Exam Date & Time: 11-Sep-2021 (02:00 PM - 05:00 PM)

MANIPAL ACADEMY OF HIGHER EDUCATION

Manipal Academy of Higher Education, Manipal MPharm Theory (II) End-Semester Examinations.

Computer Aided Drug Design [PCH-MPC203T]

Marks: 75 **Duration: 180 mins.**

SECTION - A

Answer all the questions.

Answer the following (10 marks x 5 = 50 marks)

1) Explain the different physicochemical properties that are used in predicting and analyzing ADMET of drugs. (10)

2) Explain conformational analysis and importance of local and global energy minimum.

What is virtual screening? Explain in detail the structure based virtual screening protocols. (10)

3) What is Hammett equation? How is it associated with electronic parameter? Explain with suitable examples
How do you determine the substituent Hydrophobicity constant? Explain with suitable example. (10)

4) Explain Free Wilson model. How is it different from Hansch approach? Give their advantages and disadvantages. Explain principle component analysis and partial least square regression with suitable examples. (10)

5) Enlist five important force fields used by molecular modelling softwares. Explain in detail any two force fields. Why energy minimization is important in molecular docking process? (10)

SECTION - B

Answer all the questions.

Answer the following (5 marks x 5 = 25 marks)

6) Explain the different steps used in the validation of pharmacophore model. List out the softwares used in pharmacophore mapping and mention the application of pharmacophore mapping. (5)

7) What are the stages of de novo drug design in LUDI ? Explain. (5)

8) Which are the different methods available to generate 3D structure of a protein? Explain the method of building the protein structure from scratch. (5)

9) What is CoMFA and CoMSIA? Give their advantages and disadvantages. Explain Contour mapping with suitable examples. (5)

10) Explain the experimental approaches used in the determination of partition coeffiecient. Why n-Octanol is used in the determination of Log P value? (5)

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