Scheme of examination (PGDCB)

Semester	Discipline-Specific Courses (DSC)	Skill Enhancement Courses (SEC) / Internship	Courses (VAC)	Total Credits
I	DSC 1 @ 4 credits DSC 2 @ 4 credits DSC 3 @ 4 credits	SEC1 @4 credits	VAC1 @2 credits	22
11	DSC 4 @ 4 credits DSC 5 @ 4 credits DSC 6 @ 4 credits DSC 7 @ 4 credits	Internship @4 credits	VAC2 @2 credits	22
	DSC 8 @ 4 credits			44

Semester I

S.No.	Course code	Credits	Course title Introduction to Computational Biology & Bioinformatics
1	23BIND101DS01	4	Introduction to Computational Biology & Bioline
1.	23BIND101DS02	4	Concepts of Computer Programming
2	23BIND101DS02		Principles of Genomics & Proteomics
3			Structural Biology
4	23BIND101DS04		D C Di-1- wists
5	23BIND101SE01		From the pool of courses offered by MDU/SWAYAM
6	VAC1	2	courses of same credit
	Total Credits	22	

Semester II

S.No.	Course code	Credits	Course title
1	23BIND102DS01	4	System Biology
2	23BIND102DS02	4	Programming in Perl & Python
-	23BIND102DS03	4	Datamining & Machine Learning
3	23BIND102DS04		Computer Aided Drug Designing
4	23BIND102IN01	4	
6	VAC2	2	From the pool of courses offered by MDU/SWAYAM courses of same credit
	Total Credits	22	

Page 1 of 25

Centre for Bioinformatics Introduction to Computational Biology & Bioinformatics Semester I

23BIND101DS01	Course Creates	(L: 3 T: 1 P:0)
100		3 Hours
1	23BIND101DS01 100	23BIND101D801 Course electric

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

This course aims to introduce:

- 1. Biological databases
- 2. Specialized genomic resources
- 3. Algorithms in Computing
- 4. Combinatorial Pattern Matching; Genetic Algorithm; HMM and ANN

Learning Outcomes:

Students completing this course will be able to:

- 1. Access the world of Bioinformatics and explain different types of biological data.
- 2. Explain various algorithms for computing and analyze the algorithm using different types of
- 3. Explain the concept of Genetic algorithm, Optimization & its applications in bioinformatics.
- 4. Explain the concept of machine learning in terms of HMM, ANN.

Unit - I

Introduction: Biological databases - primary, secondary and structural, Protein and Gene Information Resources - PIR, SWISSPROT, PDB, GenBank, DDBJ. Specialized genomic resources.

DNA sequence analysis: cDNA libraries and EST, EST analysis, pair wise alignment techniques, database searching, multiple sequence alignment, tools of sequence alignment. Global and local alignments, matrices, gap penalties and statistical significance.

Unit - II

Secondary database searching, building search protocol, computer aided drug design - basic principles, protein modeling and design.

Commercial databases and packages, GPL software for Bioinformatics, web-based analysis tools. System modeling and metabolomics - concepts and principles.

Unit - III

Introduction: Algorithms in Computing; Analyzing algorithms-Asymptotic notation, Standard notations, Big 'O' notations; Algorithm design techniques. Exhaustive Search- Restriction Mapping, Finding Motifs; Greedy Algorithms- Genome Rearrangements, Sorting by Reversals, Finding Motifs.

Divide-and-Conquer Algorithms- Divide-and-Conquer Approach to Sorting. Genetic Algorithm: Basic Concepts, Optimization using GAs; Applications in bioinformatics.

Unit - IV

Combinatorial Pattern Matching- Hash Tables, Repeat Finding, Exact Pattern Matching; Expectation and Maximation (EM) with forward and backward algorithms, discriminative learning. Hidden Markov Models: Markov processes and Markov Models, Hidden Markov Models, Parameter estimation for HMMs, Optimal model construction, Applications of HMMs Artificial Neural Networks: Historic evolution - Perceptron, NN Architecture, supervised and unsupervised learning, Back Propagation Algorithm.

Suggested Readings:

Vone 14

1. D. Baxevanis and F. Oulette, (2002) "Bioinformatics: A practical guide to the analysis of genes and proteins", Wiley Indian Edition

2. 2. Cynthia Gibas and Per Jambeck (2001), "Developing Bioinformatics Computer Skills".

O'Reilly press, Shorff Publishers and Distributors Pvt. Ltd., Mumbai.

3. T. K. Attwood & D. J. Parry-Smith (2001), "Introduction to Bioinformatics", Pearson Education Ltd, Low Price Edition. 2. Bioinformatics: Sequence and Genome Analysis. D. W. Mount (2001) Cold Spring Harbor Laboratory Press.

4. Arthur M. Lesk (2002) "Introduction to Bioinformatis" Oxford University Press

5. Setubal Joao and Meidanis Joao, "Introduction to Computational Molecular Biology", PWS Publishing Company (An International Thomson Publishing Company), 1997, Indian low priced edition.

6. Michael Waterman (1995), "Introduction to Computational Biology: Maps, Sequences and

Genomes"

7. Tao Jiang, Ying Xu and Michael Q. Zhnag (Editors) Current topics in computational Molecular biology. Ane Books, New Delhi 2004

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Centre for Bioinformatics **Concepts of Computer Programming** Semester I

Course Code	23BIND101DS02	Course Creates	(L: 3 T: 1 P:0)
Max. Marks		Time of end term	3 Hours
		examination	

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

- 1. To provide an introduction to computer concepts and terminology, information technology, and software applications used in business and industry.
- 2. To express algorithms and draw flowcharts in a language independent manner.
- 3. To teach how to write modular, efficient and readable C programs
- 4. To describe the techniques for creating program modules in C using functions.

Learning Outcomes:

Upon completion of the course, the students will be able to:

- 1. Identify the specifications & configurations of computer hardware.
- 2. Identify the role of an operating system.
- 3. Write, compile and debug programs in C language.
- 4. Identify the difference between call by value and call by reference.

