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 2013
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. The force field that is widely used for proteins and DNA is _____.
2. A molecule with X number of atoms contains _____ number of Internal and _____ number of Cartesian Co-ordinates.
3. Coulomb's constant can be represented as _____.
4. SMILES notation for ethane is _____.
5. Computational determination of binding affinity between the molecules is termed as _____.
6. The algorithm used to determine the hydrogen bonding terms is_____.
7. At a minimum point the second derivative of the function with respect to each variable are always _____.
8. The representation of any molecule with respect to its Internal Co-ordinate system is termed as _____.
9. The two widely used structure generator programs combined with energy minimisation are _____ and _____.
10. Drug discovery and development can broadly follow two different paradigms _____ & _____.

Answer in a line or two

11. Binding free energy
12. PMF
13. Euler's Angle
14. Inside out *denovo* drug design
15. Saddle point
16. Zeroth order Energy Minimisation.
17. QSPR
18. 3D Pharmacophore
19. What if Interface
20. Torsion Angle.

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SECTION – B

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

21. Explain the following a) Bond stretching b) Angle bending
22. How do you calculate thermodynamic properties?
23. Explain the steps involved in computer simulation.
24. Explain the various non-bonding interactions.
25. How do you do conformational changes by Molecular dynamics simulation?
26. Describe the use of Modeller.
27. Define 3D pharmacophore & its importance in drug discovery.

SECTION – C

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

28. Write an essay on energy minimization.
29. Explain the Molecular descriptor concept in QSAR.
30. Write about insilico modelling. Explain with a software tool.
31. Explain the following a)GibbsEnsemble Monte Carlo method.
    b)Differentiate Monte Carlo & MD.

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