

### ***In silico* and *in vivo* assays of a borinic DOPA-derivative for Parkinson disease**

Marvin A Soriano-Ursúa, Ana L Ocampo-Néstor, Antonio Abad-García and José G Trujillo-Ferrara

Instituto Politécnico Nacional, Mexico

The boron atom has some chemical properties which confer it advantages to be added in potential new drugs. One of these advantages has been inferred by *in silico* assays interaction on receptors or proteins with serine, threonine or tyrosine on the active site. In this sense, catecholamine receptors (belonging to the G-protein coupled receptors family) have a conserved binding site with three serine-residues involved in receptor activation. In this work, we tested the potential activity of 3-D models representing adducts of levodopa or dopamine on models of catecholamine human receptors (emphasis on beta-adrenoceptors and D2 and D3 receptors) by *in silico* docking analyses. Then, we synthesized and characterized a compound with potential activity on D2 receptor judged with the affinity score and binding mode on this receptor. Interestingly, the boron-containing compound contacts on the orthosteric site with higher affinity than Levodopa or dopamine, but its boron atom is not directed to serine residues in fifth transmembrane

domain. This compound is an adduct of levodopa and an aryl-diphenylborinic acid, which was tested in a C57/BL6-mice model of parkinsonism induced by peritoneal administration of MPTP (a well-known toxin on catecholaminergic system). The compound induced improved performance of administered mice on motor tests but several pharmacological tests are required to elucidate the putative mechanism of action.

#### **Speaker Biography**

Marvin A Soriano-Ursúa has completed his PhD from Escuela Superior de Medicina del Instituto Politécnico Nacional, México. He is a Member of the National System of Researchers, and he is Head of the Physiology Laboratory. He has focused on the rational drug design having boron-containing compounds as main moiety, as well as, the different effects of these compounds on human physiology, particularly on G-Protein coupled receptors. He has authored more than 35 publications that have been cited over 200 times, and he has been serving as an Editorial Board Member and Reviewer of repute scientific journals.

e: [soum13mx@gmail.com](mailto:soum13mx@gmail.com)

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