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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 :** | **10NT217** | **Duration :** | **3 hrs** |
| **Sub. Name :** | **CHEMINFORMATICS** | **Max. marks :** | **100** |

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| **Q. No.** | **Questions** | | **Marks** |
| **PART-A(10X1=10 MARKS)** | | | |
| 1. | An example of structure drawing software is \_\_\_\_\_\_\_\_\_\_\_\_. | | (1) |
| 2. | Write an example for a reaction database. | | (1) |
| 3. | A set of features together with their spatial orientations is known as \_\_\_\_\_\_\_\_\_\_\_\_. | | (1) |
| 4. | Define ‘clique’ in a graph. | | (1) |
| 5. | Define: Molecular Descriptor. | | (1) |
| 6. | The plots that are used to represent the results of the principal component analysis are \_\_\_\_\_\_\_\_\_\_\_\_ and \_\_\_\_\_\_\_\_\_\_\_\_. | | (1) |
| 7. | State neighbourhood principle. | | (1) |
| 8. | Write an example for an asymmetric index. | | (1) |
| 9. | An example for data visualization program is \_\_\_\_\_\_\_\_\_\_\_\_. | | (1) |
| 10. | State the aim of virtual screening? | | (1) |
| **PART B(5 X 3= 15 MARKS)** | | | |
| 11. | Write the SMILES notation for the following compounds.   1. Methane b. Ethane c. n-Propanol | | (3) |
| 12. | Define bioisosteres with examples. | | (3) |
| 13. | Write the equation for Coefficient of variation. | | (3) |
| 14. | What are the advantages of similarity searching? | | (3) |
| 15. | State the rule of five and its use in drug likeness. | | (3) |
| **PART C(5 X 15= 75 MARKS)** | | | |
| 16. | a. | What is meant by subgraph isomorphism? Discuss its importance | (9) |
| b. | Describe the various parts of the connection tables. | (6) |
| (OR) | | | |
| 17. | a. | Explain the use of graph theory in the representation of chemical structures. | (9) |
| b. | Write the aim and applications of chemoinformatics in various fields. | (6) |
| 18. |  | Discuss about the Cambridge Structural Database and Protein data bank. | (15) |
| (OR) | | | |
| 19. | a. | Explain the systematic conformational search method. | (10) |
| b. | Write a note on practical aspects of pharmacophore mapping. | (5) |
| 20. | a. | Explain the following indices.  (i) Wiener index (ii) Branching index (iii) First order chi index | (12) |
| b. | Calculate the simple and valence delta values for -CH3 and -CH2 | (3) |
| (OR) | | | |
| 21. | a. | Write a detailed account on Kappa shape indices | (10) |
| b. | Define and explain Electrotopological state indices | (5) |
| 22. | a. | Write the formula for the following similarity coefficients.  (i) Tanimato (ii) Dice (iii) Euclidean (iv) Hamming | (8) |
| b. | What is the purpose of using data fusion techniques? Discuss with any two examples.. | (7) |
| (OR) | | | |
| 23. | a. | Write the formula to find the molecular electrostatic potential and a method to improve the efficiency of the process. | (5) |
| b. | What is meant by maximum common subgraph similarity? Explain. | (10) |
| 24. |  | Write a detailed account on Protein-Ligand Docking. | (15) |
| (OR) | | | |
| 25. |  | Discuss any two data mining methods. | (15) |

ALL THE BEST