BIOINFORMATICS

Study Material for :
B.Sc. Part III
Botany Hons.
Paper V

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INTRODUCTION

- **BIOINFORMATICS is the field of science in which biology, computer science, statistics applied mathematics and information technology merge to form a single discipline**

- **It is a latest discovery of new biological insight which create a global perspective from which unifying principles in biology can be discerned**

- **Basically it is a management system of creating and restoring the information of molecular biology in the form of data, codes, graph and structure**

- **It is a result of HUMAN GENOME PROJECT and creating "GENOMIC REVOLUTION",**
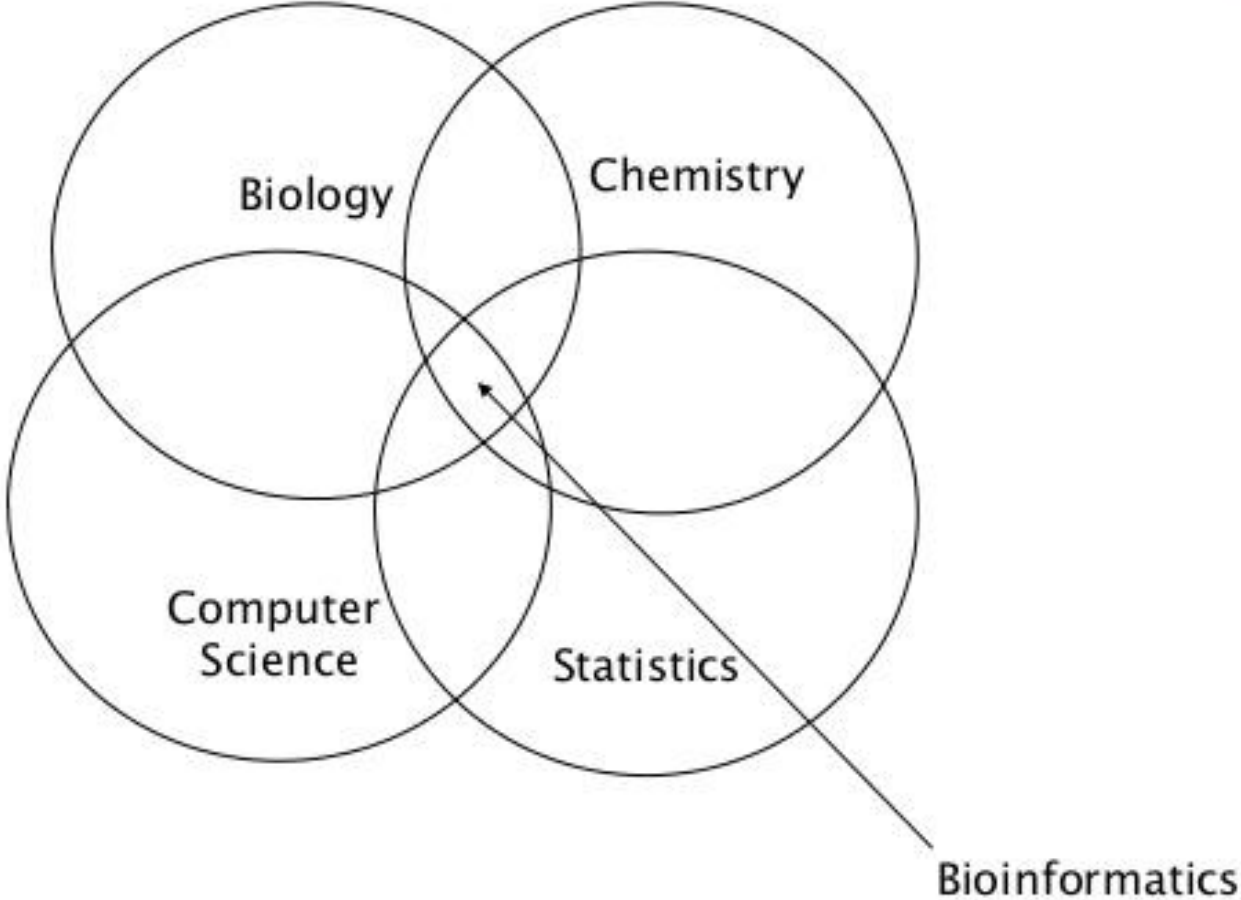
* Computer Science includes IT

