Printed Pages: 01 **Sub Code: BP807ET**

Paper Id: 231977 **Roll No.**

B.PHARM.
(SEM VIII) THEORY EXAMINATION 2022-23
COMPUTER AIDED DRUG DESIGN

Time: 3 Hours ***Total Marks: 75***

Note: Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. Attempt *all* questions in brief. **10 x 2 = 20**

(a) What various stages of drug discovery?

(b) What is Phase 0 clinical trial?

(c) What is non-classical bioisosteres?

(d) What is Taft's steric factor (Es)?

(e) Write down the drawbacks and limitations of CoMFA.

(f) What do you understand by the term Pharmacophore?

(g) Give the names of molecular docking models.

(h) What do you understand by the term "Binding mode"?

(i) What isOrangebook?

(j) What is various chemical structure representation used for chemical structures in digital databases?

SECTION B

2. Attempt any *two* parts of the following: **2 x 10 = 20**

(a) Write in detail about the drug likeness screening with the various filter used in drug likeness screening.

(b) What is cheminformatics? Write in detail about the various tools and steps involved in cheminformatics system.

(c) What do you understand by Force field? Discuss various novel technique used in molecular modeling

SECTION C

3. Attempt any *five* parts of the following: **5 x 7 = 35**

(a) Write in detail about the Free-Wilson approach to QSAR.

(b) What do you understand by conformational analysis? Write Different methods used to determine information regarding conformations.

(c) Write in detail about the Quantum mechanics methods of Molecular modelling.

(d) Discuss in detail about the De-novo drug design with steps involved in it.

(e) Differentiate between SAR and QSAR.

(f) Discuss in detail about Ligand-based pharmacophore modeling.

(g) Discuss in detail about various lead discoveries based on traditional medicine with suitable examples.