

Internal Seminar

An expedition through local and global features of IDP using computational lenses

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My research mainly centres on understanding the complex structural behaviour of intrinsically disordered proteins (IDPs) and their functional significance. I have explored the conformational landscape of hnRNPA1 through advanced sampling, revealing its structural modularity within the intrinsically disordered region. I investigated the functional role of its RGG-box domain in telomere maintenance and G-quadruplex destabilisation. I studied kinked β -strand's critical role in the formation of reversible fibrils and developed an SVM-based classifier to identify them. I have also looked into the contribution of interface residues in IDP-nucleic acid interactions. In my ongoing work, I am trying to build an accurate reconstruction of the long IDP energy landscape by integrating and reweighing all-atom and coarse-grained ensembles, which will be finally used to create a machine learning-based transferable IDP force field. Altogether, these efforts aim to advance a comprehensive, data-driven framework for decoding IDP behaviour across functional and evolutionary contexts.

Tuesday, Apr 22nd 2025

16:00 Hrs

CR-4, TIFRH