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MBJ-1603220001040500 Seat No. _____

B. Sc. (Bioinformatics) (Sem. IV) (CBCS) Examination

March / April - 2018

BI - 405 : Cheminformatics

(New Course)

Time : $2\frac{1}{2}$ Hours] [Total Marks : **70**

Instructions : (1) All questions are compulsory.

(2) The right side figures indicate total marks of the questions.

1 Attempt the following : **14**

(A) Answer the following short questions : **4**
(ALL COMPULSORY)

(1) Which algorithm has been developed to generate an inique SMILE string for every molecule?

(2) Which are two main components of graphs?

(3) How many popular line notations were there?

(4) What is CML?

(B) Answer ANY **ONE** of the following short questions : **2**

(1) How many types of line notation are there? Name them?

(2) Explain CML conventions.

(C) Answer ANY **ONE** of the following short questions : **3**

(1) Advantages and disadvantages of Matrix representation.

(2) Explain connection tables and linear notations.

(D) Explain ANY **ONE** of the following questions in detail : **5**

(1) Explain graph theory.

(2) Explain line notations.

2 Attempt the following : **14**

(A) Answer the following short questions: **4**
(ALL COMPULSORY)

(1) CHEMBL is maintained by _____

(2) Example of reaction database.

(3) BIOMET database is which kind of database?

(4) _____ is more akin to a drug encyclopedia than a drug database.

(B) Answer ANY **ONE** of the following short questions : **2**

(1) NIC

(2) Explain the chemical network of KEGG.

(C) Answer ANY **ONE** of the following short questions : **3**

(1) What is similarity search

(2) What is multi model database?

(D) Explain ANY **ONE** of the following questions in detail : **5**

(1) Explain the chemical databases.

(2) Explain a database for chemical entities of biological interest.

3 Attempt the following : **14**

(A) Answer the following short questions : **4**
(ALL COMPULSORY)

(1) Some of the reagents that are commonly used in library design are?

(2) What is homology modeling?

(3) What is descriptor statistics?

(4) The diverse library was designed without using any information about the

(B) Answer ANY **ONE** of the following short questions : **2**

(1) What are building blocks ?

(2) List out Commercial software packages for docking studies.

(C) Answer ANY **ONE** of the following short questions : **3**

(1) Generation of Virtual Library Compounds.

(2) What is Product-Based Selection?

(D) Explain ANY **ONE** of the following questions in detail : **5**

(1) How to make Selection of Candidate Molecules from Virtual Libraries?

(2) Give the general flow chart of the algorithm and detailed description of the implementation of SA in SAGE

4 Attempt following : **14**

(A) Answer the following short questions : (ALL COMPULSORY) **4**

(1) What is an agonist?

(2) _____ and _____ can guide the design of combinatorial libraries.

(3) What is QSAR?

(4) _____ enables sequenced based gene knockdown at the RNA level.

(B) Answer ANY **ONE** of the following short questions : **2**

(1) Explain in brief the process of drug discovery

(2) Target identification. Explain in brief.

(C) Answer ANY **ONE** of the following short questions : **3**

(1) Data sets in target fishing for chemical compounds. Explain

(2) Explain QSPR in brief

(D) Explain ANY **ONE** of the following questions in detail : **5**

(1) Explain: QSPR methodology.

(2) Explain genetic interaction and genomic method for target identification.

5 Attempt the following : **14**

(A) Answer the following short questions : **4**
(ALL COMPULSORY)

(1) What is ADMET?

(2) What is pharmacophore fingerprint?

(3) _____ are the most common source of structural information for drug design.

(4) Name any few docking programs in drug design.

(B) Answer ANY **ONE** of the following short questions : **2**

(1) HITS recognition

(2) The iterative process of structure-based drug design

(C) Answer ANY **ONE** of the following short questions : **3**

(1) Approaches to target identification.

(2) Ligand based drug design.

(D) Explain ANY **ONE** of the following questions in detail : **5**

(1) ADMET.

(2) Construction of pharmacophore model.
