

7179

5. (a) Differentiate between full structure and substructure search.
(b) Write SMILES for the following compounds:
Butane
Cyclohexane
Ethanol
Pyridine
Acetic acid
(c) Deduce the structure of the molecule using the following data:
Molecular Formula: C_2H_6O
IR: 3300 cm^{-1} (broad)
 1050 cm^{-1}
 $^1\text{H NMR}$ (δ ppm): 1.2 (triplet, 3H)
3.6 (quartet, 2H)
2.0 (broad singlet, 1H)
Mass: $M^+=46$
 $m/z=31$ (base peak)
6. Write short notes on any **three** of the following :
- (i) Libraries and Toolkits
 - (ii) Molecular Docking
 - (iii) Pharmacophore Modeling
 - (iv) 3D Molecular Descriptors

[This question paper contains 4 printed pages]

Your Roll No. :

Sl. No. of Q. Paper : **7179** **I**

Unique Paper Code : 2173540015

Name of the Paper : DSE-Cheminformatics

Name of the Course : **B.Sc. Prog. Analytical Chemistry**

Semester : VIII

Time : 2 Hours **Maximum Marks : 60**

Instructions for Candidates :

- (a) Write your Roll No. on the top immediately on receipt of this question paper.
 - (b) **All** questions carry equal marks.
 - (c) Each question carries **15** marks. Each subpart of a question carries **5** marks.
 - (d) Answer **four** questions in all.
 - (e) Attempt **all** parts of a question together.
1. (a) Differentiate between structure-based and ligand-based drug design.

- (b) A 33 year old man weighing 64 Kg took six 300 mg pills of Chloroquine without consulting a doctor. If the Oral LD₅₀ value for rats is 330 mg/kg, calculate the lethal dose for the man. What are the chances of his survival? Define LD₅₀.
- (c) Show the number of peaks in a plot for low and high-resolution mode of NMR for ethanol. Explain briefly.
2. (a) What is the role of IR spectroscopy in Cheminformatics? What are the characteristic peaks observed in the IR spectrum of acetone?
- (b) Explain briefly any **two** of the following terms:
- Pharmacophore keys
 - Combinatorial Library
 - 2D Finger Prints
- (c) Explain the principle of NMR spectroscopy based on nuclear spin and energy transitions.

3. (a) Define QSAR and explain its importance in drug design.
- (b) Explain the parabolic Hansch Model. Explain the terms involved in it. What is the significance of Taft's steric parameter?
- (c) Explain:
- SMILES notation
 - Molfile
4. (a) Draw the adjacency matrix for
- Butane
 - 2-methyl propane

(b) Given :

Compound	Log P (X)	Activity (Y)
A	1.0	1.5
B	1.5	2.0
C	2.0	2.8
D	2.5	3.2

Find the regression equation and predict how the biological activity varies with lipophilicity.

- (c) Explain briefly the peaks obtained in case of mass spectra of
- CH₃COOH
 - CH₃COCH₃