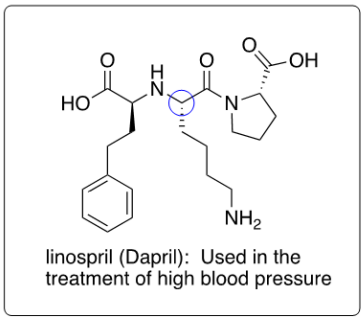
6.4: Exercise Questions

Part 1: Determining the absolute configuration of chiral centers in pharmaceuticals.

1. Please assign priorities for the groups on the indicated chiral centers and then rotate the molecule such that the lowest priority group is facing back into the plane of the paper. For help please view the chemical structures of these molecules using the supporting files.

Assign priorities to the indicated Chiral Center | **Redraw the molecule with the lowest priority to the back into the plane of the paper.**

A.

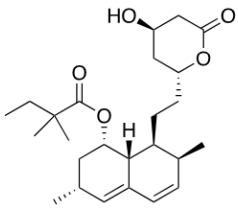


linospril (Dapril): Used in the treatment of high blood pressure

Rotate Lowest Priority to the Back →

The indicated chiral center is _____.

B.

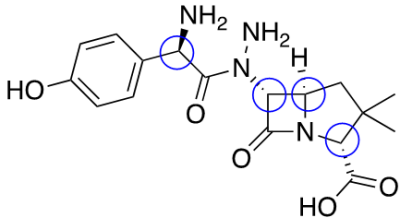


simvastatin (Zocor): used to treat high cholesterol

Rotate Lowest Priority to the Back →

The indicated chiral center is _____.

2. Using Avogadro to assist, please assign the absolute configuration all the chiral centers in the molecule amoxicillin.



Part 2: Examining the Energy Differences Between Enantiomers and Diastereomers.

3. Using the energy data provided in table 1, please determine the ΔG values for the D and L enantiomers of threonine in kcal/mol. 1 Hartree (Eh) = 627.5 kcal/mol.

$$\Delta G_{\text{Enantiomers}} = G_L - G_D$$

4. Using the energy data provided in table 1, please determine the ΔG between L-Threonine and L-Allothreonine in kcal/mol. 1 Hartree (Eh) = 627.5 kcal/mol. Is this number what you would have expected when compared to the ΔG value between the enantiomers of threonine? Explain.

$$\Delta G_{\text{Diastereomers}} = G_{\text{LThreonine}} - G_{\text{LAllothreonine}}$$

5. Examine the ground state structures L/D-Threonine and L/D-Allothreonine in Avogadro. Propose a reason why the energy values are different between enantiomers of threonine and enantiomers of allothreonine.

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