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

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

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| **Code :** | **14BI2027** | **Duration :** | **3hrs** |
| **Sub. Name :** | **CHEMINFORMATICS AND QSAR** | **Max. Marks :** | **100** |

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

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| **Q. No.** | **Sub Div.** | **Questions** | **Course**  **Outcome** | **Marks** |
| 1. | a. | Descirbe the uses of Drug Bank. | CO1 | 10 |
| b. | Write smile notation rules with structure elucidation. | CO1 | 10 |
| **(OR)** | | | | |
| 2. | a. | Explain similarity search method to find similarities between structure. | CO1 | 10 |
| b. | Mention scopes of cheminformatics in pharmaceutical development. | CO1 | 10 |
|  |  |  |  |  |
| 3. | a. | Describe process of drug development in computational aspect with example. | CO2 | 10 |
| b. | Describe need of scoring and rescoring function to analyze the molecular interaction. | CO2 | 10 |
| **(OR)** | | | | |
| 4. | a. | Define InChI. Illustrate Molfiles format. | CO2 | 10 |
| b. | Describe five binding affinity parameters of molecular interaction. | CO2 | 10 |
|  |  |  |  |  |
| 5. | a. | Descirbe 3D QSAR modeling based on pharmacophore approach. | CO3 | 10 |
| b. | Write four data optimization techniques with example. | CO3 | 10 |
| **(OR)** | | | | |
| 6. |  | Write target identification and validation by Computational approach. | CO2 | 20 |
|  |  |  |  |  |
| 7. |  | Explain lead fiding procedure in drug discovery. | CO2 | 20 |
| **(OR)** | | | | |
| 8. | a. | Discuss important aspects of drug optimization technique to improve the drug activity. | CO2 | 10 |
| b. | Write linear and nonlinear approach to analyze QSAR modeling data. | CO3 | 10 |
|  | | **Compulsory:** |  |  |
| 9. |  | Define the term QSAR. Write in detail about steps involved in QSAR and their importance in pharmaceutical development. | CO3 | 20 |