COMPONENTS OF BIOINFORMATICS

1. CREATION OF DATABASES:

- Involves the organizing, storage and management of the biological data sets

- Databases are accessible and submit new entries. Protein sequences data bank for molecular structures

2. DEVELOPMENT OF ALGORITHMS AND STATISTICS:

- Involves the development of tools and resources to determine the relationship among the members of large data sets

- Comparison of protein sequence data with the already existing protein sequences

3. ANALYSIS OF DATA INTERPRETATION:

Includes DNA, RNA and protein sequences, protein structure, gene expression profiles and biochemical pathways
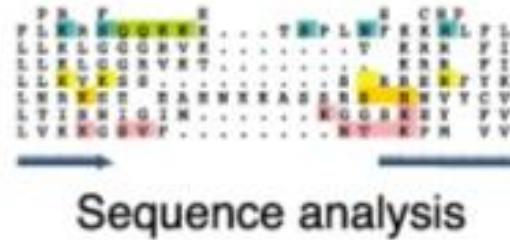
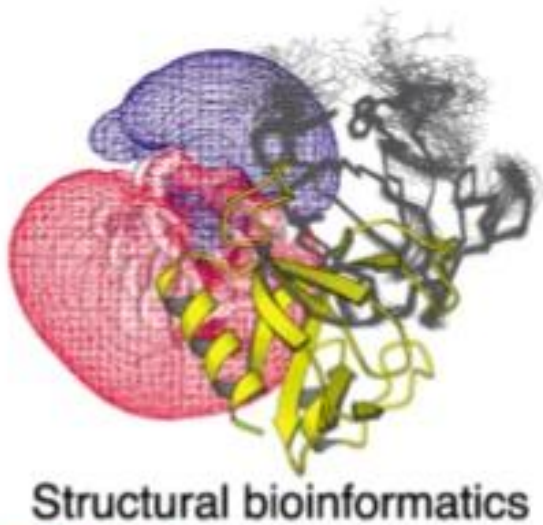# AREA OF BIOINFORMATICS
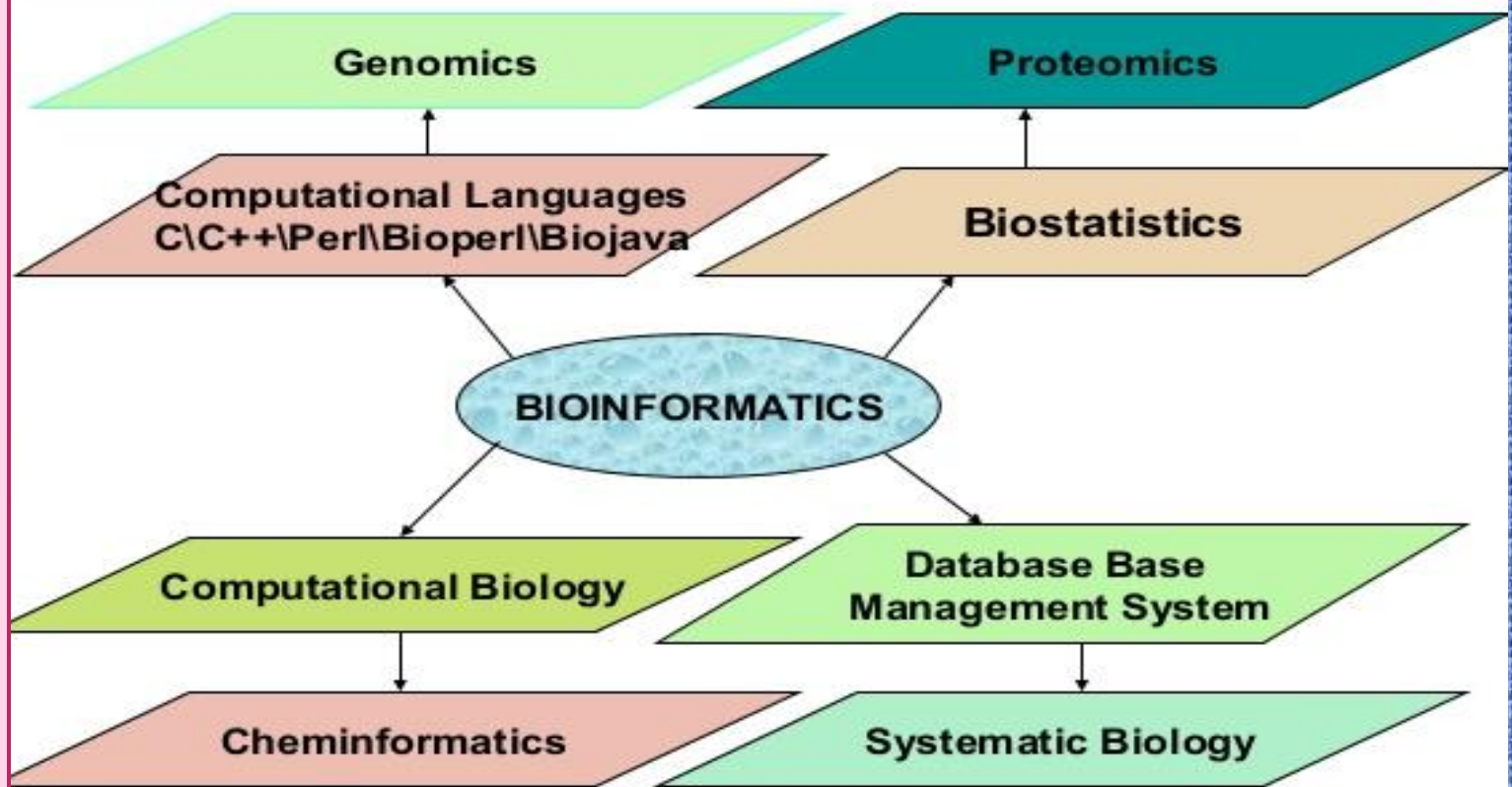
Ref: Biowits

