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In-silico and *in-vitro* evaluation of two series of isoindolines/ dioxoisoindolines derivated from phenylethylamine as inhibitors of cholinesterases

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Isoindolines and dioxoisoindolines are powerful groups of pharmacophores found in natural and non-natural products, with proven anticonvulsant, anti-inflammatory, analgesic, antihypertensive activity and antibacterial effects. In this research, two series of ligands derivated from isoindolines and dioxoisoindolines were proposed for the treatment of neurodegenerative diseases such as Alzheimer's disease. It was planned to design and synthesize both series of compounds as possible inhibitors of cholinesterases. It is proposed to determine the differences between both series of compounds: isoindolines and dioxoisoindolines. A computational study of interaction between both series of compounds with acetylcholinesterase and butyrylcholinesterase was carried out; as well as an in-vitro model to review the effectiveness and compare the activity of both families of ligands and their possible application in the treatment of Alzheimer's disease based on the cholinergic hypothesis. The inhibitors that act on the active center of the enzyme avoid the union of a substrate molecule or its hydrolysis by blocking the site by its high affinity and interacting in a reversible way with the serine, near the catalytic center; this will prevent the degradation of the neurotransmitter and increase its average life. As a result, it is a possible treatment of the pathology.

Biography

Omar Ruiz Maciel has completed his Bachelor´s Degree in Pharmacobiological Chemistry from the Michoacan University of San Nicolas de Hidalgo in Morelia, Michoacan, Mexico. He is currently completing his Master´s degree in Pharmacology with a focus on Alzheimer´s disease at the National Polytechnic Institute in Mexico City, Mexico.

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