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From Sequence to Motion: Predicting Protein Dynamics with Machine Learning

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Proteins are more than merely static structures; they are dynamic entities that facilitate a wide range of biological functions. The collective physics of proteins, including the interactions between amino acids and the propagation of forces, gives rise to their functionality. While machine learning has cracked the code of how protein sequences determine structure, the fundamental question of how sequences encode functionality remains a mystery. The missing link is the dynamics. The sequence determines the structure which is flexible and dynamic. It is this dynamic nature that ultimately determines function. Flexibility is achieved through a network of local deformations. It has been shown that local deformation is one of the key factors in protein's functionality, by allowing conformational changes and allosteric regulation. Therefore in this study we aimed to fine-tune protein language models on local deformation data obtained from molecular dynamic simulations to predict flexible regions within a sequence. These regions are essential for the transduction of force throughout the protein and thus crucial for its activity. Our model enables the user to obtain dynamic data without the need for computationally expensive simulations.