BIRLA INSTITUTE OF TECHNOLOGY
MESRA – 835215, RANCHI, INDIA

UG

Name: …… Roll No.: ……..

Branch: …… Signature of Invigilator: ……

Semester: VIth Date: 29/04/2022 (MORNING)

Subject with Code: **BE321 CHEMINFORMATICS**

Marks Obtained	Section A (30)	Section B (20)	Total Marks (50)

INSTRUCTION TO CANDIDATE

1. The booklet (question paper cum answer sheet) consists of two sections. First section consists of MCQs of 30 marks. Candidates may mark the correct answer in the space provided / may also write answers in the answer sheet provided. The Second section of question paper consists of subjective questions of 20 marks. The candidates may write the answers for these questions in the answer sheets provided with the question booklet.
2. The booklet will be distributed to the candidates before 05 minutes of the examination. **Candidates should write their roll no. in each page of the booklet.**
3. Place the Student ID card, Registration Slip and No Dues Clearance (if applicable) on your desk. All the entries on the cover page must be filled at the specified space.
4. Carrying or using of mobile phone / any electronic gadgets (except regular scientific calculator)/chits are strictly prohibited inside the examination hall as it comes under the category of unfair means.
5. No candidate should be allowed to enter the examination hall later than 10 minutes after the commencement of examination. Candidates are not allowed to go out of the examination hall/room during the first 30 minutes and last 10 minutes of the examination.
6. Write on both side of the leaf and use pens with same ink.
7. The medium of examination is English. Answer book written in language other than English is liable to be rejected.
8. All attached sheets such as graph papers, drawing sheets etc. should be properly folded to the size of the answer book and tagged with the answer book by the candidate at least 05 minutes before the end of examination.
9. The door of examination hall will be closed 10 minutes before the end of examination. Do not leave the examination hall until the invigilators instruct you to do so.
10. Always maintain the highest level of integrity. Remember you are a BITian.
11. Candidates need to **submit the question paper cum answer sheets before leaving the examination hall**.

BIRLA INSTITUTE OF TECHNOLOGY, MESRA: RANCHI
(END SEMESTER EXAMINATION)

CLASS: BE **SEMESTER: VI**

BRANCH: Biotechnology and Bioengineering **SESSION: 2021-22 (SP/22)**

TIME: 2.00 Hours **FULL MARKS: 50**

SUBJECT WITH CODE: BE321 Cheminformatics

INSTRUCTIONS:
1. All the questions are compulsory.
2. Pay attention to the marks of the questions.
3. The missing data, if any, may be assumed suitably.

1 Force can be expressed as minus the gradient of the _____ energy **1**

A. Potential
B. Kinetic
C. Total
D. Free

2 Which of the following is relatively most accurate docking protocol? **1**

A. Lock and Key
B. Rigid Docking
C. Induced Fit
D. Conformation Ensemble

3 The goal of molecular docking is to find the 3D configuration of the complex that _____ **1**

A. Maximize the energy
B. Minimize the energy
C. bring down the energy to zero
D. bring up the energy to infinity

4 Which of the following statement(s) true for Lipinski's rule of five? **2**

A. Molecular weight at least 500 Dalton
B. No more than five hydrogen bond acceptor groups
C. No more than five hydrogen bond donor group
D. No more than ten hydrogen bond donor groups
E. No more than ten hydrogen bond acceptor groups
F. logP value more than +5

5 Arrange the sequence of pharmacophore-based drug design in the right order **2**
1) Test activity 2) Buy or synthesize hits 3) Generate Pharmacophore 4) search compound library.

A. 3-->1-->4-->2-->3
B. 1-->3-->2-->4-->1

C. 3-->1-->2-->4-->3
D. 1-->3-->4-->2-->1

6 Which of the following is the correct definition of bioavailability? **2**

A. Bioavailability describes the proportion of the drug administered that is metabolised very quickly and thus is not available to induce a physiological effect.
B. Bioavailability describes the ability of the administered drug metabolites to cause undesirable physiological effects.
C. Bioavailability is used to describe the fraction of the dose of drug administered that is present within the body and facilitates the desired physiological effects.
D. Bioavailability is the length of time an administered drug is present in the body and thus is available to cause a physiological effect.

7 The rate of drug transport across a cell membrane by lipid diffusion depends on all of the following EXCEPT: **1**

A. Drug size (diffusion constant)
B. Surface area of absorption
C. Lipid partition coefficient
D. Density of transporters
E. Concentration gradient

8 What is the symbol π in a QSAR equation? **1**

A. The hydrophobicity of the molecule
B. The electronic effect of a substituent
C. The substituent hydrophobicity constant
D. A measure of the steric properties for a substituent

9 Which of the following statements best describes a lead compound? **2**

A. A compound that contains the element lead
B. A compound from the research laboratory that is chosen to go forward for preclinical and clinical trials
C. A molecule that shows some activity or property of interest and serves as the starting point for the development of a drug.
D. The first compound of a structural class of compounds to reach the market.

