Conformational and Database Study on the Intramolcular N-H···π Interaction

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In the last years, much work has been devoted to studying systems characterised by the so-called weak interactions. Between them, the N-H···π interaction has been the subject of several theoretical [1], spectroscopic [2], and structural studies [3], and has been shown to take part in the folding of biological macromolecules [4], competing with the π…π stacking interactions. In particular, intramolecular X-H…π bond has been found to influence the conformation of compounds containing both X-H and aromatic groups [5], [6].

Considering that several organic compounds, functionalized by aminic and aromatic groups linked by an aliphatic chain, are the parent structure for a variety of biologically important compounds, like dopamine or adrenaline, and have therapeutic potential [7], [8], we have decided to carried out a structural study of the intramolcular N-H···π interaction.

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