STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI –600 086
(For candidates admitted from the academic year 2002 – 03 & thereafter)

SUBJECT CODE : BI/PC/MD45

M. Sc. DEGREE EXAMINATION, APRIL 2007
BIOINFORMATICS
FOURTH SEMESTER

COURSE : MAJOR CORE
PAPER : MOLECULAR MODELLING AND DRUG DESIGNING
TIME : 3 HOURS **MAX. MARKS: 100**

SECTION – A

ANSWER ALL QUESTIONS **(20X1=20)**

I FILL IN THE BLANKS:

1. The allowed dihedral angles of a protein can be obtained from_____ plot.
2. Internal coordinates of molecules are usually written as a _____ matrix
3. The Newton-Raphson is a _____ derivative method.
4. To define a force field one must specify not only the functional form but also the _____
5. The relationship between the numerical properties and the activity is described by an equation of the form_____

II STATE WHETHER TRUE OR FALSE:

6. Force field parameters has the transferability property.
7. The molecular dynamics method is used to predict conformational changes.
8. Explicit solvent simulation can not carried out in molecular dynamics simulation.
9. Van der Waals interaction can not be described in force field methods.
10. Hydrogen bonds stabilize the protein structure.

III CHOOSE THE CORRECT ANSWER:

11. The unit or identity matrices is a special type of a diagonal matrix in which
    (a) All the non-zero elements are 2 (b) All the non-zero elements are 1
    (c) All the non-zero elements are 4 (d) None of the above
12. Molecular mechanics provides
    (a) Information about the static nature of proteins
    (b) Information about the dynamic nature of proteins
    (c) Both static and dynamic nature of proteins
    (d) None of the above
13. Docking determines
    (a) Structure of protein (b) Structure of ligand
    (c) Structure of protein-ligand intermolecular complex
    (d) None of the above
14. Clique detection is based on
    (a) Molecular mechanics (b) Molecular dynamics
    (c) Graph theory (d) Group theory
15. The development of 3D pharmacophore has spawned a new type of descriptor known as
    (a) Pharmacophore key (b) Similarity key
    (c) Docking key (d) Key

..2

IV WRITE IN ONE OR TWO SENTENCES:

16. Potential energy functions for bond stretching and angle bending
17. TIP5P
18. QSAR
19. Ensemble
20. Uses of 3D data bases

SECTION – B (4x10=40)

Answer any FOUR questions in not more than 500 words. Draw diagrams wherever necessary. Each answer carries equal marks.

21. How do you treat delocalized systems using force field approach?
22. Explain the uses of docking.
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. How do you compute the effect of long range interactions in the stabilization of protein structure?
26. How do you incorporate solvent effects into molecular dynamics simulation?
27. Explain about the various molecular descriptors used in the development of QSAR

SECTION – C (2x20=40)

Answer any TWO questions in not more than 1200 words. Draw diagrams wherever necessary. Each answer carries equal marks.

28. Give a detailed account of force field method and its applications.
29. Explain the various steps in the molecular dynamics simulation of protein with necessary theoretical background.
30. Explain in detail about the different steps in the *de novo* ligand design and drug design.
31. Explain the uses of various 2D and 3D databases and their applications.

****