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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

I. Briefly elaborate the following with suitable example wherever desired

- a) Molecular modeling
- b) Target site
- c) QSAR
- d) Molecular descriptor
- e) Finger print
- f) PubChem
- g) Pharmacoeconomics
- h) Lead optimization

(8x1½)

**UNIT – I**

II. a) What do you understand by force fields? Discuss molecular mechanics force fields methods in details.

b) Write a note on Coordinate systems.

(8,4)

III. Discuss the following:-

- a) Conformation analysis
- b) Molecular graphics

(6,6)

**UNIT – II**

IV. a) Discuss in details various concepts used in QSAR.

b) Explain details development of HANSCH QSAR equation.

(6,6)

V. Discuss the following-

- a) Target site identification and validation
- b) Comparison between high throughput and rational drug designing

(6,6)

P.T.O.

(2)

### UNIT – III

- VI. Explain the role of pharmacoinformatics in ADME. Explain with suitable example Explain genetic basis of variability in drug response. (12)
- VII. Write a note on the following:-
- Individualized drug therapy (IDT)
  - Role of genomics in drug target elucidation (6,6)

x-x-x