



**TIFR Centre for Interdisciplinary Sciences,
Narsingi, Hyderabad 500075**

Seminar

**Protein Glycosylation: From Force Field Development to
Applications.**

Sairam Swaroop Mallajosyula

**Department of Pharmaceutical Sciences,
University of Maryland
School of Pharmacy, Baltimore, Maryland, USA.**

Abstract: Glycosylation is a ubiquitous post-translational modification of proteins that involves the covalent attachment of carbohydrates to the side chains of either asparagine (N-linked) or serine/threonine (O-linked). Only 6% of protein crystal structures contain carbohydrate linked structures. In the absence of structural information molecular dynamics (MD) simulations can be used to study glycoprotein systems. To this end the development of the CHARMM all-atom additive force field parameters for glycoprotein linkages will be presented. I shall also discuss the application of the parameters together with a Hamiltonian Replica Exchange (HREX) enhanced conformational sampling methodology to develop structure-activity relationship (SAR) for antiproliferative factor (APF), a glycosylated nonapeptide involved in interstitial cystitis.

Date: Tuesday, June 11th 2013

Time: 04:00PM (Tea/Coffee at 03:30PM)

Venue: Conference Hall, TCIS

All are cordially invited