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Using Molecular Dynamics simulations and Quantum Mechanical calculations, we study the behavior of molecules with biophysical and pharmacological interest in solution and in phospholipid bilayer.

In this presentation, we will consider the interactions of a fluorescent probe, PRODAN, in several solvents and in DLPC bilayer and its polarization effect that causes an intramolecular charge transfer due to the environment [1]. Additionally, we will discuss the deprotonation/protonation process of the EMODIN in aqueous solution and in DMPC bilayer. This last molecule is a biologically active natural compound chemically classified as an anthraquinone derivative with a pKa value around 7 [2].

References:

[1] W. Nitschke, C. Vequi-Suplicy, K. Coutinho, H. Stassen, *J. Phys. Chem. B*, 116, 2713 (2012).

[2] A. R. Cunha, E. L. Duarte, M. T. Lamy, K. Coutinho, in preparation (2013).

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