

Solution State Structure of Methoxysalicylaldehyde Thiosemicarbazone Derivatives by NMR and DFT Methods

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Salicylaldehyde thiosemicarbazones and their metal complexes belong to an important class of biologically active compounds (anticancer, antiviral, antibacterial, antiinflammatory and antifungal activity) [1]. They can exist in several tautomeric forms (hydroxy-thione, hydroxy-thiol, keto-thione and keto-thiol) with both intra- and intermolecular hydrogen bonds (Fig. 1). X-ray structural analysis has confirmed the existence of intramolecular hydrogen bonds in different salicylaldehyde thiosemicarbazone derivatives [2, 3]. Bioactivity is closely related to molecular structure which is governed by the presence of hydrogen bonds. Therefore, the aim of our study was to investigate the solvent influence on molecular conformation and structure of hydrogen bonds in methoxysalicylaldehyde thiosemicarbazones by combining NMR and DFT methods. Solvents of different polarities, *i. e.* of different proton donor and acceptor abilities were used (chloroform, acetone, methanol, dimethyl sulfoxide).

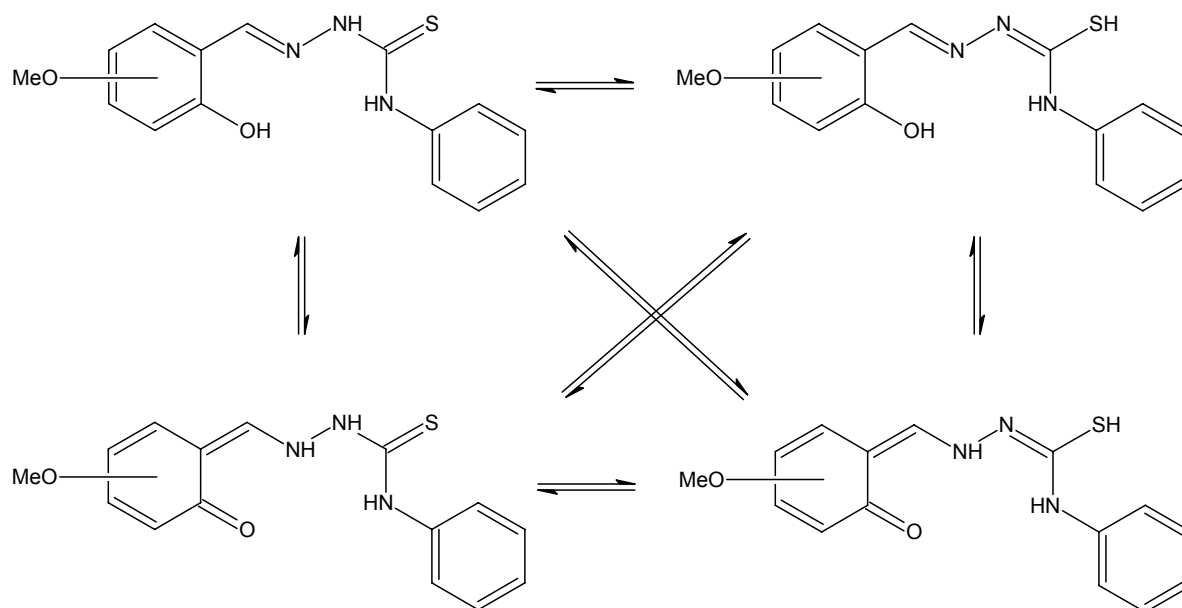


Fig. 1: Tautomerism in methoxysalicylaldehyde thiosemicarbazones.

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