

Question Paper

Exam Date & Time: 06-May-2019 (02:00 PM - 05:00 PM)



MANIPAL ACADEMY OF HIGHER EDUCATION

Manipal Academy of Higher Education, Manipal MPharm Theory End-Semester Examinations.
MPharm - Pharmaceutical Chemistry Specialization
MPharm Semester II - End-Semester Examination May 2019
Date : 06/05/2019

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 Free Wilson analysis and its relationship with Hansch analysis (10)
- 2) Explain the various drug receptor interactions involved in a docking process and what is their significance? Explain in detail the various scoring functions used in docking. (10)
- 3) Explain the role of cluster analysis and principle component analysis in 2D QSAR studies with suitable examples (10)
- 4) What is Quantum mechanics and Molecular mechanics? Mention their applications (10)
- 5) Describe the different types of pharmacophore generation methods and how the mapping of pharmacophore is done? Explain with an example. (10)

SECTION - B

Answer all the questions.

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

- 6) What is Hammett constant and Taft constant? Give their applications (5)
- 7) Explain the importance of predicting and analysing the ADMET properties of a new molecule in a drug design. (5)
- 8) What is CoMFA and CoMSIA? Explain, how they are used in QSAR model building? (5)
- 9) What is similarity based virtual screening? Explain the methodology involved in it. (5)
- 10) Write a note on Homology modelling. (5)

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