PARUL UNIVERSITY

PARUL INSTITUTE OF PHARMACY

B.PHARM EIGHTH SEMESTER

SECOND INTERNAL THEORY EXAMINATION: 2020-21

Subject Name: COMPUTER AIDED DRUG DESIGN
Subject Code: BP 807 ET   Date: 11/03/21
Time: 10:00-11:15am   **Total Marks: 30**

Instructions:
1. Figures to the right indicate full marks.
2. Make suitable assumptions wherever necessary.

Q.1		**Multiple Choice Questions:**	**[10]**
	(1)	Which of the following terms refers to the molecular modelling computational method that uses equations obeying the laws of classical physics? (a) Quantum mechanics (b) Molecular mechanics (c) Molecular calculation (d) Quantum theory	01
	(2)	Which of the following statements is true? (a) Energy minimisation is carried out using quantum mechanics. (b) Energy minimisation is used to find a stable conformation for a molecule. (c) Energy minimisation is carried out by varying only bond angles and bond lengths. (d) Energy minimisation stops when a structure is formed with a much greater stability than the previous one in the process.	01
	(3)	Which of the following operations or calculations would generally be carried out using molecular mechanics? (a) Molecular orbital energy (b) Energy minimization (b) Electrostatic potential (d) Transition state geometries	01
	(4)	Which of the following needs to be known before two drugs can be overlaid to compare their structures? (a) The pharmacophore of each (b) The active conformation of each drug (c) Both of the above (d) Neither of the above	01
	(5)	Which of the following is an example of Homology and similarity tool? (a) BLAST (b) EMBOSS (c) RasMol (d) None of above	01

	(6)	.Which of the following scientists created the first Bioinformatics database?	01
		(a) Dayhoff (c) Richard Durbin (b) Pearson (d) Michael.J.Dunn	
	(7)	The identification of drugs through the genomic study is called_____.	01
		(a) Genomics (b) Pharmacogenetics (c) Pharmacogenomics (d) Cheminformatics	
	(8)	Which of the following compounds has desirable properties to become a drug?	01
		(a) Fit drug (b) Lead (b) Fit compound (d) All of above	
	(9)	Proteomics refers to the study of_____. (a) Set of proteins in a specific region of the cell (b) Set of proteins (c) Biomolecules (d) The entire set of expressed proteins in the cell	01
	(10)	The laboratory work using computers and associated with web-based analysis generally online is referred to as _____. (a) In silico (b) Wet lab (c) Dry lab (d) All of the above	01

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SECOND INTERNAL THEORY EXAMINATION: 2020-21

Subject Name: COMPUTER AIDED DRUG DESIGN
Subject Code: BP807ET   Date: 11/03/21
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Long Answers:(Any One)

Q.2

   (1) Explain quantum mechanics and molecular mechanics.   10

   (2) Define and explain in brief about Bioinformatics. Enlist some chemical,   10
biochemical and pharmaceutical databases.

Q.3   **Short Answers:(Any Two)**

   (1) Write notes on different conformational Search algorithms.   05

   (2) What is molecular dynamics? Elaborate its application.   05
                                                                                        05
   (3) Give a brief note on ADME databases.

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