2. What are bioisosteres? Discuss the classification of bioisosteres. Mention the various approaches for bioisosteric replacement and explain any one in detail. 1+4+2+3

3. What is energy minimization? Describe the various methods of energy minimization along with their advantages and limitations. 2+8

III. Short answers (Answer seven out of nine questions) 5x7=35

1. Write a note on chemoinformatics. 5

2. Discuss*de novo* drug design with proper diagram. 5

3. Write a note on virtual screening giving emphasis on Lipinski's rule of five. 5

4. Write a note on lead discovery based on clinical observations. 5

5. Explain Born-Oppenheimer approximation method. Mention the advantages and disadvantages of *ab initio* methods. 2+2+1

6. Write a note on 'Study of Force Field' method of molecular mechanics. 5

7. Describe briefly Hansch Analysis. 5

8. Explain hydrophobic parameters of QSAR. 5

9. Describe CoMFA. 5

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B Pharm Even Semester Examination, September, 2023

PHARMACEUTICAL SCIENCES

(8th Semester)

Course No: BP-807ET
(Computer Aided Drug Design- Theory)

FM: 75
Time: 3 Hours

The figures in the right margin indicate full marks for the question

I. A. Multiple Choice questions 1x10=10

1. The primary goal of *in silico* drug designing is to:

   (a) Discover new drugs

   (b) Optimize existing drugs

   (c) Predict drug-target interactions

   (d) All of the above

2. QSAR is a method used in drug designing to:

   (a) Predict the biological activity of a compound based on its chemical structure

   (b) Determine the toxicity of a drug molecule

   (c) Study protein-ligand interactions

   (d) Analyze gene expression patterns

3. Which of the following approach is considered under the 'Ligand based drug designing'?

(a) Molecular docking

(b) Pharmacophore modeling

(c) QSAR Modeling

(d) Both b and c

4. Lipinski's rule of five is used for

(a) Docking (b) Similarity search

(c) Drug likeness (d) Dynamics simulation

5. A similarity searching programs that identify homologous DNA sequences and proteins sequence in pairwise sequence alignment is

(a) ClustalW (b) FASTA

(c) Phase (d) GLIDE

6. Which of the following is the popular force fields for protein energy minimization

(a) AMBER (b) CHARMM

(c) OPLS (d) Both a and b

7. Bupropion was discovered through

(a) Clinical observations

(b) Metabolic studies

(c) Serendipity

(d) Random screening

8. Partial Least Square (PLS) is used in

(a) SAR (b) 2D-QSAR

(c) 3D-QSAR (d) Both b and c

9. The positive value of 'π' indicates that substituent is

(a) More hydrophobic than halogen

(b) Less hydrophobic than hydrogen

(c) More hydrophobic than hydrogen

(d) Less hydrophobic than halogen

10. Which technique is based on wave properties of electrons and all material particles?

(a) Quantum mechanics

(b) Molecular mechanics

(c) Energy minimization

(d) All of the above

I. B. Objective Type Questions 2x5=10

1. What is microarray data analysis?

2. What do you mean by the term local and global energy minima?

3. Mention the full form of AMBER, CHARMM, PM3, and MOPAC.

4. Define analog design and mention the goals of analog design.

5. Write the formula to calculate the number of conformations.

II. Long answers (Answer two out of three questions) 10x2=20

1. Discuss the concept of pharmacophore mapping and pharmacophore based virtual screening with an example (give diagram). 5+5=10