Molecular dynamics simulations of a palmitoylated membrane protein

Molecular dynamics simulation of membrane protein – lipid interactions is one of our research themes. As a matter of fact, molecular dynamics simulation is a unique tool to get a detailed description (at atomic scale) of the interactions between lipids and proteins as experimental data remain difficult to obtain due to the dynamical properties of the membranes.

Some membrane proteins possess palmitoylation sites in their sequence. Palmitoylation is the covalent attachment of a 16-carbon fatty acid, palmitic acid, to cysteine and less frequently to serine and threonine residues of proteins. In the few case studies of membrane proteins, it was shown that the consequences of their palmitoylation are: altered protein conformation; association with specific membrane domains; controlled interactions with their partners; and interplay with other post-translational modifications. In fact, palmitoylation enhances the hydrophobicity of proteins which could impact its interaction with its partners (lipids and/or proteins) and itself.

During the internship, we propose to set up the molecular dynamics simulations to study the interactions of the single transmembrane helix protein with a bilayer composed of a mixture of lipids. Two systems will be studied including the protein with and without its palmitate anchor. The GROMACS program will be used with the all-atom amber force field. Deciphering the protein folding and interaction with membrane lipids would reveal the underlying information that would lead us to a better understanding of the structural role of palmitate anchors.

The internship will be performed at the I2BC (Institute for Integrative Biology of the Cell) of CEA at Saclay, Laboratory of Membrane Proteins and Membrane Systems (LPSM). Centre d'Etudes de Saclay, nearby Orsay/Gif-sur-Yvette, south of Paris.

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