"MODELLING LIPID MEMBRANE AND MEMBRANE PROTEIN PROCESSES"

Dr. Juan José Nogueira

MoBioChem
Department of Chemistry,
Universidad Autónoma de Madrid,
Calle Francisco Tomás y Valiente, 7, Madrid, Spain
juan.nogueira@uam.es

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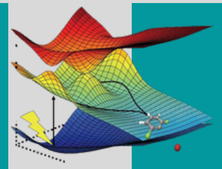
ORGANIZATION:
Prof. Dr. Antonio Carlos Borin
Instituto de Química, Universidade de São Paulo (USP), SP, Brazil

INFORMATION AND REGISTRATION:
ancborin@iq.usp.br

Registration: send a message to ancborin@iq.usp.br
with the words "Juan José Nogueira – Virtual" on the "subject"
Deadline: September 23, 2021 (Thursday), 06pm (BRT time)



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ABSTRACT

Modelling Lipid Membrane and Membrane Protein Processes

Juan J. Nogueira

Department of Chemistry, Universidad Autónoma de Madrid,
Calle Francisco Tomás y Valiente, 7, Madrid, Spain
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Lipid membranes and membrane proteins are key biological assemblies involved in many relevant functions, including cell protection, molecular transport, and signal transduction. A deep understanding of these biological processes can be achieved by means of computer simulations. However, the simulation of membrane processes is a very complex task which requires the combination of different quantum and classical mechanical techniques within a dynamic framework. In this talk, I will discuss about the simulation of two different membrane processes recently published by our group: the passive transport of the anticancer drug cisplatin through a model lipid bilayer (1,2) and the binding of photoswitches to a human voltage-gated ion channel (3).

(1) Lorena Ruano, Gustavo Cárdenas, and Juan J. Nogueira. ChemPhysChem, 2021, 22, 1-12.
(2) Gustavo Cardenas, Álvaro Pérez-Barcia, Marcos Mandado, and Juan J. Nogueira. PCCP, 2021. Advanced manuscript. DOI: 10.1039/D1CP03382D.
(3) Vito F. Palmisano, Carlos Gómez-Rodellar, Hannah Pollak, Gustavo Cárdenas, Ben Corry, Shirin Faraji, and Juan J. Nogueira. PCCP, 2020, 23, 3552-3564.