TIFR Centre for Interdisciplinary Sciences
21, Brundavan Colony, Narsingi, Hyderabad 500 075

Students' Annual Seminar

Biomolecular interaction as studied by NMR

Janeka Gartia

1. Biomolecular NMR Studies on Plant Protease Inhibitors from Capsicum annuum

Developing a peptide based eco-friendly insecticidal agents to control insect pests that adversely affect the agricultural production by destroying the crops or infesting the livestock is a major challenge. The most common Lepidoptera species that cause damage to agriculture sector is Helicoverpa. The larval stage of these species can cause a major damage to economically valuable crops such as cotton, tobacco, tomato, corn, sorghum, sunflower, wheat and other pulses. Helicoverpa species are polyphagous pests of about 200 plant species. These species are one of the most serious pests in cotton-producing countries (Australia, India and China) causing a major economic loss. Although chemical insecticides are used to control these species, H. armigera has developed the resistance to a number of insecticides. Thus, there is an urgent need for the development of eco-friendly insecticidal compounds to control Helicoverpa. Recently, it has been reported that peptide based protease inhibitors (PIs) from Capsicum annuum potently inhibit H. armigera gut proteases and also show a significant effect on its larval growth. On the other hand, very little information is currently available about the three-dimensional (3D) structure of CanPIs or the residues that mediate their interaction with insect gut proteases, and very few structural studies have quantitatively compared the activity of different CanPIs. Recently, three recombinant CanPIs (IRD7, IRD9, and IRD12) have been found to be very potent inhibitors with specific reference to their (i) stability in proteolytic environment (ii) proteinase inhibition specificities and (iii) inhibitory activity against insect proteinases. Thus, I set out to produce a panel of three recombinant CanPIs, compare their activity in-vitro and in-vivo, and determine their 3D structure with a view to selecting the best candidate for future development as a bioinsecticide proteases. During the last one year, the focus of my research has been mostly on the study of structure and dynamics of plant protease inhibitors (IRD7, IRD9, IRD12), which will be the subject matter of my talk.

2. Phase Modulated 2D HN (CACBHB) and 2D (HBCBCA) NH for fast Identification of Amino Acid type

I have also been involved in the development of a simple approach to rapidly identify amino acid types in proteins from a set of 2D spectra. The method is based on the fact that $^{13}C^{\beta}$ and $^{1}H^{\beta}$ chemical shifts of different amino acid types fall in distinct spectral regions. By evolving the $^{1}H^{\beta}/^{13}C^{\beta}$ chemical shifts in the modified HNCACB type experiment for a single specified delay period, I will show how the phase of the cross peaks of different amino acid residues are modulated depending on their $^{13}C^{\beta}$ and $^{1}H^{\beta}$ shift values and thus enable one to identify amino acids types.

Wednesday, Jun 7th 2017

4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS