

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

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

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.

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.