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Bioinformatics

INSIDE THIS ISSUE….

ANKUR

......Sprouting of thoughts

Ankur is symbol of new beginning towards growth. And Ankur is here to introduce budding writers. It would represent interesting articles in Botany, Bioinformatics and Climate Change Impacts Management. Each seed has the innate potential to grow - blossom, and display its magnificence after its dormancy has been broken. Same way this news letter would provide a platform to young researchers to share news and views, promote awareness about the subjects and generate interest in related issues. Ankur would be taken care of by a team of dedicated Student Editors who would select and edit articles for online publication.

We wish Team Ankur all the best for this endeavour.

FROM EDITOR'S DESK….

Ankur is now three years old. It has grown and established its branches. The concentrated and consistent efforts of all involved with Ankur have been really praiseworthy. The growth and development of Ankur is a reflection of the growth and progress of the students of the department. This is a platform for positive academic deliberations and we are happy that we have been getting appropriate inputs by our members. We extend our heartiest gratitude to TEAM ANKUR and all involved in the process of completing this task.

The journey began three years ago and now Ankur has blossomed and is spreading the fragrance to everyone around with the message of amalgamation of computer science and biological science as computational Biology or Bioinformatics. In this issue, we focus on various aspects of Bioinformatics.

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Patron's Message.....

Bioinformatics is an inter disciplinary science. It has become an important part of many areas of biology. In experimental molecular biology, bioinformatics techniques such as image and signal processing, allow extraction of useful results from large amounts of raw data. In the field of genetics and genomics, it aids in sequencing and annotating genomes and their observed mutations. It plays a role in the text mining of biological literature and the development of biological and gene ontologies to organize and query biological data. It also plays a role in the analysis of gene and protein expression and regulation. Bioinformatics tools aid in the comparison of genetic and genomic data and more generally in the understanding of evolutionary aspects of molecular biology. At a more integrative level, it helps analyze and catalogue the biological pathways and networks that are an important part of systems biology. In structural biology, it aids in the simulation and modelling of DNA, RNA, and protein structures as well as molecular interactions.

The primary goal of bioinformatics is to increase the understanding of biological processes. The focus is on developing and applying computationally intensive techniques like pattern recognition, data mining, machine learning algorithms, and visualization. Major research efforts in the field include sequence alignment, gene finding, genome assembly, drug design, drug discovery, protein structure alignment, protein structure prediction, prediction of gene expression, protein–protein interactions, genome-wide association studies, the modelling of evolution and cell division/mitosis.

Bioinformatics now entails the creation and advancement of databases, algorithms, computational - statistical techniques, and theory to solve formal and practical problems arising from the management - analysis of biological data. Bioinformatics also includes mapping and analyzing DNA and protein sequences, aligning DNA and protein sequences to compare them, and creating and viewing 3-D models of protein structures.

It is a science that has tremendous potential and offers new challenges and new dimensions.
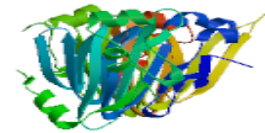Courtesy: Wikipedia
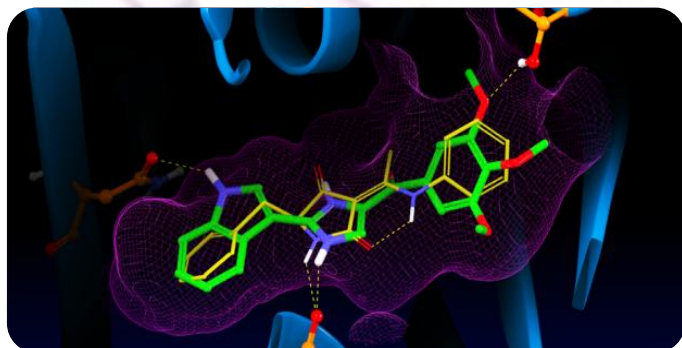
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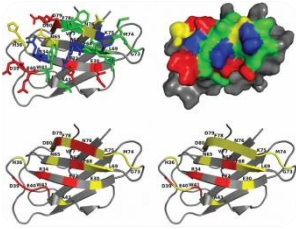
ALLERGEN BIOINFORMATICS

DR. ARCHANA MANKAD

Allergen bioinformatics isinfact the need of the hour! Experiments on genetic engineering during the last few decades have led to the production of numerous genetically modified (GM) organisms. So, proteins introduced into GM organisms through genetic engineering must be evaluated for their potential to cause allergic diseases. As a classical example, transgenic soy, that has been genetically engineered to express ground-nut 2S albumin, was found to elicit hypersensitivity reactions in groundnut allergic people (Nordlee *et al*., 1996). In 2001, the FAO/WHO suggested a procedure for performing FASTA or BLAST (Basic Local Alignment Search Tool) searches, and a threshold of greater than 35% identity in 80 or greater amino acids to identify potential allergenic cross-reactivity of transgene encoded proteins in genetically enhanced crops (Silvanovich *et al*., 2009). Given that this will not exclude all probabilities of a protein to be allergenic (and cross-reactive to known allergens), the codex guidance recognized that the assessment will evolve based on new scientific knowledge (Goodman, 2008). Bioinformatic tools are key components of the 2009 Codex Alimentarius for an overall assessment of the allergenic potential of novel proteins. Bioinformatic search comparisons between novel protein sequences, as well as potential novel fusion sequences derived from the genome and transgene or from any known allergen(s) are required by all regulatory agencies that assess the safety of genetically modified (GM) products(Ladics *et al*., 2011). Allergens were usually seen as an array of proteins with no apparent similarity in structure and function. They come from diverse sources: Plants, animals or fungi and may take different modes of exposure: inhalation, ingestion, sting or contact. They are, like their non-allergenic counterparts, structurally heterogeneous. For example, the major cat allergen Fel d 1, is an alpha-helical tropomyosin, while a major dust mite allergen Der p 2 consists predominantly of beta sheets and the major birch pollen allergen Bet v 1 contains both of these structural elements. Allergen sequences are extensively studied to find out any possible structural element or function associated with allergenicity. However, no such allergen-specific structural / functional element could be identified. High sequence identity between homologous protein allergens may result in common surface patches that may confer crossreactivity among them. Aalberse pointed out that proteins sharing less than 50% sequence identity are rarely cross-reactive(Aalberse, 2000). In contrast, proteins that share at least 70% identity often show cross-reactivity. Many IgE-binding epitopes have been identified as sequential epitopes, although for many this does

not represent the full epitope. Linear epitopes are usually part(s) of conformational epitope(s) responsible for a significant portion of IgE binding. While IgE-binding peptides can consist only of five amino acids (Banerjee *et al*., 1999), the majority of characterized IgE-linear epitopes are eight amino acids or longer (Chatchatee *et al*., 2001; Shin *et al*., 1998). Astwood recommended sequence comparisons to a database of known IgE-binding epitopes. Finally, Ivanciuc and colleagues have recently utilized mixed sequence and structure-based methods to predict IgE-binding sites. This is based on comparison of local sequence and structure to identify common features associated to allergens (Ivanciuc *et al*., 2009b).

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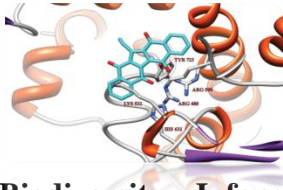
BIODIVERSITY INFORMATICS
DR. H. A. SOLANKI
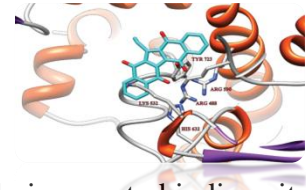
Biodiversity Informatics is the application of informatics techniques to biodiversity information for improved management, presentation, discovery, exploration and analysis. It typically builds on a foundation of taxonomic, biogeographic, or ecological information stored in digital form, which, with the application of modern computer techniques, can yield new ways to view and analyse existing information, as well as predictive models for information that does not yet exist (see niche modelling). Biodiversity informatics is a relatively young discipline (the term was coined in or around 1992) but has hundreds of practitioners worldwide, including the numerous individuals involved with the design and construction of taxonomic databases. The term "Biodiversity Informatics" is generally used in the broad sense to apply to computerized handling of any biodiversity information; the somewhat broader term "bioinformatics" is often used synonymously with the computerized handling of data in the specialized area of molecular biology.

At the 2009 e-Biosphere conference in the U.K., contributions (e.g. as posters) were grouped into the following themes, which is indicative of a broad range of current Biodiversity Informatics activities and how they might be categorized:

- Application: Conservation / Agriculture / Fisheries / Industry / Forestry
- Application: Invasive Alien Species
- Application: Systematic and Evolutionary Biology
- Application: Taxonomy and Identification Systems
- New Tools, Services and Standards for Data Management and Access
  - New Modeling Tools
  - New Tools for Data Integration
  - New Approaches to Biodiversity Infrastructure
  - New Approaches to Species Identification
  - New Approaches to Mapping Biodiversity
  - National and Regional Biodiversity Databases and Networks

A post-conference workshop of key persons with current significant Biodiversity Informatics roles also resulted in a Workshop Resolution that stressed, among other aspects, the need to create durable, global registries for the resources that are basic to biodiversity informatics (e.g., repositories, collections); complete the construction of a solid taxonomic infrastructure; and create ontologies for biodiversity data.

