Avinashilingam Institute for Home Science and Higher Education for Women

(Deemed to be University) Coimbatore – 641043

Master's Degree Examination November 2018

Semester – III

Class : II PG **Time : 3 hours**

Major : Bioinformatics **Max. marks : 60**

17MBIC16 - Molecular Modeling, Simulation and Drug Designing

Part – A **10 x ½ = 5**

Choose the correct answer

1. Which of the following crosses the blood-brain barrier?
   a. GABA b.Propranolol c.Edrophonium d.Dopamine
2. LD50 is:
   a. Median lethal dose
   b. Determined in phase I clinical trial
   c. Determined from log-dose response curve.
   d. Dose causing death in 50% of animals within ?1to24 hours
3. An alignment that essentially spans the full extents of the input sequences is called a
   a. Global alignment b.local alignment c.multiple alignment d.pairwise alignment
4. A bifurcating branch point in the phylogenetic tree is known as
   a. A Node b.A clade c.A branch d.A taxon
5. Which of these methods is/are character-based methods in Tree construction
   a. Maximum parsimony b.Maximum Likelihood
   c.Minimum evolution (ME) method d.Neighbor joining (NJ)
6. PAM stands for
   a. Point Accepted Mutation b.Percent Associated Mutation
   c.Protein Accepted Mutation d.Point Associated Mutation
7. What step of DNA sequencing is skipped during shotgun sequencing?
   a.computer analysis b.cloning of DNA fragment
   c. primer reactions d.mapping step
8. The most effective way to analyze variation at the whole genome level is to use
   a.frequency of tandem clusters
   b.number of transposons.
   c.single nucleotide polymorphisms (SNPs).
   d.segmental duplications.
9. Labeling a stretch of DNA according to its function is called
   a. recombinant DNA technology b.functional analysis.
   c.annotation d.screening.
10. Sequences that share an arbitrary, threshold level of similarity determined by alignment of matching bases are termed as
    a. Homologous sequences b.Heterologus sequences
    c.Mismatch sequences d.Bogus sequences

Part B
Answer all questions
Each answer should not exceed 200 words or one page **5x4 = 20**

11. (a) Derive the Schrödinger's equation and explain one electron atom.

Or

(b)Explain the Born-Oppenheimer approximation.

12. (a) Explain steepest descent minimization and conjugate gradient method

Or

(b) Explain in short different force field

13. (a) Explain newtonian dynamics

Or

(b) Elucidate implicit solvation model

14. (a) Explain maximum likelihood

Or

(b)What is De Novo drug designing?

15. (a) Elaborate on computer aided molecular design

Or

(b) What is regression analysis?

Part B
Answer all questions
Each answer should not exceed 600 words or three pages

5x7 = 35

16. (a) Explain in detail the four input formats for computation

Or

(b)Explain the semi empirical methods and potential energy calculation using *ab initio* methods

17. (a) Explain in detail about the molecular mechanics force field bonded interaction

Or

(b) Explain in detail about energy minimization and write brief notes on genetic algorithm

18. (a)What is simulation ? Explain various types of simulation.

Or

(b)What is Molecular dynamics? Elucidate the applications in molecular dynamics.

19. (a)What is drug discovery and its steps?.

Or

(b)What is docking? Explain in detail about types of docking.

20. (a) Explain the significance and validity of QSAR.

Or

(b) Explain partial least squares analysis and multi linear regression analysis.