Printed Pages : 1 **Roll No.** | | | | | | | | | | | **BOP485A**

B.PHARM.

THEORY EXAMINATION (SEM–VIII) 2016-17

COMPUTATIONAL METHODS IN DRUG DESIGN

Time : 3 Hours ***Max. Marks : 100***

Note : *Be precise in your answer.*

SECTION – A

1. Attempt the following: **10 x 2 = 20**

(a) What is Hansch Analysis? How is it useful in the design of drugs.

(b) Define similarity searching

(c) What is virtual screening?

(d) Give any four softwares used in molecular modeling.

(e) Define drug likeness.

(f) Define druggability.

(g) Named the software used in molecular graphics.

(h) What is CADD.

(i) Write in brief about molecular docking.

(j) What is SPSS.

SECTION – B

2. Attempt any five parts of the following question: **5 x 10 = 50**

(a) Illustrate the different physicochemical parameters which have been studied by QSAR approach.

(b) Write a note on 2D and 3D QSAR methodology.

(c) Outline the fundamental principle of structure based drug design.

(d) Discuss the role of computational chemistry in drug design.

(e) Explain Ligand based and structure based virtual screening.

(f) Outline the rational approaches of drug design.

(g) Write about molecular graphics and receptor based drug design,

(h) Discuss the method of Virtual screening like shape based screening, fingerprint based screening

SECTION – C

Attempt any two parts of the following: **2 x 15 = 30**

3. Give the principles and general methods of molecular modeling and their applications in drug design.

4. Discuss various methods of similarity searching and their applications in virtual screening like QSAR modeling and pharmacophore modeling.

5. Attempt any three**.**

(i) Protein Data Bank (ii) Bioinformatics

(iii) Molecular descriptors (iv) Protein homology modeling