Biodiversity Informatics projects of the world

- The Global Biodiversity Information Facility (GBIF), and the Ocean Biogeographic Information System (OBIS) (for marine species)
- The Species 2000, ITIS (Integrated Taxonomic Information System), and Catalogue of Life projects
- Global Names
- EOL, The Encyclopedia of Life project
- The Consortium for the Barcode of Life project
- The Map of Life project
- The uBio Universal Biological Indexer and Organizer, from the Woods Hole Marine Biological Laboratory
- The Index to Organism Names (ION) from Thomson Reuters, providing access to scientific names of taxa from numerous journals as indexed in the Zoological Record
- ZooBank, the registry for nomenclatural acts and relevant systematic literature in zoology
- The Index NominumGenericorum, compilation of generic names published for organisms covered by the International Code of Botanical Nomenclature, maintained at the Smithsonian Institution in the U.S.A.
- The International Plant Names Index
- MycoBank, documenting new names and combinations for fungi
- The List of Prokaryotic names with Standing in Nomenclature (LPSN) - Official register of valid names for bacteria and archaea, as governed by the International Code of Nomenclature of Bacteria
- The Biodiversity Heritage Library project - digitising biodiversity literature
- Wikispecies, open source (community-editable) compilation of taxonomic information, companion project to Wikipedia
- TaxonConcept.org, a Linked Data project that connects disparate species databases
- Instituto de CienciasNaturales. Universidad Nacional de Colombia. Virtual Collections and Biodiversity Informatics Unit
- ANTABIF. The Antarctic Biodiversity Information Facility gives free and open access to Antarctic Biodiversity data, in the spirit of the Antarctic Treaty.
- Genesys (website), database of plant genetic resources maintained in national, regional and international gene banks

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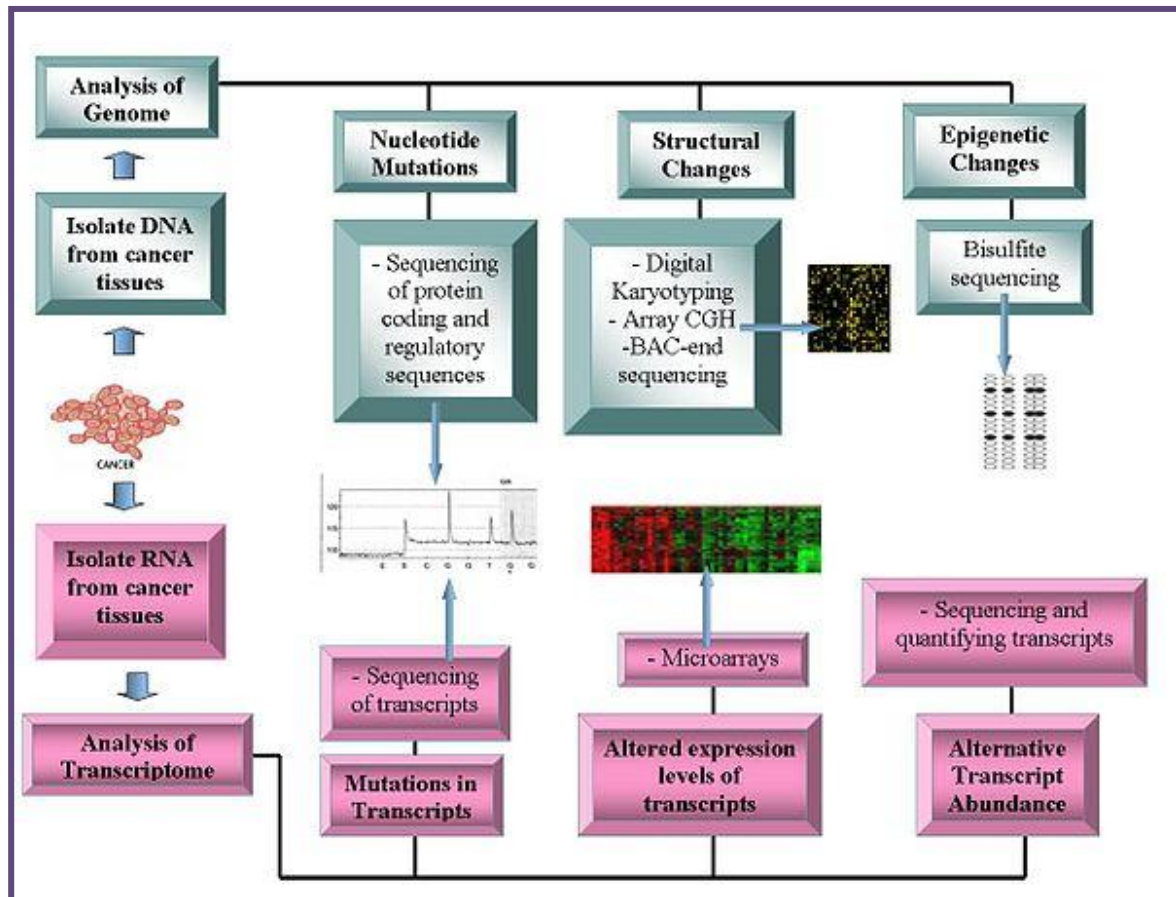
ONCOGENOMICS

DR. H.A.PANDYA

Oncogenomics is a sub-field of genomics that characterizes cancer-associated genes. It focuses on genomic, epigenomic and transcript alterations in cancer.

Cancer is a genetic disease caused by accumulation of DNA mutations leading to unrestrained cell proliferation and neoplasm formation. The goal of oncogenomics is to identify newoncogenes or tumor suppressor genes that may provide new insights into cancer diagnosis, predicting clinical outcome of cancers and new targets for cancer therapies. The success of targeted cancer therapies such as Gleevec, Herceptin and Avastin raised the hope for oncogenomics to elucidate new targets for cancer treatment.
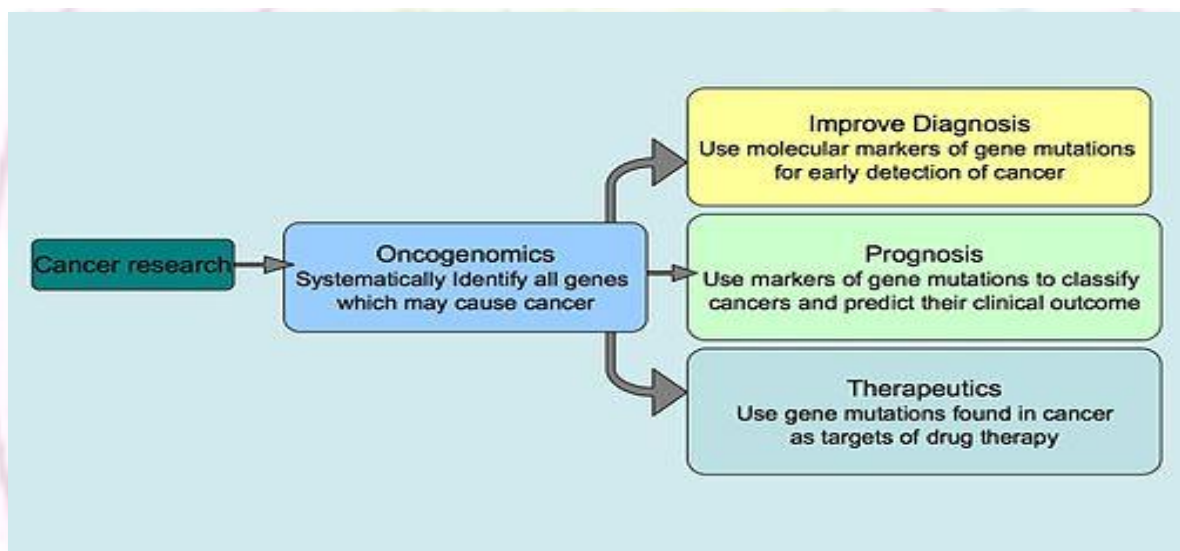
Overall goals of oncogenomics

Besides understanding the underlying genetic mechanisms that initiate or drive cancer progression, oncogenomics targets personalized cancer treatment. Cancer develops due to DNA mutations that accumulate randomly. Identifying and targeting the mutations in an individual patient may lead to increased treatment efficacy.The completion of the Human Genome Project facilitated the field of oncogenomics and increased the abilities of researchers to find oncogenes. Sequencing technologies have been applied to the study of oncogenomics.Several biomarkers can be useful in cancer staging, prognosis and treatment. They can range from single-nucleotide polymorphisms (SNPs), chromosomal aberrations, changes in DNA copy number, microsatellite instability, promoter region methylation, or even high or low protein levels.

Current technologies being used in Oncogenomics

Bioinformatics technologies allow the statistical analysis of genomic data. The functional characteristics of oncogenes has yet to be established. Potential functions include their transformational capabilities relating to tumour formation and specific roles at each stage of cancer development.

