PCH-BP 807T CADD End Semester Exam July 2021(MCQ) (PCH-BP807ET Elective 2021)

Start time: 2.30 pm
Due time: 3.00 pm
End time: 3.05 pm

* Required

* This form will record your name, please fill your name.

[   ]

1. Which of the following statement is not true with respect to a pharmacophore *
(1 Point)

○ pharmacophore represent a real molecule which is capable of binding to a specific target.

○ highest common denominator of a group of ligands exhibiting a similar biological effect recognized by the same binding site

○ a pharmacophore is an abstraction of the crucial molecular features responsible for the binding of a set of ligands to a macromolecular target

○ ensemble of steric and electronic features that is necessary to ensure the optimal supramolecular interactions with a specific biological target

2. Testosterone and 17α-Oxa-D-fomo-1,4 androstadine-3,17-dione is an example for *
(1 Point)

○ Bioisosteric replacement of C for O

○ Divalent isosteric replacement

○ Monovalent isosteric replacement

○ Ring isosteric replacement

3. The conversion of Tolbutamide to Chlorpropamide is strategically aimed *
(1 Point)

○ To increase lipid solubility

○ To prevent metabolic oxidation

○ None

○ To increase protein binding

4. In CoMFA analysis we evaluate *
(1 Point)

○ The interaction energy between a probe atom and each atom in the aligned molecules in regularly spaced grid points.

○ Calculates steric, electrostatic, and HB donor and acceptor similarity indices of aligned molecules at regularly spaced grid points occupied by a common probe atom.

○ Calculates steric, electrostatic, and HB donor and acceptor similarity indices of aligned molecules occupied by a common probe atom.

○ The interaction energy between a probe atom and each atom in the aligned molecules

5. What are Druggable genes *
   (1 Point)

   ○ Genes encoding proteins likely to possess binding domains that recognize drug-like small molecules

   ○ Genes whose altered expression is thought to be involved in the development of the disease state

   ○ Genes, mutations of which cause or predispose to the development of human disease

   ○ Genes that encode functional proteins, whose activity is altered

6. π-substituent constant is *
   (1 Point)

   ○ Measure of hydrophobic constant of a unsubstituted molecule

   ○ Measure of how hydrophobic a substituent is relative to Hydrogen

   ○ Measure of how hydrophobic a Hydrogen is relative to substitution

   ○ Measure of hydrophobic substituent of Hydrogen

7. Quantum mechanics describes molecules in terms of interactions among the following. *
   (1 Point)

   ○ Electrons and Molecular geometry

   ○ Nuclei, Electrons and Molecular geometry

   ○ Nuclei and molecular geometry

   ○ Nuclei and Electrons

8. Following drug is an example of Bioisosteric replacement to increase absorption through gut wall *
(1 Point)

○ Losartan

○ 5-Fluorouracil

○ INH

○ Alpha-tocopherol

9. De Novo Design can be used to *
(1 Point)

○ All of the above

○ generate ligand structures to virgin targets

○ generate alternative chemotypes to known active compounds

○ generate ligand structures from molecular fragments bound into the site

10. Ligand based pharmacophore program is called as: *
(1 Point)

○ Pharma Gist

○ SPORES

○ Ligand Scout

○ GOLD

11. What is the upper Polar Surface Area threshold value for oral absorption of a drug *
(1 Point)

◯ 50-60 Å2

◯ 140-150 Å2

◯ 90-100 Å2

◯ 80-90 Å2

12. Software used to detect presence or absence of water molecule is: *
(1 Point)

◯ H++

◯ PHASE

◯ GLIDE

◯ JAWS

13. Chemo informatics mainly   deals with approaches employed for the following: *
(1 Point)

◯ Chemical, Biological and Bio chemical data base concept

◯ Chemical data base concept

◯ Biochemical and chemical data base concept

◯ Chemical and Biological data base concept

14. With respect to use of NMR for screening ligands , which of the following statement is not true *
(1 Point)

◯ If the drug binds to the protein, its nuclei will have a shorter relaxation time and no NMR spectrum will be detected

◯ compounds can be tested or screened for their affinity to a macromolecular target

◯ Relaxation times of ligands bound to a macromolecule are shorter than when they are unbound

