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Modelling Lipid Membrane and Membrane Protein Processes

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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**, *23*, 20533-20540.

(3) Vito F. Palmisano, Carlos Gómez-Rodellar, Hannah Pollak, Gustavo Cárdenas, Ben Corry, Shirin Faraji, and Juan J. Nogueira. *PCCP*, **2020**, *23*, 3552-3564.