Unit - I

Components of Computer System, Basic Applications of Computer; input/output Devices, Computer Memory, Concepts of Hardware and Software; What is an Operating System; Basics of Popular Operating Systems; The User Interface; Basic of Computer networks; LAN, WAN; Concept and applications of Internet; World Wide Web; Web Browsing softwares, Search Engines.

Unit - II

Introduction to the C Language - Algorithm, Pseudo code, Flow chart, Background, C Programs, Identifiers, Data Types, Variables, Constants, Input / Output, Operators (Arithmetic, relational, logical, bitwise etc.), Expressions, Precedence and Associatively, Expression Evaluation, Type conversions.

Unit - III

Statements- Selection Statements(making decisions) - if and switch statements, Repetition statements (loops)-while, for, do-while statements, Loop examples, other statements related to looping - break, continue, go to, Simple C Program examples.

Unit - IV

Functions- Introduction to Structured Programming, Functions- basics, user defined functions, inter function communication (call by value, call by reference), Standard functions. Storage classes-auto, register, static, extern, scope rules, arrays to functions, recursive functions, example C programs.

Suggested Readings:

- 1. Computer Science: A Structured Programming Approach Using C, B.A.Forouzan and R.F. Gilberg, Third Edition, Cengage Learning.
- 2. The C Programming Language by Brian Kernighan and Dennis Ritchie 2nd edition.
- 3. Let Us C Yashavant kanetkar BPB.
- 4. Absolute beginner's guide to C, Greg M. Perry, Edition 2, Publisher: Sams Pub., 1994.
- 5. Computer Programming and Data Structures by E Balagurusamy, Tata McGraw Hill.

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Centre for Bioinformatics Principles of Genomics & Proteomics

Semester I

Course Code	23BIND101DS03	Course Credits	(L: 3 T: 1 P: 0)
Max. Marks	100	Time of end term examination	3 Hours

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives: The course aims to provide adequate knowledge about Principles of basic methods of genomic, transcriptomic and proteomic analysis.

- Extensive knowledge of various methodologies of next generation sequencing and Mass spectroscopic, and microarray technologies. Crucial concepts and techniques applied in genomics, transcriptomics and proteomics
- Formulate and assess experimental design for solving theoretical and experimental problems in Genomics and Proteomics fields.

Learning Outcomes: On completion of the course, the students will be able to

- Understand the inferring the basic concepts of genomics, transcriptomics and proteomics.
- Suggest and outline solution to theoretical and experimental problems in Genomics, Transcriptomics and Proteomics fields.
- Comprehend and solve diverse problems of genomics, transcriptomics and proteomics in human welfare, health and disease.

Unit - I

Basics of genomics and proteomics: Brief Recapitulation of prokaryotic and eukaryotic genome organization; extra-chromosomal DNA: bacterial plasmids, mitochondria and chloroplast.

Genome mapping Genetic and physical maps; markers for genetic mapping; methods and techniques used for gene mapping, physical mapping, linkage analysis, cytogenetic techniques, FISH technique in gene mapping, somatic cell hybridization, radiation hybrid maps, in situ hybridization, comparative gene mapping.

Unit - II

Genome Sequencing Projects and Genomic Techniques and Tools Human Genome Project, genome sequencing projects for microbes, plants and animals, accessing and retrieving genome project information from the web, Vectors for large scale genome projects, Cloneby-clone strategy, shotgun sequencing and Sequencing Standards.

Introduction to metabolomics, lipidomics, metagenomics and systems biology.

Unit - III

Comparative genomics Identification and classification of organisms using molecular markers-16S rRNA typing/ sequencing, SNPs and Pharmacogenomics; use of genomes to understand evolution of eukaryotes, track emerging diseases and design new drugs; determining gene location in genome sequence, Human and other vertebrate Genome.

Functional Genomics Transcriptome analysis for identification and functional annotation of gene, Contig assembly, chromosome walking and characterization of chromosomes, mining functional genes in genome, gene function- forward and reverse genetics, gene ethics; protein-protein and protein-DNA interactions; protein chips and functional proteomics; clinical and biomedical applications of proteomics.

Unit - IV

Proteomics Aims, strategies and challenges in proteomics; Protein separations, protein analyses, Quantitative proteomics, Identification and analysis of proteins by 2D gel electrophoresis, Isoelectric focusing, Spot visualization and picking, Tryptic digestion of protein and peptide fingerprinting; Mass spectrometry, mass spectrum (base peak, molecular ion, fragment ion,

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Page 5 of 25

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metastable ion), Ion source (MALDI, electrospray, chemical ionization), mass analyzer (quadrupole, TOF, Ion trap); Detector (multiplier), Clinical proteomics, Protein-protein interaction: solid ELISA, pull-down assay, co-immuno-precipitation, yeast-two hybrid system, application, proteome databases.

Suggested Readings:

- 1. Robert Weaver, Molecular Biology, 5th Edition, McGraw-Hill, 2012.
- 2. Genomes, by T.A. Brown, Garland Science, 3rd Edition, 2006
- 3. Anthony J.F. Griffiths, Susan R. Wessler, Richard C. Lewontin, William M. Gelbart, David T. Suzuki, Jeffrey H. Miller, An Introduction to Genetic Analysis, Eleventh Edition,
- 4. Primrose, S. B., Twyman, R. M., Primrose, S. B., & Primrose, S. B. (2006) Principles of Gene Manipulation and Genomics. Malden, MA: Blackwell Pub. Liebler, D. C. (2002).
- 5. Introduction to Proteomics: Tools for the New Biology. Totowa, NJ: Humana Press.
- 6. Campbell, A. M., & Heyer, L. J. (2003). Discovering Genomics, Proteomics, and Bioinformatics. San Francisco: Benjamín Cummings.

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Centre For Bioinformatics Structural Biology Semester I

Course Code	23BIND101DS04	Course Credits	(L: 3 T: 1 P: 0)
Max. Marks		Time of	3 Hours
		examination	outre le production de la constant d

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives: The course aims to provide the knowledge of the basic protein molecular architecture and then to connect it to the basic cellular processes like enzymatic activity, transport, and membrane functions.

Learning Outcomes:

Upon completion of the course, the students will be able to:

Understand the role of structural biology in life science research.

