

(Ctiff Tata Institute of Fundamental Research

Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500 046

Students' Annual Seminar

Applications of ¹⁵N CEST NMR Experiments to Study Folding of the Fast-folding Peripheral **Subunit Binding Domain**

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Protein conformational dynamics play an important role in the folding, activity, aggregation etc. of the proteins and it is therefore important to understand how these dynamics occur. ¹⁵N CEST experiments are now well established to study such conformational dynamics occurring on a second-millisecond timescale and efforts are being made to study faster dynamics using CEST. Although the use of high-power saturating magnetic fields in the ¹⁵N CEST experiment does report on the exchange parameters of such fast processes, they are poorly defined. Here we show that when the ¹⁵N CEST data is supplemented with additional experimentally derived constraints on other fitting parameters, more precise estimates of the global exchange parameters can be obtained. We have applied this approach to study the folding of the fast-folding peripheral subunit binding domain which folds on the microsecond timescale (~100 ms) and learn that while the unfolding rate shows Arrhenius behaviour, the folding rate is almost independent of temperature, a typical characteristic of fast-folding proteins. In the second part of the talk, I will briefly discuss the predicted presence of an intermediate involved in the folding/unfolding transition of the lysozyme from the T4 bacteriophage.

Friday, May 12th 2023 5:00 PM Seminar Hall, TIFR-H