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Computational Ingredients to Model Biological Processes

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The computational simulation of biological processes is a complex task which requires the combination of different quantum and classical mechanical techniques. Moreover, these hybrid calculations are often performed within a dynamic framework to account for conformational sampling. In the case where the process under investigation takes place in a long-time scale, the application of enhanced sampling approaches may also be needed. In this contribution, the modeling of several physical processes occurring in different biological media will be discussed, including the permeation of drugs across lipid membranes [1], electron-transfer events on DNA strands in terms of reduction potentials [2], and the binding of photoswitches to ion channels [3].

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[2] Jesús Lucia Tamudo, Sergio Díaz-Tendero, and Juan J. Nogueira. Phys. Chem. Chem. Phys. 2023, 25, 14578.
[3] Vito F. Palmisano, Shirin Faraji, and Juan J. Nogueira. Phys. Chem. Chem. Phys. 2023, 25, 8331.

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