Understand the basic techniques used in structural biology studies

Understand the 3Dimensional structure files of biological molecules

Understand the concept, process and applications of Molecular dynamics simulation

Unit - I

Introduction: Post NGS era, importance of structural biology, biological macromolecules, Sequence to structure to function relationship, Protein as our target study molecule.

Protein Architecture: amino acids structure and function, Primary, secondary, tertiary and quaternary structure of protein; Motifs and domains of protein structures; Conformational analysis, Protein folding.

Bonds and energies in macromolecules- Covalent, Ionic, coordinate, hydrophobic and Vander walls interactions.

Unit - II

Enzymes: introduction to enzymes, how enzyme develop magic pockets, enzyme-ligand interaction, Structure-function relationship,

Structural Biology Techniques: Basics of macromolecular crystallography, Nuclear Magnetic Resonance (NMR) and Cryo-Electron microscopy, advantages and disadvantages of all the processes: comparative discussion.

Macromolecular Crystallography: Crystallization and Data Collection Crystallization, method of protein crystallization, thermodynamics and kinetics of protein crystallization, structural genomics project.

Unit - III

Macromolecular Crystallography: Data Analysis X-ray diffraction and Bragg equation, scattering factor, Structure factor expression, Phase problem and methods for phase determination, structure determination of macromolecules by crystallography technique.

Reading and Understanding 3D structure files: Introduction to PDB data, RCSB, reading PDB files, related calculations.

3D structure Visualization: Visualization of macromolecules using Pymol and Coot.

Unit - IV

Introduction to Molecular Dynamics Simulation: Need of simulation in studying biology, Building realistic atomistic model, Size and Times scale of macromolecular movements, Atomic Interactions: bonded and non-bonded, General form of all atom force field equations, Steps in molecular dynamics, Topology and parameter files, Periodic boundary conditions, Solvation and solvation methods, Simulation programs.

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Page 7 of 25

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Suggested Readings:

- 1. Carl Ivar Branden and John Tooze., "Introduction to Protein Structure" 2nd 2001 Edition, Taylor and Francis.
- 2. Voet, D. and Voet, J. G., "Biochemistry" 3rd edition, John Wiley and Sons.
- 3. Introduction to Protein Architecture: The Structural Biology of Proteins, 2001 Arthur M. Lesk, Oxford University Press; 1st edition
- 4. Lubert Stryer, Biochemistry, 4th Edition, WH Freeman & Co
- 5. Creighton. T.E., Proteins, Structure and Molecular Properties, 2nd Edition, 1993 W.H. Freeman
- 6. McPherson, A. "Introduction to Macromolecular Crystallography", 2nd 2009 edition, Wiley-Blackwell.
- 7. Drenth, J., "Principles of Protein X-Ray Crystallography", 3rd edition, 2007 Springer.
- 8. Rhodes, G., "Crystallography Made Crystal Clear", 3rd edition, Academic Press.

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Centre for Bioinformatics R for Biologists Semester I

Course Code	23BIND101SE01	Course Credits	(L: 3 T:1 P:0)
Max. Marks	100	Time of end term examination	3 Hours

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

This course aims to introduce:

- 1. Develop proficiency in the programming language R.
- 2. Use of R to analyze and interpret biological data.
- 3. Choose appropriate analysis techniques for a variety of data types and formats.

Learning Outcomes:

Students completing this course will be able to:

- 1. Understand why programming in biology is important.
- 2. Understand basic R usage: read data, clean data, visualize data, general programming knowledge.
- 3. Troubleshoot problems with R and biological data.

Unit - I

Introduction: Why code in biology? Need of R and its approaches. R interpreter, Introduction to major R data structures like vectors, matrices, arrays, list and data frames, Control Structures, vectorized if and multiple selection, functions.

Unit - II

Installing, loading and using R packages: Read/write data from/in files, extracting data from websites, Clean data, Transform data by sorting, adding/removing new/existing columns, centring, scaling and normalizing the data values, converting types of values, using string in-built functions,

Unit - III

Statistical analysis of biological data in R, for summarizing and understanding data, Visualizing data using scatter plot, line plot, bar chart, histogram and box plot

Unit - IV

Designing GUI: Building interactive application and connecting it with database. Building Packages.

Suggested Readings:

- 1. Cotton, R., Learning R: a step by step function guide to data analysis. 1st edition. O'reilly Media Inc.
- Gardener, M. (2017). Beginning R: The statistical programming language, WILEY. 3. Lawrence, M., & Verzani, J. (2016). Programming Graphical User Interfaces in R. CRC press. (ebook)
- 3. Introduction to Statistics and Data Analysis With Exercises, Solutions and Applications in R. By Christian Heumann, Michael Schomaker and Shalabh, Springer, 2016.
- 4. The R Software-Fundamentals of Programming and Statistical Analysis -Pierre Lafaye de Micheaux, Rémy Drouilhet, Benoit Liquet, Springer 2013
- 5. A Beginner's Guide to R (Use R) By Alain F. Zuur, Elena N. Ieno, Erik H.W.G. Meesters, Springer 2009.

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Page 9 of 25

Centre for Bioinformatics Systems Biology Semester II

Course Code	23BIND102DS01	Course Credits	(L: 3 T: 1 P:0)
Max. Marks	100	Time of end term examination	3 Hours

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

This course aims to introduce the concept and applications of:

- Systems Biology Networks
- Simulation of pathways and Networks and Motifs
- Signalling & Experimental methods in systems biology
- Design of Circuits and Databases

Learning Outcomes:

Students completing this course will be able to:

- Discuss and explain the concept of systems biology and biological networks.
- · Explain the principles and levels of simulations of biological pathways upto Whole Cell Simulation and access different pathway databases.
- Understand the signalling and experimental methods in systems biology.
- Design and demonstrate the circuits in network biology.

Unit - I

Introduction: Systems Biology Networks- basics of computer networks, Biological uses and Integration. Micro array - definition, Applications of Micro Arrays in systems biology. Self organizing maps and Connectivity maps - definition and its uses. Networks and Pathways - Types and methods. Metabolic networks.

