

Identifying Antibiotic Molecules in *Ceanothus leucodermis* and Quantifying Their Antibacterial Activity with a Novel, Simulation-Aided Method

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Antibiotic-resistant bacteria have rendered many modern antibiotics ineffective. Plants, however, have traditionally provided many natural medicines. In a previous project, I discovered that the Native American herb Ishwish (*Ceanothus leucodermis*) showed antibacterial properties. This year, I purified and identified the antibiotics in Ishwish and quantified their antibacterial strength using a novel, simulation-aided method. To determine the optimal method to extract molecules from plant mass, I created several liquid extracts under varying conditions. Antibacterial strength was tested using disk diffusion assays, and an ethanolic extraction of Ishwish stems was found to be the most effective. I purified this extract with C8 and silica gel chromatography columns and evaluated the effectiveness of my purification by using a low-resource method that I developed. My method combines disk diffusion assay data with a diffusion simulation that I wrote in Python. This allowed me to find the MICs (Minimum Inhibitory Concentrations) of my active fractions despite the small amounts available. The purification was found to be successful. Finally, I applied my most purified fractions to LC-MS analysis to identify the antibacterial compounds. After comparing my LC-MS data to molecular data in the database METLIN, I determined that the active compounds were polymers of the antibiotic catechin. I successfully purified and identified the antibiotics in Ishwish and demonstrated a real-life application of my computer simulation to determine MICs. This project provides a scientific basis for the Native Americans' use of Ishwish, and the strategies developed here can be applied to examine other Native American herbs while using limited amounts of plant material.

Awards Won:

Second Award of \$1,500