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**UNIVERSITY**

(Karunya Institute of Technology & Sciences)

(Declared as Deemed-to-be University under Sec.3 of the UGC Act, 1956)

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

**End Semester Examination – Nov/Dec - 2016**

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|  |  | **Semester :** | **2016-17 ODD** |
| **Code :** | **12CH214** | **Duration :** | **3 hrs** |
| **Sub. Name :** | **CHEMINFORMATICS** | **Max. marks :** | **100** |

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| **Q. No.** | **Questions** | **Marks** |
| **PART-A(10X1=10 MARKS)** | | |
| 1. | Write one example for computer program that is used for drawing the chemical structure. | (1) |
| 2. | Write the SMILES notations for (i) methane and (ii) a triple bond. | (1) |
| 3. | Define: Pharmacophore mapping. | (1) |
| 4. | The completely connected subgraph is called \_\_\_\_\_\_\_\_\_\_\_. | (1) |
| 5. | Define: Molecular Descriptor**.** | (1) |
| 6. | What is meant by unit variance scaling? | (1) |
| 7. | State similar property principle. | (1) |
| 8. | Write the expression for Carbo coefficient. | (1) |
| 9. | An example for data visualization program is \_\_\_\_\_\_\_\_\_\_\_\_. | (1) |
| 10. | What is the aim of protein-ligand docking? | (1) |

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| **PART B(5 X 3= 15 MARKS)** | | |
| 11 | What are the various parts of connection table? | (3) |
| 12 | Write a note on structure generation programs. | (3) |
| 13 | Define: Molar refractivity. | (3) |
| 14 | Identify the Similarity coefficients among the following  (i) Tanimoto (ii) Cosine (iii) Euclidean (iv) Soergel (v) Dice (vii) Hamming | (3) |
| 15 | Based on the amount of structural and bioactivity data available, classify the Virtual screening methods. | (3) |

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| **PART C(5 X 15= 75 MARKS)** | | | |
| 16. | a. | Explain the graph theoretic representation of chemical structures. | (12) |
| b. | Aspirin-skeletal.svgAssign the connectivity value at each atom in the following structure. | (3) |
| (OR) | | | |
| 17. | a. | Explain substructure searching using subgraph isomorphism method. | (10) |
| b. | Discuss the various types of keys used in the structural key approach. | (5) |
| 18. | a. | Explain the uses of Cambridge structural database. | (3) |
| b. | Write a detailed account on 3D Pharmacophores. | (12) |
| (OR) | | | |
| 19. | a. | Describe the Constrained Systematic search method for the pharmacophore mapping. | (10) |
| b. | Write the formula to calculate score in the maximum likelihood method and explain the terms involved. | (5) |
| 20. | a. | Write a note on simple counts. | (3) |
| b. | Define topological indices. Discuss about the branching index and chi molecular connectivity indices. | (12) |
| (OR) | | | |
| 21. | a. | What are the valence angle descriptors and torsional angle descriptors in 3D fragment screen method? | (3) |
| b. | Discuss the principal component analysis method for reducing the dimensionality of a data set? | (12) |
| 22. | a. | Write a detailed account on Similarity based on 2D fingerprints. | (8) |
| b. | What is meant by maximum common subgraph similarity? Explain. | (7) |
| (OR) | | | |
| 23. |  | Explain the following similarity methods. |  |
| a. | Alignment Independent Method. | (8) |
| b. | Gnomonic Projection Method. | (7) |
| 24. | a. | Describe the stages involved in multidimensional scaling. | (10) |
| b. | Explain the discriminant analysis process. | (5) |
| (OR) | | | |
| 25. | a. | State the methods used to assess the drug likeness. Discuss any two of them. | (10) |
| b. | Explain the equation for the free energy of binding. | (5) |

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