

Internal Webinar

Multiscale Modelling of Membrane Remodelling Proteins using Monte Carlo and Molecular Simulations

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Membrane remodelling is an essential process in cells that allows biological membranes to dynamically change their shape and organisation. These shape changes are crucial for many cellular functions, including the transport of molecules, communication between cellular compartments, and the maintenance of cellular structure. For several of these biological processes to occur, membranes must bend, curve, and sometimes break or merge in a controlled manner to ensure proper functioning of the cell. Processes such as membrane fission, membrane fusion, and membrane budding play important roles in cell division, organelle transport, and maintaining cellular homeostasis. Hence, the cells possess a variety of dedicated machinery and proteins having specific domains to perform these processes. SNARE, ESCRT-III, Dynamin, EHD and BAR-domain family of proteins are a few examples. Membrane remodelling process occurs at a large temporal and spatial scales. A computational approach to understand the entire process requires the use of methods at different resolutions. Atomic-resolution can explain membrane-recognition, coarse-grained resolution for membrane curvature, and a mesoscale approach is required to investigate large-scale membrane remodelling like tubulation. In this presentation, I will show a few projects on membrane remodelling proteins. Firstly, the SNX1-SNX5 complex, that plays a role in cargo sorting and endosome remodelling. The second project is a high-throughput workflow to convert the resolutions from continuum remodelling vesicle into a Coarse-grained vesicle using N-BAR as an example.



Tuesday, Oct 13th 2026

11:30 Hrs