Code No. 6115/PCI

FACULTY OF PHARMACY

M. Pharmacy (Pharmaceutical Chemistry) II-Semester (PCI) (Suppl.) Examination, January 2020

Subject: Computer Aided Drug Design

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

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

1 (a) Discuss abt Lipophilic and electronic parameters used in QSAR .
(b) Give a hypothetical Hansch equation for predicting biological activity and explain the importance of each term. (8+7)

2 (a) Discuss the statistical terms Correlation coefficient, re-validation and cross-validation.
(b) Write the advantages of Free Wilson analysis. (8+7)

3 (a) Write a note on molecular mechanics in drug design.
(b) Discuss abt varis energy minimization techniques in molecular modeling. (8+7)

4 (a) How do y predict Abso rption of new molecules ? Discuss any three models.
(b) Write a short note on de novo drug design. (8+7)

5 (a) What is homology modeling? Enumerate steps involved in homology modeling. (9+6)
(b) Write a note on agents acting on DHFR and HMGCoA reductase.

6 Write a short note on :
(a) Drug likeness screening
(b) Structure based *in silico* virtual screening (8+7)

7 (a) Explain abt rigid docking, Flexible docking and extra -precision docking.
(b) Explain, how molecular docking is useful in rational design of new drugs? (8+7)

8 Write a short note on :
(a) Hansch analysis
(b) Statistical methods used in QSAR (8+7)

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