Sem III

VICHITRAGAD – III (2013 COURSE) (CBCS): WINTER – 2015

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

Day : Tuesday
Date : 13-10-2015

Time: 10.00 A.M. To 1.00 P.M.
Max. Marks : 60

N.B.:

1) All questions are **COMPULSORY**.
2) Figures to the right indicate **FULL** marks.
3) Answers to both the sections should be written in **SEPARATE** answer books.

SECTION – I

Q.1 Attempt **ANY TWO** of the following: **[16]**

a) Explain the chemical structure representation file format with suitable example.
b) Describe similarity metrics and their significance in Cheminformatics.
c) Discuss the Lipinski's rule for drug molecules and give its important in lead optimization process.

Q.2 Attempt **ANY TWO** of the following: **[10]**

a) Discuss role of molecular similarity and molecular diversity in virtual screening.
b) Explain the designing and analysis of combinatorial library for drug like molecules.
c) Explain in detail drug discovery process using Cheminformatics tools.

Q.3 Attempt **ANY ONE** of the following: **[04]**

a) What is graph theory? Explain its use in chemical structure representations.
b) Give applications of ADMET in drug discovery process.

SECTION – II

Q.4 Attempt **ANY TWO** of the following: **[16]**

a) Describe different tools and parameters used for analysis of receptor – ligand interactions.
b) Discuss in detail the significance of CoMFA and CoMSIA in QSAR study.
c) Explain various chemical databases and their applications in drug discovery.

Q.5 Attempt **ANY TWO** of the following: **[10]**

a) Describe the importance of flexible and rigid docking in elucidation of molecular interactions.
b) Give in detail workflow of structure based pharmacophore modeling in drug designing.
c) Explain correlation between ligand based and receptor based docking studies.

Q.6 Attempt **ANY ONE** of the following: **[04]**

a) Describe the process of target identifications and validations.
b) Discuss the role of QSPR in drug discovery process.

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VICHITRAGAD -III (2013 COURSE) (CBCS): WINTER- 2015
SUBJECT: BIOLOGICAL DATA MINING

Day: Thursday
Date: 15-10-2015

Time: 10.00 A.M. To 1.00 P.M.
Max. Marks: 60

N.B.:

1) All questions are **COMPULSORY**.
2) Figures to the right indicate **FULL** marks.
3) Answers to both the sections should be written in **SEPARATE** answer books.
4) Draw neat diagrams **WHEREVER** necessary.

SECTION-I

Q.1 Attempt the following: **(10)**

a) Define Classification Algorithms.
b) Note on: Conjugate Gradient Optimization technique.
c) BLOSUM 60 matrix.
d) What do you mean by Recombination in GA?
e) What are energy functions?

Q.2 Answer any **TWO** of the following: **(10)**

a) Explain the GA cycle. Write a pseudocode to represent it.
b) What is Clustering? Explain any one algorithm in brief.
c) Elaborate upon the prediction of protein structure using homology modeling.
d) Write a note on the Hydrophobic Lattice Model with help of suitable example.

Q.3 Answer any **TWO** of the following:

a) What is GA? Explain the Roulette Wheel method for selection in GA. **(10)**
b) Differentiate between Optimization problem and Simulation of folding.
c) Write a note on Classification and Clustering of genomic data.

SECTION-II

Q.4 Answer any **ONE** of the following: **(04)**

a) Explain in brief the Hopfield Network.
b) With the help of suitable example, write a note on four most widely used Clustering Algorithm.

Q.5 Answer any **TWO** of the following: **(10)**

a) Explain ACO for data clustering.
b) Write a note on the Interpolated Markov Model. Explain its applications in Bioinformatics.
c) Give a detailed description on Classification of Biological Data using Machine Learning.

Q.6 Answer any **TWO** of the following: **(16)**

a) How can you use SVM and ACO together for feature selection? Explain using appropriate example.
b) Explain in detail-Ant Colony Optimization with its applications in Traveling Salesman Problem.
c) How can Artificial Neural Networks be useful for B-cell epitope prediction?

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Day : Saturday
Date : 17-10-2015

Time : 10.00 A.M. To 1.00 P.M.
Max. Marks : 60

N.B.:

1) All questions are **COMPULSORY**
2) Figures to the right indicate **FULL** marks.
3) Draw well labeled diagram **WHEREVER** necessary.
4) Answers to both the sections should be written in **SEPARATE** answer books.

