# Rajiv Gandhi University of Health Sciences

Second Semester M. Pharm Degree Examination - MAY-2018 [Time: 3 Hours] [Max

## Computer Aided Drug Design -II Q.P. CODE: 5159

Your answers should be specific to the questions asked. Draw neat, labeled diagrams wherever necessary.

#### LONG ESSAY (Answer any Three)

- 1. Explain Hansch and Free Wilson method of analysis with a suitable example and relationship between them.
- 2. Discuss the approaches for 3D-QSAR analysis.
- 3. Write the protocols to be followed in In silico virtual screening.
- 4. Discuss the energy minimization methods in molecular modeling.

### SHORT ESSAY (Answer any Nine)

- 5. Describe the docking of agents on AchE.
- 6. Explain the method of generation of 3D-structure of a protein.
- 7. What is log P? How it is determined? Give its significance.
- 8. Explain the docking of agents on DHFR enzyme.
- 9. Explain pharmacopher mapping.
- 10. Discuss homology modeling of a protein.
- 11. Describe extra precision docking.
- 12. Explain the electronic parameters to be considered in QSAR.
- 13. Write a note on counter map analysis.
- 14. Discuss the role of computer aided drug design in drug discovery.

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#### 3 X 10 = 30 Marks

[Max. Marks: 75]

#### 9 X 5 = 45 Marks