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SEMINAIRE

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« Dynamic Integrative Modelling of Molecular Machines »

Adding a structural dimension to the ever-accumulating omics data presents a grand challenge to the structural biology community. Integrative modelling predicts protein assemblies under the guidance of experimental data to alleviate this challenge. During the last decade, we have observed a substantial improvement in the field of integrative modelling. Though, the field is still being challenged by numerous large, heterogeneous, and dynamic machineries. During my talk, I will present our recent efforts in modelling the structure of such an assembly. In this work, upon joining forces of molecular dynamics and integrative modelling, we explore how a specific class of transcription factor, Sox, can recognize its cognate sequence on a compact nucleosome. Our approach proposes that the productive binding of Sox transcription factor depends on the localization of its cognate sequence on the nucleosome. It also reveals that the position-dependency emanates from the differential histone-DNA interactions encoded at distinct nucleosomal positions. These striking findings came as an outcome of multiple simulation cycles, which I will discuss in detail during my presentation.

Jeudi 25 novembre 2021

14h00