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THE APPLICATION OF FMO-EDA CALCULATION TO STUDY THE SELECTIVITY OF 2-CHLOROPHENYL-PIPERAZIN DERIVATIVE TO SEROTONIN AND DOPAMINE RECEPTORS

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Long-chain arylpiperazines (LCAP) are one of the commonly studied class of bioactive compounds due to their potential therapeutic effects caused by interactions with different subtypes of serotonin receptors. A number of studies have been aimed at examining the impact of LCAP structure modifications on the affinity, selectivity and function at a given receptor protein.[1]

In this study the structure of 2-{6-[4-(2-chlorophenyl)piperazin-1-yl]hexyl}-2,3-dihydro-1H-isoindole-1,3-dione complexed with five receptors ($5\text{-}HT_{1A}R$, $5\text{-}HT_{2A}R$, $5\text{-}HT_6R$, $5\text{-}HT_7R$, D2R) has been investigated by means of quantum mechanical methods. At the beginning, the test compound was docked to receptors (homology models based on …) and next optimized with ONIOM method. For thus obtained structures FMO-EDA calculations were performed.

Results shed some lights on the interpretation of the experimental results concerning the affinity to receptors, as well as they provided the reasonable binding energies and binding patterns of ligand-protein interactions.

[1] P. Kowalski. et al., *Arch. Pharm. Chem. Life Sci*., **2013**, *346,* 339.