STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2011-12 & thereafter)

SUBJECT CODE: 11BI/PC/MC34

M. Sc. DEGREE EXAMINATION, NOVEMBER 2015
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 = 20 marks)

1. Which of the following statements best describes structure-activity relationships (SAR)?

a) The study of which functional groups are important to the chemical reactivity of the drug.
b) The study of the physicochemical properties that are important to the absorption of a drug into the blood supply.
c) The study of the structural features of a drug that are important to its biological activity.
d) The study of the structural features of a drug that are important to its chemical stability.

2. Which of the intermolecular bonding interactions below are possible for an alcohol?

a) Hydrogen bonding only
b) van der Waals interactions only
c) Ionic bonding only
d) Both hydrogen bonding and ionic bonding

3. Which of the following major aims in drug design is not related to the pharmacodynamics of a drug?

a) The reduction of side effects
b) The maximisation of activity
c) The reduction of toxicity
d) The maximisation of oral bioavailability

4. Which of the following is not true of analogues produced by a rigidification strategy?

a) They have a smaller number of conformations.
b) They are easier to synthesise.
c) They are likely to be more selective.
d) They are likely to be more active.

5. Which of the following statements is true?

a) Drugs and drug targets generally have similar molecular weights.
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

6. 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.

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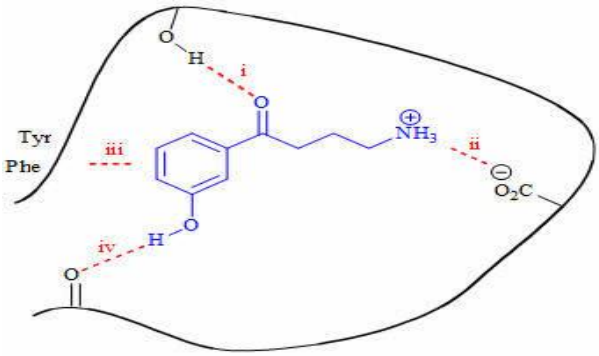
7. Consider the molecule in blue bound to a binding site. Identify the binding interactions taking place at i and iv shown.



a) hydrogen bonds b) ionic bonds c) van der Waals interactions d) None

8. Which of the following binding interactions is likely to be the most important initial interaction when a drug enters a binding site?

a) van der Waals interactions
b) hydrogen bond
c) ionic bond
d) induced dipole-dipole interactions

9. Which of the following statements is untrue?

a) Desolvation is an energy expensive process that involves the removal of water from polar functional groups prior to a drug binding to its binding site.
b) Water molecules surrounding a hydrophobic region of a drug form an ordered layer of molecules with low entropy.
c) Interaction between the non-polar regions of a drug and the non-polar regions of a target require the removal of an ordered water coat and represents a gain in binding energy due to increased entropy.
d) An increase in entropy results in a greater positive value of ΔG and a greater chance of binding.

10. Which of the following needs to be established before the search for a lead compound takes place?

a) the pharmacophore
b) Structure-activity relationships
c) a bioassay
d) patents

11. What is the term used for the automated in vitro testing of large numbers of compounds using genetically modified cells?

a) robotic testing
b) high throughput screening
c) multiscreening
d) nanotechnology

12. What is the term used for small molecules that bind to different regions of a binding site?

a) epimers b) isomers c) isotopes d) epitopes

13. What does the symbol P represent in a QSAR equation?

a) pH
b) plasma concentration
c) partition coefficient
d) prodrug

14. Which of the following statements is untrue when comparing 3D QSAR with conventional QSAR?

a) Only drugs of the same structural class should be studied by 3D QSAR or QSAR.
b) 3D QSAR has a predictive quality unlike QSAR.
c) Experimental parameters are not required by 3D QSAR, but are for QSAR.
d) Results can be shown graphically in 3D QSAR, but not with QSAR.

15. Which of the following areas of study is not part of preclinical trials?

a) Toxicology
b) Drug metabolism
c) Pharmacology
d) Structure-activity relationships

Fill in the Blanks:

16. The method which minimizes the ---------- of a system is called as energy minimization methods
17. At phase transition the heat capacity will show a dependence upon the ----------
18. The ---------- can often determine the success or failure of a simulation.
19. ---------- enable predictions to be made of the thermodynamics properties of the system.
20. Internal coordinate are usually written as a ----------.

SECTION – B

ANSWER ANY FOUR QUESTIONS **(4 x 10 = 40marks)**

21. Explain Non- bonded Interactions.
22. Briefly explain the computer simulation and its practical aspects.
23. Write a note on atom-atom pair potential
24. What are force fields? Explain with an example.
25. Explain how to simulate a phase equilibria using Gibbs Ensemble monte carlo method.
26. What is multiple linear regression? How is it applied in the field of drug designing?
27. How are computers useful in Molecular Modelling and CADD?

SECTION – C

ANSWER ANY TWO QUESTIONS IN DETAIL (2 x 20 = 40marks)

28. Explain the features of Molecular Mechanics.
29. Explain Molecular Dynamics Simulation.
30. Explain Derivative and Non- Derivative Energy Minimisation Methods.
31. Explain QSAR and QSPR.

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