(b) Given:

| Compound | logP(X) | Activity(Y) |
|---|---|---|
| A | 1.0 | 1.5 |
| B | 1.5 | 2.5 |
| C | 2.0 | 3.0 |
| D | 2.5 | 3.6 |

Find QSAR equation. Predict activity when x=2.3

(c) Deduce the structure of the molecule using the following data:

Molecular Formula: $C_4H_4O_2$

IR: 1710 $cm^{-1}$

3300 $cm^{-1}$ (broad)

'H NMR ($\delta$ ppm):

2.1 (singlet, 3H)

11-12(broad singlet, IH)

Mass: M=60

m/z = 43(base peak)

**6.** Write short notes on **any three** of the following:

(i) Virtual Screening

(ii) Differences between 2D and 3D molecular descriptors

(iii) Applications of cheminformatics in drug design

(iv) HTS

***



[This question paper contains 4 printed pages]

**Your Roll No.** : .....

**Sl. No. of Q. Paper** : **7856** **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) Attempt any **four** questions in **all.**

(c) Attempt all parts of a question together.

(d) All questions carry equal marks.

(e) Each question carries 15 marks. Each subpart of a question carries 5 marks.

**1.** (a) Differentiate between Bioinformatics and Chemoinformatics.

(b) A 40 year old man weighing 72 Kg took eight 200 mg pills of Chloroquine without consulting a doctor. If the Oral $LD_{50}$ value for rats is 250 mg/kg calculate the lethal dose for the man. What are the chances of his survival? Define $LD_{50}$.

(c) Show the number of peaks in a plot for low and high-resolution mode of NMR for $CH_3CH_2CHCl_2$. Explain briefly.

**2.** (a) Explain the principle of mass spectroscopy.

(b) Explain briefly **any two** of the following terms: (i) Similarity Search (ii) Geometry Optimization and Energy Minimization (iii)Lead Optimization

(c) Why do we observe a single strong intense band for a particular allowed vibrational mode in IR spectrum? Explain using the concept of selection rules.

**3.** (a) What are pdb files? Give one online source to obtain the same. How can one computationally model a protein whose structure is unknown?





(b) What is the general Hansch equation? Explain each term involved in the equation.

(c) Explain the principle of QSAR modeling.

**4.** (a) Write the adjacency matrix and bond order matrix for 3-chloro pent-1-ene.

(b) Given: Activity = 1.5logP - 0.8Es + 0.3.

Which parameter increases activity more: logP or steric effect? Explain.

Calculate activity for:

logP = 2.0

E = 0.5

(c) Explain briefly the peaks obtained in case of mass spectra of $CH_3CH_2CH_2CH_3$, $C_6H_5COOH$

**5.** (a) Write smiles for the following compounds:

Benzene

Formaldehyde

Phenol

Cyclohexanone

2-methyl propane