Seat No: _____ Enrollment No: _____

PARUL UNIVERSITY
FACULTY OF PHARMACY
B. Pharm. Summer-2022-23 Examination

Semester: 8 **Date: 19/04/2023**
Subject Code: BP807ET **Time: 10:00am to 1:00pm**
Subject Name: Computer Aided Drug Design **Total Marks: 75**

Instructions:
1. Figures to the right indicate maximum marks.
2. Make suitable assumptions wherever necessary.

Q.1 Multiple Choice Questions (MCQs) (1 Mark Each) **(20)**

1. Which of the following analytical techniques provides the greatest structural information on a lead compound?
   a)NMR Spectroscopy b)UV Spectroscopy
   c)IR Spectroscopy d)Elemental Analysis
2. QSAR method involves_____
   a)Target Structure b)Target Properties
   c)Ligand X-ray Structure d)Ligand Properties
3. In 3D-QSAR, green regions indicate favorable points for_____
   a)Electron-deficient groups b)Bulky groups
   c) Electron-rich groups d)Smaller groups
4. What does the symbol P represent in a QSAR?
   a)PH b)Plasma Concentration
   c) Partition Coefficient d)None of the above
5. Which of the following is associated with Conformational searching?
   a)Monte Carlo Method b)LUDI
   c)DOCK d)CoMFA
6. Which one of the following is a quantum Chemical Parameter?
   a)STERIMOL b)TAFT's Constant
   c)Highest occupied molecular orbital d)Hammets's Constants
7. Which one of the following is not the program of structural conversion and cleaning?
   a)ChemAxon b)MOE
   c)34 sybyl d)FASTA
8. Which one of the clustering techniques needs the merging approach?
   a) Hierarchical b) Partitioned
   c) Naïve Bayes d) Both A and C
9. Which one of the clustering is analogous to σ constant?
   a)Log P b)Rf value
   c)PKa d)Es
10. Semi-empirical method computes for_____
    a)Valence electron b)Proton
    c)Orbital d)None of the above
11. Which of the following is one of the rules in Lipinski's rule of five?
    a) A molecular weight more than 500 b) A calculated logP value that does not exceed 5
    c) No more than five hydrogen bond acceptor groups d) No more than 10 hydrogen bond donor groups
12. Rigid docking includes:
    a)Molecular shape representation b)Surface patch matching
    c)Filtering and Scoring d)All of the above

13. Partial Least Square (PLS) is used in:
    a)SAR b)2D-QSAR
    c)3D-QSAR d)None of the above
14. The negative value of π indicates that
    a)More hydrophobic than Hydrogen b) More hydrophobic than Halogen
    c)Less hydrophobic than Hydrogen d) Less hydrophobic than Halogen
15. Which equation helps to calculate the average position of the electron and its energy in each electronic state?
    a)Partition Coefficient b)Hammet substituent constant
    c)Schrodinger equation d)Taft Steric factor
16. Virtual screening techniques are categorized based on_____
    a)Structure-Based b)Ligand-Based
    c)Fragment-Based d)Structure and Ligand Based
17. The rotamer libraries of amino acid side chains are used for:
    a)Ligand Flexibility b)Receptor Flexibility
    c)Scoring Function d)Search Space
18. The substituents in which steric arrangements and electronic configuration are similar to those of the parent compound are known as_____
    a)Non-Classical isosteres b)Isosteres
    c)Bio-isosteres d) Classical isosteres
19. DYLOMMS (Dynamic Lattice-Oriented Molecular Modeling System) is related to:
    a)3D-QSAR b)2D-QSAR
    c)QSAR d)SAR
20. E>1 implies for_____
    a)Negative Enrichment b)Positive Enrichment
    c)Both (a) and (b) d)Constant Enrichment

Q.2 Long Answers (any 2 out of 3) (10 Mark Each) **(20)**

1. What are the various approaches involved in Lead discovery? Explain in detail
2. Define drug design. Explain in detail physicochemical parameters used in QSAR
3. Explain in detail the *de novo* drug design.

Q.3 Short Answers (any 7 out of 9) (5 Mark Each) **(35)**

1. Write a detailed note on 3D-QSAR.
2. Write a note on rigid docking.
3. Describe the different types of molecular modeling techniques.
4. Write a detailed note on Bioisosterism.
5. Write a short note on COMFA and COMSIA.
6. Write a brief note on Bioinformatics.
7. Illustrate virtual screening techniques with examples.
8. Write a brief note on chemoinformatics and ADME databases
9. Explain methods of energy minimization.