**Exam. Code : 206603**
**Subject Code : 3653**

**M.Sc. (Bio-Informatics) 3rd Semester**

# MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN

**Paper—BI–634**

Time Allowed—3 Hours] [Maximum Marks—75

**Note :**—Attempt **FIVE** questions in all. Section A is compulsory. Attempt any **FOUR** questions from Section B i.e. **ONE** question from each unit.

## SECTION—A

I. Briefly explain :

(i) CHARMM 'force field'

(ii) Hansch lipophilic descriptor

(iii) Vector system of molecular graphics

(iv) Determination coefficient

(v) cAMP as secondary messenger

(vi) Hydrogen bonding donor groups

(vii) Step size in MD simulation

(viii) Irreversible enzyme inhibitor

(ix) Drug-induced DNA damage

(x) Nucleoside reverse transcriptase inhibitors (NRTIs)

1.5×10

## SECTION—B

### UNIT—I

II. (a) Describe various types of molecular strains which are parameterized in molecular mechanics along with their mathematical expressions. 7.5

(b) Explain the Newton-Raphson and Quasi-Newton methods of energy minimization. 7.5

III. (a) Explain the principle of Monte Carlo simulation. Compare it with molecular dynamics simulation. 7.5

(b) Discuss about the identification of 'preferred conformation' of a molecular system using distance geometry. 7.5

### UNIT—II

IV. (a) Write a short note on Steric QSAR descriptors. 7.5

(b) Discuss Hansch QSAR analysis model. Comment on its advantages over other conventional QSAR models. 7.5

V. (a) What is pharmacophore ? Describe the common steps involved in pharmacophore mapping. 10

(b) Discuss selection of the most significant PLS model. 5

## UNIT—III

VI. (a) Give critical account of tyrosine kinase receptors. 7.5

(b) Classify ion channels with suitable examples. 7.5

VII. What are the various strategies which are used to target DNA by anticancer agents ? Discuss any one in detail with suitable examples. 15

## UNIT—IV

VIII. (a) What is Structure Based Drug Designing (SBDD) ? 5

(b) What is the principle of docking analysis ? Explain docking as a tool in SBDD. 10

IX. (a) Classify 3D data based search approaches used in CADD. Describe their advantages and limitations. 10

(b) How to model drug-likeness in CADD ? 5