Topic: Bioinformatics
Subject: Pharmaceutical Biotechnology
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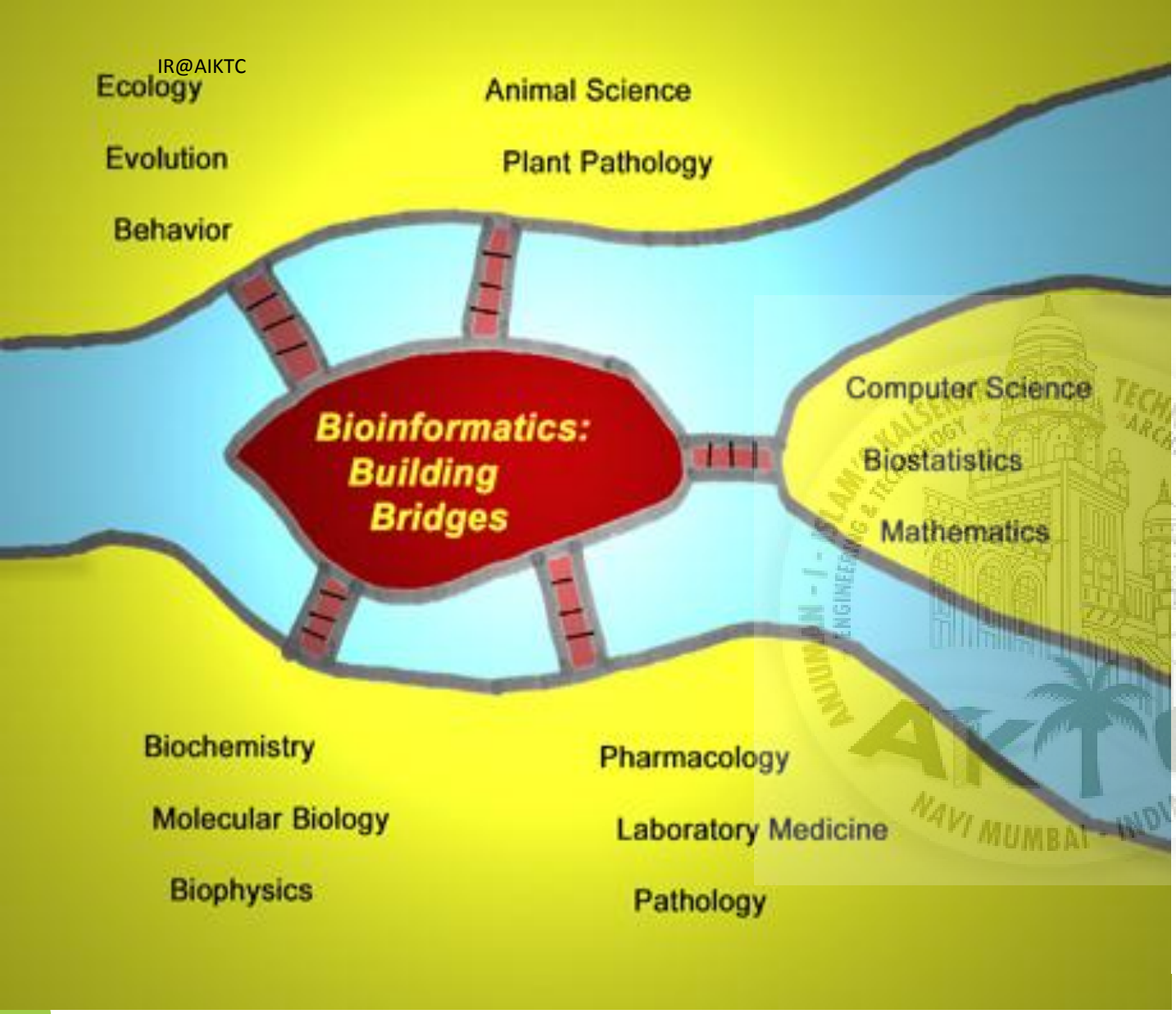
