M.Sc. Sem III

VICHITRAGAD - III (C.B.C.S.) (2013 Course) : SUMMER - 2017

Subject : Cheminformatics & Drug Design

Day : Monday
Date : 03/04/2017

34798

Time : 02.00 PM TO 05.00 PM
Max Marks : 60 Total Pages : 2

N.B:

1) **Q.No.1 and Q.No.5** are **COMPULSORY.** Out of the renaming questions solve **ANY TWO** from each section.
2) Figures to the right indicate **FULL** marks.
3) Section-I and Section-II should be solved in **SEPARATE** answer books.
4) Draw the diagram **WHEREVER** necessary.

SECTION-I

Q.1 Answer **ANY** of the **FIVE** questions in brief: **(10)**

a) Define ADMET

b) Write full form of SMARTS

c) What is Tversky Index

d) Name any four chemical file formats.

e) Define MLR

f) Define Hammet's constant

Q.2 Answer the following questions: **(ANY TWO)** **(10)**

a) What are the various 2-D descriptors used in QSAR study?

b) What is the role of cheminformatics in drug discovery?

c) Explain Vertex Partitioning algorithm

Q.3 Differentiate between: **(ANY TWO)** **(10)**

a) Topological indices and kappa shape indices.

b) SMARTS and SMIRKS.

c) Reaction databases and structure databases.

Q.4 Write a short note on: **(ANY TWO)** **(10)**

a) Combinatorial library design strategies

b) Principal Component Analysis

c) Lipinski's Rule of Five

P.T.O.

SECTION-II

Q.5 Briefly answer the following (**ANY FIVE**): **(10)**

a) What is Training set?

b) Define Rigid docking.

c) Write full form of CoMSIA

d) Define Virtual Screening.

e) Name any two softwares for QSAR studies.

f) Define Cross validation.

Q.6 Answer **ANY TWO** of the following: **(10)**

a) What are pharmacophore keys?

b) Write are a note on Free Wilson Analysis.

c) Explain the various Electronic descriptors used for QSAR studies.

Q.7 Answer **ANY TWO** of the following **(10)**

a) Differentiate between QSAR and QSPR.

b) Explain the Clique detection method for pharmacophore mapping.

c) Briefly explain CoMFA.

Q.8 Explain the process of molecular docking in detail. How flexible docking differs from rigid docking? **(10)**

OR

Explain the 3-D QSAR techniques in detail. Also explain the descriptors involved in 3D QSAR studies.

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VICHITRAGAD - III (C.B.C.S.) (2013 Course) : SUMMER - 2017

Subject : Biological Data Mining

Day : Tuesday
Date : 04/04/2017

34799

Time : 02.00 PM TO 05.00 PM
Max Marks : 60 Total Pages : 1

N.B.:

1) **Q.No.1** and **Q.No.5** are **COMPULSORY**. Out of the remaining questions attempt **ANY TWO** questions from each section.
2) Answer to both the sections should be written in **SEPARATE** answer books.
3) Figures to the right indicate **FULL** marks.

SECTION – I

Q.1 Define: **[10]**

a) Biological artifacts
b) Data optimization
c) Genetic operator
d) SOM
e) Linguistics

Q.2 Write short notes on **ANY TWO** of the following: **[10]**

a) Biological databases
b) 3D structural alignment errors.
c) Steepest - Descent method

Q.3 Answer **ANY TWO** of the following: **[10]**

a) Discuss the considerations of Genetic Algorithms.
b) Explain supervised Genetic Algorithm with example.
c) Describe the outcomes of unsupervised Genetic Algorithms.

Q.4 Discuss in brief: (**ANY TWO**) **[10]**

a) K- means clustering
b) Information Theory
c) Protein Array Data Analysis

SECTION – II

Q.5 Answer in Brief: **[10]**

a) What is twilight zone?
b) What are the basic principals behind fuzzy logic?
c) Write the basic principal of Machine Learning Technique.
d) What is dynamic programming?
e) What is similarity and identity?

Q.6 Attempt **ANY TWO** of the following: **[10]**

a) Explain dynamic programming utilization for structure alignments.
b) Differentiate between BLAST and FASTA.
c) Explain Dot Plot.

Q.7 Discuss **ANY TWO** of the following methods with example. **[10]**

a) HMM
b) NN
c) Bayesian modeling

Q.8 Write in detail on different SVM methodologies. Describe the classification algorithm used in classifying tumor categories. **[10]**

OR

Discuss the clustering algorithm in context of multidimensional data.

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VICHITRAGAD - III (C.B.C.S.) (2013 Course) : SUMMER - 2017

Subject : Systems Biology

Day : Friday
Date : 07/04/2017

34800

Time : 02.00 PM TO 05.00 PM
Max Marks : 60 Total Pages : 2

N. B.:

1) **Q. No. 1** and **Q. No.5** are **COMPULSORY**. Solve **Any Two** from the remaining questions from each section.
2) Figures to the right indicate **FULL** marks.
3) Answers to both the sections should be written in the **SEPARATE** answer book.

SECTION-I

Q.1 Define : **(10)**

a) Driving variable
b) Finite growth rate
c) Death rate
d) Stiffness
e) Structured model

Q.2 Answer in brief :

a) Explain Karplus theory for system model designing. **(05)**

b) Discuss per-capita growth rate with respect to non-linear model. **(05)**

OR

Discuss the classical Lotka – Volterra model with illustration. **(10)**

Q.3 Write short notes on : **(ANY TWO)** **(10)**

a) Open and closed network
b) Reaction matrix
c) Errors in forester diagrams

Q.4 Answer the following :

a) Define instability explain the role of bistability in metabolic networks. **(05)**

b) Discuss the role of non-linear equations in modeling and analyzing dynamic systems with proper examples. **(05)**

OR

Find the first, second and third order derivatives of the function f(x) tabulated below; at the points x = 1.5 and x = 4.0. **(10)**

X	1.5	2.0	2.5	3.0	3.5	4.0
$f(x)$	3.375	7.000	13.635	24.000	38.875	59.000

P.T.O.

SECTION- II

Q.5 Answer in brief : **(10)**

a) What are graphical probabilistic models?
b) Define modularization.
c) Explain Baye's Theorem.
d) What is Monte – Carlo error analysis?
e) What is robustness analysis?

Q.6 Answer the following :

a) Discuss certain aspects of whole organ modeling with illustrations. **(05)**

b) Discuss various constraints used for modeling biological systems with proper examples. **(05)**

OR

Discuss the validation techniques used for experiment design and verification with proper examples. **(10)**

Q.7 Propose an algorithm : **(ANY TWO)** **(10)**

a) Based on modularization for identifying meaningful groups in metabolic network.

b) Based on learning classifiers for modeling reaction kinetics.

c) For analyzing robustness of metabolic networks.

Q.8 Answer the following : **(10)**

Explain with example modularity based studies.

OR

Discuss machine-learning based modeling techniques in detail.

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