QSUN Quantum Research Group of Stellenbosch University

SA QuTI South African Quantum Technology Initiative

NITheCS National Institute for Theoretical and Computational Sciences

Stellenbosch University iYunivesithi Universiteit

SEMINAR

Ligand/Receptor Complexities and Molecular Vibrations: Insights from Nicotine and Cotinine in Flatworms

Prof Oné R. Pagán (West Chester University of Pennsylvania)

Friday, 7 June 2024 @ 14h00-15h00 SAST

Venue: Online and Physics Seminar Room, Stellenbosch University

ABSTRACT*

Molecular vibrations and quantum tunneling may affect how ligands (drugs) interact with pharmacological receptors. The well-established lock-and-key model explains how a drug binds to its receptor target in this context. Still, a general mechanism by which this binding translates to function is unclear in many cases. The Vibration Theory of Olfaction was proposed in the 1930s to explain receptor-mediated phenomena in the particular case of odorant recognition, modulated by metabotropic receptors. In the 1990s, Dr Luca Turin proposed inelastic electron tunneling as a mechanism to translate molecular vibration to odorant physiology. More recently, studies of ligands' vibrational spectra and deuterated ligand analogs, among other strategies, have provided helpful information about vibrational effects in receptors other than olfactory receptors. Based in part on published experiments from our laboratory using planarians as an experimental organism, I will present a rationale and possible experimental approach for extending this idea to another general class of receptors: the ligand-gated ion channels.

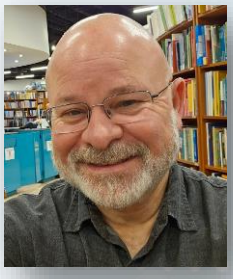
** Based on Pagán OR (2024) The complexities of ligand/receptor interactions: Exploring the role of molecular vibrations and quantum tunnelling. Bioessays. 46(5):e2300195. doi: 10.1002/bies.202300195.*

BIOGRAPHY

Dr Oné R. Pagán is an "accidental planarian biologist". He uses planarians (a type of flatworm) to explore neuropharmacology.

He earned his undergraduate degree (Natural Sciences) and his MS (Biochemistry) at the University of Puerto Rico, and his PhD (Pharmacology) from Cornell University. He is a Professor of Biology at West Chester University of Pennsylvania.

In addition to his teaching and research, he is also engaged in science communication and is a published author of academic and popular science books.



REGISTER: https://bit.ly/3V3JvG6