

## CONFORMATIONAL ANALYSIS OF OMEPRAZOLE FAMILY COMPOUNDS

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Many problems in theoretical medicinal chemistry require previous conformational analysis before studying the properties of a given set of molecules. In this work, two sets of compounds with anti- *Helicobacter pylori* activity were studied: (a) omeprazole and its derivatives; (b) the sulfide precursor of omeprazole and analogues (2-[[[(2-Pyridyl)methyl]thio]-1H-benzimidazoles). Conformational analysis was performed according to the method proposed by Bruni et al [*J. Comp. Chem.* 2002; **23**: 222]. It was observed that small differences among the compounds inside each group provide important changes in the minimum energy structures. Comparisons between the two sets of compounds showed that the presence of a S=O group for omeprazole and its derivatives was responsible for significant differences from the respective precursor sulfide minimum energy structures. The most important conclusion is that the addition of each substituent prior to the complete conformational analysis calculations is crucial in these studies.