

Bioinformatics tools and applications*

The growth of biotechnology has increased exponentially during the last decade as a result of development of high throughput techniques and parallel progress in information technology, which has led to the emergence of a novel discipline called bioinformatics. In recognition of its importance, a 'hands-on-training on bioinformatics tools and application (sponsored by BTISNet) was organized by the Department of Biotechnology, Lady Doak College, Madurai.

This programme provided a platform for focused training cum discussion by experts in the field. S. Krishnaswamy (Madurai Kamaraj University, (MKU) Madurai) in his presidential address, gave a brief introduction about bioinformatics and also mentioned some of the activities of BTISNet. He outlined the importance of systems biology and highlighted G. N. Ramachandran's contribution and its key role to validate the structure of a particular protein through *in silico* analysis. A. Thamarachelvan (Thiagarajar College, Madurai) focused on the diverse applications of bioinformatics tools and discussed the structure-based drug design and challenges in computer-aided drug design.

N. Jeyakumar (MKU) reviewed data mining, text mining and micro-array data analysis. He explained data mining as a 'science of extracting useful information from large sets or databases'. Data mining of micro array data analysis process is critical for good, reliable results, whereas text mining is knowledge-based information retrieval in the context of biological repositories. Z. A. Rafi (MKU) presented a comparative genomics approach to studying noncoding RNA in Enterobacteriaceae. He introduced how the noncoding RNAs play a key role in structural, regulatory or even catalytic mechanisms and several approaches in identification of ncRNA (non-coding RNA). P. Gowtham, (Anna University, Chennai) discussed the history of molecular modelling and the need for molecular simula-

tion. He also emphasized the mechanism of molecular dynamics simulation of lipase in selective hydrolysis at two different pH states using bioinformatics.

R. Usha (MKU) spoke on the applications of bioinformatics in plant virus research. Her talk focused on bhendi yellow mosaic virus, Indian cardamom mosaic virus, and the phylogeny derived based on genome sequence analysis in various geographical isolates from South India. S. Selvaraj (Bharathidasan University, Tiruchirapally) presented the use of various bioinformatics tools for sequence analysis and structure prediction of proteins and their applications. Sanjeev Kumar Singh (MKU) spoke on the impact of technology in the process of drug discovery and he discussed the quantum pharmacological study on HIV-1 RT and reasoned out why it is better than molecular pharmacology. R. Shenbagarathai (Lady Doak College) pointed out that systems biology is a comprehensive quantitative analysis of the manner in which all the components of a biological system interact functionally over time, and the systematic study of the cell function and physiology of the organism allowed the identification of specific metabolic targets and subsequently to significant improvements in product yield and productivity. A. Mercy Pushpalatha (Lady Doak College), delivered a lecture on combinational chemistry in drug designing and explained the drug discovery process and a flow chart of interactive refinement to get a clinically active compound.

In technical sessions, A. Mahalakshmi (Lady Doak College) gave an overview of various databases, and sequence retrieval and submission methods. The participants were introduced to different primary and secondary sequence databases and structural databases for protein by G. Thiruvartselvi (Lady Doak College). J. Asnet Mary (Lady Doak College) outlined the significance, types and methods of alignment and stressed the importance of pair-wise alignment of protein sequence, which can be more informative than DNA and to assign function to unknown proteins, to determine relatedness, to identify structural and functional elements and to predict the 3D structure

with suitable illustration. This helped the participants to understand the different types of alignments which dealt with methods like dot plot, word method and dynamic programming for DNA sequence and protein sequence alignment studies, and introduced the scoring matrices like PAM and BLOSUM. This was followed by Multiple Sequence Alignment (MSA), wherein the significance of MSA was emphasized. Progressive MSA helps to create a guide and to identify the consensus sequence using Clustal X and Clustal W. The matrix such as BLOSUM, PAM and GONNET were used to carry out similarity searches and the phylogenetic tree was constructed using Phylip, BioEdit and Phylodrew. In addition, the participants were trained to do multiple sequence alignment and protein characteristics using GCG package. Further they were exposed to TMHMM to study the transmembrane topology, secondary and tertiary prediction and structure visualization (Rasmol, SwissPDB viewer, Molmol).

Eight steps in modelling were reviewed, which encompass the entire procedure from day-one, such as detect template, get alignment, optimize alignment, optimize template, exchange side chains, deal with insertions and deletions, optimize model, validate and finally iterate to refine the model of the protein under study. The final day of the training programme was dedicated to the laboratories work, where all participants were trained to do homology modelling for the sequence that was retrieved on the first day and were also taught the method to do energy minimization steps. The instructors guided the participants to validate their model using Ramachandran plot analysis. The success of the programme was well reflected by the participants requesting the organizing committee to have an advanced-level training programme the following year.

R. Shenbagarathai, Department of Biotechnology, Lady Doak College, Madurai 625 002, India.
e-mail: shenbagarathai@gmail.com

*A report on the 'Hands-on Training on Bioinformatics Tools and Applications' organized by the Department of Biotechnology, Lady Doak College, Madurai during 2-12 May 2007 and sponsored by BTISNet.