

Seat No.: _____

Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY
B. Pharm. - SEMESTER-8 • EXAMINATION – SUMMER -2018

Subject Code: 2280006**Date: 09/05/2018****Subject Name: Computer Applications in drug discovery****Time: 10:30 AM TO 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) What do you mean by force field? Describe various methods for energy minimization. **06**
(b) What is compound library filters? Explain it. **05**
(c) Discuss potentials of in silico toxicology. **05**
- Q.2** (a) Write a note on Pharmacophore mapping **06**
(b) Discuss about Consensus – scoring function. **05**
(c) Explain in detail molecular dynamics – based detection in SBDD. **05**
- Q.3** (a) Describe multi target inhibitors using common pharmacophore models. **06**
(b) Write a note on high resolution docking. **05**
(c) Discuss about Monte Carlo Search with metropolis criterion. **05**
- Q.4** (a) Write a note on drug discovery process. Give importance of drug design. **06**
(b) Write in detail about COMFA and COMSIA Methods of QSAR. **05**
(c) Write a note on ligand databases for CADD. **05**
- Q.5** (a) Enlist methods to identify protein binding sites and explain any one in detail. **06**
(b) Write a short note on multidimensional QSAR in drug discovery. **05**
(c) Explain in brief linear regression method in QSAR models. **05**
- Q. 6** (a) Explain in detail 3D description of molecular configuration and conformation in ligand based CADD. **06**
(b) Write a note on InChIKey- the IUPAC International Chemical Identifier. **05**
(c) Explain role of octanol / water partition coefficient and polarizability as a molecular descriptors in ligand based CADD **05**
- Q.7** (a) What is pharmacophore? Explain in brief molecular superimposition in pharmacophore mapping. **06**
(b) Write a note on Receptor – dependent 3D/4D QSAR. **05**
(c) Discuss about Knowledge based scoring function. **05**
