|  |  |  |
| --- | --- | --- |
| **Student** | **Advisor** | **Poster Title, Abstract & Student Bio** |
| Benjamin Stone | Dr. Erik Sapper | Title: Developing Quantitative Structure-Activity Relationships for Antimicrobial Polymers used in Coatings Applications  Abstract: Computational models that relate chemical and structural features of materials to their performance properties have been used to aide in the discovery of active small molecules for many decades. These quantitative structure-activity relationship (QSAR) models are also important for predicting the activity of molecules that can have a range of effectiveness in biological systems. To date, however, little work has been done in the area of developing QSAR models for polymeric systems, where many traditional small-molecule descriptors do not readily translate to macromolecular length scales. This study attempts to use QSAR descriptors and machine learning techniques to predict and assess the performance of several different antimicrobial compounds which have been embedded into the covalent structure of a traditional coating resin polymer. Using this predictive data, QSAR models will then be applied to co-polymeric systems, in order to obtain structural knowledge enabling the future development of antimicrobial polymers. Results from early benchmarking studies against known biocides will be presented, along with the results from initial studies applying small-molecule QSAR methods to polymers and organic coating systems.  Bio: Benjamin Stone is a senior studying Biochemistry. He graduated from Wilson High School, Long Beach CA in 2013.  A major accomplishment is having the opportunity to study and do research at Cal Poly. His hobbies include hiking and camping. |