

Seat No.: _____

Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

M.PHARM- SEM-II-EXAMINATION – JULY 2012

Subject code: 2920201

Date: 09/07/2012

Subject Name: DRUG DESIGN AND DISCOVERY

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.

Q 1.

- a) Explain in detail concept of drug discovery. 06
- b) What do you mean by drug design, explain its applications in drug discovery 05
- c) What is 'LEAD' explain methods used for lead discovery. 05

Q 2.

- a) Explain in detail the importance stereochemistry in drug design. 06
- b) Write in detail importance of physicochemical parameters in biological activity. 05
- c) Explain the following terms 05
 - i) Bio-isosterism
 - ii) Prodrug concept

Q 3.

- a) What do you mean by QSAR, explain in detail Hanch LEFR model. 06
- b) Write a note on QSAR parameters 05
- c) What is Free Wilson analysis? Explain its significance 05

Q 4.

- a) What do mean by variables and statistical analysis in QSAR 06
- b) Explain following statistical analysis in detail 05
 - i) PLS ii) PCA iii) MFA iv) GFA
- c) Write a note on 3-D QSAR. Write differences between 2-D QSAR and 3-D QSAR. 05

Q 5.

- a) What do you mean by CADD, explain importance of molecular modeling? 06
- b) What do you mean by following terms 05
 - i) Quantum mechanics
 - ii) Molecular mechanics
 - iii) Energy minimization
- c) Explain in detail use of NMR and X-ray crystallography in CADD

Q 6.

- a) What is structure based drug design and ligand based drug design. 06
- b) What do you mean by docking study, explain different methods used in docking. 05
- c) Write a note on theory of drug action. Explain in detail about agonist and antagonist. 05

Q 7.

- a) What do you mean by virtual screening. Explain in detail about pharmacophore mapping. 06
- b) Write importance of ADME in drug discovery 05
- c) Write a note on following 05
 - i) COMFA
 - ii) COMSIA
 - iii) MSA

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