BIOINFORMATICS TOOLS

- There are certain sets of programming applications which have been designed and work as tools in the field of bioinformatics. They are:-
  1. BLASTS
  2. Fast A
  3. Emboss
  4. Clustal W
  5. Ras Mol

FORMS IN WHICH BIOLOGICAL DATA IS STORED

Sequence analysis

Structural bioinformatics

Databases

HOMOLOGY SEARCHES

PRIMARY, SECONDARY COMPOSITE DATABASE

SEQUENCE ANALYSIS

- It is the process of subjecting a DNA, RNA or peptide sequence to any of a wide range of analytical methods to understand its features, function, structure or evolution

- It includes-

- Sequencing: Sequence assembly

- Alignment: Searching (in Databases)

- On the basis of number of comparing sequencing strand, it is of two types:

  Pair wise alignment

  Multiple Sequence Alignment

TYPES OF SEQUENCE ALIGNMENT

Local Alignment

Pairwise Sequence Alignment

Target Sequence

5' ACTACTAGATTACTTACGGATCAGGTACTTTAGAGGCTTGCAACCA 3'
            |||| |||||| |||||||||||||||
Query Sequence 5' TACTCACGGATGAGGTACTTTAGAGGC 3'

Global Alignment

Target Sequence

5' ACTACTAGATTACTTACGGATCAGGTACTTTAGAGGCTTGCAACCA 3'
 ||||||||||| |||||||| ||||||||||||||| ||||||||
5' ACTACTAGATT----ACGGATC--GTACTTTAGAGGCTAGCAACCA 3'

