

Bioinformatics in Agriculture: Way Forward



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Preface

Equipped with the extraordinary technological revolution, biological and agricultural sciences both have now become data-driven science in last few decades. The promise, challenges and outcomes of this revolution is enormous and can only be looked upon over a wide span of time. Deeper insights into the basic biological mechanisms that drive the organism's progeny and their own biology can create better understanding about how biological processes are connected with the networks of genes, proteins and metabolites that regulate phenology of the organisms. Such efforts can largely affect agricultural productivity, address impact of climate change on crops, cause adaptations among organisms against stresses (biotic and abiotic), drive evolutionary mechanisms in microbes and other organisms, define pathogen interactions with host plants and animals, govern environmental processes including energy generation, next generation commercial crops and biofuels, management of global carbon and remediation of contaminated environmental resources.

Recently emerging area of –OMICS science includes genomics, transcriptomics, proteomics and metabolomics and tries to connect all the segmented science into a holistic biological approach called systems biology. Due to extensive work being carried out by several laboratories in India by different institutions in and outside NARS system, researchers working on – OMICS related research are generating huge biological data nowadays and are committed to generate even more in the future. Several whole genome sequencing projects on plants, animals, fishes and microorganisms are increasing and similar is true for proteomics and transcriptomics related projects. Because of technological, infrastructural and funding support by several funding agencies, it is anticipated that such activities will show an increasing trend in coming years. Looking into the volume of big data in the recent past in agricultural sciences, a parallel upcoming of bioinformatics support to the researchers is a must and the cyber-infrastructure as of the National Agricultural Bioinformatics Grid (NABG) was a significant effort taken up by the ICAR in this direction. Looking into the need of strengthening this interdisciplinary science, a policy framework that is coming into the form of this policy paper is an appreciable effort in documenting existing capabilities, needs, challenges and policy options for the future.



S. Ayyappan
President

Bioinformatics in Agriculture: Way Forward

PREAMBLE

Bioinformatics and computational biology are entwined employing techniques and concepts from life sciences, computer sciences and information technology. This interdisciplinary approach maintains close interactions with life sciences to realize its full potential. Bioinformatics applies concepts of information technologies to make the vast, diverse and complex biological data more readable, understandable and usable while, computational biology uses algorithms, mathematical models and computational approaches to address experimental and theoretical queries. In this way, apart from being distinct in functions and approaches, there is significant overlap in their activities to bridge the interface of the science of any biological discipline with informatics. The ultimate task of the bioinformatics in the biological system is to provide a complete computational representation of a cell (Singh et al., 2012).

Because of the complexity among the simplest to the most advanced biological systems, massive multi-dimensional data generation, analysis and interpretation is required for a critical understanding of the cellular processes. With the application of high performance data generating machines (sequencers, mass spectrometers and other instruments) for complex but interdependent biological research, wealth of diverse data are continually accumulating. Massive and fast evolving data often create problems of misleading results and inconclusive interpretations. This has also posed the difficult task of identification, characterization and integration of globally available research information and finally coming out with a conclusive end in addressing typical problems of agriculture and medical sciences, and the environment (Jones et al., 2006).

PRIORITIES FOR INDIAN AGRICULTURE

Agriculture is an assemblage of diverse physical, chemical and biological components, which in harmony with each other result in greater productivity. Present day agriculture in India is moving very fast from the *green revolution* to *evergreen revolution*. Basic priorities in the present day agriculture are to keep pace with the increasing population to meet the food requirement of the country, secure its own sustainability in the era of chemicalization and industrialization, coping with the fast emerging

technologies and withstand with the unprecedented and abrupt changes in the climate. In the era of knowledge flood, agriculture as a whole is being witnessed as own components of which, plants and soil are the most live interactive concepts followed by other biotic and abiotic interactions to which, crops are regularly exposed (Varshney et al., 2005). The overall impact of the environment can have genotypic and phenotypic short or long-lasting changes in plants and other organisms that usually open the door of the emergence of new genetic, molecular and biosynthetic pathways (Mochida and Shinozaki, 2010). Documentation of the interconnections between the conditions and representative alterations within the system can help to find out the response mechanisms behind the interactions. Equipped with this knowledge, biologists and agricultural scientists can find out the ways to mitigate the challenges of climate change, decline in the crop productivity and the issues like biosafety and biosecurity (Vassilev et al., 2005). By genome analysis, gene function can be predicted and their functional categories be defined with the interventions of bioinformatics tools. Therefore, bioinformatics can facilitate the identification of the genetic basis of agronomically important traits that can accelerate the development of improved varieties.

