(b) Name any two molecular modeling softwares and explain their brief features.

(c) How is cheminformatics different from bioinformatics?

5. Write short note on the following:

(a) HTS

(b) Lipinski's rule of 5

(c) 2D and 3D molecular descriptors

[This question paper contains 4 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 6223 **I**

Unique Paper Code : 32173904

Name of the Paper : SEC: Cheminformatics

Name of the Course : **B.Sc. (Hons.) Chemistry/ 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. Each question carries 9.5 marks.
4. First part of each question carries 3.5 marks.
5. Remaining parts of each question carries 3 marks.
6. Attempt all parts of a question together.

1. (a) Define ligand based Pharmacophore modelling. Explain its significance in drug design.

   (b) Differentiate between QSAR and QSPR.

   (c) Discuss the applications of combinatorial chemistry in drug field.

2. (a) Differentiate between 2D and 3D QSAR.

   (b) Define LD50. The LD50 value of a drug is 25mg/ Kg. Calculate the amount of dosage of a drug which is going to be lethal to a person weighing 85 kg if each pill weighs 50mg.

   (c) The general procedure in a QSPR approach consists of three steps. Explain "structure representation" with respect to QSPR.

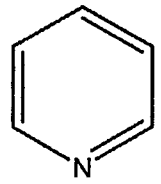
3. (a) Define similarity search. How is it different from full structure search?

   (b) Differentiate between ligand and structure based virtual screening.

   (c) Briefly explain any two chemical databases and protein databases each.

4. (a) Deabbreviate SMILES and explain its signigicance.

   Write SMILES code for the following compounds:

(i) 

(ii)