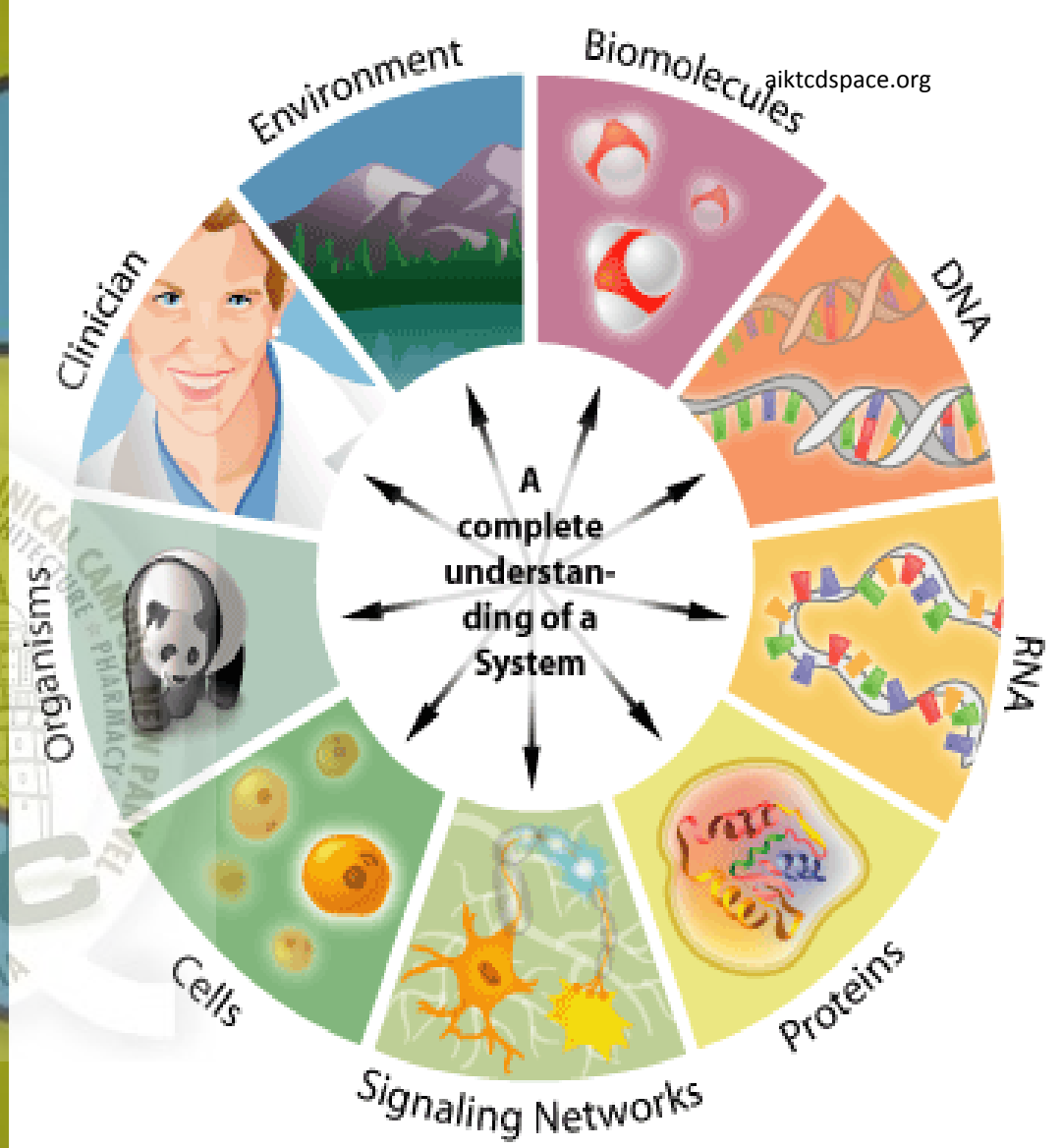
	Topic Learning Outcomes	COs	BL
1.	Explain Bioinformatics, history & applications in pharma industry	CO1	L2