Unit - II

Simulation of pathways: Whole cell: Principle and levels of simulation - Virtual Erythrocytes. Pathological analysis. Flux Balance Analysis. Biochemical metabolic pathways, Metabolomics and enzymes. Interconnection of pathways, metabolic regulation. Translating biochemical networks into linear algebra. Cellular models. Networks and Motifs: Gene Networks: basic concepts, computational models. Lambda receptor and lac operon as an example. - all types of networks and its uses

Unit - III

Signalling & Experimental methods in systems biology: Slow and auto-regulation The coherent FFL-temporal order, FIFO, DOR, Global, Development, memory and irreversibility signalling networks and neuron circuits-robust adapation-any model.

Unit - IV

Design of Circuits and Databases: Introduction to biological databases like KEGG, EMP, MetaCyc, AraCyc etc., Expression databases and various databases related to systems biology. Optional design of gene circuits I- cost and benefit: gene circuits II- selection of regulation. Stochasticity in gene expression.

Suggested Readings:

- 1 Kitano, H. (2001). Foundations of systems biology. The MIT Press Cambridge, Massachusetts London, England.
- 2. Klipp, E., Herwig, R., Kowald, A., Wierling, C., & Lehrach, H. (2005). Systems biology in practice: concepts, implementation and application. John Wiley & Sons.
- 3. Wilkinson, D. J. (2018). Stochastic modelling for systems biology. CRC press.
- 4. Soyer, O. S. (Ed.). (2012). Evolutionary systems biology (Vol. 751). Springer Science & Business Media.
- 5. Voit, E. (2017). A first course in systems biology. Garland Science.
- 6. Klipp, E., Liebermeister, W., Wierling, C., & Kowald, A. (2016). Systems biology: a textbook. John Wiley & Sons.

7. Choi, S. (Ed.). (2007). Introduction to systems biology. New Jersey:: Humana press.

Page 10 of 25

Centre for Bioinformatics Programming in Perl & Python Semester II

Course Code Max. Marks	23BIND102DS02	Time of end term	(L: 3 T: 1 P:0) 3 Hours
Max. Marks	i an in	examination total Answer to question no. 1 s	hall be compulsory

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

This course aims to introduce:

- Perl basics
- Advanced perl and bioperl
- Python programming language
- The syntax and semantics of the Python programming language.

Learning Outcomes:

Students completing this course will be able to:

- Perform the programming in PERL language.
- Solve various biological issues like pattern matching and array handling using PERL with a real-world example.
- Perform programming in Python
- Execute advance programming in Python

Unit - I

PERL: Strings, Numbers, and Variables. Variable Interpolation, Basic Input and Output, File handles, Making Decisions, Conditional Blocks, Loops, Combining Loops with Input, Standard Input and Output, Finding the Length of a Sequence File.

Unit - II

Pattern Matching in PERL: Extracting Patterns, Arrays, Arrays and Lists, Split and Join, Hashes, A Real-World Example, BioPERL; Applications. Creation, hosting and maintenance of web-site PHP, PERL and CGI. Unit - III

Introduction to Python programming: History, Features, Setting up path, Working with Python, Basic Syntax, Variable and Data Types, Operator Conditional Statements: If, If- else, Nested ifelse Looping: For, While, Nested loops Control Statements: Break, Continue, Pass String Manipulation: Accessing Strings, Basic Operations, String slices, Function and Methods Lists, Tuples, Sets, Dictionaries.

Unit - IV

Functions in Python programming: Defining a function, Calling a function, Types of functions, Function Arguments, Anonymous functions, Global and local variables Modules: Importing module, Math module, Random module, Packages, Composition Input-Output: Printing on screen, Reading data from keyboard, Opening and closing file, Reading and writing files, Functions Exception Handling: Exception, Exception Handling, Except clause, User Defined Exceptions.

Suggested Readings:

- 1. Foy, B. (2007). Mastering Perl. O'Reilly Media, Inc.
- 2. Quigley, E. (2014). Perl by example. Pearson Education.
- 3. Al Sweigart, "Automate the Boring Stuff with Python", 1st Edition, No Starch Press, 2015.
- 4. Allen B. Downey, "Think Python: How to Think Like a Computer Scientist", 2nd Edition, Page 11 of 25 Green Tea Press, 2015.

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Centre for Bioinformatics Datamining & Machine Learning

Semester II

Course Code	23BIND102DS03	Course Streets	(L: 3 T: 1 P:0)
Max. Marks		Time of end term examination	3 Hours

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

This course aims to introduce:

- Classification of datamining systems.
- Explain concept of association rule mining.
- Explain concept of classification and prediction.
- Explain and compare different clustering methods

Learning Outcomes:

- Students completing this course will be able to:
- Classify datamining systems & explain major issues in data mining.
- Describe concept of association rule mining and single dimensional boolean association
- Explain concept of classification and prediction with an emphasis on comparison of classification methods.
- Explain different clustering methods.

Unit - I

Introduction: Importance of Data Mining, Relational Databases, Data Warehouses, Transactional Databases, Advance Database Systems and Applications, Data Mining Functionalities, Classification of Data Mining Systems, Major issues in Data Mining. Primitives and System Architectures: Data Mining Primitives, Data Mining Query Language, Designing Graphical User, Interfaces Based on a Data Mining Query Language, Architectures of Data Mining Systems.

Unit - II

Concept Description and Association Rules: Concept Description, Characterization and comparison, Data Generalization and Summarization-Based Characterization, Analytical Characterization, Mining Class Comparisons, Mining Association Rules in Large Databases, Association Rule Mining, Mining Single Dimensional Boolean Association Rules from Transactional Databases.

Unit - III

Classification and Prediction: Classification and Prediction, Issues: Data preparation for classification and Prediction, Comparing classification Methods, Classification by Decision Tree Induction: Decision Trees and Decision Tress induction.

Unit - IV

Clustering Methods: Clustering Analysis, Types data in clustering analysis: Scaled variable, Binary variables, Variables of Mixed Types, Partitioning Methods: K-means and K-Medoids, Model-Based Methods, Data Mining Applications: Data mining for Biomedical and DNA Data Analysis.

