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 2017
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 Zeroth order derivative energy minimization is _____.
2. Taylor series expansion can be represented by _____.
3. The C-O bond length is _____ Angstroms.
4. The molecular force fields are _____ in nature.
5. The ideal gas equation PV=_____.
6. An algorithm that enables all pair wise non-bonded interactions is _____.
7. At phase transition the heat capacity will show a dependence upon the _____.
8. Constituents of force fields are _____ and _____.
9. The highest point on the pathway between two minima is known as_____.
10. _____ is the complex and non-linear process of refining the chemical structure of a confirmed hit to improve its drug characteristics.

II. Define

11. Order Parameters
12. Atom-atom pair potentials
13. Molecular Mechanics
14. Computer Simulation
15. Pharmacophore

III. Answer in a line or two:

16. What is active site prediction?
17. What is a lead compound?
18. What is Functional form of force field?
19. Define hydrogen bond potential
20. What is Z-matrix?

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SECTION – B

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

21. What is Energy Minimization? Explain in detail the Derivative Energy Minimization methods.
22. What are the different ways of representing a molecule and enumerate the depiction of a molecule of your choice in terms of its bond properties.
23. Explain the concept of structure based drug design.
24. Brief the Monte Carlo simulation method in molecular modeling.
25. Explain the practical aspects of computer simulation.

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