MASTER OF SCIENCE (BIOINFORMATICS) (CBCS-2019 COURSE)
M. Sc. (Bioinformatics) Sem-III : WINTER :- 2021
SUBJECT: CHEMOINFORMATICS & DRUG DESIGNING

Day : Thursday
Date 27-01-2022 **W-21176-2021**

Time : 02:00 PM-05:00 PM
Max. Marks: 60

N.B.:

1) All the questions are **COMPULSORY.**
2) Figures to right indicate **FULL** marks.
3) Answer to both sections should be written in **SAME** answer book.

SECTION-I

Q.1 Define **(ANY FIVE):** **(10)**

a) Tversky index **b)** Graph theory **c)** 2D structure descriptor
d) SMILES **e)** Catalytic resides **f)** Kappa shape index

Q.2 Answer the following **(ANY TWO):** **(10)**

a) Describe different molecular patterns.
b) Write about PDB file format.
c) Give applications of ADMET properties in drug discovery process.

Q.3 Write short note on **(ANY TWO):** **(10)**

a) Scope of chemoinformatics in pharmaceutical research.
b) Combinatorial libraries
c) Molecular descriptor

SECTION-II

Q.4 Explain in brief **(ANY FIVE):** **(10)**

a) QSPR **b)** E-state **c)** Virtual screening
d) PCA **e)** Lead optimization **f)** Cross validation techniques

Q.5 Answer the following **(ANY TWO):** **(10)**

a) Explain in detail the drug discovery process.
b) What is a concept of training set, test set and external validation dataset? Explain with example.
c) Explain in detail about various methods used for information mapping? Add a note on the applications of interaction mapping.

Q.6 Write short notes on **(ANY TWO):** **(10)**

a) What is Pharmacophose mapping? Briefly explain the various methods to derive 3D Pharmacophore.
b) What is free Wilson analysis?
c) Explain the scoring functions for protein- ligand docking.

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