Paper ID : 250294

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

BPHARMA
(SEM VIII) 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.	Define log P and explain how it relates to the partition coefficient.
b.	How does QSAR differ from SAR, and what advantages does it offer?
c.	What is a biochemical database?
d.	Compare random screening and non-random screening approaches.
e.	What is conformational analysis, and why is it important in SAR of a drug molecule?
f.	What is bioinformatics, and how is it used in modern biological research?
g.	Enlist two ADME databases.
h.	Name any two physicochemical properties commonly used to assess drug-likeness
i.	Explain COMFA and COMSIA.
j.	What is lead optimization in drug discovery?

SECTION B

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

a.	Elaborate analogue based drug design giving emphasis on objectives and categories of analogue designing.
b.	Discuss Hammet's substituent constant, Taft's steric constant and Hansch analysis and its role in predicting biological activity.
c.	Define pharmacophore. Discuss concept of pharmacophore mapping and pharmacophore-based screen.

SECTION C

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

a.	What is molecular docking? How does flexible docking differ from rigid docking in molecular docking studies?
b.	How does chemoinformatics contribute to drug discovery? Explain steps involved in chemical data curation.
c.	Discuss various energy minimization techniques used in molecular modelling study.
d.	How do similarity-based methods in virtual screening help identify potential drug candidates? Discuss key techniques used to measure molecular similarity.
e.	Define and classify bio-isosters. Explain bio-isosterism approach with examples.
f.	Discuss the role of molecular mechanics in drug design.
g.	Write an elaborative note on De novo drug design with example.