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Experimental and Theoretical Studies on Conformations of Arylpiperazines with Pyrimido[5,4-c]quinolin-4(3H)-one Terminal.

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Arylpiperazine derivatives of cyclic amides and imides are big and intensively investigated group of serotonin receptor ligands. Our study concentrates on pyrimido[5,4-c]quinolin-4(3*H*)-ones connected with arylpiperazine via 2–4 carbon spacer developed as 5-HT_{1A} receptor agents. Conformational behavior of the investigated compounds was studied experimentally in solid state (crystallographic structure), and theoretically in vacuum and in solution (semi-empirical methods) as well as in the rhodopsin-based homology model of 5-HT_{1A} receptor.

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