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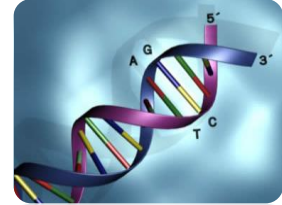
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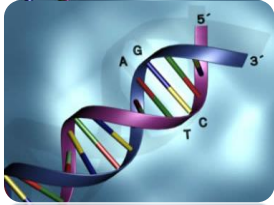
GENOMICS

DRUSHTI BHATT

Bioinformatics was invented by Paulien Hogeweg and Ben Hesper in 1970 as "the study of informatic processes in biotic systems". Paulien Hogeweg is a Dutch theoretical biologist and complex systems researcher studying biological systems as dynamic information processing systems at many interconnected levels. Bioinformatics is an interdisciplinary field mainly involving molecular biology and genetics, computer science, mathematics, and statistics. Data intensive, large-scale biological problems are addressed from a computational point of view. The most common problems are modeling biological processes at the molecular level and making inferences from collected data. Bioinformatics studies include analysis and integration of -omics data, prediction of gene or protein function from sequence and structural information, and cheminformatics comparisons of protein ligands to identify off-target effects of drugs.

Genetics is the study of DNA-based inheritance and variation of individuals, while genomics is the study of the structure and function of the genome. Both apply bioinformatics and computational techniques using data generated from methods such as DNA and RNA sequencing, microarrays, proteomics, and electron microscopy, or optical methods for nucleic acid structure determination. Availability of these and many other new technologies, such as those that can conduct deep sequencing or sequencing of entire microbial communities, is generating massive amounts of data faster than informatics and computational methods can be developed to manage and query them. This opens opportunities for genetics and genomics scientists to develop and apply new cutting-edge technologies to analyze these data.

Genomics includes:

- Functional genomics -- the characterization of genes and their mRNA and protein products.
- Structural genomics -- the dissection of the architectural features of genes and chromosomes.
- Comparative genomics -- the evolutionary relationships between the genes and proteins of different species.
- Epigenomics (epigenetics) -- DNA methylation patterns, imprinting and DNA packaging.

- Pharmacogenomics -- new biological targets and new ways to design drugs and vaccines.

The ongoing genomics revolution, highlighted by the sequencing of the human genome, promises to change how diseases are diagnosed, prevented, and treated. There are tremendous potential to improve health globally. It has been widely predicted that genomics will soon allow us to unravel the genetics of most common diseases and will provide a mechanism for risk prediction for individuals susceptible to a variety of complex disorders.
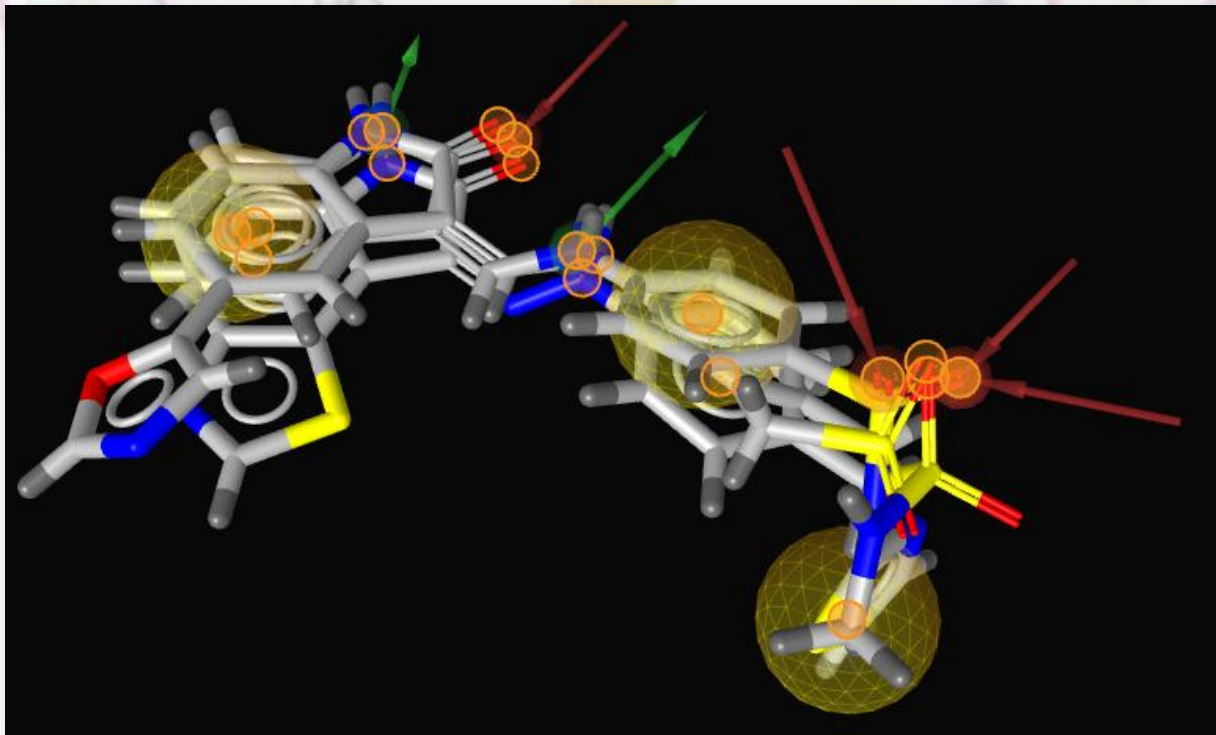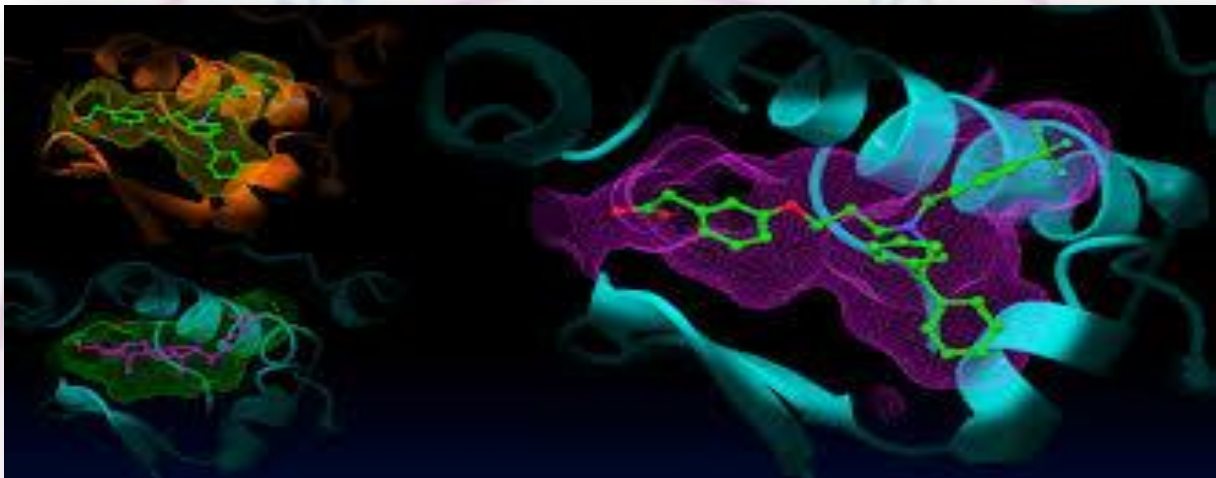
IN SILICO DRUG DESIGN

CHIRAG N. PATEL AND HIMANSHU A. PANDYA

Drug discovery is usually depicted as a continuous, ensuring procedure that starts with target and lead analysis, pursued by lead optimization and pre-clinical *in vitro* and *in vivo* studies to regulate if such compounds satisfy a number of pre-set criteria for triggering clinical evolution. Time and cost required for designing a new drug are massive and at an offensive level. According to time estimates it costs about $880 million and 14 years of research to establish a new drug before it is introduced in the market intervention of computers at some possible steps is important to bring down the cost and time recommended in the drug discovery process.

Today, the process of drug discovery has been revolutionized with the advent of genomics, proteomics, bioinformatics and powerful technologies like, combinatorial chemistry, high throughput screening (HTS), virtual screening, *de novo* design, *in vitro*, *in silico* ADMET screening and structure-based drug design. *In silico* methods can help in analyzing drug targets through bioinformatics tools.

