STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2010-11)

SUBJECT CODE: BI/PC/MC33

M. Sc. DEGREE EXAMINATION, NOVEMBER 2011
BIOINFORMATICS
THIRD SEMESTER

COURSE : CORE
PAPER : MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGNING
TIME : 3 HOURS **MAX. MARKS: 100**

SECTION – A

ANSWER ALL QUESTIONS **(20 x 1 = 20marks)**

1. The de Broglie relations show that the _____is inversely proportional to the momentum of a particle
   a. frequency b. wavelength c. photons d. electrons

2. A covalent bond is sharing of ---------- between atoms.
   a. neutrons b. photons c. electrons d. positrons

3. The valance of carbon is
   a. 4 b. 5 c. 6 d.3

4. The time-independent Schrödinger equation are commonly used to calculate the _____.
   a. time b. quantum c. energy level d. molecular level

5. The hydrogen bonds are
   a. stronger than van der walls b. weaker than covalent
   c. weaker than ionic d. All the above

6. The van der Waals force is the sum of the attractive or repulsive forces between molecules of
   a. ions b. neutral atoms c. both a and b correct d. both a and b incorrect

7. The Lennard-Jones potential referred as interaction between
   a. atoms b. ions c. molecules d. neutral atoms and molecules

8. Bond lengths are measured by
   a. nanometer b. picometer c. micron d. millimeter

9. The process of determining whether a given conformation and orientation of a ligand fits the active site is
   a. docking b. locking c. scoring d. posing

10. The simulation which apply forces to a protein in order to manipulate its structure by pulling it along desired degrees of freedom_____.
    a. Free energy enrolling dynamics b. conventional molecular dynamics
    c. nonconventional molecular dymanics d. steered molecular dynamics

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11. **NVE** ensemble means the system is isolated from changes in
    a. numerical, liter, kcal b. number, weight and energy
    c. moles, volume and energy d. number, volume and energy

12. If two systems are each in thermal equilibrium with a third, they are also in thermal equilibrium with each other is _____ law of thermodynamics.
    a. First b. second c. zero d. none

13. The backbone –dependent rotomer library is helped to study _____ of proteins.
    a. Hydrogen bond b. peptide bond c. side chains d. folding pattern

14. The blind docking (BD) approach is used for
    a. design of inhibitor b. comparison of microtubule-stabilizing agent
    c. exploring substrate binding d. All the above

15. Force field is calculated by_____
    a. sum of van der Waals and electrostatic interactions b. sum of covalent bonds
    c. sum of ionic bonds d. sum of hydrogen bonds

16. The protein threading, is a method of protein modeling by
    a. same fold as proteins of known structures, but do not have homologous proteins with known structure
    b. same fold as proteins of known structures, but have homologous proteins with known structure
    c. same fold as proteins of unknown structures, but have homologous proteins with known structure
    d. same fold as proteins of unknown but do not have homologous proteins with known structure

17. The large number of potential ligand molecules are screened to find those fitting the binding pocket of the receptor is called _____.
    a. building" ligands b. finding" ligands c. active''ligands d. reference ''ligands

18. In the molecular modeling, the scoring functions are used to predict the strength of the _____ interaction of two molecules after they have been docked.
    a. non-covalent b. covalent c. ionic d. van der waals force

19. It is assumed that hydrophobicity changes from protein interior to exterior according to Gauss distribution is _____.
    a. maximum to minimum b. evenly distributed c. minimum to maximum d. neutral

20. The large libraries of compounds evaluating automatically is called _____"
    a. virtual screening b. Online screening
    c. computer based screening d. offline screening

SECTION – B

ANSWER ANY 4 FROM THE FOLLOWING QUESTIONS: (4 x 10 = 40marks)

21. Lagrangian equations of motions are cyclic coordinates ones – why?
22. Write the salient feature of Bohr model for Hydrogen atom
23. Explain the role of electrostatic potential for stabilization of protein structure.
24. What are the descriptors used for QSAR?
25. How to generate ligand libraries for drug design?
26. Explain the methods used for detection of 3D pharmacophore.
27. Write short notes on salient features of in silico modeling

SECTION – C

ANSWER ANY 2 FROM THE FOLLOWING QUESTIONS IN DETAIL

(2 x 20 = 40marks)

28. Define energy minimization. Describe the techniques used for minimization of energy in globular proteins
29. Describe in detail about molecular dynamics simulation of constant temperature and pressure.
30. Describe the various approaches involved in Molecular docking and explain limitations of molecular docking for protein-ligand interactions
31. What is SBDD? Explain the steps involved in the SBDD for drug design.

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