Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Students' Annual Seminar

Stratification of Solid-state NMR Spectra of Proteins based on their Aminoacid Side-chains

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Solid-state Nuclear Magnetic Resonance (ssNMR) is a powerful tool for studying the structure and dynamics of solids, including polymers, proteins, and other complex systems. Peak assignment in ssNMR can be challenging due to limited resolution resulting from several factors such as broad peaks, anisotropic interactions, misalignment of spinning-angle from magic-angle and multiple other interactions. Multi-dimensional NMR experiments are often employed to overcome spectral overlap and increase resolution. However, these experiments require time-intensive sophisticated pulse sequences and data processing techniques, adding complexity to the assignment process. Spectral simplification has been addressed by employing various isotope labelling schemes (2-^{13}C-Glycerol, 1,3-^{13}C-Glycerol, SAIL, ILV, etc). In solution-state NMR, sequences like MUSIC (Multiplicity Selective In-phase Coherence transfer) were developed for filtering peaks based on the amino-acid type. This study demonstrates that side-chain differences amongst different amino acids can be exploited to distinguish peaks in 2D CH/NH solid-state HETCOR spectra. Although sequential resonance assignment is still required, we expect these experiments to reduce ambiguities and hasten resonance assignment approaches. We will showcase the latest results on the GB1 protein (6.2 kDa).

Friday, Mar 15th 2024

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Seminar Hall, TIFR-H