

Modelling protein mechanics: From structure to function.

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It is now widely accepted that protein function depends not only on structure, but also on flexibility. However, the way protein mechanical properties contribute to their biological activity remains unclear. In this perspective, we developed the ProPHet (Probing Protein Heterogeneity) program for investigating local flexibility within protein structures, which combines a reduced representation with Brownian dynamics simulations. The analysis of the residue fluctuations during the dynamic simulations yields a rigidity profile for the protein made up of force constants describing the ease of displacing each residue with respect to the rest of the structure. This mechanical response, which is highly heterogeneous along the protein sequence, can be related to the protein structure (and in particular to its secondary structure elements), but also to its biological activity.