

M.Sc. (Bio-Informatics) Fourth Semester
MBIN-8018: Molecular Modeling and Pharmacoinformatics

Time allowed: 3 Hours

Max. Marks: 60

NOTE: Attempt five questions in all, including Question No. I which is compulsory and selecting atleast one question from each Unit.

x-x-x

I. Briefly define or discuss the following:-

- a) Molecular modeling
- b) Force fields
- c) Objectives of QSAR
- d) Pub Chem
- e) Active site
- f) Molecular descriptors
- g) Genetic algorithm
- h) Genome

(8x1½)

UNIT - I

- II. a) Discuss various energy minimization methods help of suitable example.
b) Write a note on basic concepts in molecular modeling.

(6,6)

III. Discuss the following:-

- a) Conformation analysis
- b) Empirical potential energy

(6,6)

UNIT - II

- IV. a) Discuss the various concepts used in QSAR with the help of suitable example.
b) Write a note on "lead optimization".

(8,4)

V. Discuss the following:-

- a) Compare high throughput versus rational drug designing.
- b) Target identification and target validation

(6,6)

P.T.O.

(2)

UNIT - III

- VI. a) Discuss genetic basis for variability in drug response with the help of suitable example.
- b) Write a note on "Chemo informatics". (8,4)
- VII. Explain the following:-
- a) Tools used for searching chemicals on the internet
- b) Use of Genome in drug target identification (6,6)

x-x-x