Drug discovery through has been implemented by the use of computers and computational methods today. High-performance computing, data management software and internet are aiding the approach of enormous amount of data provoked and converted the huge complex biological data into workable knowledge in current day drug discovery process. The use of integral experimental and informatics techniques development the chance of success in many stages of the discovery process, from the identification of novel targets and elucidation of their functions to the discovery and development of lead compounds with desired properties. Computational tools offer the advantage of delivering new drug candidates more quickly and at a lower cost. Major roles of computation in drug discovery are; (1) Virtual screening & *de novo* design, (2) *in silico* ADME/T prediction and (3) Advanced methods for determining protein-ligand binding. Also to combat life-threatening diseases such as AIDS, Tuberculosis, Malaria etc., a global push is essential.
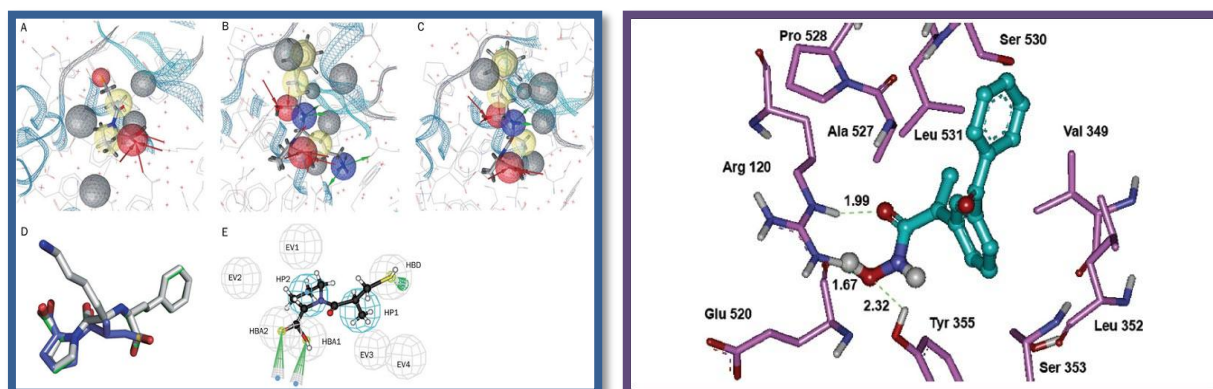
COMPARATIVE ANALYSIS IN BIOINFORMATICS

SHETTY SHILPA S.

Bioinformatics is defining as the application of tools and analysis to capture and interpretation of biological data. It is an interdisciplinary field, which include computer science, mathematics, physics, and biology. Bioinformatics is important for management of data in modern biology and medicine. The main weapon of a bioinformatician is computer software programs and the internet. A primary activity is sequence analysis of DNA and proteins using various programs and databases available on the World Wide Web. Bioinformatics is an growing discipline, where professional bioinformaticians use complex software programs for retrieving, sorting out, analysing, predicting, and storing DNA and protein sequence data. Paulien Hogeweg, a Dutch system-biologist, was the first person who used the term "Bioinformatics" in 1970, as the use of information technology for studying biological systems.

Bioinformatics is the study of the application of computer and statistical techniques to manage biological information, including development of methods to search databases quickly, to analyze DNA sequence information, and to predict protein sequence and structure from DNA sequence data. Comparative genomics is the study of comparison between genomes across species, which includes structural or functional genomics and evolutionary genomics.
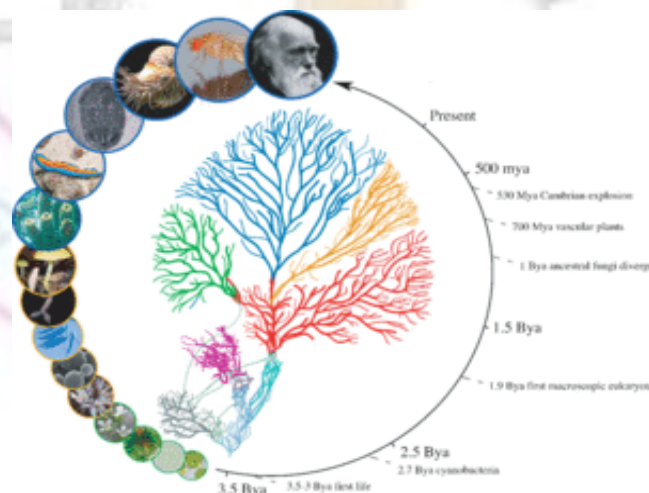

In bioinformatics, it is used to compare gene numbers, gene locations & biological functions of gene, in the genomes of different organisms. One of the main objectives is to being to identify groups of genes that play a distinctive biological role in a particular organism.

Computational approaches to genome comparison have in recent times become a widespread research topic in computer science. Two very large issues are immediately apparent in undertaking the sequencing of entire genomes are (i) The huge numbers of species and the much larger size of some genomes which makes the entire sequencing of all genomes a non-optimal approach for understanding genome structure. (ii) Second, within a given species most individuals are genetically distinct in a various way.

These two problems, and the potential for other novel applications, have given rise to new approaches which, taken together, form the field of comparative genomics. Because all modern genomes have arisen from common ancestral genomes, the relationships between genomes can be studies with this information in mind. This union means that information gained in one organism can have relevance in other even distantly related organisms. The nature and significance of differences between genomes also provides a potent tool for determining the relationship between genotype and phenotype through comparative genomics and morphological and physiological studies. It provides a potent way in which to analyze sequence data. Using comparative genomics, the genome sequences of different species - human, mouse and a wide variety of other organisms from yeast to chimpanzees are compared. Another application of comparative analysis is comparative proteomics which is to analyze proteome changes in response to development, disease, or environment.

Comparative information has the capability to both decrease the cost and accelerate mapping and sequencing projects by reducing experimental attempt. Various comparative mapping and sequencing methods have previously been set in practice. Future requirement for comparative mapping and assembly is responsible to be driven by two trends: the increasing accessibility of reference genomes as potential templates for assembly and advances in sequencing technology. If existing trends continue, comparative assembly of individual human genomes and even diagnostic sequencing of individual tumor samples will become an everyday practice.

Various challenges will have to be beat along the way to efficient gigabase-scale sequence assembly. Other is the development of computational means for fast and accurate sequence anchoring based on all against all comparisons of exponentially rising sequence databases. Another major challenge is the development of comparative mapping and assembly methods and their organized characterization and validation.
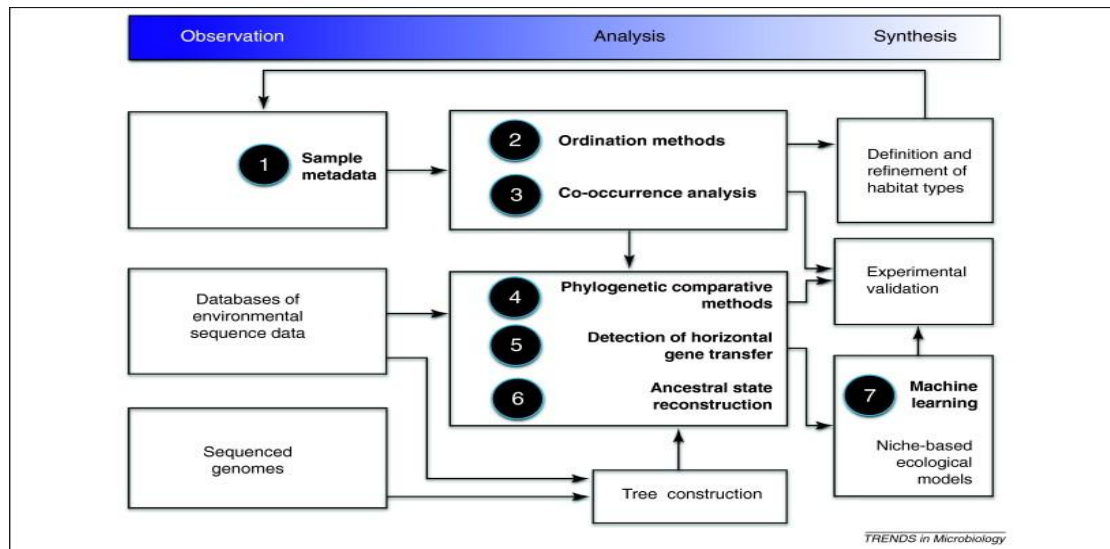
Many databases and computational tools were available for comparative analysis of prokaryotic genomes like: BacMap, CMR, IMG, MicrobesOnline, PUMA2, GenoMycDB, LEGER, xBASE, ShiBASE, HAMAP, IslandPath, KEGG, MetaCyc, OMA Browser, ProtRepeatsDB, ORFanage, SEED, STRING, TransportDB, BPhyOG, Phydbac, Genome Properties, ACT, CGATGeneOrder3.0, GECO, GenomeViz, MuGeN, GenomeBlast, MUMmer, GenomePixelizer, PipMaker, PipTools, MultiPipMaker, zPicture, VISTA, etc and many more.
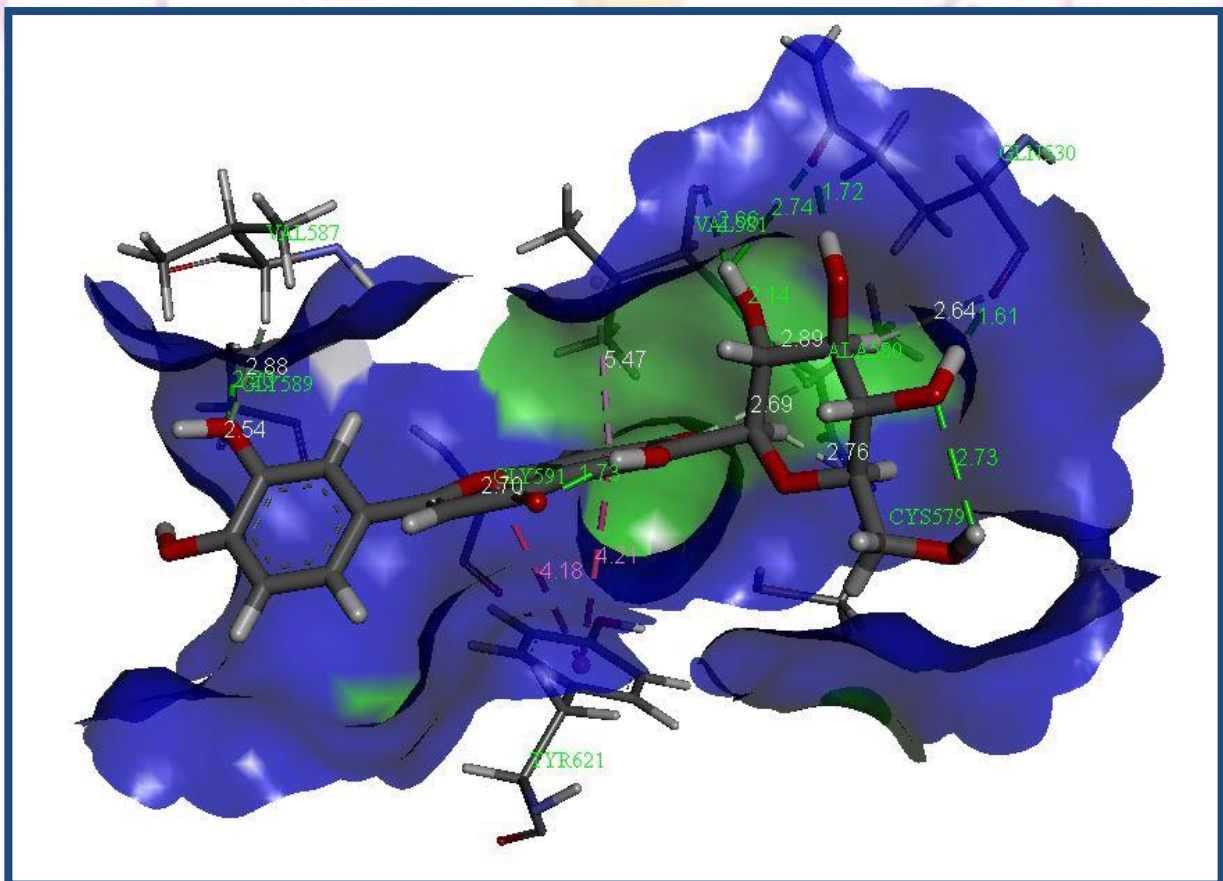
HUMAN MICROBIOME PROJECT

