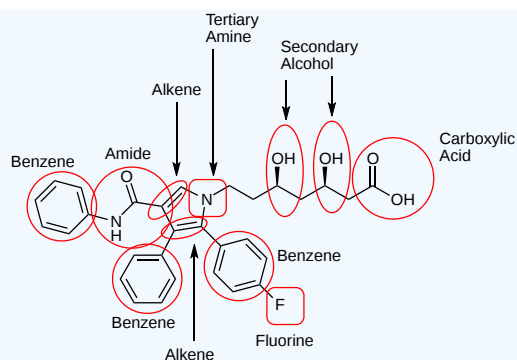
SUMMARY PROBLEMS

? EXERCISE 3.S.1

Atorvastatin (Lipitor) is a synthetic pharmaceutical marketed by Pfizer for lowering blood cholesterol and is one of the top selling drugs in the world. Circle and label all functional groups in Lipitor. (Be sure to label any amines or alcohols as primary, secondary, or tertiary.)

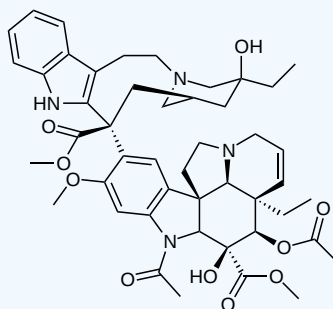


Answer

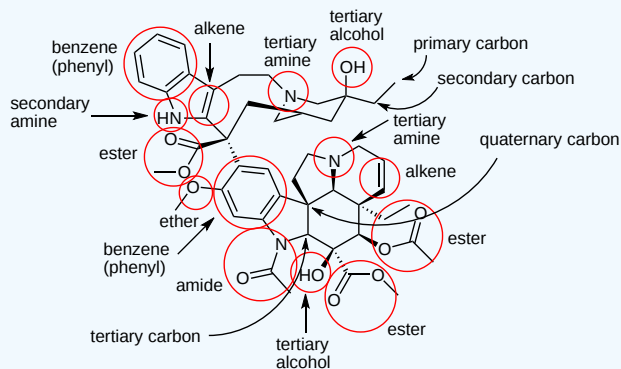


? EXERCISE 3.S.2

Vincristine is a natural product that was originally isolated in 1958 and has been studied as an anticancer agent. Answer the following questions related to this molecule. a) Circle and label all functional groups. (Be sure to label any amines or alcohols as primary, secondary, or tertiary.) b) Clearly label one primary carbon, one secondary carbon, one tertiary carbon, and one quaternary carbon.

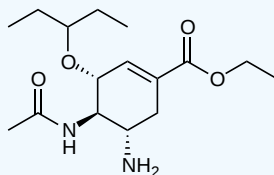


Answer

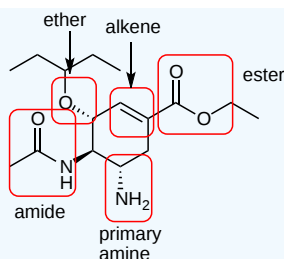


? EXERCISE 3.S.3

Tamiflu (oseltamivir) is an anti-influenza medication that was discovered by Gilead Sciences and is marketed by the pharmaceutical company Genentech. Circle and label all functional groups in Tamiflu. (Be sure to label any amines or alcohols as primary, secondary, or tertiary.)



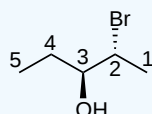
Answer



Notes: Alkanes are not functional groups, so there is no reason to circle groups like methyl or ethyl. (They are structural fragments.) Also, this molecule does not contain an aromatic ring. This is a cyclohexene ring. An aromatic ring is benzene and requires three double bonds in a six-membered ring.

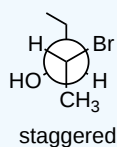
? EXERCISE 3.S. 4

For the following structure, a) Draw a Newman projection looking down the C2-C3 bond. (C2 should be in front.) b) Rotate the C2-C3 bond by 180 degrees (keep 3, 4, and 5 in the same orientation as the original structure). Draw the new skeletal structure and the new Newman projection looking down the C2-C3 bond. c) Label the Newman projections from parts a and b as staggered or eclipsed.

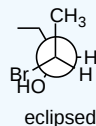
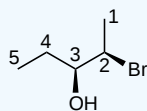


Answer

a)



b)



SKILLS TO MASTER

- Skill 3.1 Identify the following functional groups that are present in a given organic molecule: alkanes, alkenes, alkynes, arenes, (alkyl and aryl) halides, alcohols, ethers, aldehydes, ketones, esters, carboxylic acids, acid chlorides, amides, amines, nitriles, and nitro compounds.
- Skill 3.2 Name and draw structures of straight chain alkanes up to ten carbons in length.
- Skill 3.3 Name and draw structures for all the structural isomers of a given molecular formula.
- Skill 3.4 Identify methyl, primary, secondary, tertiary, and quaternary carbons in organic structures.
- Skill 3.5 Provide the IUPAC name of any given alkane or cycloalkane structure.
- Skill 3.6 Draw the structure of an alkane or cycloalkane given its IUPAC name.
- Skill 3.7 Arrange a series of alkanes in order of increasing or decreasing boiling point.
- Skill 3.8 Be able to draw Newman Projections of different conformers of alkanes.
- Skill 3.9 be able evaluate a conformer in terms of torsional and steric strain.
- Skill 3.10 Be able to identify the staggered, eclipsed, anti and gauche conformers of alkanes and to order them with respect to relative energy.

MEMORIZATION TASKS (MT)

- MT 3.1 Memorize the name and structure of each of the common functional groups listed in Skill 3.1.
- MT 3.2 Memorize the names and be able to draw the first ten straight chain alkanes.
- MT 3.3 Memorize the structures and common names of the alkyl substituent groups - isopropyl, *sec*-butyl, isobutyl,, and *tert*-butyl.

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