STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2019 – 2020 & thereafter)

SUBJECT CODE: 19BI/PC/MC34

M. Sc. DEGREE EXAMINATION, NOVEMBER 2021
BIOINFORMATICS
THIRD SEMESTER

COURSE: CORE
PAPER : MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN
TIME : 3 HOURS MAX. MARKS: 100

SECTION - A

ANSWER ALL THE QUESTIONS IN A LINE OR TWO (10 x 2 = 20 MARKS)

1. Define PES and draw the graph.

2. Write about torsion angle potential.

3. What are the three basic kinds of moves in simplex method?

4. Define order parameters.

5. Mention any two tools for determining force field.

6. Comment on 3D pharmacophore.

7. What is Widom approach in computer simulation?

8. What is the use of Gibbs Ensemble in Monte Carlo Simulation?

9. What is molecular dynamic simulation using simple model?

10. Comment on protein structure validation tools.

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SECTION - B

ANSWER ANY TWO QUESTIONS. EACH ANSWER SHOULD NOT EXCEED 500 WORDS. ALL QUESTIONS CARRY EQUAL MARKS. DRAW DIAGRAMS WHEREVER NECESSARY (2 x 20 = 40 MARKS)

11. Explain the protein secondary structure prediction methods and write notes on homology modeling.

12. Discuss briefly on the bonded and non-bonded interactions to determine the force fields.

13. Enumerate the algorithms used in molecular dynamics simulation.

14. Comment on derivative and non-derivative energy minimization methods

SECTION - C

ANSWER ANY ONE QUESTION. EACH ANSWER SHOULD NOT EXCEED 1200 WORDS. ALL QUESTIONS CARRY EQUAL MARKS. DRAW DIAGRAMS WHEREVER NECESSARY (1 x 40 = 40 MARKS)

15. Brief about the following:

    a) periodic boundary conditions

    b) non-periodic boundary conditions

16. Explain the process of structure based drug design. Write notes on softwares used for docking and visualization of results.

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