

EFFECT OF CALCIUM REMOVAL AND IONIC STRENGTH VARIATION ON THE CONFORMATION CHANGE IN CALMODULIN PROTEIN AT PHYSIOLOGICAL pH

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ABSTRACT

It is well known that there are many conformational sub-states of proteins which are determined by their folded structures. External factors like solvent type, temperature, pH and ionic strength play a very important role in this conformational sampling of the protein. In this manuscript, we investigate the response of the Calmodulin (CaM) protein as a function of calcium removal and ionic strength at physiological pH. CaM plays a very important role in different physiological processes as it can bind to a variety of other proteins. One hundred nanosecond simulations are carried out on the extended form of CaM. Changing the ionic strength came out to be one of the possible routes for observing a conformation change in the protein. This behavior is similar to the conformation change observed in our previous study where a change in the pH was observed to trigger a conformation change in this protein. As the calciums are removed from the protein, the protein is observed to become more flexible and acquires a more compact form as compared to its extended initial structure. The N and the C-lobes are observed to come as close as to a distance of 20-25 Angstroms. At a lower ionic strength of 150 nM, this conformation change is observed to take place at a much shorter time duration.