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Study of self-assembly features in 4H-pyrans: Synthesis, Hirshfeld surface, and energy framework analysis

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ABSTRACT

In this study, the 4H-pyran derivatives were synthesized and crystallized, and their structures were established by the single-crystal x-ray diffraction method. The importance of noncovalent interactions in the supramolecular framework of the 4H-pyrans was investigated and demonstrated. The supramolecular framework analysis showed that 4H-pyrans expand their network in crystal packing mainly by N–H···N, N–H···O, C–H···N, C–H···O hydrogen bonds, and C–H···π interactions. The energy framework calculations showed the high contribution of electrostatic energy for the molecular pairs connected by N–H···N interactions. Further, the molecular docking study was performed to study the noncovalent interactions between the 4H-pyran derivatives and the beta-adrenoreceptors (β1-AR and β2-AR). This gave insights about the antagonistic property of 4H-pyrans as anti-ischemic agents.

1. Introduction

The study and understanding of noncovalent interactions are crucial in the field of supramolecular chemistry and crystal engineering to generate robust and novel three-dimensional structures with desirable properties [1–6]. The study of noncovalent interactions is also important for understanding the molecular recognition processes in biological systems [7,8]. Moreover, in the field of medicinal chemistry, designing and developing novel drugs requires a thorough understanding of their nature of noncovalent interactions with biological targets [9–11]. Although noncovalent interactions are generally weak, they act as cohesive forces for the association of drugs with the proteins. It is also responsible for forming solid-state materials [12,13].

4H-pyran is a class of six-membered oxygen-containing heterocycles with diverse biological properties. Since the 4H-pyran core is found in many natural products and has several pharmacological properties, the synthesis and study of 4H-pyran derivatives have caught the interest of many chemists [14]. The pharmacological properties of 4H-pyran derivatives include anticancer [15–17], antimicrobial [18,19], anti-HIV [20], antimalarial [21], anti-inflammatory [22], anti-diabetic [23,24], antianaphylactic, anticoagulants, spasmolytic, anti-leukemic and anti-Alzheimer activities [25,26]. Moreover, the application of 4H-pyran derivatives includes its usage as photoactive materials, laser dyes, optical brighteners, cosmetics, and biodegradable agrochemicals [27–30]. Further, 4H-Pyran derivatives such as cyano(ethoxycarbonyl)methylene-4H-pyran and dicyanomethylene-4H-pyran derivatives have been reported to be useful entities for developing donor-π-acceptor (D-π-A) fluorescent materials [31].

Therefore, due to their structural importance and varied applications, we have synthesized 4H-pyran derivatives, and their structures have been characterized using SC-XRD. Further, their supramolecular framework has been analyzed, studied, and reported. The molecular docking study has also been incorporated to study and predict the biological relevance of the synthesized 4H-pyrans.

1.1. X-ray crystallography investigation

The suitable single crystals of compounds **1**-**5** formed by the slow evaporation of ethanol solvent are collected and then subjected to SC-XRD analysis. The molecular structures of compounds **1**-**5** are presented in ellipsoid-style at 40% probability in Fig. 1, and crystallography details are given in Table 1. The geometrical parameters of **1**-**5** are given in Table S1-S3. Compounds **1 & 4**

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