Total No. of printed pages = 4

MPC 203 T

Roll No. of candidate | | | | | | | | | | |

23/08/22.

2022

M.Pharm 2nd Semester End-Term Examination

COMPUTER AIDED DRUG DESIGN

Full Marks – 75 Time – Three hours

The figures in the margin indicate full marks for the questions.

1. Answer the following (MCQ) : (20 × 1 = 20)

(i) QSAR Method includes

(a) Target Structure

(b) Target Properties

(c) Ligand properties

(d) Ligand X-ray Structure

(ii) Bupropion was discovered through

(a) Clinical Observations (b) Metabolic Studies

(c) Serendipity (d) Random Screening

(iii) The biological Activity of most of the drug is related to a combination of physico-chemical properties. This statement is relevant to

(a) Hammett's Substitution Constant

(b) Taft Steric Constant

(c) Hansch Analysis

(d) Free Wilson Analysis

(iv) The Partial Least Square (PLS) is used in

(a) SAR (b) 2-D QSAR

(c) 3-D QSAR (d) None of these

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(v) Multiple Protein structures are utilized as an ensemble for docking with ligand in one of the following technique:

(a) Induced fit Docking (b) Lock and key docking

(c) Ensemble Docking (d) Rigid Docking

(vi) Name of the programme in which frequents from bioactive conformation are joint with spacer to generate a new structure to fit the model

(a) SCROUT (b) UNITY

(c) NEWLEAD (d) QSAR

(vii) The molecular mechanics deals with

(a) Number of atoms (b) Number of orbitals

(c) Number of protons (d) Number of molecules

(viii) Which one of the following helps to calculate the average position of the electron and its energy in each electronic state:

(a) Partition Coefficient

(b) Hammett Substituent Constant

(c) Schrodinger Equation

(d) Taft Steric Factor

(ix) Serendipitious Drug Discovery Meaning

(a) Drug Developed on basis of target

(b) Accidentally or non-intentionally drug finding

(c) Random Screening

(d) All of the above

(x) Assessment of safety, pharmacokinetic and pharmacodynamics of molecule occur in

(a) Phase 0 (b) Phase 1

(c) Phase 2 (d) Phase 3

(xi) Ionization of benzoic acid is used in

(a) Hydrophobic parameter (b) Steric Parameter

(c) Electronic Parameter (d) None of the above

(xii) 3-D geometry of Interaction features that a molecule must have in order to bind in a protein's active site is called as

(a) Inactive Compound (b) Active Compound

(c) Pharmacophore (d) Bioprecursor

(xiii) Rigid Docking includes:

(a) Molecular Shape representation

(b) Surface patch matching

(c) Filter and scoring

(d) All of above

(xiv) Challenges stand up during De-novo design

(a) Structure Generation (b) Scoring

(c) Optimization (d) All of the above

(xv) Which of the following approach is considered under the 'Ligand based drug designing'?

(a) Molecular docking (b) Pharmacophore modelling

(c) QSAR Modelling (d) (b) and (c) both

(xvi) What does MR represent in a QSAR equation?

(a) Molar refractivity is an steric factor

(b) Molar refractivity is an electronic factor

(c) Molar refractivity is a hydrophobic factor

(d) Molar refractivity is an stereoelectronic factor

(xvii) Which programme is using as shape based super position for identifying compound that have similar shape

(a) CSD (b) DOCK

(c) DBS-3D (d) ROCS

(xviii) Semi empirical method computes for

(a) Valence Electron (b) Electron

(c) Proton (d) Orbital

(xix) Force field energy estimation is most often used for:

(a) Ligand Flexibility (b) Scoring Function

(c) Receptor Flexibility (d) Search Space

(xx) Bond stretching, Bond Angle Bending and torsion angle rotation are considered under the

(a) Hydrophobic Interaction

(b) Non-bonded Interaction

(c) Bonded Interaction

(d) Intermolecular Interaction

2. Answer any Seven questions: (7 × 5 = 35)

(a) Discuss about similarity-based methods used in virtual screening.

(b) Explain Lipinski rule of 5.

(c) Give example of lead discovery based on clinical observation.

(d) What properties a lead compound should possess to develop as an orally active compound?

(e) Briefly explain quantum mechanical approach in drug design.

(f) Explain the importance of charge and electrostatic environment of molecule in molecular modeling and Drug design.

(g) Write the methods for handling ligand flexibility.

(h) Write short notes on COMFA and COMSIA.

3. Answer any two questions: (2 × 10 = 20)

(a) Explain the Hansch analysis and Free Wilson analysis and relationship between them.

(b) Write a brief note on De-Novo Drug Design.

(c) What is a lead molecule? Discuss the various stages involved in identification of a lead molecule.