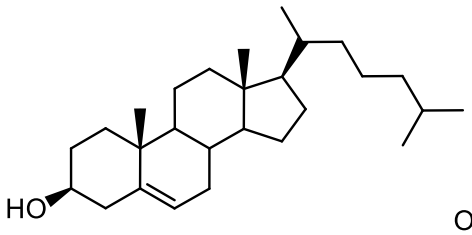
MOLECULAR STRUCTURES AND MODELS:
CONFORMATIONAL ANALYSIS OF CYCLOALKANES

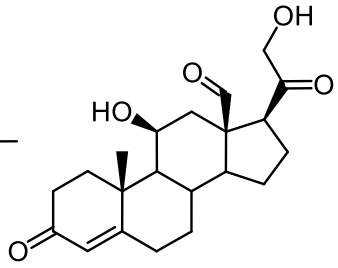
Note: There will be no pre-laboratory quiz for this experiment. However, you may should make sure you have studied the lecture(s) on the topics, and / or reviewed Chapter 3 in the online e course etext. The laboratory period will run more like a tutorial, when you will be provided with a worksheet to work through. The worksheet activity is "open book", you can work in groups and ask your TA about any concepts you don't understand.

Your grade for this laboratory is assessed based on an individual quiz at the end of the laboratory period (run under examination conditions).

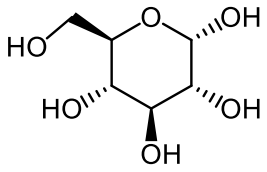
Cyclic structures are widespread in natural materials and biologically active compounds. A few examples are shown below:



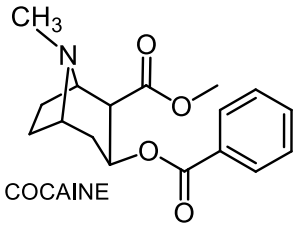
CHOLESTEROL



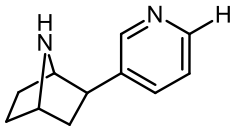
ALDOSTERONE



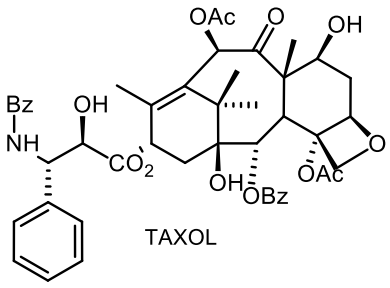
GLUCOSE



COCAINE



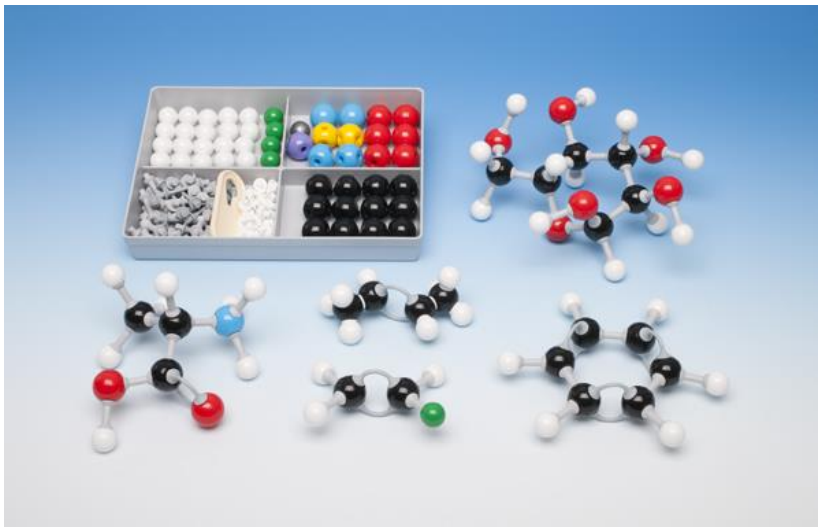
EPIBATIDINE



TAXOL

This activity is an extension of the first molecular models activity but the focus this time is on cycloalkanes which are clearly widespread and therefore of interest and important. A key learning goal is to help students with the visualization of cyclic molecules and to learn how to use model kits. Model kits are a tool that chemists will use to visualize and explain aspects of chemical structure. Molecular models are designed to reproduce molecular structures in three dimensions, allowing many subtle features concerning shapes of molecule to become clearer. Learning how to use a model kit and/or computational modelling correctly can help you to realise how models may be able to help you answer questions about molecular structure. They are very useful for helping students develop the ability to visualize molecules in 3 dimensions (after all, very few molecules are flat). Some students certainly struggle to grasp and manage the 3D shapes of molecules without the use of model kits (like the one

shown below which it the type we typically recommend) and it is a topic that becomes increasingly important. Since we regard model kits as a valuable tool, and a tool a chemist might use, for many years we have allowed and encouraged model kits to be used during examinations and assignments. That doesn't change with COVID. We also know that many students don't really know how to use model kits correctly and effectively, so this activity tries to show that while also exploring some to the topics related to conformations of cyclic structures that many students often struggle with. We always ask UofC Bookstore to stock model kits. While the kits might appear expensive, they are worth the investment and can retain most of their resale value.



During COVID times, the primary tool will be the "online model kit" at https://chemagic.org/molecules/amini.html and you will need to draw structures by selecting LOAD MODELS (left side, half way down) and then DRAW,. This will open a familiar face, the same drawing tool we use in Moodle. Draw what you need to in the window and then "LOAD MODEL" (bottom left) which will create a 3D interactive model of the molecule you had drawn. This 3D model can then be used like a hand-built model. *Almost…* Alternatively, we will make use of preexisting structure files from CheMagic (diagonal down and left from DRAW).

We will also be making use some measurement features (right side, under "Other Model Actions") such as length, angle and torsion and energy measurements (left side bottom "Other Model Actions") OPTIMIZE and ENERGY.

An important fundamental principle is that a molecule tends to position its atoms to give the arrangement with the lowest possible energy (*i.e*. most stable). This allows us to predict the shape of a molecule, and the subsequent physical and chemical properties to a very good approximation.

In this laboratory activity you will use the model kits to help answer questions and investigate:

- Shapes of cycloalkanes
- Conformational analysis of cycloalkanes
- Conformations of cyclohexane
- Substituent preferences in cyclohexanes

- Drawing substituted cyclohexanes
- Predicting the most stable conformation of substituted cyclohexanes

In preparation you should review the following concepts and terms from 1st year chemistry, 351 lectures and / or tutorial materials:

- Newman projections; eclipsed/staggered, anti/gauche etc.,
- conventions used in the two-dimensional representation of molecules and add that all important third dimension.
- interpretation of potential energy diagrams
- definitions of the terminology of conformational analysis (esp. strains)