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Molecular Hospitality: The Interactions of Brooker's Merocyanine with Modified Cyclodextrins

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The binding of a guest molecule to a host system occurs through weak molecular interactions instead of through the formation of chemical bonds. The relative strength of these interactions can be understood by comparing the binding constant in related host-guest systems. B-cyclodextrin (β-CD) is a seven-membered ring of glucose units which was used as the host molecule due to its basket-like shape. This shape allows Brooker's merocyanine (BM), a highly conjugated guest molecule that is sensitive to its environment, to enter the cavity and interact with substituents located along the primary and secondary rims of the CD. This project measured the changes in the equilibrium binding constant due to different modifications to the CD, as well as the isomerization of BM within the cavity using UV-Vis and fluorescence spectroscopy. Binding constants were determined for different CD modifications, including β-CD, hydroxypropyl-β-CD, hydroxyethyl-β-CD, and sulfated β-CD (sodium salt). The largest effect of these substituents was the hindrance of the binding by the sulfate groups due to either steric effects or ionic interactions. A better understanding of these factors that affect binding and how molecules behave within the cavity will allow for more accurate predictions of their behavior under different conditions.

Information about the Authors:
Ben Averill is a senior chemistry major planning on attending graduate school to pursue a doctorate in food chemistry. He has worked on this project since September 2012. This topic allows him to focus on analytical chemistry, the area in which he plans on focusing in graduate school. Apart from research and classes, Ben is also involved in VU Science Olympiad, Chemistry Club, Luce Band, Phi Lambda Upsilon, and Gamma Theta Upsilon. Kelsey Larson is a junior chemistry/physics double major and is drawn to projects that overlap the two fields. This project is a way to explore molecular dynamics from both an Experimental and First Principles method that will be incredibly useful for future graduate studies.

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