Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Seminar

When Molecular Dynamics met Spin Resonance (and several other experiments)

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Purdue University, USA &
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I will cover three projects that we currently pursue in the Laboratory of bio-NMR. First, I will speak about ESR spectra of MTSL-tagged proteins. We have simulated these spectra using μs-timescale MD trajectories and compared the simulations with experiment. This type of analysis provides new insight into the role of ESR labels as a probe of protein dynamics. Second, I will speak about pulsed-field-gradient NMR experiments to measure diffusion of amyloid fibrils. We have constructed a new theory of these experiments, taking into consideration both translational and rotational diffusion of fibrils. In doing so, we dispelled certain misconceptions that existed in this field and demonstrated that the idea of diffusion filter can be successfully implemented also for amyloid fibrils, such as Sup35NM fibrils investigated in our study. Finally, I will also discuss refinement of x-ray coordinates using Amber MD platform. We have shown that using state-of-the-art MD model of protein crystal, including faithful representation of crystal contacts, explicit interstitial water, realistic representation of conformational dynamics, etc. allows one to consistently achieve better R_{free} indicators and better MolProbity scores compared to crystallographic coordinates refined via the industry standard program Phenix.

Tuesday, Apr 16th 2019

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H