

# Question Paper

Exam Date & Time: 07-May-2018 (02:00 PM - 05:00 PM)



**MANIPAL ACADEMY OF HIGHER EDUCATION**

**MANIPAL COLLEGE OF PHARMACEUTICAL SCIENCES**

**END SEMESTER THEORY EXAMINATIONS - MAY 2018**

**PROGRAM: MPHARM SEMESTER 2 (PHARMACEUTICAL CHEMISTRY)**

**DATE: 07/05/2018**

**TIME: 02:00 PM - 5:00 PM**

**Computer Aided Drug Design [PCH-MPC203T]**

**Marks: 50**

**Duration: 180 mins.**

**a**

**Answer all the questions.**

Answer the following (5 marks x 8 = 40 marks)

- 1) Explain the principle of Molecular mechanics. (5)
- 2) Explain the different virtual screening methods. (5)
- 3) Enlist the methods used in QSAR studies and explain any one of them. (5)
- 4) Discuss the different in silico drug design techniques. (5)
- 5) Explain Free Wilson model and give its relationship with Hansch analysis (5)
- 6) How ADMET properties are predicted and analysed? What is their importance in drug design? (5)
- 7) Explain the various descriptors used in QSAR studies. Mention their uses (5)
- 8) Discuss the various similarity based methods of screening. (5)

**b**

**Answer all the questions.**

Answer the following with specific answers (2 marks x 5 = 10 marks)

- 9) What is quantum mechanics? Mention the methods used in quantum mechanics. (2)
  - A)
  - B)
- B) Define docking and list out the softwares which help in docking. (2)

- C) What is COMFA and energy minimisation? (2)
- D) Enlist the various statistical methods used in QSAR studies (2)
- E) Define pharmacophore with the help of two examples. (2)

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