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Structural Characterization of New Potential 5-HT_{1A} Receptor Ligands

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The discovery of new 5-HT_{1A} receptor ligands with high affinity and selectivity is an area of research in medicinal chemistry. Structural investigations of them are very important for the designing of new, effective and safe drugs. Long chain arylpiperazines with an amide or imide moiety represent one of the most important classes of the 5-HT_{1A} receptor ligands. They are regarded as potential drugs in the therapy of anxiety, depression, memory dysfunction and learning. The most frequently investigated member of them is buspirone.
As a part of our work on the development of novel piperazine derivatives with central nervous system activity, new analoques of buspirone have been obtained and their crystal and molecular structures have been determined by X-ray structure analysis.

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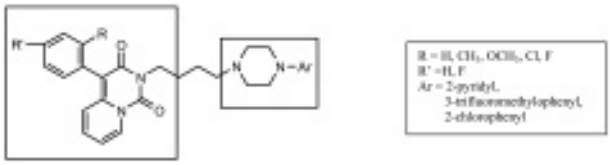

New 4-aryl-2H-pyrido[1,2-cπyrimidine-1,3-dione deriva-tives of arylpiperazine are expected to be pharmacologically active and structural characterization of them is necessary to determine the parameters important for ligand-receptor interactions. The results presented in this report concern the crystal and molecular structures of some of these derivatives.
Crystals were obtained in the Medical University of Warsaw.

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A Topological Analysis of the Intra/Intermolecular Interactions of 5-Methylbenzo-Phenanthrene

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The 5-methylbenzo-phenanthrene molecule consists of four fused aromatic rings that take up an α-helical staircase geometry. It is this geometry that brings two hydrogen atoms into close proximity too each other and allows for the possibility of an intramolecular H-H bond to be formed in the bay region of the molecule. There are a number of intermolecular interactions, such as C-H•••C and C-H•••H-C, involved in packing of this molecule in the crystalline state. These interactions all have the potential of being either hydrogen bonds, van der Waals interactions or H-H bonds. All this leads to a better understanding of the role these weak interactions play in the formation of small organic molecules.