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Hosted by Marina Guenza

Computational models for intrinsically disordered proteins

Abstract:

Understanding the conformational preference of an intrinsically disordered protein (IDP) is of great interest due to its relevance to critical intracellular functions and diseases. It could be challenging to investigate IDPs with solely experimental techniques considering its flexible conformations. Computational models in different resolutions can provide complementary information.

In this presentation, I will first present our efforts on modeling the liquid-liquid phase separation of IDPs using coarse-grained and polymer models. I will further introduce our recent work on understanding the binding between an IDP and its folded ligand.

