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

* * * * *