Classical and Quantum Mechanical Study of Binol-based Receptors for Discrimination of Carboxylic Acids

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Synthetic Binol-based receptors have been designed to selectively bind and fluorometrically discriminate between several di- and tricarboxylic acids. The detection of di- and tricarboxylic acids is important due to the role they play in several metabolic pathways. Classical and quantum mechanical methods have been implemented to determine the conformational and spectrochemical behavior of the receptors as they interact with the guests. The lowest energy modes of receptor- guest binding were determined and analysis of the low energy ensembles found that the receptors are capable of orienting themselves in several different ways so as to facilitate optimal binding with the guests. Regardless of guest size the receptors were able to encompass and bind with the guest. Experimental results indicated that receptor fluorescence increases or decreases depending on the interacting guest. This is believed to be the result of conformational changes upon guest complexation that result in changes in π-π interactions between the receptor. Increased π-π interactions result in quenching of fluorescence while decrease in π-π interactions result in greater fluorescence.