SWETA TRIPATHI

The human body hosts contains diverse microbial population. Human microbial cells are plays a important role in genetic contribution of development, physiology, immunity, and nutrition. The United States National Institutes of Health initiative with the goal of identifying and characterizing the microorganisms which are found in association with both healthy and diseased humans (the human microbiome). Human contains enormous number of micro-organism in their gastrointestinal flora which is known as "a virtual organ of human body". Human Microbial Project (HMP) aims to generate resources to define these microbial communities and to investigate their roles in health and disease.

The HMP is an interdisciplinary area in which researchers isolating pathogens and growing them in a culture. This tedious process identifies only few microbial species. Now, they will go for the DNA sequencing. On the basis of these results researchers conclude that the human microbiome contributes 8 million unique protein-coding genes or 360 times more bacterials genes than human genes.

Numerous medical studies has been done by NIH using HMP data and techniques, including the role of the gut microbiome in Crohn's disease, ulcerative colitis and oesophageal cancer; skin microbiome in psoriasis, atopic dermatitis and immunodeficiency and a number of childhood disorders, including paediatric abdominal pain, intestinal inflammation, and a severe condition in premature infants in which the intestine actually dies.

A series of studies has been carried out to evaluate the ethical, legal and social implications of microbiome research. A number of serious issues already have been identified, ranging from how products designed to manipulate the microbiome such as probiotic concoctions that include live beneficial microorganisms useful for economically, medicinally purposes.

DATABASE CREATION IN BIOINFORMATICS

RIKIN D. PATEL

Bioinformatics is merger of biology with information technology. It includes computational tools to manage, analyse and manipulate large collection of biological data. Bioinformatics include many types of biological data like nucleotide sequence, protein structure, gene expression profiles, protein interaction and system biology. The term bioinformatics coined by Paulien Hogeweg in 1979 for the study of informatics processes in bioitic system.

In the early time of computer technology, the main use of computer programs was to store and manipulate data. These programs recorded the data on disk according to their own structures. All programs that were not familiar with the structure of the data were not capable to use them. If various programs needed to share data from the same file or needed to change the data structure, all other programs would have to be changed, even if the alteration took place in data that was not manipulated by all the programs. In order to stay away from this problem, an intermediate system was set up to convert the data from the format they were recorded in the file to the specific format renowned by each program.

With this intermediate program, the following circumstances occurs: (a) The programs "see" only the data that they have to interact with; (b)The programs don't need to be familiar with the details of the physical recording of their data; (c)The programs don't have to be customized when the data structure is modified; (d)The alterations are determined in this intermediate system. Ultimately, these intermediate systems were able to administer many different files. This group of files was named **Database** and the intermediate system became known as **Database Management System** (or **DBMS**).
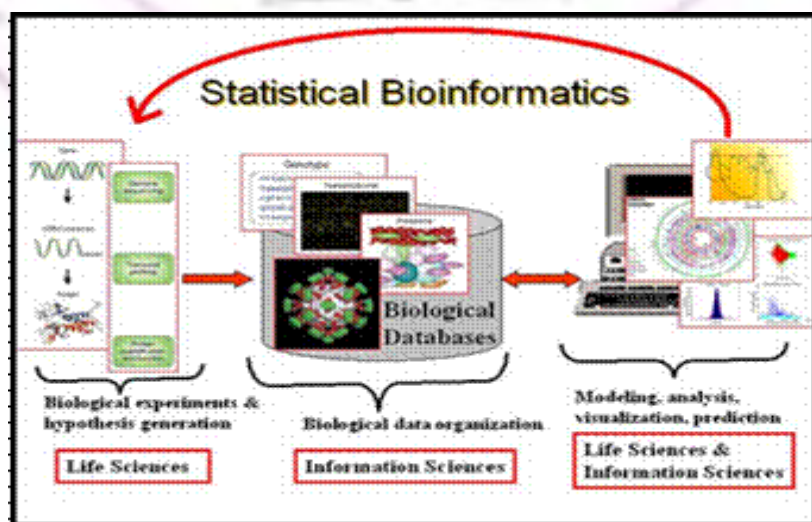
According to the contents and distinctiveness of bioinformatics database, they can be classified as a primary or secondary database. Primary databases consist of gene related data as well as nucleic acid, protein sequences, with information regarding features of the nucleic acid, amino acid sequences and biochemical reactions, metabolic pathway, etc. On the other hand, secondary databases are created based on primary databases and the information derived from the primary databases.

In short, Bioinformatics deals with database creation, data analysis and modeling. Data capturing is done not only from printed stuff but also from network resources. Databases in biology are usually in the multimedia form organized in relational database model. Modeling is done not only on lone biological molecule but also on multiple systems thus requiring a use of high recital computing systems.

It is useful in various fields linking biological data. One of its uses is in pharmaceutical companies to design modern prescription drugs modified to the specific needs of individual people and doctors could take action more rapidly to changes in bacteria and viruses that effect them to become drug-resistant. On the basis of the recent press release of IBM, "One day, you're going to be able to walk into a doctor's office and have a computer analyse a tissue sample, identify the offending pathogen, and then instantly prescribe a treatment best suited your specific illness and your genetic makeup."

According to the pharmaceutical industry, bioinformatics is the key to rational drug discovery. It reduces the number of trials in the screening of drug compounds and in identifying potential drug targets for a exacting disease using high power computing workstations and software. This reflective application of bioinformatics in genome sequence has led to a new area in pharmacology – Pharmacogenomics, where potential targets for drug development is hypothesized from the genome sequences. Molecular modeling which needs a lot of calculations has turn out to be faster due to the advances in computer processors and its architecture.

METABOLOMICS - AN ARRAY OF POTENTIAL OPPORTUNITIES
PUJAN N. PANDYA

In the current scientific research era with -omics, being a buzzword Metabolomics, turns out to be a rapidly emerging omics field being primarily concerned with the comprehensive characterization of the biological molecules in a wide array of living systems, often beingreferred to as a large scale study of small molecules. Development of metabolomics in an integrated field of life sciences offers a growing heap of opportunities in the world of scientific and technological research and advancements.

As a matter of fact, each type of cells and tissues has its unique fingerprint that helps in elucidation of organ or tissue specific information. This data is biologically dynamic and extensively deep rooted, which further plays a major role in qualitative measurement of a system's metabolic activities. Historically as well, it is known that each individual possesses a metabolic profile that reflects in their biological and biochemical makeup. Currently, through the rapid advancements in technological evolution of instrumentation and biotechnological arenas, metabolomics and the other related bioinformatics fields have an important role to play in various fields of research ranging from environmental science to the diverse pathological fields.

Metabolomics through its diverse techniques has a major emphasis on Metabolic profiling from cellular to the organ level and to the further integrated organ system level. The gene expression data and its further proteomic analysis, reveals a set of gene products produced in a cell, however through the lens of metabolic profiling one can instantly have a quick insight through the physiology of that cell and the further organ and organ system. Furthermore, one of i its major focus is on widely and rapidly growing diseases such as diabetes, cancer etc. that is rampant worldwide. With the help of bioinformatics and technological advancements the potential of metabolomics is being explored in early detection of severe diseases, which plays a commendable role in systematic treatment of fatal diseases. Metabolomics thus

accurately gathers information from the other related -omics fields and gleans the relevant data for further analysis and development of novel techniques such as disease screening, its network analysis, novel biomarker development etc. for further research and methodological treatment at varied stages of disease progression and metastasis.

