PAPER ID-411347

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

MPHARM
(SEM II) THEORY EXAMINATION 2023-24
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 CADD? Explain its advancements.
b.	Explain the Importance of the partition coefficient (log P).
c.	Define QSAR with COMSIA & COMFA.
d.	What is Taft constant?
e.	Which are the softwares used for ADMET calculations.
f.	What is the significance of Docking? Mention any two software used for Docking.
g.	What is Craig plot? Mention any one application.
h.	What is Lipinski's rule of five?
i.	What is the Virtual screening?
j.	Define Pharmacophore and De novo drug design.

SECTION B

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

a.	Explain various stages involved in De Novo drug design in drug discovery.
b.	Define & Classify Molecular Docking? Discuss the overall steps in Docking.
c.	What are the concept of Quantitative structure activity relationship (QSAR)? Discuss the different QSAR Applications.

SECTION C

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

a.	Explain the basic model of QSAR given by Hansch.
b.	Explain Hammet constant.
c.	Explain the importance of prediction and analysis of ADME properties in drug design
d.	Explain 3D QSAR approach in drug design.
e.	Explain Molecular & Quantum mechanics in drug design. (Molecular modeling).
f.	Describe the virtual screening techniques.
g.	Explain Pharmacophore Mapping in detail & its applications.