STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2015 – 2016 & thereafter)

SUBJECT CODE: 15BI/PC/MC34

M. Sc. DEGREE EXAMINATION, NOVEMBER 2019
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)**

1. List out a few Software used in CADD, specifically in Docking
2. What is meant by a Binding site
3. What are the major interatomic forces that determine protein structure?
4. Characteristic feature/s of Protein Data Bank.
5. Applications of Monte Carlo Simulations
6. Computer simulations are extensively utised in Energy Minimization (True/ False)
7. Statisitical parameter "Linear Regression" have less role to play in Str.Bioinformatics (True/ False)
8. Van der Waals Force is type of Non-bonded Interaction (True/ False)
9. No Descriptors, can be tried in QSAR (True/ False)
10. Each Protein has a X-ray Diffraction pattern (True/ False)
11. How to determine the success or failure of a Simulation
12. Define : Structure-activity relationships (SAR)
13. Define : Pharmacophore
14. List out a few Databases used in Computer Aided Drug Design
15. Advantages of Lead Optimization Process.
16. Define : Gibbs Ensemble
17. Write down the significance of active site prediction in CADD.
18. List few of the molecular viewers
19. Differentiate : Derivative & the Non.derivative Energy Minimization Methods
20. Advantages of Computer Simulations in Molecular Modeling.

SECTION – B

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

21. Discuss any three Search Algorithms used in Molecular Docking.
22. Define Energy Minimization and add a note on various methods adopted in it.
23. What are force fields? Explain with an example.
24. Explain QSAR and QSPR with an example
25. Elaborate "Drug Target validation"

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