Exam.Code:0442
Sub. Code: 3512

1058

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. Attempt the following:-

a) Define empirical energy.

b) Write formula for estimation of energy term for bonded atoms?

c) Explain genetic algorithm.

d) Define pharmacophore keys.

e) Define QSAR.

f) Discuss 3D Fingerprints.

g) What is Tanimoto coefficient?

h) Discuss phase I clinical trial stage. (8x1½)

UNIT – I

II. a) Define molecular modeling and what can we learn from it.

b) Write a note on confonnational analysis. (2x6)

III. a) Discuss role of molecular mechanism & its application.

b) What is ideal minimization technique and why.

UNIT –II

IV. a) What are the different approaches for drug designing?

b) Differentiate between high throughputs vs. rational drug design methods. (2x6)

V. a) What is the importance of molecular descriptor in QSAR?

b) Why indicator variable is used in QSAR models? (2x6)

P.T.O.

UNIT – III

VI. a) Discuss Pharmacogenomics & its applications.

b) What a note on using genomics for target identification. (2x6)

VII. a) What are molecular descriptor & name three descriptors?

b) Write a note on molecular similarity & its applications. (2x6)

x-x-x