Tata Institute of Fundamental Research
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Seminar

Structure of the Intrinsically Disordered Viral VPg protein in free and bound forms

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The conformational transitions of intrinsically disordered proteins are of current interest for understanding virulence, pathogenesis and disease in plants, livestock and humans and importantly, to understand how these proteins fold. Viral proteins exhibit a propensity towards structural disorder because they are less compact, have fewer hydrophobic contacts and possess large disordered segments. These properties have hampered the determination of structures of viral proteins. We have recently determined the structure of an intrinsically disordered plant VPg protein in its protease bound conformation using data driven docking protocols. Restraints for docking include the NMR derived structure of VPg, H/D exchange data, RDC restraints of the complex and mutational and other biochemical data. The VPg protein folds into a three stranded β-sheet, one face of which binds to the protease though essential aromatic – aromatic and CH···π interactions. The structure of the protease-VPg heterocomplex is in excellent agreement with mutational data and shows an excellent correlation with residual dipolar coupling data (R = 0.995; N = 129). The importance of aromatic and CH···π interactions are analyzed with special emphasis on anisotropic interactions originating from aromatic ring current shifts of methyl protons and residual dipolar couplings of aromatic ring protons in VPg and Pro respectively. The results of these studies will be presented.

Wednesday, Dec 26th 2018

12:00 PM (Tea/Coffee at 11:30 AM)

Auditorium, TIFR-H