**SPECTROSCOPIC AND DFT STUDIES ON CRYSTALLINE**

**3,4',5-TRIHYDROXYSTILBENE – PLANT ANTIBIOTIC**

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3,4',5-Trihydroxystilbene is phytoalexin generated by plants i.a. peanuts, berries, most notably in the skin of red grapes [1]. The title compound exists as *cis*- and *trans*-isomers, which may have different biological effects. *Trans-*isomer is characterized by multi-faceted potential to act as: anticarcinogenic, antioxidant, anti-inflammatory as well as anti-estrogenic agent. It is also archetype innovation in arena of anti-ageing therapy [2], and play a crucial protective role in disorders neurodegeneration in aging-related dysfunctions like Alzheimer's or Parkinson's diseases [3]. Another data indicate that 3,4',5-trihydroxystilbene is a PAH antagonist, which can inhibit the proliferation of carcinogens through its interaction with the cytochrome P450 enzyme system [4]. While, physiological activity of *cis*-isomer concerns to inhibit kinase activity, a factor related to cancer [5, 6]. It also shows anti-aggregation properties [7].

Herein, we present the spectroscopic investigations combined with the DFT quantum chemical calculations. FT-IR spectroscopy has been used as a way to study the nature of HBs in the 3,4',5-trihydroxystilbene. Theoretical calculations were carried out with the Gaussian 09 software package using DFT at the B3LYP level and with 6-311++G(d,p) basis set (all computations have been carried out in gas phase). To discussion of the intermolecular interactions in a molecular crystals of 3,4',5-trihydroxystilbene have also been used Hirshfeld Surfaces technique (HS), which is based on the calculation of the promolecular electron density both crystal and in gas phase. To obtain the fingerprint plots the CrystalExplorer program has been used. The fingerprint plots are generated based on the *de* and *di* distances, the distance from the HS to the nearest nucleus outside and inside the surface, respectively. The 2-D fingerprint plots have been also used for visualizing, exploring and quantifying intermolecular interactions. It has been shown that the major intermolecular interactions, i.e. O-H…O hydrogen bonds, stabilize the crystal structure of 3,4',5-trihydroxystilbene. Here, the difference in molecular behavior of two isomers of 3,4',5-trihydroxystilbene has been also discussed. Finally, it was shown that the frequencies are in good agreement with the calculated values, and the analysis of the Hirshfeld surface is well correlated to the spectroscopic studies.

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