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Design of new drugs: Challenges for the rational development of novel ligands with affinity for G-protein-coupled receptors

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G-protein-coupled receptors (GPCRs) are a heterogeneous group of proteins that form a physiological and pharmacological perspective results fascinating; their large number of functions and locations in vertebrates make them key pharmacological targets for the development of new drugs, emphasizing those that impact over public health problems in our environment. Within this group, we highlight those GPCRs that are regulated by neurotransmitters derived from amino acids: dopamine, noradrenaline and serotonin receptors are important in the epidemiological context of the country where our workgroup resides because they represent an option to treat diseases such as obesity, depression or Parkinson's disease. However, the phylogenetical similarity between them and the complexity to obtain new crystallized models of GPCRs, slow down the development of new drugs. To obtain highly potent or selective molecules, our workgroup uses an algorithm for pharmacological design that includes the use of computational tools that allows us to obtain the molecular homology model of the receptors and explore the amino acids that are important for its activation or inactivation, along with the calculation of basic pharmacological properties, as well as the evaluation of the docking among the designed ligands and receptors, evaluating the affinity between them, just to complete the experimental design with different *in vivo* and *in vitro* techniques, all with the aim of reduce the time of investigation and increase the possibility of develop useful drugs. Several examples of the application of this methodology with the attainment of successful results will be presented.

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