WHY BIOINFORMATICS?

Worldwide, research activities in experimental molecular biology and whole genome sequencing projects have generated large volume nucleotide and protein sequencing data. Traditional molecular biology research is still carried out making use as advanced machines, that has led to increase in generation of large and varied data sets needing the involvement of computational power to make valid interpretations (Caschi, 2012).

Voluminous data in genomics, proteomic, transcriptomic and metabolomics has been witnessed in the recent past. Therefore projects use computational techniques to glean biological knowledge from literature and from other public databases to address challenges of analysis and interpretation. To pin point specify and identify the problems of the present day agriculture and to implement solutions at the right time, computing applications are the upcoming viable options for agricultural sciences (BPI, 2004).

The integration of information on the key biological processes allows us to achieve complete understanding of the biology of organisms as a long-term goal. The rationale behind strengthening the fast emerging field of Bioinformatics therefore, lies in.

- ◆ Bioinformatics and computational biology are parallel to the high-data generation in molecular biology at global scale.
- ◆ This field has grown as a cross-boundary research and development sector in the area of biology, agriculture, molecular biology, genetics, chemistry, health, environment and biostatistics.
- ◆ Bioinformatics is not only an area of primary research but its technological embedding makes this area critically applicable for work in all fields of biological, chemical and physical fields related to, agriculture and environment.

HANDLING MASSIVE BIOLOGICAL DATA-FLOW

Worldwide, big-data flow in the biological research coming out from the technologically-driven wet-lab experiments are accumulating at a phenomenal rate. India is obviously a part of this phenomenon because Indian researchers are taking integrative approaches to generate big-data in plant, microbe, fish and animal genomics, proteomics and phenomics. Currently, the data from the myriad of whole genome, transcriptome, proteome, metabolome and other interrelated projects are increasing with the fast pace from all the domains of biological, medical and agricultural sciences (Jimenez-Lopez et al., 2013). Since, the data are wide ranging and of diverse quality addressing signatures within the organisms or their networks, the process of extracting information lying within it becomes critical. The information dynamics, quantity and variety of information within a single experiment that includes the study of gene expression can be imagined from the fact that it involves analysis of genes, determination of protein structures encoded by the genes and details of how these products interact with each other. The ease with which computers can handle large amount of diverse data at a time and probe complex dynamics observed, makes computers indispensable to assist in biological research.

In the era of fast accumulating biological data coming out from the phenotypic analysis of many crop plants, live-stocks, microbes, climates, habitats and other interrelated entities and from the massive data generation from the – omics research (genomics, proteomics and metabolomics), bioinformatics has come forward across the globe to solve the problems of analysis, prediction, storage, management, pattern recognition, submission, retrieval and storage of the data to find out fruitful outcome. Complete whole genome sequencing projects on various crop plants along with more than 300 on-going projects, livestock (742 on-going

projects) and microbes (4000 completed, >8000 ongoing) have generated huge data resources at a large pace in many parts of the world (Source: NCBI). A core collection of 3,000 rice accessions from 89 countries were re-sequenced in China (<http://www.gigasciencejournal.com/content/3/1/7>). Bioinformatics-driven analysis and interpretations of huge data can help in finding out novel alleles for important rice phenotypes and serves to understand genomic diversity within rice. Such big data in biological and agricultural sciences has attracted biologists to look at the cellular, molecular and metabolic levels to decipher agriculturally important traits (Bansal, 2005).

The size of data generated on each and every aspect of the organisms is too large to decipher, analyze, store, manage and retrieve. Therefore, the need of bioinformatics and its integration in the present days of agricultural research and education with high end computer applications, tools and softwares, database development and management, computational biology, biotechnology and bio-statistics is inevitable.