Query Sequence

Multiple Sequence Alignment (MSA)

| Species/Abbrv |
| --- |
| 1. Rhizobium_leguminosarum_bv._viciae_3841_g115254414 |
| 2. Sinorhizobium_medicae_WSM419_g150026743 |
| 3. Agrobacterium_fabrum_str._C58_g159139455 |
| 4. Agrobacterium_fabrum_str._C58_g159140696 |
| 5. Rhizobium_etli_CIAT_652_g190694918 |
| 6. Rhizobium_leguminosarum_bv._trifolii_WSM2304_g209533368 |
| 7. Agrobacterium_radiobacter_K84_g221721649 |
| 8. Agrobacterium_vitis_S4_g221737306 |
| 9. Sinorhizobium_fredii_NGR234_g227339586 |
| 10. Rhizobium_leguminosarum_bv._trifolii_WSM1325_g240856645 |
| 11. Sinorhizobium_meliloti_1021_g30407155 |
| 12. Candidatus_Liberibacter_solanacearum_CLso-ZC1_g313495152 |
| 13. Agrobacterium_sp._H13-3_g325062059 |
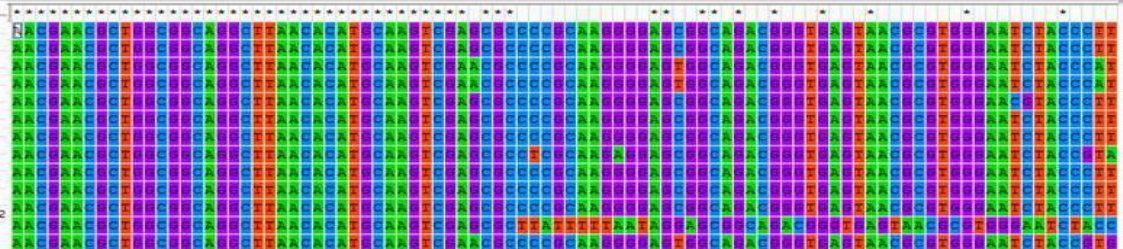
STRUCTURAL BIOINFORMATICS

▸ Prediction of structure from sequence
  - secondary structure
  - homology modelling, threading
  - ab initio 3D prediction
▸ Analysis of 3D structure
  - structure comparison/ alignment
  - prediction of function from structure
  - molecular mechanics/ molecular dynamics
  - prediction of molecular interactions, docking
▸ Structure databases (RCSB)

