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

CLASS: MPHARM **SEMESTER : II**
BRANCH: PHARMACY **SESSION : SP/18**

SUBJECT: MPH2015 COMPUTER AIDED DRUG DESIGN

TIME: 3.Hours **FULL MARKS: 60**

INSTRUCTIONS:
1. The question paper contains 7 questions each of 12 marks and total 84 marks.
2. Candidates may attempt any 5 questions maximum of 60 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) Distinguish between 2D QSAR and 3D QSAR and enumerate their advantages and disadvantages. [6]
Q.1(b) Elaborate with the help of diagram (i) Craig Plot (ii) Topliss tree for aromatic substituents. [6]

Q.2(a) Explain the terms: (i)Molecular Modelling (ii)Basic Modules required in a molecular modeling system. [6]
Q.2(b) Explain energy minimization with examples. [6]

Q.3(a) Elaborate the (i) Ab initio methods (ii) Semi empirical methods. [6]
Q.3(b) How will you identify the bioactive conformation? Detail the procedure. [6]

Q.4(a) Discuss in detail about various statistical methods generally adopted for developing ADMET models. [6]
Q.4(b) Discuss in detail the problems associated with *de novo* drug design. Discuss the means to handle them. [6]

Q.5(a) Briefly list the applications of comparative homology modeling. Discuss in detail regarding the *Alignment of Target Sequence*. [6]
Q.5(b) How will you define a Pharmacophore? Write a note on ROC. [6]

Q.6(a) Make a flow diagram for Pharmacophore modelling and Similarity Search. Differentiate on the basis of the protocol used for practicing them. [6]
Q.6(b) Explain *Deformation* in detail. [6]

Q.7(a) Write short notes on Docking. [6]
Q.7(b) Write a note on model validation methods used for ADMET models. [6]

:::::27-04-2018 E:::::