

Editorial

Dear Readers,

The present copy of the journal Current Bioinformatics (CBio) is the inaugural issue of the journal. Current Bioinformatics is a review journal which has been started to provide the scientific community involved in computational molecular/structural biology with a comprehensive and cohesive coverage on different topics of fast developing bioinformatics, encompassing the areas such as computing in biomedicine and genomics, computational proteomics and systems biology, and metabolic pathway engineering. Developments in these fields have direct implications on key issues related to health care, medicine, genetic disorder, development of agricultural products, renewable energy, environmental protection, etc. The journal will focus on reviews on knowledge discovery from biological data, computing in biomedicine and genomics, computational proteomics and systems biology. So far no such journal has been available that may provide a comprehensive coverage with critical assessment of the day-to-day developments in these topics. The Bentham Science has now taken this step starting the journal "Current Bioinformatics", wherein the leading scientists from all over the world are invited to contribute the review articles on topics in which they have expertise. The journal would cover a wide range of the integration of biology with computer and information science. The present issue contains ten articles covering a variety of interesting topics.

The issue starts with an article by Ambesi-Impiombato and Bernardo on computational biology and drug discovery. Computational biology and bioinformatics have the potential not only to speed up the drug discovery process, thus reducing the costs, but also to change the way drugs are designed. In this review, authors have focused on the different computational and bioinformatics approaches that have been proposed and applied to the different steps involved in the drug development process. In drug design and drug discovery, the functional features of proteins play very important roles. In article 2, Pazos and Bang discuss computational methods for predicting protein functional features, which can be coupled to the pipelines of genome sequencing and structure determination. This review focuses on current *in-silico* methods for predicting regions in proteins with some functional importance (catalytic sites, binding sites, protein interaction regions, etc.) using sequence and/or three-dimensional structure information. Determining functional features of a protein experimentally is expensive, time consuming and difficult to automate. The stability of protein structure and function at a desired temperature is of crucial importance and the possibility of maintaining the structure and function of a protein at a temperature above that of its native state has been the objective of many researchers ever since mutating a protein became a relatively easy process. In article 3, therefore, Mozovilliarías and Querol present the most recent theoretical and computer advances related to the problem of thermally stabilizing proteins.

Since proteins are the major players in most processes of living cells, knowledge of the proteome has great relevance to the study of cells and organisms at the molecular level. Proteome analysis linked to genome sequence information is very useful for functional genomics. For its analysis, therefore, Komatsu presents in article 4, the rice proteome database and other plant proteome databases with a fruitful discussion. Similarly, in article 5, Pham *et al.* discuss several main research directions and methods in the analysis of microarray gene expression data. Microarrays provide the biological research community with tremendously rich, sensitive and detailed information on gene expression profiles. Related to this theme is an article by Asyali *et al.* on gene expression profile classification (article 6) in which the authors have discussed the class-prediction and discovery methods that are applied to gene expression data, along with the implications of the findings.

Databases of three-dimensional macromolecular structures became so large that fast search tools and comparison methods were needed and were actually designed. In article 7, Carugo presents a review on the algorithms that allow fast structure comparison, particularly suitable to handle large databases, and should provide a comprehensive picture, useful for the

development and the assessment of novel tools. Our understanding of biological systems has improved dramatically due to decades of exploration and has been accelerated further during the past ten years, mainly due to the genome projects, new technologies such as microarray, and developments in proteomics. Still, integrating this knowledge to reconstruct a biological system *in silico* has been a significant challenge for biologists, computer scientists, engineers, mathematicians and statisticians. In article 8, Zheng discusses engineering approaches towards biological information integration at the systems level, which can provide many advantages and capture both the static and dynamic information of a biological system. Thompson and Poch present an article (article 9) on multiple sequence alignment as a workbench for molecular systems biology. In a multiple sequence alignment, structural and functional data can be combined with evolutionary information to allow reliable data validation, consensus predictions and rational propagation of information from known to unknown sequences.

One of the main topics in genomics is to determine the relevance of DNA variations with some genetic disease. Single nucleotide polymorphism (SNP) is the most frequent and important form of genetic variation which involves a single DNA base. The values of a set of SNPs on a particular chromosome copy define a haplotype. Because of its importance in the studies of complex disease association, haplotyping is one of the central problems in bioinformatics. In the last article (article 10), Zhang *et al.* give an account of the existing models and algorithms for haplotyping problems, report the recent progresses from the computational viewpoint, and discuss the future research trends. I thank all the authors of this issue for their excellent stimulating contributions and hope that readers will greatly enjoy reading these articles as I did and that these contributions will be of great value to the researchers involved in the area of bioinformatics.

Satya P. Gupta
(*Editor-in-Chief*)

Department of Chemistry
Birla Institute of Technology and Science
Pilani-333031
India
E-mail: spg@bits-pilani.ac.in