



P-ISSN: 2349-8528

E-ISSN: 2321-4902

IJCS 2019; 7(5): 282-286

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Received: 16-07-2019

Accepted: 18-08-2019

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Basics of bioinformatics and it's application for applied life sciences: A national training workshop report-2019

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Abstract

A variety of bioinformatics tools in the areas of basic and applied life sciences has altered the worldview of bioscience studies over the years. The creation of new and strong bioinformatics techniques devoted to the acquisition, information mining and analysis of biological data enabled basic and applied research in life sciences from molecular biology to the creation of new biomedical tools. These bioinformatics advances cover the emerging biomedical research areas including the development of newer algorithms with predictive applications, genome annotation tools and prediction of function, gene expression analysis, and biological data in the form of advanced databases. Bioinformatics Sub-DIC, at department of molecular biology & genetic engineering, CBSH, Govind ballabh Pant University of Agriculture & Technology, Pantnagar, Uttarakhand, India having expertise in bioinformatics and conducting training, novel research projects, workshops with the UG, PG and doctorate courses of bioinformatics. Started in 1998 we have been conducting workshops and successfully trained hundreds of attendees including researchers, faculty, scientists etc. The workshop including lectures of eminent scientist and hands on practical sessions of various bioinformatics software/tools thus participants can perform by themselves on their own computer/laptop using bioinformatics. We have conducted more than 20 workshops around the country on latest technologies of bioinformatics especially NGS data analysis, Gene & genome annotation, drug discovery & designing, and MD Simulations. From these perspectives and a huge demand in the region a three days training course & hands-on workshop entitled "Basics of Bioinformatics and its Application for Applied Life Sciences" has been organized by Bioinformatics Sub-DIC Pantnagar to provide the emerging aspects of bioinformatics for agriculture and life sciences.

Keywords: Insilico, molecular modeling, docking, pathway, tools

Introduction

Researchers in life sciences bring together and evaluate a large number of distinct kinds of data, including sequences of DNA, RNA and amino acids, in situ and microarray information, protein structures, gene expression, biological signals, biological pathways, and pictures of varied scientific origin (Bumgarner *et al.*, 2013). Advances of bioinformatics applications in the areas of basic as well as applied life sciences in latest years have changed the way of life sciences research paradigm. These innovations in bioinformatics range from genome annotation and prediction of gene function, analyzes of gene expression, and biological data and databases to the emerging areas of life sciences and agriculture (Alemu 2015) [15]. Agriculture plays an essential role in human progress and development of civilization. The objective of plant molecular biology is to study cellular mechanisms, their genetic control and relationships with modifications in the environment. Such a multi-dimensional and comprehensive study needs extensive experiments involving whole genetic, structural or functional elements. Big-data flows from technologically driven wet-lab studies in biological researches are accumulating at a phenomenal pace worldwide (Leonelli 2019) [16]. In the age of rapidly accumulating biological information from the phenotypic as well as genotypic assessment of many plant crops, and from the-omics research's huge information generation. Bioinformatics has entered all major biological fields today. Bioinformatics uses computer technology to help researchers keep track of the genetic information they find and researchers can obtain, store, assess and match biological data rapidly and precisely (He, *et al.*, 2017) [9]. Bioinformatics tools have developed beyond limits, creating latest biotechnology techniques for genetically modifying and improving the availability of food for an ever-increasing world population.

This workshop can now be leveraged to speed the conversion of fundamental knowledge into agriculture and life sciences (Roy *et al.*, 2016)^[22].

The main goal of this workshop is to gather recent advances in bioinformatics applications in the broad area biosciences and make them available to the academia and research. The current workshop is an important effort in the right direction to help students and appreciate the integration of physical sciences in gainfully exploring the complexities of a biological system. Keeping in view of above, National Training Workshop on “Basics of Bioinformatics and It’s Application for Applied Life Sciences” from April 27-29, 2019 was organized for the benefits of academic fraternity. The organizing team consists of Dr. Gohar Taj (Organizer), Dr. Sundip Kumar (Coordinator) and staff of Bioinformatics Sub-DIC Mr. Apoorv Tiwari (SRF), Mr. Ganga Datt Sharma, Mr. Ram Pratap Singh and Mrs Neelam.

Objectives of the workshop

The workshop's primary goals were to comprehend the basic applications of bioinformatics in order to meet the concurrent challenges of agriculture and life sciences. In this the main objectives covered by the 3-day national workshop were as follows:

- Comparative Omics (genomics, transcriptomics and proteomics).
- In silico methods for modulation of regulatory networks and metabolic pathways.
- Structural bioinformatics.

- Informatics of disease diagnosis and drug design.

Content and Outline of the workshop

The details of contents covered in the workshop were as follows

Bio-prospecting and Metabolomics: Identification of novel molecules and their metabolic pathways/regulatory networks using different pathway database and tools.

Molecular and Structure biology: The study of biological micro/macromolecules' architecture, shape, and dynamics is important in understanding the fundamental mechanisms that drive the vital functions of all life. The driving forces and interactions which characterize the three dimensional forms and dynamics of biomolecules are dealt with in structural biology. Use of different structure databases for modeling of 3-D structures of target and ligand molecules and visualization.

