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

SUBJECT CODE: 19BI/PE/CD23

M.A/M.Com/M.Sc. DEGREE EXAMINATION, NOVEMBER 2022
BIOINFORMATICS
THIRD SEMESTER

COURSE   : ELECTIVE
PAPER   : COMPUTER AIDED DRUG DESIGN
TIME   : 3 HOURS   MAX. MARKS: 100

SECTION – A

ANSWER ALL THE QUESTIONS: **(20x1=20)**

1. What is a lead compound?
2. Define pre – clinical research.
3. List the phases in the drug discovery process.
4. List the types of pre – clinical studies.
5. What are special populations?
6. List the types of non – covalent interactions.
7. Expand SMILES.
8. What is docking?
9. What do you understand by the term "biosynthesis"?
10. What is conformational change?
11. What is *bioactivity*?
12. What is Pubchem?
13. What are chemical file formats?
14. What is active site?
15. What do you understand by *bioavailability*?
16. List the steps involved in an FDA approval.
17. Name two antibiotics.
18. What are target molecules?
19. What is a force field?
20. What is binding affinity?

SECTION – B

ANSWER ANY FOUR OF THE FOLLOWING   **(4x10=40)**

21. Write notes on ADME Prediction.
22. Discuss pharmacodynamics in detail.
23. Elaborate on the Lipinski's rule of five.
24. Write notes on drug regulation in India.
25. Elaborate on the most used databases for drug targets.
26. Write notes on the uses of the DrugBank.
27. What are phytochemicals? Add a note on secondary metabolites.

SECTION – C

ANSWER ANY TWO OF THE FOLLOWING   **(2x20 =40)**

28. Discuss the FDA regulations in drug development.
29. Elaborate on the mechanics and evaluation of molecular docking.
30. Enumerate the steps of ligand based drug design.
31. Elucidate the drug discovery time line with its prominent milestones.

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