

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



Internal Examination: S.Y.B. Sc

Total marks: 20

Subject Code: US03IDBOT01 (T) Subject Name: Chemoinformatics in Plant Sciences

Date: 25-09-2025, (THURSDAY)

Time: 2:45 to 3:45 PM

Q-1 Write the most appropriate answer from the following multiple-choice [06] questions.

(1) Which organization maintains the PubChem database?

- A) The Royal Society of Chemistry B) The National Institutes of Health (NIH)
C) The United Nations B) The World Health Organization (WHO)

(2) What is SMILES?

- A) A graphical representation B) A linear text notation for chemical structures
C) A type of file format D) A 3D model

(3) What does SAR stand for?

- A) Structure-Activity Relationship B) Systematic-Analysis Report
C) Substance-Aromatic Regulation D) Synthetic-Activity Reaction

(4) The ClogP descriptor is a measure of a molecule's:

- A) Size B) Lipophilicity C) Electronic charge D) Shape

(5) Which database is a comprehensive repository of drugs and drug targets?

- A) ChemSpider B) PubChem C) DrugBank D) PDB

(6) Which plant-derived compound is a case study for its antioxidant and anti-inflammatory properties?

- A) Water B) Resveratrol C) Plastic D) Ethanol

Q-2 Describe the following

- A) Define chemoinformatics in your own words. What are the core disciplines that it integrates, and what is its primary objective? [4]
B) What is Structure-Activity Relationship (SAR) analysis? [3]

OR

Q-2 Describe the following

- A) Explain what a SMILES string is. Provide an example and describe the rules for representing linear, branched, and ring structures. [4]
B) How does chemoinformatics help in virtual screening? [3]

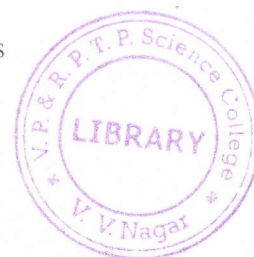
Q-3 Describe the following

- A) Explain what molecular descriptors are and why they are essential for chemoinformatics. [4]
B) Define molecular docking and explain its basic principle. [3]

OR

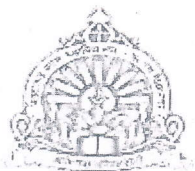
Q-3 Describe the following

- A) Discuss the importance of databases like PubChem and ChEMBL. [4]
B) Explain the concept of QSAR modeling. What is its primary goal? [3]



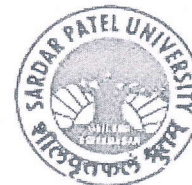
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PART A Quiz – 2025

Bachelor of Science (Semester III)

Internal Examination - 2025

Subject Code: US03IDBOT01 SUBJECT NAME: Chemoinformatics in Plant Sciences

Date: 25/09/2025

Day: Thursday

Total marks : 05

Time: 2:45 to 2:55 PM

Time: 10 minutes

Q.1 Answer the MCQ by selecting the correct option or Mark the true/false statements as either true (✓) or false (x)

05

1. PubChem is a database of:

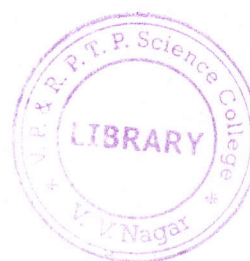
- A. Historical events
- B. Chemical molecules and their activities
- C. Musical scores
- D. Recipes

2. The PDB file format stores:

- A. 2D structure
- B. Sequence data
- C. 3D atomic coordinates
- D. Vendor information

3. Which of these is a common file format for chemical data?

- A. MP4
- B. PDF
- C. SDF
- D. JPEG



Tick mark () True or False (x) against the following sentences

4. To serve as a virtual screening library for purchasable compounds is the main purpose of the ZINC database

[True/False]

5. Molecular formula is the most basic representation of a chemical compound

[True/False]