Metabolomics has gained commendable success in bridging the gap between its varied sub branches, by demonstrating its worth in linking different metabolomes by overcoming several challenges in molecular pharmacology and pharmacokinetic studies for multi-component therapeutics for different diseases. Metabolomics, surely offers a bright ray of hope on horizon with creative possibilities, clenched in its fist, which is about to open new frontiers in upsurging the marvels in the field of research.
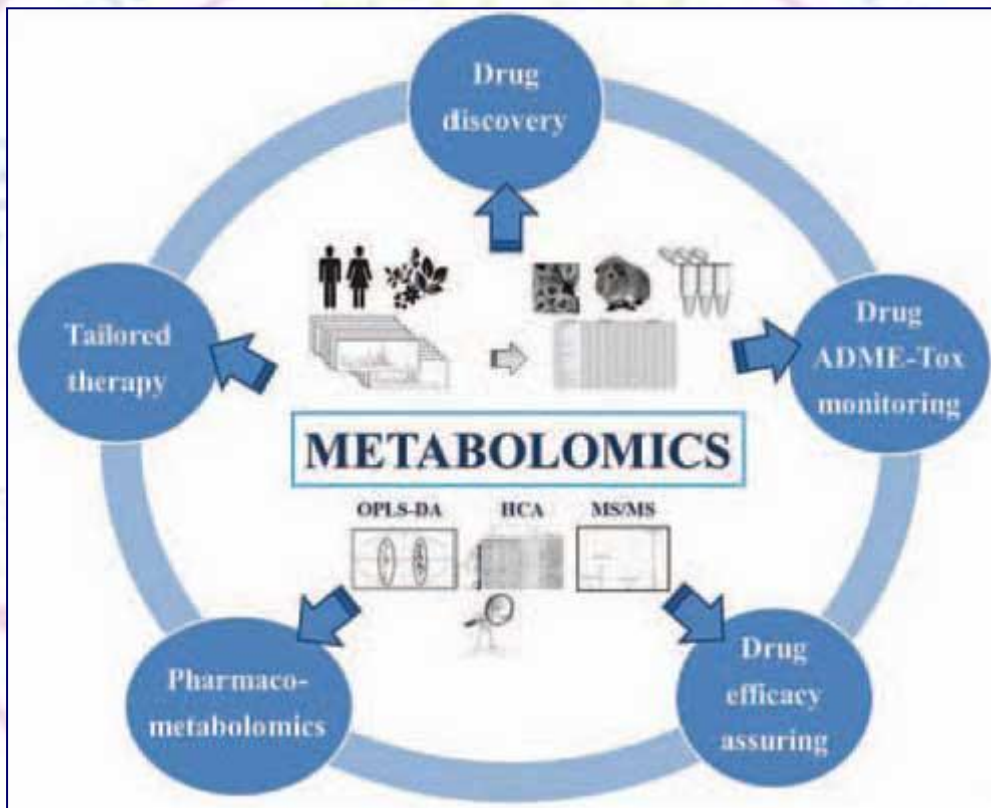
*Courtesy: www.benthamscience.com

JOURNEY OF MEDICINAL WORLD

WITH BIOINFORMATICS

KUMARI RASHMI

Bioinformatics is the application of tools of computation and analysis to the capture and interpretation of biological data.

Research in Bioinformatics focuses on development of novel algorithms and architectures for genomics, proteomics, and microarray analysis. The interested areas include protein-protein interaction network analysis, microarray data analysis, high dimensional data visualization, computational analysis and interpretation of Genomes, protein structure prediction, comparison, and modeling, evolutionary studies of Genomic ORFans, molecular recognition and docking of ligands onto receptors.Useful bioinformatic websites which are available freely on the internet are National Center for Biotechnology Information which maintains bioinformatic tools and databases, Genbank, Unigene , European Bioinformatic Institute, Ensembl, SWISS-PROT.Bioinformatics is very important for the use of genomic information to understand human diseases and to identify new ways for gene-based drug discovery and development. **Genomics** is the study of complex sets of genes, their expression and the most vital role they play in biology. Genomics has greatly accelerated fundamental research in molecular biology.The most important application of bioinformatics in genomics is the **Human Genome Project** through which more than **30,000 genes** have been identified and secured through the sequencing. It has thus enabled us to obtain necessary knowledge as to how these genes inter-relate and what functions they perform. Furthermore, next-generation sequencing (NGS) provides researchers with complete gene and genome sequences. Much of the data that are produced by the genomics community become freely available and this resulted in the development of many biological databases. The two most important applications of genomic medicine are as follows: The identification of genes and pathways and the elucidation of their role in health and disease. This will enhance our basic understanding of the molecular processes underlying disease and identify new targets for drug development. The millions DNA sequences fragments produced by new generation sequencers are sorted and assembled with sophisticated bioinformatics software.

VIRTUAL SCREENING IS BLESSING FOR DRUG DISCOVERY

MEHUL SONI AND JANKI GORJI

The drug discovery is the process through which potential new medicines are identified and reduce mortality and morbidity of the disease. This drug development process is a complex process, which can take 12–15years, and cost in excess of $1 billion. It's a time taking and costly procedure.The process of drug discovery/ design mainly stages Target and lead identification and optimization after clinical trials and FDA approval. The drug discovery has an initial stage of target and lead identification and optimization process are made easy, fast and time consuming by virtual screening.
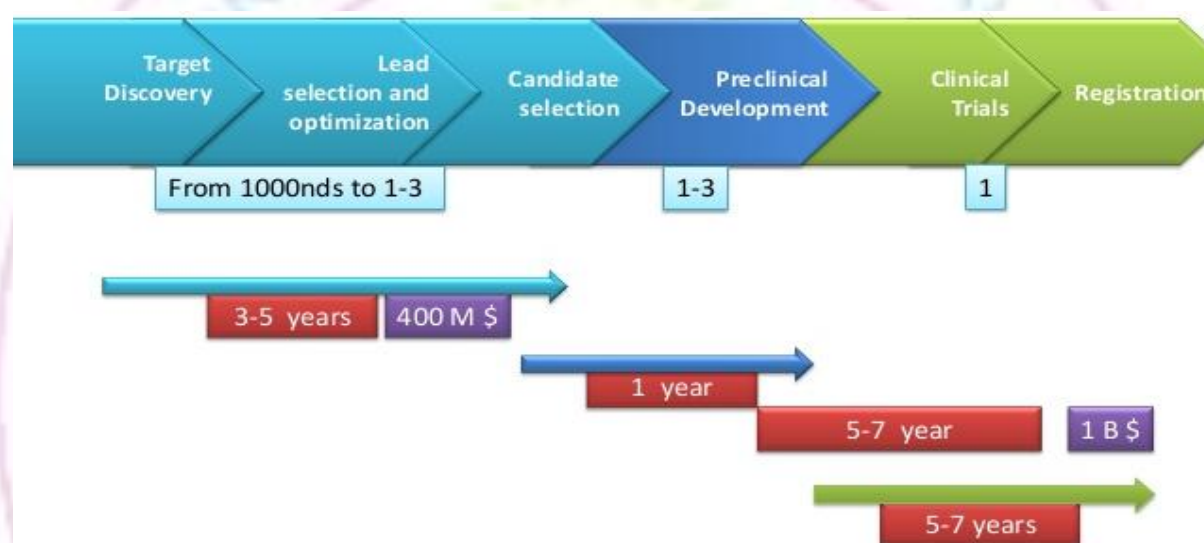

Figure: Drug Discovery pipeline

The virtual Screening is a computational approach to assess the interaction of an *in-silico* library of small molecules and the structure of a target macromolecule to rapidly identify new drug leads. It's also defined as the "automatically evaluating very large libraries of compounds" using computer programs. There is a wide range of comparative and contrasting methodological protocols available in screening databases for the lead compound identification using the number of methods and software packages. The virtual screening evaluates drug likeliness of small molecules, drug like molecules exhibit favourable absorption, distribution, metabolism, excretion, toxicological (ADMET) parameters. There are two generally accepted approaches for virtual screening: structure-based and ligand-based methods.

The structural based virtual screening methods begin available protein target which determined by NMR, X-ray crystallography or homology modelling and with the

identification of a potential ligand-binding site also called the active site on the target molecule. In this method, the protein structure as a biological target, the small molecules of library candidate drugs that are predicted to bind with high affinity and selectivity to the target using computer software and tools. This process is also called docking process. Many computational software and tools such as GOLD, autodock, YASARA, V-life, Flex, Hex, etc. are used for docking.

In ligand-based methods, the most effective biologically active lead molecule is detected using structural or topological similarity or pharmacophoric similarity search. Taking into consideration several criteria such as structure as well as shape of individual fragment or electrostatic properties of the molecule carries out the similarity comparisons. The leads generated are ranked based on their similarity score, obtained using different methods or algorithms.

