

Internal Seminar

**Optimization of Tracked AuTOMated
Assignments in PROteins (TATAPRO)
algorithm: Identification of amino acid type
from NMR spectral data using kernel density
estimations and neural networks**

Gopi Krishna Guntupalli

TCIS, Hyderabad

Sequence-specific resonance assignment is a prelude for the 3D structure determination of proteins using NMR spectroscopy. The automated algorithm, Tracked AuTOMated Assignments in PROteins (TATAPRO) proposed earlier utilizes the peak-lists from a pre-defined suite of triple-resonance spectra (for example CBCANH, CBCA(CO)NH, HNCO and HN(CA)CO) and the protein primary structure, which then correlate ^1HN and ^{15}N chemical shifts for a given amino acid residue with those of self and sequential ^{13}CA , ^{13}CB and ^{13}CO . Identification of amino acid type using the experimental data is the primary task in implementing TATAPRO algorithm. In my presentation, I will demonstrate the utility of “Kernel Density Estimations and Neural Networks”, in making identification of amino acid residue type robust and thus improving accuracy of the assignment process in TATAPRO algorithm.

Tuesday, Oct 3rd 2017

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

Auditorium, TIFR-H (FReT-B)