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

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

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| **Code :** | **MOLECULAR MODELING AND CADD** | **Duration :** | **3hrs** |
| **Sub. Name :** | **17BI2012** | **Max. Marks :** | **100** |

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

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| **Q. No.** | **Sub Div.** | **Questions** | **Course**  **Outcome** | **Marks** |
| 1. |  | Explain 3D structure prediction procedure by homology modeling. | CO1 | 20 |
| **(OR)** | | | | |
| 2. |  | Describe Protein Databank file format of 3D structure of Protein. | CO2 | 20 |
|  |  |  |  |  |
| 3. |  | Define Molecular simulation. Write Molecular Simulation methods with example. | CO3 | 20 |
| **(OR)** | | | | |
| 4. |  | Justify the statement “Molecular Mechanics Force Field is used to determine potential energy”. | CO4 | 20 |
|  |  |  |  |  |
| 5. | a. | Explain energy minimization and related methods for exploring the Energy surface. | CO3 | 10 |
| b. | Mention drug properties based on Lipinski’s rule of 5. | CO2 | 10 |
| **(OR)** | | | | |
| 6. | a. | Define Docking. Explain need of docking and scoring function in biological response. | CO5 | 10 |
| b. | Explain uses of computer graphics in Molecular Simulation. | CO1 | 10 |
|  |  |  |  |  |
| 7. |  | Define Hydrogen bonding. Describe hydrogen bonding importance in molecular mechanics. | CO6 | 20 |
| **(OR)** | | | | |
| 8. | a. | Describe role of Computer aided Molecular modeling for the designing of novel Inhibitor. | CO5 | 10 |
| b. | Define QSAR. Explain QSAR approach to predict antiviral drug activity based on physiochemical properties. | CO4 | 10 |
|  | | **Compulsory:** |  |  |
| 9. |  | Describe structure and ligand based drug design approach to identify the lead molecules. | CO6 | 20 |