The combination of the above mentioned structure and ligand-based strategies are also becoming a desired and common path for researchers and different methods, including sequential and parallel approaches. Hybrid approaches, in which ligand- and structure-based applications are truly moulded together (protein-ligand pharmacophores) and integrated into one standalone technique to enhance accuracy and performance.

The advantages of virtual screening are fast process and to reduce the enormous virtual space of chemical compounds (a practical virtual library might comprise $\sim 10^{15}$ molecules) to a more manageable number for further synthesis and screening against biological targets, which could lead to potential drug candidates. Some disadvantages of virtual screening are limited number of available compounds and synthetic accessibility of virtual hits is a problem. In addition to pointing out the recent developments, some major pitfalls and challenges still need to be solved in order to handle the exponentially increased volume of data compound and biological activity information expected soon to be unleashed as a consequence of entering the new genomic era.

LESSONS FROM NATURE

Dr. Archana Mankad

Fire devastates..fire destroys. Yet it is also a reason for life. Fire grows, and as it spreads, it creates new fires that spread out and make new fires of their own. Fire fights for territory, it loves and hates. Fire doesn't settle; fire doesn't tolerate. After a wild fire in the forest there are species that bloom, others germinate their seeds, while most grow. Because life has to go on. Plants that perished made way for others to take over. The scorching made the seeds germinate and the buds bloom.

Difficult times in our lives are like fire. They test our patience, our conviction and our strength. Holding on to our ideals and principles inspite of all odds is a courageous act. Each one of us has a fire in our hearts burning for something. It's our responsibility in life to find it and keep it lit. This is our life and it's a short one. Let us not let others extinguish the flame. Let us TRY what we wanted to try. Let us GO where we wanted to go. Let us Follow our own intuition and realize our dreams.
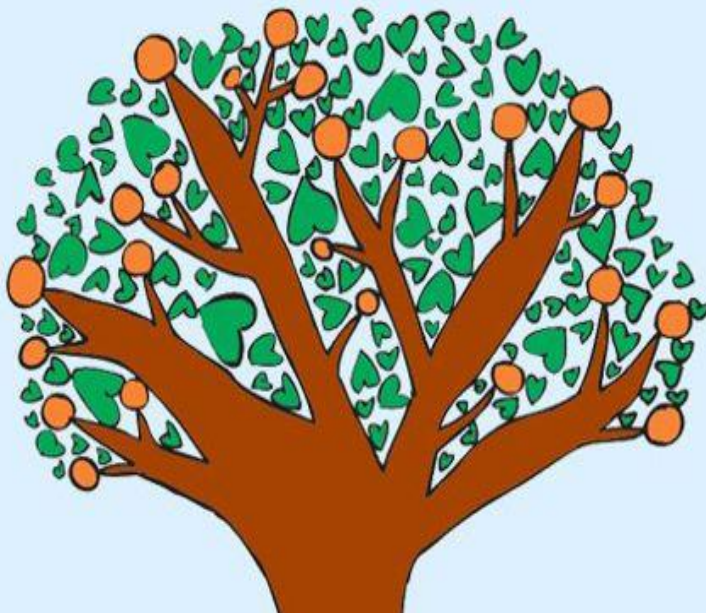
Set your life on fire. Seek those who fan your flames.

GLIMPSES OF GUJARAT UNIVERSITY BOTANICALS SOCIETY ACTIVITIES   DECEMBER 2015-MAY-2016

Visit to Science City- 1st September, 2015.

Students reached Science city around 10 a.m. accompanied by Megha mam. Following her instructions, they first decided to see "Energy Park". This park had different sources of energy production from wind energy, solar energy, solar energy, geothermal energy. At the entrance of the park, there was a board. The board was divided into 12 subparts. So each part was designed in such a way you can easily compare how technology from Ancient time to our time. Alpesh one of the research scholars read and described the story of a Grandmother which described how she used to live in the early stages and how technology has changed our lives so much. Then Megha mam started explaining to the students how turbine works, she told them that each street light they saw in Science city had solar panel above it so basically solar panel above the light takes the energy from the sun and use it. Then the students were taken towards Petroleum oil rings where they were explained how the production of petroleum takes place, then to Bio-gas plant, project of Sardar Sarovar dam, then the students also saw the Solar cooker. Atlast, students visited solar house where they explained all about energy generation i.e. solar house had 24 panels above it which is directly attached to 12v battery, so that the stored energy in that battery can be utilized in the house. Thereafter, students visited "Life science" Park, where they saw different forms of life. In Life Science Park, they saw Aromatics and Medicinal plants. All these activities were interesting and gave them hands on experience. Thereafter, they reached IMAX. IMAX is a big 3D theatre with advanced technology. Students collected their 3D glasses from the counter and went inside the theatre and decided to watch Hubble. Hubble is actually space telescope, so, the documentary described the NASA Astronauts mission to perform maintenance and repair Hubble telescope. The documentary was never seen before experience as it described the life of scientists, problems faced by them. Then, students had a break. After little rest, students moved for lunch into "Planet Earth". Planet Earth was a unique dome structure and it was surprising for all to know that it is one of the largest dome in India. In the planet Earth, we started with coal mine, for that we went to ground floor of the dome, but part of the dome was that one could feel as if you are going at the depth of around 3000 feet from the Ground level. The guide-in charge explained how mining process is done. He told that how different mine workers and machine are used to dig the wall of coal. How the cutting machine and other equipments were used. After that students visited the "Planetarium". Planetarium was basically semi-circular made dome where they explored the universe through space film, film

described how the universe is made, what are stars, comets and how the energy get transformed when one star crossed the other. Then the students went to the third floor of the building which included the information related to different types of rocks and minerals. How different soils give the production of different crops and pulses. Then, the student had an activity that is "Earthquake experience" where they get into the room in order to feel the earthquake. Room had television installed where professor explained how earthquake happens and the types of Earthquake. The students enjoyed their visit to science city and the day ended with both knowledge and fun. The entire trip was very informative and created huge interest among the students.

Students at Gujarat Science City with Dr. Megha Bhatt

Visit to Polo Forest-15th September, 2015

The students of climate change and impact management, Department of Botany, Bioinformatics and Climate Change and impacts management were taken for field visit at polo forest by the professor Dr. Megha Bhatt, accompanied by other administrators and research scholars. Polo forest is in Vijaynagar which comes under district Himmatnagar is a great heritage and a natural scenic place between a town. It is 80 km away from Ahmedabad and it takes 2.5 hours to reach the destination. It is surrounded by Aravalli ranges. It is a mixed deciduous forest and gives shelter to a lot of wild species of plants and animals. It is a beautiful place to visit during weekends. Students left for Polo forest on 15th September, 2015 early in the morning. At around 12 pm students reached the forest. The campsite at Polo forest was looked after by Mr. Mayur Rathod. He is a biodiversity Naturalist, who took care of a part of forest and also, conducts camps for students and youngsters. The students had an interaction session with Mayur sir and they were introduced with some rules and regulations which they had to follow in campsite. The students then visited the base of the forest. They started inside the forest and walked along the line safely. The students were accompanied by

a tribal person, Megha mam and research scholars who introduced them to the wild plant and animal species. The most amazing experience was to walk along those big stones seeing *Gloriosa superba*, a rare plant species and it also looked like flames. They saw a signature spider too. The students saw Shikakai tree with dried fruits. This place also had a lake like water body in which the local children came to swim. The students played and swayed on the entrance of the campsite where there was a huge banyan tree. In the evening, they visited a local dairy. In the dairy, they saw a machine which tells how much water is added in the milk. It allowed only some acceptable amounts but not more than that. The students were explained that after supplying enough milk to the villager the extra only went to the dairy and then to bigger processing unit for further supply. After returning to the base camp, students taught meditation and they interacted with each other regarding the dairy industries, agriculture and also talked regarding meditation. After the interaction, students had dinner. Then they went for star gazing. For all the students, it was the first experience of star gazing in an informative manner with the help of lazer beam, sir introduced them the famous constellations. The students saw constellations like Cassiopeia, Gandhi star, Saptarishi, Jesus cross etc. Next day students were lucky to watch bird like grey hornbill. After breakfast students left for trekking and with great efforts students reached the top and saw the amazing scene of the whole place. They saw a variety of species of butterflies. On the way downwards students saw amla trees. Students reached the polo heritage in the afternoon. After that, they visited Harnav dam. The students saw millions of fireflies there. The sight was magical. They also felt fireflies on their palms. The students had an amazing time amidst nature and experiencing and gaining knowledge.

Students at the Polo forest with Dr. Megha Bhatt

Visit to BISAG- 5th January , 2016

On 5th January, 2016, the students of Gujarat University Botanical Society had visited GEER Foundation and BISAG. At around 2.30 pm students reached BISAG, situated in Gandhinagar near infocity. BISAG stands for Bhaskaracharya Institute for Space

Applications and Geoinformatics. BISAG is a state level agency by Govt. of Gujarat to facilitate, to provide service and solution in implementing map based geospatial information system. Dr. Megha Bhatt accompanied the students. She explained about the infrastructure of BISAG and students were shown the display session and presentation regarding the establishment of BISAG, its ownership, how it came under work and more. After the presentation, Director of BISAG taught the students about BISAG, its SATCOM Network and the mechanism. They were given knowledge about various satellites and Remote Sensing Applications. The lecture was very much informative and fruitful to the students. After the lecture, students went to see the different system and technical working part of BISAG. There they found that it comprised of 2 studios from where Honourable Prime Minister and our state's Chief Minister deliver the speech and also, some of the issues and programmes that are directly telecast from there. Dr. Megha Bhatt also showed a demo on the same by saying a few lines on camera. The clarity and resolution of the entire system was amazing. The visit to BISAG was a very informative experience for the students.