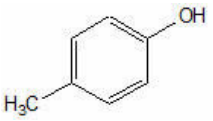
10 Which of the following approach is considered under the ‘Ligand based drug designing’ ? **2**

A. Molecular docking
B. Pharmacophore modeling
C. QSAR Modeling
D. A and B both
E. A and C both
E. B and C both
F. A, B and C

11 Which of the following statements is true? **2**

A. The most stable conformation of a drug is also the active conformation.
B. The active conformation is the most reactive conformation of a structure.
C. The active conformation is the conformation adopted by a drug when it binds to its target binding site.
D. The active conformation can be determined by conformational analysis.

12 Calculate the logP value for the structure shown; logP for benzene = 2.13; π(OH) -0.67; π(CH3) 0.52. **2**

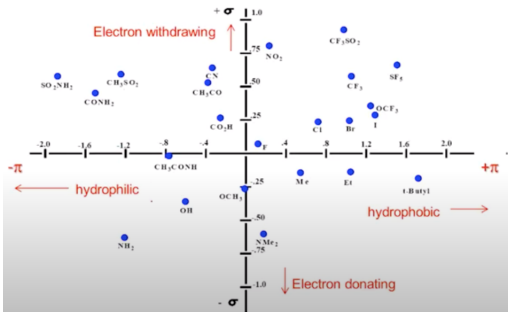


A. 3.32
B. 0.94
C. 1.98
D. 2.13

13 Which of the following statements is untrue when comparing 3D QSAR with conventional QSAR? **1**

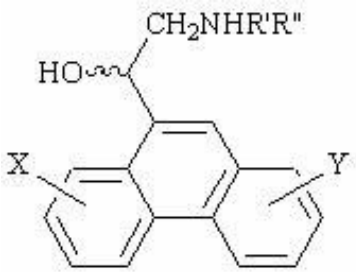
A. Only drugs of the same structural class should be studied by 3D QSAR or QSAR.
B. 3D QSAR has a predictive quality unlike QSAR.
C. Experimental parameters are not required by 3D QSAR, but are for QSAR.
D. Results can be shown graphically in 3D QSAR, but not with QSAR.

14 A Hansch analysis is being carried out in order to relate biological activity to σ and π. Which of the following substituents would best suit the study? **2**



A. SO_2NH_2, $CONH_2$, CH_3SO_2, CH_3CO, CN
B. NH_2, OH, F, Cl, CF_3
C. NO_2, CO_2H, F, OCH_3, NMe_2
D. SO_2NH_2, Br, NMe_2, NH_2, CF_3SO_2

15 A series of 102 phenanthrene aminocarbinols (see structure below) were tested for antimalarial activity and found to fit the following Hansch equation: **2**



$$\log\left(\frac{1}{C}\right) = -0.015(\pi_{sum})^2 + 0.14\pi_{sum} + 0.27\Sigma\pi_X + 0.40\Sigma\pi_Y + 0.65\Sigma\sigma_X + 0.88\Sigma\sigma_X + 2.34$$

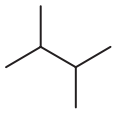
What is the significance of $-0.015(\pi_{sum})^2 + 0.14\pi_{sum}$ in the equation? (π_{sum} indicates the sum of the π constants for all the substituents in the molecule)?

A. It indicates that activity falls to a minimum value as πsum increases to an optimum value, then rises again as πsum increases beyond that value.
B. It indicates that activity falls to a minimum value as πsum decreases to a certain value, then rises again as πsum increases beyond that value.
C. It indicates that activity rises to a maximum value as π sum increases to an optimum value, then falls again as sum increases beyond that value.
D. It indicates that activity rises to a maximum value as πsum decreases to a certain value, then falls again as πsum decreases beyond that value.

16 QSAR method involves **2**

A. Target Structure
B. Target Properties
C. Ligand X-ray structure
D. Ligand Properties
E. None of the above

17 For the structure given below, how many paths of length 3 are present? **1**



A. 2
B. 3
C. 4
D. 5

18 Which of the following statement is correct for Hammett Substituent Constant σ? **2**

A. Electron donating substituents have negative (σ) values since they destabilize the carboxylate anion and shift the equilibrium to the left.
B. Electron withdrawing substituents have negative (σ) values since they destabilize the carboxylate anion and shift the equilibrium to the right.

C. Electron donating substituents have negative (σ) values since they stabilize the carboxylate anion and shift the equilibrium to the right.
D. Electron withdrawing substituents have positive (σ) values since they stabilize the carboxylate anion and shift the equilibrium to the left.

19 Roughly _____ percent of drug candidate fails due to poor pharmacokinetic properties **1**

A. 20
B. 30
C. 40
D. 50

16 Discuss the advantages and limitations of bitstring representation of a query substructure. **2**

17 Enlist five important databases of cheminformatics along with their description **5**

18 What are PK and PD? Which one is more relevant for ADME/T and why? **2**

19 Discuss two pharmacophore mapping algorithms with their advantages and limitations. **4**

20 How drug dosage amount and drug dosage frequency affect by the ADME/T properties of the substance? **2**

21 Discuss the critical factors considered for selecting the target for structure-based virtual screening based on the articles you presented during the class. **5**