Dr. B. C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206

Add on Course Continuous Assessment-I

Paper – Computational Drug Design using QSAR/Cheminformatics & Bioinformatics

Time – 1 hour **Full Marks – 50**

MCQs (Answer all) **[50x1=50]**

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

a) Molecular docking c) Pharmacophore modeling

b) QSAR Modeling d) b and c both

2) Which of the following software is used for Phylogenetic analysis?

a) LUDI b) MEGA c) CHEM3D d) CoMFA

3) Which of these is gene prediction algorithm?

a) UPGMA c) Hidden Markov Model

b) Maximum parsimony d) None

4) Procheck tool is use for

a) Alignment b) Protein Validation c) Simulation d) None of these

5) ARSA is search engine of

a) DDBJ b) GENBANK c) EMBL d) UNIPROT

6) Which one is the application of bioinformatics

a) Design of primers c) Reconstructing genes from EST sequences

b) Grouping of proteins into families d) All

7) Which of the following method used for virtual screening

a) ADMET analyses b) QSAR modeling c) Pharmacophore modeling d) All of them

8) Lipinski's rule of five is used for

a) Dynamics simulation b) Similarity search c) Drug likeness d) Docking

9) CoMFA method is used for

a) 4D-QSAR b) 3D-QSAR c) 5D-QSAR d) 6D-QSAR

10) Periodic table window in ChemDraw can appear using ..... toolbar

a) File b) Object c) Structure d) View

11) How is permeability predicted in Molinspiration software?

a) ClogP b) LlogP c) KlogP d) TlogP

12) Which of the following function is not observed in ChemDraw Professional?

a) Convert structure to name
c) Convert name to structure
b) Shows enhanced geometry
d) Show analysis window

13) Symbol A -A in ChemDraw toolbar refers to

a) letter b) Query tool c)Addition d) None

14) Which of the following tool is not present in ChemDraw toolbar?

a) Query tools b) Arrow tool c) Chromatography tool d) Reaction Tool

15) Fragmentation tool is present in ChemDraw software

a) True b) False c)May be correct d) None

16) Marquee section in ChemDraw helps to

a) Erase the drawing
c) Select the structures
b) Draw double bonds
d) Draw phenyl rings

17) Convert structure to name icon is present in which of the following toolbars

a) File b) Edit c) View d) Structure

18) Chromatography tool is present in ChemDraw software

a) True b) False c)May be correct d) None

19) Which of the following template is not present in ChemDraw toolbar?

a) Microorganisms b) Bioinstruments c) Shapes d) Walls

20) Choose the incorrect statement about the SMILES generation of compound

a) Drawing the compound in the Molinspiration software
b) Directly from Google
c) Copy paste from the chemical drawing software
d) Typing the SMILES of the compound on your own

21) Which of the following are not chemical drawing softwares?

a) ChemDraw b) ChemDraw 3D c) Chem sketch d)Chem Art

22) Which of the following would NOT be regarded as part of the science of informatics?

a) Storage of information about chemical properties
b) Storage of information about physical properties
c) Storage of information about synthetic methods
d) Storage of information about chemical structures

23) Which of the following SMILES codes does NOT represent a cyclic structure?

a) C1CCCCC1 c) O1CCOCC1

b) CC(=O)OC(C)(C)C d) n1CCCCC1

24) Which of the following databases CANNOT be used to store 3D structures?

a) SMILES b) Alchemy c) Sybyl d) Chem3D

25) A QSAR study is only valid if

a) It comprises of two inputs: biological data and physicochemical parameters

b) It involves a group of closely related structures

c) It involves an appropriate number of structures

d) It predicts the activity of new molecules, not within the original data set

26) In order to be used in a QSAR study, biological data must

a) Use information from the same biological test system

b) Have been obtained in the same laboratory

c) Have been produced by the same operator

d) Use a quantitative measure of potency

27) Which of the following is NOT a hydrophobic parameter?

a) Partition coefficient (*P*) c) Substituent constant (*Π*)

b) Molecular connectivity d) Log *P*

28) Which of the following is NOT an electronic parameter?

a) Hammett substituent constant c) Molecular connectivity

b) Dipole moment d) HOMO/LUMO

29) Which of the following is NOT used by molecular modelling software packages?

a) Relative molecular mass c) Bond lengths

b) Bond angles d) Torsion angles

30) Which of the following is NOT a useful statistical indicator of the goodness of fit of a regression analysis equation?

a) Regression coefficient (r) b) r^2 c) Standard error (s) d) F tests

31) Which of the following is NOT usually used as a steric parameter?

