W 016/011

20/5/24

Enrolment Number										

Total No. of printed pages = 01

Winter, 2024

M. Pharm 2nd Semester Examination

COMPUTER AIDED DRUG DESIGN

Course Code: MPC203T

Full Marks – 75 **Time – 03 hours**

The figure in the margin indicates full marks for the questions.

A. Answer all (30 words) (100 words) **(2×10=20)**

1. Write the disadvantages of 2D QSAR.
2. Mention about some softwares used for drug design.
3. Explain the need of energy minimization in drug design.
4. Mention the importance of energy minimization in molecular modeling.
5. Define Pharmacophore.
6. Explain about hydrogen bond donor.
7. Mention the parameters of Lipinski's rule of five.
8. Explain the importance of determining ADMET parameters in drug design.
9. Mention some descriptors used in QSAR studies.
10. Explain how LogP value plays important role in drug design.

B. Answer any seven (500 words) **(5×7=35)**

1. Explain the experimental approach to determine logP value.
2. Explain the concept of Hansch analysis and compare with Free Wilson approach.
3. Write a note on history of QSAR.
4. Define molecular mechanics. Mention some forcefields used in drug design.
5. Write the experimental approach to determine hammett electronic parameter.
6. Write a note on homology *modeling*.
7. Define rigid and flexible docking.
8. Write a note on agents acting on DHFR.
9. Write a note on prediction ADMET properties.

C. Answer any two (1000 words) **(10×2=20)**

1. Explain the different types of ligand-receptor active site interactions. Elaborate the steps involved in molecular docking experiment. **(5+5=10)**
2. Write an elaborate note on *de novo* drug design. **(10)**
3. Define CADD. Explain the different methodologies used in CADD. **(2+8=10)**