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SEMINAR
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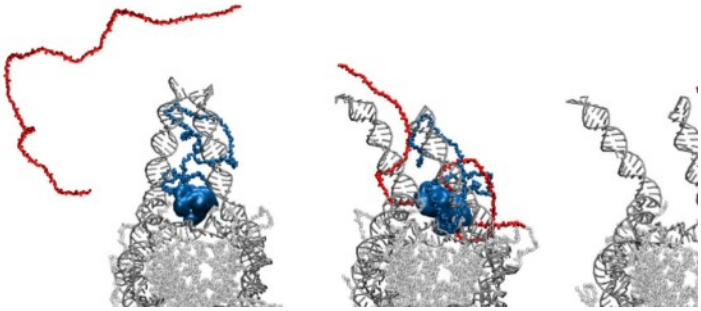
"Characterizing protein ensembles and designing protein resilience through experimentally aided computational efforts "



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O-030, Department of Biotechnology

Host: Miranda Mladenić Pejatović

Characterizing protein ensembles and designing protein resilience through experimentally aided computational efforts

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Abstract

Evolved to perform a large set of functions related to their many folds, proteins are the workhorses of cells. The ability to understand, control or design proteins is linked to our capacity to characterize their behavior at an exhaustive level of detail.
For this, the combination of experiments and simulations represents a powerful coupling: while tackling protein characterization and design solely by experiments is destined to fail.
Similarly, theoretical protein scientists "walk in the dark" without the aid of experiments, which shed light on a meaningful characterization of molecular behavior.
Within this premise, and especially for a multi-resolution investigation of protein intrinsic disorder and protein design, computational methods and their tight and direct integration with experiments are paramount. I will delve into the methodological advancements proposed for the determination of intrinsically disordered protein dynamics, directly combining MD simulations and observables from single-molecules Förster Resonance Energy Transfer (smFRET) spectroscopic data. I will then briefly talk about how to design new protein variants for industrial applications by combining computational and experimental workflows. More generally, the talk hopes to provide an overview of strategies useful to directly combine experimental and theoretical efforts for protein understanding and design.