

Nature has an amazing ability to create a huge number of interesting and complex molecules. Among such works of creation are terpenes—unique kinds of compounds that are made by many plants and often possess important biological activities with the potential to have a great influence on health and well-being, such as their ability to kill unwanted bacteria, to reduce inflammation in the body, or even to work to inhibit the formation of cancer. One such terpene that is of particular interest is borneol, a small but significant molecule present in many essential oils. Why borneol is of specific interest is that it exists in four forms known as stereoisomers, each of which can have different behaviors and interactions within biological systems, exerting different types of effects on health and physiology.

The main objective of this project is to gain a detailed understanding of the complex interactions between four different forms of borneol and cyclodextrins, naturally occurring substances composed of glucose molecules linked together in a truncated cone shape. Cyclodextrins have a special characteristic of "hosting" or trapping other molecules within their central cavities similar to a glove receiving a hand inside it. Such molecules are already being used in a wide range of industries like medicine, cosmetics, and food in an attempt to significantly enhance the solubility, stability, and effective delivery of active ingredients and hence enhancing their overall efficacy.

To thoroughly investigate these fascinating interactions, I will be employing the technique of NMR spectroscopy, a highly sophisticated and powerful analytical instrument that enables us to take a close look at the behavior of molecules and their movement in various solutions. My experiment will involve quantifying the strength of the binding interactions of borneol with several types of cyclodextrins and also determine the rate at which these particular molecules bind to each other. Given that cyclodextrins possess the remarkable ability of distinguishing between different stereoisomers, I will also conduct an in-depth study to ascertain whether some forms or variants of borneol exhibit a greater degree of selective binding compared to others.

In addition to experiments, I will use computer modeling to calculate the 3D structures of borneols and simulate how they are included in the cyclodextrins (molecular docking). The simulations will complement the experimental results and give a better picture of how the complexes are formed.

This is an important project that elegantly combines state-of-the-art experimental techniques with cutting-edge computational techniques in a bid to create an improved understanding of the way that plant-derived molecules interact when they are in the proximity of natural sugar hosts. The data that is generated from this work has the potential to assist and ease the creation of far more effective systems for drug delivery, or they might even assist in the development of new materials.