

CiQUS Lecture

**Dr. Juan José Nogueira Pérez****Quantum and Classical Modelling of Biological Events**FONDO EUROPEO DE DESENVOLVIMENTO REGIONAL
PO FEDER Galicia 2014-202 - *Unha maneira de facer Europa***Thursday, January 25, 2024**
12:15 pm - CiQUS Seminar Room**Dr. Juan José Nogueira Pérez**
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Universidad Autónoma de Madrid<https://www.mobiochem.com/>**Abstract:**

The computational simulation of biological processes is a complex task which requires the combination of different quantum and classical mechanical approaches. Moreover, these hybrid calculations must often be performed within a dynamic framework to account for conformational sampling. In this contribution, the modeling of chemical and physical processes occurring in different biological media will be discussed, including the permeation of drugs across lipid membranes, charge transfer events on DNA, and the binding of photoswitches to membrane proteins, among others.