UNIVERSITY OF RHODE ISLAND
Department of Chemistry
CHM644
SEMINAR

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URI

"Design, Synthesis and Evaluation of Dissymmetric Macrocycles for Benzo[a]pyrene Detection"

HOST

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Since 1987, synthetic macrocycles have gained much attention in supramolecular chemistry, especially for their use in the extraction and/or detection of specific guests. The binding of a guest within the host leads to the formation of a host-guest complex. These host-guest complexes are governed by a variety of non-covalent interactions such as π-π stacking, electrostatic, Van der Waals forces, and hydrophobic interactions. Herein we report the rational design and synthesis of a series of dissymmetric organic macrocycles as hosts for the evaluation of binding and detection of carcinogenic polycyclic aromatic hydrocarbons including benzo[*a*]pyrene. Benzo[*a*]pyrene is the one of the most carcinogenic, mutagenic and teratogenic polycyclic aromatic hydrocarbon, and persists in the environment ubiquitously.

Current detection methods involve tedious procedures and require multiple instruments for analysis. Hence, there is a need to find more efficient detection methods for this carcinogenic benzo[*a*]pyrene. The synthesized macrocycle hosts were evaluated for the efficient binding of benzo[*a*]pyrene and a high quantum yield fluorophore in the cavity of the macrocycle to generate ternary complexes. Proximity-induced energy transfer from the benzo[*a*]pyrene to a fluorophore resulted in a bright, turn-on fluorescence signal that can be used for benzo[*a*]pyrene detection. These complex systems also provided key information about the intermolecular interactions that are required for efficient energy transfer to occur, including hydrophobic binding and π-π stacking. While synthesizing these macrocycles, we explored the development of new organic reactions such as green bromination of benzylic alcohols to their benzylic bromides, to optimize and complete the macrocyclization reaction and minimize the generation of environmentally toxic waste products. We have also explored highly efficient and sensitive detection methods for cesium metal ions in aqueous media and hydrogen peroxide, both in solution and vapor phase, via fluorescence quenching.