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

SUBJECT CODE: 15BI/PC/MC34

M. Sc. DEGREE EXAMINATION, NOVEMBER 2018
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. In only one co-ordinate is used in PES, then the surface is called ____
2. Say true or false; Electrostatic force works depending on a particle's initial and final position.
3. Interaction between highly electron deficient hydrogen and highly electronegative atom is called ___
   a. Covalent bond, b. Ionic bond, c. Dipole-dipole interaction d. hydrogen bond.
4. Strength of intermolecular forces from ionic or covalent bond is
   a. Weaker, b. Stronger, c. Equal, d. None of the above
5. Mention any one force field.
6. ___ is the method used to study the energetic of ionic crystals.
7. ___ and ___ are non-derivative methods of energy minimization.
8. Consider the following thermodynamic properties.
   i) Work done on a system
   ii) Heat absorbed
   iii) Entropy
   iv) Enthalpy

   Which of these properties are state functions?
   a. i) and ii) only
   b. i) and iii) only
   c. i) only
   d. iii) and iv) only
9. In the practical application of molecular dynamics simulations which fundamental equation is used:
   a. Law of gravity
   b. Schrodinger equation from quantum mechanics
   c. Newton's equation of motion
   d. Thermodynamic equations of state
10. SMILES notation represents
    a. Molecular structural details c. Chemical details
    b. Data collection d. Reaction

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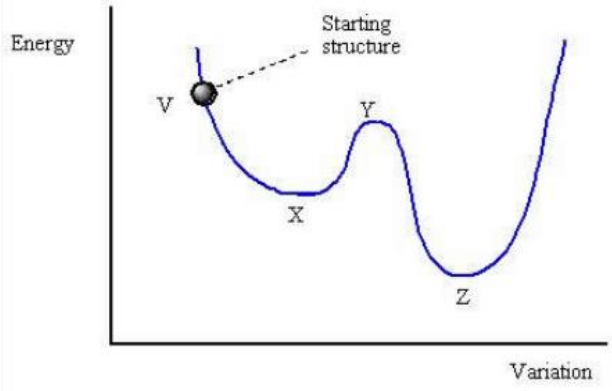
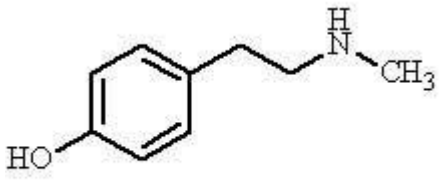
11. Molecular dynamics simulations can be used to
    a. Follow the time dependence of a biomolecule
    b. Calculate thermodynamics quantities
    c. Calculate spectroscopic quantities
    d. All the above
12. Mention any one molecular docking software.
13. Which of the following is not a crucial requirement for a drug to act as an agonist?
    a. Functional groups,b. Metabolic stability, c. Pharmacophore d. Size
14. What is the symbol π in a QSAR equation?
    a. The hydrophobicity of the molecule
    b. The electronic effect of a substituent
    c. The substituent hydrophobicity constant
    d. A measure of the steric properties for a substituent
15. The following graph shows the stability of a molecule as its structure is varied during conformational analysis.



What term is used to describe the point on the graph marked X?
a. Global energy minimum
b. Transition state
c. Local energy minimum
d. Conformational minimum

16. What does the symbol P represent in a QSAR equation?
    a. pH, b. plasma concentration, c. partition coefficient, d. prodrug
17. Which of the following statements is true?
    a. Drugs and drug targets generally have similar molecular weight
    b. Drugs are generally smaller than drug targets
    c. Drugs are generally larger than drug targets
    d. There is no general rule regarding the relative size of drugs and their targets
18. Mention any two criteria to choose the protein structure for docking analysis.

19. What is meant by a binding site?
    a. The area of a macromolecular target that is occupied by a drug when it binds
    b. The portion of the drug to which a drug target binds
    c. The functional groups used by a drug in binding to a drug target
    d. The bonds involved in binding a drug to its target
20. Structure I has a highly flexible side chain



I

    a. A flexible molecule is more likely to be in its active conformation when it approaches its target binding site. This results in increased activity.
    b. A flexible molecule is more likely to adopt conformations that will bind to different targets, resulting in side effects
    c. A flexible molecule may be able to bind to its target binding site in different binding modes, resulting in an increase in activity
    d. A flexible molecule is more likely to show target selectivity.

SECTION – B

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

21. Explain the features of molecular mechanics in detail.
22. Write in detail about derivatives and non-derivative minimization methods.
23. Describe the Gibbs ensemble Monte Carlo method in detail.
24. Give a detailed account on QSAR.
25. Write a note on protein-ligand docking and explain its steps involved in detail.

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