STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2015 - 16)

SUBJECT CODE: 15BI/PC/MC34

M. Sc. DEGREE EXAMINATION, NOVEMBER 2016
BIOINFORMATICS
THIRD SEMESTER

COURSE : CORE
PAPER : MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGNING
TIME : 90 MINUTES **MAX. MARKS: 50**

SECTION – A

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

1. The dipole moment of molecules depends on
   a. Bonds having different electro negativity b. The separation of charges is larger
   c. Multiple polar bonds pointing in the same direction d. All the above

2. Select the correct order of strong interaction between atoms
   a. Ion-dipole forces ≤ ion-induced dipole forces ≤ dipole-dipole interactions
   b. dipole-dipole interactions ≤ Ion-dipole forces ≤ ion-induced dipole forces
   c. Ion-dipole forces ≤ dipole-dipole interactions ≤ ion-induced dipole forces
   d. ion-induced dipole forces ≤ dipole-dipole interactions ≤ Ion-dipole forces

3. The hydrogen bond is one of the poor electrostatic dipole-dipole interaction
   True or False

4. Keesom interaction indicated
   a. permanent-permanent dipoles b. permanent-induced dipoles
   c. dipole-induced dipoles interaction d. Ionic Lattice Energy

5. The process of finding an arrangement in space of a collection of atoms where, according to some computational model of chemical bonding is called
   a. energy minimization b. energy optimization
   c. geometry minimization d. All the above

6. The following computer simulation method used for studying the physical movements of atoms and molecules is
   a. Molecular dynamics b. Atomic simulation
   c. Molecular simulation d. noe of the above

7. Markov Chain Monte Carlo method was invented by
   a. Markov b. Monte Carlo
   c. Markov and Monte Carlo d. Stanislaw Ulam

8. Graph invariants is measured by
   a. 0D-descriptors b. 1D-descriptors c. 2D-descriptors d. 3D-descriptors

9. The 4D-descriptors derived from
   a. GRID b. CoMFA c. Volsurf d. All the above

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10. Arrange the sequence of QSAR/QSPR method
(i) variable selection (ii) validation evaluation
(iii) Selection of Data and extraction of descriptors (iv) model construction
a. I, ii, iii, iv b. iii, I, iv, iii c. I, iii, iv, ii d. iii, ii, I, iv

11. Protein – lead simulation done by the computer simulation tool is
a. Modeller b. Swiss PDB viewer c. Autodock d. Rasmol

12. The Zeta potential is the indicator of
a. stability b. molecular reaction c. kinetic energy d. current force

13. The process of heat transfer from object to another because of molecular motion and interaction is called:
a. Convection b. Conduction c. Radiation d. Induction

14. The average molecular kinetic energy of a gas depends on:
a. Pressure b. Volume c. Temperature d. Number of moles

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

16. 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

17. System biology is the field of science deals the
a. Plants and animals b. Enzymes
c. Systems of organism d. Metabolic pathway

18. Which of the following statements is true?
a) The most stable conformation of a drug is also the active conformation.
b) The active conformation is the most reactive conformation of a structure.
c) The active conformation is the conformation adopted by a drug when it binds to its target binding site.
d) The active conformation can be determined by conformational analysis.

19. What is meant by *de novo* drug design?
a) The synthesis of a compound from simple starting materials.
b) The design of the synthesis required to generate a novel range of structures.
c) The design of a novel drug based on molecular modelling studies of a binding site.
d) The modification of a drug based on molecular modelling studies into how it binds to its target binding site.

20. Which of the following software programmes is used for automated *de novo* drug design?
a) DOCK b) LUDI c) CHEM3D d) CoMFA

SECTION – B

ANSWER ANY THREE QUESTIONS (3 x 10 = 30marks)

21. Describe the various features of molecular descriptors on Quantitative structure activity relation ship
22. Elaborate the methods adopted for Protein – Ligand in molecular docking in Drug design
23. Write the brief account on Gibbs Ensemble Monte Carlo method for chemical Equilibrium.
24. Write any five computer simulation method for Energy minimization technique.

25. Describe the various features of molecular mechanics on molecular modeling

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