Séminaire

CONFÉRENCIER INVITÉ

Vendredi 1er Septembre 2017 à 11h

Salle des séminaires

Institut de biologie structurale - 71 avenue des Martyrs CS 10090 38044 Grenoble Cedex 9 - T.+33 (0)4 57 42 85 00

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Lipid-protein interactions through a «computational microscope»: molecular simulation studies of complex biological membranes

Membrane proteins account for ca. 20% of all genes, 40% of drug targets, and are mutated in many human diseases. The past decade has witnessed an exponential rise in the number of high resolution membrane protein structures and recent developments in cryo-electron microscopy have accelerated the rate of structure determination. However, the structures do not often reveal interactions with lipid molecules present in their native membrane environments. Interactions with lipids are of crucial importance for the stability, regulation, and targeting of membrane proteins. Notably, specific lipid binding sites provide potential allosteric druggable targets, and thus these protein-lipid interactions are of immense biomedical importance. While advances in membrane lipidomics and mass spectrometry are beginning to uncover the diversity and importance of lipid/protein interactions, there is a paucity of detailed structural and biophysical/biochemical characterization of protein/lipid interactions for many families of membrane proteins. Molecular dynamics (MD) simulations provide a key tool for probing the interactions of lipids with membrane proteins. Recent advances in MD make reliable prediction and analysis of lipid interactions possible. Building upon our database of membrane proteins simulated in simple lipid bilayers, MemProtMD (http://memprotmd.bioch.ox.ac.uk), we are able to use 'computational biochemistry' to probe the strength and specificity of the interactions of lipids with key membrane proteins, including ion channels and GPCRs. Larger scale simulations allow us to address a number of aspects of the dynamic organization of lipids and proteins in models of bacterial, viral, and mammalian cell membranes.

Hôte : Eva Pebay-Peyroula (IBS/Membrane)