

Course: Computer Aided Drug Design

(02 Credits)

Code: BIN 465

Time: 1 hour

Section - A (All questions are compulsory) (5x1=5)

1. Write a note on following:

- Pharmacokinetics?
- Pharmacophore?
- Isostere?
- Discuss Lead vs Hit compound?

e. SAR? *Structure activity relationship*

Section - B (Attempt any two questions)

(2 x 2.5 = 5)

2. What is hydrophobic substituent constant ( $\pi$ )?

3. What is QSAR? Name 3 most important parameters of QSAR preferably studied for drug design. *Steric, Electronic, Hydrophobicity*

4. What is serendipity, discuss with example? *Penicillin, Squalene*

5. Discuss Bioisosterism in light of one case study.

Section - C (Attempt any two questions)

(2 x 5 = 10)

*Absorption, Distribution, Metabolism, Excretion, Toxicity.*

6. What do you mean by ADMET? How are these drug likeliness properties important in drug design?

7. Discuss historical events in the development of CADD. Draw flow chart showing sequential events in Drug Discovery starting from Target Identification. (Flow chart only)

8. Discuss partition coefficient (P). Discuss significance of log P vs log (1/C) graph.

9. Discuss atleast 3 approaches used for Optimisation of Lead Structure.