Ref: Biowits

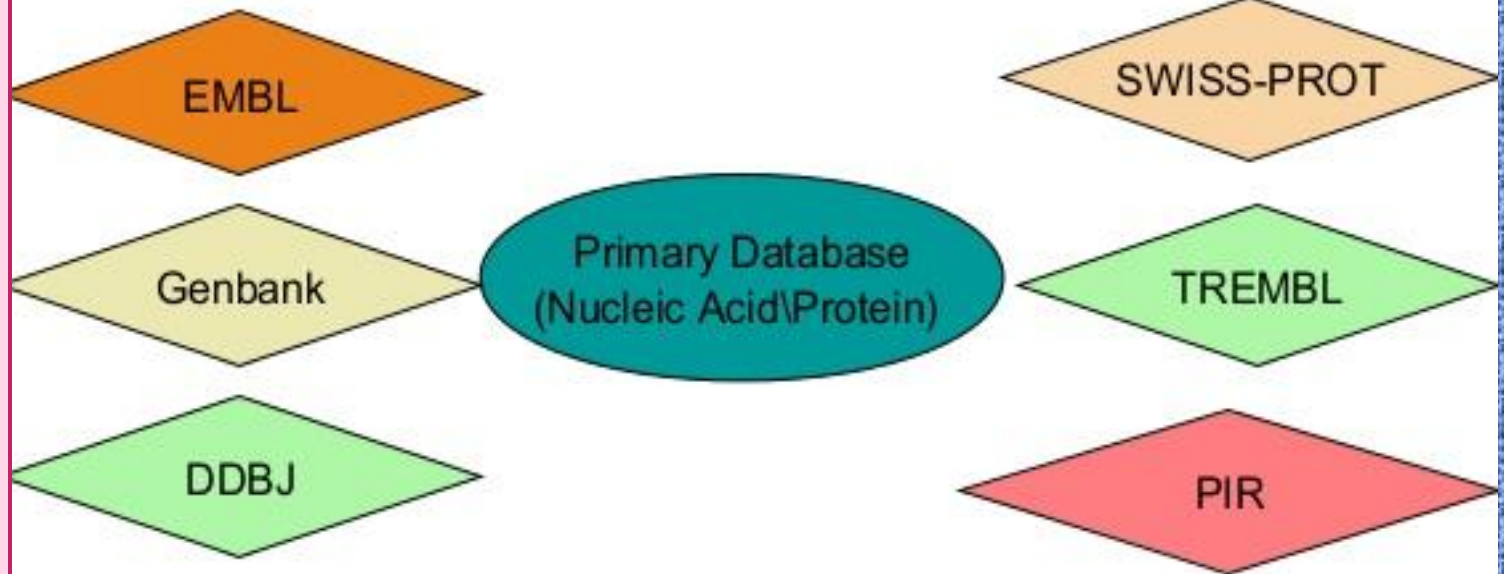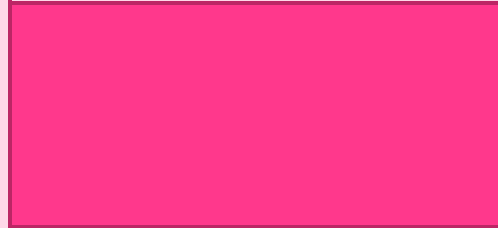# STRUCTURAL BIOINFORMATICS
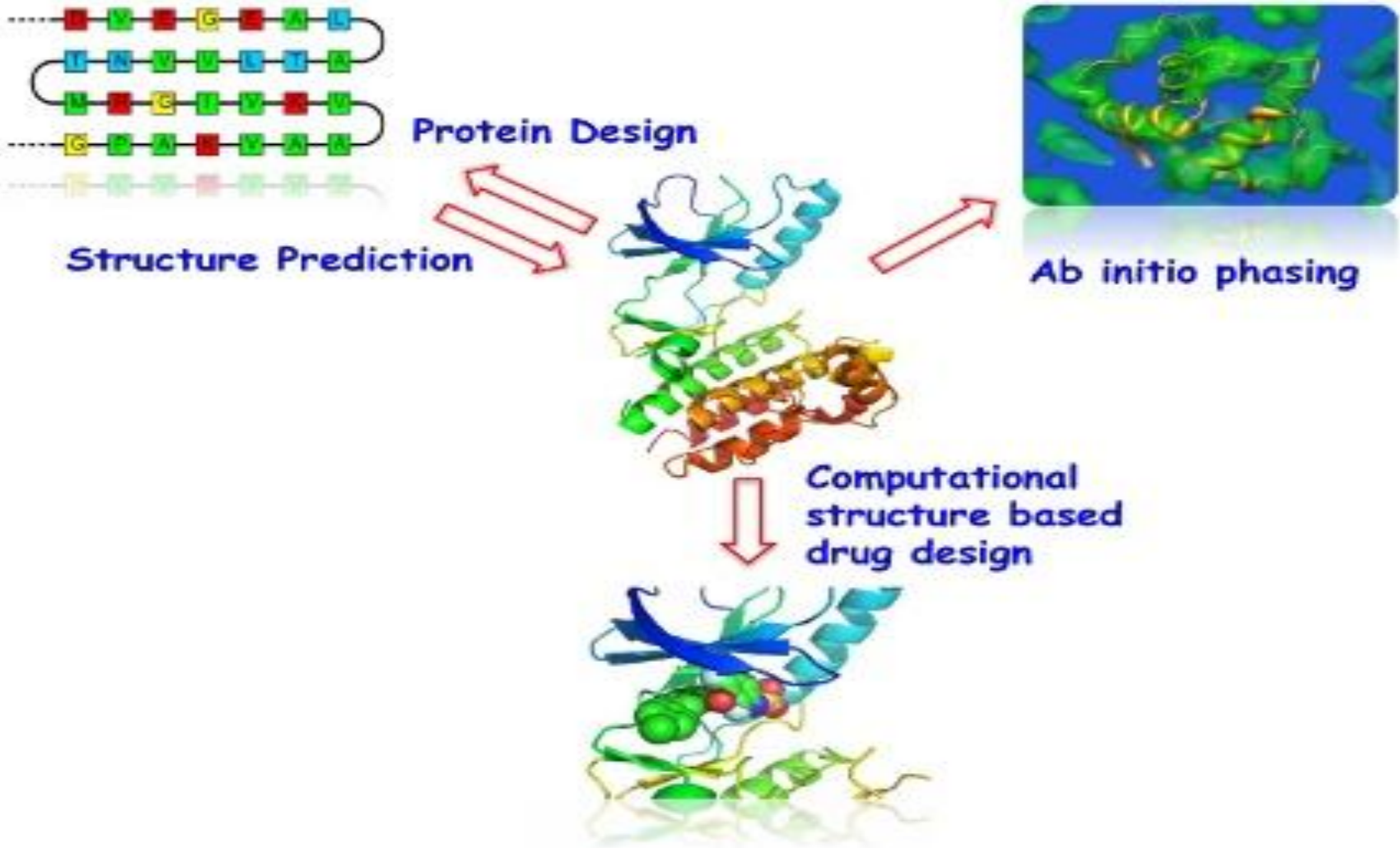
DATABASE

