Code No. 13325/PCI

FACULTY OF PHARMACY

M. Pharmacy (Pharmaceutical Chemistry) II-Semester (PCI) (Main) Examination, August 2019

Subject: Computer Aided Drug Design

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

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

1 (a) Discuss in detail abt varis parameters used in QSAR.
(b) How substituent hydrophobicity constant is used in the QSAR? Discuss with an example equation. (10+5)

2 (a) What is Hansch analysis and Discuss how it is used in predicting the biological activity?
(b) Give the advantages and disadvantages of Hansch analysis. (9+6)

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

4 (a) What is Homology modeling? Discuss its importance in drug design. (8+7)
(b) Write a note on fragment based drug design.

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

6 (a) Write a note on Scoring techniques in Molecular docking.
(b) Discuss varis models for predicting ADMET properties . (7+8)

7 (a) What is virtual screening ? Discuss abt druglikeness screening .
(b) Write a note on Privileged structures. (8+7)

8 (a) What is bioactive conformation ? Discuss varis energy minimization techniques. (8+7)
(b) Write a note on application of Free Wilson analysis in drug design.

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