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Roll No.

<https://pharmacyindia.co.in/>

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

Time: 3 Hours

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Total Marks: 75

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

SECTION A

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

- (a) What various stages of drug discovery? <https://pharmacyindia.co.in/>
- (b) What is Phase 0 clinical trial?
- (c) What is non-classical bioisosteres?
- (d) What is Taft's steric factor (E_s)?
- (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. <https://pharmacyindia.co.in/>
- (h) What do you understand by the term "Binding mode"?
- (i) What is Orangebook?
- (j) What is various chemical structure representation used for chemical structures in digital databases?

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SECTION B

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

- (a) Write in detail about the drug likeness screening with the various filter used in 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

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

- (a) Write in detail about the Free-Wilson approach 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. <https://pharmacyindia.co.in/>
- (g) Discuss in detail about various lead discoveries based on traditional medicine with suitable examples.