Suggested Readings:

- Kevin P. Murphey, "Machine Learning, a probabilistic perspective", The MIT Press, 2012.
- Jiawei Han and MichelineKamber, Jian Pei, "Data Mining: Concepts and Techniques", Third Edition, Elsevier, 2012.
- 3. Pang-Ning Tan, Michael Steinbach and Vipin Kumar, "Introduction to Data Mining", First Edition, Pearson Education, 2006.
- 4. Tom Mitchael, "Machine Learning", McGraw Hill, 1997

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Page 12 of 25

Centre for Bioinformatics Computer Aided Drug Designing Semester II

Course Code	23BIND102DS04	Course Credits	(L: 3 T: 1 P:0)
Max. Marks	100	Time of end term examination	3 Hours

Note: Examiner will set nine questions in total. Answer to question no. 1 shall be compulsory comprising questions from all four units and remaining eight questions shall be set by taking two questions from each unit. The students have to attempt five questions in total, first being compulsory and selecting one from each unit.

Learning Objectives:

This subject is designed to provide the concept of:

- Rational drug design process
- Various techniques used in rational drug design process.
- The process of QSAR
- Molecular modelling and Virtual screening methods

Learning Outcomes:

Upon completion of the course, the student shall be able to understand

- · Design and discovery of lead molecules
- The role of drug design in drug discovery process
- The concept of QSAR and docking
- Various strategies to develop new drug like molecules.
- The design of new drug molecules using molecular modeling software.

Unit - I

Introduction to Drug Discovery and Development: Stages of drug discovery and development Lead discovery and Analog Based Drug Design: Rational approaches to lead discovery based on traditional medicine, Random screening, Non-random screening, serendipitous drug discovery, lead discovery based on drug metabolism, lead discovery based on clinical observation. Analog Based Drug Design: Bioisosterism, Classification, Bioisosteric replacement. Any three case studies

Unit - II

Quantitative Structure Activity Relationship (QSAR): SAR versus QSAR, History and development of QSAR, Types of physicochemical parameters, experimental and theoretical approaches for the determination of physicochemical parameters such as Partition coefficient, Hammet's substituent constant and Tafts steric constant. Hansch analysis, Free Wilson analysis, 3D-QSAR approaches like COMFA and COMSIA.

Unit - III

Molecular Modeling and virtual screening techniques

Virtual Screening techniques: Drug likeness screening, Concept of pharmacophore mapping and phar-macophore based Screening,

Molecular docking: Rigid docking, flexible docking, manual docking, Docking based screening. De novo drug design.

Unit - IV

Informatics & methods in drug design Introduction to Bioinformatics, chemoinformatics. ADME databases, chemical, biochemical and pharmaceutical databases.

Suggested Readings:

- 1. Robert GCK, ed., "Drug Action at the Molecular Level" University Prak Press Baltimore.
- 2. Martin YC. "Quantitative Drug Design" Dekker, New York.
- 3. Delgado JN, Remers WA eds "Wilson & Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry" Lippincott, New York.

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Page 13 of 25

4. Foye WO "Principles of Medicinal chemistry 'Lea & Fibiger.

5. Koro lkovas A, Burckhalter JH. "Essentials of Medicinal Chemistry" Wiley Interscience.

6. Wolf ME, ed "The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry" John Wiley&

7. Patrick Graham, L., An Introduction to Medicinal Chemistry, Oxford University Press. 8. Smith HJ, Williams H, eds, "Introduction to the Principles of Drug Design" Wright Boston.

9. Silverman R.B. "The Organic Chemistry of Drug Design and Drug Action" Academic Press New York.

Centre for Bioinformatics Computer Aided Drug Designing Semester II

IVIAA. IVIAI II	23BIND102IN01	Course Credits	(L: 0 T: 0 P:4)
	100	Time of end term	
		examination	
	1: 1-t- will submit an Interr	nship report to the Director with such	ccessful completion

and evaluated report from the organization where internship was carried out.

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Learning Objectives:

This subject is designed to develop a professional ability through an appropriate learning.

Learning Outcomes:

Upon completion of the course, the student shall be able to understand

The application of theoretical concepts of computational biology.

The duration of Internship is of 120 hours for 4 credits during summer vacation.

1.0. Definition of keywords

Course refers to a paper having specified credits mentioning its learning objectives and learning outcomes. A course may be designed comprising credits for lectures/ tutorials/laboratory work/field work/outreach activities/project work/internship/ vocational training etc. or combination thereof.

Credit is the weightage given to each course of the study. It is the numerical value assigned to a course according to the contact hours required to teach the prescribed syllabi of the program.

As per prescribed UGC standards: 1 credit = 15 hours of lectures

Mechanism for Computation of Work-load:

The following mechanism shall be adopted for computation of work-load:

- (a) 1 Credit = 1 Theory period of one hour duration/week/semester;
- (b) 1 Credit: 1 Tutorial period of one hour duration/week/semester;
- (c) 1 Credit: 1 Practical period of two hours duration/week/semester;
- (d) 1 Credit: Internship of 30 hours per semester.

The marks distribution according to the credit hours is 25 marks per credit.

Discipline Specific Course (DSC):

Discipline specific course is the discipline or subject of main focus in which the diploma will be awarded.

Skill Enhancement Course (SEC):

Skill Enhancement Course aims to promote skills pertaining to a particular field of study, impart practical skills, hands-on training, soft skills, etc., in order to enhance the student's employability.

Value Added Course (VAC):

Value Added Course aims to add the knowledge of the learner beyond academic disciplines.

Internship is a course to develop a professional ability through an appropriate learning. The duration of Internship is of 120 hours for 4 credits during summer vacation.

Semester/Academic Year A semester comprises of atleast 15 weeks of study within 90 working days (excluding the time spent for the conduct of final examination of each semester) and an academic year is divided into two semesters.

Page 15 of 25

Academic Bank of Credit (ABC)

Academic Bank of credit is an academic service mechanism to facilitate students to become its academic account holders, thereby paving the way for seamless student's mobility between or within degree-granting Higher Educational Institutions through a formal system of credit recognition, credit accumulation, credit transfers and credit redemption to promote distributed and flexible teachinglearning. ABC will digitally store the academic credits earned by students from HEIs registered with ABC for awarding degrees / diplomas / certificates taking into account credits earned by the students.

