

Supramolecular assembly in designing co-crystals of fumaric acid and pyrimidine/picolinate derivatives

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ABSTRACT

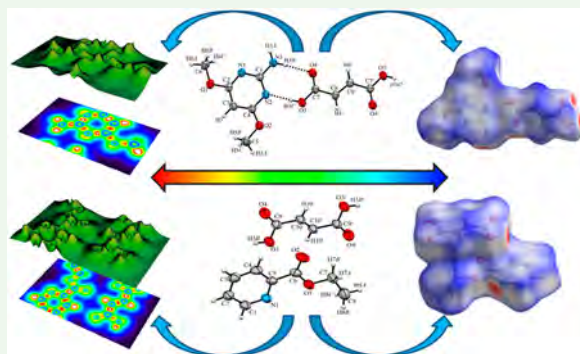
Two co-crystals possessing fumaric acid and 2-amino-4,6-dimethoxypyrimidine (**1**) and fumaric acid and ethyl 2-picolinate (**2**) were prepared. The structure of both compounds was determined using single-crystal X-ray crystallography. The asymmetric unit of cocrystal **1** formed in a triclinic system with space group *P*-1 consists of one 2-amino-4,6-dimethoxypyrimidine and one half of fumarate, whereas cocrystal of **2** formed in a monoclinic system with space group *P*₂₁/*c* consists of an ethyl-2-picolinate and a half of fumarate. Co-crystal **1** exhibits intramolecular O–H...N and N–H...O hydrogen bonds as well as intermolecular N–H...O hydrogen bonds, whereas co-crystal **2** exhibits intermolecular C–H...O and O–H...N hydrogen bonds as well as weak π ... π stacking interactions. Intermolecular interactions were investigated using Hirshfeld surface analyses. H...H (40.9%), O...H (32.9%), and C...H (8.2%) are the major interactions in **1** and H...H (41.6%), O...H (34.8%), and C...H (8.5%) are the most common in **2**. Furthermore, density functional theory (DFT) was used to investigate the structural features of the molecules using the B3LYP-D3/6-311G(d,p) basis set. Molecular electrostatic potential (MEP) surface and global reactivity descriptors for molecules were determined to explain the reactivity of molecular behavior, structural activity, and hydrogen bonds.

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Synthesis; Supramolecular assembly; single crystal; DFT; Hirshfeld surface analyses



Introduction

Crystal engineering, which is the application of the concepts of supramolecular chemistry to the solid state with the assumption that crystalline solids are in fact self-assembling systems, provides an excellent opportunity for studying and comprehending the hierarchy of intermolecular interactions between the various functional groups in order to construct new solid-state structures with desired physical and chemical characteristics (1–4). Over the years, organic

supramolecular frameworks have attracted a lot of interest in supramolecular chemistry because of their ability to use hydrogen bonds (H-bonds) as a prominent driving force (1–5). Research on organic entities based on supramolecular synthons is rapidly progressing using crystal engineering techniques (6,7). Hydrogen bonds, halogen bonds, and stacking interactions have been used extensively in the construction of these synthons, with hydrogen bonding being the most common due to its strength, directionality, and

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