

Question Paper

Exam Date & Time: 17-May-2024 (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) Explain any three important physico-chemical parameters used in QSAR studies with their significance in detail (10)
- 2) Illustrate homology modelling and explain the different steps involved in homology modelling. (10)
- 3) Enlist various approximations given to the Schrödinger equation and briefly explain each of them. (5)
 - A)
 - B) Enlist five important force fields used by molecular modelling soft wares. Explain in detail about DRIEDING and AMBER force fields (5)
- 4) What are regression-based and classification-based methods used in QSAR? Explain in detail Multiple linear regression and cluster analysis (10)
- 5) What is Hansch's analysis? Give the applications with suitable illustrations. (5)
 - A)
 - B) What is pharmacophore mapping? Write in detail about pharmacophore feature search and modelling (5)

SECTION - B

Answer all the questions.

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

- 6) Outline the Structure based drug design concept. Name some related software. (5)
- 7) What is De novo Drug design. Write a note on connection methods in Denovo design. (5)
- 8) Write briefly about the structure-based virtual screening protocols. (5)
- 9) Explain fingerprint-based molecular similarity measurement with suitable examples. (5)
- 10) Give the historical development of HMG CoA reductase inhibitors with suitable examples. (5)

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