Institut Européen de Chimie et Biologie

I E C B

Molecular simulations of lipid membranes.

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Biological membranes are heterogeneous assemblies of lipids and proteins with a complex lateral organization. In their physiologically relevant state, most biological membranes are highly fluid – which makes it difficult to characterize experimentally their structural properties with high resolution. Molecular simulations can provide structural and dynamic information on model membranes with atomic-level resolution, and therefore can aid in the interpretation of experiments, and sometimes even predict the outcome of experiments. During my presentation I will introduce some basic concepts on molecular simulations of lipid membranes, then I will describe two examples of how simulations can be used to predict and to interpret experiments. The first example will be about the lateral organization of ternary lipid mixtures, and the effect of hydrophobic pollutants on such organization. Simulations indicate that relatively small concentrations of hydrophobic pollutants can have a broad impact on membrane lateral organization, and suggest possible mechanisms for the biological activity of common hydrophobic compounds. The second example will deal with one fundamental property of lipid membranes: their capacity to dissolve apolar solutes. I will show how molecular simulations can be used to interpret the different solubility of C60 fullerene in alkanes *vs* lipid membranes.