Credit Point

It is the product of the grade point and the number of credits for a course.

Grade Point

It is a numerical weight allotted to each letter grade on a 10-point scale.

Letter Grade

It is an index of the performance of students in a said course. Grades are denoted by letters O, A+, A, B+, B, C, P and F.

Semester Grade Point Average (SGPA)

The SGPA is the ratio of total credit points secured by a student in various courses registered in a semester and the total course credits taken during that semester. It shall be expressed up to two decimal places.

Cumulative Grade Point Average (CGPA)

The CGPA is the ratio of total credit points secured by a student in various courses in all semesters and the sum of the total credits of all courses in all the semesters. It is expressed up to two decimal places.

2.0. Components of course/program of study

The following types of courses/activities may be used to build program of study. Each of them will require specific number of hours of teaching/guidance/practicum/ laboratory/studio/workshop activities, field-based learning/projects, internships and community engagement and service.

Lecture courses: Courses involving lectures relating to a field or discipline by an expert or qualified personnel in a field of learning, work/vocation, or professional practice.

Tutorial courses: Courses involving problem-solving and discussions relating to a field or discipline under the guidance of qualified personnel in a field of learning, work/vocation, or professional practice.

Practicum or Laboratory work: A course requiring students to participate in a project or practical or lab activity that applies previously learned/studied principles/theory related to the chosen field of learning, work/vocation, or professional practice under the supervision of an expert or qualified individual in the field of learning, work/vocation or professional practice.

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Seminar: A course requiring students to participate in structured discussion/conversation or debate focused on assigned tasks/readings, current or historical events, or shared experiences guided or led by an expert or qualified personnel in a field of learning, work/vocation, or professional practice.

Internship: A course requiring students to participate in a professional activity or work experience, or cooperative education activity with an entity external to the education institution, normally under the supervision of an expert of the given external entity. A key aspect of the internship is induction into actual work situations. Internships involve working with local industry, government or private organizations, business organizations, artists, crafts persons, and similar entities to provide opportunities for students to actively engage in on-site experiential learning.

Studio activities: Studio activities involve the engagement of students in creative or artistic activities. Every student is engaged in performing a creative activity to obtain a specific outcome. Studio-based activities involve visual- or aesthetic focused experiential work.

Field practice/projects: Courses requiring students to participate in field-based learning/projects generally under the supervision of an expert of the given external entity.

Community engagement and service: Courses requiring students to participate in field-based learning/projects generally under the supervision of an expert of the given external entity. The curricular component of 'community engagement and service' will involve activities that would expose students to the socio-economic issues in society so that the theoretical learnings can be supplemented by actual life experiences to generate solutions to real-life problems.

3.0 Course/Program Structure

3.1 Structure of PG Diploma Program

Semester	Discipline-Specific Courses (DSC)	Skill Enhancement Courses (SEC) / Internship	Value-Added Courses (VAC)	Total Credits
Ι	DSC 1 @ 4 credits DSC 2 @ 4 credits DSC 3 @ 4 credits DSC 4 @ 4 credits	SEC1 @4 credits	VAC1 @2 credits	22
II DSC 5 @ 4 credits DSC 6 @ 4 credits DSC 7 @ 4 credits DSC 8 @ 4 credits	Internship @4 credits	VAC2 @2 credits	22	
				44

3.2 Issuance of Certificate

Students who are declared to have qualified all the course work as prescribed for concerned Certificate/Diploma Program will be awarded relevant certificate.

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Page 17 of 25

3.3 Maximum Duration to complete Certificate Course/Diploma Program

Duration of Certificate Course/Diploma Program + Two years.

4.0. Course Curriculum, Syllabus and Pedagogical Practices

The course curriculum and syllabus of every Certificate Course and Diploma Program shall be developed by the concerned Board of Studies (BOS) and be implemented after obtaining approval of the Academic Council. The course content and structure of Discipline Specific Courses (DSC) may vary from discipline to discipline depending upon the learning requirement of the program. However, the total credit to be earned for award of diploma shall be 44 credits. The concerned BOS may decide the mode of delivery of course i.e. offline/online/blended.

Pedagogical Practices

Effective learning requires an appropriate curriculum, an apt pedagogy, continuous formative assessment and adequate student support. The intention is to contextualize curriculum through meaningful pedagogical practices, which determine learning experiences directly influencing learning outcomes. Active, cooperative, collaborative and experiential learning pedagogies are some of the examples. The use of technology in creating a learning environment that connects learners with content, peers and instructors all through the learning process, respecting learners' pace is the need of the hour.

- a) Classroom processes must encourage rigorous thinking, reading and writing, debate, discussion, peer learning and self-learning.
- b) The emphasis is on critical thinking and challenge to current subject orthodoxy and develops innovative solutions. Curricular content must be presented in ways that invite questions, not as a body of ready knowledge to be assimilated or reproduced. Faculty should be facilitators of questioning and not authorities on expertise.
- c) Classroom pedagogy should focus on the 'how' of things, i.e. applying theory and ideas. All courses, including social sciences and humanities, should design projects and practicums to enable students to get relevant hands-on experiences.
- d) Learning must be situated in the Indian context to ensure no sense of alienation from their context, country and culture.
- e) Classroom processes must address issues of inclusion and diversity since students are likely to be from diverse cultural, linguistic, socio-economic and intellectual backgrounds.
- f) Cooperative and peer-supported activities must be part of empowering students to take charge of their own learning.
- g) Faculty will have the freedom to identify and use the pedagogical approach best suited to a particular course and student.
- h) Pedagogies like PBL (Problem/Project Based Learning) and Service Learning be brought into practice as part of the curriculum. Experiential learning in an internship with a specified number of credits is to be made mandatory.

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age 18 of 25

i) UGC suggests implementing Blended Mode (BL) as a new mode of teaching-learning in higher education. BL is not a mere mix of online and face-to-face mode, but it refers to an well-planned combination of meaningful a activities in both modes. The blend demands consideration of several factors, mainly focusing on learning outcomes and the learner- centered instructional environment.

