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- (ii) Ligand Based Drug design
- (iii) Pharmacophore Modeling
- (iv) Lipinski's rule of five

(500)

[This question paper contains 4 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 3273

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Unique Paper Code : 32173904

Name of the Paper : SEC – Cheminformatics

Name of the Course : **B.Sc. (Hons.) / B.Sc. (Prog)**

Semester : IV/VI

Duration : 2 Hours

Maximum Marks : 38

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Answer **four** questions in all.
3. Question number **1** is compulsory. It carries **11** marks.
4. Question Numbers 2-5 carry 9 marks each.
5. Attempt **all** parts of a question together.

P.T.O.

1. (a) What are CT Files? Explain giving suitable examples. (2)
 - (b) The concentration of a drug was found to be 4.51×10^{-5} M. Comment on its activity? How is QSAR different from QSTR and QSPR? (4)
 - (c) Show the number of peaks in a plot for low and high-resolution mode of NMR for acetone and methanol. Explain briefly. (5)
2. (a) How is LD_{50} different from ED_{50} ?
 - (b) Differentiate between OD QSAR and ID QSAR.
 - (c) Based on fragmentation, predict the values of m/z for any three peaks of pentane obtained in case of its mass spectra.
3. (a) Deabbreviate SMILES. Give the code for (i) Ethanol (ii) Butanone.
 - (b) Give a generalized expression for Schrodinger Wave Equation, stating its significance. Can it be solved for multielectronic systems?

- (c) Write (pointwise) the protocol to be followed while performing QSAR.
4. (a) Draw the HMO matrix for (i) Cyclobutadiene (ii) Propenyl radical ion.
 - (b) The pK_a for para-substituted benzoic acids at room temperature is given as

Para substituent	pK_a
A	4.9
B	4.01

Evaluate the Hammett's constant and comment on the nature of the substituents.

(Given: pK_a value of benzoic acid = 4.201 at room temperature)

- (c) Why is TMS used as a reference compound for recording NMR spectra?
5. Write short notes on **any three** of the following :
 - (i) Partition coefficient as a descriptor