

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.

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|-------------|-----|--|-----------|
| 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 |