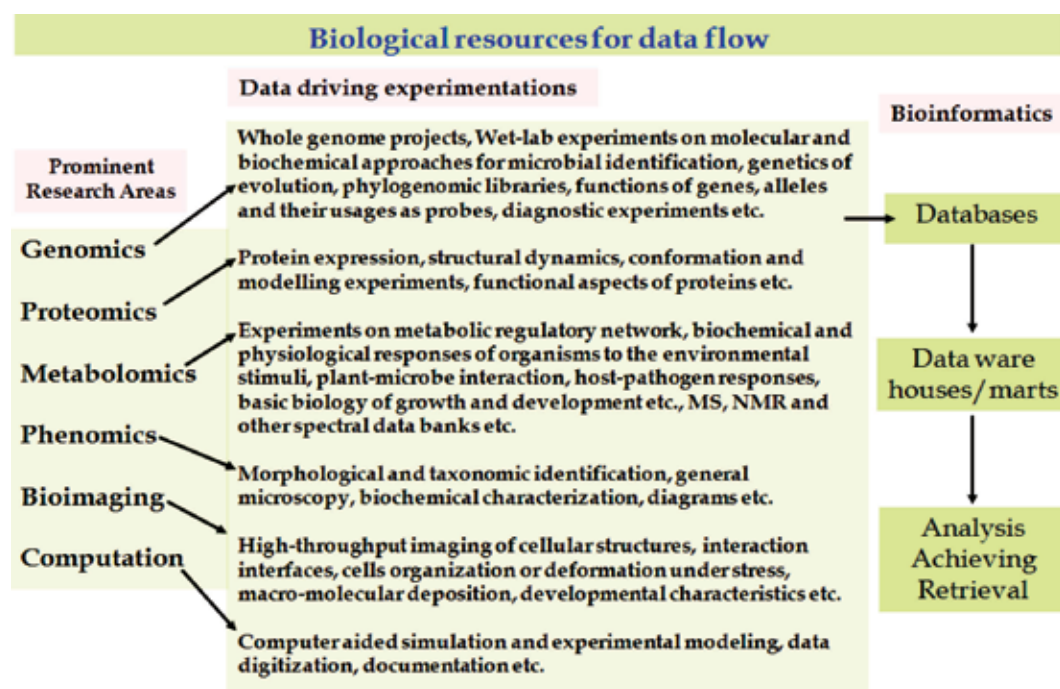


Fig. Experimental resources for data flow in biological research and their connectivity with bioinformatics

As there is an enormous increase of raw sequenced data, there is an increasing need of annotation that converts raw data into a significant form that is handy to biologists and can be interpreted into biological information (Fraser et al., 2000). At present genome annotation is a combined approach of experimental and computational tools where computational methods represent a noteworthy fraction of the intensifying area of bioinformatics. Bioinformatics also facilitates the analysis of huge quantity of genome expression data generated by the technologies as microarrays and SAGE (Jones et al., 2006).

RESEARCH AND DEVELOPMENTAL CONCERNS

With the advent of widespread, fast growing, very complex and often interdependent research data in the field of biological and agricultural sciences, the problem of non-concluding analysis and interpretation is increasingly felt. Since these data sets are different and regularly generated by different methods and sets of models, their integration at a common platform is not feasible. Responses of organisms with complex systems to the environment, pathogens and abiotic stresses and interactions with other organisms are among the few examples on which huge information has been gathered during the past several decades. This has posed a tough task of identifying, characterizing and integrating globally available research information to the field of agriculture, medical, pharmaceutical, biochemical and environmental etc. In reality, this would have been the greatest problem in biological research where computational systems, biostatistics and information technologies are finding their increasing applications (Ouzounis, 2012) However, these technologies developing parallel to the biological research enabled scientists in interpreting results. The assembling and integration of these technologies in solving the problems related to biological systems has given rise to “bioinformatics” (NABG, 2010).

Experimental biologists are more likely to create new technologies that are emerging with a very fast pace to enable high throughput collection of useful biological data. The complex cellular data will in turn be correlated with higher levels of phenotypic data based on the observations of the nature of cells, organs and organisms. This is why the establishment of connectivity between what is being observed at the molecular level with that of the phenotypic characters of the organisms under the environmental conditions is among the most emerging research areas. The mount and variety of biological data from recently developed methods enabled bioinformatics to perform the study of entire system at a single time (real time) rather than in individual components (genes, proteins, metabolites etc.). This has opened a new

area of Systems Biology that is basically “Integrative Biology”, which means for the integration of biological data for a better and meaningful understanding of the functioning of biological systems. Bioinformatics for Systems Biology links and connects many disciplines. It brings scientists from different areas like life sciences, computational biology, biomedical sciences and mathematics under a common framework (Jones et al., 2006).