Biologists
collect molecular data:
DNA & Protein sequences,
gene expression, etc.

Bioinformaticians
Study biological questions by analyzing molecular data

Computer scientists
(+Mathematicians, Statisticians, etc.)
Develop tools, softwares, algorithms to store and analyze the data.

- Definition: Is the science concerned with the development and application of computer hardware and software to the acquisition, storage, analysis and visualization of biological information.
- Three core areas :
  1. Molecular biology database
  2. Seq. comparison & seq. Analysis
  3. The emerging technology of microarrays.
- In short bioinformatics is the management and analysis of biological information stored in database.

History of Bioinformatics:

- National Biomedical Research Foundation :The first comprehensive collection of amino acid sequences was compiled in the “Atlas of Protein sequence and structure”.

- 1965-1978: the above collection was edited by Margaret O. Dayhoff. Dayhoff and coworkers made notable contribution to the comparison of amino acid seq. by developing computer s/w for detecting distantly related seq., relationships, etc.

- 1980: European Molecular Biology Lab (EMBL) established data library to collect, organize and distribute nucleotide seq. data and related information. Now by EBI, Hinxton, U.K.

- 1980: National Centre for Bioinformatics Institute (NCBI) USA. It serve as Primary information databank and provider of information.
- Japan: DNA data bank
- 1984: Protein information Resource (PIR) established by National Biomedical Research Foundation. It helps researchers in the identification and interpretation of protein sequence information.
- All these databanks operate in close collaboration and regularly exchange data.
- Databanks serve as an imp. resource to all who are having the interest in biological phenomena, particularly molecular aspects.

Applications:

- Medical : Bioinformatics and drug design can be highly useful for diagnosis and treatment of various neurological disorders. It has been found that many neurological disorders are due to unusual gene structures like the triple 'A' formation "AAA" (the A of "ATGC" nucleotides) in the genes. The problem becomes more complex with multiple repeats or occurrences of triple 'A'. More than eight such repeats are known and in such cases children are permanently bed ridden or has to use wheel chairs.

- Waste cleanup: Microbial Genome Program (MGP) scientists are determining the DNA sequence of the genome of C. crescentus, the organisms responsible for sewage treatment.

- Gene therapy : Gene therapy is the approach used to treat, cure or even prevent disease by changing the expression of a person's gene.

- Forensic analysis of microbes Scientists used their genomic tools to help distinguish between the strain of Bacillus anthracis that was used in the summer of 2001 terrorist attack in Florida with that of closely related anthrax strains.

- Biotechnology: The archaeon Archaeoglobus fulgidus and the bacterium “ Thermotoga maritima” have potential for practical applications in industry and government-funded environmental remediation. These microorganisms thrive in water temperatures above the boiling point and therefore may provide the DOE, the Department of Defence, and private companies with heat-stable enzymes suitable for use in industrial processes.

- Drug development:

-Genomics, proteomics, combinatorial chemistry and high-throughput screening (HTS) have all contributed to a massive increase in the amount of data generated by the pharmaceutical industry.

-The role of bioinformatics is to store, track and provide tools for the analysis of these data - some thing like an automated environment.

-modeling of protein interactions with small molecules allowing rational drug design, the association of genotype and drug response patterns (pharmacogenomics), the design and assessment of chemical diversity in combinatorial libraries, and the processing and storage of data from high-throughput screens of lead compounds

Areas of biology

Application	Role of bioinformatics
Genomics/proteomics (human genome project)	
•Characterization of human genes and proteins	•Target identification/ validation in the human genome •Cataloging SNPs and association with drug response patterns (pharmacogenomics)
Genomics/proteomics (human pathogen genome project)	
•Characterization of genes and proteins of organisms that are pathogenic to humans	•Target identification/ validation in pathogens
Functional genomics (protein structures)	
•Analysis of protein structures (humans and their pathogens)	•Prediction of drug/target interactions •Rational drug design

Application	Role of bioinformatics
Functional genomics (expression profiling)	
•Determining gene expression patterns in disease and health	•Gene classification based on drug responses •Pathway reconstruction
Functional genomics (genome-wide mutagenesis)	
•Determining the mutant phenotypes for all genes in the genome	•Databases of animal models •Target identification/ validation
Functional genomics (protein interactions)	
•Determining interactions among all proteins	•Characterization of protein interactions •Reconstruction of pathways •Prediction of binding sites

Approaches in functional genomics

Approach	Functional annotation method
Homology searching	Comparison to related sequences with known function
Protein structure determination (structural genomics)	Comparison to molecules with related structure and known function
Comparative genomics	Functional annotation by domain conservation, conserved phylogeny or conserved genomic organization
Expression analysis	Similar expression profiles indicate conserved function
Mutagenesis	Function based on mutant phenotype, e.g. knockout mice
Protein interaction screening	Function based on presence in multi-subunit complex or on interaction with proteins of known function
Small molecule informatics	Interaction with small molecules

References:

-R. C. Dubey, A textbook of Biotechnology
-B. D. Singh, Biotechnology
-K. Sambamurthy, Ashutosh Kar; Pharmaceutical Biotechnology Fundamentals and Applications

Review questions to ensure attainment of TLOs/ Cos

1. Define Bioinformatics.
2. Write down the applications of Bioinformatics.
3. Discuss the History of Bioinformatics.