Sr. No. 325503

December 2023
B.Sc (LS)- V SEMESTER
Chemistry V Cheminformatics (BLS503)

Time: 3 Hours   Max. Marks:75

Instructions:
1. *It is compulsory to answer all the questions (1.5 marks each) of Part -A in short.*
2. *Answer any four questions from Part -B in detail.*
3. *Different sub-parts of a question are to be attempted adjacent to each other.*

PART –A

Q1 (a) What does the term Chem-informatics refer to?   (1.5)

(b) Exaplain Molecular modelling .   (1.5)

(c) Write a concise overview of data visualization.   (1.5)

(d) What are the key characteristics and principles of the three-dimensional searcl (1.5)
method?

(e) What is Mass Spectra?   (1.5)

(f) What is role of Model building in structure determination of compounds? (1.5)

(g) Describe drug design in brief.   (1.5)

(h) Explain two terms: Target identification and Validation   (1.5)

(i) What is Matrix representation ?   (1.5)

(j) Enumerate three key significance of infrared (IR) spectra in predicting compounds. (1.5)

PART –B

Q2 (a) Explain the term: representation of molecules and chemical reactions.   (10)

(b) What role does Nuclear Magnetic Resonance (NMR) play in the identification of (5)
compounds and why is it significant?

Q3 (a) Describe full structure search and sub structure search in detail.   (5)

(b) What is basics of computation of physical and chemical data?   (10)

Q4   Write down the details of recent developments in chem-informatics.   (15)

Q5 (a) What are the various technique used in structure elucidations of ompounds? (5)

(b) Explain the computer assisted structure determination .   (10)

Q6 (a) Define two terms: ligand-based drug design and structure-based drug design. (10)

(b) Define term: QSAR (5)

Q7 Explain how Chem-informatics is utilized in the process of designing drugs and its (15) various applications?

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