- There are various types of data base designed to study and store different molecular information. The different databases are:
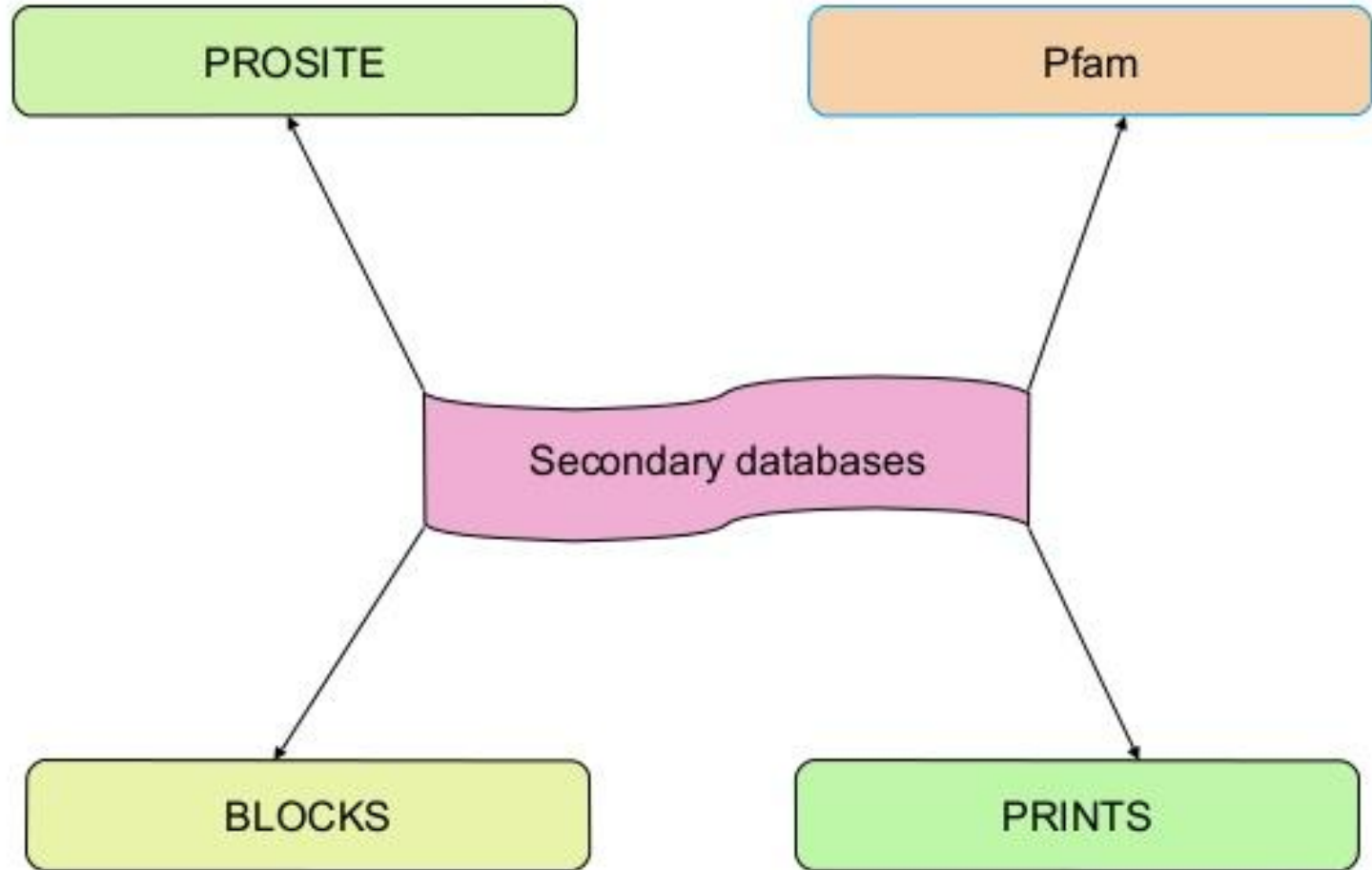
  Primary Database