Computer Aided Drug Designing: Identification of potential drug targets for lead molecules/peptides to know their mode of action through ligand-protein and/or protein-protein interaction (molecular modeling, docking and simulation studies).

Next Generation Sequencing: Introduction of Next Generation Sequencing, Read/contig assembly methods, popular Next Generation Technologies, Tools for NGS data analysis, Application of NGS in agriculture and life sciences.



Fig 1: Inaugural Function of the Three days national training workshop

Dr. Tej Partap ji, Vice Chancellor of our university was the Chief Guest of inaugural function and inaugurated three-days training/workshop entitled “Basics of Bioinformatics and It’s Application for Applied Life Sciences” organized by Sub-DIC Bioinformatics at Department of molecular biology and genetic engineering, CBSH on 27th April 2019 and delivered an Inaugural address and highlighted the importance of bioinformatics tools and high throughput sequencing and omics in the area of applied life sciences and agriculture (Figure 1). Dr. Tej Partap said that the backbreaking work by the University on green revolution based agriculture to enhance the productivity has been plateaued off. From being the Harbinger of Green Revolution, the G B Pant University

is now moving towards the ‘Gene Revolution’. Biotechnology, being one of the important branches of science, has the potential to create new products for the welfare of human race and provide gainful employment to millions of our farmers. The large volumes of data that has been produced through the advance biotechnological approaches, needs to be converted into useful information for the ultimate use by all the stake holders (Sharma, D *et al.*, 2018)^[21]. Towards this end, we need to appreciate that the biological system is a complex one and understanding the complexities of the biological system involves developing newer algorithms and bionetworks (Chin *et al.*, 2008)^[6]. System biology approaches brings around greater integration

of mathematical modelling for understanding the biological system and its complex regulatory networks (Najafi *et al.*, 2014) ^[19]. Therefore, there is a big challenge in front of agricultural scientists to further increase quality agricultural production. He said that it has been possible to successfully enhance the production with the use of latest bioinformatics and computational biology techniques (Koyutürk (2010, Oulas *et al.*, 2019) ^[12, 4]

Dr. Partap further emphasized in his address that it is possible to map the genes responsible for important agricultural trait with the use of bioinformatics techniques and develop the crop of high nutraceutical values. These high quality crops will not only increase the income of farmers but also increase both quality and quantity of agriculture produce (Oulas *et al.*, 2019) ^[4]. Bioinformatics tools can be used for identification of the useful genes and proteins which can be exploited to develop the disease resistant organic crop varieties that can use soil nutrients efficiently (Nicola *et al.*, 2018) ^[5]. Therefore every agricultural scientist must have essential knowledge of bioinformatics.

The guest of honour of the inaugural function Dr. Manoj Prasad, Principal Scientist NIIPGR, New Delhi said that knowledge of computational techniques is very important to understand the mechanisms of biological problems. Along with that, Dr. Prasad also told that organisms of agricultural importance should be identified by the dissolution of genome sequences by the use of bioinformatics techniques.

Dr. A. K. Shukla, Dean College of Basic Science and Humanities, welcomed all the participants of workshop and highlighted about different activities of the college and university. Dr. A.K. Gaur Head of department Molecular Biology and Genetic Engineering welcomed the privileged guests and participants and highlighted about different aspects of workshop. Dr. Sundip Kumar, Coordinator, Bioinformatics centre has discussed the importance of the workshop and told about the workshop's objectives. Dr. Gohar Taj Scientist Incharge presented the vote of thanks to all the organizing team members, participants and faculty members along with the DBT. At the time of inauguration, Esteemed scientist, Dr. Jitendra Thakur, Dr. Jitendra Giri from NIPGR, Dean, Directors, Head of the departments of various departments; faculty members, Dr. Veer Singh, Dr. J P N Rai, Dr. Dinesh Pandey, Dr. Gohar Taj and all the staff of Sub-DIC Bioinformatics were present.

On first day of workshop Dr. Manoj Prasad, Scientist VI was the Guest of honor and delivered an informative lecture talk on Multi-omics tools for crop improvement and described briefly about different approaches of crop genomics of barley, wheat, millets, bean etc. (Mir *et al.*, 2012) ^[17]. He described how the novel sets of markers are used for a multitude of features of crop species the genetic and compared mapping, molecular genetic diversity studies and the identification of QTLs (Sood *et al.*, 2019) ^[23]. He said that food security is one of the major global challenges of the 21st century agriculture, and it is characterized by ever-growing population, limited food nutrition, ever increasing cost of cultivation, climate change and many persisting biotic and abiotic stresses. Millets retain excellent hope for food security and nutrition despite ever-increasing agricultural expenses and climate change. They are nutritious, have extra health advantages, involve considerably lower production input expenses and are obviously tolerant of most biotic and abiotic stresses (Tiwari *et al.*, 2017) ^[25]. These characteristics accentuate millets as plants of preference for the world population in the face of increasing climate change concerns. In this scenario, foxtail

