Exam. Code: 0442
Sub. Code: 3512

2054

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. 1 which is compulsory and selecting atleast one question from each Unit.*

x-x-x

1 **Briefly define or discuss the following** 8 ×1.5

i) Force fields
ii) Pharmacoinformatics and its significance
iii) Molecular modeling
iv) Lead optimization
v) Molecular graphics
vi) Coordinate system
vii) Rational Drug designing
viii) Pub Chem

UNIT I

2 a) Discuss various concepts in molecular modeling with the help of suitable example 8,4

b) Write a note on Molecular graphic and its significance

3 Discuss the following- 8,4

a) Briefly discuss various energy minimization methods
b) Write a note on Empirical potential energy

UNIT II

4 a) Discuss the basic principle of similarity and complementarity with the help of suitable example 6,6

b) Write a note on high throughput screening and its wide applications

5 Discuss the following- 6,6

a) Basic concept and principles use in QSAR
b) Target identification and validation

UNIT III

6 a) Discuss the genetic basis for variability in drug response and metabolism with the help of suitable example 8,4

b) Write a note gene-drug interaction

7 Explain the following 6,6

a) Pharmacogenomics in individualized drug response
b) Chemoinformatics and its importance in drug development

x-x-x