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B TECH

(SEM VI) THEORY EXAMINATION 2017-18

MOLECULAR MODELLING AND DRUG DESIGNING

Time: 3 Hours *Total Marks: 100*

Note: Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. **Attempt *all* questions in brief.** **2 x10 = 20**

(a) Note down the numerous applications of protein folding.

(b) What do you mean by molecular modeling?

(c) How Ramachandran plot is used for validation of protein models?

(d) What is conformational searching?

(e) Explain the ADME properties of lead.

(f) Give some molecular orbital theories with examples.

(g) Define combination libraries.

(h) What is free energy & salvation?

(i) Discuss the postulates of quantum mechanics.

(j) What are electrostatic interaction?

SECTION B

2. **Attempt any *three* of the following:** **10 x 3 = 30**

(a) What do you mean by linear and nonlinear QSAR model?

(b) What is drug designing? Explain the various steps involved in this process?

(c) Discuss the *ab initio* method for computational modeling of protein.

(d) What are artificial neural network? Explain its applications.

(e) What do you mean by virtual screening? Why it is important?

SECTION C

3. **Attempt any *one* part of the following:** **10 x 1=10**

(a) What is molecular docking? Discuss the protein – ligand docking with example.

(b) Draw a setup of MD simulation system. Also explain molecular similarity and similarity searching.

4. **Attempt any *one* part of the following:** **10 x 1=10**

(a) Give an overview of different strategies used for the search of new potential drug.

(b) What are pharmacophores? Explain antihistamine 3D pharmacophore with a suitable diagram.

5. **Attempt any *one* part of the following:** **10 x 1=10**

(a) Keeping in mind the mechanics of molecular modeling, show the number of force field involved in the process of modeling with the use of its various parameters for force field calculation.

(b) Database searching is attractive way to discover new compound. Prove this statement with the structure based de-novo Ligand design.

6. **Attempt any *one* part of the following:** **10 x 1=10**

(a) What is the minimal input for molecular modeling process?

(b) Show the structure based design of templates for zeolite synthesis.

7. **Attempt any *one* part of the following:** **10 x 1=10**

(a) How QSAR relates numerical properties of molecular structure to its activity?

(b) What are molecular descriptors? Explain the Jack knifing process in detail.

B.Tech

(SEM VIII) THEORY EXAMINATION 2017-18

METABOLIC ENGINEERING

Time: 3 Hours *Total Marks: 100*

Note: Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. **Attempt *all* questions in brief.** **2 x10 = 20**

(a) What is HMP shunt?

(b) What is difference in dark and light reaction?

(c) Differentiate between active and passive transport.

(d) Differentiate between osmosis and diffusion.

(e) What are the high energy compounds?

(f) Differentiate between catabolism and anabolism.

(g) What meant by term intermediary metabolism?

(h) What are saturated fatty acids?

(i) Define ATP and ADP.

(j) What is Phosphorylation?

SECTION B

2. **Attempt any *three* of the following:** **10x 3 = 30**

(a) Write differences between fatty acid biosynthesis and fatty acid degradation.

(b) Discuss gluconeogenesis steps in detail. Write down its significance in human body.

(c) What do you mean by transport channels? Explain various types of transport processes in detail.

(d) Explain electron transport chain in detail.

(e) Elaborate mechanism of beta oxidation of fatty acids in detail and its significance.

SECTION C

3. **Attempt any *one* part of the following:** **10 x 1= 10**

(a) Discuss mechanism of protein targeting with its significance.

(b) Explain the structure of plasma membrane given by Singer and Nicolson.

4. **Attempt any *one* part of the following:** **10 x 1 = 1**

(a) Describe oxidative Phosphorylation. Name two inhibitors of ETC.

(b) Discuss various type of photosynthetic material in detail.

5. **Attempt any *one* part of the following:** **10x 1 =**

(a) Write regulation of fatty acid biosynthesis in detail.

(b) Describe regulation of the ETS in detail.

6. **Attempt any *one* part of the following:** ***10x 1 =10***

(a) What is Glycolysis? Explain regulation of glycolysis in detail.

(b) What do you mean by TCA cycle? Explain regulation of TCA.

7. **Attempt any *one* part of the following:** ***10 x 1 =10***

(a) Explain the process of ATP-ADP exchange across the mitochondrial membrane.

(b) Explain reversible and irreversible phases of pentose phosphate pathways.