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

CLASS: M.PHARM **SEMESTER : II**
BRANCH: PHARMACY **SESSION : SP/19**

SUBJECT: MPC203T COMPUTER AIDED DRUG DESIGN

TIME: 3.00 Hrs **FULL MARKS: 75**

INSTRUCTIONS:
1. The question paper contains 7 questions each of 15 marks and total 105 marks.
2. Candidates may attempt any 5 questions maximum of 75 marks.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

Q.1(a)	Elaborate the steps required in a 3D QSAR analysis	[7]
Q.1(b)	Explain the terms: (i)P (ii)Pi (iii) Sigma (iv) Es	[8]
Q.2(a)	Elaborate the Hansch equation	[7]
Q.2(b)	Elaborate the Craig plot and describe it in reference to Hansch equation	[8]
Q.3(a)	Elaborate the Topliss scheme for aromatic susbtituents.	[7]
Q.3(b)	Define QSAR and explain the various physicochemical parameters associated with it.	[8]
Q.4(a)	Explain the terms(i) Bootstrapping (ii) Simulated annealing (iii)Training and Test set	[7]
Q.4(b)	Elaborate the methods used in conformational analyses in details	[8]
Q.5(a)	What is the importance of study of CADD in field of drug discovery and development?	[7]
Q.5(b)	Mention and explain the major factors in drug design.	[8]
Q.6(a)	What are the major physical factors which play a role in rational planning of ligands in context to (i) H-bonding (ii) complexation?	[7]
Q.6(b)	What are the factors linked to drug receptor interaction studies of therapeutic ligands?	[8]
Q.7(a)	Write a short note on drug receptor theories linked to:(i) Induced fit theory. (ii) macromolecular aggregations theory.	[7]
Q.7(b)	Write a short note on SBDD and drug design.	[8]

:::::26/04/2019 M:::::