Crystal engineering of the seventh polymorph of Gallic acid monohydrate: A structural comparative study with previous polymorphs

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Gallic acid (GA) (3,4,5-trihydroxybenzoic acid) is one of the abundant, therapeutic and bioactive phenolic compounds found in Choerospondiatis fructus, a Mongolian medicinal plant, used to treat some diseases, particularly myocardial infarction and angina pectoris. Gallic acid is an active pharmaceutical element (API) containing two of API's most omnipresent functional groups: phenols and carboxylic acids. According to US FDA Gallic acid is a GRAS molecule that exhibits anticholesterol, antitubercular, antifungal, antibacterial, antiviral, antiobesity, antitumor, immunomodulatory activities [1]. It also displays antimicrobial, anticancer and antioxidant properties [2]. Gallic acid has three hydroxyl groups which can act as both donors and acceptors of hydrogen bonds. The O-H carboxy hydrogen atom has a strong hydrogen bonding donor property and the C=O moiety of acid function has a strong hydrogen bonding acceptor property. Moreover, GA has many possible conformers depending on the orientations of its three OH and COOH groups. Thus, all these characteristics and properties of GA allow for exhibiting polymorphism and pseudopolymorphism [3].

In the present study, the low-temperature structural properties of the seventh polymorph of Gallic acid monohydrate (GAM-VII) are discussed and compared with those of the six polymorphs reported previously. Further, Hirshfeld surface analysis was extensively carried out for the seven polymorphs to understand the various intermolecular interactions. Moreover, to learn more about the stacking modes’ effect on molecular properties in GAM polymorphs, we employed computational quantum chemistry approaches.

Figure 1. The asymmetric unit of GA-VII with displacement ellipsoids shown at the 50% probability level.