

End Semester Examinations - 2015-16 Even Semester - May 2016

15BI3004 Cheminformatics and QSAR

Set A

Time : 3 hrs
Total Marks: 100

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1. A. Define Cheminformatics? Write a detail note on cheminformatics for modern drug discovery.(10)
 B. Give an overview of application of cheminformatics in various fields.(10)
 - OR**
 2. A. Describe about the various Prospects of cheminformatics(10)
 B. Briefly describe the History and Evolution of cheminformatics (10)
 3. A. Explain Detail about Molecular mechanics and Quantum mechanics.(10)
 B. Write a complete note on Computational molecular structure prediction.(10)
 - OR**
 4. A. What is modelling? Describe the different methods used for molecular modelling.(10)
 B. Explain briefly about experimental methods used for molecular structure elucidation.(10)
 5. A. Discuss the different type of chemical molecular file formats.(5)
 B. Explain in detail about SMILE, molfile ,sdf file structure and application in cheminformatics fields .(15)
 - OR**
 6. Define Electronic effect? Elaborate different types of electronic effect take place in chemical reaction (20)
 7. A. Briefly describe the reaction mechanism of inductive effect and electrometric effect(10)
 B. Write a complete note on following
 - I. Resonance(5)
 - II. Hyper conjugation(5)
 - OR**
 8. A. Define QSAR? Detail the Outline of Conformational molecular field analysis.(10)
 B. Write a methods used in PLS Regression and post regression in CoMFA.(10)
 9. A. Define 3DQSAR? Elaborate the basic principle of QSAR modelling in chemical molecules.(10)
 B. Briefly describe the statistical tools routinely required in QSAR methodologies.(10)

Wishing you All the Best
