

Seat No.: _____

Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

M. Pharm. Semester – IIND Examination – June/July- 2011

Subject code: 920201

Subject Name: Drug Design and Discovery

Date: 04/07/2011

Time: 10:30 am – 01:30 pm

Total Marks: 80

Instructions:

- 1. Attempt any five questions.**
- 2. Make suitable assumptions wherever necessary.**
- 3. Figures to the right indicate full marks.**

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|-------------|-----|---|-----------|
| Q.1 | (a) | Explain the term ‘Lead molecule’? Describe the traditional ways of finding lead molecule. | 06 |
| | (b) | Discuss the role of drug design concept in drug discovery. | 05 |
| | (c) | Explain various steps involved in drug design concept. | 05 |
| Q.2 | (a) | Explain the concept of enzyme inhibition in drug design. Justify giving the proper explanation why mechanism based inhibitors have potential advantages over affinity labels? | 06 |
| | (b) | Explain the concept enzyme in drug design. | 05 |
| | (c) | What are goals of Analog design? Discuss the strategy of analog design by making geometrical isomers | 05 |
| Q.3 | (a) | What is bio-isosterism? Discuss classical bioisosters with examples. | 06 |
| | (b) | Explain role of stereochemistry in relation to drug design. | 05 |
| | (c) | Why racemic mixtures of drug are not preferred for clinical use. | 05 |
| Q.4 | (a) | Discuss how site specific action can be achieved by using pro-drug concept with suitable examples. | 06 |
| | (b) | What are micromolecular pro-drugs? Discuss the benefits of such pro-drugs with suitable example. | 05 |
| | (c) | What is 3D-QSAR. Discuss the importance of COMFA and DISCO models of 3D-QSAR. | 05 |
| Q.5 | (a) | What do you mean QSAR? Discuss various physiochemical and electronic parameters in detail. | 06 |
| | (b) | What are the advantages of 3D-QSAR over 2D-QSAR. | 05 |
| | (c) | Discuss the merits and demerits of Free Wilson Analysis. | 05 |
| Q. 6 | (a) | What is molecular modeling? Discuss the application of molecular docking in drug design. | 06 |
| | (b) | Discuss Topliss Decision Tree Method used for designing drugs | 05 |
| | (c) | Discuss advantages and disadvantages of Quantum Mechanics and Molecular Mechanics in CADD. | 05 |
| Q.7 | (a) | What is virtual screening? Explain the methodology of virtual screening by pharmacophore mapping. | 06 |
| | (b) | What is de-novo drug designing? Discuss its requirement and different steps involved in it. | 05 |
| | (c) | Justify, importance of pharmacokinetics in new drug delivery. | 05 |
