Dynamic approaches to structural ensembles of intrinsically disordered proteins

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Abstract. Intrinsically disordered proteins and complex multidomain proteins are characterized by dynamic ensembles of conformations that cannot be unequivocally described by traditional static terms of structural biology. These states of proteins are critical in understanding their function at the atomic level, which will eventually lead to extending the structure-function paradigm to establish "unstructural biology" as a new field [1]. The functional importance of structural dynamics and complexity necessitates new standards and protocols for the description of structural ensembles, also termed "supertertiary" structure in the case of very large proteins composed of a combination of folded and disordered elements [2]. Here we will 1) outline the development of a new database (pE-DB) that is designed to hold structural ensembles of proteins [3], 2) show through a few examples (PSD95, CBP) current experimental efforts to describe structural complexity at the supertertiary structural level, and 3) describe a novel bioinformatics tool, DynaMine, developed for predicting backbone dynamics from amino acid sequence.

References

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