Printed Pages: 01
Paper Id: 231977

Sub Code: BP807ET
Roll No.: _____

BPHARM
(SEM VIII) THEORY EXAMINATION 2021-22
COMPUTER AIDED DRUG DESIGN

Time: 3 Hours Total Marks: 75

Note: Attempt all Sections. If requireanymissingdata;thenchoosesuitably.

SECTION A

1. Attempt all questions in brief. 10 × 2 = 20
(a) Write a note on serendipitous discovery of drugs?
(b) Define the term lead optimization?
(c) Differentiate between SAR and QSAR?
(d) Write about Free-Wilson analysis.
(e) What is virtual screening?
(f) What is rigid docking?
(g) Define the terms: Bioactive conformation & Force field.
(h) What is global conformational minima?
(i) Enlist the applications of bioinformatics tools in drug design.
(j) Give examples for pharmaceutical databases.

SECTION B

2. Attempt any two parts of the following: 2 × 10 = 20
(a) What is 3D QSAR? Write about CoMFA and CoMSIA methods.
(b) Describe the concept of pharmacophore-based virtual screening in drug design.
(c) Define and classify bioisosteres. Explain its significance in drug design with suitable examples.

SECTION C

3. Attempt any five parts of the following: 5 × 7 = 35
(a) Explain about Hansch analysis with a model QSAR equation.
(b) Highlight the significance of partition coefficient in QSAR analysis and write its determination.
(c) Describe metabolism-based lead discovery with specific examples.
(d) Explain the steps involved in molecular docking.
(e) Explain drug-likeness screening along with the tools used for its determination.
(f) List out various protein databases. Explain the significance of these databases in drug design with a specific example.
(g) Discuss the significance of in silico ADME databases in drug design.

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(SEM VIII) THEORY EXAMINATION 2022-23
COMPUTER AIDED DRUG DESIGN

Time: 3Hours ***Total Marks: 75***

Note: Attemptall Sections. If require anymissingdata; then choose suitably.

SECTION A

1. Attempt all questions in brief. **10 x 2 = 20**

(a) What various stages of drug discovery?

(b) What is Phase 0 clinical trial?

(c) What is non-classical bioisosteres?

(d) What is Taft's steric factor (Es)?

(e) Write down the drawbacks and limitations of CoMFA.

(f) What do you understand by the term Pharmacophore?

(g) Give the names of molecular docking models.

(h) What do you understand by the term "Binding mode"?

(i) What isOrangebook?

(j) What is various chemical structure representation used for chemical structures in digital databases?

SECTION B

2. Attempt any *two* parts of the following: **2 x 10 = 20**

(a) Write in detailaboutthe druglikenessscreening with the various filterusedin drug likeness screening.

(b) What is cheminformatics? Write in detail about the various tools and steps involved in cheminformatics system.

(c) What do you understand by Force field? Discuss various novel technique used in molecular modeling

SECTION C

3. Attempt any *five* parts of the following: **5 x 7 = 35**

(a) Write in detail abouttheFree-Wilsonapproach to QSAR.

(b) What do you understand by conformational analysis? Write Different methods used to determine information regarding conformations.

(c) Write in detail about the Quantum mechanics methods of Molecular modelling.

(d) Discuss in detail about the De-novo drug design with steps involved in it.

(e) Differentiate between SAR and QSAR.

(f) Discuss in detail about Ligand-based pharmacophore modeling.

(g) Discuss in detail about various lead discoveries based on traditional medicine with suitable examples.

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Roll No: | | | | | | | | | | | | | |

Subject Code: BP807ET

BPHARM
(SEM VIII) THEORY EXAMINATION 2024-25
COMPUTER AIDED DRUG DESIGN

TIME: 3 HRS **M.MARKS: 75**

Note: 1. Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. Attempt *all* questions in brief. **10 x 2 = 20**

a.	
b.	How lead moleculeplay a vital rolein drug discovery?
c.	What do you understand from non-random screening?
d.	Write the importance of *de novo* drug design.
e.	Write the importance of partition coefficient.
f.	Write the outcomes of docking based screening.
g.	Write the purpose of conformational analysis.
h.	Define Pharmacophore mapping.
i.	Write the applications of bio-informatics.
j.	Define random screening.
	Define COMSIA.

SECTION B

2. Attempt any *two* parts of the following: **2 x 10 = 20**

a.	Give the stagesof drugdiscovery and development.
b.	Write the history and development of QSAR.
c.	Discuss the energy minimization methods.

SECTION C

3. Attempt any *five* parts of the following: **7 x 5 = 35**

a.	
b.	Howtraditional medicinesbecome the source of drug discovery? Explain.
c.	Describe the physicochemical parameters used in QSAR studies.
d.	Compare between rigid docking and flexible docking.
e.	Write the role of ADME databases in drug discovery.
f.	Write a note on bio-isosterism.
g.	Explain lead discovery based on clinical observation.
	Describe principle and applications of COMFA.