SECTION - I

Q.1 **a)** Derive the immigration rate equation for island biogeography model. **[03]**

b) Differentiate between linear & non -linear parameters. **[03]**

OR

Discuss the process of bifurcation with an example.

c) Define: **i)** Odum Energy Flow Diagrams **ii)** Structured Models **[04]**

Q.2 Differentiate between the following: **[10]**

a) Top - down & Bottom - up approach

b) Open & Closed networks

OR

Suppose a population is modeled by the equation **[10]**

$N_{t+1} = N_t + 1.2N_t (1 - N_t/500000)$, when N_t is measured in individuals.

i) Find an equation of the same form, describing the same model, but with the population measured in thousands of individuals.

ii) Find an equation of the same form, describing the same model, but with the population measured in units chosen so that carrying capacity is 1 in those units.

Q.3 **a)** Explain the role of bistability in metabolic networks. **[03]**

b) Explain the Gauss – Jorden Method. **[03]**

OR

Explain Jacobi's iteration method.

c) Define: **i)** Instability **ii)** Stiffness **[04]**

SECTION – II

Q.4 Explain with an example: **[10]**

a) Multilevel modeling

b) Role of prior probability in Bayes' theorem

c) System – level modeling

d) Spatial extended systems

e) Control Theory

Q.5 Answer **ANY TWO** of the following: **[10]**

a) Discuss the method of Monte-Carlo error analysis with proper examples.

b) How can generative topographic mapping be used to model gene regulatory networks? Discuss with an example.

c) Can perceptrons be used to model internal architecture of metabolic networks? Justify.

Q.6 Propose an algorithm based on learning classifiers for modeling reaction kinetics. **[10]**

OR

Propose an algorithm for analyzing robustness of metabolic networks.

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VICHITRAGAD -III (2013 COURSE) (CBCS): WINTER- 2015

SUBJECT: ELECTIVE –IV: a) RECENT TRENDS IN BIOINFORMATICS

Day: Monday
Date: 19-10-2015

Time: 10.00 A.M. To 1.00 P.M
Max. Marks: 60

N.B.:

1) All questions are **COMPULSORY**.
2) Figures to the right indicate **FULL** marks.
3) Answers to both the sections should be written in **SEPARATE** answer books.
4) Draw neat diagrams **WHEREVER** necessary.

SECTION-I

Q.1 Answer any **TWO** of the following: **(10)**

a) What is Linux? Mention different commands with their utilities.
b) Explain use of various bioinformatics tools in NGS analysis.
c) What is Genome browser? Give its significance in genome sequence analysis.

Q.2 Answer any **TWO** of the following: **(10)**

a) Explain use of statistical and logical functions of EXCEL in biological data analysis.
b) What is differential gene expression? How it is determined using RNA-seq analysis.
c) Describe salient features of ENSEMBLE in gene / genome analysis.

Q.3 Answer any **FIVE** of the following: **(10)**

a) Define FASTQ sequence format for read alignment.
b) Explain difference between SAM and BAM.
c) What is PHRED quality score?
d) Applications of SQL in creating biological databases.
e) Explain use of arithmetic functions in Excel.
f) Enlist various Next Generation Sequencing platforms.
g) Give significance of UCSC genome browser in genome visualization.

SECTION-II

Q.4 Answer any **ONE** of the following: **(04)**

a) Write a short note on available Microarray databases. Explain any one in detail.
b) What kinds of networks data can be visualized in Cytoscape?

Q.5 Answer any **TWO** of the following: **(10)**

a) Mention the process implemented to normalize a Microarray data.
b) Explain role of MSA in Phylogenetic Analysis.
c) Write a short note on TRANSFAC as a tool to search for transcription factors in Eukaryotes.

Q.6 Answer any **TWO** of the following: **(16)**

a) Describe maximum likelihood, neighbor joining and minimum evolution methods of Phylogenetic tree construction.
b) What is Microarray? Mention about the platforms and probes available for Microarray.
c) Explain the syntax for coding and manipulating a simple network in Cytoscape. Add a note on the basic functions available in the Cytoscape.

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