M. PHARM. (PHARMACEUTICAL CHEMISTRY) SEM –II
(CBCS- 2019 COURSE): Winter - 2021.
SUBJECT: COMPUTER AIDED DRUG DESIGN

Day: Wednesday
Date: 01-12-2021

Time. 02:00 PM-05:00 PM
Max. Marks: 75

W-20784-2021

N.B.:

1) **Q. No.1** and **Q. No.5** are **COMPULSORY.** Out of remaining questions attempt **ANY TWO** questions from each section.
2) Answer to both the sections should be written in **SEPARATE** answer book.
3) Figures to the right indicate **FULL** marks.

SECTION-I

Q.1 What are physiochemical properties? List out the different physiochemical properties and describe the importance of any two of them. **(08)**

Q.2 Explain in detail Hansch and Free Wilson model with examples. **(15)**

Q.3 Describe detailed methodical process of molecular docking. Write different mathematical components of scoring functions. **(15)**

Q.4 Write short notes on **ANY TWO** of the following: **(15)**

a) Energy minimization
b) HIV protease structure and binding interactions with any one HIV protease inheritors
c) Topless approach of substitution

SECTION-II

Q.5 What is pharamceophore model and explain in detail. **(07)**

Q.6 Explain importance of ADMET properties of new molecules in view with drug design. **(15)**

Q.7 What are the methods to predict binding cavity size of an enzyme or receptor? **(15)**

Q.8 Write short notes on **ANY TWO** of the following: **(15)**

a) Fragment based screening
b) Importance of drug design
c) Strategies for virtual screening

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