Dr. Megha Bhatt with the students at BISAG

Days Celebrations and New Year Celebrations-2016

The Gujarat University Botanical Society celebrated its annual cultural festival and the New Year in the form of purposeful theme days. Each day witnessed participation of the members in various competitions coordinated by different student groups. The group day- "Hum Saath Saath Hain"-6th January,2016, Sports Day-Khiladiyon ka Khiladi-7th January, Food Mad- "Food Festival 2016"-8th January, Rangoli, Toran Making, Mehndi, Best from Waste, Vegetable carving, flower arrangement competition-9th January, Traditional wear day-11th January, Each one teach one, Kite flying Day, Share and Care-12th January, 2016. The **FOOD FESTIVAL** on 8th January-2016 was a big hit with one and all as visitors enjoyed the mouthwatering delicacies prepared by the students. The students got a hands-on-experience of handling, managing and coordinating various aspects of the festival. The

students participated with great enthusiasm and the thrust was on entrepreneurship and teamwork. The whole event was managed by students.

"Hum Saath Saath Hain"- Group Day Celebration through group activities and plays.

3- legged Race   Football games
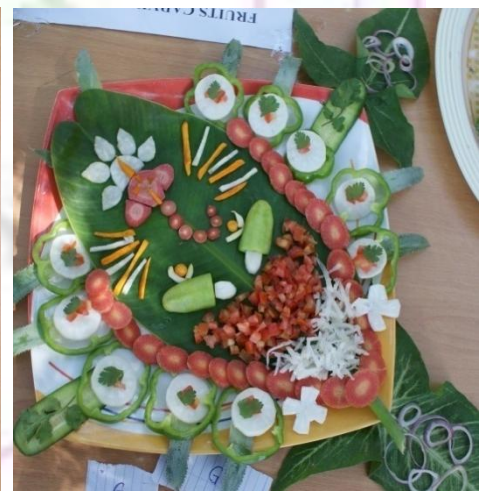
Darts Game

Badminton

Khiladiyon Ka Khiladi- Sports Day 2016

Salad decoration, Fruit and Vegetable carving competition

The people enjoying various delicacies at the food fest

Judges tasting and judging the various delicacies during the competition

Workshop on Financial Planning-Ms. Palak Lotiya (SEBI)-12th February, 2016

The **Workshop on financial Planning for Young Investors** was organized with the help of Ms.Palak Lotiya-12th February, 2016, certified trainer from SEBI. The session started with a video presentation of "One Idiot-an IDFC initiative" which conveyed the essence of the workshop very effectively. Ms.Palak explained the need for saving, appropriate investment and the risks to be taken care of to the participants.

Ms. Palak Lotiya explaining about financial planning and investment

Visit to ISRO- 9th March,2016

Students of Climate Change Impacts Management had gone on a visit to ISRO (Indian Space Research Organization) on 9th March, 2016, where they visited VSSE- Vikram Sarabhai Space Exhibition. VSSE was created by Dr. Vikram Sarabhai in the year 1962.Around 11.30 am students gathered at ISRO. The students were accompanied by Dr. Kashyap Mankad, who explained to students all about the history of ISRO, working of ISRO and various branches of ISRO in our country. Ahmedabad branch is known as SAC. SAC-ISRO is a communication centre. Dr. Kashyap Mankad, gave brief introduction about satellites, uses of payloads, sensors, fuel requirements and other features, types of satellites according to their range of rotation and disturbance, PSLV, GSLV and ASLV Rockets. He also mentioned that GSLV and PSLV are sent from Trivandrum and their fuel is obtained from TamilNadu. He also explained about ISRO's role in making MANGALYAAN and gave the students knowledge about Remote Sensing and its applications. The visit to ISRO was a fruitful one as it created curiosity and increased the knowledge and interest for Space Science, Applications and Remote Sensing among the students.

Students at SAC-ISRO   Students learning about satellites

Students visiting the Exhibition at SAC-ISRO

Annual Function of GUBS-12th April, 2016

The Annual Function of Gujarat University Botanical Society was arranged on 12th April, 2016. Shri S.N. Tyagi, IFS (Mission Director, Gujarat State Biotechnology Mission) was the Chief Guest. The function witnessed over 100 prizes and certificates distributed to the winners and the participation in various events throughout the year like Quiz, One Minute Games, Elocution and much more. This year the prestigious **GOLDEN PETAL AWARDS** were awarded to meritorious students by Tyagi sir.

Dr. Archana Mankad addressing the audience   Dr. Himanshu Pandya welcoming the Chief Guest

Fulesh welcoming Dr. Hitesh Solanki   Shri S. N. Tyagi,IFS addressing the students

Winners being felicitated with certificates and prizes

Golden Petal Awards : 2015-16

Congratulations to the winners

A) GOLDEN PETAL AWARD FOR EXCELLENCE:

- The Golden Petal award for excellence in Management was awarded to SHIRIN QURESHI
- The Golden Petal award for excellence in Management was awarded to ALAY MEHTA
- The Golden Petal award for excellence in Management was awarded to DHARMESH JAISWAL

B) GOLDEN PETAL AWARD FOR ENTREPRENEUR OF THE YEAR:

- The Golden Petal award for Entrepreneur of the year was awarded to COLACO IMANUEL FRANCIS

C) GOLDEN PETAL AWARD FOR ACADEMIC ACHIEVEMENT:

- The Golden Petal award for Academic Achievement was awarded to ROHAN THAKKER for JRF to SRF upgradation and Prize in Science Excellence 2015.
- The Golden Petal award for Academic Achievement was awarded to NIRMAL DESAI for JRF to SRF upgradation and Prize in Science Excellence 2015.
- The Golden Petal award for Academic Achievement was awarded to MONA PARMAR for JRF to SRF upgradation and Prize in Science Excellence 2015.
- The Golden Petal award for Academic Achievement was awarded to QURESHIMATVA UMERFARUQ for JRF to SRF upgradation and Prize in Science Excellence 2015.
- The Golden Petal award for Academic Achievement was awarded to RIKIN PATEL for JRF to SRF upgradation.
- The Golden Petal award for Academic Achievement was awarded to CHARVI PANDYA –Topper Internal Exam, Prize-Science Excellence 2015.
- The Golden Petal award for Academic Achievement was awarded to MADHAVI SINGH- Topper Internal Exam, Prize-Science Excellence 2015.
- The Golden Petal award for Academic Achievement was awarded to HARSHIDA GADHAVI- Topper Internal Exam, Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to DIVYANI PANCHAL- Topper Internal Exam, Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to PATHIK BHATT - Topper Internal Exam.

- The Golden Petal award for Academic Achievement was awarded to JALJA CHAVDA - Topper Internal Exam, Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to NEHA JHA-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to MEHUL SONI-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to PUJAN PANDYA-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to MITI PANCHOLI-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to VINAL PATEL-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to VIDHI PATEL-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to ZARNESH KANOJIA-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to BHOOMIKA VAGHELA-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to SHILPA SHETTY-Prize-Science Excellence 2015.

- The Golden Petal award for Academic Achievement was awarded to KAJAL SHAH - Prize-Science Excellence 2015

D) GOLDEN PETAL AWARD FOR OUTSTANDING ACHIEVEMENT

- The Golden Petal award for Outstanding Achievement was awarded to RENUKA DESAI, ACF, Govt. of GUJARAT.

- The Golden Petal award for Outstanding Achievement was awarded to SHILPA SHETTY, Prize -National Symposium-Rajkot.

- The Golden Petal award for Outstanding Achievement was awarded to MEHUL SONI, Prize -National Symposium-Rajkot.
- The Golden Petal award for Outstanding Achievement was awarded to KAJAL SHAH, Prize -National Symposium-Rajkot.
- The Golden Petal award for Outstanding Achievement was awarded to ANJANI PANDEY, Prize -National Symposium-Rajkot.

E) GOLDEN PETAL AWARD FOR STUDENT OF THE YEAR

- The Golden Petal award for Student of the Year was awarded to CHARVI PANDYA.

F) GOLDEN PETAL AWARD FOR RESEARCHER OF THE YEAR

- The Golden Petal award for Researcher of the Year was awarded to UMERFARUQ QURESHIMATVA.

G) GOLDEN PETAL AWARD FOR PRIDE OF DEPARTMENT

- The Golden Petal award for Pride of Department was awarded to S. PRASANTHKUMAR for DBT- RA.
- The Golden Petal award for Pride of Department was awarded to Dr. SAUMYA PATEL-NPDF-SERB (SCIENCE AND ENGINEERING RESEARCH BOARD), DST

Recipients of GOLDEN PETAL AWARDS

S.N. Tyagi sir giving the GOLDEN PETAL AWARDS to students

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