CENTER FOR BIOINFORMATICS
PONDICHERRY UNIVERSITY

SEMINAR NOTICE

NEW APPROACHES FOR COMPUTATIONAL INFERENCE OF PROTEIN MOLECULAR FUNCTION

by

Dr. Debnath Pal

Department of Computational and Data Sciences
Indian Institute of Science
Bangalore 560 012, Karnataka, India
dpal@cds.iisc.ac.in

Date and Time: 19-10-2016 (Wednesday) 3.45 PM
Interaction with the speaker and tea 3.30 PM to 3.45 PM
Venue: Seminar Hall, Center for Bioinformatics

ABSTRACT OF THE TALK

Computational inference of protein molecular function is an urgent need given that the bioinformatic data on sequence and structure is increasing by the day. However, the task is not easy because the conundrum of function annotation of proteins is not a simple extension of inference by comparative analysis of sequence and structure alignments. The outcome of a functional activity requires juxtaposition of several physicochemical features of the protein molecule, whose combinations could be context specific. Therefore, it is necessary to understand the prerequisites for a functional activity, which is not often possible through simple alignments of sequence and structure. We have developed a method for de novo inference of function for a protein molecule through its structural dynamics. A long timescale coarse grained dynamics of protein is used to capture its mobile regions and the autocorrelation vector profile is used to fingerprint the dynamics of these segments. The dynamics fingerprint of equivalent segments were found to match for orthologous proteins suggesting existence of a specific dynamics-function link that can be exploited for function annotation. Benchmark studies evaluating the dynamics-function relationship showed that it can be used for correct recall in 87% cases in positive dataset and 93% in negative dataset. We have shown that mixing dynamics based function inference in traditional annotation pipeline improves the specificity of annotation. The work establishes a generalized proof-of-principle of using dynamics data for protein function inference

Dr. R. Krishna
Seminar coordinator

Dr. R. KRISHNA
Assistant Professor
Centre for Bioinformatics
Pondicherry University
Pondicherry-605 014

ALL ARE WELCOME

12/10/2016

Dr. H. Surya Prakash Rao
Center Head

Prof. H. Surya Prakash Rao,
Centre Head (i/c)
Centre for Bioinformatics,
School of Life Sciences,
Pondicherry University, Puducherry-14.