BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: M. Pharm **SEMESTER: IInd**
BRANCH: PHARMACY **SESSION: SP2022**

SUBJECT: MPC203T COMPUTER AIDED DRUG DESIGN

TIME: 3.00 Hours **FULL MARK: 75**

INSTRUCTIONS:
1. The missing data, if any, may be assumed suitably.
2. Before attempting the question paper, be sure that you have got the correct question paper.
3. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

Q.1(a)	Explain molecular modeling in the context of historical times and in the applications in modern times.	[7]
Q.1(b)	Elaborate the terms:(1) Visualization (ii) Molecular Mechanics (iii)Conformational Search	[8]
Q.2(a)	Define QSAR and explain the requirements for a QSAR study with detail references to descriptors	[7]
Q.2(b)	Describe Craig Plot with the diagram	[8]
Q.3(a)	Analyze the differences between 2D QSAR and 3D QSAR. Explain the preparation of a molecule for 3 D QSAR studies	[7]
Q.3(b)	Define the following(i)Contour Plots (ii) ComSIA	[8]
Q.4(a)	Define the following: (i) Direct Drug Design (ii) Monte Carlo Search (iii)Systematic Search	[7]
Q.4(b)	Explain Topliss tree for aromatics and aliphatics related to drug design	[8]
Q.5(a)	Discuss the Pharmacophore modeling protocol in detail.	[7]
Q.5(b)	Briefly discuss of defects in PDB files of proteins and how to rectify the same	[8]
Q.6(a)	Discuss in detail the various statistical tools in building PK predictive models?	[7]
Q.6(b)	Write a note on Alphafold. How it is different from traditional homology modeling?	[8]
Q.7(a)	Discuss in detail on various parameters used for the validationof Pharmacophore model	[7]
Q.7(b)	Enumerate the steps involved in homology modeling with a brief discussion on each step.	[8]