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Study of the Intermolecular Interactions in the Biologically Relevant Thiosemicarbazones. Jesús Valdés-Martínez, Simón Hernández-Ortega, Inst. de Química, Univ. Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, 04510, Coyoacán, México, D.F. MEXICO, jvaldes@servidor.unam.mx.

A family of compounds with beneficial biological activity is the thiosemicarbazones; they have shown to have antitumor, antiviral and antimalarial activity. Thiosemicarbazones are very good ligands, and it has been shown that their biological activity is related to their ability to coordinate to metal centers in enzymes. One interesting thing is that the more pharmaceutically promising thiosemicarbazone possess an additional functional groups that is not coordinated to their “primary” metal ion, suggesting that the biological activity of thiosemicarbazones may also depend to the molecular recognition ability of the non-coordinating groups. To contribute not only to the understanding of the activity of thiosemicarbazones, but also to a better understanding of the intermolecular interaction of the relatively common small molecule compounds containing sulfur in biological system, in this paper we discuss our recent results in the supramolecular chemistry of thiosemicarbazones and related compounds.