Total No. of Pages : 02

Total No. of Questions : 13

B.Pharmacy (Sem.-8) COMPUTER AIDED DRUG DESIGN Subject Code : BP-807ET M.Code : 79770 Date of Examination : 09-01-2023

Time: 3 Hrs.

Max. Marks: 75

INSTRUCTIONS TO CANDIDATES :

- 1. SECTION-A is COMPULSORY consisting of TEN questions carrying TWO marks each.
- 2. SECTION-B contains THREE questions carrying TEN marks each and student has to attempt any TWO questions.
- 3. SECTION-C contains NINE questions carrying FIVE marks each and student has to attempt any SEVEN questions.

SECTION-A

- 1. Write briefly :
 - a) Define Pharmacophore.
 - b) Discuss Hammett's Substituent constant.
 - c) What is analog Based Drug Design? Explain with suitable examples.
 - d) Define Comparative Molecular Field Analysis (CoMFA)
 - e) Compare SAR and QSAR.
 - f) Define Random screening for lead optimization.
 - g) Define Free Wilson Analysis with examples.
 - h) Enlist two ADME databases.
 - i) What is Lipinski's Rule of five?
 - j) Define the terms Bioinformatics and Chemoinformatics.

SECTION-B

- 2. What is a lead molecule? Discuss the various stages involved in identification of a lead molecule.
- 3. Define and classify Molecular docking and discuss various steps involved in the flexible docking.
- 4. Discuss concept of pharmacophore mapping and pharmacophore based Screening.

SECTION-C

- 5. Explain the process of global conformational minima determination.
- 6. Explain the different approaches of de novo drug design.
- 7. Discuss in brief various parameters of quantum mechanics.
- 8. Write a note on different stages of drug discovery.
- 9. Define bioisosterism. Classify bioisosterism with examples.
- 10. Write experimental method of determination of log P.
- 11. Explain in detail the history and development of QSAR.
- 12. Define the term virtual screening. Explain the concept.
- 13. Enlist the various databases applications in drug design.

NOTE : Disclosure of Identity by writing Mobile No. or Marking of passing request on any paper of Answer Sheet will lead to UMC against the Student.