Shape-shifting Molecules: The Search for Low Cost, Ring-shaped Drugs

The shape of a drug will determine how it interacts in the body. For it to work, it must dissolve, be absorbed into the bloodstream, avoid breakdown, enter the cell and bind to its target. Each of these steps likely requires a different shape. The pharmaceutical industry has historically only focused on the shape required to bind the target. This research has identified molecules that can readily adopt multiple shapes. These ring-shaped molecules (called macrocycles) represent a new model for drug design. Usual drugs (ie ibuprofen) are small and interact with a specific target to stop a chemical reaction. Macrocycles can work by an additional mechanism. They are larger and can interfere with interactions between proteins but are still small enough to travel the body. The preparation of these macrocycles is inexpensive and quick, properties that are important for the pharmaceutical industry. This poster describes the design and synthesis of a macrocycle and an analysis of the shapes that it adopts.