Reg. No. \_\_\_\_\_\_\_\_\_\_\_\_

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**End Semester Examination – Nov / Dec – 2019**

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| **Code :** | **14BI2008** | **Duration :** | **3hrs** |
| **Sub. Name :** | **MOLECULAR MODELING AND CADD** | **Max. Marks :** | **100** |

**ANSWER ALL QUESTIONS (5 x 20 = 100 Marks)**

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| **Q. No.** | **Sub Div.** | **Questions** | **Course**  **Outcome** | **Marks** |
| 1. |  | Describe molecular modeling concept in Quantum and Molecular Mechanics. | CO1 | 20 |
| **(OR)** | | | | |
| 2. |  | Justify the statement “Molecular mechanics force field is used to determine the potential energy”. | CO1 | 20 |
|  |  |  |  |  |
| 3. |  | Describe energy minimization and related methods for exploring the Energy surface. | CO2 | 20 |
| **(OR)** | | | | |
| 4. |  | Explain Molecular Simulation methods with example. | CO2 | 20 |
|  |  |  |  |  |
| 5. | a. | Write 3D structure prediction by homology modeling method. | CO2 | 10 |
|  | b. | Describe drug development process with example. | CO1 | 10 |
| **(OR)** | | | | |
| 6. |  | Describe importance of Computer Aided Drug Design (CADD) approach in Pharmaceutical Development. | CO3 | 20 |
|  | | | | |
| 7. |  | Describe steps involved in QSAR modeling. | CO2 | 20 |
| **(OR)** | | | | |
| 8. |  | Write pharmacophore modeling features and applications with an example. | CO3 | 20 |
|  | | **Compulsory:** |  |  |
| 9. |  | Describe molecular docking process and scoring function to identify the lead molecule. | CO3 | 20 |