Our understanding of basic biology is being facilitated through comparison of organisms at different evolutionary distances, in order to reconstruct both the tree of life and the emergence of important phenotypic traits. Also, there is a growing expectation that bioinformatics will help fuel the creation of computational models (both qualitative and quantitative) which will allow us to capture, store and maintain biological models that help explain experimental observations. Algorithms in bioinformatics cover research in all aspects of computational biology. The emphasis is on discrete algorithms that address important problems in molecular biology, genomics, and proteomics that are computationally efficient, implemented and tested in simulations and on real datasets and provide new biological results and insights. Exact and approximate algorithms pertain to genomics, sequence analysis, gene and signal recognition, alignment, molecular evolution, phylogenetics, structure determination or prediction, gene expression and gene networks, proteomics, functional genomics, and drug design. In particular, bioinformatics tools include the BLAST program (homology searching), GENSCAN, GENIE (gene-finding), SAPS (statistical analysis of protein sequences), CLUSTAL, ITERALIGN, (multiple sequence alignment), r-SCAN STATISTICS (target array clustering, over-dispersion), etc (Cochrane and Galperin, 2009). These programs are used by thousands of researchers every day in molecular biology and medicine. The BLAST protocol currently serves more than one lakh queries per day at the National Center for Biotechnology Information (NCBI) in Washington, DC.

DEVELOPMENTS AND INITIATIVES

Looking into the needs of Indian researchers certain landmark efforts have been taken-up in India in the past at various platforms to address the problems of biological data management, transfer and applications. India is credited in the whole world to establish a BioTechnology Information System (BTIS) network in 1987 for creating an infrastructure aimed to harness biotechnological applications through the use of bioinformatics. Department of Biotechnology (DBT) has successfully established a high-speed and high-bandwidth network in the form of Virtual Public Network (VPN) named as BIOGRID INDIA. Eleven nodes for this

system have been established in the first phase and now being actively used for pursuing bioinformatics activities such as human resource development and R&D in bioinformatics and dissemination of biotechnology information to the researchers in the country. The nodes are interconnected through 2mbps dedicated leased circuit line at each location and 4Mbps Internet bandwidth shared from the central server by all the nodes. The BIOGRID allows exchange of database and softwares which have been created/acquired by the individual centers/nodes of BTIS. This resource-sharing helps in enhancing the value and usefulness of the BTIS, a true resource sharing network in India. The Department of Information Technology (DIT), India established Centre for Development of Advanced Computing (C-DAC) to deploy the nation-wide computational grid GARUDA which connected many cities across the country with an aim to bring Grid Network Computing for research laboratories and industry. Another network, GARUDA is a collaborative program of scientific and technological researchers on a nation-wide grid comprising of computational nodes, mass storage and scientific instruments. GARUDA aims to provide the technological advances required to enable data and compute intensive science. DBT has also provided support for the development of a highly curated international database entitled 'Manually Curated Database of Rice Proteins' (www.genomeindia.org/biocuration) based on semantic digitization of published experimental data on rice (BPI, 2004).

In Indian agricultural system, ICAR has taken an stepping-up initiative to establish National Agricultural Bioinformatics Grid (NABG) coupled with a high-end supercomputing facility and large data storage device to support agricultural research for all purposes of bioinformatics tasks right from sequence submission and retrieval to the annotation of whole genome sequencing projects, comparative genomics, transcriptomics, proteomics and metabolomics. This grid-based supercomputing facility has been established in 2013 at Indian Agricultural Statistics Research Institute, New Delhi with extensions at five National Bureaux of the ICAR including National Bureau of Plant Genetic Resources (NBPGR), New Delhi, National Bureau of Fish Genetic Resources (NBFGR), Lucknow, National Bureau of Animal Genetic Resources (NBAGR), Karnal, National Bureau of Agriculturally Important Microorganisms (NBAIM), Mau (UP) and National Bureau of Agriculturally Important Insects (NBAII), Bangalore for the integration and curation of biological data in the specific domains with an aim to provide bioinformatics services to the Indian scientists in a similar manner in which NCBI, EMBL, KEGG or other international public databases are providing. At the same time, to strengthen the capacity of Indian scientists, several National level training programs are regularly being organized at a mission mode.

Masters level academic course in Agricultural Bioinformatics has been started in Indian Agricultural Statistics Research Institute, New Delhi and the Ph.D. program is underway (NABG, 2010).

GOALS FOR BIOINFORMATICS

Sequencing projects worldwide have resulted in a unique wealth of biological data for which bioinformatics has met the huge demand for analysis, storage and interpretation. The first row of genome and protein sequence information flow created demand for computational tools for search, comparison and analysis of nucleic acid, protein sequences and macromolecular structures (Allen, 2004). The second type of data flow related to the expression profiling (gene, protein, metabolite and ultrastructure) similarly generated demand for such tools that allowed the data to be minimized, understood and integrated. Future waves of data will support innovations in phenomic, genomic, proteomic and metabolomic research including large scale genomic comparisons, protein structures, simulation models, interactions, taxonomy, compartmentalization and overall turnover of metabolic pathways and regulatory networks (Al-Haggar, 2013).