a) Molecular surface area c) Relative molecular mass

b) Molar volume d) Taft's steric parameter

32) Which of the following scientists created the first Bioinformatics database?

a) Dayhoff b) Pearson c) Richard Durbin d) Michael.J.Dunn

33) What is the deposition of cDNA into the inert structure called?

a) DNA probes b) DNA fingerprinting c) DNA polymerase d) DNA microarrays

34) The identification of drugs through the genomic study is called_____.

a) Genomics c) Pharmacogenetics

b) Pharmacogenomics d) Cheminformatics

35) Which of the following compounds has desirable properties to become a drug?

a) Fit drug b) Lead c) Fit compound d) All of the above

36) Proteomics refers to the study of _____.

a) Set of proteins in a specific region of the cell c) Biomolecules

b) The entire set of expressed proteins in the cell d) Set of proteins

37) The process of finding the relative location of genes on a chromosome is called

a) Gene tracking c) Genome mapping

b) Chromosome walking d) Genome walking

38) The computational methodology that tries to find the best matching between two molecules, a receptor and ligand are called _____.

a) Molecular fitting b) Molecular matching

c) Molecule affinity checking d) Molecular docking

39) Which of the following is not the application of bioinformatics?

a) Understand the relationships between organisms c) Drug designing

b) Data storage and management d) None of the above

40) The term "*in vivo*" is the Latin word which refers to_____.

a) Within the lab c) Within the glass

b) Outside the lab d) Outside the glass

41) The stepwise method for solving problems in computer science is

a) Flowchart b) Algorithm c) Procedure d) Sequential design

42) The laboratory work using computers and associated with web-based analysis generally

a) In silico b) Dry lab c) Wet lab d) All of the above

43) The computer simulation refers to

a) In silico b) Dry lab c) Wet lab d) All of the above

44) Which of the following tools is used for the identification of motifs?

a) BLAST b) COPIA c) PROSPECT d) Pattern hunter

45) Which of the following tools is used for the identification of motifs?

a) BLAST b) COPIA c) PROSPECT d) Pattern hunter

46) The term Bioinformatics was coined by _____.

a) J.D Watson b) Pauline Hogeweg

c) Margaret Dayhoff d) Frederic Sanger

47) The human genome contains approximately_____ base pairs

a) 6 billion b) 5 billion c)3 billion d) 4 billion

48) Which of the following is analogous to σ constant?

a) logP b) Rf c)pKa d) Es

49) Which of the following is analogous to π constant?

a) MW b) k' c)pKa d) Es

50) Which QSAR technique is performed manually?

a) Hansch approach c) Free Wilson approach

b) Fujita Ban approach d) Topliss approach

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Add on Course Continuous Assessment-II

Paper – Computational Drug Design using QSAR/Cheminformatics & Bioinformatics

Time – 1 hour **Full Marks – 50**

MCQs (Answer all) **[25x2=50]**

1. **Lipinski rule of 5 includes**
   a) Molecular weight less than 300 daltons
   b) logP value can exceed 5
   c) All nitrogen and oxygen atoms may be more than 10
   d) Hydrogen bond donors must not be more than 5
2. **Drug likeliness means**
   a) How drug like a substance is with respect to factors like bioavailability
   b) How a drug likes the receptor
   c) Property of drug similar to receptor
   d) Affinity of drug to become a lead
3. **ADME of a drug does not include**
   a) Adsorption
   b) Distribution
   c) Metabolism
   d) Excretion
4. **Molinspiration software provides details like**
   a) Drug likeliness
   b) Bioactivity score
   c) Bioavailability
   d) All of these
5. **Chemical drawing softwares are**
   a) ChemDraw
   b) Chemical draw
   c) Chem academy
   d) ChemMaster
6. **Which of the following template is not present in ChemDraw toolbar?**
   a) Microorganisms
   b) Bioinstruments
   c) Shapes
   d) Walls

7. **In 3D QSAR blue regions indicate favorable points for**
    a) Bulky groups
    b) Electron rich groups
    c) Electron deficient groups
    d) Smaller groups
8. **In 3D QSAR green regions indicate favorable points for**
    e) Bulky groups
    f) Electron rich groups
    g) Electron deficient groups
    h) Smaller groups
9. **In 3D QSAR yellow regions indicate favorable points for**
    i) Bulky groups
    j) Electron rich groups
    k) Electron deficient groups
    l) Smaller groups
10. **One of the following is a quantum chemical parameter**
    a) STERIMOL
    b) Taft c constant
    c) HOMO
    d) Hammett's constant
11. **One of the following is not used in QSAR**
    a) Molecular connectivity index
    b) Molecular similarity index
    c) Topological Polar surface area
    d) Partition Coefficient
12. **Which of the following are not bioisosteres of -NH2**
    a) -OH
    b) –SH
    c) $-CH_3$
    d) H_2S
13. **Choose the compound which can be drug like with respect to their molecular weight**
    a) Naphthalene
    b) Anthracene
    c) Phenanthrene
    d) All of these