  Secondary Database

  Composite Database

PRIMARY DATABASE
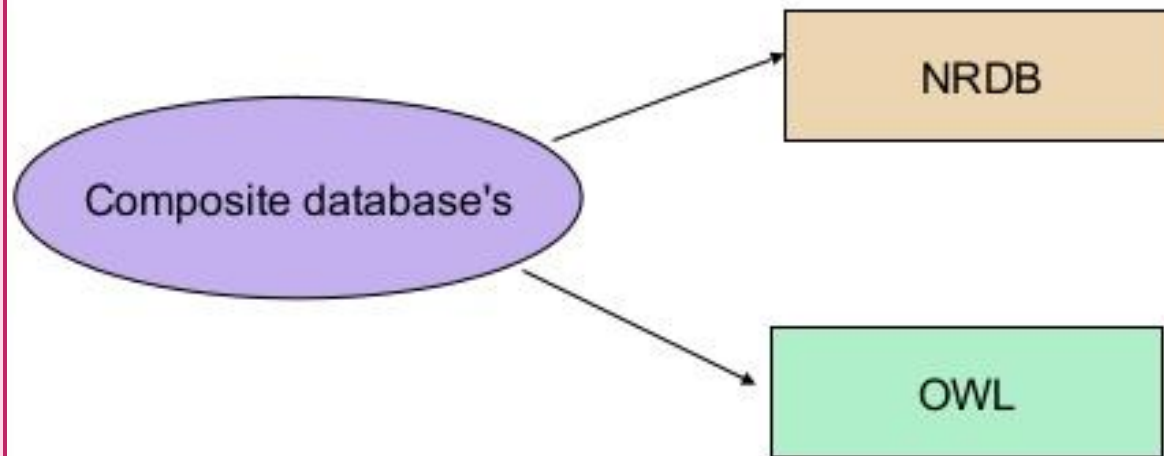

EMBL

SWISS-PROT

Genbank

Primary Database
(Nucleic Acid\Protein)

TREMBL

DDBJ

PIR

Ref: BII

SECONDARY DATABASE

PROSITE

Pfam

Secondary databases

BLOCKS

PRINTS

Ref: BII

COMPOSITE DATABASE

COMBINES DIFFERENT FORMS OF PRIMARY DATA BASE

APPLICATION OF BIOINFORMATICS

- Sequence mapping of biomolecules (DNA,RNA and proteins)

- Identification of nucleotide sequences of functional gene

- Finding of sites that can be cut by restriction enzymes

- Prediction of functional gene products

- To trace the evolutionary trees of genes

- For the prediction of 3-dimensional structure of proteins

- Molecular modelling of biomolecules

- Designing of drugs for medical treatment

- Handling of vast biological data which otherwise is not possible

- Development of models for the functioning of various cells, tissues and organs

- Designing bioweapons

THANK YOU

- Students are requested to share their queries on **whatsapp group** of class: **MMC botany(D2)**
- OR
- Khare.pushpanjali2@gmail.com
- OR
- # 9708063491