Med chem 2015, 5:10
http://dx.doi.org/10.4172/2161-0444.C1.016

Designing compounds with probable serotoninergic activity: *In silico* and *in vivo* evaluation over a stress model

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Both 5HT1A receptor and serotonin transporter SERT have an essential role in the homeostasis of serotonergic pathway. Deregulation of these proteins leads to complex mental disorders, making them an attractive pharmacological target for the development of new antipsychotics or antidepressive drugs. Therefore, elucidate essential interactions for ligand-receptor recognition and the discovery of compounds with affinity over them, is a topic of interest for pharmacology. In this study, we aim for the rational design of a novel series of isoindoline-based molecules with dual action over 5HT1A receptor and SERT. The *in silico* results suggest that our molecules share the binding mode with serotonin, fluoxetine and vilazodone, interacting with the aminoacid residues ASP116, ILE 113, CYS 187, SER 199 and TRP 35 for 5HT1A receptor, and with TYR95, ILE 172, TYR 176, SER 336, VAL 343 and THR 439 for SERT. Ligands MD20, MD22 and MD1 presents the highest affinity over both receptors; our molecules might be metabolized by CYP450 and they fulfill the Lipinski's rule of five. A newfangled route of synthesis for the designed molecules was completed with a novel reaction. *In vivo* open field test in CD1 mice with acute administration of ligand MD1 demonstrated that this molecule presents an interesting anxiogenic-like effect. We propose that the designed drugs are likely to interact with the studied receptors. Future experiments will be performed in order to determine *in vitro* and *in vivo* behavior of this molecules and their metabolites.

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Synthesis & anti-inflammatory screening of some novel 2-azetidinones/4-thiazolidinones bearing 1,3,4-thiadiazole nucleus

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The oxidative cyclization of thiosemicarbazone (I) was carried out using ferric chloride as an oxidative agent to get 2-amino-5-styryl-1,3,4-thiadiazole (II). 2-amino-5-styryl-1,3,4-thiadiazole (II) reacted with aromatic aldehydes in methanol to give the new product N-(4-sustituted)-5-styryl-1,3,4-thiadiazol-2-amine (IIIa-h). Compound (IIIa-h) reacted with chloroacetyl chloride in triethylamine to give 2-azetidinone derivatives bearing 1,3,4-thiadiazole nucleus (IVa-h). Compound (IIIa-h) on cyclo condensation with mercaptoacetic acid leads to the formation with 4-thiazolidinone derivatives bearing 1,3,4-thiadiazole ring (Va-h). Synthesis of all titled compounds were confirmed by melting point, IR, 1H-NMR and mass spectrum and evaluated for their anti-inflammatory activity. Out of the synthesized compound IVa and IVb were capable of showing very good anti-inflammatory activity almost on compared with that of the standard ibuprofen, followed by IVc while the rest of compounds were found to be mild in their potency.

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