

# Question Paper

Exam Date & Time: 16-May-2023 (02:00 PM - 05:00 PM)



## MANIPAL ACADEMY OF HIGHER EDUCATION

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

### COMPUTER AIDED DRUG DESIGN [PCH-MPC203T-S1]

Marks: 75

Duration: 180 mins.

#### SECTION - A

Answer all the questions.

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

- 1) A. 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)  
B. Explain classical free Wilson model and Fujita ban model. Mention their merits and demerits.
- 2) A. Enlist the various molecular descriptors used in QSAR studies and explain any one of them. (10)  
B. Explain the theoretical and experimental approaches used in the determination of Partition coefficient.
- 3) A. Enlist various approximations given to the Schrödinger equation and briefly write about each of them. (10)  
B. Enlist five important force field used by molecular modelling soft wares. Explain in detail about DRIEDING and AMBER force field.
- 4) A. Explain the development of Acetyl choline esterase inhibitors as an example for structure based drug design. (10)  
B. Explain in detail the Montecarlo multiple minimum method , Genetic and evolutionary algorithm methods with suitable examples.
- 5) A. Explain how absorption and metabolism of drugs is predicted and analyzed using Insilco techniques. (10)  
B. What are the stages of de novo drug design in LUDI? Explain.

#### SECTION - B

Answer all the questions.

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

- 6) A. What is the use of following programs: a) GASTROPLUS b) TOPKAT c) CATALYST d) METEOR e) QIKPROP. (5)  
B. What is meant by threading and fold recognition in homology modelling? What is Ab initio method?.
- 7) How do pharmacophore maps help in identifying potential drug targets? What are some of the limitations of pharmacophore mapping?. (5)
- 8) What is virtual screening? Explain in detail the similarity based virtual screening protocols. (5)
- 9) What is CoMFA and CoMSIA? Explain, how they are used in QSAR model building?. (5)
- 10) Illustrate contour map analysis with suitable example. (5)

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