Contribution ID: **6** Type: **Oral Presentation**

Protein dynamics as a function of ionic strength, calcium ion concentration and temperature: Calmodulin as a first step

Monday, 11 July 2016 12:20 (20 minutes)

Abstract content
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Calmodulin protein plays a very crucial role in the calcium signaling inside the eukaryotic cell structure as it can also bind to other proteins/targets and facilitate various activities inside the cell. The response of CaM protein as a function of ionic strength, calcium ion removal and temperature at physiological pH condition is investigated using classical Molecular dynamics simulations. Changing the ionic strength and temperature came out to be two possible routes for observing a conformation change in the protein. As the calcium ions are removed from the protein, it is observed to acquire more flexibility. This flexibility is observed to be more prominent at a higher ionic strength. At a lower ionic strength of 150 mM with all the four calcium ions intact, the N and C-lobes are observed to come close to a distance of 30 Å starting from an initial separation distance of 48 Å. This conformation change is observed to take place around 50 ns in a simulation of 100 ns. As a second parameter, temperature is observed to play a key role in the conformation change of the protein. Earlier these kind of studies have been performed experimentally using fluorescence measurements as in. The calcium bound form of CaM is observed to undergo a reversible conformation change in the range 295-301 K at calcium ion concentration 150 mM. The transition temperature was observed to depend on the calcium ion concentration of the protein. We perform MD simulations of 100 ns each for the temperature range 300-500 K on the apo form of CaM, 3CLN and 1CFD. A remarkable dependence of the temperature is observed on the overall dynamics of the protein as reported in our earlier study. 1CFD shows a much flexible linker as compared to 3CLN whereas the overall dynamics of the lobes mainly N-lobe is observed to be more in later case.

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Session Classification: Parallel Track B

Track Classification: Computational Biology