5.0. Learning assessment

A variety of assessment methods that are appropriate to a given discipline/subject area and a program of study will be used to assess progress towards the course/program learning outcomes. Priority will be accorded to formative and summative assessment. Evaluation will be based on continuous assessment, in which sessional and the terminal examinations will contribute to the final grade. Sessionals will consist of class tests, mid-semester examination(s), homework assignments, class presentations etc., as determined by the concerned Board of Studies.

5.1. Examination and Internal Assessment

The internal assessment work and the End-Semester examination shall have the weightage of 30% and 70%, respectively. For practical examination also, 70 percent of the marks will be awarded through an end semester practical exam and remaining 30 percent of the marks will consist of internal assessment to be awarded by concerned faculty member(s) of the department.

- a. Internal Assessment shall be done on the basis of student's class attendance, submission of assignments, seminar presentations and performance at the two compulsory sessional tests to be conducted in a semester.
- b. First Internal Assessment Test shall be held around the sixth week of the semester for the syllabi covered till then. Second Internal Assessment Test shall be held around the twelfth week for the syllabi covered between seventh and twelfth week. Third Internal Assessment Test, if required, may be held around the fourteenth week for the syllabi covered between seventh and fourteenth week. However, the best scores in any two sessional tests shall be counted.
- c. The Internal Assessment for theory shall consist of the following components with marks indicated against each:

Credit Hours	4	3	2	1	
Total Marks	100	75	50	25	
Criteria					
Attendance		5	5	5	5
% of attendance Marks					
Below 65	0				
65 to < 70	2				
70 to < 75	3				
75 to < 80	4				
80 and above	5				

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Page 19 of 25

Assignments/Seminars Presentations	5	5	-	-
Assignments/Schimars 1100	20	15	10	-
Sessional Examination Total	30	25	15	5

d. The Internal Assessment for practical shall consist of the following components with marks indicated against each:

dicated against each			4	3	2	1
Credit Hours 1 Total Marks 1				75 75	50 50	25 25
Attendance						
% of attendance	Marks				P B	
Below 65	0					
65 to < 70	2					
70 to < 75	3				188.1	
75 to < 80	4					
80 and above	5		25	20	10	
Practical Assignment	ents/ Practical Fil	e Total	30	25	15	5

- e. The HOD/Director shall display the internal assessment awards of each course on the notice board of the Department/Institute/Centre atleast fifteen days before the commencement of the end semester examinations to give an opportunity to the students to make representation, if any regarding the dispute of sessional marks within two days of notification which shall be addressed by a three member appellate committee constituted by the concerned HOD/Director. The appellate committee shall submit its recommendation within three days and the corrective measures if any based on the recommendation of the committee shall be taken by the HOD/Director within next three days.
 - The HOD/Director shall forward the internal assessment marks awarded by the concerned teacher on the basis of class test, written assignment/ presentation/seminar and attendance in the classes to the Controller of Examinations as per the following schedule: (i) The Internal Heads the by supplied be should Assessment/Sessional marks Departments/Directors/Principals of the Colleges invariably within 20 days after the commencement of the examination. (ii) Thereafter, a late fee @ Rs.100/ per student per subject shall be levied upon the Department/ College/ Institute upto 10 days from the expiry of 20 days of the commencement of the examinations. This penalty/late fee shall not be charged from the student by the Department/College/Institute. (iii) If still, internal assessment/ sessional marks are not supplied by the Department/College/institute, then the result of the candidate(s) shall be declared by proportionating the marks of concerned theory/practical paper in which he/she has been declared as pass. Marks of candidates having reappear shall not be proportionate in this

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- g. The internal assessment awards as well as viva-voce awards of a candidate who fails in any semester examination shall be carried forward to the next examination.
- h. The end semester examination for the odd semesters shall ordinarily be held in the month of December/January and for the even semesters in the month of May/June on such dates as may be notified by the Controller of Examinations.
- i. The examination schedule containing the dates of receipt of examination forms with and without late fee, shall be notified by the Controller of Examinations from time to time.
- j. Students failing in one or more courses of end semester examinations will be entitled to clear them during the regular semester examinations of courses to be held in subsequent years.
- k. The examination fee to be paid by the candidate for each semester shall be as prescribed by the University from time to time.
- I. Every student shall be examined in the courses as prescribed in the syllabus and scheme of examination approved by the Academic Council from time to time. The fail/re-appear candidates will appear in the exam as per the syllabus applicable to regular students at that time.
- m. The HOD/Director shall preserve the records pertaining to internal assessment awards for verification, if needed, by the University up to three months from the date of declaration of the semester examination results.
- n. The candidate shall be allowed to appear in the examination if he/she fulfils the following requirements: -
- i. Bears a good character
- ii. Has been on the rolls of the Department/College/Institution during the semester.
- Has attended not less than 65% of lectures delivered in theory as well as practicals. Relaxation in shortage of lectures up to 20% will be allowed by the Head of the Department/Principal of the College/institute on the following grounds: (i) Self-illness; (ii) Illness/death of parents, brother, sister or any other close family member; (iii) Any other reason beyond the control of the student to the satisfaction of the HOD/Director/Principal.
- o. The minimum percentage of marks to pass the examination in each semester shall be:
 - (i) 40% in each theory paper
 - (ii) 40% in each practical examination.
 - (iii) 40% in the aggregate of each theory paper and internal assessment (and practical where practical is a component of theory paper).
- p. The grace marks will be allowed as per University rules.
- q. Letter Grades and Grade Points: The Semester Grade Point Average (SGPA) is computed from the grades as a measure of the student's performance in a given semester. The SGPA is

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Page 21 of 25

based on the grades of the current term, while the Cumulative GPA (CGPA) is based on the grades in all courses taken after joining the program of study. University may also mention marks obtained in each course and a weighted average of marks based on marks obtained in all the semesters taken together for the benefit of students.

Marks (%)	Letter Grade	Grade Point
> 90	O(outstanding)	10
> 75 to 90	A+(Excellent)	9
> 65 to 75	A(Very good)	8
> 55 to 65	B+(Good)	7
> 50 to 55	B(Above average)	6
> 40 to 50	C(Average)	5
40	P (Pass)	4
Less than 40	F(Fail)	0
	Ab(Absent)	0

r. Computation of SGPA and CGPA

The SGPA is the ratio of the sum of the product of the number of credits with the grade points scored by a student in all the courses taken by a student in a semester and the sum of the number of credits of all the courses undergone by a student, i.e.

