M. Sc. Bioinformatics Sem.-III (2013 Course) (Choice Based Credit Systems) : WINTER - 2018

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

Day : Thursday
Date : 25/10/2018

Time : 02.00 PM TO 05.00 PM
Max. Marks : 60

W-2018-1260

N.B.:

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

SECTION – I

Q.1 Define: **[10]**

a) SMIRKS **c)** KNN **e)** PLS
b) Euclidean distance **d)** Huckel charge

Q.2 Answer the following: **[10]**

a) Explain the role of cheminformatics in pharmaceutical and chemical research.
b) Discuss about molecular descriptors.

Q.3 Write short notes on: **[10]**

a) Virtual Screening
b) Chemical databases

Q.4 Explain in detail molecular properties. **[10]**

OR

How to design and analyze combinatorial libraries.

SECTION – II

Q.5 Write in brief on: **[10]**

a) Activities and toxicities
b) Structure based drug design

Q.6 Explain in short: **[10]**

a) CoMFA **c)** QSPRs **e)** Cross validation techniques
b) CoMSIA **d)** Pubchem Bioassay

Q.7 Write short notes on: **[10]**

a) Receptor based and ligand based pharmacophore modeling
b) Similarity matrices and scoring functions

Q.8 Discuss in detail all docking procedure. Comment on its types. **[10]**

OR

What is QSAR? Explain in detail the various properties studied while doing QSAR analysis.

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