Exam. Code : 206603

Subject Code : 4771

M.Sc. Bio-Informatics 3rd Semester (Batch 2020-22)

MOLECULAR MODELING & COMPUTER AIDED DRUG DESIGN

Paper—BI-634

Time Allowed—3 Hours] [Maximum Marks—75

Note :— Attempt **FIVE** questions in all, selecting at least **ONE** question from each section. The **FIFTH** question may be attempted from any section. All questions carry equal marks.

SECTION—A

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

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

II. (a) Sketch a Ramachandran plot for a typical Protein containing α-helix and β-sheet secondary structure. Label the axes of the plot and indicate the regions corresponding to the different types of secondary structure. 7.5

(b) What are rotamers ? How to model side chain of amino acids in protein structure ? 7.5

SECTION—B

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

IV. (a) Write note on oncogene and tumor suppressor genes. 10

(b) Discuss the principle and methods of Molecular Docking. 5

SECTION—C

V. (a) What is pharmacophore ? Describe the common steps involved in pharmacophore mapping. 7.5

(b) Discuss various 3D database search approaches. 7.5

VI. Explain both structure based and ligand based drug design approach. 15

SECTION—D

VII. (a) Discuss the Lipinski rule of five and its applications. 5

(b) What is partial least square regression analysis ? Give its advantages over other regression methods. 10

VIII. (a) Describe the development and evaluation of Hansch QSAR model. 10

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