14. The chem draw files can be renamed to pdb file using ……software

a) Pymol
b) Discovery Studio Visualizer
c) Protein Data Bank
d) ChemSketch

15. The structures in the Auto Dock file can be opened using

a) Load structure
b) Ligand-Input
c) Load molecule
d) Upload structure

16. The features like 'add Kollman charges' and 'compute gasteiger' are used for

a) Ligand
b) Protein
c) Both a and b
d) None

17. What is the principle of AutoDock?

a) A tool designed to predict how small molecules and drug candidates bind to a receptor
b) Helps to find syntax errors, spelling mistakes, missing code, and other issues in your Python code
c) An interactive source code debugger for Python programs
d) Identification of new protein structures via in silico approaches or can be used in protein nucleic acid interaction studies.

18. Why are protein databases important?

a) It can be used in sequence analysis
b) It identifies homologous sequences of programs
c) It predicts protein functions based on non-sequence similarity
d) None of the above

19. Lead optimization helps in

a) Enhancing the most promising compound to improve the toxicity
b) Obtaining lower RMSD values
c) Building the target protein model
d) Generating the Pharmacophore models

20. Choose the compound with best docking score

a) Compound 47- Score -5.5
b) Compound 45- Score -6.8
c) Compound 46- Score -7.1
d) Compound 48- Score -4.3

21. Select the wrong pair

a) **MOL INSPIRATION -** Lipinsky Rule of 5
b) **MOL SOFT-** Drug Likeliness
c) **ADMET SAR-** Toxicity evaluation
d) **CANIMOTO INDEX-** Dissimilarity index

22. Choose the incorrect statement

a) The grid box includes the entire protein in blind docking
b) The docking result is analyzed using Discovery Studio Visualizer software
c) The desired protein can be easily downloaded from Protein Data Bank
d) Binding Energy and Docking score are same parameters to determine binding

23. The file must be converted to pdbqt before using command in …….

a) CHEMDRAW
b) AUTODOCK VINA
c) MOL INSPIRATION
d) PYMOL

24. nON and nOHNH refers to …….. respectively

a) Hydrogen bond donors and acceptors
b) Hydrogen bond acceptors and donors
c) Virtual screening and ligand design
d) Ligand design and virtual screening

25. Choose the correct statement

a) A compound with 1.34 milogP passes Lipinski rule of 5
b) Human oral bioavailability can be determined by *in silico* toxicity study
c) Ligand energy minimization is essential before docking
d) Development of protein is not required for running AUTODOCK

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Add on Course Continuous Assessment-III

Paper – Computational Drug Design using QSAR/Cheminformatics & Bioinformatics

Time – 1 hour **Full Marks – 50**

Fill in the Blanks: - (Answer all) **[4x1=4]**

1. **Full form of MEGA ……**
2. **In …….. to complete an analysis the user is not required to move between different subprograms while keeping modifying names of the intermediate output files.**
3. **…….. deals with the interaction between computers and humans using the natural language**
4. **……. model were developed and incorporated in machines which mimicked the functionalities of human origin.**

Short Answer Questions: - (Answer all) **[23x2=46]**

1. **Define Free Wilson Analysis with examples.**
2. **Write the applications of QSAR.**
3. **Enlist two ADME databases.**
4. **Mention two Biochemical databases.**
5. **Define Lead molecule with examples.**
6. **Define Random screening for lead optimization.**
7. **Define COMFA and COMSIA.**
8. **Write applications of pharmaceutical databases.**
9. **Mention any two lead optimization techniques.**
10. **Define bioisosteres with examples.**
11. **Explain Hansch analysis.**
12. **Compare SAR and QSAR.**
13. **Define COMSIA with its two applications.**
14. **Explain Lipinski rule of 5.**
15. **Protein processing for Docking in AutoDock Vina.**
16. **Enlist any two pharmaceutical databases.**
17. **How binding sites are located in PDB and Discovery studio Visualizer**
18. **Importance of Grid Box in docking**
19. **Docking in Virtual screening of compounds.**
20. **BLAST and gene ontology finding.**
21. **Multiple Sequence Alignment and protein function assessment**
22. **Homology modelling and use of MODELLER.**
23. **Semi empirical methods and energy minimization.**