



Design of Small Molecule and Polymer-Based Receptors for Removal of Pharmaceutical Contaminants

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Abstract

Pharmaceuticals and personal care products are widely available and utilized daily throughout the world. Some of these medications are incompletely metabolized in the body and excreted as waste, while unused medications are often improperly disposed by consumers. The usage of these products has resulted in pharmaceuticals and other products entering the water supply, and we currently lack effective methods to remove them.

While many pharmaceutical compounds are well-studied, some are underexplored and minimal structural information or intermolecular bonding behavior studies have been conducted. We hypothesized that characterization of intermolecular bonding behavior between a contaminant and receptor in the crystalline state could provide a pathway for determining what types of functional groups to incorporate into a material (i.e. polymer) for removing contaminants. We, thus, investigated the chemical bonding behavior of some pharmaceutical contaminants in the presence of potential receptor molecules. The pharmaceuticals are in the anti-inflammatory or anti-cholesterol classes, namely naproxen (Figure 1), mefenamic acid, and bezafibrate. Here, we discuss co-crystallization of these pharmaceuticals, synthesis of polymer materials, and solution-state binding studies involving receptor candidates.

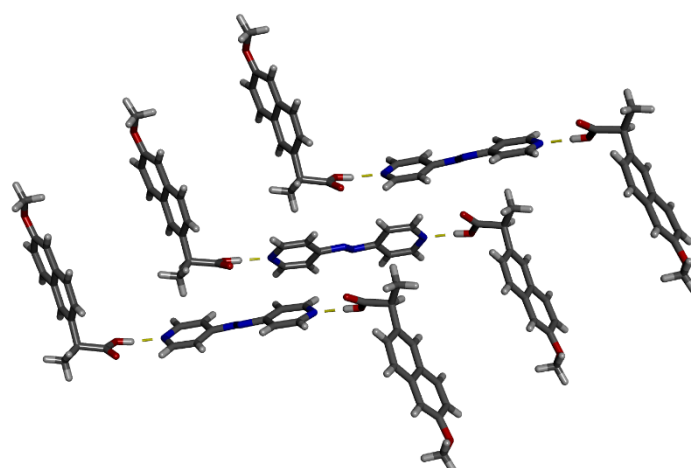


Figure 1: X-ray crystal structure of naproxen·4,4'-azopyridine.

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