Rajiv Gandhi University of Health Sciences

Second Semester M. Pharm Degree Examination - JAN-2019

[Time: 3 Hours] [Max. Marks: 75]

Computer Aided Drug Design

Q.P. CODE: 5159

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

LONG ESSAY (Answer any Three) **3 X 10 = 30 Marks**

1. Explain briefly different physiochemical used to determine the Quantitative structure activity relationship of drug molecules.
2. Explain different energy minimization methods and compare global minimum conformation and bioactive conformation.
3. Discuss the fragment based drug design and homology modeling.
4. Explain the pharmacophore based and structure based In-silico virtual screening protocols.

SHORT ESSAY (Answer any Nine) **9 X 5 = 45 Marks**

5. Explain in brief Hammett equation and sigma parameters.
6. Enumerate the different methods in the calculation of partition co-efficient.
7. Discuss the Free Wilson analysis and give its applications.
8. What are the various statistical methods adopted for the QSAR analysis.
9. Discuss the different approaches of 3D QSAR.
10. Discuss the agents used in the inhibition of HMG Co-A reductase enzyme.
11. Discuss the different types of drug receptor interactions.
12. Explain how ADMET properties are predicted for new molecules.
13. Write a note on receptor/enzyme interaction and its analysis.
14. How do you identify features of pharmacophore?

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