For such integrated and cumulative efforts, research, education and services in bioinformatics need to be interdependent and mutually supportive. Future developments in the area need to have following goals-

1. Research goals should fulfill nationally and internationally recognized capabilities to strengthen multidisciplinary research tasks within and outside NARS system in India. Multiplicity and plurality in the bioinformatics research and development is essential in order to establish this area as a mainstream of scientific research.
2. Educational goals should aim to develop an established system of educational offerings in the area of bioinformatics at different levels including Masters and Ph D programs as well as high end orientation programs for scientific and technical staff.
3. Service-oriented goals should be user-centric to support research efforts and develop bioinformatics tools and techniques as per the research needs and without any barrier of physical location where the actual research is being carried out. Participatory programs should be initiated with software developing companies, institutions, research departments and/or individuals that can support researchers in developing algorithms, databases and analytical as per the demand of the experiments to fetch maximum information.

4. Infrastructure resources should be aimed at maintaining efficient physical and technical infrastructure with full capability to allow fast and efficient computation, analysis, modeling, visualization and retrieval of biological data.
5. Organizational capabilities need to be created for the integration of research, education and service-oriented missions garner requisite institutional resources, leadership and back-up resources to realize these goals.
6. Development of data storage models and schemas with the capacity of digitizing every aspect of data generated by agricultural research including phenotypes, traits (molecular/biochemical), environmental conditions, plant development stage, tissue etc.

PRIORITIES

National level priorities for bioinformatics should address the problems and perspectives of the current day biological and agricultural research. Major foreseen areas are as under:

1. Prioritize to cater the needs of the people who are engaged in generating data from biological experimentation related to agriculture.
2. Integration with the educational system should be given due priority to produce well-trained bioinformatics professionals and contribute to bioinformatics service.
3. Creation of bioinformatics research community involving extensive collaborations between the bioinformatics and life sciences researchers across the country.
4. Establishment of a high-end computational and statistical bioinformatics support system.
5. Establishing a nation-wide capacity building system for conveying bioinformatics techniques and information.
6. Increasing the practice of data digitization at institutional level for conversion of the same in databases with uniform platforms for end-use access.
7. Increase in the computational and data storage facilities and its upgradation should be addressed to accommodate bioinformatics and biological sciences researchers.
8. Recruiting and hiring support personnel working with the high-end clusters and high-performance computational environments, and large-scale storage systems commensurate with the infrastructure.

9. Gaining visibility by not only producing high quality research papers but also through developing novel bioinformatics tools, softwares and other integrated packages for data management.
10. Attracting appropriate funding from various National funding sources to cater the needs of infrastructure, man power and capacity building.

STRATEGIES FOR FUTURE BIOINFORMATICS INFRASTRUCTURES

- ◆ Extensive and wide spread competence development of man-power to handle challenges in data analysis.
- ◆ Serve the needs and priorities of a very complex community of users.
- ◆ Respond to the distinct demands of biological researchers.
- ◆ Provide a biological information environment with information about other biological (or biology-related) data and not simply genetic and molecular information.
- ◆ Comprehensive and multi-disciplinary data environment for integrative disciplines (e.g. systems biology, metagenomics, drug discovery etc.).
- ◆ Overcome several bottle-necks in bioinformatics resources exploitation such as lack of resource interoperability, programmatic access, input/output format standardization and user-friendly web interfaces.
- ◆ Establish optimal community synergy between resource providers/developers and users.
- ◆ Involvement of future users during resource development phase, efficient capture of users' feedback information, development of resources documentation and tutorials.

NEEDS TO SUPPORT BIOINFORMATICS SERVICES

Overarching needs

- ◆ *Recognition among leadership that bioinformatics is essential for agricultural research*

Such leadership supported envisioned programs are essentially required to establish bioinformatics resources to support high throughput-based Indian agricultural research

◆ *Strengthening of organizational framework support for bioinformatics*

Initiatives are needed to equip NARS with world class bioinformatics centers with at least minimum of bioinformatics resources and capacity building.

