2819

Unique Paper Code	:	32173904
Name of the paper	:	Cheminformatics
Name of the course	:	B.Sc. (Hons.) Chemistry/B.Sc. (Prog.)
Semester	:	IV/VI
Duration	:	2.5 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.

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

b) Difference between QSAR and QSPR.

c) Discuss the application of combinatorial chemistry in drug field.

Q.2 a) Define chemical shift in NMR. Arrange the following compounds in increasing order of chemical shift

CH_3I, CH_3Br, CH_3I

b) Elaborate on basic steps of molecular docking.

c) Mention the difference between LC_{50} Vs. IC_{50}

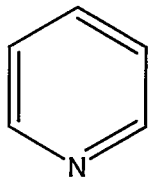
Q.3 a) Define similarity search. How is it different from full structure search?

b) Difference between ligand and structure based virtual screening.

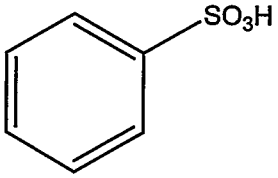
c) Mention and explain two chemical database and protein database each.

Q.4 a) Write SMILES code for the following compounds:

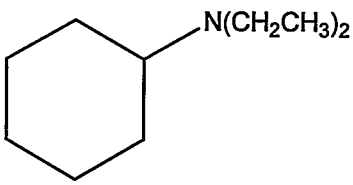
i



ii



iii



Q.5 Write short note on the following:

a) Potential energy surface

b) 2D and 3D molecular descriptors

c) Lipinski's rule of 5