SGPA (Si) =
$$\Sigma$$
(Ci x Gi) / Σ Ci

Where Ci is the number of credits of the ith course and Gi is the grade point scored by the student in the ith course.

Example for Computation of SGPA

Semester	Course	Credit	Letter Grade	Grade point	Credit Point (CreditxGrade)
I	Course 1	3	A	8	3X8= 24
I	Course 2	4	B+	7	4X7= 28
I	Course 3	3	В	6	3X6= 18
I	Course 4	3	0	10	3X 10 =30
I	Course 5	3	· C	5	3X5= 15
I	Course 6	4	В	6	4X6= 24
		20			139
			SGI	PA	139/20=6.95

The Cumulative Grade Point Average (CGPA) is also calculated in the same manner taking into account all the courses undergone by a student in all the semesters of a program, i.e.

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where Si is the SGPA of the ith semester and Ci is the total number of credits in that semester.

Example for Computation of CGPA

Credit:22
Credit.22
SGPA:7.8

The SGPA and CGPA shall be rounded off to 2 decimal points and reported in the transcripts.

5.2. Setting of Question Papers and Evaluation

- a. The question papers for the End-Semester theory examination shall be set and evaluation of answer books shall be done by the examiners (Internal and/or External ordinarily) out of the Panel of Examiners recommended by the Board of Studies of the Department concerned on the basis of their expertise/ specialization/area of interest.
- b. In the case of the practical examination of the courses, the assessment shall be jointly undertaken by the internal and external examiners. The External examiners shall be invited from amongst the panel of examiners recommended by the concerned Board of Studies. In case of unavailability of external examiners due to unavoidable circumstances, the Controller of Examinations may allow the conduct of practical examination by the internal examiners so that the conduct of examination and declaration of results is not delayed.
- c. The pattern of Question Papers for End-Semester theory examinations shall be as under:

Question 1: Answer to Question no. 1 shall be compulsory	Short answer type questions from all units				
Question 2 and 3	Two questions from Unit-I and the student shoul answer one question				
Question 4 and 5 Two questions from Unit-II and t answer one question					
Question 6 and 7	Two questions from Unit-III and the student should answer one question				
Question 8 and 9	Two questions from Unit-IV and the student should answer one question				

All the questions shall carry equal marks

5.3. Improvement of Grades: For improvement of grades, a student shall have to apply on the prescribed form available on the University Website or the Examination Branch of the University, along

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Page 23 of 25

with the original Detailed Marks Certificate or the copy of the result sheet and the prescribed fee, as revised from time to time.

- After passing each semester examination, a candidate will be allowed to appear for improvement of result in one or more theory papers only once within the period prescribed for completion of the Program. Only improved marks (higher score) will be taken into account.
- A student improving the Division/grade shall not be considered for award of Gold Medal/Rank Certificate.

6.0. Removal of the Name of a Student from the Program: .

- a. The name of a student remaining absent for 15 consecutive days (excluding Sunday/Holiday) after the start or during the academic session without any notice shall be struck off from the rolls of the Department/ Institute. A fine of Rs.20/- per lecture/day shall be charged on account of remaining absent from the classes.
- b. Re-admission may be allowed on payment of Rs. 2000/- alongwith required fine within 15 days with the permission of the Dean Academic Affairs. If a student fails to report within this time limit, the seat will be declared vacant and will be filled according to University rules. In respect of an applicant seeking re-admission, his/her previous record shall be carefully scrutinized and the decision of the Dean Academic Affairs in this regard shall be final.
- c. Re-admission may be allowed by the Dean Academic Affairs only once on the recommendations of the concerned HOD/Director on payment of prescribed re- admission fee and fine as applicable. However, while giving his/her specific recommendations, the concerned Head of the Department/Director must ensure that the student will fulfill the minimum requirement of attendance for appearing in the examinations as per Ordinance.

6.1. For Detained Student:

A student, who had been detained in semester end examination on account of shortage of attendance, will not be promoted to the next semester till he/she completes the requirements as mentioned (i) and (ii) below in the preceding semester:

- (i) he/she seeks re-admission within the prescribed date in the relevant semester in the next academic session.
- (ii) his/her conduct has been satisfactory; and he/she shows sufficient cause to the satisfaction for not having put in the requisite percentage of attendance.
- (ii). However, such students will have to pay fee being charged for that semester. If such a student had been detained in 1st semester of a program, he/she may be readmitted next year without competing with the other students seeking admission to the 1st semester. Supernumerary

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Page 24 of 25

seat(s) be created for readmitting such student(s) in the corresponding semester.

7.0 Credit Transfer through Academic Bank of Credits (ABC):

- a. The University shall provide the facility of Academic Bank of Credits in consonance with UGC (Establishment and Operationalization of Academic Bank of Credits (ABC) Scheme in Higher Education) Regulations, 2021, as amended from time to time.
- b. Each student shall have to register on Academic Bank of Credits (ABC) portal for creation of the unique ABC ID.
- c. Credits earned and deposited with Academic Bank of Credits (ABC) shall be valid for the purpose of redemption to a Certificate/Diploma/Degree, for varying duration as specified in the Ordinance subject to a maximum duration of 7 years.
- d. Provided that once any credit is redeemed for the award of a degree, diploma or certificate, such credit shall be irrevocably debited from the student's Academic Bank Account and cannot be reused for the award of any other formal academic qualifications.
- e. A student can take the courses of any other university subject to equivalence of the DSC courses and availability of seats, adopting due administrative process and formal consent of the University/Universities through the Equivalence Committee(s).

8.0. Power to Remove Difficulties:

If any difficulty arises in giving effect to the provisions of this Ordinance, the Vice Chancellor may, by order, make such provisions not inconsistent with the Act, Statutes, Ordinances or other Regulations, as appears to be necessary or expedient to remove the difficulty, however subject to ratification of such order by the Statutory bodies of the University.