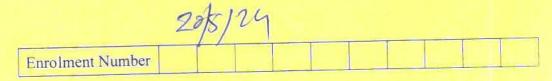
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Winter, 2024

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)

 $(2 \times 10 = 20)$

- 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.
- 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)

 $(5 \times 7 = 35)$

- 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)

 $(10 \times 2 = 20)$

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

(2+8=10)

3. Define CADD. Explain the different methodologies used in CADD.