Tata Institute of Fundamental Research
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Internal Seminar

A quantitative approach towards molecular recognition and protein folding

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Biomolecular recognition and protein folding are two important fields in biological chemistry. However, a quantitative approach to elucidate the kinetic pathways is a desirable and one of the emerging topics in the field of biomolecular computer simulation. In this talk, I will discuss about an approach based on Markov state model (MSM), which is gaining popularity in recent time worldwide. In my presentation, I will illustrate two useful application of MSM. In the first application, we will use MSM to extract the kinetically important states and their rate of interconversion in the context of binding of benzene to a buried and solvent-inaccessible cavity of L99A T4-lysozyme. In the second application, I will emphasize the use of MSM to obtain the optimum collective variable for getting underlying free energy surfaces of small protein GB1.

Tuesday, Sep 26th 2017

02:00 PM (Tea/Coffee at 01:45 PM)

Auditorium, TIFR-H (FReT-B)