◯ If the drug does not binds to the protein, its nuclei will have a shorter relaxation time and no NMR spectrum will be detected

15. Micro array provides massive amount of data about the following: *
(1 Point)

◯ Gene activity in the absence of certain biological samples under specific conditions

◯ Protein activity in the presence of certain biological samples under specific conditions

◯ Protein activity in the absence of certain biological samples under specific conditions

◯ Gene activity in the presence of certain biological samples under specific conditions

16. Benzoic acid having electron donating substituent will have *
(1 Point)

◯ Higher Kx value than benzoic acid

◯ Equal Kx like substituted Benzoic acid

◯ σX for an electron withdrawing substituent will be negative

◯ Smaller Kx value than benzoic acid

17. AMBER is the force field used for the simulation for the following: *
   (1 Point)

   ◯ Proteins

   ◯ Proteins

   ◯ Carbohydrates

   ◯ Nucleic acids and Proteins

18. The biggest challenges (protein folding problems) of structural bioinformatics reside in the prediction of *
   (1 Point)

   ◯ Secondary structure from primary structure

   ◯ Tertiary structure from secondary structure

   ◯ Quaternary structure from secondary structure

   ◯ Tertiary structure from Primary structure

19. Which of the following functional groups can be considered as structural alerts used to detect compounds with potential mutagenicity and carcinogenicity *
   (1 Point)

   ◯ alkylnitrosamines

   ◯ ring epoxides

   ◯ all of the above

   ◯ arylamine function

20. Binding site for a protein target is selected on the basis of which of the following *
(1 Point)

○ Site score

○ Binding site volume

○ Druggability score

○ All of the above

Manipal College of Pharmaceutical Sciences
MAHE, Manipal
8ᵗʰ Semester B-Pharm – End semester Examination, July 2021

Course Code. PCH-BP807ET Course Title. CADD

Date: 12-07-2021	Duration: 2hr	Max. Marks: 50

Instructions to the students

1. The duration of semester/annual sessional examination is from 3.05PM to 4.45 PM Indian Standard Time. This includes the time for answering the questions and uploading the document to the Microsoft Teams.
2. Candidate shall use A4 size plain white paper to write the answers.
3. The answer sheets used by the candidate shall not have watermark/logos or any other printed matter.
4. Candidate shall use only blue or black ink pen while answering the papers.
5. Candidate must write in each page Class, Register No. Name, Signature with date and the **camera in on mode.**
6. Candidate must write the correct question and number and then answer.
7. At the end, candidate must scan the answer pages using CamScan or any other suitable means in the order ensuring that the written matter is clearly visible in the image captured.
8. The entire document shall be submitted as a Single PDF. The file name of the PDF shall be your **Registration number-Subject code** (For example **190000009.pdf**)
9. Press turn in button after uploading answer file before Due time or Close time. Besides, the submission of the scripts is through MST only and the **submissions through emails are not acceptable.** System will not allow you to upload answer file after close time. Hence advised to submit before Due time preferably.
10. Before uploading the PDF file to MST, the candidate must ensure that all the written pages are included in sequence as per question number.
11. The candidate must open the PDF file to ensure that there are no technical problems and contents of all the pages are clearly visible. The file size is should NOT be more than 45MB.
12. **Candidates must take care to upload the pdf document that contains the answers pertaining to the examination of concerned subject only.**
13. Candidate do hereby agree that they have received and read the detailed instructions from the college regarding their obligation/conduct during sessional examination.

Answer ALL questions.

Q.1-20 MCQ		20 Marks
Section B: Shor Answer Questions (6 × 5 marks = 30 marks)		
21.	Explain lead discovery through CADD and serendipity	5 Marks
22	Explain the various stages involved in molecular docking and add a note on fundamental steps involved in pharmacophore modelling	5 Marks
23	Write the principle involved in quantum mechanics and molecular mechanics	5 Marks
24	Justify, how Bioinformatics and Chemo informatics together support new drug discovery program	5 Marks
25	Taking Benzoic acid and its derivatives as example, explain Hammett substituent constant as an electronic parameter in QSAR.	5 Marks
26	With a case study explain the development of antihypertensive drug analogues to Clonidine using bioisosteric strategy.	5 Marks
	End of question paper"	