

The Department of Chemistry Presents:

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Title: Molecular Baskets as Abiotic Sequesters of Toxic Drugs

Molecular baskets with amino acids at their rim (Figure 1) are cup-shaped molecules capable of forming inclusion complexes with a variety of complementary guests^{1,2} in water. As an example, baskets holding anticancer drug mitoxantrone³ and stimulant ephedrine⁴ via p-p, C-H...p and hydrogen bonding contacts are shown in Figure 1. Our most recent computational and experimental efforts center on developing baskets capable of including toxic anticancer methotrexate⁵ and synthetic opioid fentanyl in their binding pockets. My lecture will describe discoveries related to the preparation of such hosts and the role of noncovalent interactions and hydrophobic effect for their assembly/recognition characteristics in abiotic and biotic environments.

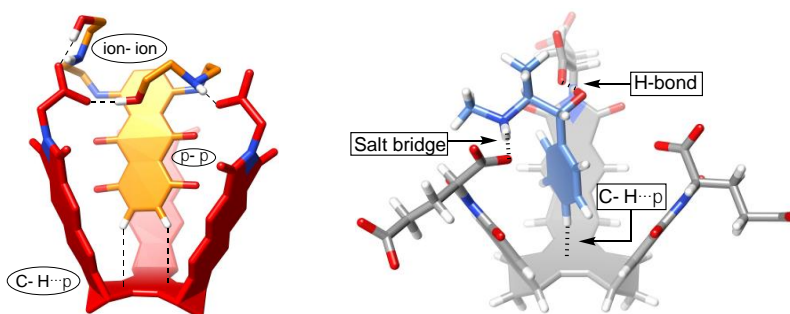


Figure 1. Stick representations of inclusion complexes of molecular baskets with anticancer drug mitoxantrone (left) and (1*R*, 2*S*)-ephedrine (right).

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