Code No: 13169/PCI

FACULTY OF PHARMACY

M. Pharmacy (Pharmaceutical Chemistry) II-Semester (PCI) (Suppl.) Examination, February 2019

Subject: Computer Aided Drug Design

Time : 3 Hrs **Max. Marks: 75**

Note: Answer any Five questions. All questions carry equal marks

1. a) What is QSAR? Describe the physicochemical parameters used in QSAR.
   b) Explain how hydrophobicity constant and Hammet comnstants of a substituent are measured experimentally? (10+5)

2. a) Discuss in detail abt Hansch analysis and its applications.
   b) Write a note on 3D QSAR studies. (9+6)

3. a) What is quantum mechanics? Describe the use of quantum mechanics in drug design.
   b) What is molecular docking? Discuss the general method of molecular docking. (8+7)

4. a) Describe the steps involved in Homology modeling of a protein. (8+7)
   b) Discuss the concept of predicting ADMET properties and its importance in drug design.

5. a) What is known as pharmacophore? Discuss the concept of Pharmacophore based virtual screening.
   b) Write a note on Similarity based Virtual screening (8+7)

6. a) Write a note on Scoring techniques in Molecular docking.
   b) Write a note on Fragment based drug design. (7+8)

7. a) What is virtual screening? Enumerate varis virtual screening techniques .
   b) Write a note on Privileged structures. (8+7)

8. a) Discuss the importance of molecular Mechanics in drug design.
   b) What is Free Wilson analysis? What are the advantages and disadvantages over hansch analysis?

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