



CALIFORNIA STATE SCIENCE FAIR  
2013 PROJECT SUMMARY

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<b>Project Title</b> Achiral GC Analysis Using Alpha- and Beta-cyclodextrins as Chiral Selectors to Separate Diastereomers of Cypermethrin	
<b>Objectives/Goals</b> Cypermethrin is a highly chiral synthetic pyrethroid pesticide. Despite having desired insecticidal effects, it is harmful to the environment because certain stereoisomers induce sharp levels of toxicity in aquatic wildlife and cause hyperactivity in voltage-sensitive sodium channels in the animal nervous system. In this study, cypermethrin was used in spiked water samples to determine whether chiral selectors, alpha- and beta-cyclodextrin would assist in isolation of insecticidal cis-cypermethrin diastereomers to prevent this environmental stress. Because of its larger cavity, beta-cyclodextrin should show greater resolution.	
<b>Abstract</b> Cypermethrin is a highly chiral synthetic pyrethroid pesticide. Despite having desired insecticidal effects, it is harmful to the environment because certain stereoisomers induce sharp levels of toxicity in aquatic wildlife and cause hyperactivity in voltage-sensitive sodium channels in the animal nervous system. In this study, cypermethrin was used in spiked water samples to determine whether chiral selectors, alpha- and beta-cyclodextrin would assist in isolation of insecticidal cis-cypermethrin diastereomers to prevent this environmental stress. Because of its larger cavity, beta-cyclodextrin should show greater resolution.	
<b>Methods/Materials</b> Emulsifiable CP-concentrate (100 mg) was immersed in 100 mL hexane/acetone (1:1 v/v) stock solution with cyclodextrin to create spiked solutions with 1:1 guest-to-host molar ratios. Magnetic stirrers mechanically included analyte in cyclodextrin buckets; the hydrophobic guest binds to CD's chiral cavity through lateral interactions with hydroxyl groups. Unselected isomer formed in top layer, selected in the bottom, which was extracted using hexane/acetone to "pull" analyte from cavity. Using Thermo-Fisher's TR-5MS, each sample was injected in Autosystem XL GC at 2 microliters for 50 min at 260 C inlet temperature and FID detector at 290 C.	
<b>Results</b> Four peaks were resolved at the baseline with retention times similar to those in previous research journals. Two peaks represented two cis-diastereomer pairs, while two peaks represented two trans-diastereomer pairs. In cross-comparison with samples, little visible effect of cyclodextrin-assisted separation occurred. However, elution order marked visible separation of diastereomers.	
<b>Conclusions/Discussion</b> Chemical reasoning seems to show that the H on the cyano-carbon H-bonded with carbonyl oxygen at one chiral center which created a 5-member ring structure reducing rotatability of the cyanocarbon. Rigidity increased, decreasing vapor pressure as retention time increases, such that molecules with greater linear stability adsorb onto stationary phase due to stronger IMFs while other more volatile diastereomers pass through mobile phase. Modifications with procedure like increasing host to guest ratio, using stronger non-polar extraction solvent like ethyl acetate, concentrating solution to near dryness, will help for future experimentation to ensure cyclodextrin participation in chiral separation.	
<b>Summary Statement</b> With the intent of creating more potent and less toxic pesticide, cis-cypermethrin diastereomers with insecticidal properties were separated from environmentally harmful trans-cypermethrin using different cyclodextrins as chiral selectors.	
<b>Help Received</b> Used Autosystem XL Gas Chromatograph and TR-5MS Column at Thermo-Fisher Inc. under the supervision of Mr. Jinhua Chen and Dr. Chris Pohl	