STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2006-07 thereafter)

SUBJECT CODE: BI/PC/MM35

M. Sc. DEGREE EXAMINATION, NOVEMBER 2008
BIOINFORMATICS
THIRD SEMESTER

COURSE : CORE
PAPER : MOLECULAR MODELLING
TIME : 3 HOURS **MAX. MARKS: 100**

SECTION – A **1x20=20**

I. FILL IN THE BLANKS.

1. …… of the functional form and ……. is an important feature of a force field.
2. …….. coordinates are commonly used as input to quantum mechanics.
3. At minimum point in the potential energy surface, second derivative is …….
4. Even at absolute zero temperature molecule undergo vibrations due to ……..
5. ……. and …… are required for the substructure searching in lead discovery.

II. STATE WHETHER TRUE OR FALSE

6. NVE is a canonical ensemble.
7. CHRAMM force field can be used for molecular dynamics simulation.
8. Molecular dynamics simulation is based on Ergodic hypothesis.
9. Phenylalanine and tryptophan are hydrophilic amino acids.
10. Alpha helical structure is proposed by Gibbs.

III. CHOOSE THE CORRECT ANSWSER

11. …….. is a square matrix with all non-diagonal elements zero
    a) Diagonal matrix b) Unit matrix
    c) Null matrix d) Identity matrix
12. Phase space for N atoms
    a) 3N b) N c) 6N d) N-1
13. The biologically active conformation of a drug molecule may not correspond to
    a) Global minimum b) Local minimum
    c) Both (a) & (b) d) Unstable
14. The average position of a particle in a liquid is determined by
    a) Heat capacity b) Radial distribution function
    c) Boltzmann law d) Hooke's law
15. Among the following which one is related to QSAR
    a) logP b) log(P-1)
    c) log(1-P) d) logPG

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IV. WRITE IN ONE OR TWO SENTENCES

16. van der Waal's interaction.
17. SPDBV
18. Partition coefficient
19. Ensemble
20. Pharmacaphore

SECTION – B 4x10=40

ANSWER THE FOLLOWING QUESTIONS IN 500 WORDS:

21. What is meant by multiple referencing problem in the force field development of metal complexes.
22. Explain the salient features of secondary structural elements of proteins.
23. State the uses of clique detection method in the 3D pharmacophore searching
24. Explain the merits and demerits of first and second derivative energy minimization techniques.
25. What you mean by periodic boundary condition? And explain its significance in molecular dynamics simulation.
26. Explain: Partition functions
27. Explain the uses of various molecular descriptors in the development of QSAR.

SECTION – C 2x20=40

ANSWER THE FOLLOWING QUESTIONS IN 1200 WORDS:

28. Explain the uses of molecular mechanics and dynamics methods in the prediction of protein-ligand interactions.
29. Give a detailed account of various algorithms used in molecular dynamics simulation.
30. Give a detailed account of molecular modeling in the de novo drug design.
31. Explain data mining and visualization tools in bioinformatics.

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