Exam Date & Time: 18-Jul-2022 (10:00 AM - 01:00 PM)

MANIPAL ACADEMY OF HIGHER EDUCATION

Manipal Academy of Higher Education, Manipal MPharm Theory 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 in detail the various steps involved in homology modelling of a protein. (10)

2) A. Enlist various approximations given to the Schrödinger equation and briefly write about each of them.

B. Enlist five important force fields used by molecular modelling soft wares. Explain in detail about MM2 and AMBER force fields. (10)

3) A. Explain Free Wilson analysis and its relationship with Hansch analysis.

B Mention the various statistical methods used in QSAR .Explain the role of cluster analysis and principle component analysis in 2D QSAR studies with suitable examples. (10)

4) A. Explain the development of HIV protease and HMG COA inhibitors as examples of structure based drug design.

B. Write in detail about two important methods used for conformation generation. (10)

5) A.Discuss the experimental approaches used in the determination of Partition coefficient.

B. Explain how LogP, Polar surface area and Solubility determination help in predicting the ADMET of a drug molecule. (10)

SECTION - B

Answer all the questions.

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

6) How do you validate a pharmacophore model? Explain. Name atleast five softwares used in pharmacophore mapping. (5)

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

8) What is virtual screening? Explain in detail the structure based virtual screening protocols. (5)

9) What is Hammet constant and Taft constant? Give their applications. (5)

10) A. What are the various methods used in 3D QSAR analysis? Explain any one method in detail (5)

B. What is active site interaction in 3D QSAR?

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