Specific needs

Research

- ◆ Identifying truly national priorities in agricultural bioinformatics.
- ◆ Human resource development to strengthen human capital knowledge in bioinformatics.
- ◆ Parallel funding for collaborative research support for both wet- and dry-lab work.
- ◆ Support for partnering development in IT sector for new algorithms, tools, software and database to cater analytical needs of biological researchers.
- ◆ Centralized space to support bioinformatics research and cohesive research environment.

Education

- ◆ Mass awareness about the necessities, capabilities and services on bioinformatics.
- ◆ Masters, doctoral and post-doctoral programs and associated administrative support.
- ◆ Capacity building through orientation courses among NARS and university people.
- ◆ Bioinformatics courses:
 - Should be updated to include new aspects like systems biology, biocuration.
 - Emphasize the importance and functioning of various algorithms used in bioinformatics analysis. Competence development should be emphasized to inculcate the capacity to design and modify algorithms based on a biological problem.

Service

- ◆ Develop sustainable funding models to support public-private partnership services

- ◆ Space for bioinformatics services especially connected with the biological/agricultural sciences
- ◆ Cloud-computing concept should be implemented where a centralized high-end infrastructure and highly qualified and motivated personnel may offer project/job wise assistance to various labs involved in wet-lab analysis over high speed internet.

POLICY OPTIONS

- ◆ Developing a cohesive understanding in the wet-lab and dry-lab (bioinformatics) scientists.
- ◆ Partnering among the NARS scientists for data generation, sharing and management.
- ◆ Providing translational bioinformatics services for the NARS people.
- ◆ Maintenance of large-scale genomics and other biological databases.
- ◆ Audit and control of databases that are increasingly becoming larger and larger.
- ◆ Ensuring security in stretched and quickly changing computing environment.
- ◆ Proper internet network and computational infrastructure to work with high end servers.
- ◆ Management and design of large-scale genotype and phenotypic data.
- ◆ In-house curriculum development and pro-bioinformatics environment for institutions.
- ◆ Systematic government or inter-government funding to support upcoming programs.
- ◆ Closing-up the gaps between the intellectual haves and have-nots for bioinformatics and computational biology.
- ◆ Developing interface research coupling bioinformatics and systems biology.
- ◆ A dynamic interface (with active participation) with the international bioinformatics community to keep abreast with latest and path-defining bioinformatics implementation.

RECOMMENDATIONS

- ◆ Priority areas for biological tasks assisted by the bioinformatics in agricultural research with a better understanding of genomic, proteomic, metabolomic and phenomic data may be identified at national level. The work within these areas may be distributed across the country at a diverse level but, it need to be integrated.
- ◆ The importance of the application of the subject in routine research programs should be propagated among the Indian researchers especially the young researchers.
- ◆ To cater the need of Indian researchers, high-end infrastructure fully capable of handling processing of huge data at a time and storage of the processed data at the same time may be developed at National level and be maintained regularly.
- ◆ Targeted orientation and focused approach for database generation based on the work of Indian scientists may be initiated as a long-term goal to generate huge databases on Indian work. The concept of 'Biocuration' should be extensively explored to enable the development of highly intricate databases.
- ◆ Promotion of bioinformatics research and education in India in the specific context of agricultural system is a basic need these days. Looking into this need, focus on the Human Resource Development Programs, that too primarily based on sensitization about the subject and the latter related to specific issues in the subject should be designed and popularized.
- ◆ A greater understanding about how to digitize phenotypic data into a computer readable form is essentially required and this may be integrated. Extensive use of various ontologies as well as development of new ontologies to efficiently digitize all kinds of agricultural data such as phenotype, environmental conditions etc. are required.
- ◆ For targeted applications of bioinformatics in crop improvement programs, genomics of important crop plants, animals, fishes, insects and microbes, systems biology of organisms and impact assessment of climatic changes on crops, biologists may be trained in different aspects of computational biology. This may help in fetching down the specific and targeted information.

- ◆ Service-oriented bioinformatics tasks may be started in the NARS system by making and implementing National level guidelines.
- ◆ Projects integrating data generation by laboratory experimentation and its integration with the bioinformatics need financial support to make a scope of the biological data generation at faster.

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NAAS Documents on Policy Issues

61. Mastitis Management in Dairy Animals	- 2013
62. Biopesticides – Quality Assurance	- 2013
63. Nanotechnology in Agriculture: Scope and Current Relevance	- 2013
64. Improving Productivity of Rice Fallows	- 2013
65. Climate Resilient Agriculture in India	- 2013
66. Role of Millets in Nutritional Security of India	- 2013
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