PAPER ID-312119

Roll No: | | | | | | | | | | | | | |

MPHARM
(SEM II) THEORY EXAMINATION 2024-25
COMPUTER AIDED DRUG DESIGN

TIME: 3 HRS **M.MARKS: 75**

Note: 1. Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. Attempt *all* questions in brief. **10 x 2 = 20**

a.	What is the significance of molecular weight in drug design?
b.	Why is the concept of polarity important when designing drugs?
c.	What is the importance of hydrogen bonding in drug-receptor interactions?
d.	What is Quantitative Structure-Activity Relationship (QSAR)?
e.	What are molecular descriptors, and how are they used in QSAR studies?
f.	Define "activity" in the context of a 2D-QSAR model.
g.	How do 2D-QSAR models differ from 3D-QSAR models?
h.	What is cross-validation in QSAR analysis, and why is it important?
i.	How do the principles of quantum mechanics apply to understanding molecular interactions in drug design?
j.	What role do atomic orbitals play in determining the reactivity of a drug molecule during the binding process?

SECTION B

2. Attempt any *two* parts of the following: **2 x 10 = 20**

a.	What is Computer-Aided Drug Design (CADD), and how does it contribute to the drug discovery process?
b.	What is homology modeling in the context of protein structure prediction? How does it help in understanding the 3D structure of a protein when the experimental structure is unavailable?
c.	What does the acronym ADMET stand for in the context of drug discovery? Explain why each of the ADMET properties is crucial for the successful development of a new drug.

SECTION C

3. Attempt any *five* parts of the following: **7 x 5 = 35**

a.	What is molecular docking, and how is it used in the context of CADD to predict the interaction between a drug molecule and its target protein?
b.	What is a pharmacophore, and how does it relate to the biological activity of a drug molecule?
c.	What is *in silico* drug design? How does it differ from traditional drug discovery methods, and what are the primary advantages of using computational approaches in drug design?
d.	What is virtual screening, and how is it used in drug discovery? Describe its importance in the identification of potential drug candidates.
e.	Briefly describe the role of HMG-CoA reductase in cholesterol biosynthesis and its importance in cellular metabolism. Why is it a target for drug discovery?
f.	What is lipophilicity, and how does it affect the pharmacokinetics and pharmacodynamics of a drug? Explain the role of partition coefficient (logP) in predicting drug behavior.
g.	How does solubility influence the drug's bioavailability? What are the strategies used to enhance the solubility of poorly water-soluble drugs?