



A Charutar Vidya Mandal's Institution  
**V.P. & R.P.T.P. SCIENCE COLLEGE**

(AUTONOMOUS) (Grant-in-Aid)  
Affiliated to Sardar Patel University  
VALLABH VIDYANAGAR-388120



**Bachelor of Science (Semester -III) External Examination - 2025**

Subject Code: US03IDBOT01

Subject Name: Chemoinformatics in Plant Sciences

Date: 8-10-2025, (WEDNESDAY)

Time: 2:00 PM to 3:30 PM (1.5 HRS.)

Total marks: 25

Q-1 Write the most appropriate answer from the following multiple-choice questions. [05]

- (1) The C logP descriptor is a measure of a molecule's:  
A) Size      B) Lipophilicity      C) Electronic charge      D) Shape
- (2) What is ADMET in the context of drug design?  
A) Adsorption, Distribution, Metabolism, Excretion & Toxicity  
B) Absorption, Digestion, Metabolism, Excretion & Toxicity  
C) Absorption, Distribution, Metabolism, Excretion & Toxicity  
D) Absorption, Distribution, Metabolism, Expectance & Toxicity
- (3) Which of these is a 1D molecular representation?  
A) SMILES      B) InChIKey  
C) Molecular Graph      D) 3D Structure Visualization
- (4) What kind of curation does ChEMBL use?  
A) Automatic only      B) Community-based  
C) Manually curated      D) Robot-assisted only
- (5) Which database provides detailed information on FDA-approved drugs, including their mechanism of action and adverse effects?  
A) ChemSpider      B) PubChem      C) DrugBank      D) PDB

Q-2 Describe the following

- A) Describe the role of Chemoinformatics in modern plant science, with a focus on its applications. [5]
- B) Write short note on chemoinformatics databases and its application. [5]

OR

Q-2 Describe the following

- A) What are molecular databases? Explain the types of information they store and their overall importance in chemical research [5]
- B) Explain what a SMILES string is. Provide an example and describe the rules for representing linear, branched, and ring structures. [5]

Q-3 Describe the following

- A) What is the Protein Data Bank (PDB)? Discuss its purpose, key features, and the experimental methods used to obtain its structural data. [5]
- B) Define molecular docking and explain its basic principle. [5]

OR

Q-3 Describe the following

- A) Discuss the challenges and opportunities for Chemoinformatics in India, including aspects like syllabus modernization and industry-academia collaboration. [5]
- B) Explain the concept of Structure-Activity Relationship (SAR) analysis and QSAR modeling [5]