millet has lately been considered a traceable experimental C4 plant for genomics of cereals and grasses. In addition, its prospective abiotic stress tolerance has attracted considerable scientific attention and has tried to create genomic resources and decipher the molecular stress tolerance mechanism (Jaiswal *et al.*, 2019) ^[10, 11]. While a number of attempts have led to considerable knowledge of the structural and functional genomics of foxtail millets, the publishing of the genome sequence has significantly boosted genome research to a fresh dimension. As is shown by comprehensive genome asset development, web-base development, genome-wide association, genome-wide functionality and standardized genomic studies. Recent researches have now led to the conversion of orphan plant into a nutrient rich plant with wealthy genomic and genetic resources. These assets would promises to promote crop improvement programs that include millet and grass species, thereby aiming at the global food safety situation under climate change (Garg, V. K *et al.*, 2016, Tiwari *et al.*, 2017 and Jaiswal *et al.*, 2019, Akbar N, 2018) ^[7, 25, 10-11, 1].

In Afternoon Session Dr. Jitendra Thakur, Staff Scientist V, Plant Mediator Lab, NIPGR delivered a lecture on topic "Taking Advantage of Bioinformatics in Basic Experimental Research" and described about several transcription factor sequence-specific regulations for organism development and functionality. An important multi-protein complex that functions as an adapter between regulatory transcription factors and the transcription machinery is a co-factor-based mediator. In spite of its primary significance, we do not understand the molecular detailed functioning of the Mediator due to the complex network of numerous respondents in the transcription machine (Kumar V *et al.*, 2018) ^[14]. He has outlined various methods of understanding how distinct sub-units contribute to the maintenance of the complicated structural integrity through bioinformatics tools and databases (Samanta S *et al.*, 2017, Nagulapalli M *et al.*, 2016) ^[20, 18].

Later Research staff of Bioinformatics Sub-DIC, Mr. Apoorv Tiwari presented hands on module on basics of bioinformatics. After that the participants visited to departmental labs of OMICS such as Genomics, Proteomics and Metabolomics and various instruments applied in agriculture and life sciences (Tiwari, A. *et al.*, 2016 and Taj G. *et al.*, 2018) ^[26, 24].

In the 2nd day of workshop Mr. Apoorv Tiwari performed practical modules on Bioinformatics analysis of Transcriptome data for identification, and annotation of genes by standalone BLAST. In this practical module he performed different types of BLAST and their applications (Altschul *et al.*, 1990) ^[2].

In the afternoon session Dr. Rohit Saluja, Scientist D (Ramalingaswamy Fellow) (AIIMS), Bhopal delivered a very informative lecture on topic "Application of Bioinformatics in different fields of sciences", and performed different practical sessions on Primer Designing, BLAST, PIR, Phylogenetic analysis, Multiple sequence alignment and other related databases and tools which are frequently used in the area of life sciences (Ye *et al.*, 2012, Kumar 2018) ^[27, 14].

In the 3rd i.e. last day of workshop Dr. Dev Buksh Singh, Assistant Professor, CSJM University, Kanpur delivered a very informatics lecture on topic "Protein structure modeling and validation" and briefly described about different approaches of structure prediction (Gaur M, 2018 and Jabeen *et al.*, 2019) ^[8, 3]. In his lecture he also described about online server and tools for secondary and tertiary structure prediction and visualization. In his second lecture on topic "Natural

Product and lead optimization approaches” he described about drug discovery and its different modules. He described in detail about the ligand and protein interaction and different tools like Autodock and Chemscketch are used to play an

important role in the molecular design and interaction. In the 3 days national training workshop total of 5 lectures practical modules were covered to provide directional flow of information for applied life sciences.



Fig 2: Group photograph of Scientists, Research Scholars and Academic staff during workshop on 27-29th April, 2019.

Feedback analysis and conclusions

With response to our publicity we tend to received several applications and twenty one participants were selected based on 1st come 1st serve basis. Participants’ feedback was also asked to judge the end result of the workshop. The feedback consisted of sub-domains, starting from technical experience to learning expertise to active coaching to cordial reception rendered. The fields include practical needs and interests, effective activities, use online resources and training materials, knowledge of the instructor, style of the lecturer, the material covered by the teacher, instructor answered the questions well and how the workshop can be enhanced. Participants exceeded the expectations of the organizers and were most gratifying. All agreed that this workshop was an outstanding success. The Organizer of the workshop Dr. Gohar Taj devoted her sincere thanks to Dean CBSH Dr. A.K. Shukla, for his valuable guidance, Dr Anil Kumar Gaur, Head MBGE, Dr. Sundip Kumar, Coordinator, Bioinformatics Sub-DIC, Panatnagar (Figure 2) and all the teaching and non-teaching staff for successful completion of the workshop.

Acknowledgements

The authors are grateful for the financial support provided by the BTISNet, department of biotechnology, the government of India to the Bioinformatics Sub-DIC Pantnagar to conducting training and provide quality teaching and research.

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