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 <u>five</u> 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.

<u>UNIT – I</u>

II.	a) Define molecular modeling and what can we learn from it.	
	b) Write a note on conformational 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)

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<u>UNIT – III</u>

VI. a) Discuss Pharmacogenomics & its applications.

- b) What a note on using genomics for target identification.
- VII. a) What are molecular descriptor & name three descriptors?
 - b) Write a note on molecular similarity & its applications.

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(2x6)

(2x6)

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 a) Petina molecular modeling and what can we leave from b) Write a new or conformational manarity.

a) Diarses role of molecular neovembers & in application by What 's ident minimization technique and why

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a) What was the different approaches fourfully designing?
b) Effectuations between bigh Encounteres vs. rational those design wellaws.

(• What is the importance of enforting deterior in OS What is the importance of enforcement in OSA & models?

(2)