

MS36-P6 The intramolecular hydrogen bond analysis in biologically active 5-fluoro-1*h*-indole-2,3-dione-3-thiosemicarbazones derivatives by experimental and theoretical methods

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There are several reports on the anticancer, antiviral and antibacterial activities of isatin-3-thiosemicarbazone derivatives (1-5). Investigations regarding the structure-activity relationships of 2-indolinones revealed that 5-halojenation and 3-thiosemicarbazone formations were efficient in increasing activity against a range of human cancer cells and various bacteria and viruses (3-8). In the light of these findings, 5-fluoro-1*H*-indole-2,3-dione 3-thiosemicarbazone derivatives were synthesized by reaction of *N*-substituted thiosemicarbazids with 5-fluoro-1*H*-indole-2,3-dione and evaluated for in vitro antituberculosis activity against *Mycobacterium tuberculosis* H37Rv. Their structures were confirmed by the spectral data elemental analysis and three of them were analysed by X-ray diffraction method. Due to playing a central role in the molecular structure and interactions of biologically molecules, the intramolecular hydrogen bonds (IHBs) were also calculated at the DFT level. Natural bond orbitals (NBO) calculations were used to examine the electronic characteristics of the intra-molecular hydrogen bonds. Experimental X-ray and NMR data were correlated with theoretical results. NBO energies show that the main contributions to energy stabilization correspond to LP → σ^* interactions for IHBs, O1...N3-H3 and N2...N4-H4; the delocalization LP → π^* for N₃-N₂=C₂ and N₃-C₉=S₁.

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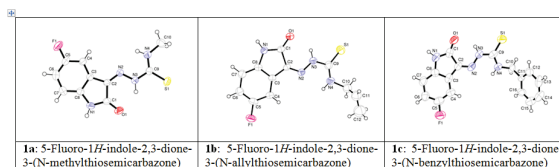


Figure 1. X-Ray Structures of 1a, 1b and 1c.

Keywords: 5-fluoro-1*H*-indole-2,3-dione, thiosemicarbazone, intramolecular hydrogen bonds, DFT, NBO