CALIFORNIA STATE SCIENCE FAIR
2015 PROJECT SUMMARY

Name(s)

Rochelle Ellison; Bernard Moon

Project Number

35814

Project Title

The Effect of Various Human Body Conditions on the Racemization of Doxylamine Succinate

Abstract

Objectives/Goals

The objective of this project was to demonstrate the racemization of Doxylamine Succinate, an active ingredient of NyQuil, when exposed to simulated human body conditions including body temperature, liver enzymatic action and stomach pH.

Methods/Materials

Aliquots of Vicks NyQuil Cough Syrup were incubated for 48 hours at 37.5°C with: no treatment, mouse liver extract, or 3.0M HCl (pH 1.5). These samples, controls, and doxylamine succinate standards were prepared in 100% ethanol. Samples were analyzed by High Performance Liquid Chromatography with a Chiralcel OX-RH column to separate the enantiomers of doxylamine succinate. A mobile phase of 10:90 (v/v) 100% isopropanol and hexane with 0.1% Diethanolamine was used at a flow rate of 1 mL min-1. The eluent was monitored at 258 ± 4 nm and run for 15 minutes. Chromatograms and 3D spectra were used to analyze the enantiomers based on retention time and peak area.

Results

NyQuil (no treatment) presented the enantiomer S(+). Nyquil incubated at 37.5°C or in presence of mouse liver enzymes for 48 hours showed no racemization. However, it racemized when incubated in the presence of 3.0M HCl. 42.9 % of the R(-) and 57.1% of S(+) were found in the 2 peaks that corresponded to each enantiomers (appropriate retention time and wavelength absorption when compared to doxylamine succinate enantiomers retention time). Enantiomeric excess after exposure to HCl was calculated to be 14.2%.

Conclusions/Discussion

This experiment showed that prior to consumption the active enantiomer, S(+) doxylamine succinate, is present in NyQuil. However, a racemic mixture was created as a result of exposure to simulated stomach acidity. This may have occurred due to reactions between the acids H+ ions, which dissociate in solution, and unstable chiral center of NyQuil. The molecular bonds of the doxylamine succinate break and when reformed both enantiomers were produced. Yet in conflict with our hypothesis were results that demonstrated that human body temperature and mouse liver enzymes did not cause racemization. Nevertheless since the NyQuil must pass through the stomach during the digestion process, it is exposed to this acidic pH and racemization likely occurs. The presence of the R(-) enantiomer could make NyQuil either less active than intended or toxic. Further work conducted will examine the effect of each enantiomer on living organisms.

Summary Statement

This project analyzes the degree of racemization of doxylamine succinate, an active ingredient in NyQuil Cough Suppressant, when exposed to various simulated human body conditions.

Help Received

Research was conducted in high school laboratory supervised by Dr. Nikki Malhotra; HPLC chiral column was donated by Amgen Inc; Doxylamine Succinate standard was given by Thermo Fisher Scientific.